



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:24 AM GMT

PDB ID : 3AIE  
Title : Crystal Structure of glucansucrase from Streptococcus mutans  
Authors : Ito, K.; Ito, S.; Shimamura, T.; Iwata, S.  
Deposited on : 2010-05-12  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

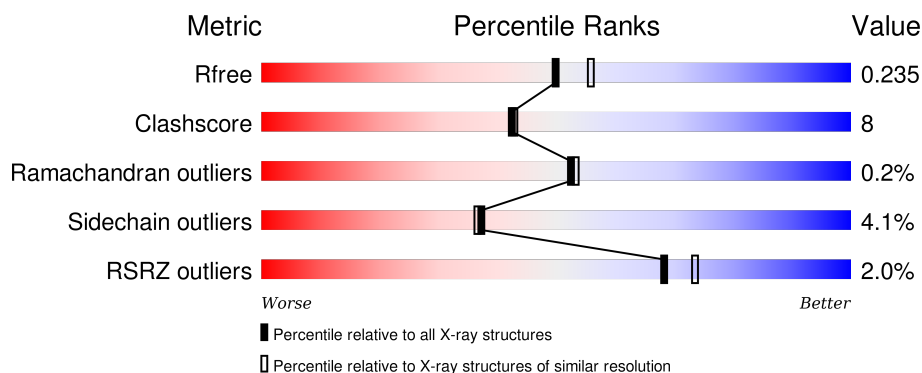
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	844	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>
1	B	844	<div> <div>3%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	C	844	<div> <div>%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	D	844	<div> <div>%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	E	844	<div> <div>2%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	844	 3% 80% 18% •
1	G	844	 2% 82% 15% ••
1	H	844	 2% 81% 16% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MES	B	5001	-	-	-	X
3	MES	C	5001	-	-	-	X
3	MES	D	5001	-	-	-	X
3	MES	H	5001	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 57830 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glucosyltransferase-SI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	B	844	Total	C	N	O	S	0	0	0
			6659	4196	1143	1304	16			
1	C	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	D	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	E	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	F	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	G	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	H	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	597	ASP	ASN	SEE REMARK 999	UNP P13470
A	600	LYS	ARG	SEE REMARK 999	UNP P13470
A	727	ILE	THR	SEE REMARK 999	UNP P13470
A	734	VAL	ALA	SEE REMARK 999	UNP P13470
B	597	ASP	ASN	SEE REMARK 999	UNP P13470
B	600	LYS	ARG	SEE REMARK 999	UNP P13470
B	727	ILE	THR	SEE REMARK 999	UNP P13470
B	734	VAL	ALA	SEE REMARK 999	UNP P13470
C	597	ASP	ASN	SEE REMARK 999	UNP P13470
C	600	LYS	ARG	SEE REMARK 999	UNP P13470
C	727	ILE	THR	SEE REMARK 999	UNP P13470
C	734	VAL	ALA	SEE REMARK 999	UNP P13470
D	597	ASP	ASN	SEE REMARK 999	UNP P13470

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Chain	Residue	Modelled	Actual	Comment	Reference
D	600	LYS	ARG	SEE REMARK 999	UNP P13470
D	727	ILE	THR	SEE REMARK 999	UNP P13470
D	734	VAL	ALA	SEE REMARK 999	UNP P13470
E	597	ASP	ASN	SEE REMARK 999	UNP P13470
E	600	LYS	ARG	SEE REMARK 999	UNP P13470
E	727	ILE	THR	SEE REMARK 999	UNP P13470
E	734	VAL	ALA	SEE REMARK 999	UNP P13470
F	597	ASP	ASN	SEE REMARK 999	UNP P13470
F	600	LYS	ARG	SEE REMARK 999	UNP P13470
F	727	ILE	THR	SEE REMARK 999	UNP P13470
F	734	VAL	ALA	SEE REMARK 999	UNP P13470
G	597	ASP	ASN	SEE REMARK 999	UNP P13470
G	600	LYS	ARG	SEE REMARK 999	UNP P13470
G	727	ILE	THR	SEE REMARK 999	UNP P13470
G	734	VAL	ALA	SEE REMARK 999	UNP P13470
H	597	ASP	ASN	SEE REMARK 999	UNP P13470
H	600	LYS	ARG	SEE REMARK 999	UNP P13470
H	727	ILE	THR	SEE REMARK 999	UNP P13470
H	734	VAL	ALA	SEE REMARK 999	UNP P13470

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	529	Total	O	0	0
			529	529		
4	B	528	Total	O	0	0
			528	528		
4	C	593	Total	O	0	0
			593	593		
4	D	592	Total	O	0	0
			592	592		

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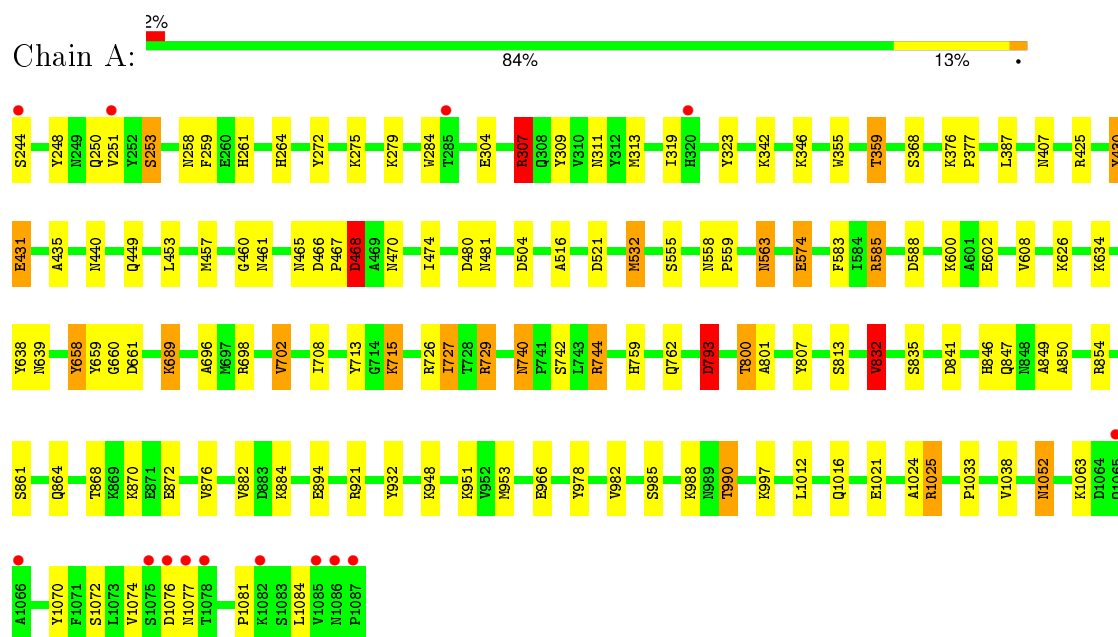
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	523	Total 523	O 523	0	0
4	F	485	Total 485	O 485	0	0
4	G	622	Total 622	O 622	0	0
4	H	575	Total 575	O 575	0	0

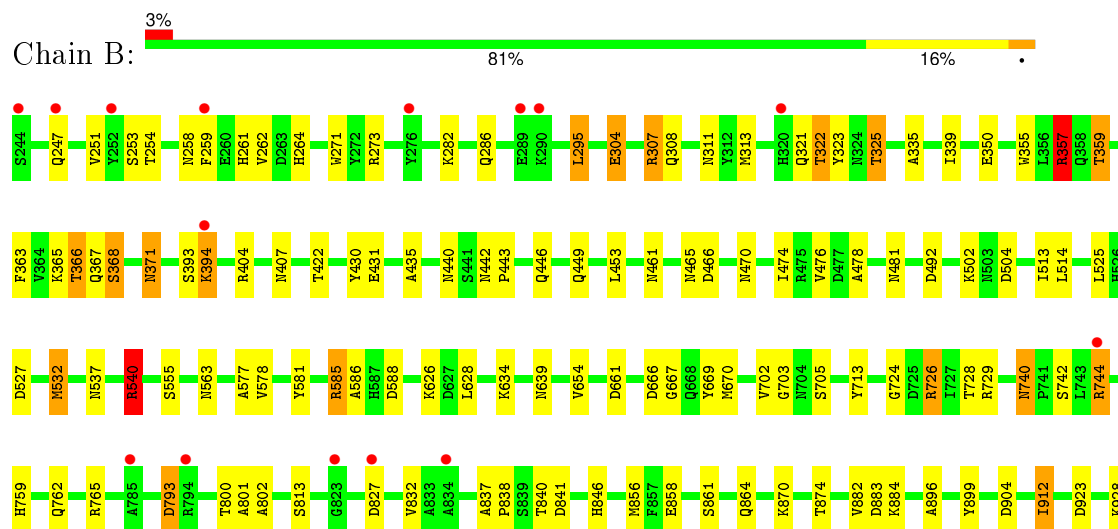
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

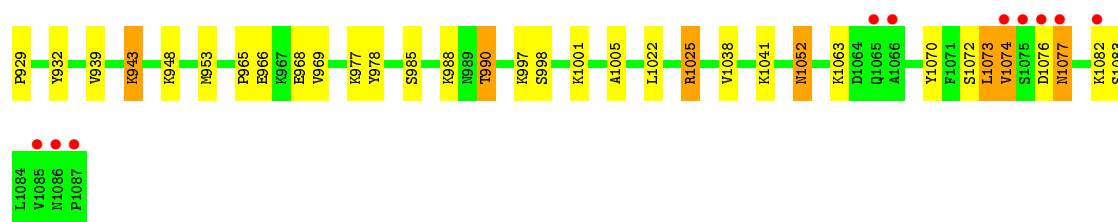
#### • Molecule 1: Glucosyltransferase-SI



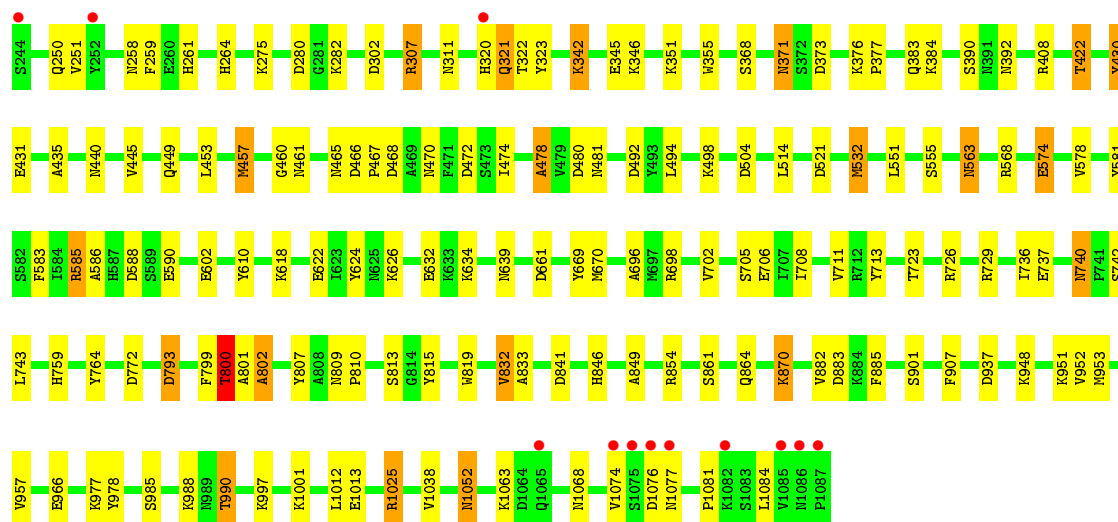
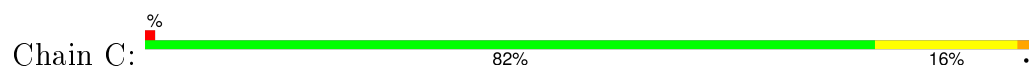
#### • Molecule 1: Glucosyltransferase-SI



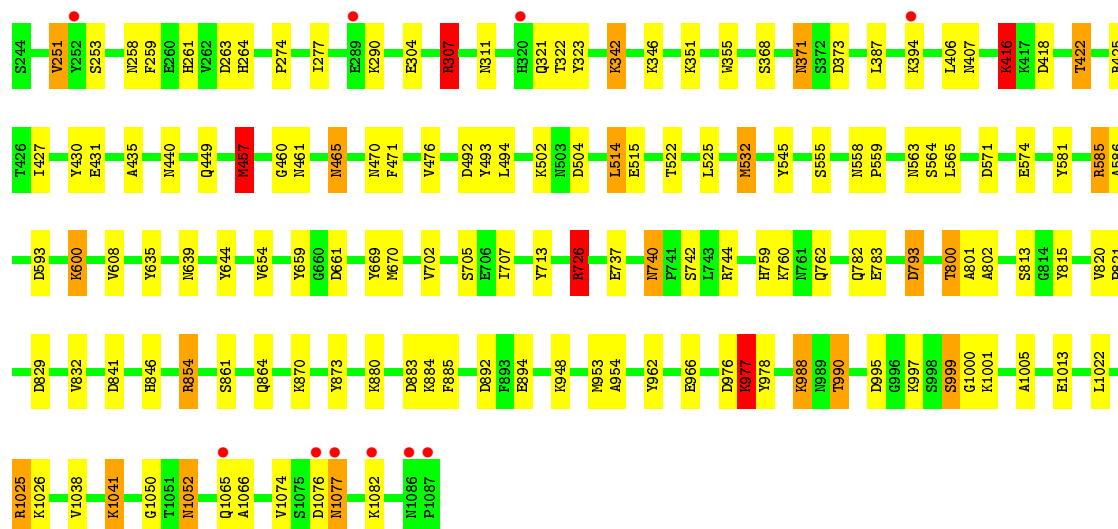
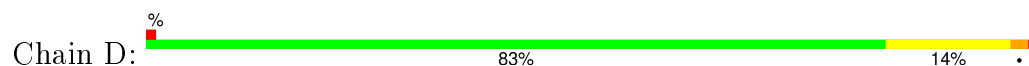




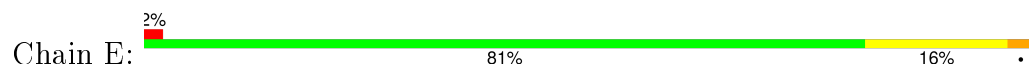
• Molecule 1: Glucosyltransferase-SI

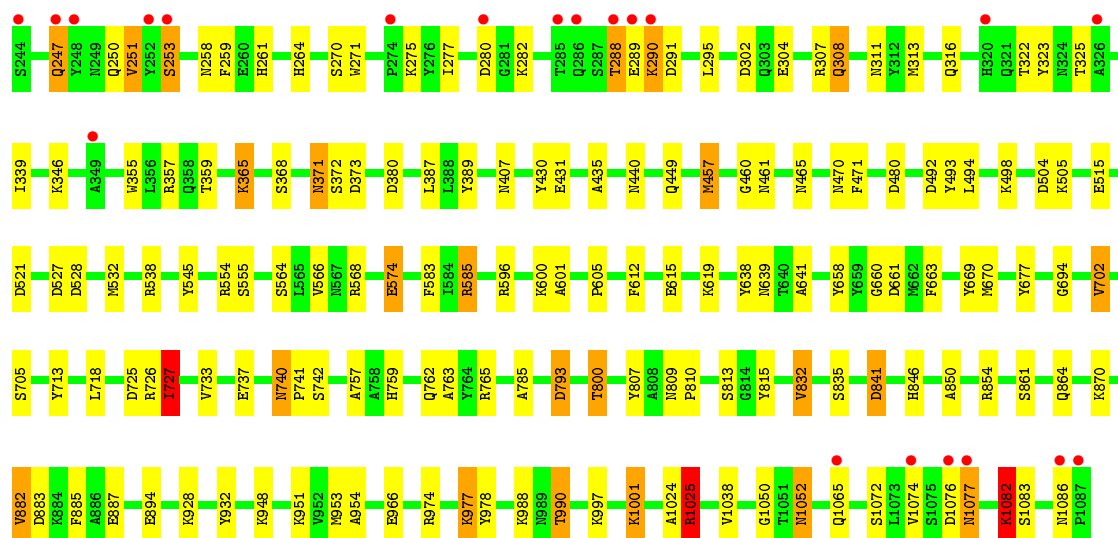


• Molecule 1: Glucosyltransferase-SI

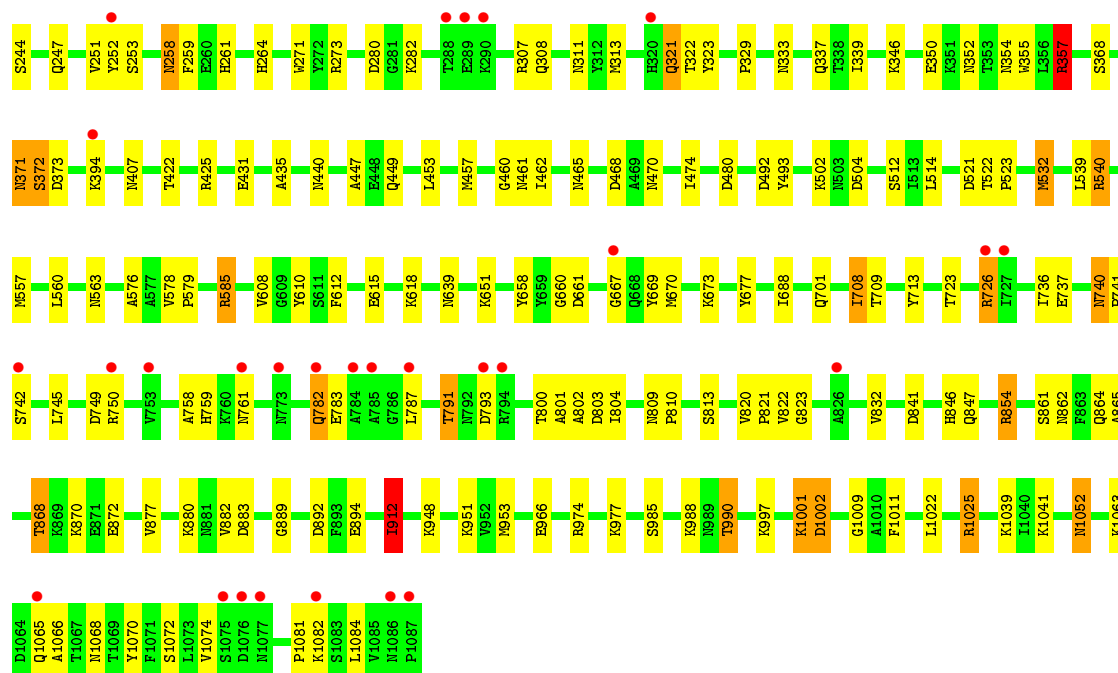
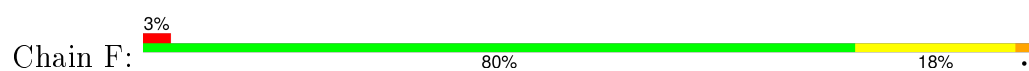


• Molecule 1: Glucosyltransferase-SI

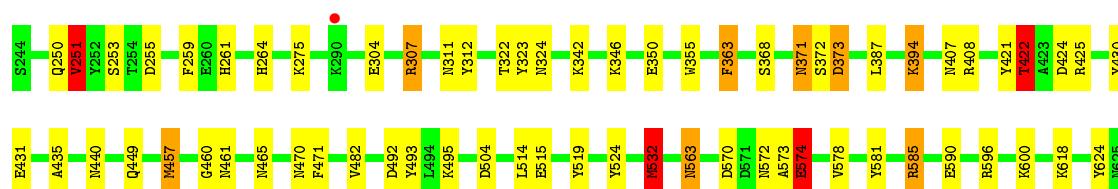
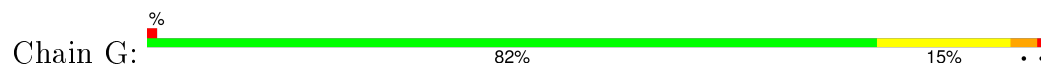


