



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:26 AM GMT

PDB ID : 2D40  
Title : Crystal Structure of Z3393 from Escherichia coli O157:H7  
Authors : Adams, M.A.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)  
Deposited on : 2005-10-05  
Resolution : 2.41 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

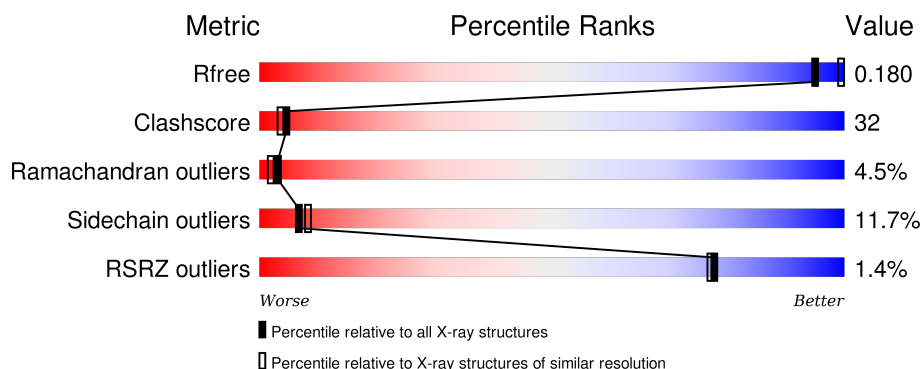
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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	354	<div> <div>32%</div> <div>33%</div> <div>14%</div> <div>•</div> <div>18%</div> </div>
1	B	354	<div> <div>27%</div> <div>33%</div> <div>15%</div> <div>5%</div> <div>20%</div> </div>
1	C	354	<div> <div>31%</div> <div>34%</div> <div>14%</div> <div>•</div> <div>18%</div> </div>
1	D	354	<div> <div>30%</div> <div>32%</div> <div>13%</div> <div>5%</div> <div>19%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9579 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 putative gentisate 1,2-dioxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	Se	0	0	0
			2280	1447	399	426	2	6			
1	B	284	Total	C	N	O	S	Se	0	0	0
			2235	1418	392	417	2	6			
1	C	289	Total	C	N	O	S	Se	0	0	0
			2281	1447	399	427	2	6			
1	D	287	Total	C	N	O	S	Se	0	0	0
			2263	1437	396	422	2	6			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	EXPRESSION TAG	UNP Q8X655
A	-10	GLY	-	EXPRESSION TAG	UNP Q8X655
A	-9	SER	-	EXPRESSION TAG	UNP Q8X655
A	-8	SER	-	EXPRESSION TAG	UNP Q8X655
A	-7	HIS	-	EXPRESSION TAG	UNP Q8X655
A	-6	HIS	-	EXPRESSION TAG	UNP Q8X655
A	-5	HIS	-	EXPRESSION TAG	UNP Q8X655
A	-4	HIS	-	EXPRESSION TAG	UNP Q8X655
A	-3	HIS	-	EXPRESSION TAG	UNP Q8X655
A	-2	HIS	-	EXPRESSION TAG	UNP Q8X655
A	-1	GLY	-	EXPRESSION TAG	UNP Q8X655
A	0	SER	-	EXPRESSION TAG	UNP Q8X655
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
A	96	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
A	131	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
A	199	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
A	241	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
A	253	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
A	256	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
B	-11	MSE	-	EXPRESSION TAG	UNP Q8X655
B	-10	GLY	-	EXPRESSION TAG	UNP Q8X655

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	SER	-	EXPRESSION TAG	UNP Q8X655
B	-8	SER	-	EXPRESSION TAG	UNP Q8X655
B	-7	HIS	-	EXPRESSION TAG	UNP Q8X655
B	-6	HIS	-	EXPRESSION TAG	UNP Q8X655
B	-5	HIS	-	EXPRESSION TAG	UNP Q8X655
B	-4	HIS	-	EXPRESSION TAG	UNP Q8X655
B	-3	HIS	-	EXPRESSION TAG	UNP Q8X655
B	-2	HIS	-	EXPRESSION TAG	UNP Q8X655
B	-1	GLY	-	EXPRESSION TAG	UNP Q8X655
B	0	SER	-	EXPRESSION TAG	UNP Q8X655
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
B	96	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
B	131	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
B	199	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
B	241	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
B	253	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
B	256	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
C	-11	MSE	-	EXPRESSION TAG	UNP Q8X655
C	-10	GLY	-	EXPRESSION TAG	UNP Q8X655
C	-9	SER	-	EXPRESSION TAG	UNP Q8X655
C	-8	SER	-	EXPRESSION TAG	UNP Q8X655
C	-7	HIS	-	EXPRESSION TAG	UNP Q8X655
C	-6	HIS	-	EXPRESSION TAG	UNP Q8X655
C	-5	HIS	-	EXPRESSION TAG	UNP Q8X655
C	-4	HIS	-	EXPRESSION TAG	UNP Q8X655
C	-3	HIS	-	EXPRESSION TAG	UNP Q8X655
C	-2	HIS	-	EXPRESSION TAG	UNP Q8X655
C	-1	GLY	-	EXPRESSION TAG	UNP Q8X655
C	0	SER	-	EXPRESSION TAG	UNP Q8X655
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
C	96	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
C	131	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
C	199	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
C	241	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
C	253	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
C	256	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
D	-11	MSE	-	EXPRESSION TAG	UNP Q8X655
D	-10	GLY	-	EXPRESSION TAG	UNP Q8X655
D	-9	SER	-	EXPRESSION TAG	UNP Q8X655
D	-8	SER	-	EXPRESSION TAG	UNP Q8X655
D	-7	HIS	-	EXPRESSION TAG	UNP Q8X655
D	-6	HIS	-	EXPRESSION TAG	UNP Q8X655

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	EXPRESSION TAG	UNP Q8X655
D	-4	HIS	-	EXPRESSION TAG	UNP Q8X655
D	-3	HIS	-	EXPRESSION TAG	UNP Q8X655
D	-2	HIS	-	EXPRESSION TAG	UNP Q8X655
D	-1	GLY	-	EXPRESSION TAG	UNP Q8X655
D	0	SER	-	EXPRESSION TAG	UNP Q8X655
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
D	96	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
D	131	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
D	199	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
D	241	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
D	253	MSE	MET	MODIFIED RESIDUE	UNP Q8X655
D	256	MSE	MET	MODIFIED RESIDUE	UNP Q8X655

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

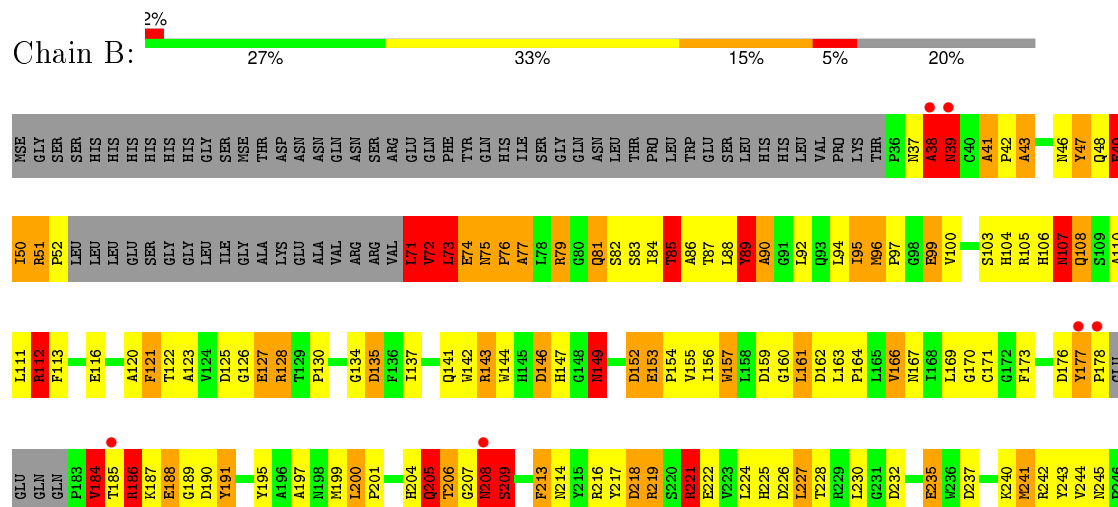
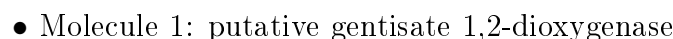
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

- Molecule 3 is water.

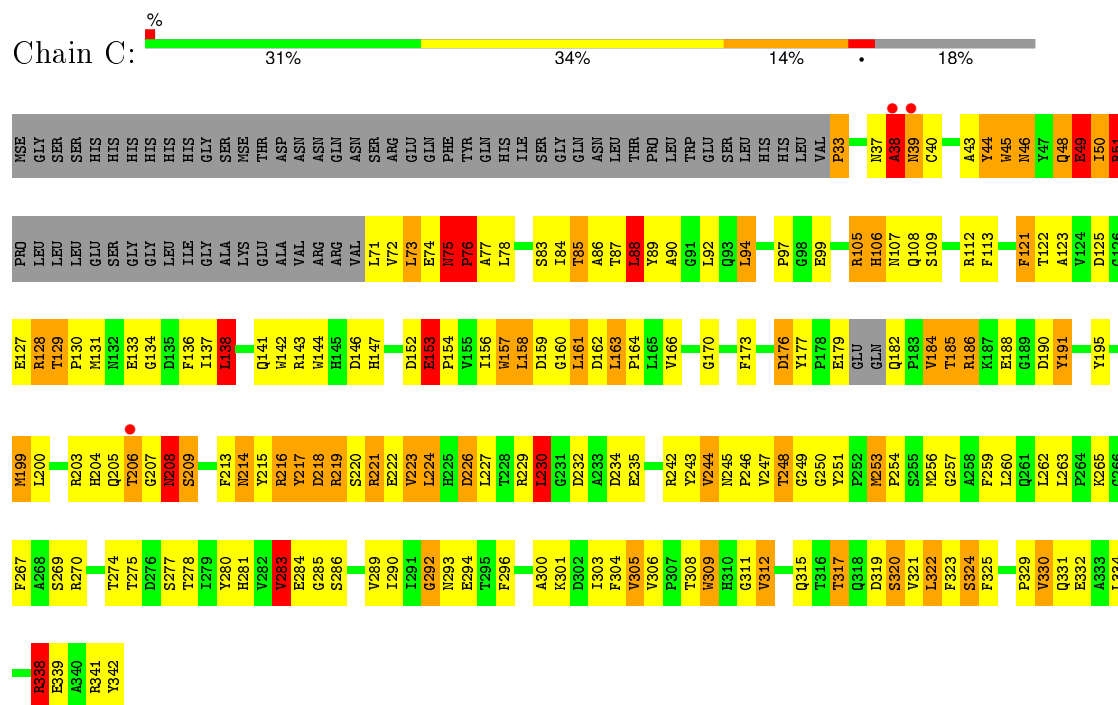
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	110	Total O 110 110	0	0
3	B	129	Total O 129 129	0	0
3	C	130	Total O 130 130	0	0
3	D	147	Total O 147 147	0	0



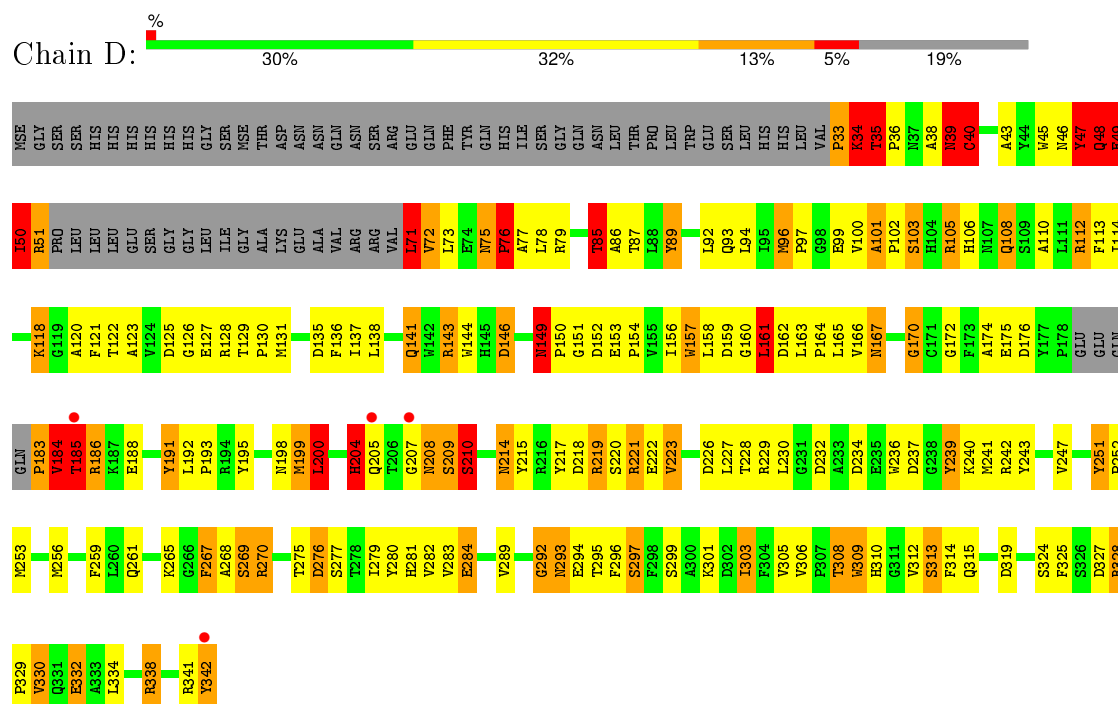
- Molecule 1: putative gentisate 1,2-dioxygenase



