



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:51 AM GMT

PDB ID : 3N9H  
Title : Crystal Structural of mutant Y305A in the copper amine oxidase from  
hansenula polymorpha  
Authors : Chen, Z.; Datta, S.; DuBois, J.L.; Klinman, J.P.; Mathews, F.S.  
Deposited on : 2010-05-30  
Resolution : 2.50 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

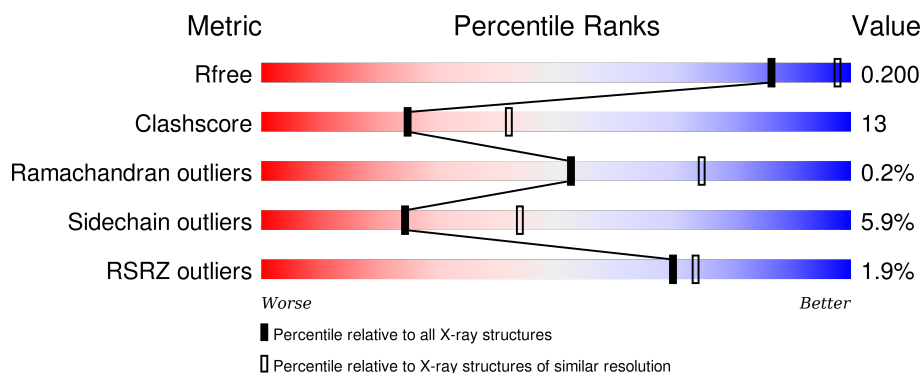
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	692	<div> <div>73%</div> <div>19%</div> <div>• 5%</div> </div>
1	B	692	<div> <div>72%</div> <div>20%</div> <div>• 5%</div> </div>
1	C	692	<div> <div>4%</div> <div>73%</div> <div>19%</div> <div>• 5%</div> </div>
1	D	692	<div> <div>3%</div> <div>73%</div> <div>19%</div> <div>• 5%</div> </div>
1	E	692	<div> <div>73%</div> <div>18%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	692	<div><div></div><div>2%</div><div>72%</div><div>20%</div><div>• 5%</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 34296 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 Peroxisomal primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	2	0
			5203	3309	895	975	24			
1	B	655	Total	C	N	O	S	0	2	0
			5203	3309	895	975	24			
1	C	655	Total	C	N	O	S	0	2	0
			5203	3309	895	975	24			
1	D	655	Total	C	N	O	S	0	2	0
			5203	3309	895	975	24			
1	E	655	Total	C	N	O	S	0	2	0
			5203	3309	895	975	24			
1	F	655	Total	C	N	O	S	0	2	0
			5203	3309	895	975	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	ALA	TYR	ENGINEERED MUTATION	UNP P12807
B	305	ALA	TYR	ENGINEERED MUTATION	UNP P12807
C	305	ALA	TYR	ENGINEERED MUTATION	UNP P12807
D	305	ALA	TYR	ENGINEERED MUTATION	UNP P12807
E	305	ALA	TYR	ENGINEERED MUTATION	UNP P12807
F	305	ALA	TYR	ENGINEERED MUTATION	UNP P12807

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cu	0	0
			1	1		
2	E	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Cu 1	0	0
2	A	1	Total 1	Cu 1	0	0
2	F	1	Total 1	Cu 1	0	0