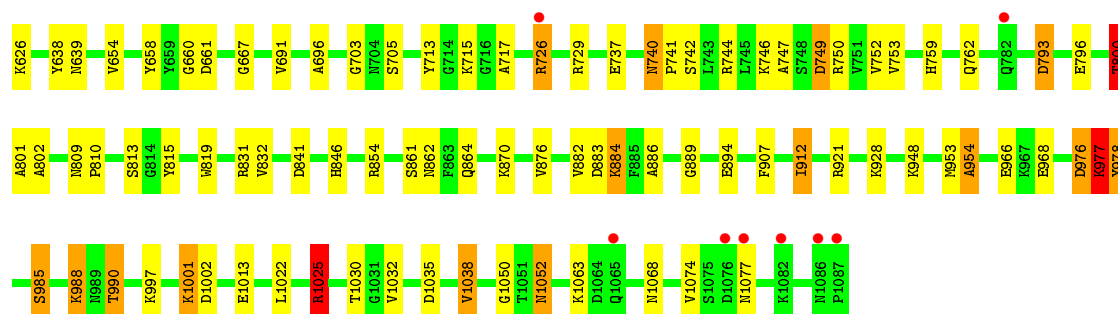


• Molecule 1: Glucosyltransferase-SI

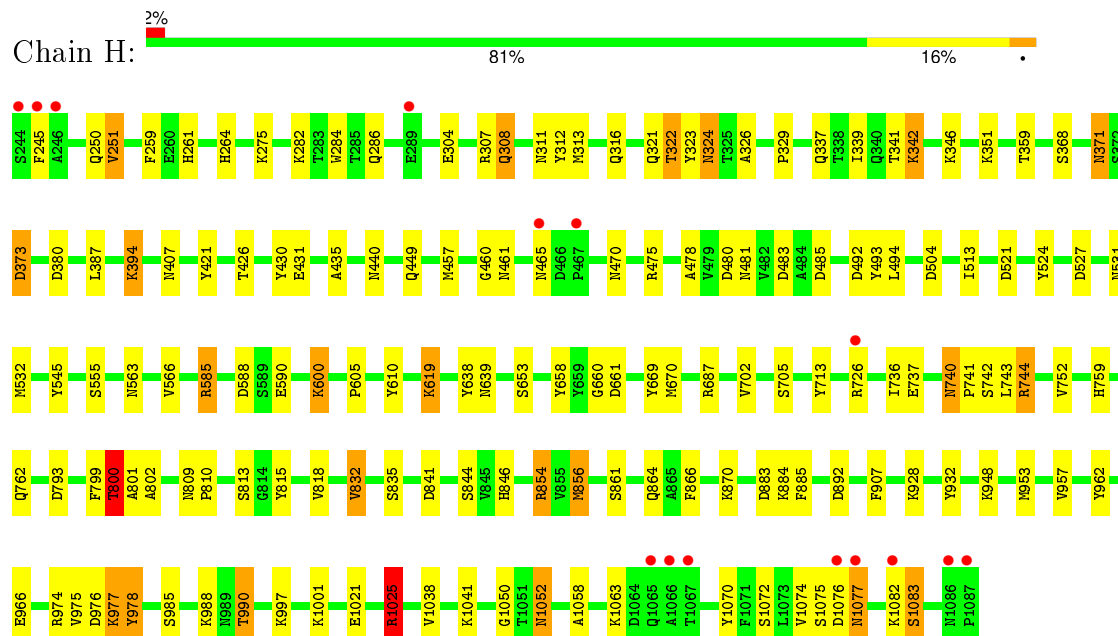


• Molecule 1: Glucosyltransferase-SI





● Molecule 1: Glucosyltransferase-SI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	293.88Å 215.42Å 218.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.10) 99.6 (50.00-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.91 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.203 , 0.236 0.208 , 0.235	Depositor DCC
$R_{free}$ test set	39655 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.1	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 792885 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	57830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.73 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6894e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.34	30/6802 (0.4%)	1.20	30/9237 (0.3%)
1	B	1.19	11/6801 (0.2%)	1.15	30/9237 (0.3%)
1	C	1.32	39/6802 (0.6%)	1.17	31/9237 (0.3%)
1	D	1.31	27/6802 (0.4%)	1.22	31/9237 (0.3%)
1	E	1.37	37/6802 (0.5%)	1.23	34/9237 (0.4%)
1	F	1.13	10/6802 (0.1%)	1.12	30/9237 (0.3%)
1	G	1.42	47/6802 (0.7%)	1.30	36/9237 (0.4%)
1	H	1.28	26/6802 (0.4%)	1.18	29/9237 (0.3%)
All	All	1.30	227/54415 (0.4%)	1.20	251/73896 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	1	0

All (227) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1083	SER	CB-OG	12.42	1.58	1.42
1	E	574	GLU	CB-CG	-10.80	1.31	1.52
1	C	574	GLU	CB-CG	-10.38	1.32	1.52
1	G	421	TYR	CD2-CE2	9.85	1.54	1.39
1	H	371	ASN	CB-CG	-9.70	1.28	1.51
1	F	540	ARG	C-N	9.61	1.56	1.34
1	A	307	ARG	CG-CD	8.47	1.73	1.51
1	A	555	SER	CB-OG	-8.43	1.31	1.42
1	D	854	ARG	CD-NE	-8.34	1.32	1.46
1	C	807	TYR	CD2-CE2	8.23	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	667	GLY	N-CA	8.20	1.58	1.46
1	C	478	ALA	CA-CB	7.99	1.69	1.52
1	B	540	ARG	CD-NE	-7.95	1.32	1.46
1	H	566	VAL	CB-CG1	7.88	1.69	1.52
1	A	638	TYR	CD2-CE2	7.86	1.51	1.39
1	C	854	ARG	CD-NE	-7.83	1.33	1.46
1	H	1021	GLU	CB-CG	7.68	1.66	1.52
1	B	555	SER	CB-OG	-7.64	1.32	1.42
1	E	854	ARG	CD-NE	-7.48	1.33	1.46
1	G	372	SER	CB-OG	-7.43	1.32	1.42
1	G	251	VAL	CB-CG2	-7.42	1.37	1.52
1	C	602	GLU	CG-CD	-7.41	1.40	1.51
1	D	608	VAL	CB-CG2	7.40	1.68	1.52
1	H	800	THR	CB-CG2	-7.36	1.28	1.52
1	G	371	ASN	CB-CG	-7.21	1.34	1.51
1	G	854	ARG	CD-NE	-7.21	1.34	1.46
1	E	372	SER	CB-OG	-7.15	1.32	1.42
1	C	371	ASN	CA-CB	7.14	1.71	1.53
1	C	555	SER	CB-OG	-7.11	1.33	1.42
1	C	590	GLU	CB-CG	7.10	1.65	1.52
1	C	849	ALA	CA-CB	7.06	1.67	1.52
1	A	876	VAL	CB-CG1	7.03	1.67	1.52
1	D	1025	ARG	CD-NE	-7.03	1.34	1.46
1	A	696	ALA	CA-CB	7.01	1.67	1.52
1	C	422	THR	CB-CG2	-6.90	1.29	1.52
1	B	371	ASN	CB-CG	-6.89	1.35	1.51
1	G	624	TYR	CD2-CE2	6.86	1.49	1.39
1	B	476	VAL	CB-CG2	6.85	1.67	1.52
1	E	545	TYR	CD2-CE2	6.84	1.49	1.39
1	C	371	ASN	CB-CG	-6.82	1.35	1.51
1	G	793	ASP	CB-CG	-6.78	1.37	1.51
1	F	371	ASN	CB-CG	-6.78	1.35	1.51
1	G	876	VAL	CB-CG1	6.77	1.67	1.52
1	D	545	TYR	CD2-CE2	6.74	1.49	1.39
1	D	962	TYR	CD1-CE1	6.71	1.49	1.39
1	G	574	GLU	CG-CD	-6.67	1.42	1.51
1	G	886	ALA	CA-CB	6.65	1.66	1.52
1	A	574	GLU	CD-OE2	-6.56	1.18	1.25
1	H	818	VAL	CB-CG2	6.45	1.66	1.52
1	D	585	ARG	CD-NE	-6.43	1.35	1.46
1	C	711	VAL	CB-CG1	6.39	1.66	1.52
1	G	573	ALA	CA-CB	6.35	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	654	VAL	CB-CG2	6.26	1.66	1.52
1	E	1082	LYS	CB-CG	6.26	1.69	1.52
1	G	371	ASN	CA-CB	6.26	1.69	1.53
1	H	304	GLU	CG-CD	6.24	1.61	1.51
1	D	555	SER	CB-OG	-6.21	1.34	1.42
1	C	585	ARG	CD-NE	-6.20	1.35	1.46
1	G	977	LYS	CB-CG	-6.17	1.35	1.52
1	A	608	VAL	CB-CG2	6.17	1.65	1.52
1	H	793	ASP	CB-CG	-6.16	1.38	1.51
1	E	515	GLU	CB-CG	6.10	1.63	1.52
1	G	978	TYR	CD2-CE2	6.10	1.48	1.39
1	C	430	TYR	CD1-CE1	6.10	1.48	1.39
1	B	899	TYR	CD2-CE2	6.07	1.48	1.39
1	G	1025	ARG	CD-NE	-6.05	1.36	1.46
1	G	1025	ARG	CG-CD	6.04	1.67	1.51
1	H	555	SER	CB-OG	-6.02	1.34	1.42
1	E	887	GLU	CG-CD	6.00	1.60	1.51
1	A	431	GLU	CG-CD	6.00	1.60	1.51
1	E	807	TYR	CD2-CE2	6.00	1.48	1.39
1	C	802	ALA	CA-CB	5.97	1.65	1.52
1	B	896	ALA	CA-CB	5.97	1.65	1.52
1	G	696	ALA	CA-CB	5.97	1.65	1.52
1	G	618	LYS	CE-NZ	5.97	1.64	1.49
1	F	1025	ARG	CD-NE	-5.96	1.36	1.46
1	H	653	SER	CB-OG	5.95	1.50	1.42
1	A	1021	GLU	CG-CD	5.95	1.60	1.51
1	G	618	LYS	CB-CG	5.94	1.68	1.52
1	C	800	THR	CB-CG2	-5.94	1.32	1.52
1	G	667	GLY	N-CA	5.92	1.54	1.46
1	E	566	VAL	CB-CG2	5.92	1.65	1.52
1	F	608	VAL	CB-CG2	5.92	1.65	1.52
1	A	932	TYR	CD1-CE1	5.92	1.48	1.39
1	E	583	PHE	CE1-CZ	5.89	1.48	1.37
1	C	957	VAL	CB-CG2	5.89	1.65	1.52
1	G	1002	ASP	CB-CG	5.88	1.64	1.51
1	F	1002	ASP	CB-CG	-5.88	1.39	1.51
1	A	468	ASP	CB-CG	-5.86	1.39	1.51
1	G	819	TRP	CG-CD1	5.86	1.45	1.36
1	H	1041	LYS	CD-CE	5.85	1.65	1.51
1	E	793	ASP	CB-CG	-5.84	1.39	1.51
1	A	563	ASN	CB-CG	5.83	1.64	1.51
1	E	585	ARG	CD-NE	-5.82	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	590	GLU	CB-CG	5.82	1.63	1.52
1	A	847	GLN	CB-CG	5.81	1.68	1.52
1	G	638	TYR	CD2-CE2	5.80	1.48	1.39
1	C	833	ALA	CA-CB	5.79	1.64	1.52
1	C	624	TYR	CD1-CE1	5.79	1.48	1.39
1	C	953	MET	C-N	-5.78	1.20	1.34
1	A	658	TYR	CD2-CE2	5.77	1.48	1.39
1	H	978	TYR	CD1-CE1	5.77	1.48	1.39
1	G	854	ARG	CB-CG	5.77	1.68	1.52
1	C	764	TYR	CD1-CE1	-5.76	1.30	1.39
1	D	581	TYR	CD1-CE1	5.76	1.48	1.39
1	D	515	GLU	CG-CD	5.73	1.60	1.51
1	H	545	TYR	CD2-CE2	5.72	1.48	1.39
1	F	447	ALA	CA-CB	5.71	1.64	1.52
1	G	752	VAL	CB-CG2	5.71	1.64	1.52
1	C	793	ASP	CB-CG	-5.70	1.39	1.51
1	A	982	VAL	CB-CG1	5.70	1.64	1.52
1	E	757	ALA	CA-CB	5.70	1.64	1.52
1	D	457	MET	CB-CG	-5.69	1.33	1.51
1	D	854	ARG	CB-CG	5.69	1.68	1.52
1	E	564	SER	CB-OG	5.69	1.49	1.42
1	A	793	ASP	CB-CG	-5.68	1.39	1.51
1	H	752	VAL	CB-CG2	5.68	1.64	1.52
1	G	590	GLU	CB-CG	5.65	1.62	1.52
1	B	968	GLU	CG-CD	5.65	1.60	1.51
1	G	585	ARG	CD-NE	-5.64	1.36	1.46
1	H	977	LYS	CB-CG	-5.63	1.37	1.52
1	B	540	ARG	CG-CD	5.61	1.66	1.51
1	F	1002	ASP	CA-CB	5.60	1.66	1.53
1	A	849	ALA	CA-CB	5.59	1.64	1.52
1	E	882	VAL	CB-CG2	-5.59	1.41	1.52
1	E	555	SER	CB-OG	-5.57	1.35	1.42
1	F	372	SER	CB-OG	-5.57	1.35	1.42
1	G	578	VAL	CB-CG2	5.56	1.64	1.52
1	F	512	SER	CB-OG	5.55	1.49	1.42
1	G	907	PHE	CE2-CZ	5.54	1.47	1.37
1	C	901	SER	CB-OG	5.54	1.49	1.42
1	E	365	LYS	CD-CE	5.53	1.65	1.51
1	C	574	GLU	CG-CD	-5.52	1.43	1.51
1	D	800	THR	CB-CG2	-5.51	1.34	1.52
1	E	515	GLU	CG-CD	5.51	1.60	1.51
1	E	641	ALA	CA-CB	5.51	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	785	ALA	CA-CB	5.51	1.64	1.52
1	D	371	ASN	CA-CB	5.50	1.67	1.53
1	E	1025	ARG	CD-NE	-5.49	1.37	1.46
1	E	585	ARG	CG-CD	5.49	1.65	1.51
1	H	962	TYR	CD1-CE1	5.49	1.47	1.39
1	C	586	ALA	CA-CB	5.49	1.64	1.52
1	D	793	ASP	CB-CG	-5.49	1.40	1.51
1	H	371	ASN	CA-CB	5.48	1.67	1.53
1	D	644	TYR	CD2-CE2	5.46	1.47	1.39
1	E	677	TYR	CD1-CE1	5.46	1.47	1.39
1	B	307	ARG	CG-CD	5.45	1.65	1.51
1	H	426	THR	CB-CG2	5.45	1.70	1.52
1	G	307	ARG	CG-CD	5.44	1.65	1.51
1	C	610	TYR	CD2-CE2	5.44	1.47	1.39
1	C	563	ASN	CB-CG	5.42	1.63	1.51
1	G	954	ALA	CA-CB	5.40	1.63	1.52
1	E	850	ALA	CA-CB	5.40	1.63	1.52
1	D	977	LYS	CD-CE	5.40	1.64	1.51
1	A	850	ALA	CA-CB	5.39	1.63	1.52
1	C	632	GLU	CG-CD	5.39	1.60	1.51
1	G	717	ALA	CA-CB	5.39	1.63	1.52
1	H	932	TYR	CE2-CZ	5.38	1.45	1.38
1	G	519	TYR	CD1-CE1	5.38	1.47	1.39
1	D	635	TYR	CE2-CZ	5.38	1.45	1.38
1	D	465	ASN	CB-CG	-5.37	1.38	1.51
1	A	602	GLU	CG-CD	-5.36	1.44	1.51
1	H	866	PHE	CE2-CZ	5.36	1.47	1.37
1	B	939	VAL	CB-CG1	5.35	1.64	1.52
1	C	696	ALA	CA-CB	5.34	1.63	1.52
1	C	706	GLU	CG-CD	5.34	1.59	1.51
1	E	638	TYR	CD1-CE1	5.34	1.47	1.39
1	C	431	GLU	CB-CG	5.33	1.62	1.52
1	D	783	GLU	CB-CG	-5.33	1.42	1.52
1	E	800	THR	CB-CG2	-5.32	1.34	1.52
1	H	957	VAL	CB-CG2	5.31	1.64	1.52
1	C	819	TRP	CG-CD1	5.29	1.44	1.36
1	G	884	LYS	CB-CG	-5.29	1.38	1.52
1	C	907	PHE	CD2-CE2	5.29	1.49	1.39
1	D	586	ALA	CA-CB	5.29	1.63	1.52
1	C	583	PHE	CE1-CZ	5.29	1.47	1.37
1	G	563	ASN	CB-CG	5.28	1.63	1.51
1	G	638	TYR	CD1-CE1	5.28	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	638	TYR	CD1-CE1	5.28	1.47	1.39
1	D	726	ARG	CG-CD	5.28	1.65	1.51
1	C	307	ARG	CG-CD	5.27	1.65	1.51
1	G	363	PHE	CE2-CZ	5.27	1.47	1.37
1	G	921	ARG	CD-NE	5.26	1.55	1.46
1	H	975	VAL	CB-CG2	5.25	1.63	1.52
1	E	1025	ARG	CG-CD	5.24	1.65	1.51
1	C	622	GLU	CG-CD	5.22	1.59	1.51
1	A	1038	VAL	C-N	-5.22	1.22	1.34
1	A	585	ARG	CG-CD	5.22	1.65	1.51
1	C	581	TYR	CD2-CE2	5.21	1.47	1.39
1	A	1024	ALA	C-N	5.21	1.46	1.34
1	G	889	GLY	N-CA	5.21	1.53	1.46
1	A	430	TYR	CD1-CE1	5.19	1.47	1.39
1	A	807	TYR	CD2-CE2	5.18	1.47	1.39
1	D	1041	LYS	CD-CE	5.17	1.64	1.51
1	C	952	VAL	C-N	-5.16	1.22	1.34
1	D	659	TYR	CD2-CE2	5.16	1.47	1.39
1	H	1058	ALA	CA-CB	5.16	1.63	1.52
1	D	564	SER	CB-OG	5.16	1.49	1.42
1	E	1024	ALA	CA-CB	5.14	1.63	1.52
1	G	968	GLU	CG-CD	5.14	1.59	1.51
1	A	457	MET	CB-CG	-5.13	1.34	1.51
1	G	482	VAL	CB-CG2	5.13	1.63	1.52
1	E	733	VAL	CB-CG2	5.13	1.63	1.52
1	A	659	TYR	CD2-CE2	5.13	1.47	1.39
1	E	574	GLU	CG-CD	-5.13	1.44	1.51
1	E	601	ALA	CA-CB	5.11	1.63	1.52
1	E	615	GLU	CB-CG	5.11	1.61	1.52
1	E	932	TYR	CD1-CE1	5.10	1.47	1.39
1	G	800	THR	CB-CG2	-5.10	1.35	1.52
1	E	763	ALA	CA-CB	5.09	1.63	1.52
1	G	515	GLU	CB-CG	5.09	1.61	1.52
1	G	408	ARG	CZ-NH1	5.08	1.39	1.33
1	A	272	TYR	CD2-CE2	5.07	1.47	1.39
1	H	854	ARG	CG-CD	5.05	1.64	1.51
1	G	977	LYS	CD-CE	-5.05	1.38	1.51
1	G	691	VAL	CB-CG1	5.05	1.63	1.52
1	E	371	ASN	CA-CB	5.05	1.66	1.53
1	A	481	ASN	CG-ND2	-5.04	1.20	1.32
1	A	583	PHE	CE1-CZ	5.04	1.47	1.37
1	E	663	PHE	CE1-CZ	5.04	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	726	ARG	CG-CD	5.04	1.64	1.51
1	G	519	TYR	CE1-CZ	-5.04	1.31	1.38
1	A	832	VAL	CB-CG2	5.04	1.63	1.52
1	F	912	ILE	CB-CG2	5.03	1.68	1.52
1	D	476	VAL	CB-CG2	5.02	1.63	1.52
1	D	515	GLU	CD-OE2	-5.02	1.20	1.25
1	C	445	VAL	CB-CG1	5.01	1.63	1.52