- Molecule 1: putative gentisate 1,2-dioxygenase



- Molecule 1: putative gentisate 1,2-dioxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.13Å 76.08Å 85.46Å 114.08° 94.93° 108.11°	Depositor
Resolution (Å)	34.50 – 2.41 34.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.50-2.41) 78.7 (34.48-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.71 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.173 , 0.249 0.188 , 0.180	Depositor DCC
$R_{free}$ test set	2048 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 41628 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: FE

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	2.32	88/2340 (3.8%)	1.67	39/3182 (1.2%)
1	B	2.31	92/2294 (4.0%)	1.63	41/3118 (1.3%)
1	C	2.31	90/2341 (3.8%)	1.77	49/3181 (1.5%)
1	D	2.38	100/2323 (4.3%)	1.73	55/3156 (1.7%)
All	All	2.33	370/9298 (4.0%)	1.70	184/12637 (1.5%)

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	A	0	1
1	B	0	2
1	D	0	2
All	All	0	5

All (370) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	ALA	CA-CB	-14.93	1.21	1.52
1	D	50	ILE	CA-CB	12.29	1.83	1.54
1	B	289	VAL	CB-CG2	-11.71	1.28	1.52
1	D	267	PHE	CD2-CE2	-10.95	1.17	1.39
1	D	76	PRO	CA-CB	10.78	1.75	1.53
1	B	39	ASN	CB-CG	10.58	1.75	1.51
1	A	40	CYS	C-O	10.41	1.43	1.23
1	A	251	TYR	CE2-CZ	10.41	1.52	1.38
1	D	39	ASN	CB-CG	10.38	1.75	1.51
1	D	89	TYR	CE2-CZ	-10.04	1.25	1.38
1	D	40	CYS	CB-SG	-9.96	1.65	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	GLU	CD-OE1	9.78	1.36	1.25
1	A	90	ALA	CA-CB	-9.78	1.31	1.52
1	A	280	TYR	CE1-CZ	-9.62	1.26	1.38
1	D	283	VAL	CB-CG1	-9.56	1.32	1.52
1	D	50	ILE	N-CA	9.51	1.65	1.46
1	C	209	SER	CA-CB	9.35	1.67	1.52
1	A	215	TYR	CZ-OH	9.32	1.53	1.37
1	C	217	TYR	CE1-CZ	-9.32	1.26	1.38
1	C	312	VAL	CB-CG1	9.17	1.72	1.52
1	D	101	ALA	CA-CB	9.10	1.71	1.52
1	A	213	PHE	CE2-CZ	-8.98	1.20	1.37
1	C	330	VAL	CB-CG2	-8.96	1.34	1.52
1	A	293	ASN	CB-CG	8.88	1.71	1.51
1	C	143	ARG	CG-CD	8.74	1.73	1.51
1	B	41	ALA	CA-CB	8.74	1.70	1.52
1	B	142	TRP	CE3-CZ3	-8.66	1.23	1.38
1	A	243	TYR	CE2-CZ	-8.64	1.27	1.38
1	B	321	VAL	CA-CB	-8.58	1.36	1.54
1	B	149	ASN	CB-CG	-8.51	1.31	1.51
1	D	33	PRO	N-CA	8.48	1.61	1.47
1	B	38	ALA	CA-CB	8.44	1.70	1.52
1	C	244	VAL	CB-CG1	-8.44	1.35	1.52
1	D	282	VAL	CB-CG2	-8.38	1.35	1.52
1	D	45	TRP	CB-CG	-8.38	1.35	1.50
1	C	305	VAL	CB-CG1	-8.34	1.35	1.52
1	B	319	ASP	CB-CG	-8.34	1.34	1.51
1	D	297	SER	CA-CB	8.34	1.65	1.52
1	C	324	SER	CB-OG	8.32	1.53	1.42
1	B	249	GLY	C-O	8.32	1.36	1.23
1	B	184	VAL	CB-CG2	8.30	1.70	1.52
1	B	267	PHE	CE2-CZ	8.29	1.53	1.37
1	B	314	PHE	CG-CD1	8.26	1.51	1.38
1	A	72	VAL	CB-CG2	-8.21	1.35	1.52
1	D	222	GLU	CD-OE2	8.18	1.34	1.25
1	D	96	MSE	SE-CE	8.17	2.43	1.95
1	C	195	TYR	CE1-CZ	-8.16	1.27	1.38
1	D	309	TRP	CZ3-CH2	8.04	1.52	1.40
1	B	90	ALA	CA-CB	-8.02	1.35	1.52
1	A	155	VAL	CB-CG2	7.97	1.69	1.52
1	A	251	TYR	CD2-CE2	-7.87	1.27	1.39
1	D	100	VAL	C-O	-7.86	1.08	1.23
1	B	49	GLU	CD-OE2	7.83	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	112	ARG	NE-CZ	-7.80	1.23	1.33
1	D	209	SER	CA-CB	7.78	1.64	1.52
1	C	99	GLU	CD-OE2	7.78	1.34	1.25
1	C	72	VAL	CB-CG2	7.76	1.69	1.52
1	D	105	ARG	NE-CZ	7.74	1.43	1.33
1	A	305	VAL	CB-CG1	-7.73	1.36	1.52
1	A	341	ARG	CD-NE	-7.72	1.33	1.46
1	A	107	ASN	CB-CG	-7.70	1.33	1.51
1	B	113	PHE	CD2-CE2	-7.68	1.23	1.39
1	D	229	ARG	CG-CD	7.68	1.71	1.51
1	B	235	GLU	CD-OE2	-7.66	1.17	1.25
1	D	108	GLN	CG-CD	7.57	1.68	1.51
1	C	235	GLU	CD-OE1	7.53	1.33	1.25
1	C	50	ILE	CB-CG2	7.51	1.76	1.52
1	B	309	TRP	CB-CG	-7.50	1.36	1.50
1	C	38	ALA	CA-CB	7.48	1.68	1.52
1	B	191	TYR	CD1-CE1	7.47	1.50	1.39
1	D	342	TYR	CE1-CZ	7.47	1.48	1.38
1	D	284	GLU	CD-OE2	-7.46	1.17	1.25
1	D	296	PHE	CG-CD1	-7.45	1.27	1.38
1	B	280	TYR	CE1-CZ	-7.45	1.28	1.38
1	C	75	ASN	CG-ND2	7.45	1.51	1.32
1	A	247	VAL	CB-CG2	-7.39	1.37	1.52
1	A	152	ASP	C-O	7.37	1.37	1.23
1	D	243	TYR	CE1-CZ	7.36	1.48	1.38
1	B	191	TYR	CZ-OH	-7.33	1.25	1.37
1	B	337	PHE	CE2-CZ	7.30	1.51	1.37
1	B	209	SER	CA-CB	7.29	1.63	1.52
1	A	300	ALA	C-O	-7.27	1.09	1.23
1	D	105	ARG	CB-CG	-7.27	1.32	1.52
1	B	188	GLU	C-O	7.23	1.37	1.23
1	C	309	TRP	CB-CG	-7.20	1.37	1.50
1	A	76	PRO	CA-CB	7.19	1.68	1.53
1	B	273	ARG	CG-CD	-7.15	1.34	1.51
1	D	332	GLU	CG-CD	7.14	1.62	1.51
1	C	323	PHE	CE2-CZ	7.13	1.50	1.37
1	C	285	GLY	C-O	-7.11	1.12	1.23
1	A	223	VAL	CB-CG2	-7.03	1.38	1.52
1	C	243	TYR	CB-CG	-7.03	1.41	1.51
1	B	143	ARG	CZ-NH1	7.01	1.42	1.33
1	C	311	GLY	C-O	-7.00	1.12	1.23
1	C	283	VAL	CB-CG2	-6.99	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	THR	CA-CB	6.99	1.71	1.53
1	A	321	VAL	CA-CB	-6.96	1.40	1.54
1	D	204	HIS	C-O	6.96	1.36	1.23
1	B	188	GLU	CD-OE2	6.93	1.33	1.25
1	A	243	TYR	CG-CD2	-6.91	1.30	1.39
1	C	249	GLY	C-O	-6.90	1.12	1.23
1	D	144	TRP	C-O	-6.87	1.10	1.23
1	A	44	TYR	CE2-CZ	-6.86	1.29	1.38
1	C	76	PRO	CA-CB	6.85	1.67	1.53
1	B	184	VAL	CB-CG1	6.83	1.67	1.52
1	B	267	PHE	CD1-CE1	6.83	1.52	1.39
1	A	314	PHE	CE2-CZ	-6.82	1.24	1.37
1	A	253	MSE	CG-SE	6.79	2.18	1.95
1	A	37	ASN	C-O	6.79	1.36	1.23
1	A	121	PHE	CE1-CZ	6.76	1.50	1.37
1	D	342	TYR	CG-CD2	6.76	1.48	1.39
1	B	208	ASN	CB-CG	6.75	1.66	1.51
1	D	306	VAL	CB-CG1	6.74	1.67	1.52
1	B	85	THR	CB-CG2	-6.74	1.30	1.52
1	C	153	GLU	CD-OE2	6.70	1.33	1.25
1	A	136	PHE	CD1-CE1	-6.69	1.25	1.39
1	D	128	ARG	CZ-NH2	-6.69	1.24	1.33
1	A	121	PHE	CE2-CZ	-6.66	1.24	1.37
1	D	312	VAL	CA-CB	-6.66	1.40	1.54
1	C	157	TRP	CE3-CZ3	6.60	1.49	1.38
1	D	118	LYS	CE-NZ	6.58	1.65	1.49
1	B	121	PHE	CE2-CZ	6.58	1.49	1.37
1	D	110	ALA	CA-CB	-6.57	1.38	1.52
1	D	85	THR	CB-CG2	-6.57	1.30	1.52
1	B	274	THR	C-O	-6.55	1.10	1.23
1	D	267	PHE	CE1-CZ	-6.55	1.25	1.37
1	B	298	PHE	CA-C	-6.55	1.35	1.52
1	C	209	SER	CB-OG	6.54	1.50	1.42
1	B	315	GLN	CG-CD	6.53	1.66	1.51
1	A	121	PHE	CD2-CE2	6.53	1.52	1.39
1	D	223	VAL	CB-CG1	-6.50	1.39	1.52
1	C	222	GLU	CG-CD	6.48	1.61	1.51
1	B	269	SER	CB-OG	6.48	1.50	1.42
1	C	50	ILE	CA-CB	-6.43	1.40	1.54
1	B	298	PHE	C-O	-6.41	1.11	1.23
1	D	45	TRP	CG-CD1	-6.40	1.27	1.36
1	C	51	ARG	NE-CZ	-6.40	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	296	PHE	CB-CG	-6.40	1.40	1.51
1	C	113	PHE	CE1-CZ	6.39	1.49	1.37
1	C	223	VAL	CB-CG2	-6.36	1.39	1.52
1	C	141	GLN	CD-OE1	6.34	1.38	1.24
1	B	261	GLN	CB-CG	-6.34	1.35	1.52
1	A	260	LEU	CG-CD2	-6.31	1.28	1.51
1	C	142	TRP	CG-CD1	6.31	1.45	1.36
1	B	326	SER	C-O	-6.30	1.11	1.23
1	D	48	GLN	N-CA	6.29	1.58	1.46
1	B	43	ALA	CA-CB	-6.29	1.39	1.52
1	C	216	ARG	NE-CZ	-6.28	1.24	1.33
1	A	298	PHE	CE1-CZ	6.27	1.49	1.37
1	A	327	ASP	CB-CG	6.26	1.64	1.51
1	C	153	GLU	CD-OE1	6.21	1.32	1.25
1	C	304	PHE	CD2-CE2	6.21	1.51	1.39
1	C	128	ARG	CB-CG	-6.20	1.35	1.52
1	C	153	GLU	CG-CD	6.19	1.61	1.51
1	D	99	GLU	CD-OE1	6.19	1.32	1.25
1	A	124	VAL	CB-CG2	-6.18	1.39	1.52
1	B	130	PRO	C-O	-6.18	1.10	1.23
1	B	227	LEU	CG-CD2	6.17	1.74	1.51
1	D	35	THR	CB-CG2	6.16	1.72	1.52
1	B	243	TYR	CZ-OH	6.15	1.48	1.37
1	A	236	TRP	CZ3-CH2	6.14	1.49	1.40
1	B	314	PHE	CE2-CZ	6.12	1.49	1.37
1	D	185	THR	CA-CB	6.12	1.69	1.53
1	B	209	SER	CB-OG	6.11	1.50	1.42
1	B	206	THR	CA-CB	6.10	1.69	1.53
1	B	251	TYR	CE2-CZ	6.09	1.46	1.38
1	A	284	GLU	CG-CD	6.09	1.61	1.51
1	D	200	LEU	N-CA	-6.09	1.34	1.46
1	D	269	SER	CB-OG	6.07	1.50	1.42