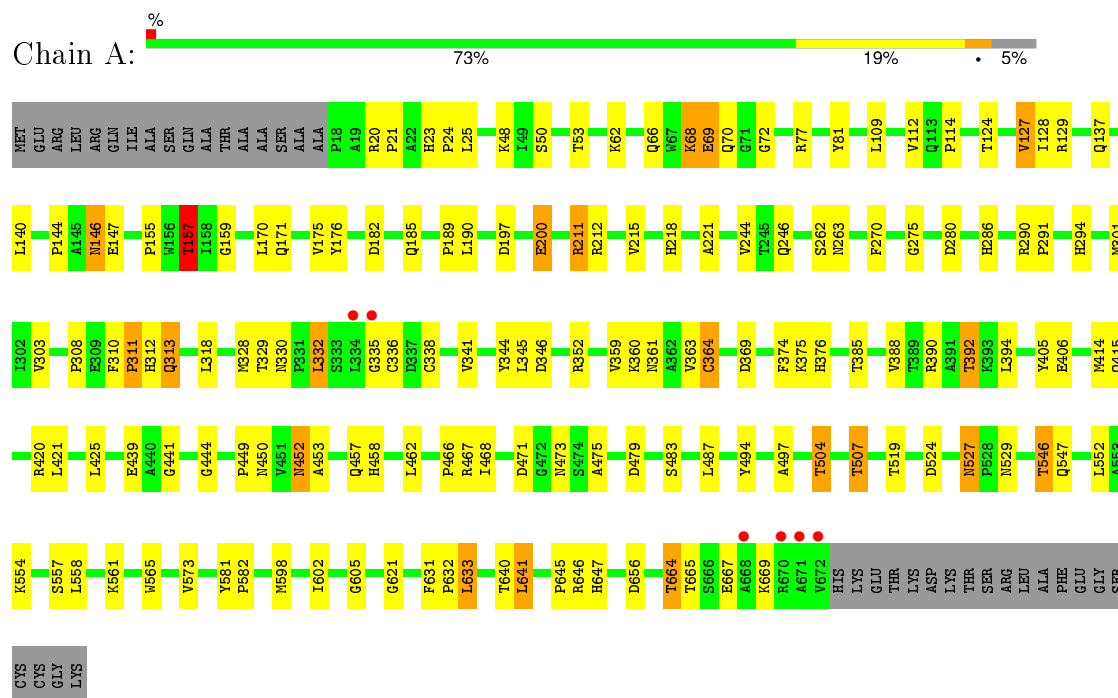
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	507	Total 507	O 507	0	0
3	B	517	Total 517	O 517	0	0
3	C	515	Total 515	O 515	0	0
3	D	509	Total 509	O 509	0	0
3	E	506	Total 506	O 506	0	0
3	F	518	Total 518	O 518	0	0