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	854	ARG	NE-CZ-NH2	-35.02	102.79	120.30
1	A	854	ARG	NE-CZ-NH2	-33.32	103.64	120.30
1	D	854	ARG	NE-CZ-NH2	-33.26	103.67	120.30
1	E	854	ARG	NE-CZ-NH2	-32.09	104.26	120.30
1	B	540	ARG	NE-CZ-NH2	-31.61	104.50	120.30
1	G	1025	ARG	NE-CZ-NH2	-31.34	104.63	120.30
1	E	1025	ARG	NE-CZ-NH2	-27.68	106.46	120.30
1	D	1025	ARG	NE-CZ-NH2	-27.22	106.69	120.30
1	H	854	ARG	NE-CZ-NH2	-26.76	106.92	120.30
1	C	854	ARG	NE-CZ-NH2	-26.17	107.21	120.30
1	G	854	ARG	NE-CZ-NH1	25.05	132.82	120.30
1	H	1025	ARG	NE-CZ-NH2	-24.61	108.00	120.30
1	C	1025	ARG	NE-CZ-NH2	-24.14	108.23	120.30
1	F	1025	ARG	NE-CZ-NH2	-23.04	108.78	120.30
1	A	854	ARG	NE-CZ-NH1	22.28	131.44	120.30
1	D	1025	ARG	NE-CZ-NH1	21.84	131.22	120.30
1	H	1025	ARG	NE-CZ-NH1	21.79	131.19	120.30
1	G	585	ARG	NE-CZ-NH2	-21.69	109.45	120.30
1	E	854	ARG	NE-CZ-NH1	21.15	130.88	120.30
1	A	585	ARG	NE-CZ-NH2	-20.61	109.99	120.30
1	G	1025	ARG	NE-CZ-NH1	20.21	130.40	120.30
1	G	585	ARG	NE-CZ-NH1	20.17	130.38	120.30
1	B	1025	ARG	NE-CZ-NH2	-19.76	110.42	120.30
1	E	1025	ARG	NE-CZ-NH1	19.21	129.90	120.30
1	H	854	ARG	NE-CZ-NH1	18.95	129.77	120.30
1	F	854	ARG	NE-CZ-NH2	-18.27	111.17	120.30
1	H	585	ARG	NE-CZ-NH1	17.21	128.91	120.30
1	D	854	ARG	NE-CZ-NH1	17.17	128.89	120.30
1	B	540	ARG	NE-CZ-NH1	17.07	128.84	120.30
1	H	585	ARG	NE-CZ-NH2	-17.07	111.77	120.30
1	D	585	ARG	NE-CZ-NH2	-16.93	111.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1025	ARG	NE-CZ-NH1	16.37	128.49	120.30
1	C	1025	ARG	NE-CZ-NH1	16.36	128.48	120.30
1	E	585	ARG	NE-CZ-NH2	-16.35	112.12	120.30
1	C	854	ARG	NE-CZ-NH1	15.95	128.27	120.30
1	A	585	ARG	NE-CZ-NH1	15.76	128.18	120.30
1	F	307	ARG	NE-CZ-NH2	-15.51	112.54	120.30
1	D	585	ARG	NE-CZ-NH1	14.70	127.65	120.30
1	F	357	ARG	NE-CZ-NH1	14.45	127.52	120.30
1	E	585	ARG	NE-CZ-NH1	14.21	127.41	120.30
1	C	585	ARG	NE-CZ-NH1	13.96	127.28	120.30
1	F	585	ARG	NE-CZ-NH2	-13.91	113.34	120.30
1	F	357	ARG	NE-CZ-NH2	-13.88	113.36	120.30
1	C	585	ARG	NE-CZ-NH2	-13.61	113.50	120.30
1	B	1025	ARG	NE-CZ-NH1	13.55	127.07	120.30
1	B	585	ARG	NE-CZ-NH1	13.28	126.94	120.30
1	B	357	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	A	793	ASP	CB-CG-OD1	-13.14	106.48	118.30
1	B	585	ARG	NE-CZ-NH2	-12.97	113.81	120.30
1	F	585	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	F	1002	ASP	CB-CG-OD1	-11.99	107.51	118.30
1	F	1002	ASP	CB-CG-OD2	11.39	128.56	118.30
1	G	793	ASP	CB-CG-OD1	-10.59	108.77	118.30
1	G	307	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	D	371	ASN	CB-CA-C	-10.47	89.45	110.40
1	A	854	ARG	CD-NE-CZ	10.42	138.19	123.60
1	G	408	ARG	NE-CZ-NH2	-10.25	115.17	120.30
1	B	666	ASP	C-N-CA	-10.15	100.99	122.30
1	H	856	MET	CG-SD-CE	-10.12	84.02	100.20
1	E	977	LYS	CD-CE-NZ	-9.73	89.32	111.70
1	F	854	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	D	1025	ARG	CD-NE-CZ	9.25	136.55	123.60
1	C	302	ASP	CB-CG-OD1	9.23	126.61	118.30
1	G	1025	ARG	CD-NE-CZ	9.22	136.50	123.60
1	G	1025	ARG	CG-CD-NE	-9.20	92.48	111.80
1	F	357	ARG	CD-NE-CZ	8.91	136.07	123.60
1	G	831	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	B	540	ARG	CD-NE-CZ	8.73	135.83	123.60
1	E	854	ARG	CD-NE-CZ	8.56	135.59	123.60
1	G	408	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	E	1025	ARG	CD-NE-CZ	8.46	135.44	123.60
1	B	295	LEU	CA-CB-CG	8.41	134.65	115.30
1	G	854	ARG	CD-NE-CZ	8.41	135.37	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1025	ARG	CD-NE-CZ	8.30	135.22	123.60
1	B	357	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	D	854	ARG	CD-NE-CZ	8.10	134.93	123.60
1	H	832	VAL	CG1-CB-CG2	7.98	123.67	110.90
1	C	1025	ARG	CG-CD-NE	-7.96	95.09	111.80
1	F	793	ASP	CB-CG-OD1	-7.84	111.25	118.30
1	E	1025	ARG	CG-CD-NE	-7.83	95.35	111.80
1	F	974	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	F	307	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	H	854	ARG	CG-CD-NE	-7.66	95.71	111.80
1	G	912	ILE	CA-CB-CG1	-7.59	96.58	111.00
1	E	727	ILE	CG1-CB-CG2	7.35	127.57	111.40
1	D	854	ARG	CG-CD-NE	-7.33	96.41	111.80
1	D	263	ASP	CB-CG-OD2	7.25	124.83	118.30
1	H	793	ASP	N-CA-CB	-7.23	97.59	110.60
1	D	1025	ARG	CG-CD-NE	-7.22	96.63	111.80
1	A	1025	ARG	O-C-N	7.21	134.23	122.70
1	B	977	LYS	CA-CB-CG	7.21	129.25	113.40
1	C	854	ARG	CG-CD-NE	-7.19	96.71	111.80
1	C	1025	ARG	CD-NE-CZ	7.18	133.65	123.60
1	F	357	ARG	CG-CD-NE	7.16	126.84	111.80
1	H	585	ARG	CD-NE-CZ	7.12	133.57	123.60
1	B	540	ARG	CG-CD-NE	-7.11	96.88	111.80
1	G	585	ARG	CD-NE-CZ	7.10	133.54	123.60
1	A	532	MET	CA-CB-CG	7.05	125.28	113.30
1	E	585	ARG	CD-NE-CZ	7.04	133.46	123.60
1	G	715	LYS	CD-CE-NZ	-7.02	95.55	111.70
1	A	1024	ALA	O-C-N	-7.01	111.48	122.70
1	H	854	ARG	CD-NE-CZ	6.92	133.29	123.60
1	D	307	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	E	951	LYS	CD-CE-NZ	-6.86	95.93	111.70
1	B	357	ARG	CD-NE-CZ	6.85	133.19	123.60
1	F	372	SER	CB-CA-C	-6.81	97.16	110.10
1	B	295	LEU	CB-CG-CD1	-6.81	99.43	111.00
1	C	634	LYS	CD-CE-NZ	-6.79	96.08	111.70
1	D	593	ASP	CB-CG-OD2	6.76	124.38	118.30
1	H	371	ASN	CB-CG-OD1	-6.76	108.08	121.60
1	D	514	LEU	CB-CG-CD2	6.72	122.43	111.00
1	E	841	ASP	CB-CG-OD1	6.71	124.33	118.30
1	E	568	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	H	527	ASP	CB-CG-OD2	6.63	124.26	118.30
1	A	585	ARG	CD-NE-CZ	6.62	132.87	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	772	ASP	CB-CG-OD1	6.62	124.26	118.30
1	H	977	LYS	CD-CE-NZ	-6.60	96.53	111.70
1	F	912	ILE	CG1-CB-CG2	6.59	125.90	111.40
1	B	588	ASP	CB-CG-OD1	6.58	124.23	118.30
1	F	1025	ARG	CG-CD-NE	-6.54	98.06	111.80
1	G	1038	VAL	CG1-CB-CG2	6.52	121.33	110.90
1	C	568	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	502	LYS	CD-CE-NZ	-6.47	96.83	111.70
1	A	744	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	H	1025	ARG	CG-CD-NE	-6.46	98.24	111.80
1	G	307	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	G	744	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	E	527	ASP	CB-CG-OD2	6.37	124.03	118.30
1	G	854	ARG	CG-CD-NE	-6.34	98.48	111.80
1	A	425	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	C	854	ARG	CD-NE-CZ	6.30	132.43	123.60
1	F	1025	ARG	CD-NE-CZ	6.29	132.41	123.60
1	D	726	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	E	832	VAL	CG1-CB-CG2	6.26	120.92	110.90
1	H	588	ASP	CB-CG-OD1	6.26	123.93	118.30
1	H	687	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	E	702	VAL	CB-CA-C	-6.16	99.69	111.40
1	G	1035	ASP	CB-CG-OD1	6.15	123.84	118.30
1	G	532	MET	CB-CG-SD	6.15	130.85	112.40
1	A	951	LYS	CD-CE-NZ	-6.13	97.61	111.70
1	E	727	ILE	CB-CA-C	-6.12	99.36	111.60
1	A	832	VAL	CG1-CB-CG2	6.12	120.69	110.90
1	C	793	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	A	948	LYS	CD-CE-NZ	-6.10	97.67	111.70
1	G	422	THR	OG1-CB-CG2	6.10	124.03	110.00
1	D	585	ARG	CD-NE-CZ	6.08	132.12	123.60
1	G	424	ASP	CB-CG-OD1	6.07	123.77	118.30
1	H	307	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	G	372	SER	CB-CA-C	-6.06	98.59	110.10
1	B	912	ILE	CG1-CB-CG2	6.05	124.71	111.40
1	C	371	ASN	CB-CG-OD1	-6.03	109.55	121.60
1	E	251	VAL	CG1-CB-CG2	6.02	120.53	110.90
1	A	715	LYS	CD-CE-NZ	-6.00	97.91	111.70
1	G	373	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	359	THR	OG1-CB-CG2	-5.94	96.34	110.00
1	D	585	ARG	CG-CD-NE	-5.92	99.36	111.80
1	D	999	SER	C-N-CA	-5.91	109.88	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	502	LYS	CB-CG-CD	-5.88	96.31	111.60
1	B	765	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	976	ASP	CB-CG-OD1	5.85	123.57	118.30
1	F	1001	LYS	C-N-CA	5.85	136.33	121.70
1	B	1025	ARG	CG-CD-NE	-5.84	99.53	111.80
1	E	765	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	B	1025	ARG	CD-NE-CZ	5.83	131.76	123.60
1	A	727	ILE	CG1-CB-CG2	-5.81	98.61	111.40
1	A	854	ARG	CG-CD-NE	-5.78	99.66	111.80
1	A	1025	ARG	CA-C-N	-5.77	104.51	117.20
1	C	371	ASN	CB-CA-C	-5.75	98.89	110.40
1	E	854	ARG	CG-CD-NE	-5.75	99.73	111.80
1	B	904	ASP	CB-CG-OD2	5.74	123.47	118.30
1	E	288	THR	CB-CA-C	-5.72	96.17	111.60
1	D	854	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	D	571	ASP	CB-CG-OD2	-5.69	113.17	118.30
1	A	634	LYS	CD-CE-NZ	-5.69	98.62	111.70
1	G	800	THR	N-CA-CB	-5.67	99.53	110.30
1	G	373	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	E	800	THR	CA-CB-CG2	5.63	120.29	112.40
1	E	800	THR	OG1-CB-CG2	5.63	122.95	110.00
1	F	651	LYS	CD-CE-NZ	-5.63	98.76	111.70
1	E	800	THR	N-CA-CB	-5.60	99.67	110.30
1	A	835	SER	N-CA-CB	-5.59	102.11	110.50
1	E	974	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	282	LYS	CD-CE-NZ	5.57	124.52	111.70
1	H	976	ASP	CB-CG-OD1	5.56	123.31	118.30
1	D	999	SER	N-CA-C	-5.56	96.00	111.00
1	H	974	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	F	371	ASN	CB-CA-C	-5.54	99.32	110.40
1	C	422	THR	CA-CB-CG2	5.54	120.16	112.40
1	A	990	THR	OG1-CB-CG2	-5.52	97.31	110.00
1	H	483	ASP	CB-CG-OD1	5.51	123.25	118.30
1	G	371	ASN	CB-CA-C	-5.50	99.40	110.40
1	H	380	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	588	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	585	ARG	CD-NE-CZ	5.48	131.27	123.60
1	C	953	MET	O-C-N	-5.48	113.94	122.70
1	G	255	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	E	498	LYS	CD-CE-NZ	-5.44	99.18	111.70
1	B	404	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	B	923	ASP	CB-CG-OD1	5.43	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	C	588	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	702	VAL	CB-CA-C	-5.41	101.12	111.40
1	F	1041	LYS	CD-CE-NZ	-5.40	99.28	111.70
1	B	540	ARG	NH1-CZ-NH2	5.40	125.34	119.40
1	E	793	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	H	371	ASN	CB-CA-C	-5.36	99.68	110.40
1	B	527	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	921	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	585	ARG	CD-NE-CZ	5.33	131.07	123.60
1	C	498	LYS	CD-CE-NZ	-5.32	99.47	111.70
1	A	1021	GLU	OE1-CD-OE2	-5.32	116.92	123.30
1	F	578	VAL	CB-CA-C	-5.31	101.31	111.40
1	E	380	ASP	CB-CG-OD1	5.31	123.08	118.30
1	G	371	ASN	CB-CG-OD1	-5.31	110.98	121.60
1	G	976	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	574	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	E	554	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	527	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	H	485	ASP	CB-CG-OD1	5.27	123.04	118.30
1	F	468	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	C	618	LYS	CD-CE-NZ	5.23	123.73	111.70
1	D	829	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	951	LYS	CD-CE-NZ	-5.21	99.71	111.70
1	H	373	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	468	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	F	307	ARG	CG-CD-NE	-5.20	100.88	111.80
1	A	387	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	H	977	LYS	N-CA-CB	-5.17	101.29	110.60
1	D	995	ASP	CB-CG-OD1	5.16	122.94	118.30
1	D	418	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	793	ASP	CB-CG-OD2	5.15	122.93	118.30
1	G	422	THR	N-CA-CB	-5.14	100.53	110.30
1	C	870	LYS	CD-CE-NZ	-5.13	99.89	111.70
1	C	408	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	472	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	628	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	G	912	ILE	CG1-CB-CG2	5.10	122.62	111.40
1	C	578	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	D	995	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	E	585	ARG	CG-CD-NE	-5.09	101.11	111.80
1	E	538	ARG	NE-CZ-NH1	-5.08	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	416	LYS	CD-CE-NZ	-5.08	100.01	111.70
1	G	749	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	C	832	VAL	CG1-CB-CG2	5.04	118.96	110.90
1	B	977	LYS	CB-CA-C	-5.04	100.33	110.40
1	F	560	LEU	CB-CG-CD2	-5.04	102.44	111.00
1	H	928	LYS	CD-CE-NZ	5.04	123.28	111.70
1	E	528	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	522	THR	CA-CB-CG2	-5.02	105.37	112.40
1	F	1002	ASP	N-CA-CB	-5.01	101.58	110.60
1	F	502	LYS	CD-CE-NZ	-5.01	100.19	111.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	800	THR	CB