1	B	208	ASN	C-O	6.05	1.34	1.23
1	B	315	GLN	CB-CG	6.02	1.68	1.52
1	B	157	TRP	C-O	-6.01	1.11	1.23
1	D	144	TRP	CB-CG	6.01	1.61	1.50
1	D	113	PHE	CD1-CE1	-6.00	1.27	1.39
1	B	77	ALA	CA-CB	-5.98	1.39	1.52
1	D	167	ASN	CB-CG	-5.98	1.37	1.51
1	D	252	PRO	CB-CG	-5.95	1.20	1.50
1	D	191	TYR	CE2-CZ	-5.95	1.30	1.38
1	C	85	THR	CA-CB	5.93	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	PRO	N-CA	5.93	1.57	1.47
1	C	224	LEU	CG-CD2	-5.92	1.29	1.51
1	D	157	TRP	CB-CG	-5.92	1.39	1.50
1	D	270	ARG	CZ-NH2	-5.92	1.25	1.33
1	B	330	VAL	CB-CG2	-5.92	1.40	1.52
1	B	321	VAL	CB-CG2	5.92	1.65	1.52
1	C	203	ARG	NE-CZ	5.91	1.40	1.33
1	D	268	ALA	C-O	-5.91	1.12	1.23
1	B	103	SER	CB-OG	-5.90	1.34	1.42
1	D	209	SER	CB-OG	5.89	1.50	1.42
1	A	330	VAL	CA-CB	5.89	1.67	1.54
1	D	342	TYR	CB-CG	-5.89	1.42	1.51
1	A	342	TYR	CE1-CZ	-5.89	1.30	1.38
1	B	287	GLY	C-O	-5.89	1.14	1.23
1	B	171	CYS	CB-SG	5.87	1.92	1.82
1	C	223	VAL	CA-CB	5.87	1.67	1.54
1	A	84	ILE	CB-CG2	-5.86	1.34	1.52
1	C	217	TYR	CB-CG	-5.86	1.42	1.51
1	D	280	TYR	CD2-CE2	5.86	1.48	1.39
1	B	47	TYR	CE1-CZ	5.86	1.46	1.38
1	C	121	PHE	CE1-CZ	-5.85	1.26	1.37
1	C	303	ILE	CB-CG2	5.85	1.71	1.52
1	C	43	ALA	CA-CB	-5.85	1.40	1.52
1	C	83	SER	CA-CB	-5.84	1.44	1.52
1	B	79	ARG	CG-CD	5.84	1.66	1.51
1	C	286	SER	CB-OG	5.84	1.49	1.42
1	C	206	THR	CA-CB	5.82	1.68	1.53
1	B	169	LEU	N-CA	5.82	1.57	1.46
1	C	156	ILE	CA-CB	5.82	1.68	1.54
1	A	96	MSE	SE-CE	5.81	2.29	1.95
1	A	277	SER	CA-CB	5.81	1.61	1.52
1	A	242	ARG	CZ-NH1	-5.79	1.25	1.33
1	A	342	TYR	CG-CD1	-5.79	1.31	1.39
1	C	182	GLN	N-CA	5.79	1.57	1.46
1	D	330	VAL	CB-CG1	-5.78	1.40	1.52
1	C	33	PRO	CB-CG	5.78	1.78	1.50
1	D	265	LYS	CG-CD	5.78	1.72	1.52
1	A	196	ALA	C-O	-5.77	1.12	1.23
1	D	191	TYR	CB-CG	-5.76	1.43	1.51
1	A	137	ILE	CA-CB	5.75	1.68	1.54
1	B	166	VAL	CA-CB	-5.74	1.42	1.54
1	D	299	SER	C-O	-5.72	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	184	VAL	CB-CG1	5.72	1.64	1.52
1	D	183	PRO	CA-CB	-5.70	1.42	1.53
1	A	124	VAL	C-O	-5.69	1.12	1.23
1	A	251	TYR	CZ-OH	5.67	1.47	1.37
1	B	156	ILE	CB-CG2	5.67	1.70	1.52
1	C	130	PRO	C-O	-5.66	1.11	1.23
1	C	294	GLU	CD-OE1	5.65	1.31	1.25
1	B	187	LYS	CB-CG	5.64	1.67	1.52
1	A	185	THR	N-CA	5.63	1.57	1.46
1	B	283	VAL	CB-CG1	-5.63	1.41	1.52
1	C	185	THR	N-CA	5.62	1.57	1.46
1	C	229	ARG	CZ-NH1	5.61	1.40	1.33
1	B	322	LEU	CG-CD1	-5.61	1.31	1.51
1	D	296	PHE	CD1-CE1	5.61	1.50	1.39
1	A	247	VAL	C-O	-5.60	1.12	1.23
1	B	195	TYR	CD1-CE1	-5.60	1.30	1.39
1	A	328	ARG	C-O	-5.60	1.12	1.23
1	C	45	TRP	CB-CG	-5.59	1.40	1.50
1	C	75	ASN	CG-OD1	5.58	1.36	1.24
1	C	199	MSE	SE-CE	-5.58	1.62	1.95
1	D	217	TYR	CG-CD2	5.58	1.46	1.39
1	A	203	ARG	C-O	5.58	1.33	1.23
1	D	51	ARG	CZ-NH2	5.58	1.40	1.33
1	D	45	TRP	CE3-CZ3	5.57	1.48	1.38
1	B	79	ARG	NE-CZ	5.57	1.40	1.33
1	B	47	TYR	CE2-CZ	5.56	1.45	1.38
1	D	125	ASP	CG-OD2	5.56	1.38	1.25
1	C	152	ASP	C-O	5.56	1.33	1.23
1	B	205	GLN	CG-CD	5.55	1.63	1.51
1	A	77	ALA	CA-C	5.55	1.67	1.52
1	C	254	PRO	C-O	-5.54	1.12	1.23
1	C	280	TYR	CB-CG	5.54	1.59	1.51
1	D	103	SER	CB-OG	-5.53	1.35	1.42
1	A	157	TRP	C-O	-5.53	1.12	1.23
1	B	241	MSE	C-O	-5.53	1.12	1.23
1	D	195	TYR	CG-CD1	-5.53	1.31	1.39
1	D	110	ALA	C-O	-5.53	1.12	1.23
1	A	229	ARG	NE-CZ	5.53	1.40	1.33
1	D	159	ASP	CG-OD2	5.53	1.38	1.25
1	D	209	SER	C-O	-5.51	1.12	1.23
1	A	215	TYR	CD2-CE2	-5.50	1.31	1.39
1	D	284	GLU	CD-OE1	5.50	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	320	SER	C-O	-5.49	1.12	1.23
1	B	127	GLU	CD-OE1	-5.48	1.19	1.25
1	A	258	ALA	CA-CB	-5.48	1.41	1.52
1	A	316	THR	C-O	-5.48	1.12	1.23
1	A	304	PHE	CE1-CZ	-5.45	1.26	1.37
1	D	239	TYR	CG-CD1	-5.44	1.32	1.39
1	C	76	PRO	CA-C	5.44	1.63	1.52
1	A	281	HIS	CA-CB	-5.43	1.42	1.53
1	A	265	LYS	CD-CE	5.43	1.64	1.51
1	D	280	TYR	CB-CG	5.43	1.59	1.51
1	B	71	LEU	CG-CD2	5.43	1.72	1.51
1	A	329	PRO	CG-CD	5.42	1.68	1.50
1	D	236	TRP	CD2-CE2	5.41	1.47	1.41
1	B	99	GLU	CD-OE2	5.40	1.31	1.25
1	A	71	LEU	N-CA	5.40	1.57	1.46
1	C	72	VAL	CB-CG1	5.40	1.64	1.52
1	D	48	GLN	CB-CG	5.40	1.67	1.52
1	B	243	TYR	CE2-CZ	-5.40	1.31	1.38
1	D	342	TYR	CE2-CZ	5.39	1.45	1.38
1	B	324	SER	CB-OG	5.39	1.49	1.42
1	C	163	LEU	C-O	5.39	1.33	1.23
1	B	51	ARG	NE-CZ	5.37	1.40	1.33
1	C	270	ARG	CG-CD	5.37	1.65	1.51
1	A	208	ASN	CB-CG	5.34	1.63	1.51
1	B	306	VAL	CB-CG1	5.33	1.64	1.52
1	D	170	GLY	C-O	-5.32	1.15	1.23
1	C	262	LEU	CA-CB	-5.31	1.41	1.53
1	C	121	PHE	CB-CG	-5.31	1.42	1.51
1	D	118	LYS	CD-CE	5.30	1.64	1.51
1	D	251	TYR	CE2-CZ	5.30	1.45	1.38
1	A	210	SER	CA-CB	5.30	1.60	1.52
1	A	45	TRP	CA-CB	-5.30	1.42	1.53
1	D	199	MSE	N-CA	-5.30	1.35	1.46
1	C	277	SER	CB-OG	5.29	1.49	1.42
1	B	77	ALA	N-CA	5.29	1.56	1.46
1	A	52	PRO	CA-C	5.29	1.63	1.52
1	D	198	ASN	N-CA	5.29	1.56	1.46
1	D	247	VAL	CA-CB	5.29	1.65	1.54
1	C	284	GLU	CG-CD	5.28	1.59	1.51
1	D	123	ALA	CA-CB	5.27	1.63	1.52
1	C	289	VAL	CB-CG2	-5.26	1.41	1.52
1	D	121	PHE	CG-CD1	-5.26	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	SER	CA-CB	5.26	1.60	1.52
1	C	133	GLU	C-O	-5.25	1.13	1.23
1	C	133	GLU	CD-OE1	-5.25	1.19	1.25
1	C	191	TYR	CE1-CZ	-5.24	1.31	1.38
1	D	143	ARG	CD-NE	5.24	1.55	1.46
1	A	283	VAL	CB-CG1	-5.24	1.41	1.52
1	B	282	VAL	CB-CG1	5.23	1.63	1.52
1	C	342	TYR	CD1-CE1	5.22	1.47	1.39
1	D	195	TYR	CE1-CZ	-5.22	1.31	1.38
1	D	261	GLN	CB-CG	-5.22	1.38	1.52
1	B	127	GLU	CB-CG	-5.22	1.42	1.52
1	D	314	PHE	CD2-CE2	5.22	1.49	1.39
1	B	329	PRO	CA-CB	-5.21	1.43	1.53
1	B	128	ARG	C-O	-5.21	1.13	1.23
1	C	44	TYR	CZ-OH	5.20	1.46	1.37
1	B	89	TYR	CE1-CZ	5.19	1.45	1.38
1	A	144	TRP	CD2-CE2	-5.19	1.35	1.41
1	A	40	CYS	CB-SG	-5.19	1.73	1.81
1	D	188	GLU	CD-OE2	5.18	1.31	1.25
1	B	195	TYR	CE2-CZ	-5.18	1.31	1.38
1	C	77	ALA	N-CA	5.17	1.56	1.46
1	B	49	GLU	CD-OE1	5.17	1.31	1.25
1	B	141	GLN	N-CA	-5.16	1.36	1.46
1	B	280	TYR	CD1-CE1	-5.15	1.31	1.39
1	D	47	TYR	CD1-CE1	5.14	1.47	1.39
1	C	39	ASN	C-O	-5.14	1.13	1.23
1	C	128	ARG	N-CA	-5.14	1.36	1.46
1	D	267	PHE	CG-CD1	-5.13	1.31	1.38
1	C	191	TYR	CD2-CE2	5.13	1.47	1.39
1	A	314	PHE	C-O	5.13	1.33	1.23
1	B	242	ARG	CA-CB	-5.13	1.42	1.53
1	A	105	ARG	CB-CG	-5.13	1.38	1.52
1	B	37	ASN	CB-CG	5.12	1.62	1.51
1	A	196	ALA	CA-CB	-5.12	1.41	1.52
1	D	325	PHE	CD1-CE1	-5.12	1.29	1.39
1	C	76	PRO	CG-CD	5.11	1.67	1.50
1	C	51	ARG	CG-CD	-5.11	1.39	1.51
1	A	267	PHE	CD1-CE1	-5.11	1.29	1.39
1	B	77	ALA	CA-C	5.10	1.66	1.52
1	C	130	PRO	CB-CG	-5.08	1.24	1.50
1	A	318	GLN	CB-CG	5.08	1.66	1.52
1	A	45	TRP	CZ3-CH2	5.07	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	ARG	C-O	-5.07	1.13	1.23
1	A	314	PHE	CD1-CE1	-5.07	1.29	1.39
1	B	329	PRO	CG-CD	5.07	1.67	1.50
1	C	208	ASN	C-O	-5.06	1.13	1.23
1	A	76	PRO	N-CA	5.06	1.55	1.47
1	A	232	ASP	N-CA	-5.05	1.36	1.46
1	D	265	LYS	C-O	-5.05	1.13	1.23
1	C	157	TRP	CA-CB	-5.05	1.42	1.53
1	A	341	ARG	CG-CD	-5.04	1.39	1.51
1	D	153	GLU	CD-OE1	5.04	1.31	1.25
1	C	49	GLU	CA-C	5.03	1.66	1.52
1	C	94	LEU	CG-CD1	-5.03	1.33	1.51
1	A	271	VAL	CA-CB	-5.03	1.44	1.54
1	D	342	TYR	CD1-CE1	-5.02	1.31	1.39
1	A	267	PHE	CE1-CZ	-5.01	1.27	1.37
1	B	79	ARG	CZ-NH1	5.01	1.39	1.33
1	A	132	ASN	CB-CG	5.01	1.62	1.51
1	C	136	PHE	CD1-CE1	-5.01	1.29	1.39
1	D	265	LYS	CE-NZ	5.01	1.61	1.49
1	A	229	ARG	C-O	-5.00	1.13	1.23
1	B	86	ALA	C-O	5.00	1.32	1.23
1	A	188	GLU	CD-OE2	5.00	1.31	1.25
1	D	146	ASP	CB-CG	5.00	1.62	1.51