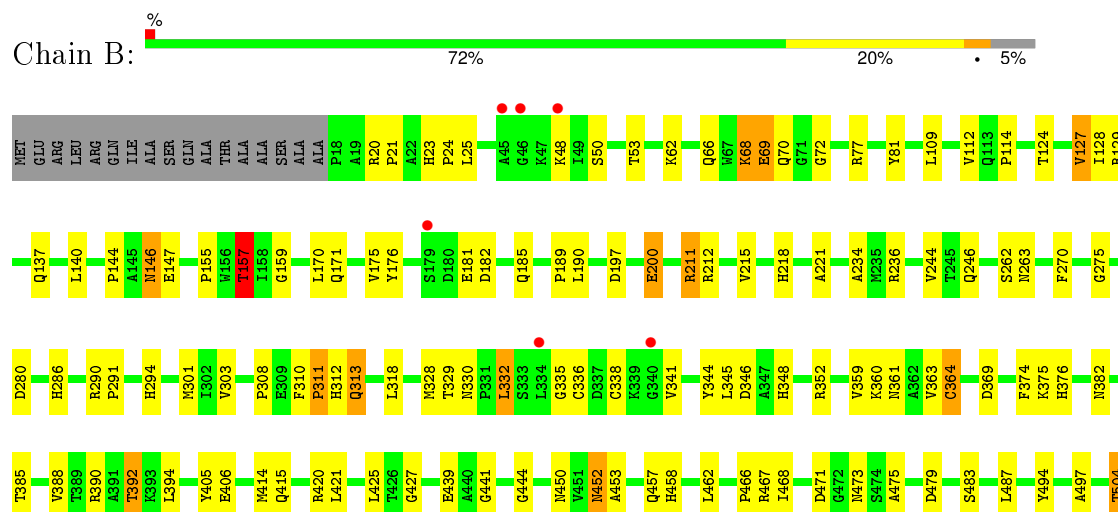
### 3 Residue-property plots

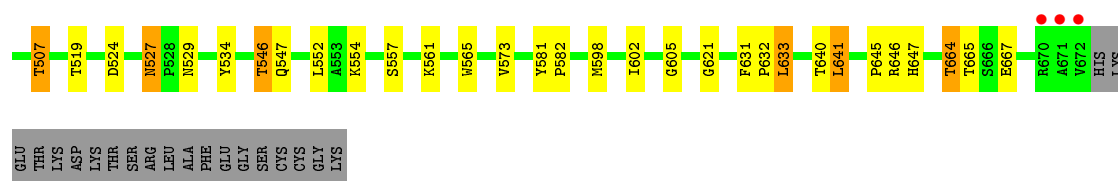
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Peroxisomal primary amine oxidase