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6660	0	6489	79	0
1	B	6659	0	6489	117	0
1	C	6660	0	6487	98	0
1	D	6660	0	6489	107	0
1	E	6660	0	6489	110	0
1	F	6660	0	6489	139	0
1	G	6660	0	6489	110	0
1	H	6660	0	6489	117	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1	0	0	0	0
3	A	12	0	12	0	0
3	B	12	0	12	2	0
3	C	12	0	12	0	0
3	D	12	0	12	1	0
3	E	12	0	12	0	0
3	F	12	0	12	0	0
3	G	12	0	12	0	0
3	H	12	0	12	1	0
4	A	529	0	0	8	0
4	B	528	0	0	13	0
4	C	593	0	0	10	0
4	D	592	0	0	15	0
4	E	523	0	0	2	0
4	F	485	0	0	10	0
4	G	622	0	0	13	0
4	H	575	0	0	5	0
All	All	57830	0	52006	878	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (878) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:475:ARG:HB2	1:H:953:MET:CE	1.39	1.52
1:G:394:LYS:CD	1:G:394:LYS:H	1.44	1.27
1:H:475:ARG:CB	1:H:953:MET:HE2	1.69	1.20
1:E:277:ILE:CD1	1:E:291:ASP:HB3	1.69	1.20
1:A:250:GLN:NE2	1:A:275:LYS:HE3	1.56	1.18
1:B:394:LYS:H	1:B:394:LYS:CE	1.55	1.18
1:A:250:GLN:HE21	1:A:275:LYS:HE3	1.08	1.13
1:H:475:ARG:CB	1:H:953:MET:CE	2.26	1.12
1:H:250:GLN:HE21	1:H:275:LYS:HE3	1.03	1.12
1:H:250:GLN:NE2	1:H:275:LYS:HE3	1.65	1.11
1:B:304:GLU:OE1	1:B:307:ARG:HD3	1.49	1.11
1:F:726:ARG:H	1:F:726:ARG:HD3	1.13	1.10
1:E:250:GLN:NE2	1:E:275:LYS:HE2	1.67	1.09
1:C:251:VAL:HG21	1:C:259:PHE:CZ	1.87	1.09
1:E:1082:LYS:HD3	1:E:1083:SER:H	1.14	1.08
1:H:475:ARG:HB2	1:H:953:MET:HE1	1.30	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:GLN:HE21	1:E:275:LYS:HE2	0.96	1.07
1:H:513:ILE:HG12	1:H:953:MET:HE3	1.24	1.07
1:F:759:HIS:O	1:F:791:THR:HG21	1.53	1.07
1:F:726:ARG:HG2	1:F:726:ARG:NH1	1.58	1.06
1:B:513:ILE:HD13	1:B:856:MET:HE2	1.37	1.06
1:E:288:THR:HG22	1:E:289:GLU:H	1.20	1.06
1:H:669:TYR:CE2	1:H:670:MET:HE3	1.93	1.04
1:D:669:TYR:CE2	1:D:670:MET:HE3	1.93	1.03
1:B:394:LYS:H	1:B:394:LYS:HE3	1.24	1.02
1:H:669:TYR:HE2	1:H:670:MET:HE3	1.23	1.02
1:F:726:ARG:N	1:F:726:ARG:HD3	1.66	1.02
1:G:394:LYS:HD2	1:G:394:LYS:H	1.19	1.02
1:H:475:ARG:HB2	1:H:953:MET:HE2	1.09	1.02
1:F:800:THR:HG22	1:F:801:ALA:N	1.74	1.02
1:H:670:MET:HE1	1:H:885:PHE:HZ	1.21	1.01
1:F:726:ARG:HH11	1:F:726:ARG:CG	1.73	1.01
1:C:669:TYR:CE2	1:C:670:MET:HE3	1.97	1.00
1:F:726:ARG:HH11	1:F:726:ARG:HG2	0.84	1.00
1:G:394:LYS:H	1:G:394:LYS:HD3	1.24	1.00
1:F:1063:LYS:HE2	1:F:1068:ASN:HD21	1.27	1.00
1:E:669:TYR:CE2	1:E:670:MET:HE3	1.97	0.99
1:C:861:SER:H	1:C:864:GLN:HE21	1.08	0.99
1:E:277:ILE:HD11	1:E:291:ASP:HB3	1.45	0.99
1:F:1063:LYS:HE2	1:F:1068:ASN:ND2	1.76	0.98
1:A:251:VAL:HG21	1:A:259:PHE:CZ	1.98	0.98
1:H:251:VAL:HG21	1:H:259:PHE:CZ	1.99	0.98
1:G:394:LYS:N	1:G:394:LYS:HD2	1.77	0.97
1:F:861:SER:H	1:F:864:GLN:HE21	1.04	0.97
1:D:416:LYS:HE2	4:D:2790:HOH:O	1.62	0.97
1:B:800:THR:HG22	1:B:802:ALA:H	1.27	0.96
1:C:1081:PRO:HG2	1:C:1084:LEU:HD12	1.48	0.96
1:G:394:LYS:N	1:G:394:LYS:CD	2.22	0.95
1:B:669:TYR:CE2	1:B:670:MET:CE	2.50	0.94
1:D:1013:GLU:HG2	4:D:3867:HOH:O	1.65	0.94
1:H:504:ASP:OD1	1:H:846:HIS:HD2	1.51	0.94
1:A:861:SER:H	1:A:864:GLN:HE21	1.15	0.94
1:C:351:LYS:HE3	4:C:3968:HOH:O	1.67	0.94
1:B:466:ASP:OD2	1:B:943:LYS:HE2	1.68	0.93
1:E:250:GLN:HE21	1:E:275:LYS:CE	1.81	0.93
1:F:251:VAL:HG21	1:F:259:PHE:HZ	1.33	0.93
1:E:457:MET:HE2	1:E:493:TYR:HE2	1.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:639:ASN:HD21	1:D:813:SER:H	1.14	0.93
1:B:639:ASN:HD21	1:B:813:SER:H	1.15	0.93
1:D:669:TYR:CE2	1:D:670:MET:CE	2.52	0.92
1:B:669:TYR:CE2	1:B:670:MET:HE2	2.03	0.92
1:H:861:SER:H	1:H:864:GLN:HE21	1.09	0.92
1:D:492:ASP:HB3	1:D:1022:LEU:HD22	1.51	0.92
1:E:288:THR:HG22	1:E:289:GLU:N	1.83	0.92
1:F:251:VAL:HG21	1:F:259:PHE:CZ	2.05	0.91
1:E:861:SER:H	1:E:864:GLN:HE21	1.13	0.91
1:C:670:MET:CE	1:C:885:PHE:HZ	1.83	0.90
1:D:861:SER:H	1:D:864:GLN:HE21	1.18	0.90
1:A:250:GLN:HE21	1:A:275:LYS:CE	1.83	0.90
1:H:250:GLN:HE21	1:H:275:LYS:CE	1.85	0.90
1:E:440:ASN:HD21	1:E:449:GLN:HE21	1.19	0.90
1:D:669:TYR:HE2	1:D:670:MET:CE	1.85	0.90
1:G:861:SER:H	1:G:864:GLN:HE21	1.19	0.89
1:B:394:LYS:CE	1:B:394:LYS:N	2.35	0.89
1:B:669:TYR:HE2	1:B:670:MET:CE	1.84	0.89
1:H:1074:VAL:HG23	1:H:1077:ASN:HB3	1.54	0.89
1:G:492:ASP:HB3	1:G:1022:LEU:HD22	1.52	0.89
1:E:1082:LYS:HD3	1:E:1083:SER:N	1.86	0.89
1:E:669:TYR:CE2	1:E:670:MET:CE	2.55	0.89
1:E:670:MET:HE1	1:E:885:PHE:HZ	1.36	0.89
1:C:261:HIS:HD2	1:C:264:HIS:H	1.20	0.88
1:F:800:THR:CG2	1:F:801:ALA:N	2.37	0.88
1:H:513:ILE:HG12	1:H:953:MET:CE	2.04	0.87
1:H:670:MET:HE1	1:H:885:PHE:CZ	2.09	0.87
1:D:563:ASN:HB3	4:D:1180:HOH:O	1.74	0.87
1:C:311:ASN:HD21	1:C:323:TYR:H	1.23	0.87
1:B:1074:VAL:CG1	1:B:1077:ASN:HB3	2.05	0.87
1:C:251:VAL:HG21	1:C:259:PHE:HZ	1.39	0.86
1:C:440:ASN:HD21	1:C:449:GLN:HE21	1.22	0.86
1:E:1082:LYS:CD	1:E:1083:SER:H	1.87	0.86
1:H:669:TYR:CE2	1:H:670:MET:CE	2.59	0.86
1:H:639:ASN:HD21	1:H:813:SER:H	1.22	0.86
1:D:440:ASN:HD21	1:D:449:GLN:HE21	1.20	0.86
1:B:861:SER:H	1:B:864:GLN:HE21	1.16	0.86
1:G:800:THR:HG22	1:G:802:ALA:H	1.40	0.86
1:C:639:ASN:HD21	1:C:813:SER:H	1.23	0.85
1:E:669:TYR:HE2	1:E:670:MET:HE3	1.41	0.85
1:B:440:ASN:HD21	1:B:449:GLN:HE21	1.18	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:GLN:HG3	4:C:3192:HOH:O	1.76	0.85
1:A:440:ASN:HD21	1:A:449:GLN:HE21	1.20	0.84
1:F:667:GLY:O	1:F:865:ALA:HB3	1.78	0.84
1:H:513:ILE:CG1	1:H:953:MET:HE3	2.06	0.84
1:E:639:ASN:HD21	1:E:813:SER:H	1.23	0.84
1:G:639:ASN:HD21	1:G:813:SER:H	1.23	0.84
1:A:261:HIS:HD2	1:A:264:HIS:H	1.24	0.84
1:H:669:TYR:HE2	1:H:670:MET:CE	1.91	0.84
1:A:460:GLY:H	1:A:470:ASN:HD22	1.25	0.84
1:H:251:VAL:HG21	1:H:259:PHE:HZ	1.40	0.83
1:B:1074:VAL:HG11	1:B:1077:ASN:HB3	1.61	0.83
1:B:988:LYS:H	1:B:990:THR:HG23	1.44	0.83
1:F:247:GLN:HG3	4:F:4174:HOH:O	1.78	0.82
1:C:670:MET:HE2	1:C:885:PHE:CZ	2.15	0.82
1:E:1072:SER:OG	1:E:1074:VAL:HG12	1.80	0.82
1:F:1063:LYS:CE	1:F:1068:ASN:ND2	2.42	0.82
1:A:870:LYS:HD2	4:A:3971:HOH:O	1.77	0.82
1:E:457:MET:HE2	1:E:493:TYR:CE2	2.13	0.82
1:H:1074:VAL:CG2	1:H:1077:ASN:HB3	2.10	0.82
1:F:514:LEU:HD21	1:F:532:MET:HG3	1.62	0.81
1:G:311:ASN:HD21	1:G:323:TYR:H	1.27	0.81
1:B:271:TRP:CZ2	1:B:357:ARG:HG3	2.16	0.81
1:A:311:ASN:HD21	1:A:323:TYR:H	1.26	0.81
1:G:261:HIS:HD2	1:G:264:HIS:H	1.28	0.81
1:F:639:ASN:HD21	1:F:813:SER:H	1.26	0.80
1:D:883:ASP:OD1	1:D:948:LYS:HE3	1.81	0.80
1:A:639:ASN:HD21	1:A:813:SER:H	1.29	0.80
1:C:626:LYS:HE2	4:C:1985:HOH:O	1.79	0.80
1:E:841:ASP:OD1	1:E:846:HIS:HE1	1.65	0.80
1:B:251:VAL:HG21	1:B:259:PHE:CZ	2.17	0.80
1:A:261:HIS:CD2	1:A:264:HIS:H	2.00	0.80
1:D:988:LYS:H	1:D:990:THR:CG2	1.94	0.80
1:D:1082:LYS:HB2	4:D:3996:HOH:O	1.81	0.80
1:H:475:ARG:CA	1:H:953:MET:HE2	2.12	0.79
1:F:261:HIS:HD2	1:F:264:HIS:H	1.28	0.79
1:A:504:ASP:OD1	1:A:846:HIS:HD2	1.66	0.79
1:E:277:ILE:CD1	1:E:291:ASP:CB	2.57	0.79
1:B:563:ASN:HB3	4:B:3514:HOH:O	1.81	0.79
1:D:988:LYS:N	1:D:990:THR:HG23	1.98	0.79
1:D:800:THR:HG22	1:D:802:ALA:H	1.45	0.79
1:H:563:ASN:HB3	4:H:1162:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:669:TYR:HE2	1:D:670:MET:HE3	1.38	0.78
1:H:430:TYR:CD1	1:H:977:LYS:HG2	2.18	0.78
1:C:261:HIS:CD2	1:C:264:HIS:H	2.02	0.78
1:F:667:GLY:O	1:F:865:ALA:CB	2.32	0.78
1:D:311:ASN:HD21	1:D:323:TYR:H	1.31	0.78
1:C:460:GLY:H	1:C:470:ASN:HD22	1.32	0.77
1:C:504:ASP:OD1	1:C:846:HIS:HD2	1.66	0.77
1:F:407:ASN:ND2	1:F:431:GLU:H	1.81	0.77
1:G:261:HIS:CD2	1:G:264:HIS:H	2.02	0.77
1:F:841:ASP:OD1	1:F:846:HIS:HE1	1.68	0.77
1:F:492:ASP:HB3	1:F:1022:LEU:HD22	1.66	0.77
1:C:669:TYR:HE2	1:C:670:MET:HE3	1.46	0.77
1:C:371:ASN:HB3	1:C:373:ASP:H	1.49	0.77
1:H:670:MET:CE	1:H:885:PHE:HZ	1.95	0.77
1:B:304:GLU:OE1	1:B:307:ARG:CD	2.30	0.76
1:E:669:TYR:HE2	1:E:670:MET:CE	1.95	0.76
1:F:261:HIS:CD2	1:F:264:HIS:H	2.03	0.76
1:B:713:TYR:O	1:B:759:HIS:HE1	1.69	0.76
1:F:435:ALA:HA	1:F:1052:ASN:ND2	1.99	0.76
1:D:342:LYS:CE	4:D:2496:HOH:O	2.34	0.76
1:B:504:ASP:OD1	1:B:846:HIS:HD2	1.69	0.76
1:B:669:TYR:CE2	1:B:670:MET:HE3	2.19	0.76
1:G:985:SER:HB2	4:G:3639:HOH:O	1.86	0.76
1:G:440:ASN:HD21	1:G:449:GLN:HE21	1.33	0.75
1:F:440:ASN:HD21	1:F:449:GLN:HE21	1.33	0.75
1:E:311:ASN:HD21	1:E:323:TYR:H	1.32	0.75
1:A:251:VAL:HG21	1:A:259:PHE:HZ	1.50	0.75
1:G:1063:LYS:HE2	1:G:1068:ASN:ND2	2.02	0.75
1:C:1076:ASP:OD2	1:C:1077:ASN:HB2	1.87	0.75
1:B:1076:ASP:O	1:B:1077:ASN:HB2	1.87	0.75
1:C:670:MET:HE2	1:C:885:PHE:HZ	1.47	0.74
1:D:639:ASN:ND2	1:D:813:SER:H	1.83	0.74
1:B:1072:SER:OG	1:B:1074:VAL:HG12	1.87	0.74
1:F:726:ARG:H	1:F:726:ARG:CD	1.97	0.74
1:H:883:ASP:OD1	1:H:948:LYS:HE3	1.87	0.74
1:G:251:VAL:HG21	1:G:259:PHE:HZ	1.51	0.74
1:F:861:SER:H	1:F:864:GLN:NE2	1.83	0.74
1:D:461:ASN:H	1:D:470:ASN:HD21	1.31	0.74
1:C:713:TYR:O	1:C:759:HIS:HE1	1.71	0.74
1:F:311:ASN:HD21	1:F:323:TYR:H	1.35	0.73
1:F:563:ASN:HB3	4:F:3413:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:504:ASP:OD1	1:G:846:HIS:HD2	1.71	0.73
1:E:288:THR:CG2	1:E:289:GLU:H	2.01	0.73
1:E:504:ASP:OD1	1:E:846:HIS:HD2	1.72	0.73
1:F:726:ARG:CD	1:F:726:ARG:N	2.50	0.73
1:B:639:ASN:ND2	1:B:813:SER:H	1.86	0.73
1:B:435:ALA:HA	1:B:1052:ASN:ND2	2.04	0.73
1:D:504:ASP:OD1	1:D:846:HIS:HD2	1.71	0.73
1:C:670:MET:HE1	1:C:885:PHE:HZ	1.53	0.72
1:B:669:TYR:HE2	1:B:670:MET:HE2	1.46	0.72
1:H:460:GLY:H	1:H:470:ASN:HD22	1.38	0.72
1:C:321:GLN:CG	4:C:3192:HOH:O	2.36	0.72
1:G:639:ASN:ND2	1:G:813:SER:H	1.87	0.72
1:E:460:GLY:H	1:E:470:ASN:HD22	1.38	0.72
1:B:988:LYS:H	1:B:990:THR:CG2	2.03	0.72
1:G:988:LYS:H	1:G:990:THR:HG23	1.55	0.72
1:F:708:ILE:HD11	1:F:737:GLU:HB2	1.71	0.72
1:H:440:ASN:HD21	1:H:449:GLN:HE21	1.38	0.72
1:E:988:LYS:H	1:E:990:THR:CG2	2.03	0.71
1:G:800:THR:CG2	1:G:802:ALA:H	2.04	0.71
1:H:461:ASN:H	1:H:470:ASN:HD21	1.38	0.71
1:H:342:LYS:HE2	4:H:2642:HOH:O	1.88	0.71
1:E:261:HIS:CD2	1:E:264:HIS:H	2.08	0.71
1:G:883:ASP:OD1	1:G:948:LYS:HE3	1.90	0.71
1:E:639:ASN:ND2	1:E:813:SER:H	1.89	0.71
1:C:988:LYS:H	1:C:990:THR:CG2	2.02	0.71
1:G:457:MET:HE2	1:G:493:TYR:HE2	1.53	0.71
1:D:342:LYS:HE2	4:D:2496:HOH:O	1.90	0.71
1:B:394:LYS:H	1:B:394:LYS:HE2	1.53	0.70
1:B:800:THR:HG22	1:B:801:ALA:N	2.04	0.70
1:E:247:GLN:H	1:E:247:GLN:HE21	1.37	0.70
1:H:475:ARG:CA	1:H:953:MET:CE	2.67	0.70
1:B:705:SER:HA	4:B:3521:HOH:O	1.91	0.70
1:B:286:GLN:HB3	4:B:2568:HOH:O	1.91	0.70
1:B:393:SER:HA	1:B:394:LYS:HE2	1.72	0.70
1:C:988:LYS:H	1:C:990:THR:HG23	1.56	0.69
1:E:261:HIS:HD2	1:E:264:HIS:H	1.41	0.69
1:E:250:GLN:HG3	1:E:275:LYS:HG3	1.74	0.69
1:E:670:MET:HE1	1:E:885:PHE:CZ	2.25	0.69
1:B:800:THR:HG22	1:B:802:ALA:N	2.05	0.69
1:F:861:SER:N	1:F:864:GLN:HE21	1.85	0.69
1:D:514:LEU:HD21	1:D:532:MET:HG3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:639:ASN:ND2	1:H:813:SER:H	1.90	0.69
1:H:513:ILE:HD11	1:H:953:MET:HE1	1.74	0.68
1:C:861:SER:H	1:C:864:GLN:NE2	1.86	0.68
1:B:394:LYS:CD	1:B:394:LYS:N	2.56	0.68
1:G:841:ASP:OD1	1:G:846:HIS:HE1	1.76	0.68
1:C:461:ASN:H	1:C:470:ASN:HD21	1.41	0.68
1:A:585:ARG:CD	1:A:661:ASP:OD1	2.41	0.68
1:D:585:ARG:HD3	1:D:661:ASP:OD1	1.94	0.68
1:G:703:GLY:HA2	1:G:746:LYS:HD2	1.75	0.68
1:D:726:ARG:H	1:D:726:ARG:NE	1.92	0.68
1:C:670:MET:CE	1:C:885:PHE:CZ	2.70	0.67
1:F:514:LEU:CD2	1:F:532:MET:HG3	2.23	0.67
1:E:988:LYS:N	1:E:990:THR:HG23	2.10	0.67
1:E:461:ASN:H	1:E:470:ASN:HD21	1.42	0.67
1:B:988:LYS:N	1:B:990:THR:HG23	2.08	0.67
1:F:787:LEU:HD12	1:F:787:LEU:N	2.10	0.67
1:F:708:ILE:CD1	1:F:737:GLU:HB2	2.25	0.67
1:G:457:MET:CE	1:G:493:TYR:HE2	2.08	0.66
1:F:557:MET:HE1	1:F:708:ILE:HD13	1.77	0.66
1:B:311:ASN:HD21	1:B:323:TYR:H	1.43	0.66
1:C:250:GLN:NE2	1:C:275:LYS:NZ	2.43	0.66
1:F:709:THR:HG22	1:F:736:ILE:HD12	1.75	0.66
1:D:422:THR:HG23	4:G:1164:HOH:O	1.96	0.66
1:E:1076:ASP:O	1:E:1077:ASN:HB2	1.95	0.66
1:C:988:LYS:N	1:C:990:THR:HG23	2.11	0.66
1:D:304:GLU:OE2	1:D:307:ARG:NH1	2.28	0.66
1:F:800:THR:CG2	1:F:801:ALA:H	2.08	0.66
1:A:639:ASN:ND2	1:A:813:SER:H	1.94	0.66
1:E:302:ASP:HB3	1:E:1065:GLN:HE21	1.59	0.66
1:H:743:LEU:O	1:H:744:ARG:HD3	1.95	0.66
1:F:800:THR:HG22	1:F:802:ALA:H	1.59	0.66
1:D:760:LYS:HE2	4:D:2980:HOH:O	1.95	0.66
1:A:585:ARG:HD3	1:A:661:ASP:OD1	1.95	0.65
1:H:261:HIS:CD2	1:H:264:HIS:H	2.15	0.65
1:C:1063:LYS:HE2	1:C:1068:ASN:HD21	1.59	0.65
1:G:371:ASN:HB3	1:G:373:ASP:H	1.61	0.65
1:E:346:LYS:HE2	1:E:355:TRP:CE3	2.32	0.65
1:A:861:SER:H	1:A:864:GLN:NE2	1.91	0.65
1:A:346:LYS:HE2	1:A:355:TRP:CD2	2.31	0.65
1:G:988:LYS:H	1:G:990:THR:CG2	2.10	0.65
1:D:261:HIS:HD2	1:D:264:HIS:H	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:988:LYS:H	1:E:990:THR:HG23	1.60	0.65
1:H:988:LYS:H	1:H:990:THR:HG23	1.61	0.65
1:B:366:THR:HG21	4:B:3624:HOH:O	1.96	0.65
1:B:492:ASP:HB3	1:B:1022:LEU:HD22	1.79	0.65
1:A:1081:PRO:HG2	1:A:1084:LEU:HD12	1.79	0.65
1:E:1052:ASN:H	1:E:1052:ASN:HD22	1.43	0.65
1:D:1052:ASN:H	1:D:1052:ASN:HD22	1.44	0.65
1:D:854:ARG:HD3	1:D:892:ASP:OD2	1.96	0.65
1:C:1063:LYS:CE	1:C:1068:ASN:ND2	2.60	0.64
4:D:1230:HOH:O	1:G:422:THR:HG23	1.97	0.64
1:G:713:TYR:O	1:G:759:HIS:HE1	1.80	0.64
1:H:585:ARG:HD3	1:H:661:ASP:OD1	1.97	0.64
1:C:585:ARG:HD3	1:C:661:ASP:OD1	1.96	0.64
1:E:670:MET:CE	1:E:885:PHE:HZ	2.11	0.64
1:C:841:ASP:OD1	1:C:846:HIS:HE1	1.80	0.64
1:C:883:ASP:OD1	1:C:948:LYS:HE3	1.98	0.64
1:F:407:ASN:HD22	1:F:431:GLU:H	1.46	0.64
1:F:740:ASN:C	1:F:740:ASN:HD22	2.01	0.64
1:H:513:ILE:CG1	1:H:953:MET:CE	2.72	0.64
1:G:251:VAL:HG21	1:G:259:PHE:CZ	2.31	0.64
1:E:280:ASP:OD2	1:E:282:LYS:NZ	2.31	0.64
1:B:514:LEU:HD21	1:B:532:MET:HG3	1.79	0.64
1:B:726:ARG:NH2	4:B:3637:HOH:O	2.31	0.64
1:D:713:TYR:O	1:D:759:HIS:HE1	1.80	0.64
1:F:761:ASN:N	1:F:791:THR:HG22	2.13	0.64