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	ARG	NE-CZ-NH1	-16.78	111.91	120.30
1	A	341	ARG	NE-CZ-NH1	15.39	128.00	120.30
1	C	128	ARG	NE-CZ-NH2	15.21	127.91	120.30
1	A	341	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	D	237	ASP	CB-CG-OD1	-12.19	107.33	118.30
1	A	319	ASP	CB-CG-OD2	12.18	129.26	118.30
1	C	51	ARG	NE-CZ-NH1	-12.06	114.27	120.30
1	D	270	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	A	229	ARG	NE-CZ-NH1	11.35	125.97	120.30
1	C	186	ARG	NE-CZ-NH1	-11.18	114.71	120.30
1	C	229	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	C	319	ASP	CB-CG-OD2	10.76	127.98	118.30
1	D	128	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	C	40	CYS	N-CA-C	-10.44	82.83	111.00
1	D	105	ARG	NE-CZ-NH2	9.90	125.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ASP	CB-CG-OD2	9.73	127.06	118.30
1	C	88	LEU	CB-CG-CD1	9.73	127.53	111.00
1	D	234	ASP	CB-CG-OD2	9.35	126.72	118.30
1	A	327	ASP	CB-CG-OD2	9.24	126.62	118.30
1	A	152	ASP	CB-CG-OD2	9.12	126.50	118.30
1	D	125	ASP	CB-CG-OD1	-9.09	110.12	118.30
1	D	71	LEU	CB-CG-CD2	-9.02	95.66	111.00
1	D	338	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	C	341	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	B	162	ASP	CB-CG-OD2	8.82	126.24	118.30
1	C	105	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	B	327	ASP	CB-CG-OD2	8.74	126.17	118.30
1	C	143	ARG	NE-CZ-NH2	8.47	124.54	120.30
1	C	125	ASP	CB-CG-OD2	8.36	125.82	118.30
1	D	146	ASP	CB-CG-OD2	8.34	125.81	118.30
1	D	128	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	D	176	ASP	CB-CG-OD2	8.31	125.78	118.30
1	B	79	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	D	276	ASP	CB-CG-OD1	8.04	125.53	118.30
1	B	146	ASP	CB-CG-OD2	7.99	125.49	118.30
1	C	218	ASP	CB-CG-OD2	7.83	125.35	118.30
1	B	319	ASP	CB-CG-OD1	7.74	125.27	118.30
1	D	330	VAL	CG1-CB-CG2	-7.67	98.63	110.90
1	C	85	THR	OG1-CB-CG2	-7.66	92.38	110.00
1	C	190	ASP	CB-CG-OD2	7.66	125.19	118.30
1	A	242	ARG	NE-CZ-NH2	7.65	124.13	120.30
1	B	221	ARG	NE-CZ-NH2	7.65	124.12	120.30
1	C	71	LEU	CA-CB-CG	7.52	132.60	115.30
1	B	49	GLU	N-CA-C	-7.50	90.77	111.00
1	A	128	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	C	186	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	B	218	ASP	CB-CG-OD2	7.39	124.95	118.30
1	D	237	ASP	CB-CG-OD2	7.37	124.93	118.30
1	C	341	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	C	71	LEU	CB-CG-CD2	7.32	123.45	111.00
1	C	133	GLU	OE1-CD-OE2	-7.31	114.53	123.30
1	B	135	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	341	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	C	51	ARG	NH1-CZ-NH2	7.15	127.27	119.40
1	B	276	ASP	CB-CG-OD2	7.14	124.73	118.30
1	D	284	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	B	73	LEU	CB-CA-C	-7.00	96.91	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	ILE	CA-CB-CG2	6.99	124.88	110.90
1	B	122	THR	OG1-CB-CG2	-6.97	93.97	110.00
1	C	50	ILE	CG1-CB-CG2	6.92	126.63	111.40
1	D	232	ASP	CB-CG-OD2	6.91	124.52	118.30
1	D	289	VAL	CG1-CB-CG2	-6.90	99.87	110.90
1	C	138	LEU	CB-CG-CD2	-6.88	99.31	111.00
1	A	218	ASP	CB-CG-OD1	6.87	124.48	118.30
1	C	232	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	338	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	A	176	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	A	203	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	C	73	LEU	CB-CG-CD1	-6.59	99.79	111.00
1	C	152	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	72	VAL	CB-CA-C	-6.57	98.92	111.40
1	A	319	ASP	CB-CG-OD1	-6.54	112.41	118.30
1	C	77	ALA	CB-CA-C	-6.47	100.39	110.10
1	D	219	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	105	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	D	242	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	D	226	ASP	CB-CG-OD1	6.44	124.09	118.30
1	A	138	LEU	CA-CB-CG	6.42	130.06	115.30
1	B	79	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	D	50	ILE	CG1-CB-CG2	-6.40	97.33	111.40
1	B	319	ASP	N-CA-C	-6.35	93.85	111.00
1	A	295	THR	OG1-CB-CG2	-6.32	95.46	110.00
1	A	138	LEU	CB-CG-CD1	-6.29	100.30	111.00
1	C	215	TYR	CG-CD2-CE2	6.27	126.31	121.30
1	D	208	ASN	N-CA-C	-6.23	94.17	111.00
1	C	253	MSE	CA-CB-CG	-6.23	102.71	113.30
1	C	143	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	C	248	THR	OG1-CB-CG2	-6.18	95.78	110.00
1	A	284	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	C	51	ARG	CG-CD-NE	-6.12	98.94	111.80
1	C	76	PRO	C-N-CA	6.12	137.00	121.70
1	C	162	ASP	CB-CG-OD1	6.10	123.79	118.30
1	D	328	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	C	216	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	226	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	78	LEU	CB-CG-CD2	5.98	121.16	111.00
1	A	329	PRO	N-CD-CG	-5.97	94.25	103.20
1	D	303	ILE	CA-CB-CG2	5.97	122.83	110.90
1	B	96	MSE	CG-SE-CE	5.95	111.99	98.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	ASP	CB-CG-OD1	5.94	123.64	118.30
1	B	213	PHE	CB-CG-CD1	-5.92	116.65	120.80
1	B	73	LEU	CB-CG-CD1	-5.91	100.95	111.00
1	A	290	ILE	CG1-CB-CG2	-5.90	98.42	111.40
1	B	186	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	95	ILE	CG1-CB-CG2	-5.90	98.43	111.40
1	C	128	ARG	CA-CB-CG	5.88	126.33	113.40
1	B	232	ASP	CB-CG-OD2	5.85	123.57	118.30
1	D	210	SER	N-CA-CB	5.84	119.26	110.50
1	D	334	LEU	C-N-CA	-5.83	110.06	122.30
1	A	229	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	107	ASN	CB-CA-C	5.77	121.94	110.40
1	D	234	ASP	CB-CG-OD1	-5.77	113.10	118.30
1	C	219	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	D	308	THR	OG1-CB-CG2	-5.77	96.73	110.00
1	A	330	VAL	CG1-CB-CG2	-5.77	101.67	110.90
1	A	276	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	232	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	C	226	ASP	CB-CG-OD1	5.76	123.48	118.30
1	D	223	VAL	CG1-CB-CG2	-5.75	101.71	110.90
1	A	289	VAL	CB-CA-C	-5.74	100.49	111.40
1	D	183	PRO	N-CD-CG	-5.74	94.59	103.20
1	D	338	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	C	48	GLN	CB-CA-C	-5.72	98.95	110.40
1	D	125	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	112	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	289	VAL	CG1-CB-CG2	-5.70	101.78	110.90
1	D	143	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	152	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	269	SER	N-CA-CB	-5.64	102.04	110.50
1	A	308	THR	OG1-CB-CG2	-5.63	97.06	110.00
1	B	330	VAL	CG1-CB-CG2	-5.62	101.91	110.90
1	D	219	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	135	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	270	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	71	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	B	81	GLN	CA-CB-CG	5.57	125.65	113.40
1	A	111	LEU	CB-CG-CD2	5.57	120.46	111.00
1	B	128	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	C	234	ASP	CB-CG-OD1	5.53	123.27	118.30
1	D	114	ILE	CG1-CB-CG2	-5.51	99.28	111.40
1	A	178	PRO	N-CD-CG	5.50	111.45	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	PRO	N-CD-CG	-5.48	94.97	103.20
1	D	301	LYS	CD-CE-NZ	5.48	124.31	111.70
1	D	161	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	328	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	C	188	GLU	OE1-CD-OE2	5.47	129.86	123.30
1	B	237	ASP	CB-CG-OD2	5.46	123.22	118.30
1	D	332	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	D	72	VAL	CG1-CB-CG2	-5.43	102.21	110.90
1	B	317	THR	OG1-CB-CG2	-5.42	97.53	110.00
1	C	283	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	D	49	GLU	C-N-CA	5.41	135.22	121.70
1	C	186	ARG	CG-CD-NE	-5.41	100.45	111.80
1	D	105	ARG	CG-CD-NE	5.39	123.12	111.80
1	B	289	VAL	CB-CA-C	-5.38	101.17	111.40
1	D	209	SER	C-N-CA	5.37	135.13	121.70
1	A	159	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	303	ILE	CA-CB-CG2	5.37	121.63	110.90
1	B	155	VAL	CG1-CB-CG2	-5.36	102.32	110.90
1	C	230	LEU	CB-CG-CD1	5.35	120.10	111.00
1	A	200	LEU	CB-CG-CD1	5.35	120.10	111.00
1	A	141	GLN	O-C-N	-5.33	114.17	122.70
1	D	162	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	128	ARG	CD-NE-CZ	5.28	130.99	123.60
1	A	305	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	A	77	ALA	CA-C-O	5.24	131.11	120.10
1	D	232	ASP	OD1-CG-OD2	-5.23	113.36	123.30
1	D	176	ASP	OD1-CG-OD2	-5.17	113.47	123.30
1	D	34	LYS	N-CA-C	-5.16	97.06	111.00
1	B	100	VAL	CG1-CB-CG2	-5.16	102.65	110.90
1	D	342	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	D	342	TYR	CB-CA-C	-5.14	100.11	110.40
1	B	71	LEU	N-CA-C	5.14	124.87	111.00
1	A	230	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	D	165	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	B	88	LEU	CB-CG-CD2	5.12	119.69	111.00
1	C	215	TYR	CB-CG-CD1	5.11	124.06	121.00
1	B	184	VAL	CG1-CB-CG2	5.10	119.06	110.90
1	D	334	LEU	CA-C-N	5.10	126.39	116.20
1	A	136	PHE	CB-CG-CD1	5.09	124.36	120.80
1	B	206	THR	OG1-CB-CG2	-5.08	98.31	110.00
1	D	328	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	A	317	THR	O-C-N	-5.07	114.59	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	89	TYR	CZ-CE2-CD2	5.01	124.31	119.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	ASN	Peptide
1	B	39	ASN	Peptide
1	B	76	PRO	Peptide
1	D	149	ASN	Mainchain
1	D	47	TYR	Peptide

## 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	2280	0	2134	129	0
1	B	2235	0	2093	180	0
1	C	2281	0	2135	137	0
1	D	2263	0	2122	144	2
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
3	A	110	0	0	9	0
3	B	129	0	0	26	0
3	C	130	0	0	21	0
3	D	147	0	0	25	2
All	All	9579	0	8484	565	2

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 32.