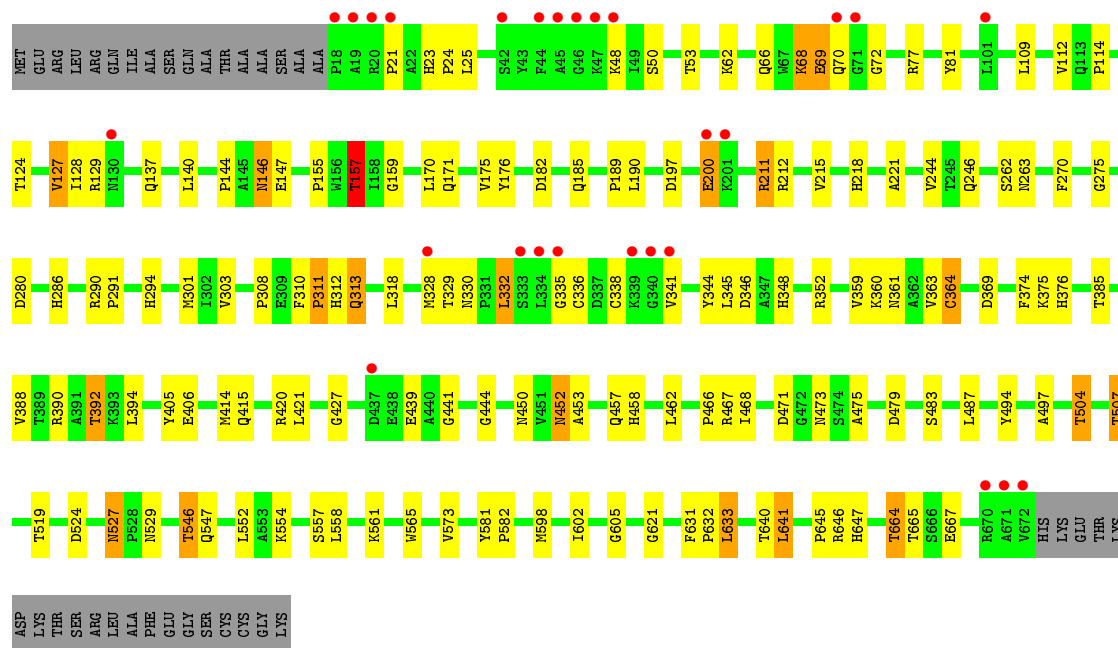


- Molecule 1: Peroxisomal primary amine oxidase

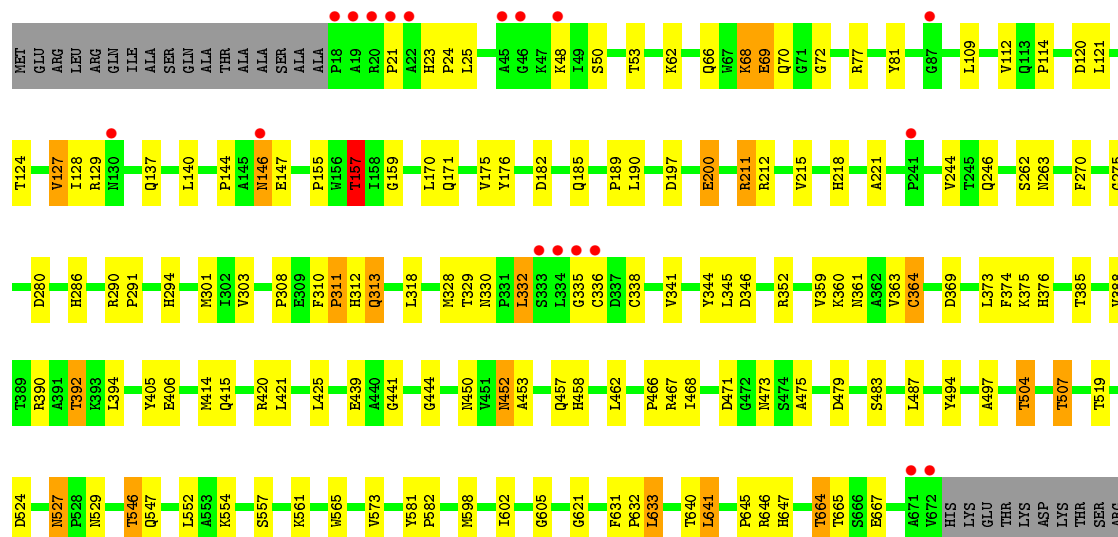
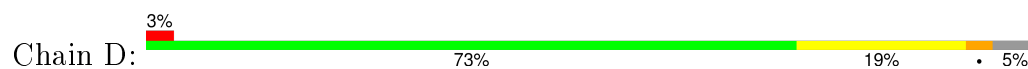




• Molecule 1: Peroxisomal primary amine oxidase



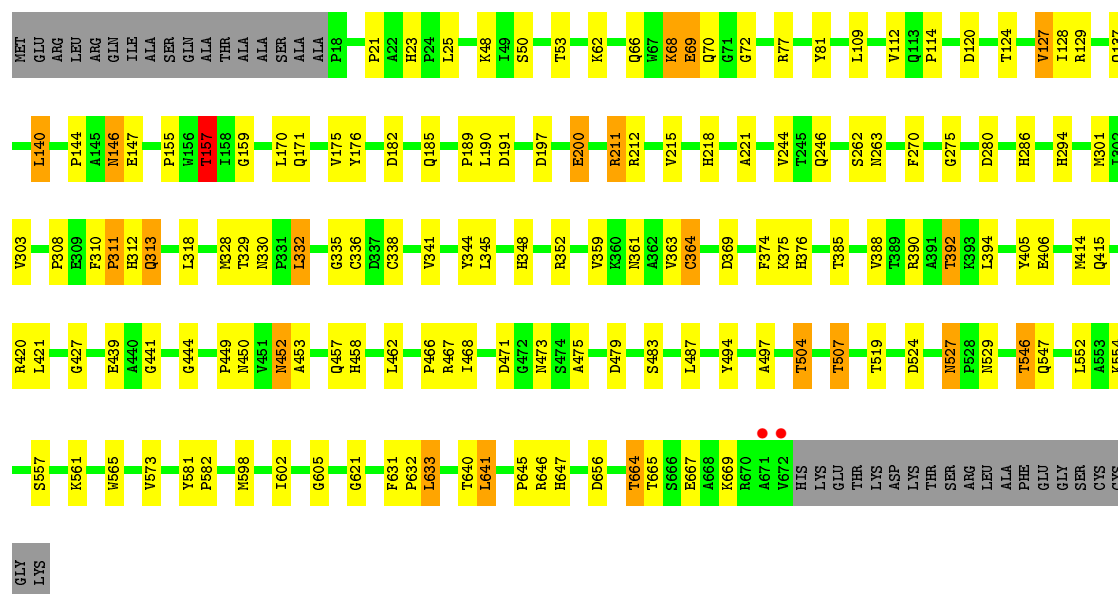
• Molecule 1: Peroxisomal primary amine oxidase