1:E:669:TYR:CE2	1:E:670:MET:HE2	2.33	0.63
1:E:251:VAL:HG13	1:E:253:SER:O	1.98	0.63
1:H:245:PHE:CD1	1:H:284:TRP:HZ2	2.15	0.63
1:D:669:TYR:CE2	1:D:670:MET:HE2	2.31	0.63
1:B:1074:VAL:HG13	1:B:1077:ASN:HB3	1.79	0.63
1:H:261:HIS:HD2	1:H:264:HIS:H	1.44	0.63
1:E:883:ASP:OD1	1:E:948:LYS:HE3	1.99	0.63
1:H:371:ASN:HB3	1:H:373:ASP:H	1.63	0.63
1:B:585:ARG:HD3	1:B:661:ASP:OD1	1.99	0.63
1:D:371:ASN:HB3	1:D:373:ASP:H	1.63	0.63
1:C:1063:LYS:HE3	1:C:1068:ASN:ND2	2.13	0.63
1:G:457:MET:HE2	1:G:493:TYR:CE2	2.33	0.63
1:E:435:ALA:HA	1:E:1052:ASN:ND2	2.14	0.63
1:F:670:MET:HE3	1:F:877:VAL:HG12	1.81	0.63
1:B:461:ASN:H	1:B:470:ASN:HD21	1.47	0.63
1:D:966:GLU:HB2	1:D:997:LYS:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:VAL:CG2	1:C:259:PHE:CZ	2.76	0.62
1:E:277:ILE:HD13	1:E:291:ASP:HB3	1.76	0.62
1:G:460:GLY:H	1:G:470:ASN:HD22	1.48	0.62
1:G:574:GLU:HG2	4:G:2941:HOH:O	1.99	0.62
1:F:311:ASN:ND2	1:F:323:TYR:H	1.98	0.62
1:C:280:ASP:OD2	1:C:282:LYS:HE3	2.00	0.62
1:E:277:ILE:HD12	1:E:291:ASP:HB3	1.72	0.62
1:A:440:ASN:HD21	1:A:449:GLN:NE2	1.95	0.62
1:A:1052:ASN:H	1:A:1052:ASN:HD22	1.48	0.62
1:E:861:SER:H	1:E:864:GLN:NE2	1.93	0.62
1:D:261:HIS:CD2	1:D:264:HIS:H	2.17	0.62
1:D:435:ALA:HA	1:D:1052:ASN:ND2	2.15	0.62
1:E:585:ARG:HD3	1:E:661:ASP:OD1	1.99	0.62
1:G:457:MET:CE	1:G:493:TYR:CE2	2.83	0.61
1:D:1076:ASP:O	1:D:1077:ASN:HB2	1.99	0.61
1:D:670:MET:CE	1:D:885:PHE:HZ	2.13	0.61
1:H:337:GLN:O	1:H:341:THR:HG23	2.00	0.61
1:C:514:LEU:HD21	1:C:532:MET:HG3	1.82	0.61
1:E:313:MET:HB2	1:E:339:ILE:HD13	1.80	0.61
1:D:600:LYS:HE3	4:D:3768:HOH:O	2.01	0.61
1:H:740:ASN:ND2	1:H:742:SER:H	1.99	0.61
1:B:800:THR:CG2	1:B:801:ALA:N	2.63	0.61
1:A:461:ASN:H	1:A:470:ASN:HD21	1.47	0.61
1:D:669:TYR:CD2	1:D:670:MET:HE3	2.36	0.61
1:F:658:TYR:CE2	1:F:660:GLY:HA3	2.36	0.61
1:G:492:ASP:OD2	1:G:1025:ARG:HD2	2.00	0.61
1:F:1081:PRO:HG2	1:F:1084:LEU:HD12	1.82	0.61
1:E:492:ASP:OD2	1:E:1025:ARG:HD2	1.99	0.61
1:B:407:ASN:ND2	1:B:431:GLU:H	1.98	0.61
1:G:988:LYS:N	1:G:990:THR:HG23	2.15	0.61
1:F:252:TYR:HB3	1:F:258:ASN:HD21	1.65	0.61
1:G:435:ALA:HA	1:G:1052:ASN:ND2	2.16	0.60
1:B:363:PHE:O	1:B:366:THR:HG22	2.01	0.60
1:B:251:VAL:HG21	1:B:259:PHE:HZ	1.67	0.60
1:E:247:GLN:N	1:E:247:GLN:HE21	2.00	0.60
1:C:311:ASN:ND2	1:C:323:TYR:H	1.97	0.60
1:F:740:ASN:ND2	1:F:742:SER:H	1.99	0.60
1:E:585:ARG:CD	1:E:661:ASP:OD1	2.49	0.60
1:H:1052:ASN:HD22	1:H:1052:ASN:H	1.50	0.60
1:D:585:ARG:CD	1:D:661:ASP:OD1	2.48	0.60
1:G:251:VAL:CG2	1:G:259:PHE:CZ	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:VAL:CG2	1:F:259:PHE:CZ	2.82	0.60
1:D:460:GLY:H	1:D:470:ASN:HD22	1.50	0.60
1:D:670:MET:HE1	1:D:885:PHE:HZ	1.65	0.59
1:E:1074:VAL:HG13	1:E:1077:ASN:HB3	1.84	0.59
1:E:371:ASN:HB3	1:E:373:ASP:H	1.66	0.59
1:B:729:ARG:NH2	1:B:762:GLN:HB2	2.17	0.59
1:C:440:ASN:HD21	1:C:449:GLN:NE2	1.96	0.59
1:G:461:ASN:H	1:G:470:ASN:HD21	1.51	0.59
1:G:407:ASN:ND2	1:G:431:GLU:H	2.00	0.59
1:B:514:LEU:CD2	1:B:532:MET:HG3	2.32	0.59
1:F:460:GLY:H	1:F:470:ASN:HD22	1.48	0.59
1:C:585:ARG:CD	1:C:661:ASP:OD1	2.50	0.59
1:B:313:MET:HB2	1:B:339:ILE:HD13	1.84	0.59
1:A:1076:ASP:OD2	1:A:1077:ASN:HB2	2.02	0.59
1:G:250:GLN:OE1	1:G:275:LYS:HE3	2.03	0.59
1:A:868:THR:HG22	1:A:868:THR:O	2.02	0.59
1:C:311:ASN:HD21	1:C:323:TYR:N	1.97	0.59
1:G:800:THR:HG22	1:G:802:ALA:N	2.13	0.59
1:G:883:ASP:OD1	1:G:948:LYS:CE	2.51	0.59
1:D:351:LYS:HE2	4:D:2565:HOH:O	2.03	0.59
1:E:440:ASN:HD21	1:E:449:GLN:NE2	1.96	0.59
1:A:841:ASP:OD1	1:A:846:HIS:HE1	1.86	0.59
1:D:514:LEU:CD2	1:D:532:MET:HG3	2.33	0.59
1:D:407:ASN:ND2	1:D:431:GLU:H	2.01	0.59
1:C:346:LYS:HE2	1:C:355:TRP:CE3	2.38	0.58
1:F:713:TYR:O	1:F:759:HIS:HE1	1.87	0.58
1:B:669:TYR:CD2	1:B:670:MET:HE3	2.37	0.58
1:B:883:ASP:OD1	1:B:948:LYS:CE	2.51	0.58
1:H:988:LYS:N	1:H:990:THR:HG23	2.19	0.58
1:H:713:TYR:O	1:H:759:HIS:HE1	1.86	0.58
1:B:394:LYS:HE3	1:B:394:LYS:N	2.07	0.58
1:G:311:ASN:ND2	1:G:323:TYR:H	2.00	0.58
1:A:253:SER:HB2	4:A:4186:HOH:O	2.02	0.58
1:B:793:ASP:OD1	1:B:793:ASP:N	2.36	0.58
1:H:800:THR:HG22	1:H:802:ALA:H	1.69	0.58
1:G:884:LYS:HG3	4:G:3691:HOH:O	2.03	0.58
1:C:492:ASP:OD2	1:C:1025:ARG:HD2	2.04	0.58
1:F:321:GLN:HG2	1:F:323:TYR:CZ	2.39	0.57
1:A:440:ASN:ND2	1:A:449:GLN:HE21	1.97	0.57
1:G:430:TYR:CD1	1:G:977:LYS:HG2	2.39	0.57
1:F:726:ARG:CG	1:F:726:ARG:NH1	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:5001:MES:H51	4:H:2109:HOH:O	2.04	0.57
1:H:658:TYR:CE2	1:H:660:GLY:HA3	2.40	0.57
1:F:333:ASN:O	1:F:337:GLN:HG3	2.05	0.57
1:H:861:SER:H	1:H:864:GLN:NE2	1.90	0.57
1:E:311:ASN:HD21	1:E:323:TYR:N	2.02	0.57
1:H:800:THR:HG23	1:H:801:ALA:N	2.19	0.57
1:D:440:ASN:ND2	1:D:449:GLN:HE21	1.96	0.57
1:G:585:ARG:HD3	1:G:661:ASP:OD1	2.05	0.57
1:H:513:ILE:HD13	1:H:856:MET:CE	2.35	0.57
1:E:600:LYS:HE2	1:E:605:PRO:O	2.05	0.57
1:H:475:ARG:N	1:H:953:MET:HE2	2.20	0.57
1:H:251:VAL:CG2	1:H:259:PHE:CZ	2.84	0.57
1:B:563:ASN:CB	4:B:3514:HOH:O	2.48	0.56
1:H:585:ARG:CD	1:H:661:ASP:OD1	2.53	0.56
1:C:368:SER:HA	1:C:371:ASN:HB2	1.88	0.56
1:B:325:THR:HG21	4:B:2752:HOH:O	2.05	0.56
1:B:261:HIS:HD2	1:B:264:HIS:H	1.54	0.56
1:B:840:THR:HG21	1:C:723:THR:OG1	2.06	0.56
1:C:457:MET:HE3	1:C:494:LEU:CD2	2.35	0.56
1:D:311:ASN:ND2	1:D:323:TYR:H	2.01	0.56
1:F:457:MET:CE	1:F:493:TYR:HE2	2.19	0.56
1:F:966:GLU:HB2	1:F:997:LYS:HB2	1.88	0.56
1:H:504:ASP:OD1	1:H:846:HIS:CD2	2.43	0.56
1:F:639:ASN:ND2	1:F:813:SER:H	2.00	0.55
1:F:321:GLN:HG3	1:F:322:THR:N	2.21	0.55
1:E:316:GLN:HG2	1:E:359:THR:HG23	1.88	0.55
1:H:286:GLN:HG3	4:H:1200:HOH:O	2.06	0.55
1:E:368:SER:HA	1:E:371:ASN:HB2	1.88	0.55
1:D:800:THR:CG2	1:D:801:ALA:N	2.69	0.55
1:H:988:LYS:H	1:H:990:THR:CG2	2.18	0.55
1:F:461:ASN:H	1:F:470:ASN:HD21	1.53	0.55
1:F:540:ARG:HD2	4:F:1142:HOH:O	2.06	0.55
1:A:988:LYS:H	1:A:990:THR:HG23	1.71	0.55
1:F:585:ARG:HD3	1:F:661:ASP:OD1	2.06	0.55
1:F:740:ASN:HD22	1:F:741:PRO:N	2.03	0.55
1:E:759:HIS:HD2	1:E:762:GLN:OE1	1.90	0.55
1:C:726:ARG:NH2	4:C:1110:HOH:O	2.38	0.55
1:D:820:VAL:HB	1:D:821:PRO:HD2	1.89	0.55
1:A:460:GLY:N	1:A:470:ASN:HD22	1.99	0.55
1:E:713:TYR:O	1:E:759:HIS:HE1	1.89	0.55
1:C:321:GLN:CD	4:C:3192:HOH:O	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ASN:HD21	1:A:323:TYR:N	2.01	0.55
1:F:407:ASN:HD22	1:F:431:GLU:N	2.03	0.55
1:H:740:ASN:HD22	1:H:740:ASN:C	2.09	0.55
1:G:740:ASN:ND2	1:G:742:SER:H	2.05	0.55
1:H:513:ILE:HD13	1:H:856:MET:HE1	1.87	0.55
1:H:311:ASN:HD21	1:H:323:TYR:H	1.52	0.55
1:F:618:LYS:HE3	4:F:149:HOH:O	2.07	0.55
1:D:440:ASN:HD21	1:D:449:GLN:NE2	1.96	0.54
1:F:557:MET:HE1	1:F:708:ILE:CD1	2.36	0.54
1:D:311:ASN:HD21	1:D:323:TYR:N	2.02	0.54
1:A:689:LYS:HE3	4:A:3634:HOH:O	2.06	0.54
1:A:504:ASP:OD1	1:A:846:HIS:CD2	2.54	0.54
1:F:809:ASN:HB2	1:F:810:PRO:CD	2.37	0.54
1:B:1005:ALA:O	1:B:1041:LYS:HD2	2.08	0.54
3:B:5001:MES:C7	4:B:2759:HOH:O	2.55	0.54
1:H:435:ALA:HA	1:H:1052:ASN:ND2	2.23	0.54
1:A:715:LYS:HZ1	1:A:832:VAL:HG23	1.72	0.54
1:E:440:ASN:ND2	1:E:449:GLN:HE21	1.97	0.54
1:C:966:GLU:HB2	1:C:997:LYS:HB2	1.90	0.54
1:B:365:LYS:HD3	4:B:3556:HOH:O	2.08	0.54
1:E:277:ILE:HD12	1:E:291:ASP:CB	2.32	0.54
1:G:574:GLU:CG	4:G:2941:HOH:O	2.54	0.54
1:E:430:TYR:CD1	1:E:977:LYS:HD3	2.43	0.54
1:D:251:VAL:HG13	1:D:253:SER:O	2.08	0.54
1:G:563:ASN:HB3	4:G:1128:HOH:O	2.08	0.54
1:A:868:THR:CG2	1:A:868:THR:O	2.56	0.54
1:F:670:MET:CE	1:F:877:VAL:HG12	2.38	0.53
1:E:407:ASN:ND2	1:E:431:GLU:H	2.06	0.53
1:E:966:GLU:HB2	1:E:997:LYS:HB2	1.89	0.53
1:D:800:THR:HG22	1:D:801:ALA:N	2.23	0.53
1:B:261:HIS:CD2	1:B:264:HIS:H	2.26	0.53
1:E:669:TYR:CD2	1:E:670:MET:HE3	2.43	0.53
1:B:525:LEU:HD11	1:B:532:MET:HG2	1.90	0.53
1:H:457:MET:HE2	1:H:493:TYR:HE2	1.73	0.53
1:F:782:GLN:HG3	1:F:783:GLU:N	2.24	0.53
1:C:563:ASN:HB3	4:C:1770:HOH:O	2.07	0.53
1:A:346:LYS:HE2	1:A:355:TRP:CE3	2.43	0.53
1:F:894:GLU:HA	1:F:953:MET:HB3	1.90	0.53
1:D:988:LYS:O	1:D:988:LYS:HG3	2.08	0.53
1:C:460:GLY:N	1:C:470:ASN:HD22	2.04	0.53
1:C:1063:LYS:HE2	1:C:1068:ASN:ND2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:862:ASN:O	1:G:912:ILE:HG12	2.08	0.53
1:D:841:ASP:OD1	1:D:846:HIS:HE1	1.91	0.53
1:C:1063:LYS:CE	1:C:1068:ASN:HD21	2.20	0.53
1:A:435:ALA:HA	1:A:1052:ASN:ND2	2.23	0.53
1:A:585:ARG:HD2	1:A:661:ASP:OD1	2.07	0.53
1:C:351:LYS:CE	4:C:3968:HOH:O	2.39	0.53
1:B:440:ASN:HD21	1:B:449:GLN:NE2	1.98	0.52
1:H:800:THR:CG2	1:H:801:ALA:N	2.72	0.52
1:E:504:ASP:OD1	1:E:846:HIS:CD2	2.60	0.52
1:G:746:LYS:O	1:G:749:ASP:HB2	2.10	0.52
1:D:1074:VAL:CG2	1:D:1077:ASN:HB3	2.40	0.52
1:A:868:THR:HB	1:A:872:GLU:OE1	2.09	0.52
1:D:1082:LYS:CB	4:D:3996:HOH:O	2.51	0.52
1:D:457:MET:HE2	1:D:493:TYR:HE2	1.74	0.52
1:H:368:SER:HA	1:H:371:ASN:HB2	1.91	0.52
1:C:800:THR:HG22	1:C:802:ALA:H	1.75	0.52
1:B:368:SER:HA	1:B:371:ASN:HB2	1.92	0.52
1:F:346:LYS:HE2	1:F:355:TRP:CE3	2.45	0.51
1:A:800:THR:HG23	1:A:801:ALA:N	2.26	0.51
1:H:513:ILE:CD1	1:H:953:MET:HE1	2.41	0.51
1:B:726:ARG:NH2	4:B:3961:HOH:O	2.43	0.51
1:D:457:MET:HE2	1:D:493:TYR:CE2	2.46	0.51
1:F:688:ILE:HD11	1:F:889:GLY:CA	2.40	0.51
1:E:311:ASN:ND2	1:E:323:TYR:H	2.05	0.51
1:G:425:ARG:HG2	4:G:1748:HOH:O	2.10	0.51
1:C:1052:ASN:HD22	1:C:1052:ASN:H	1.59	0.51
1:C:440:ASN:ND2	1:C:449:GLN:HE21	2.00	0.51
1:H:948:LYS:NZ	4:H:2486:HOH:O	2.44	0.51
4:D:1230:HOH:O	1:G:422:THR:CG2	2.55	0.51
1:B:355:TRP:O	1:B:359:THR:HG23	2.09	0.51
1:F:244:SER:N	4:F:2541:HOH:O	2.44	0.51
1:E:302:ASP:HB3	1:E:1065:GLN:NE2	2.26	0.51
1:F:371:ASN:HB3	1:F:373:ASP:H	1.75	0.51
1:B:740:ASN:HD22	1:B:742:SER:H	1.59	0.51
1:F:667:GLY:O	1:F:865:ALA:N	2.39	0.51
1:E:480:ASP:OD1	1:E:521:ASP:OD2	2.28	0.51
1:H:669:TYR:CE2	1:H:670:MET:HE2	2.44	0.51
1:G:311:ASN:HD21	1:G:323:TYR:N	2.03	0.51
1:F:618:LYS:CE	4:F:149:HOH:O	2.59	0.51
1:A:460:GLY:H	1:A:470:ASN:ND2	2.02	0.51
1:B:357:ARG:HA	4:B:2535:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:GLY:N	1:D:470:ASN:HD22	2.09	0.51
1:E:883:ASP:OD1	1:E:948:LYS:CE	2.58	0.51
1:C:551:LEU:HD21	4:C:3907:HOH:O	2.10	0.51
1:F:1052:ASN:H	1:F:1052:ASN:HD22	1.59	0.50
1:B:883:ASP:OD1	1:B:948:LYS:HE3	2.10	0.50
1:C:435:ALA:HA	1:C:1052:ASN:ND2	2.25	0.50
1:E:288:THR:HB	1:E:290:LYS:H	1.76	0.50
1:B:366:THR:HG23	1:B:367:GLN:OE1	2.11	0.50
1:A:884:LYS:CE	4:A:1171:HOH:O	2.58	0.50
1:E:304:GLU:OE2	1:E:307:ARG:NH2	2.43	0.50
1:C:457:MET:HE3	1:C:494:LEU:HD21	1.93	0.50
1:C:669:TYR:HE2	1:C:670:MET:CE	2.21	0.50
1:C:251:VAL:HG21	1:C:259:PHE:CE1	2.43	0.50
1:G:504:ASP:OD1	1:G:846:HIS:CD2	2.59	0.50
1:G:394:LYS:N	1:G:394:LYS:HD3	2.07	0.50
1:F:868:THR:OG1	1:F:872:GLU:OE1	2.29	0.50
1:E:1001:LYS:O	1:E:1001:LYS:HG3	2.11	0.50
1:G:324:ASN:HB2	4:G:2423:HOH:O	2.12	0.50
1:E:270:SER:HB2	1:E:295:LEU:HD12	1.93	0.50
1:G:966:GLU:HB2	1:G:997:LYS:HB2	1.92	0.50
1:B:586:ALA:HA	1:B:858:GLU:OE1	2.12	0.50
1:G:492:ASP:HB3	1:G:1022:LEU:CD2	2.34	0.50
1:D:988:LYS:N	1:D:990:THR:CG2	2.61	0.49
1:B:841:ASP:OD1	1:B:846:HIS:HE1	1.94	0.49
1:B:800:THR:CG2	1:B:802:ALA:H	2.13	0.49
1:D:988:LYS:O	1:D:990:THR:HG22	2.11	0.49
1:H:460:GLY:N	1:H:470:ASN:HD22	2.07	0.49
1:F:854:ARG:HD3	1:F:892:ASP:OD2	2.12	0.49
1:E:988:LYS:O	1:E:990:THR:HG22	2.12	0.49
1:F:504:ASP:OD1	1:F:846:HIS:HD2	1.95	0.49
1:F:723:THR:O	1:F:758:ALA:HB2	2.11	0.49
1:H:457:MET:HE1	1:H:494:LEU:HD21	1.95	0.49
1:G:471:PHE:CG	1:G:954:ALA:HB2	2.46	0.49
1:D:1065:GLN:HG3	1:D:1066:ALA:N	2.27	0.49
1:D:274:PRO:HG2	1:D:277:ILE:HD12	1.94	0.49
1:F:669:TYR:CE2	1:F:670:MET:HE3	2.47	0.49
1:E:505:LYS:NZ	4:E:2897:HOH:O	2.44	0.49
1:A:516:ALA:HB1	1:A:521:ASP:OD2	2.12	0.49
1:D:427:ILE:HG12	3:D:5001:MES:H82	1.95	0.49
1:C:740:ASN:ND2	1:C:742:SER:H	2.11	0.49
1:B:563:ASN:HB3	4:B:3350:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:988:LYS:H	1:F:990:THR:CG2	2.25	0.49
1:A:251:VAL:HG21	1:A:259:PHE:CE1	2.46	0.49
1:A:870:LYS:CD	4:A:3971:HOH:O	2.49	0.49
1:E:365:LYS:HE3	4:E:3590:HOH:O	2.13	0.49
1:F:883:ASP:OD1	1:F:948:LYS:CE	2.61	0.49
1:C:809:ASN:HB2	1:C:810:PRO:HD2	1.94	0.49
1:F:457:MET:HE2	1:F:493:TYR:HE2	1.78	0.48
1:B:304:GLU:HA	1:B:307:ARG:HG2	1.94	0.48
1:C:670:MET:HE2	1:C:885:PHE:CE1	2.48	0.48
1:D:1076:ASP:O	1:D:1077:ASN:CB	2.61	0.48
1:H:457:MET:HE2	1:H:493:TYR:CE2	2.46	0.48
1:A:248:TYR:HB3	1:A:284:TRP:CZ3	2.48	0.48
1:A:311:ASN:ND2	1:A:323:TYR:H	2.02	0.48
1:F:557:MET:HE2	1:F:708:ILE:HD12	1.95	0.48
1:A:715:LYS:NZ	1:A:832:VAL:HG23	2.28	0.48
1:F:453:LEU:CD1	1:F:474:ILE:HG21	2.43	0.48
1:F:749:ASP:C	1:F:750:ARG:HG2	2.33	0.48
1:B:861:SER:H	1:B:864:GLN:NE2	1.98	0.48
1:B:740:ASN:ND2	1:B:742:SER:H	2.12	0.48
1:H:966:GLU:HB2	1:H:997:LYS:HB2	1.96	0.48
1:G:750:ARG:CD	4:G:1546:HOH:O	2.61	0.48
1:B:394:LYS:HD3	1:B:394:LYS:N	2.27	0.48
1:G:800:THR:HG23	1:G:801:ALA:N	2.27	0.48
1:F:669:TYR:HE2	1:F:670:MET:CE	2.26	0.48
1:G:740:ASN:C	1:G:740:ASN:HD22	2.16	0.48
1:E:725:ASP:OD1	1:E:727:ILE:CD1	2.62	0.48
1:B:966:GLU:HB2	1:B:997:LYS:HB2	1.96	0.48
1:D:1026:LYS:NZ	4:D:3568:HOH:O	2.45	0.48
1:B:1052:ASN:HD22	1:B:1052:ASN:H	1.62	0.48
1:F:457:MET:CE	1:F:493:TYR:CE2	2.97	0.48
1:D:565:LEU:HD11	4:D:3922:HOH:O	2.12	0.48
1:C:460:GLY:H	1:C:470:ASN:ND2	2.08	0.47
1:F:1065:GLN:HG3	1:F:1066:ALA:N	2.29	0.47
1:A:1025:ARG:O	1:A:1033:PRO:HA	2.13	0.47
1:F:800:THR:HG23	1:F:801:ALA:H	1.80	0.47
1:D:461:ASN:H	1:D:470:ASN:ND2	2.07	0.47
1:F:557:MET:CE	1:F:708:ILE:CD1	2.92	0.47
1:F:745:LEU:HD13	1:F:804:ILE:O	2.13	0.47
1:F:462:ILE:HD13	1:F:1011:PHE:CZ	2.49	0.47
1:A:250:GLN:NE2	1:A:275:LYS:CE	2.48	0.47
1:B:513:ILE:HG12	1:B:953:MET:HE1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:894:GLU:HA	1:E:953:MET:HB3	1.96	0.47