All (565) 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:D:76:PRO:CB	1:D:76:PRO:CA	1.75	1.61
1:C:50:ILE:CB	1:C:50:ILE:CG2	1.76	1.59
1:B:227:LEU:CD2	1:B:227:LEU:CG	1.74	1.59
1:D:50:ILE:CA	1:D:50:ILE:CB	1.83	1.56
1:C:33:PRO:CB	1:C:33:PRO:CG	1.78	1.53
1:D:39:ASN:CG	1:D:39:ASN:CB	1.74	1.52
1:B:39:ASN:CG	1:B:39:ASN:CB	1.75	1.49
1:C:253:MSE:CE	1:C:253:MSE:SE	2.15	1.44
1:A:36:PRO:CB	1:A:36:PRO:CG	1.74	1.44
1:A:253:MSE:SE	1:A:253:MSE:CG	2.18	1.41
1:A:253:MSE:CE	1:A:253:MSE:SE	2.19	1.40
1:D:253:MSE:SE	1:D:253:MSE:CE	2.24	1.35
1:A:96:MSE:SE	1:A:96:MSE:CE	2.29	1.29
1:C:209:SER:HA	3:C:1103:HOH:O	1.31	1.28
1:D:185:THR:HG21	3:D:1049:HOH:O	1.42	1.17
1:D:96:MSE:CE	1:D:96:MSE:SE	2.43	1.16
1:B:149:ASN:HD22	1:B:149:ASN:N	1.37	1.15
1:A:241:MSE:HE2	1:B:201:PRO:HA	1.28	1.14
1:A:240:LYS:O	1:A:241:MSE:HE3	1.42	1.14
1:B:39:ASN:HB3	3:B:1111:HOH:O	1.49	1.13
1:D:71:LEU:HD22	1:D:72:VAL:N	1.68	1.09
1:B:265:LYS:HG2	1:B:266:GLY:H	0.98	1.07
1:C:85:THR:HB	3:C:1069:HOH:O	1.57	1.04
1:B:265:LYS:HG2	1:B:266:GLY:N	1.70	1.04
1:D:209:SER:N	3:D:1078:HOH:O	1.58	1.03
1:B:207:GLY:HA2	3:B:1070:HOH:O	1.56	1.01
1:B:120:ALA:HB2	1:B:149:ASN:HB3	1.40	1.01
1:D:75:ASN:HD22	1:D:75:ASN:H	1.08	1.00
1:B:149:ASN:H	1:B:149:ASN:ND2	1.61	0.97
1:D:71:LEU:C	1:D:71:LEU:HD22	1.82	0.96
1:D:85:THR:HG22	1:D:87:THR:H	1.30	0.96
1:C:331:GLN:O	1:C:334:LEU:O	1.83	0.96
1:B:149:ASN:N	1:B:149:ASN:ND2	2.11	0.96
1:D:207:GLY:C	3:D:1079:HOH:O	2.02	0.96
1:B:248:THR:HG23	1:B:250:GLY:H	1.30	0.96
1:C:37:ASN:O	1:C:38:ALA:O	1.84	0.96
1:A:248:THR:HG21	3:A:1041:HOH:O	1.67	0.94
1:B:38:ALA:HB2	1:B:308:THR:HB	1.50	0.92
1:B:319:ASP:N	3:B:1043:HOH:O	2.02	0.92
1:C:50:ILE:CA	1:C:50:ILE:CG2	2.49	0.91
1:C:275:THR:HA	1:C:308:THR:HG23	1.52	0.90
1:B:106:HIS:HB2	1:B:108:GLN:NE2	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:THR:HA	1:B:308:THR:HG23	1.53	0.90
1:A:40:CYS:O	1:A:76:PRO:HB2	1.72	0.89
1:B:184:VAL:HG23	1:B:185:THR:H	1.33	0.89
1:A:142:TRP:N	3:A:1043:HOH:O	2.03	0.89
1:B:96:MSE:HE3	1:B:97:PRO:HD2	1.53	0.89
1:B:227:LEU:CD2	1:B:227:LEU:CD1	2.51	0.88
1:C:248:THR:HG23	1:C:250:GLY:H	1.36	0.88
1:B:49:GLU:O	1:B:50:ILE:HB	1.74	0.87
1:B:96:MSE:HE3	1:B:97:PRO:CD	2.05	0.86
1:C:108:GLN:HG3	1:C:166:VAL:HG21	1.55	0.86
1:A:40:CYS:O	1:A:76:PRO:CB	2.24	0.85
1:D:49:GLU:O	1:D:51:ARG:HG3	1.79	0.83
1:B:108:GLN:H	1:B:108:GLN:HE21	1.23	0.83
1:A:73:LEU:HD12	1:A:73:LEU:H	1.43	0.83
1:A:317:THR:O	1:A:318:GLN:HB2	1.76	0.82
1:B:149:ASN:HD22	1:B:149:ASN:H	0.86	0.82
1:D:75:ASN:N	1:D:75:ASN:HD22	1.69	0.80
1:D:127:GLU:HB2	1:D:186:ARG:HG2	1.63	0.80
1:B:227:LEU:CD2	1:B:227:LEU:CB	2.60	0.80
1:B:207:GLY:CA	3:B:1070:HOH:O	2.20	0.80
1:B:327:ASP:O	1:B:330:VAL:HG22	1.80	0.80
1:C:206:THR:HG21	1:C:247:VAL:HG11	1.63	0.79
1:B:99:GLU:HB2	3:B:1088:HOH:O	1.82	0.79
1:C:105:ARG:HG2	1:C:144:TRP:CZ3	2.18	0.78
1:B:240:LYS:HG3	1:B:261:GLN:HB3	1.66	0.78
1:A:38:ALA:O	1:A:39:ASN:OD1	2.02	0.78
1:D:208:ASN:O	3:D:1079:HOH:O	2.01	0.77
1:B:75:ASN:ND2	1:B:83:SER:H	1.81	0.77
1:B:248:THR:HG23	1:B:250:GLY:N	2.00	0.77
1:B:38:ALA:CB	1:B:308:THR:HB	2.14	0.77
1:D:208:ASN:C	3:D:1079:HOH:O	2.22	0.77
1:A:163:LEU:HB2	1:A:164:PRO:HD3	1.67	0.76
1:A:327:ASP:O	1:A:330:VAL:HG22	1.85	0.76
1:C:51:ARG:C	3:C:1130:HOH:O	2.24	0.76
1:A:191:TYR:OH	1:A:214:ASN:HB3	1.86	0.76
1:B:47:TYR:O	1:B:48:GLN:HB2	1.86	0.75
1:B:85:THR:HG22	1:B:87:THR:H	1.52	0.75
1:D:267:PHE:CE2	1:D:269:SER:HB3	2.22	0.75
1:B:73:LEU:HD11	1:B:89:TYR:CE2	2.23	0.74
1:D:208:ASN:HA	3:D:1102:HOH:O	1.86	0.74
1:B:208:ASN:O	1:B:209:SER:HB3	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ASN:H	1:D:149:ASN:HD22	1.35	0.74
1:B:265:LYS:HA	1:B:318:GLN:O	1.88	0.74
1:D:50:ILE:HB	1:D:50:ILE:CA	2.10	0.74
1:D:75:ASN:N	1:D:75:ASN:ND2	2.35	0.74
1:A:103:SER:OG	1:A:181:GLN:O	2.05	0.73
1:D:270:ARG:HH21	1:D:342:TYR:HE1	1.35	0.73
1:C:223:VAL:HG21	1:D:199:MSE:HE3	1.69	0.73
1:A:241:MSE:HE2	1:B:201:PRO:CA	2.14	0.73
1:A:160:GLY:C	1:A:161:LEU:HD12	2.09	0.73
1:A:105:ARG:HB2	1:A:144:TRP:CE3	2.24	0.72
1:B:76:PRO:HD3	1:B:84:ILE:HA	1.71	0.72
1:A:181:GLN:O	1:A:182:GLN:HB2	1.89	0.72
1:B:120:ALA:CB	1:B:149:ASN:HB3	2.20	0.71
1:B:49:GLU:O	1:B:50:ILE:CB	2.38	0.71
1:B:160:GLY:O	1:B:161:LEU:HD23	1.91	0.71
1:D:106:HIS:O	1:D:141:GLN:O	2.06	0.71
1:D:76:PRO:CB	1:D:76:PRO:C	2.59	0.71
1:A:89:TYR:C	1:A:89:TYR:CD1	2.62	0.71
1:B:216:ARG:HD3	1:B:219:ARG:HD2	1.71	0.71
1:D:75:ASN:H	1:D:75:ASN:ND2	1.85	0.71
1:D:327:ASP:O	1:D:330:VAL:HG12	1.90	0.71
1:B:160:GLY:C	1:B:161:LEU:HD23	2.10	0.70
1:D:135:ASP:HB3	1:D:214:ASN:HD21	1.56	0.70
1:C:184:VAL:O	1:C:185:THR:HB	1.92	0.70
1:B:265:LYS:CG	1:B:266:GLY:H	1.89	0.69
1:B:206:THR:HG23	3:B:1070:HOH:O	1.92	0.69
1:B:116:GLU:HA	3:B:1052:HOH:O	1.91	0.69
1:C:33:PRO:N	3:C:1080:HOH:O	2.25	0.69
1:C:220:SER:HA	1:D:199:MSE:HE1	1.75	0.69
1:D:167:ASN:OD1	3:D:1031:HOH:O	2.09	0.69
1:A:85:THR:HG22	1:A:88:LEU:H	1.57	0.69
1:D:79:ARG:NE	3:D:1146:HOH:O	2.24	0.69
1:D:208:ASN:N	3:D:1079:HOH:O	2.22	0.69
1:C:248:THR:HG21	3:C:1034:HOH:O	1.92	0.69
1:B:71:LEU:N	3:B:1027:HOH:O	2.26	0.69
1:A:292:GLY:O	1:A:293:ASN:HB2	1.92	0.68
1:D:79:ARG:HH11	1:D:79:ARG:HG3	1.58	0.68
1:A:317:THR:O	1:A:318:GLN:CB	2.36	0.68
1:D:126:GLY:O	1:D:186:ARG:HB3	1.94	0.68
1:C:51:ARG:HH22	1:C:94:LEU:HB2	1.58	0.68
1:D:270:ARG:NH2	1:D:342:TYR:OH	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:PRO:HA	3:B:1042:HOH:O	1.92	0.68
1:D:305:VAL:HG21	3:D:1126:HOH:O	1.92	0.68
1:A:73:LEU:HD12	1:A:73:LEU:N	2.09	0.68
1:B:245:ASN:HB3	1:B:248:THR:HG22	1.76	0.68
1:B:184:VAL:CG2	1:B:185:THR:H	2.05	0.68
1:A:308:THR:HG21	1:D:170:GLY:O	1.94	0.68
1:D:85:THR:HG22	1:D:87:THR:N	2.08	0.67
1:B:108:GLN:H	1:B:108:GLN:NE2	1.90	0.67
1:D:149:ASN:N	1:D:149:ASN:HD22	1.87	0.67
1:A:75:ASN:ND2	3:A:1049:HOH:O	2.26	0.67
1:D:184:VAL:HG23	3:D:1059:HOH:O	1.93	0.67
1:B:47:TYR:O	1:B:48:GLN:CB	2.37	0.67
1:C:163:LEU:HB2	1:C:164:PRO:HD3	1.77	0.67
1:D:43:ALA:HB3	1:D:305:VAL:CG1	2.24	0.67
1:D:208:ASN:HB3	3:D:1109:HOH:O	1.94	0.67
1:C:161:LEU:HD12	1:C:163:LEU:CD1	2.25	0.66
1:B:170:GLY:HA2	3:C:1108:HOH:O	1.96	0.66
1:B:184:VAL:HG23	1:B:185:THR:N	2.09	0.66
1:D:183:PRO:HD2	3:D:1085:HOH:O	1.95	0.66
1:D:85:THR:HG21	3:D:1068:HOH:O	1.94	0.66
1:B:126:GLY:O	1:B:184:VAL:O	2.13	0.66
1:D:49:GLU:O	1:D:51:ARG:CG	2.44	0.66
1:C:226:ASP:O	1:C:230:LEU:HD22	1.95	0.65
1:B:52:PRO:O	3:B:1057:HOH:O	2.14	0.65
1:A:85:THR:CG2	1:A:88:LEU:H	2.09	0.65
1:B:208:ASN:O	1:B:208:ASN:CG	2.34	0.65
1:B:338:ARG:HH21	1:B:338:ARG:HB2	1.61	0.65
1:A:46:ASN:HB3	1:A:49:GLU:CG	2.27	0.65
1:C:275:THR:CA	1:C:308:THR:HG23	2.27	0.65
1:D:108:GLN:HG2	1:D:163:LEU:HD23	1.78	0.65
1:A:108:GLN:HG2	1:A:163:LEU:HD23	1.78	0.65
1:A:240:LYS:O	1:A:241:MSE:CE	2.33	0.64
1:C:46:ASN:ND2	1:C:48:GLN:HB3	2.11	0.64
1:D:163:LEU:HB2	1:D:164:PRO:HD3	1.80	0.64
1:A:45:TRP:CZ2	1:A:74:GLU:HB2	2.32	0.64
1:B:127:GLU:HB3	1:B:186:ARG:HB3	1.80	0.64
1:A:240:LYS:HG3	1:A:261:GLN:HB3	1.80	0.63
1:C:85:THR:HG22	1:C:88:LEU:HB2	1.80	0.63
1:B:106:HIS:HB2	1:B:108:GLN:HE21	1.62	0.63
1:C:206:THR:CG2	1:C:247:VAL:HG11	2.28	0.63
1:A:127:GLU:HG3	1:A:213:PHE:HZ	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ASN:HD21	1:B:83:SER:H	1.44	0.62
1:B:235:GLU:HG2	3:B:1048:HOH:O	2.00	0.62
1:C:208:ASN:C	3:C:1097:HOH:O	2.37	0.62
1:B:92:LEU:HD22	1:B:92:LEU:N	2.14	0.62
1:B:248:THR:CG2	1:B:250:GLY:H	2.10	0.62
1:C:204:HIS:NE2	1:C:206:THR:HB	2.14	0.61
1:D:191:TYR:OH	1:D:214:ASN:HB3	2.00	0.61
1:B:308:THR:HG21	1:C:170:GLY:O	2.00	0.61
1:B:209:SER:HA	3:B:1114:HOH:O	2.00	0.61
1:D:79:ARG:HA	3:D:1150:HOH:O	2.00	0.61
1:A:46:ASN:HB3	1:A:49:GLU:HG3	1.81	0.61
1:A:230:LEU:HD21	1:B:190:ASP:HA	1.81	0.61
1:D:50:ILE:C	1:D:50:ILE:CB	2.65	0.61
1:A:248:THR:HG23	1:A:250:GLY:H	1.66	0.61
1:B:279:ILE:O	1:B:324:SER:HA	1.99	0.61
1:C:248:THR:HG23	1:C:250:GLY:N	2.13	0.61
1:A:199:MSE:HE2	1:B:241:MSE:HB3	1.83	0.61
1:C:50:ILE:CG2	1:C:50:ILE:HB	2.16	0.61
1:C:292:GLY:O	1:C:293:ASN:HB2	2.01	0.61
1:B:216:ARG:HB3	1:B:218:ASP:OD1	1.99	0.60
1:C:184:VAL:O	1:C:185:THR:CB	2.48	0.60
1:B:84:ILE:HG21	1:B:90:ALA:CB	2.31	0.60
1:D:108:GLN:HG3	1:D:166:VAL:HG21	1.83	0.60
1:B:330:VAL:HG23	1:B:331:GLN:N	2.15	0.60
1:C:45:TRP:O	1:C:46:ASN:HB3	2.01	0.60