LEU  
ALA  
PHE  
GLU  
GLY  
SER  
CYS  
GLY  
LYS

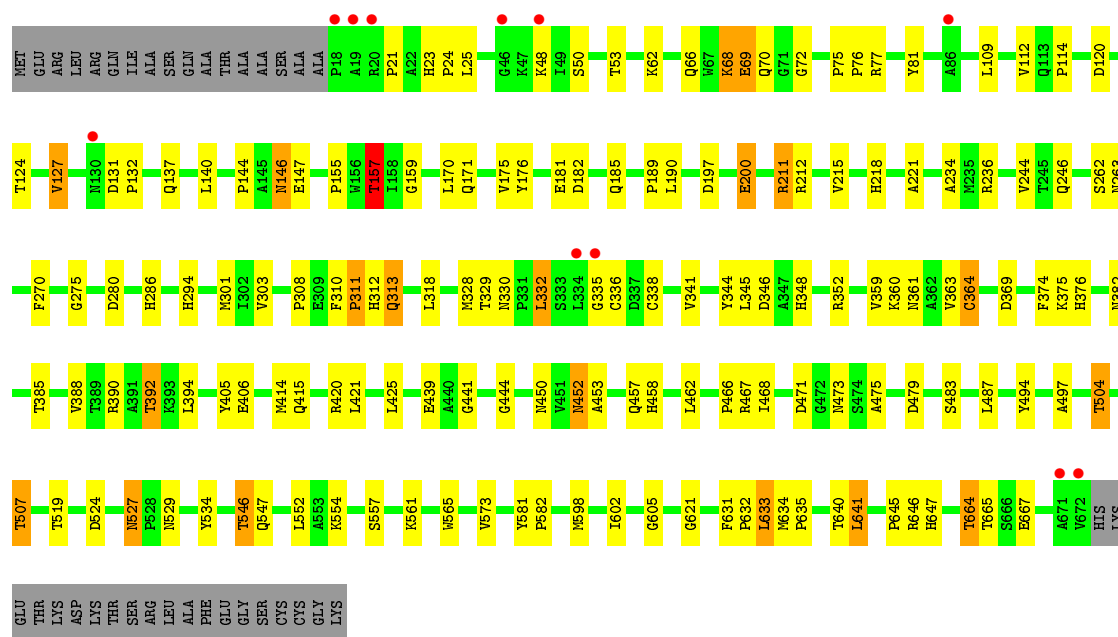
- Molecule 1: Peroxisomal primary amine oxidase

Chain E:  73% 18% 5%



- Molecule 1: Peroxisomal primary amine oxidase

Chain F:  72% 20% 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.91Å 147.15Å 233.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.10 – 2.50 30.10 – 2.41	Depositor EDS
% Data completeness (in resolution range)	81.0 (30.10-2.50) 75.4 (30.10-2.41)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.185 , 0.198 0.187 , 0.200	Depositor DCC
$R_{free}$ test set	13398 reflections (9.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 138872 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	34296	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 2.87% 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: TPQ, CU