1:B:394:LYS:HE2	1:B:394:LYS:N	2.21	0.47
1:F:761:ASN:H	1:F:791:THR:HG22	1.77	0.47
1:G:759:HIS:HD2	1:G:762:GLN:OE1	1.98	0.47
1:E:740:ASN:C	1:E:740:ASN:HD22	2.17	0.47
1:G:626:LYS:HB3	1:G:626:LYS:HE3	1.54	0.47
1:F:669:TYR:CE2	1:F:670:MET:CE	2.98	0.47
1:C:740:ASN:C	1:C:740:ASN:HD22	2.17	0.47
1:D:759:HIS:HD2	1:D:762:GLN:OE1	1.98	0.47
1:G:261:HIS:CD2	1:G:264:HIS:N	2.78	0.47
1:B:978:TYR:CD1	3:B:5001:MES:H31	2.50	0.47
1:H:324:ASN:ND2	1:H:326:ALA:H	2.12	0.47
1:B:1070:TYR:HE2	4:B:2873:HOH:O	1.98	0.47
1:E:740:ASN:ND2	1:E:742:SER:H	2.12	0.46
1:F:615:GLU:HG2	4:F:1620:HOH:O	2.14	0.46
1:G:740:ASN:HD22	1:G:741:PRO:N	2.13	0.46
1:A:319:ILE:HD11	1:A:342:LYS:HG3	1.97	0.46
1:F:280:ASP:OD2	1:F:282:LYS:HE3	2.15	0.46
1:C:430:TYR:HB3	1:C:978:TYR:CE1	2.50	0.46
1:C:250:GLN:NE2	1:C:275:LYS:HZ2	2.13	0.46
1:F:440:ASN:HD21	1:F:449:GLN:NE2	2.07	0.46
1:H:245:PHE:CD2	1:H:337:GLN:HG2	2.50	0.46
1:F:1072:SER:OG	1:F:1074:VAL:HG12	2.16	0.46
1:H:421:TYR:OH	1:H:524:TYR:HA	2.15	0.46
1:D:883:ASP:OD1	1:D:948:LYS:CE	2.60	0.46
1:B:492:ASP:HB3	1:B:1022:LEU:CD2	2.46	0.46
1:E:308:GLN:HE21	1:E:308:GLN:HB3	1.39	0.46
1:A:1072:SER:OG	1:A:1074:VAL:HG12	2.15	0.46
1:C:705:SER:HB3	1:C:743:LEU:HD13	1.96	0.46
1:B:577:ALA:C	1:B:578:VAL:HG23	2.36	0.46
1:H:883:ASP:OD1	1:H:948:LYS:CE	2.60	0.46
1:H:440:ASN:HD21	1:H:449:GLN:NE2	2.09	0.46
1:G:600:LYS:HB3	1:G:600:LYS:HE3	1.61	0.46
1:F:1063:LYS:HA	1:F:1070:TYR:HA	1.98	0.46
1:E:457:MET:HE3	1:E:494:LEU:HD23	1.98	0.46
1:G:861:SER:O	1:G:864:GLN:HG3	2.15	0.46
1:H:311:ASN:HD21	1:H:323:TYR:N	2.14	0.46
1:C:809:ASN:HB2	1:C:810:PRO:CD	2.45	0.46
1:D:894:GLU:HA	1:D:953:MET:HB3	1.96	0.46
1:B:740:ASN:C	1:B:740:ASN:HD22	2.19	0.46
1:D:740:ASN:ND2	1:D:742:SER:H	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:PHE:CG	1:E:954:ALA:HB2	2.51	0.46
1:G:726:ARG:HG2	4:G:2598:HOH:O	2.15	0.46
1:F:988:LYS:H	1:F:990:THR:HG23	1.80	0.45
1:F:522:THR:HB	1:F:523:PRO:CD	2.46	0.45
1:C:861:SER:N	1:C:864:GLN:HE21	1.92	0.45
1:B:407:ASN:HD22	1:B:431:GLU:N	2.15	0.45
1:C:740:ASN:HD22	1:C:742:SER:H	1.63	0.45
1:H:312:TYR:O	1:H:316:GLN:HG2	2.16	0.45
1:F:329:PRO:HD2	4:F:2953:HOH:O	2.17	0.45
1:F:709:THR:HG22	1:F:736:ILE:CD1	2.46	0.45
1:E:740:ASN:HD22	1:E:741:PRO:N	2.14	0.45
1:F:460:GLY:N	1:F:470:ASN:HD22	2.13	0.45
1:G:740:ASN:HD22	1:G:742:SER:H	1.64	0.45
1:F:1065:GLN:HG3	1:F:1066:ALA:H	1.81	0.45
1:H:313:MET:HB2	1:H:339:ILE:HD13	1.99	0.45
1:A:460:GLY:N	1:A:470:ASN:ND2	2.64	0.45
1:E:725:ASP:OD1	1:E:727:ILE:HD12	2.17	0.45
1:H:600:LYS:HE2	1:H:605:PRO:O	2.17	0.45
1:D:1000:GLY:C	1:D:1001:LYS:HG3	2.37	0.45
1:B:308:GLN:HB3	1:B:308:GLN:HE21	1.62	0.45
1:F:610:TYR:HA	1:F:612:PHE:CE2	2.52	0.45
1:C:639:ASN:ND2	1:C:813:SER:H	2.03	0.45
1:B:435:ALA:HA	1:B:1052:ASN:HD22	1.79	0.45
1:E:1052:ASN:N	1:E:1052:ASN:HD22	2.13	0.45
1:A:304:GLU:OE2	1:A:307:ARG:NH1	2.49	0.45
1:G:460:GLY:N	1:G:470:ASN:HD22	2.12	0.45
1:H:740:ASN:HD22	1:H:742:SER:H	1.63	0.45
1:A:988:LYS:N	1:A:990:THR:HG23	2.32	0.45
1:F:368:SER:HA	1:F:371:ASN:HB2	1.99	0.45
1:A:740:ASN:HD22	1:A:740:ASN:C	2.20	0.45
1:F:809:ASN:HB2	1:F:810:PRO:HD2	1.99	0.45
1:F:425:ARG:H	1:F:425:ARG:HG2	1.60	0.45
1:G:861:SER:H	1:G:864:GLN:NE2	2.01	0.45
1:E:430:TYR:HB3	1:E:978:TYR:CE1	2.52	0.45
1:F:311:ASN:HD21	1:F:323:TYR:N	2.07	0.44
1:G:570:ASP:HB3	1:G:572:ASN:HD21	1.81	0.44
1:C:870:LYS:NZ	1:C:937:ASP:OD2	2.44	0.44
1:B:407:ASN:ND2	1:B:431:GLU:N	2.64	0.44
1:C:800:THR:CG2	1:C:801:ALA:N	2.80	0.44
1:G:809:ASN:HB2	1:G:810:PRO:CD	2.47	0.44
1:G:1001:LYS:HB2	1:G:1001:LYS:HE2	1.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:GLN:HG3	1:H:275:LYS:HG3	1.99	0.44
1:D:726:ARG:H	1:D:726:ARG:HE	1.62	0.44
1:D:346:LYS:HG2	1:D:355:TRP:CE2	2.53	0.44
1:G:800:THR:CG2	1:G:801:ALA:N	2.78	0.44
1:G:457:MET:HE3	1:G:493:TYR:CE2	2.52	0.44
1:D:457:MET:HE1	1:D:494:LEU:HD21	1.99	0.44
1:D:999:SER:O	1:D:1001:LYS:N	2.50	0.44
1:B:827:ASP:N	1:B:827:ASP:OD1	2.46	0.44
1:D:1052:ASN:N	1:D:1052:ASN:HD22	2.13	0.44
1:H:387:LEU:O	1:H:1050:GLY:HA3	2.17	0.44
1:C:376:LYS:HB3	1:C:377:PRO:HA	1.99	0.44
1:B:258:ASN:ND2	1:B:273:ARG:HB3	2.33	0.44
1:A:1012:LEU:O	1:A:1016:GLN:HG3	2.18	0.44
1:A:713:TYR:O	1:A:759:HIS:HE1	2.01	0.44
1:E:1001:LYS:O	1:E:1001:LYS:CG	2.66	0.44
1:A:466:ASP:HA	1:A:467:PRO:HD2	1.80	0.44
1:C:383:GLN:O	1:C:384:LYS:HB2	2.17	0.44
1:F:435:ALA:HA	1:F:1052:ASN:HD22	1.81	0.44
1:B:262:VAL:HG12	1:B:969:VAL:HG23	2.00	0.44
1:B:724:GLY:HA3	1:B:728:THR:OG1	2.17	0.44
1:H:394:LYS:HB2	1:H:394:LYS:HE2	1.41	0.44
1:A:430:TYR:HB3	1:A:978:TYR:CE1	2.53	0.44
1:E:271:TRP:CZ2	1:E:357:ARG:HD3	2.53	0.44
1:G:304:GLU:OE2	1:G:307:ARG:NH1	2.50	0.44
1:A:658:TYR:CE2	1:A:660:GLY:HA3	2.52	0.44
1:H:619:LYS:HE2	1:H:619:LYS:HB3	1.44	0.44
1:F:313:MET:HB2	1:F:339:ILE:HD13	2.00	0.44
1:F:1063:LYS:HE3	1:F:1068:ASN:ND2	2.28	0.44
1:H:854:ARG:HD3	1:H:892:ASP:OD2	2.18	0.44
1:C:392:ASN:ND2	4:C:3574:HOH:O	2.48	0.44
1:H:861:SER:N	1:H:864:GLN:HE21	1.93	0.43
1:G:596:ARG:NH2	1:G:600:LYS:HD2	2.34	0.43
1:G:793:ASP:HB2	4:G:3607:HOH:O	2.17	0.43
1:F:492:ASP:OD2	1:F:1025:ARG:HD2	2.18	0.43
1:D:274:PRO:HG2	1:D:277:ILE:CD1	2.47	0.43
1:F:352:ASN:OD1	1:F:354:ASN:N	2.51	0.43
1:B:703:GLY:HA3	1:B:744:ARG:O	2.19	0.43
1:B:311:ASN:ND2	1:B:323:TYR:H	2.12	0.43
1:F:669:TYR:HE2	1:F:670:MET:HE2	1.83	0.43
1:H:394:LYS:H	1:H:394:LYS:CE	2.31	0.43
1:A:966:GLU:HB2	1:A:997:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:658:TYR:CE2	1:E:660:GLY:HA3	2.53	0.43
1:G:495:LYS:NZ	4:G:3377:HOH:O	2.51	0.43
1:G:658:TYR:CE2	1:G:660:GLY:HA3	2.52	0.43
1:A:453:LEU:CD1	1:A:474:ILE:HG21	2.48	0.43
1:H:430:TYR:HB3	1:H:978:TYR:CE1	2.53	0.43
1:D:1074:VAL:HG22	1:D:1077:ASN:HB3	2.00	0.43
1:D:884:LYS:HE3	4:D:1112:HOH:O	2.18	0.43
1:D:425:ARG:HD3	1:D:425:ARG:HH11	1.65	0.43
1:G:261:HIS:CD2	1:G:264:HIS:HA	2.54	0.43
1:E:737:GLU:HA	1:E:815:TYR:O	2.18	0.43
1:G:1074:VAL:CG2	1:G:1077:ASN:HB3	2.49	0.43
1:H:475:ARG:HA	1:H:953:MET:HE3	2.00	0.43
1:E:841:ASP:OD1	1:E:846:HIS:CE1	2.57	0.43
1:G:894:GLU:HA	1:G:953:MET:HB3	2.00	0.43
1:C:737:GLU:HA	1:C:815:TYR:O	2.19	0.43
1:D:1005:ALA:O	1:D:1041:LYS:HD2	2.19	0.43
1:F:673:LYS:HE2	1:F:677:TYR:CZ	2.53	0.43
1:H:1076:ASP:N	1:H:1076:ASP:OD1	2.49	0.43
1:B:440:ASN:ND2	1:B:449:GLN:HE21	1.98	0.43
1:C:460:GLY:N	1:C:470:ASN:ND2	2.67	0.43
1:F:688:ILE:HD11	1:F:889:GLY:HA3	2.00	0.43
1:C:466:ASP:HA	1:C:467:PRO:HD2	1.89	0.43
1:E:585:ARG:HD2	1:E:661:ASP:OD1	2.19	0.43
1:H:740:ASN:HD22	1:H:741:PRO:N	2.17	0.43
1:B:478:ALA:HB1	1:B:481:ASN:HD22	1.84	0.43
1:H:308:GLN:HE21	1:H:308:GLN:HB3	1.68	0.43
1:E:1072:SER:HG	1:E:1074:VAL:HG12	1.83	0.42
1:H:461:ASN:H	1:H:470:ASN:ND2	2.11	0.42
1:C:800:THR:HG23	1:C:801:ALA:N	2.34	0.42
1:G:753:VAL:O	1:G:796:GLU:HA	2.19	0.42
1:B:874:THR:HB	1:B:932:TYR:HB3	2.01	0.42
1:H:1063:LYS:HA	1:H:1070:TYR:HA	2.01	0.42
1:H:809:ASN:HB2	1:H:810:PRO:CD	2.49	0.42
1:H:736:ILE:HD11	1:H:799:PHE:CE2	2.54	0.42
1:B:928:LYS:HB2	1:B:929:PRO:CD	2.49	0.42
1:H:884:LYS:HD2	1:H:884:LYS:HA	1.83	0.42
1:B:504:ASP:OD1	1:B:846:HIS:CD2	2.60	0.42
1:G:977:LYS:HB2	1:G:977:LYS:HE2	1.78	0.42
1:G:346:LYS:HG2	1:G:355:TRP:CE2	2.54	0.42
1:H:737:GLU:HA	1:H:815:TYR:O	2.19	0.42
1:D:988:LYS:HE3	1:D:988:LYS:HB2	1.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:460:GLY:N	1:E:470:ASN:HD22	2.13	0.42
1:D:304:GLU:CD	1:D:307:ARG:HH11	2.22	0.42
1:G:407:ASN:HD22	1:G:431:GLU:H	1.66	0.42
1:G:1030:THR:HB	1:G:1032:VAL:HG22	2.00	0.42
1:B:442:ASN:O	1:B:446:GLN:HG3	2.19	0.42
1:C:736:ILE:HD11	1:C:799:PHE:CE2	2.55	0.42
1:B:321:GLN:HG3	1:B:322:THR:N	2.34	0.42
1:A:1063:LYS:HE3	1:A:1070:TYR:CZ	2.54	0.42
1:F:480:ASP:OD1	1:F:521:ASP:OD2	2.37	0.42
1:C:342:LYS:HE2	1:C:345:GLU:OE1	2.19	0.42
1:H:1072:SER:OG	1:H:1074:VAL:HG22	2.19	0.42
1:G:440:ASN:HD21	1:G:449:GLN:NE2	2.10	0.42
1:G:585:ARG:CD	1:G:661:ASP:OD1	2.67	0.42
1:H:421:TYR:CZ	1:H:524:TYR:HA	2.55	0.42
1:F:576:ALA:HB3	1:F:847:GLN:HB3	2.01	0.42
1:H:610:TYR:HB2	1:H:907:PHE:CE1	2.54	0.42
1:B:537:ASN:OD1	1:B:540:ARG:HD3	2.20	0.42
1:F:701:GLN:HG2	4:F:3429:HOH:O	2.18	0.42
1:F:585:ARG:CD	1:F:661:ASP:OD1	2.66	0.42
1:G:737:GLU:HA	1:G:815:TYR:O	2.19	0.42
1:E:389:TYR:CE2	1:E:1050:GLY:HA2	2.54	0.42
1:E:387:LEU:O	1:E:1050:GLY:HA3	2.19	0.42
1:G:976:ASP:OD1	1:G:976:ASP:C	2.58	0.42
1:C:453:LEU:CD1	1:C:474:ILE:HG21	2.50	0.42
1:C:1076:ASP:OD2	1:C:1077:ASN:N	2.53	0.42
1:F:258:ASN:ND2	1:F:273:ARG:HB3	2.34	0.42
1:F:457:MET:HE3	1:F:493:TYR:HE2	1.84	0.42
1:F:271:TRP:CZ2	1:F:357:ARG:HD2	2.54	0.42
1:F:820:VAL:HB	1:F:821:PRO:HD2	2.01	0.42
1:D:870:LYS:HD2	1:D:873:TYR:HD2	1.85	0.42
1:H:492:ASP:OD2	1:H:1025:ARG:HD2	2.20	0.42
1:A:759:HIS:HD2	1:A:762:GLN:OE1	2.03	0.42
1:B:837:ALA:HA	1:B:838:PRO:HD3	1.94	0.42
1:G:368:SER:HA	1:G:371:ASN:HB2	2.01	0.42
1:G:250:GLN:CG	1:G:275:LYS:HE2	2.48	0.42
1:F:457:MET:HE2	1:F:493:TYR:CE2	2.55	0.42
1:E:304:GLU:O	1:E:308:GLN:HG2	2.20	0.42
1:A:376:LYS:HA	1:A:377:PRO:C	2.40	0.42
1:D:258:ASN:HB3	1:D:259:PHE:CE2	2.55	0.42
1:H:475:ARG:CA	1:H:953:MET:HE3	2.48	0.41
1:C:311:ASN:HD22	1:C:311:ASN:HA	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:740:ASN:HD22	1:D:742:SER:H	1.67	0.41
1:C:698:ARG:O	1:C:708:ILE:HA	2.20	0.41
1:A:563:ASN:HB3	4:A:1115:HOH:O	2.19	0.41
1:G:387:LEU:O	1:G:1050:GLY:HA3	2.19	0.41
1:B:261:HIS:HB3	1:B:1073:LEU:HD23	2.02	0.41
1:A:480:ASP:OD1	1:A:521:ASP:OD2	2.38	0.41
1:H:321:GLN:HG3	1:H:322:THR:H	1.85	0.41
1:H:531:ASN:ND2	1:H:844:SER:OG	2.53	0.41
1:A:729:ARG:HD2	1:A:729:ARG:HH11	1.72	0.41
1:E:694:GLY:HA3	1:E:718:LEU:O	2.20	0.41
1:E:247:GLN:O	1:E:250:GLN:HG2	2.19	0.41
1:B:861:SER:N	1:B:864:GLN:HE21	2.00	0.41
1:A:884:LYS:HE3	4:A:1171:HOH:O	2.18	0.41
1:H:478:ALA:HB1	1:H:481:ASN:HD22	1.85	0.41
1:D:471:PHE:CG	1:D:954:ALA:HB2	2.55	0.41
1:E:258:ASN:HB3	1:E:259:PHE:CE2	2.56	0.41
1:B:581:TYR:HA	1:B:654:VAL:O	2.20	0.41
1:C:478:ALA:HB1	1:C:481:ASN:HD22	1.84	0.41
1:H:513:ILE:CD1	1:H:953:MET:CE	2.99	0.41
1:E:669:TYR:CD2	1:E:670:MET:HG3	2.55	0.41
1:H:841:ASP:OD1	1:H:846:HIS:HE1	2.02	0.41
1:D:504:ASP:OD1	1:D:846:HIS:CD2	2.62	0.41
1:B:430:TYR:HB3	1:B:978:TYR:CE1	2.55	0.41
1:A:894:GLU:HA	1:A:953:MET:HB3	2.02	0.41
1:A:558:ASN:N	1:A:559:PRO:HD2	2.36	0.41
1:G:324:ASN:OD1	1:G:324:ASN:C	2.58	0.41
1:G:514:LEU:HD21	1:G:532:MET:HG3	2.02	0.41
1:F:862:ASN:O	1:F:912:ILE:HG12	2.21	0.41
1:C:1012:LEU:HA	1:C:1012:LEU:HD23	1.87	0.41
1:G:430:TYR:HB3	1:G:978:TYR:CE1	2.56	0.41
1:F:539:LEU:O	1:F:540:ARG:C	2.58	0.41
1:E:809:ASN:HB2	1:E:810:PRO:CD	2.51	0.41
1:H:407:ASN:ND2	1:H:431:GLU:H	2.19	0.41
1:B:965:PRO:HD2	1:B:998:SER:HA	2.03	0.41
1:D:430:TYR:HB3	1:D:978:TYR:CE1	2.56	0.41
1:F:870:LYS:HG3	4:F:3278:HOH:O	2.21	0.41
1:F:951:LYS:HA	1:F:951:LYS:HD3	1.94	0.41
1:H:759:HIS:HD2	1:H:762:GLN:OE1	2.04	0.41
1:D:670:MET:HE1	1:D:885:PHE:CZ	2.52	0.41
1:A:251:VAL:CG2	1:A:259:PHE:CZ	2.88	0.41
1:G:407:ASN:HD22	1:G:431:GLU:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:LEU:HD22	1:D:431:GLU:HG2	2.03	0.41
1:A:689:LYS:CE	4:A:3634:HOH:O	2.68	0.41
1:D:430:TYR:CD1	1:D:977:LYS:HD3	2.55	0.41
1:F:822:VAL:HG12	1:F:823:GLY:N	2.35	0.41
1:A:698:ARG:O	1:A:708:ILE:HA	2.21	0.41
1:G:524:TYR:CD2	1:G:524:TYR:C	2.94	0.41
1:D:492:ASP:HB3	1:D:1022:LEU:CD2	2.37	0.41
1:B:311:ASN:HD21	1:B:323:TYR:N	2.14	0.41
1:F:740:ASN:HD22	1:F:742:SER:H	1.65	0.41
1:B:335:ALA:O	1:B:339:ILE:HG13	2.21	0.41
1:A:309:TYR:CZ	1:A:313:MET:HG3	2.56	0.41
1:D:558:ASN:N	1:D:559:PRO:CD	2.84	0.41
1:C:988:LYS:O	1:C:990:THR:HG22	2.22	0.40
1:D:457:MET:CE	1:D:493:TYR:HE2	2.34	0.40
1:C:376:LYS:HA	1:C:377:PRO:C	2.41	0.40
1:F:579:PRO:HA	1:F:847:GLN:OE1	2.21	0.40
1:F:322:THR:CG2	1:F:323:TYR:N	2.84	0.40
1:G:1052:ASN:HD22	1:G:1052:ASN:H	1.68	0.40
1:G:750:ARG:HD3	4:G:1546:HOH:O	2.21	0.40
1:H:313:MET:CE	1:H:359:THR:HG22	2.51	0.40
1:G:581:TYR:HA	1:G:654:VAL:O	2.22	0.40
1:D:394:LYS:HB2	1:D:394:LYS:HE2	1.60	0.40
1:D:525:LEU:HD11	1:D:532:MET:HG2	2.03	0.40
1:H:480:ASP:OD1	1:H:521:ASP:OD2	2.39	0.40
1:F:1009:GLY:O	1:F:1039:LYS:HE2	2.21	0.40
1:E:596:ARG:HB2	1:E:612:PHE:HZ	1.87	0.40
1:G:729:ARG:HH11	1:G:729:ARG:HD2	1.72	0.40
1:A:466:ASP:C	1:A:468:ASP:H	2.25	0.40
1:D:870:LYS:HD2	1:D:873:TYR:CD2	2.56	0.40
1:G:312:TYR:CD2	1:G:363:PHE:HB2	2.56	0.40
1:C:480:ASP:OD1	1:C:521:ASP:OD2	2.40	0.40
1:B:453:LEU:HD13	1:B:474:ILE:HG21	2.03	0.40
1:H:346:LYS:HB3	1:H:346:LYS:HE3	1.91	0.40
1:C:251:VAL:HG22	1:C:258:ASN:HD22	1.86	0.40
1:D:1013:GLU:H	1:D:1013:GLU:HG2	1.60	0.40
1:G:250:GLN:HG2	1:G:275:LYS:HE2	2.04	0.40
1:D:1065:GLN:HG3	1:D:1066:ALA:H	1.86	0.40
1:B:442:ASN:HA	1:B:443:PRO:HD3	1.93	0.40
1:D:387:LEU:O	1:D:1050:GLY:HA3	2.22	0.40
1:A:244:SER:OG	1:A:244:SER:O	2.36	0.40
1:A:407:ASN:ND2	1:A:431:GLU:H	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:737:GLU:HA	1:D:815:TYR:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	842/844 (100%)	816 (97%)	25 (3%)	1 (0%)	56	58
1	B	842/844 (100%)	812 (96%)	29 (3%)	1 (0%)	56	58
1	C	842/844 (100%)	817 (97%)	24 (3%)	1 (0%)	56	58
1	D	842/844 (100%)	815 (97%)	25 (3%)	2 (0%)	52	53
1	E	842/844 (100%)	815 (97%)	25 (3%)	2 (0%)	52	53
1	F	842/844 (100%)	818 (97%)	24 (3%)	0	100	100
1	G	842/844 (100%)	817 (97%)	23 (3%)	2 (0%)	52	53
1	H	842/844 (100%)	817 (97%)	23 (3%)	2 (0%)	52	53
All	All	6736/6752 (100%)	6527 (97%)	198 (3%)	11 (0%)	52	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1077	ASN
1	D	1077	ASN
1	E	1077	ASN
1	C	793	ASP
1	G	747	ALA
1	D	705	SER
1	A	793	ASP
1	E	705	SER
1	H	1077	ASN