1:C:85:THR:CG2	1:C:88:LEU:HB2	2.32	0.59
1:A:267:PHE:CE2	1:A:269:SER:HB3	2.37	0.59
1:C:138:LEU:N	1:C:138:LEU:HD12	2.18	0.59
1:C:38:ALA:CB	1:C:308:THR:HB	2.32	0.59
1:A:181:GLN:O	1:A:182:GLN:CB	2.51	0.59
1:B:288:GLN:NE2	1:B:295:THR:OG1	2.34	0.59
1:D:48:GLN:CG	1:D:48:GLN:O	2.50	0.59
1:D:135:ASP:HB3	1:D:214:ASN:ND2	2.18	0.58
1:D:192:LEU:HB2	1:D:193:PRO:CD	2.34	0.58
1:C:244:VAL:HG21	1:D:200:LEU:HD22	1.85	0.58
1:A:78:LEU:O	1:A:81:GLN:HB2	2.04	0.58
1:B:224:LEU:HD11	1:B:260:LEU:HG	1.85	0.58
1:A:73:LEU:CD1	1:A:73:LEU:H	2.14	0.58
1:A:244:VAL:HG21	1:B:200:LEU:HB2	1.86	0.58
1:B:104:HIS:HD2	3:B:1095:HOH:O	1.85	0.58
1:B:127:GLU:HG3	1:B:213:PHE:HZ	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ASN:CA	1:D:39:ASN:CG	2.69	0.58
1:B:96:MSE:HE3	1:B:97:PRO:HD3	1.85	0.58
1:C:199:MSE:HE3	1:D:223:VAL:HG21	1.86	0.58
1:A:230:LEU:CD2	1:B:190:ASP:HA	2.34	0.58
1:C:245:ASN:HB3	1:C:248:THR:HG22	1.86	0.57
1:D:160:GLY:O	1:D:161:LEU:HD23	2.04	0.57
1:A:228:THR:HG22	1:A:239:TYR:CE1	2.39	0.57
1:D:341:ARG:O	1:D:342:TYR:CG	2.57	0.57
1:A:49:GLU:O	1:A:50:ILE:HB	2.04	0.57
1:D:48:GLN:HG2	1:D:48:GLN:O	2.04	0.57
1:B:253:MSE:CE	1:B:256:MSE:HE3	2.35	0.56
1:A:38:ALA:CB	1:A:308:THR:HB	2.36	0.56
1:A:244:VAL:HG21	1:B:200:LEU:HD22	1.86	0.56
3:B:1128:HOH:O	1:C:208:ASN:HB3	2.04	0.56
1:D:137:ILE:C	1:D:138:LEU:HD12	2.24	0.56
1:A:53:LEU:HG	1:A:72:VAL:CG2	2.35	0.56
1:B:48:GLN:O	1:B:49:GLU:HB2	2.03	0.56
1:C:161:LEU:HD12	1:C:163:LEU:HD12	1.88	0.56
1:C:121:PHE:CE1	1:C:128:ARG:HD2	2.41	0.56
1:D:101:ALA:HB1	1:D:102:PRO:HD2	1.87	0.56
1:C:37:ASN:O	1:C:38:ALA:C	2.44	0.56
1:B:338:ARG:HH21	1:B:338:ARG:CB	2.19	0.56
1:D:43:ALA:HB3	1:D:305:VAL:HG12	1.87	0.56
1:B:226:ASP:O	1:B:230:LEU:HD13	2.06	0.56
1:B:76:PRO:CA	3:B:1042:HOH:O	2.51	0.55
1:C:216:ARG:HG2	1:C:216:ARG:NH2	2.21	0.55
1:D:267:PHE:HE2	1:D:269:SER:HB3	1.67	0.55
1:B:111:LEU:HD12	1:B:111:LEU:C	2.26	0.55
1:A:275:THR:HA	1:A:308:THR:HG23	1.88	0.55
1:C:129:THR:HG22	1:C:213:PHE:CE2	2.41	0.55
1:B:208:ASN:O	1:B:209:SER:CB	2.52	0.55
1:A:40:CYS:O	1:A:76:PRO:CG	2.54	0.55
1:B:89:TYR:C	1:B:89:TYR:CD1	2.80	0.55
1:D:275:THR:HA	1:D:308:THR:HG23	1.88	0.55
1:D:143:ARG:HA	3:D:1125:HOH:O	2.05	0.55
1:B:85:THR:HG21	3:B:1017:HOH:O	2.06	0.55
1:D:183:PRO:CG	3:D:1085:HOH:O	2.53	0.55
1:B:272:ALA:O	1:B:311:GLY:HA2	2.07	0.55
1:B:285:GLY:HA3	1:B:320:SER:HB3	1.89	0.55
1:C:308:THR:HG22	1:C:309:TRP:N	2.21	0.55
1:C:191:TYR:OH	1:C:214:ASN:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:TYR:CD1	1:A:90:ALA:N	2.75	0.54
1:B:253:MSE:HE3	1:B:256:MSE:HE3	1.89	0.54
1:D:183:PRO:CD	3:D:1085:HOH:O	2.52	0.54
1:A:184:VAL:O	1:A:185:THR:HB	2.07	0.54
1:D:106:HIS:HB2	1:D:108:GLN:OE1	2.06	0.54
1:A:76:PRO:HG2	1:A:78:LEU:HG	1.89	0.54
1:D:223:VAL:O	1:D:227:LEU:HG	2.07	0.54
1:B:84:ILE:HG21	1:B:90:ALA:HB3	1.89	0.54
1:C:107:ASN:ND2	1:C:173:PHE:HB2	2.22	0.54
1:A:248:THR:HG23	1:A:250:GLY:N	2.23	0.54
1:D:50:ILE:CG1	1:D:50:ILE:CA	2.81	0.54
1:C:281:HIS:HE1	3:C:1052:HOH:O	1.91	0.54
1:C:163:LEU:CB	1:C:164:PRO:HD3	2.38	0.54
1:C:129:THR:HG22	1:C:213:PHE:HE2	1.73	0.54
1:A:248:THR:CG2	1:A:250:GLY:H	2.21	0.53
1:B:39:ASN:CB	1:B:39:ASN:ND2	2.64	0.53
1:A:85:THR:HG23	1:A:87:THR:H	1.73	0.53
1:B:293:ASN:O	1:B:294:GLU:C	2.46	0.53
1:D:308:THR:O	1:D:310:HIS:HD2	1.90	0.53
1:B:46:ASN:ND2	1:B:47:TYR:O	2.42	0.53
1:B:334:LEU:HB2	1:B:336:LEU:HD12	1.91	0.53
1:A:35:THR:N	1:D:174:ALA:H	2.06	0.53
1:C:127:GLU:HB2	1:C:186:ARG:HB3	1.91	0.53
1:D:85:THR:HG22	1:D:86:ALA:N	2.22	0.53
1:A:177:TYR:CD1	1:A:178:PRO:HD2	2.44	0.53
1:C:109:SER:HB2	1:C:256:MSE:HE2	1.90	0.53
1:A:94:LEU:HD21	1:A:96:MSE:SE	2.59	0.53
1:A:274:THR:HB	1:A:276:ASP:OD1	2.09	0.53
1:D:214:ASN:HD22	1:D:214:ASN:C	2.11	0.53
1:B:127:GLU:OE1	1:B:186:ARG:NH2	2.42	0.52
1:A:328:ARG:N	1:A:329:PRO:CD	2.71	0.52
1:D:292:GLY:O	1:D:293:ASN:HB2	2.09	0.52
1:A:97:PRO:HB3	1:A:151:GLY:O	2.08	0.52
1:B:265:LYS:CG	1:B:266:GLY:N	2.52	0.52
1:C:208:ASN:HD22	1:C:208:ASN:C	2.12	0.52
1:A:289:VAL:HG23	1:A:298:PHE:CD2	2.45	0.52
1:C:251:TYR:CG	1:C:329:PRO:HG3	2.44	0.52
3:A:1088:HOH:O	1:B:227:LEU:HD13	2.08	0.52
1:B:184:VAL:CG2	1:B:185:THR:N	2.72	0.52
1:A:85:THR:HG22	1:A:88:LEU:HB2	1.91	0.52
1:D:103:SER:HA	1:D:146:ASP:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:HIS:HB2	1:B:108:GLN:HE22	1.68	0.52
1:B:328:ARG:N	1:B:329:PRO:CD	2.73	0.52
1:D:85:THR:CG2	1:D:86:ALA:N	2.73	0.52
1:D:267:PHE:O	1:D:315:GLN:HA	2.10	0.52
1:C:50:ILE:CG1	1:C:50:ILE:O	2.57	0.51
1:C:338:ARG:CD	3:C:1027:HOH:O	2.58	0.51
1:A:123:ALA:HB3	1:A:146:ASP:OD1	2.10	0.51
1:A:170:GLY:O	1:D:308:THR:HG21	2.11	0.51
1:C:283:VAL:HG22	1:C:321:VAL:HB	1.91	0.51
1:A:253:MSE:SE	1:A:253:MSE:CB	3.04	0.51
1:B:163:LEU:HB2	1:B:164:PRO:HD3	1.93	0.51
1:A:127:GLU:HG3	1:A:213:PHE:CZ	2.45	0.51
1:B:305:VAL:O	1:B:305:VAL:HG13	2.11	0.51
1:D:76:PRO:C	1:D:78:LEU:H	2.13	0.51
1:C:94:LEU:HD11	1:C:154:PRO:HB3	1.92	0.51
1:D:138:LEU:HD12	1:D:138:LEU:N	2.26	0.51
1:C:163:LEU:HD23	3:C:1096:HOH:O	2.10	0.51
1:B:197:ALA:O	1:B:199:MSE:HG3	2.09	0.51
1:C:208:ASN:HA	3:C:1097:HOH:O	2.10	0.51
1:D:89:TYR:O	1:D:160:GLY:HA2	2.11	0.51
1:B:188:GLU:HG2	1:B:189:GLY:N	2.25	0.51
1:C:121:PHE:CD1	1:C:121:PHE:C	2.83	0.51
1:D:328:ARG:N	1:D:329:PRO:CD	2.74	0.51
1:B:275:THR:CA	1:B:308:THR:HG23	2.35	0.50
1:A:37:ASN:CG	1:A:38:ALA:H	2.13	0.50
1:C:161:LEU:HD12	1:C:163:LEU:HD11	1.93	0.50
1:C:208:ASN:N	3:C:1081:HOH:O	2.43	0.50
1:D:160:GLY:C	1:D:161:LEU:HD23	2.31	0.50
1:D:184:VAL:O	1:D:185:THR:C	2.46	0.50
1:C:90:ALA:HA	1:C:159:ASP:O	2.11	0.50
1:B:72:VAL:HG23	3:B:1124:HOH:O	2.10	0.50
1:B:123:ALA:HB2	1:B:128:ARG:HB3	1.93	0.50
1:C:137:ILE:HA	1:C:213:PHE:O	2.11	0.50
1:C:45:TRP:O	1:C:46:ASN:CB	2.58	0.50
1:C:112:ARG:HH22	1:C:147:HIS:CD2	2.28	0.50
1:D:149:ASN:N	1:D:149:ASN:ND2	2.58	0.50
1:B:161:LEU:HD12	1:B:163:LEU:HD12	1.94	0.50
1:B:112:ARG:HH21	1:B:147:HIS:HD2	1.59	0.50
1:B:308:THR:O	1:B:310:HIS:HD2	1.95	0.50
1:D:136:PHE:HB3	1:D:215:TYR:HB2	1.93	0.50
1:B:75:ASN:HD21	1:B:82:SER:CA	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:TYR:CD1	1:C:329:PRO:HG3	2.47	0.49
1:B:90:ALA:HA	1:B:159:ASP:O	2.13	0.49
1:A:206:THR:HG23	1:A:207:GLY:N	2.26	0.49
1:C:275:THR:HA	1:C:308:THR:CG2	2.33	0.49
1:C:257:GLY:O	1:C:325:PHE:HA	2.12	0.49
1:C:332:GLU:HG2	3:C:1110:HOH:O	2.12	0.49
1:B:75:ASN:ND2	1:B:83:SER:N	2.57	0.49
1:D:228:THR:HG22	1:D:239:TYR:CE1	2.46	0.49
1:D:105:ARG:HH11	1:D:175:GLU:CD	2.16	0.49
1:B:75:ASN:HD21	1:B:83:SER:N	2.10	0.49
1:D:192:LEU:CB	1:D:193:PRO:CD	2.91	0.49
1:D:112:ARG:HD3	1:D:131:MSE:CE	2.43	0.49
1:A:292:GLY:O	1:A:293:ASN:CB	2.55	0.49
1:C:199:MSE:HE1	1:D:220:SER:HA	1.95	0.49
1:D:79:ARG:HG3	1:D:79:ARG:NH1	2.27	0.49
1:D:46:ASN:O	1:D:48:GLN:N	2.44	0.49
1:D:39:ASN:ND2	1:D:39:ASN:CB	2.66	0.48
1:D:163:LEU:O	1:D:167:ASN:HB2	2.13	0.48
1:B:178:PRO:HA	3:B:1035:HOH:O	2.13	0.48
1:A:182:GLN:N	3:A:1038:HOH:O	2.45	0.48
1:A:228:THR:HA	1:A:239:TYR:CZ	2.48	0.48
1:C:106:HIS:HB2	1:C:108:GLN:OE1	2.13	0.48
1:D:305:VAL:CG2	3:D:1126:HOH:O	2.57	0.48
1:C:45:TRP:CE2	1:C:74:GLU:HG3	2.49	0.48
1:D:97:PRO:HB3	1:D:151:GLY:O	2.12	0.48
1:A:173:PHE:CE2	1:D:338:ARG:HD3	2.49	0.48
1:A:85:THR:HG21	3:A:1021:HOH:O	2.14	0.48
1:D:328:ARG:HB3	1:D:329:PRO:HD3	1.96	0.48
1:D:240:LYS:C	1:D:241:MSE:HG2	2.33	0.48
1:C:214:ASN:C	1:C:214:ASN:HD22	2.17	0.48
1:C:85:THR:HG23	1:C:87:THR:H	1.79	0.48
1:A:53:LEU:HG	1:A:72:VAL:HG21	1.95	0.48
1:B:43:ALA:HB3	1:B:305:VAL:HG12	1.96	0.48
1:B:105:ARG:HD3	1:B:144:TRP:CE2	2.49	0.48
1:C:267:PHE:O	1:C:315:GLN:HA	2.14	0.47
1:D:108:GLN:HG2	1:D:163:LEU:CD2	2.42	0.47
1:D:228:THR:HA	1:D:239:TYR:CZ	2.49	0.47
1:C:76:PRO:HG3	1:C:84:ILE:O	2.14	0.47
1:D:208:ASN:CA	3:D:1078:HOH:O	2.61	0.47
1:B:73:LEU:HD11	1:B:89:TYR:HE2	1.70	0.47
1:A:289:VAL:HG23	1:A:298:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD12	1:A:111:LEU:C	2.35	0.47
1:D:50:ILE:CG1	1:D:72:VAL:HG21	2.45	0.47
1:A:164:PRO:O	1:A:168:ILE:HG23	2.14	0.47
1:B:73:LEU:CD1	1:B:89:TYR:CE2	2.97	0.47
1:C:216:ARG:HH21	1:C:216:ARG:HG2	1.79	0.47
1:A:104:HIS:C	1:A:104:HIS:CD2	2.87	0.47
1:C:224:LEU:HD11	1:C:260:LEU:HG	1.95	0.47
1:B:330:VAL:CG2	1:B:331:GLN:N	2.78	0.47
1:C:89:TYR:C	1:C:89:TYR:CD1	2.87	0.47
1:D:151:GLY:HA3	3:D:1010:HOH:O	2.13	0.47
1:C:38:ALA:HB3	1:C:308:THR:HB	1.96	0.47
1:C:123:ALA:HB2	1:C:128:ARG:HB3	1.96	0.47
1:C:177:TYR:HB3	3:C:1116:HOH:O	2.13	0.47
1:D:78:LEU:O	1:D:79:ARG:C	2.53	0.47
1:C:138:LEU:CD1	1:C:138:LEU:N	2.78	0.47
1:B:251:TYR:CD2	1:B:329:PRO:HG3	2.50	0.47
1:D:221:ARG:NH2	1:D:284:GLU:OE1	2.44	0.47
1:D:251:TYR:OH	1:D:332:GLU:OE2	2.27	0.47
1:D:341:ARG:O	1:D:342:TYR:CD1	2.68	0.46
1:C:129:THR:HB	3:C:1021:HOH:O	2.15	0.46
1:A:71:LEU:HD12	1:A:93:GLN:HG3	1.97	0.46
1:B:217:TYR:CE2	1:B:283:VAL:HG21	2.51	0.46
1:B:318:GLN:C	3:B:1043:HOH:O	2.43	0.46
1:B:127:GLU:HG3	1:B:213:PHE:CZ	2.48	0.46
1:B:137:ILE:HA	1:B:213:PHE:O	2.16	0.46
1:B:41:ALA:HB1	1:B:42:PRO:HD2	1.97	0.46
1:B:276:ASP:OD1	1:B:276:ASP:N	2.42	0.46
1:C:217:TYR:O	1:C:218:ASP:C	2.51	0.46
1:A:90:ALA:HA	1:A:159:ASP:O	2.15	0.46
1:D:183:PRO:HB3	3:D:1106:HOH:O	2.15	0.46
1:C:134:GLY:C	1:C:217:TYR:HB2	2.36	0.46
1:B:205:GLN:NE2	3:B:1108:HOH:O	2.48	0.46
1:B:121:PHE:CD1	1:B:121:PHE:C	2.89	0.46
1:A:107:ASN:HD22	1:A:107:ASN:C	2.15	0.46
1:B:207:GLY:O	1:B:208:ASN:C	2.54	0.46
1:A:216:ARG:HD2	3:A:1105:HOH:O	2.15	0.46
1:B:184:VAL:O	1:B:185:THR:HB	2.16	0.45
1:A:108:GLN:HE21	1:A:166:VAL:HG21	1.81	0.45
1:C:51:ARG:HG2	1:C:51:ARG:H	1.32	0.45
1:B:84:ILE:HG21	1:B:90:ALA:HB2	1.98	0.45
1:C:158:LEU:HD13	1:C:159:ASP:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ARG:NH1	3:D:1092:HOH:O	2.49	0.45
1:C:246:PRO:HB2	3:C:1075:HOH:O	2.15	0.45
1:C:207:GLY:CA	3:C:1081:HOH:O	2.64	0.45
1:B:291:ILE:O	1:B:293:ASN:O	2.34	0.45
1:A:51:ARG:O	1:A:53:LEU:N	2.48	0.45
1:D:143:ARG:NH1	3:D:1098:HOH:O	2.47	0.45
1:C:219:ARG:CZ	3:C:1032:HOH:O	2.65	0.45
1:B:134:GLY:C	1:B:217:TYR:HB2	2.37	0.45
1:A:161:LEU:HD12	1:A:161:LEU:N	2.31	0.45
1:D:105:ARG:NH1	1:D:175:GLU:OE2	2.45	0.45
1:B:216:ARG:CD	1:B:219:ARG:HD2	2.45	0.45
1:B:338:ARG:HD2	1:C:173:PHE:CZ	2.52	0.45
1:B:144:TRP:HZ3	1:B:177:TYR:H	1.65	0.45
1:A:71:LEU:CD1	1:A:93:GLN:HG3	2.46	0.45
1:B:143:ARG:NH1	3:B:1112:HOH:O	2.40	0.45
1:C:219:ARG:NH1	3:C:1065:HOH:O	2.49	0.45
1:B:338:ARG:NH2	1:B:338:ARG:HB2	2.28	0.45
1:A:282:VAL:HG21	1:A:298:PHE:CD1	2.51	0.45
1:B:51:ARG:N	1:B:52:PRO:HD2	2.31	0.45
1:C:45:TRP:HZ2	1:C:75:ASN:O	2.00	0.45
1:A:127:GLU:HB3	1:A:186:ARG:HB2	1.99	0.45
1:C:89:TYR:CD1	1:C:90:ALA:N	2.84	0.45
1:C:265:LYS:HG3	1:C:317:THR:O	2.17	0.45
1:C:44:TYR:CE2	1:C:46:ASN:HB2	2.52	0.44
1:C:216:ARG:HH21	1:C:216:ARG:CG	2.30	0.44
1:A:36:PRO:HA	1:D:172:GLY:O	2.17	0.44
1:C:108:GLN:CG	1:C:166:VAL:HG21	2.37	0.44
1:A:103:SER:HB2	1:A:177:TYR:HB2	1.98	0.44
1:B:74:GLU:HB2	1:B:90:ALA:O	2.17	0.44
1:A:129:THR:HG22	1:A:213:PHE:HE2	1.82	0.44
1:A:202:LEU:N	1:A:202:LEU:HD12	2.32	0.44
1:A:337:PHE:N	3:A:1018:HOH:O	2.49	0.44
1:D:39:ASN:O	1:D:40:CYS:CB	2.66	0.44
1:D:112:ARG:HD3	1:D:131:MSE:HE1	2.00	0.44
1:B:105:ARG:NE	1:B:144:TRP:CZ2	2.86	0.44
1:B:207:GLY:C	3:B:1070:HOH:O	2.53	0.44
1:A:199:MSE:CE	1:B:241:MSE:HB3	2.46	0.44
1:C:134:GLY:HA3	1:C:217:TYR:CG	2.53	0.44
1:C:121:PHE:O	1:C:147:HIS:HB2	2.18	0.44
1:D:39:ASN:O	1:D:40:CYS:HB3	2.18	0.44
1:A:290:ILE:O	1:A:312:VAL:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ASN:ND2	1:B:173:PHE:H	2.16	0.44
1:A:241:MSE:HB3	1:B:199:MSE:HE2	1.99	0.43
1:C:267:PHE:CE2	1:C:269:SER:HB3	2.53	0.43
1:C:263:LEU:HB2	1:C:320:SER:HB2	2.00	0.43
1:C:278:THR:CG2	1:C:324:SER:HB2	2.48	0.43
1:A:285:GLY:HA3	1:A:320:SER:HA	1.99	0.43
1:B:206:THR:HG22	1:B:247:VAL:HG11	2.00	0.43
1:D:270:ARG:NH2	1:D:342:TYR:CZ	2.87	0.43
1:D:94:LEU:HD11	1:D:154:PRO:HB3	2.00	0.43
1:A:289:VAL:HG12	1:A:290:ILE:N	2.31	0.43
1:C:33:PRO:CA	3:C:1080:HOH:O	2.67	0.43
1:C:160:GLY:O	1:C:161:LEU:HD23	2.19	0.43
1:D:120:ALA:HA	1:D:149:ASN:HB3	2.00	0.43
1:C:46:ASN:HD22	1:C:48:GLN:HB3	1.82	0.43
1:A:163:LEU:CB	1:A:164:PRO:HD3	2.43	0.43
1:A:112:ARG:HH22	1:A:147:HIS:HD2	1.66	0.43
1:B:104:HIS:CD2	3:B:1095:HOH:O	2.64	0.43
1:B:221:ARG:HG2	1:B:221:ARG:HH21	1.83	0.43
1:D:281:HIS:HD2	1:D:303:ILE:HG22	1.82	0.43
1:C:199:MSE:CE	1:D:223:VAL:HG21	2.48	0.43
1:B:48:GLN:O	1:B:49:GLU:CB	2.67	0.43
1:D:214:ASN:ND2	1:D:214:ASN:C	2.72	0.43
1:D:138:LEU:CD1	1:D:138:LEU:N	2.82	0.43
1:A:122:THR:HG22	1:A:123:ALA:N	2.33	0.43
1:C:221:ARG:HG2	1:C:221:ARG:HH21	1.84	0.43
1:C:259:PHE:CD1	1:C:259:PHE:N	2.86	0.43
1:A:308:THR:O	1:A:310:HIS:HD2	2.02	0.42
1:B:166:VAL:HG23	1:B:167:ASN:N	2.34	0.42
1:D:214:ASN:HD22	1:D:215:TYR:N	2.17	0.42
1:A:85:THR:HG22	1:A:88:LEU:N	2.30	0.42
1:A:122:THR:OG1	1:A:131:MSE:HE3	2.19	0.42
1:C:274:THR:HG22	1:C:339:GLU:HB3	2.00	0.42
1:B:184:VAL:O	1:B:185:THR:CB	2.66	0.42
1:A:38:ALA:O	1:A:39:ASN:CG	2.57	0.42
1:D:46:ASN:OD1	1:D:48:GLN:HB3	2.19	0.42
1:A:202:LEU:N	1:A:202:LEU:CD1	2.82	0.42
1:C:122:THR:OG1	1:C:131:MSE:HE3	2.19	0.42
1:A:267:PHE:HE2	1:A:269:SER:HB3	1.80	0.42
1:C:224:LEU:O	1:C:227:LEU:HB2	2.19	0.42
1:C:290:ILE:O	1:C:312:VAL:HA	2.19	0.42
1:D:209:SER:HB2	1:D:210:SER:H	1.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLU:O	1:B:295:THR:O	2.36	0.42
1:A:43:ALA:HB3	1:A:305:VAL:HG12	2.01	0.42
1:C:38:ALA:N	3:C:1108:HOH:O	2.38	0.42
1:B:143:ARG:HA	3:B:1059:HOH:O	2.19	0.42
1:B:265:LYS:HA	1:B:318:GLN:C	2.40	0.42
1:B:330:VAL:O	1:B:334:LEU:HG	2.19	0.42
1:B:94:LEU:HD11	1:B:154:PRO:HB3	2.02	0.42
1:B:318:GLN:CA	3:B:1043:HOH:O	2.68	0.42
1:A:112:ARG:HA	1:A:158:LEU:O	2.19	0.42
1:D:276:ASP:O	1:D:277:SER:C	2.53	0.42
1:D:279:ILE:O	1:D:324:SER:HA	2.20	0.42
1:A:118:LYS:HE3	1:A:118:LYS:HB2	1.84	0.42
1:D:270:ARG:NH2	1:D:342:TYR:CE1	2.79	0.42
1:D:112:ARG:NH1	1:D:122:THR:CG2	2.83	0.42
1:A:141:GLN:HG2	1:A:142:TRP:N	2.35	0.41
1:C:221:ARG:CG	1:C:221:ARG:HH21	2.34	0.41
1:A:152:ASP:O	1:A:153:GLU:HB2	2.20	0.41
1:D:204:HIS:CE1	3:D:1151:HOH:O	2.72	0.41
1:B:293:ASN:C	1:B:293:ASN:OD1	2.58	0.41
1:B:112:ARG:HB3	1:B:157:TRP:CD1	2.55	0.41
1:A:174:ALA:O	1:D:34:LYS:HG3	2.19	0.41
1:C:263:LEU:HD11	1:C:322:LEU:HD22	2.02	0.41
1:C:306:VAL:HG21	1:C:312:VAL:HG21	2.02	0.41
1:B:153:GLU:HA	1:B:154:PRO:HD3	1.82	0.41
1:A:96:MSE:O	1:A:97:PRO:C	2.59	0.41
1:C:85:THR:OG1	1:C:86:ALA:N	2.54	0.41
1:A:166:VAL:HG23	1:A:167:ASN:N	2.34	0.41
1:A:103:SER:HB2	1:A:177:TYR:CB	2.50	0.41
1:B:95:ILE:CG1	1:B:157:TRP:CZ3	3.03	0.41
1:D:157:TRP:C	1:D:157:TRP:CD1	2.94	0.41
1:B:288:GLN:HB3	1:B:288:GLN:HE21	1.29	0.41
1:C:112:ARG:HH22	1:C:147:HIS:HD2	1.66	0.41
1:B:252:PRO:HD3	3:B:1029:HOH:O	2.20	0.41
1:A:223:VAL:O	1:A:224:LEU:C	2.58	0.41
1:C:85:THR:CG2	1:C:88:LEU:H	2.34	0.41
1:B:163:LEU:HA	1:B:166:VAL:HG22	2.03	0.41
1:B:217:TYR:CZ	1:B:283:VAL:HG21	2.56	0.41
1:D:253:MSE:CE	1:D:256:MSE:HE3	2.51	0.41
1:A:101:ALA:HA	1:A:102:PRO:HD2	1.84	0.41
1:A:200:LEU:HB2	1:B:244:VAL:HG11	2.02	0.41
1:C:247:VAL:HG12	1:C:247:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ALA:HB1	1:A:308:THR:HB	2.02	0.41
1:D:313:SER:HB2	1:D:315:GLN:HE22	1.86	0.41
1:C:45:TRP:CE2	1:C:74:GLU:CG	3.04	0.41
1:B:288:GLN:NE2	1:B:295:THR:HG1	2.18	0.41
1:C:112:ARG:HG2	1:C:157:TRP:NE1	2.36	0.41
1:C:242:ARG:HD2	1:C:251:TYR:CE1	2.55	0.41
1:D:129:THR:HA	1:D:130:PRO:HD3	1.92	0.41
1:C:300:ALA:O	1:C:301:LYS:HB2	2.20	0.41
1:A:92:LEU:HA	1:A:92:LEU:HD12	1.76	0.41
1:B:170:GLY:O	1:C:308:THR:HG21	2.21	0.41
1:C:51:ARG:NH2	1:C:94:LEU:HB2	2.32	0.41
1:C:292:GLY:O	1:C:293:ASN:CB	2.66	0.41
1:A:328:ARG:HB3	1:A:329:PRO:HD3	2.03	0.40
1:A:118:LYS:HG3	3:A:1079:HOH:O	2.20	0.40
1:A:301:LYS:N	1:A:301:LYS:HD3	2.35	0.40
1:D:47:TYR:CG	1:D:47:TYR:O	2.74	0.40
1:B:135:ASP:HB3	1:B:214:ASN:OD1	2.21	0.40
1:B:248:THR:HG23	1:B:250:GLY:CA	2.51	0.40
1:A:265:LYS:HD2	1:A:318:GLN:H	1.86	0.40
1:D:218:ASP:OD1	1:D:219:ARG:N	2.54	0.40
1:C:49:GLU:OE1	1:C:49:GLU:CA	2.70	0.40
1:D:93:GLN:O	1:D:156:ILE:HA	2.21	0.40
1:D:35:THR:HA	1:D:36:PRO:HD3	1.85	0.40
1:B:225:HIS:O	1:B:228:THR:OG1	2.36	0.40
1:B:120:ALA:CA	1:B:149:ASN:HB3	2.51	0.40
1:B:47:TYR:OH	1:B:116:GLU:OE2	2.21	0.40
1:B:110:ALA:HA	1:B:160:GLY:O	2.22	0.40
1:C:216:ARG:NH2	1:C:216:ARG:CG	2.82	0.40
1:B:75:ASN:HD21	1:B:82:SER:N	2.18	0.40
1:C:163:LEU:CB	1:C:164:PRO:CD	3.00	0.40
1:B:191:TYR:C	1:B:191:TYR:CD1	2.95	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:THR:N	3:D:1122:HOH:O[1_455]	1.91	0.29
1:D:33:PRO:CB	3:D:1136:HOH:O[1_455]	1.98	0.22