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Mol	Chain	Res	Type
1	G	705	SER
1	H	705	SER

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	715/715 (100%)	689 (96%)	26 (4%)	42	43
1	B	715/715 (100%)	673 (94%)	42 (6%)	24	20
1	C	715/715 (100%)	690 (96%)	25 (4%)	43	44
1	D	715/715 (100%)	686 (96%)	29 (4%)	37	36
1	E	715/715 (100%)	687 (96%)	28 (4%)	39	39
1	F	715/715 (100%)	686 (96%)	29 (4%)	37	36
1	G	715/715 (100%)	688 (96%)	27 (4%)	40	40
1	H	715/715 (100%)	685 (96%)	30 (4%)	36	35
All	All	5720/5720 (100%)	5484 (96%)	236 (4%)	37	36

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	SER
1	A	258	ASN
1	A	279	LYS
1	A	307	ARG
1	A	359	THR
1	A	368	SER
1	A	465	ASN
1	A	468	ASP
1	A	532	MET
1	A	574	GLU
1	A	600	LYS
1	A	626	LYS
1	A	689	LYS

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Mol	Chain	Res	Type
1	A	702	VAL
1	A	726	ARG
1	A	727	ILE
1	A	729	ARG
1	A	740	ASN
1	A	742	SER
1	A	744	ARG
1	A	793	ASP
1	A	800	THR
1	A	832	VAL
1	A	882	VAL
1	A	985	SER
1	A	1052	ASN
1	B	247	GLN
1	B	253	SER
1	B	254	THR
1	B	295	LEU
1	B	304	GLU
1	B	322	THR
1	B	325	THR
1	B	350	GLU
1	B	357	ARG
1	B	359	THR
1	B	366	THR
1	B	368	SER
1	B	394	LYS
1	B	422	THR
1	B	465	ASN
1	B	502	LYS
1	B	532	MET
1	B	540	ARG
1	B	626	LYS
1	B	634	LYS
1	B	702	VAL
1	B	726	ARG
1	B	740	ASN
1	B	744	ARG
1	B	793	ASP
1	B	832	VAL
1	B	870	LYS
1	B	882	VAL
1	B	884	LYS

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Mol	Chain	Res	Type
1	B	912	ILE
1	B	943	LYS
1	B	985	SER
1	B	990	THR
1	B	1001	LYS
1	B	1025	ARG
1	B	1038	VAL
1	B	1052	ASN
1	B	1063	LYS
1	B	1073	LEU
1	B	1074	VAL
1	B	1082	LYS
1	B	1083	SER
1	C	307	ARG
1	C	320	HIS
1	C	321	GLN
1	C	322	THR
1	C	342	LYS
1	C	390	SER
1	C	422	THR
1	C	457	MET
1	C	465	ASN
1	C	532	MET
1	C	574	GLU
1	C	702	VAL
1	C	729	ARG
1	C	740	ASN
1	C	800	THR
1	C	832	VAL
1	C	882	VAL
1	C	977	LYS
1	C	985	SER
1	C	990	THR
1	C	1001	LYS
1	C	1013	GLU
1	C	1038	VAL
1	C	1052	ASN
1	C	1074	VAL
1	D	251	VAL
1	D	290	LYS
1	D	307	ARG
1	D	321	GLN

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Mol	Chain	Res	Type
1	D	322	THR
1	D	342	LYS
1	D	368	SER
1	D	416	LYS
1	D	422	THR
1	D	457	MET
1	D	465	ASN
1	D	532	MET
1	D	574	GLU
1	D	600	LYS
1	D	702	VAL
1	D	707	ILE
1	D	726	ARG
1	D	740	ASN
1	D	744	ARG
1	D	782	GLN
1	D	793	ASP
1	D	832	VAL
1	D	880	LYS
1	D	977	LYS
1	D	988	LYS
1	D	990	THR
1	D	1025	ARG
1	D	1038	VAL
1	D	1052	ASN
1	E	247	GLN
1	E	253	SER
1	E	290	LYS
1	E	308	GLN
1	E	322	THR
1	E	325	THR
1	E	457	MET
1	E	465	ASN
1	E	532	MET
1	E	574	GLU
1	E	619	LYS
1	E	702	VAL
1	E	727	ILE
1	E	740	ASN
1	E	793	ASP
1	E	800	THR
1	E	832	VAL

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Mol	Chain	Res	Type
1	E	835	SER
1	E	870	LYS
1	E	882	VAL
1	E	928	LYS
1	E	990	THR
1	E	1001	LYS
1	E	1025	ARG
1	E	1038	VAL
1	E	1052	ASN
1	E	1082	LYS
1	E	1086	ASN
1	F	253	SER
1	F	258	ASN
1	F	308	GLN
1	F	321	GLN
1	F	350	GLU
1	F	357	ARG
1	F	372	SER
1	F	394	LYS
1	F	422	THR
1	F	465	ASN
1	F	532	MET
1	F	708	ILE
1	F	726	ARG
1	F	740	ASN
1	F	782	GLN
1	F	791	THR
1	F	803	ASP
1	F	832	VAL
1	F	868	THR
1	F	880	LYS
1	F	882	VAL
1	F	912	ILE
1	F	977	LYS
1	F	985	SER
1	F	990	THR
1	F	1001	LYS
1	F	1002	ASP
1	F	1052	ASN
1	F	1082	LYS
1	G	251	VAL
1	G	253	SER

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Mol	Chain	Res	Type
1	G	322	THR
1	G	342	LYS
1	G	350	GLU
1	G	394	LYS
1	G	422	THR
1	G	457	MET
1	G	465	ASN
1	G	532	MET
1	G	574	GLU
1	G	726	ARG
1	G	740	ASN
1	G	800	THR
1	G	832	VAL
1	G	870	LYS
1	G	882	VAL
1	G	928	LYS
1	G	977	LYS
1	G	985	SER
1	G	988	LYS
1	G	990	THR
1	G	1001	LYS
1	G	1013	GLU
1	G	1025	ARG
1	G	1038	VAL
1	G	1052	ASN
1	H	251	VAL
1	H	282	LYS
1	H	308	GLN
1	H	322	THR
1	H	324	ASN
1	H	329	PRO
1	H	342	LYS
1	H	351	LYS
1	H	394	LYS
1	H	465	ASN
1	H	532	MET
1	H	600	LYS
1	H	619	LYS
1	H	702	VAL
1	H	726	ARG
1	H	740	ASN
1	H	744	ARG

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Mol	Chain	Res	Type
1	H	800	THR
1	H	832	VAL
1	H	835	SER
1	H	870	LYS
1	H	985	SER
1	H	990	THR
1	H	1001	LYS
1	H	1025	ARG
1	H	1038	VAL
1	H	1052	ASN
1	H	1075	SER
1	H	1082	LYS
1	H	1083	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (171) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	261	HIS
1	A	308	GLN
1	A	311	ASN
1	A	367	GLN
1	A	407	ASN
1	A	440	ASN
1	A	470	ASN
1	A	481	ASN
1	A	531	ASN
1	A	572	ASN
1	A	639	ASN
1	A	740	ASN
1	A	759	HIS
1	A	773	ASN
1	A	782	GLN
1	A	846	HIS
1	A	864	GLN
1	A	960	GLN
1	A	1052	ASN
1	A	1068	ASN
1	B	247	GLN
1	B	258	ASN
1	B	261	HIS
1	B	308	GLN

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Mol	Chain	Res	Type
1	B	311	ASN
1	B	407	ASN
1	B	440	ASN
1	B	461	ASN
1	B	470	ASN
1	B	481	ASN
1	B	531	ASN
1	B	572	ASN
1	B	639	ASN
1	B	740	ASN
1	B	759	HIS
1	B	773	ASN
1	B	846	HIS
1	B	864	GLN
1	B	881	ASN
1	B	960	GLN
1	B	1003	GLN
1	B	1052	ASN
1	C	250	GLN
1	C	261	HIS
1	C	308	GLN
1	C	311	ASN
1	C	367	GLN
1	C	407	ASN
1	C	440	ASN
1	C	470	ASN
1	C	481	ASN
1	C	531	ASN
1	C	572	ASN
1	C	639	ASN
1	C	740	ASN
1	C	759	HIS
1	C	782	GLN
1	C	846	HIS
1	C	864	GLN
1	C	881	ASN
1	C	1003	GLN
1	C	1052	ASN
1	C	1068	ASN
1	D	261	HIS
1	D	308	GLN
1	D	311	ASN

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Mol	Chain	Res	Type
1	D	367	GLN
1	D	407	ASN
1	D	440	ASN
1	D	470	ASN
1	D	481	ASN
1	D	531	ASN
1	D	572	ASN
1	D	639	ASN
1	D	699	ASN
1	D	740	ASN
1	D	759	HIS
1	D	782	GLN
1	D	846	HIS
1	D	864	GLN
1	D	881	ASN
1	D	960	GLN
1	D	1052	ASN
1	D	1068	ASN
1	E	247	GLN
1	E	250	GLN
1	E	261	HIS
1	E	308	GLN
1	E	311	ASN
1	E	367	GLN
1	E	407	ASN
1	E	440	ASN
1	E	470	ASN
1	E	481	ASN
1	E	531	ASN
1	E	572	ASN
1	E	639	ASN
1	E	740	ASN
1	E	759	HIS
1	E	846	HIS
1	E	864	GLN
1	E	881	ASN
1	E	960	GLN
1	E	1003	GLN
1	E	1052	ASN
1	E	1065	GLN
1	F	258	ASN
1	F	261	HIS

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Mol	Chain	Res	Type
1	F	308	GLN
1	F	311	ASN
1	F	367	GLN
1	F	407	ASN
1	F	440	ASN
1	F	470	ASN
1	F	481	ASN
1	F	531	ASN
1	F	572	ASN
1	F	639	ASN
1	F	699	ASN
1	F	740	ASN
1	F	759	HIS
1	F	846	HIS
1	F	864	GLN
1	F	960	GLN
1	F	1052	ASN
1	F	1068	ASN
1	G	261	HIS
1	G	308	GLN
1	G	311	ASN
1	G	367	GLN
1	G	407	ASN
1	G	440	ASN
1	G	470	ASN
1	G	481	ASN
1	G	531	ASN
1	G	572	ASN
1	G	639	ASN
1	G	699	ASN
1	G	740	ASN
1	G	759	HIS
1	G	846	HIS
1	G	864	GLN
1	G	881	ASN
1	G	960	GLN
1	G	1003	GLN
1	G	1052	ASN
1	G	1068	ASN
1	H	250	GLN
1	H	261	HIS
1	H	308	GLN

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Mol	Chain	Res	Type
1	H	311	ASN
1	H	324	ASN
1	H	337	GLN
1	H	367	GLN
1	H	407	ASN
1	H	440	ASN
1	H	461	ASN
1	H	470	ASN
1	H	481	ASN
1	H	531	ASN
1	H	572	ASN
1	H	639	ASN
1	H	740	ASN
1	H	759	HIS
1	H	846	HIS
1	H	864	GLN
1	H	960	GLN
1	H	1003	GLN
1	H	1052	ASN
1	H	1068	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	MES	A	5001	-	11,12,12	1.32	2 (18%)	14,16,16	7.53	8 (57%)
3	MES	B	5001	-	11,12,12	0.67	0	14,16,16	7.27	11 (78%)
3	MES	C	5001	-	11,12,12	0.72	0	14,16,16	9.61	9 (64%)
3	MES	D	5001	-	11,12,12	2.02	1 (9%)	14,16,16	9.44	8 (57%)
3	MES	E	5001	-	11,12,12	0.83	0	14,16,16	4.34	10 (71%)
3	MES	F	5001	-	11,12,12	1.11	1 (9%)	14,16,16	2.93	5 (35%)
3	MES	G	5001	-	11,12,12	0.78	0	14,16,16	6.83	8 (57%)
3	MES	H	5001	-	11,12,12	0.73	0	14,16,16	9.61	9 (64%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	5001	-	-	0/6/14/14	0/1/1/1
3	MES	B	5001	-	-	0/6/14/14	0/1/1/1
3	MES	C	5001	-	-	0/6/14/14	0/1/1/1
3	MES	D	5001	-	-	0/6/14/14	0/1/1/1
3	MES	E	5001	-	-	0/6/14/14	0/1/1/1
3	MES	F	5001	-	-	0/6/14/14	0/1/1/1
3	MES	G	5001	-	-	0/6/14/14	0/1/1/1
3	MES	H	5001	-	-	0/6/14/14	1/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5001	MES	O3S-S	-6.20	1.30	1.46
3	A	5001	MES	O2S-S	-2.52	1.37	1.45
3	A	5001	MES	O3S-S	-2.45	1.40	1.46
3	F	5001	MES	O3S-S	-2.07	1.41	1.46

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5001	MES	O2S-S-C8	-29.07	82.10	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5001	MES	O2S-S-C8	-24.42	86.07	106.91
3	H	5001	MES	O1S-S-C8	-24.38	86.11	106.91
3	C	5001	MES	O1S-S-C8	-24.37	86.11	106.91
3	H	5001	MES	O2S-S-C8	-24.36	86.12	106.91
3	B	5001	MES	O1S-S-C8	-22.45	87.75	106.91
3	A	5001	MES	O2S-S-C8	-21.41	88.64	106.91
3	G	5001	MES	O1S-S-C8	-19.26	90.47	106.91
3	A	5001	MES	O1S-S-C8	-15.63	93.57	106.91
3	D	5001	MES	O1S-S-C8	-15.06	94.06	106.91
3	G	5001	MES	O2S-S-C8	-14.02	94.94	106.91
3	B	5001	MES	O2S-S-C8	-10.37	98.05	106.91
3	E	5001	MES	O2S-S-C8	-8.68	99.50	106.91
3	E	5001	MES	O1S-S-C8	-7.15	100.80	106.91
3	D	5001	MES	C6-C5-N4	-4.51	103.29	110.12
3	H	5001	MES	C2-C3-N4	-4.26	103.66	110.12
3	H	5001	MES	C6-C5-N4	-3.44	104.91	110.12
3	C	5001	MES	C6-C5-N4	-3.38	105.00	110.12
3	C	5001	MES	C2-C3-N4	-3.37	105.02	110.12
3	B	5001	MES	O1-C2-C3	-2.83	105.36	111.84
3	B	5001	MES	C2-C3-N4	-2.39	106.50	110.12
3	A	5001	MES	C2-C3-N4	-2.39	106.50	110.12
3	E	5001	MES	O3S-S-O2S	2.11	116.51	111.61
3	D	5001	MES	C2-C3-N4	2.12	113.34	110.12
3	E	5001	MES	C6-O1-C2	2.36	117.84	109.89
3	E	5001	MES	C2-C3-N4	2.51	113.93	110.12
3	E	5001	MES	O1-C6-C5	2.78	118.21	111.84
3	B	5001	MES	O3S-S-O1S	2.90	118.36	111.61
3	B	5001	MES	C6-C5-N4	2.95	114.59	110.12
3	G	5001	MES	O3S-S-O1S	3.09	118.81	111.61
3	F	5001	MES	C6-C5-N4	3.17	114.93	110.12
3	G	5001	MES	C7-N4-C5	3.29	119.71	111.27
3	A	5001	MES	C7-N4-C5	3.31	119.75	111.27
3	H	5001	MES	O3S-S-O2S	3.39	119.50	111.61
3	C	5001	MES	O3S-S-O1S	3.40	119.52	111.61
3	C	5001	MES	C7-N4-C5	3.40	120.00	111.27
3	C	5001	MES	C7-N4-C3	3.41	120.00	111.27
3	C	5001	MES	O3S-S-O2S	3.41	119.54	111.61
3	H	5001	MES	O3S-S-O1S	3.41	119.55	111.61
3	G	5001	MES	C7-N4-C3	3.50	120.24	111.27
3	G	5001	MES	O3S-S-O2S	3.52	119.80	111.61
3	A	5001	MES	C5-N4-C3	3.52	116.53	108.90
3	H	5001	MES	C7-N4-C3	3.56	120.40	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	5001	MES	C7-N4-C5	3.58	120.46	111.27
3	B	5001	MES	C7-N4-C3	3.61	120.53	111.27
3	G	5001	MES	C2-C3-N4	3.83	115.93	110.12
3	B	5001	MES	C7-N4-C5	3.86	121.16	111.27
3	A	5001	MES	O3S-S-O2S	3.86	120.60	111.61
3	A	5001	MES	O3S-S-O1S	3.89	120.66	111.61
3	E	5001	MES	C6-C5-N4	4.01	116.20	110.12
3	F	5001	MES	O1S-S-C8	4.25	110.53	106.91
3	B	5001	MES	C5-N4-C3	4.34	118.30	108.90
3	B	5001	MES	C7-C8-S	4.48	126.37	112.51
3	F	5001	MES	C7-N4-C3	4.49	122.78	111.27
3	D	5001	MES	O3S-S-O1S	4.66	122.45	111.61
3	G	5001	MES	C5-N4-C3	4.70	119.07	108.90
3	H	5001	MES	C5-N4-C3	4.73	119.14	108.90
3	A	5001	MES	C7-N4-C3	4.86	123.72	111.27
3	B	5001	MES	O3S-S-O2S	4.97	123.18	111.61
3	E	5001	MES	C7-N4-C5	5.05	124.23	111.27
3	F	5001	MES	O2S-S-C8	5.10	111.25	106.91
3	E	5001	MES	O3S-S-O1S	5.11	123.50	111.61
3	C	5001	MES	C5-N4-C3	5.13	120.00	108.90
3	D	5001	MES	C7-N4-C5	5.55	125.50	111.27
3	F	5001	MES	C5-N4-C3	5.80	121.46	108.90
3	D	5001	MES	C5-N4-C3	6.01	121.93	108.90
3	E	5001	MES	C5-N4-C3	6.46	122.89	108.90
3	D	5001	MES	O3S-S-O2S	7.57	129.22	111.61

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	5001	MES	C2-C3-C5-C6-N4-O1

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5001	MES	2	0
3	D	5001	MES	1	0
3	H	5001	MES	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	844/844 (100%)	-0.18	14 (1%) 73 78	19, 30, 49, 66	0
1	B	844/844 (100%)	-0.04	25 (2%) 54 62	27, 37, 52, 70	0
1	C	844/844 (100%)	-0.21	12 (1%) 78 82	22, 30, 45, 61	0
1	D	844/844 (100%)	-0.23	10 (1%) 81 85	21, 30, 47, 64	0
1	E	844/844 (100%)	-0.17	21 (2%) 61 67	19, 29, 53, 70	0
1	F	844/844 (100%)	0.01	28 (3%) 50 59	26, 38, 54, 65	0
1	G	844/844 (100%)	-0.18	9 (1%) 82 86	19, 28, 45, 62	0
1	H	844/844 (100%)	-0.20	15 (1%) 71 76	21, 30, 44, 61	0
All	All	6752/6752 (100%)	-0.15	134 (1%) 68 73	19, 32, 50, 70	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1087	PRO	5.7
1	B	1087	PRO	5.3
1	B	1076	ASP	5.2
1	A	1087	PRO	5.2
1	G	1087	PRO	5.0
1	B	1077	ASN	4.9
1	F	785	ALA	4.9
1	A	1076	ASP	4.8
1	C	1086	ASN	4.7
1	B	1075	SER	4.6
1	E	1086	ASN	4.6
1	A	1077	ASN	4.5
1	A	1086	ASN	4.4
1	D	1076	ASP	4.4
1	H	1065	GLN	4.3
1	H	1087	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	1087	PRO	4.3
1	F	320	HIS	4.3
1	F	1077	ASN	4.2
1	F	1086	ASN	4.2
1	A	320	HIS	4.2
1	H	1086	ASN	4.2
1	H	1076	ASP	4.1
1	H	245	PHE	4.0
1	F	667	GLY	3.9
1	D	1087	PRO	3.9
1	B	289	GLU	3.8
1	F	1087	PRO	3.7
1	F	1076	ASP	3.6
1	G	1086	ASN	3.6
1	E	1076	ASP	3.5
1	B	1086	ASN	3.5
1	D	1086	ASN	3.5
1	F	1075	SER	3.5
1	B	1065	GLN	3.5
1	B	785	ALA	3.5
1	C	1077	ASN	3.5
1	A	1075	SER	3.5
1	E	248	TYR	3.5
1	F	726	ARG	3.4
1	C	1076	ASP	3.3
1	C	1082	LYS	3.3
1	E	289	GLU	3.3
1	F	1082	LYS	3.2
1	C	1065	GLN	3.1
1	B	1074	VAL	3.1
1	D	394	LYS	3.1
1	B	1085	VAL	3.1
1	H	1082	LYS	3.1
1	G	1076	ASP	3.0
1	A	285	THR	3.0
1	E	252	TYR	3.0
1	F	727	ILE	3.0
1	B	244	SER	3.0
1	G	782	GLN	3.0
1	C	252	TYR	2.9
1	F	1065	GLN	2.9
1	E	288	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	467	PRO	2.9
1	C	320	HIS	2.9
1	A	1065	GLN	2.9
1	C	1075	SER	2.9
1	E	1077	ASN	2.9
1	F	252	TYR	2.8
1	A	1082	LYS	2.8
1	C	244	SER	2.8
1	B	320	HIS	2.8
1	F	784	ALA	2.8
1	H	244	SER	2.8
1	G	290	LYS	2.8
1	H	246	ALA	2.8
1	B	1082	LYS	2.7
1	B	827	ASP	2.7
1	E	244	SER	2.7
1	G	1077	ASN	2.7
1	B	823	GLY	2.6
1	H	1077	ASN	2.6
1	E	285	THR	2.6
1	F	782	GLN	2.6
1	G	1082	LYS	2.6
1	E	1065	GLN	2.6
1	E	274	PRO	2.6
1	F	289	GLU	2.6
1	D	1082	LYS	2.6
1	B	247	GLN	2.5
1	E	290	LYS	2.5
1	F	794	ARG	2.5
1	A	244	SER	2.5
1	D	1077	ASN	2.5
1	H	289	GLU	2.5
1	B	290	LYS	2.5
1	A	1078	THR	2.4
1	E	280	ASP	2.4
1	E	349	ALA	2.4
1	G	726	ARG	2.4
1	F	793	ASP	2.4
1	B	744	ARG	2.4
1	D	289	GLU	2.4
1	E	247	GLN	2.3
1	F	753	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	288	THR	2.3
1	E	320	HIS	2.3
1	F	750	ARG	2.3
1	B	834	ALA	2.3
1	E	1074	VAL	2.2
1	D	320	HIS	2.2
1	B	794	ARG	2.2
1	C	1074	VAL	2.2
1	B	1066	ALA	2.2
1	B	252	TYR	2.2
1	B	276	TYR	2.2
1	E	253	SER	2.2
1	G	1065	GLN	2.2
1	H	726	ARG	2.2
1	H	1067	THR	2.2
1	B	259	PHE	2.2
1	D	252	TYR	2.2
1	F	826	ALA	2.2
1	F	773	ASN	2.1
1	E	286	GLN	2.1
1	F	742	SER	2.1
1	H	1066	ALA	2.1
1	C	1085	VAL	2.1
1	A	1066	ALA	2.1
1	E	326	ALA	2.1
1	F	394	LYS	2.1
1	H	465	ASN	2.1
1	A	251	VAL	2.1
1	F	290	LYS	2.0
1	D	1065	GLN	2.0
1	F	787	LEU	2.0
1	F	761	ASN	2.0
1	A	1085	VAL	2.0
1	B	394	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MES	B	5001	12/12	0.94	0.17	6.65	6,13,15,16	0
3	MES	C	5001	12/12	0.94	0.23	6.01	2,2,7,10	0
3	MES	D	5001	12/12	0.97	0.15	4.78	2,6,13,14	0
3	MES	H	5001	12/12	0.92	0.17	3.59	5,22,93,99	0
3	MES	G	5001	12/12	0.98	0.09	-0.92	4,8,15,21	0
2	CA	G	4001	1/1	1.00	0.10	-1.53	16,16,16,16	0
2	CA	H	4001	1/1	0.99	0.10	-1.55	18,18,18,18	0
3	MES	E	5001	12/12	0.99	0.08	-2.60	19,24,27,28	0
2	CA	E	4001	1/1	0.99	0.07	-2.75	18,18,18,18	0
2	CA	A	4001	1/1	1.00	0.08	-2.88	17,17,17,17	0
2	CA	B	4001	1/1	0.95	0.04	-4.14	19,19,19,19	0
2	CA	C	4001	1/1	1.00	0.05	-4.43	17,17,17,17	0
2	CA	F	4001	1/1	0.99	0.03	-5.68	16,16,16,16	0
2	CA	D	4001	1/1	0.98	0.06	-5.75	18,18,18,18	0
3	MES	A	5001	12/12	0.96	0.10	-	22,22,62,81	0
3	MES	F	5001	12/12	0.90	0.14	-	2,16,32,98	0

### 6.5 Other polymers

There are no such residues in this entry.