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	283/354 (80%)	257 (91%)	13 (5%)	13 (5%)	3	2
1	B	278/354 (78%)	248 (89%)	15 (5%)	15 (5%)	2	1
1	C	283/354 (80%)	251 (89%)	25 (9%)	7 (2%)	7	6
1	D	281/354 (79%)	249 (89%)	16 (6%)	16 (6%)	2	1
All	All	1125/1416 (79%)	1005 (89%)	69 (6%)	51 (4%)	3	2

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	A	50	ILE
1	A	77	ALA
1	A	141	GLN
1	A	182	GLN
1	B	38	ALA
1	B	49	GLU
1	B	77	ALA
1	B	209	SER
1	B	265	LYS
1	B	295	THR
1	C	38	ALA
1	C	184	VAL
1	D	50	ILE
1	D	77	ALA
1	D	186	ARG
1	D	210	SER
1	A	292	GLY
1	B	184	VAL
1	B	204	HIS
1	B	205	GLN
1	B	292	GLY

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Mol	Chain	Res	Type
1	C	76	PRO
1	D	40	CYS
1	D	47	TYR
1	D	205	GLN
1	D	292	GLY
1	A	76	PRO
1	A	79	ARG
1	B	50	ILE
1	B	79	ARG
1	B	319	ASP
1	C	292	GLY
1	D	38	ALA
1	D	185	THR
1	D	293	ASN
1	D	319	ASP
1	A	36	PRO
1	A	41	ALA
1	A	52	PRO
1	A	153	GLU
1	B	153	GLU
1	B	177	TYR
1	C	46	ASN
1	C	153	GLU
1	D	76	PRO
1	D	184	VAL
1	C	97	PRO
1	D	35	THR
1	D	204	HIS
1	A	318	GLN

### 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	232/293 (79%)	210 (90%)	22 (10%)	11	15
1	B	227/293 (78%)	196 (86%)	31 (14%)	4	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	232/293 (79%)	204 (88%)	28 (12%)	6	7
1	D	230/293 (78%)	203 (88%)	27 (12%)	7	8
All	All	921/1172 (79%)	813 (88%)	108 (12%)	7	8

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	51	ARG
1	A	53	LEU
1	A	74	GLU
1	A	75	ASN
1	A	89	TYR
1	A	92	LEU
1	A	104	HIS
1	A	107	ASN
1	A	141	GLN
1	A	150	PRO
1	A	152	ASP
1	A	200	LEU
1	A	214	ASN
1	A	241	MSE
1	A	260	LEU
1	A	283	VAL
1	A	286	SER
1	A	309	TRP
1	A	317	THR
1	A	322	LEU
1	A	338	ARG
1	B	49	GLU
1	B	71	LEU
1	B	72	VAL
1	B	73	LEU
1	B	74	GLU
1	B	75	ASN
1	B	81	GLN
1	B	85	THR
1	B	89	TYR
1	B	107	ASN
1	B	108	GLN
1	B	112	ARG

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Mol	Chain	Res	Type
1	B	125	ASP
1	B	146	ASP
1	B	149	ASN
1	B	152	ASP
1	B	161	LEU
1	B	176	ASP
1	B	184	VAL
1	B	186	ARG
1	B	200	LEU
1	B	208	ASN
1	B	219	ARG
1	B	221	ARG
1	B	265	LYS
1	B	288	GLN
1	B	293	ASN
1	B	319	ASP
1	B	322	LEU
1	B	338	ARG
1	B	341	ARG
1	C	39	ASN
1	C	49	GLU
1	C	51	ARG
1	C	73	LEU
1	C	75	ASN
1	C	88	LEU
1	C	92	LEU
1	C	106	HIS
1	C	129	THR
1	C	138	LEU
1	C	146	ASP
1	C	153	GLU
1	C	158	LEU
1	C	161	LEU
1	C	176	ASP
1	C	179	GLU
1	C	200	LEU
1	C	205	GLN
1	C	208	ASN
1	C	214	ASN
1	C	221	ARG
1	C	230	LEU
1	C	283	VAL

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Mol	Chain	Res	Type
1	C	305	VAL
1	C	317	THR
1	C	322	LEU
1	C	330	VAL
1	C	338	ARG
1	D	34	LYS
1	D	39	ASN
1	D	40	CYS
1	D	48	GLN
1	D	49	GLU
1	D	71	LEU
1	D	73	LEU
1	D	75	ASN
1	D	85	THR
1	D	92	LEU
1	D	118	LYS
1	D	141	GLN
1	D	149	ASN
1	D	150	PRO
1	D	152	ASP
1	D	158	LEU
1	D	161	LEU
1	D	200	LEU
1	D	214	ASN
1	D	221	ARG
1	D	230	LEU
1	D	259	PHE
1	D	294	GLU
1	D	295	THR
1	D	297	SER
1	D	309	TRP
1	D	313	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	198	ASN
1	A	214	ASN
1	A	281	HIS
1	A	310	HIS
1	A	318	GLN

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Mol	Chain	Res	Type
1	A	331	GLN
1	B	37	ASN
1	B	46	ASN
1	B	75	ASN
1	B	93	GLN
1	B	104	HIS
1	B	107	ASN
1	B	108	GLN
1	B	141	GLN
1	B	147	HIS
1	B	149	ASN
1	B	205	GLN
1	B	288	GLN
1	B	310	HIS
1	B	318	GLN
1	B	331	GLN
1	C	37	ASN
1	C	46	ASN
1	C	93	GLN
1	C	107	ASN
1	C	147	HIS
1	C	167	ASN
1	C	205	GLN
1	C	208	ASN
1	C	214	ASN
1	C	281	HIS
1	C	310	HIS
1	C	318	GLN
1	C	331	GLN
1	D	75	ASN
1	D	93	GLN
1	D	149	ASN
1	D	198	ASN
1	D	208	ASN
1	D	214	ASN
1	D	281	HIS
1	D	293	ASN
1	D	310	HIS
1	D	315	GLN
1	D	318	GLN
1	D	331	GLN

### 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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	283/354 (79%)	-0.49	3 (1%) 82 82	13, 26, 47, 55	0
1	B	278/354 (78%)	-0.45	6 (2%) 65 64	15, 27, 51, 64	0
1	C	283/354 (79%)	-0.45	3 (1%) 82 82	17, 28, 50, 66	0
1	D	281/354 (79%)	-0.51	4 (1%) 78 77	14, 26, 49, 65	0
All	All	1125/1416 (79%)	-0.48	16 (1%) 78 77	13, 27, 49, 66	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	207	GLY	5.4
1	B	208	ASN	2.7
1	B	38	ALA	2.7
1	B	177	TYR	2.7
1	C	38	ALA	2.7
1	D	185	THR	2.6
1	B	185	THR	2.6
1	D	342	TYR	2.5
1	A	181	GLN	2.4
1	C	206	THR	2.4
1	B	39	ASN	2.4
1	A	184	VAL	2.4
1	D	205	GLN	2.3
1	A	35	THR	2.3
1	B	178	PRO	2.2
1	C	39	ASN	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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
2	FE	A	1001	1/1	1.00	0.08	-	27,27,27,27	0
2	FE	D	1004	1/1	1.00	0.13	-	31,31,31,31	0
2	FE	C	1003	1/1	1.00	0.11	-	31,31,31,31	0
2	FE	B	1002	1/1	0.99	0.17	-	26,26,26,26	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.