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	0.47	0/5337	0.76	2/7262 (0.0%)
1	B	0.47	0/5337	0.76	2/7262 (0.0%)
1	C	0.47	0/5337	0.76	2/7262 (0.0%)
1	D	0.47	0/5337	0.76	2/7262 (0.0%)
1	E	0.47	0/5337	0.76	2/7262 (0.0%)
1	F	0.47	0/5337	0.76	2/7262 (0.0%)
All	All	0.47	0/32022	0.76	12/43572 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	641	LEU	CA-CB-CG	6.82	130.99	115.30
1	F	641	LEU	CA-CB-CG	6.81	130.96	115.30
1	A	641	LEU	CA-CB-CG	6.79	130.92	115.30
1	B	641	LEU	CA-CB-CG	6.79	130.91	115.30
1	D	641	LEU	CA-CB-CG	6.79	130.91	115.30
1	C	641	LEU	CA-CB-CG	6.78	130.89	115.30
1	B	157	THR	CB-CA-C	-5.93	95.58	111.60
1	C	157	THR	CB-CA-C	-5.93	95.58	111.60
1	F	157	THR	CB-CA-C	-5.93	95.59	111.60
1	D	157	THR	CB-CA-C	-5.93	95.59	111.60
1	A	157	THR	CB-CA-C	-5.93	95.59	111.60
1	E	157	THR	CB-CA-C	-5.93	95.59	111.60

There are no chirality outliers.

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	5203	0	5044	144	3
1	B	5203	0	5044	148	1
1	C	5203	0	5044	149	0
1	D	5203	0	5044	148	2
1	E	5203	0	5044	146	1
1	F	5203	0	5044	148	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
3	A	507	0	0	15	0
3	B	517	0	0	18	0
3	C	515	0	0	16	0
3	D	509	0	0	16	1
3	E	506	0	0	15	0
3	F	518	0	0	18	0
All	All	34296	0	30264	782	4

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 13.

All (782) 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:E:546:THR:HG21	1:F:546:THR:CG2	1.41	1.50
1:C:546:THR:HG21	1:D:546:THR:CG2	1.40	1.50
1:A:546:THR:HG21	1:B:546:THR:CG2	1.42	1.49
1:C:546:THR:CG2	1:D:546:THR:HG21	1.40	1.48
1:A:546:THR:CG2	1:B:546:THR:HG21	1.41	1.48
1:E:546:THR:CG2	1:F:546:THR:HG21	1.40	1.46
1:D:211:ARG:HD3	1:D:211:ARG:H	1.09	1.15
1:C:546:THR:CG2	1:D:546:THR:CG2	2.11	1.13
1:A:211:ARG:H	1:A:211:ARG:HD3	1.09	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:ARG:H	1:F:211:ARG:HD3	1.09	1.12
1:C:211:ARG:H	1:C:211:ARG:HD3	1.09	1.12
1:E:211:ARG:HD3	1:E:211:ARG:H	1.09	1.12
1:E:546:THR:CG2	1:F:546:THR:CG2	2.11	1.10
1:B:211:ARG:H	1:B:211:ARG:HD3	1.09	1.08
1:E:494:TYR:CD1	1:F:313:GLN:HG2	1.88	1.07
1:A:546:THR:CG2	1:B:546:THR:CG2	2.13	1.05
1:E:313:GLN:HG2	1:F:494:TYR:CD1	1.93	1.03
1:A:311:PRO:HA	1:A:313:GLN:HE22	1.24	1.02
1:E:311:PRO:HA	1:E:313:GLN:HE22	1.24	1.02
1:A:494:TYR:CD1	1:B:313:GLN:HG2	1.94	1.02
1:D:311:PRO:HA	1:D:313:GLN:HE22	1.24	1.02
1:B:311:PRO:HA	1:B:313:GLN:HE22	1.24	1.01
1:C:313:GLN:HG2	1:D:494:TYR:CD1	1.96	1.01
1:C:494:TYR:CD1	1:D:313:GLN:HG2	1.95	1.00
1:C:311:PRO:HA	1:C:313:GLN:HE22	1.24	1.00
1:F:311:PRO:HA	1:F:313:GLN:HE22	1.24	1.00
1:A:313:GLN:HG2	1:B:494:TYR:CD1	1.98	0.98
1:A:23:HIS:HD2	1:A:25:LEU:H	1.07	0.98
1:E:23:HIS:HD2	1:E:25:LEU:H	1.07	0.98
1:B:23:HIS:HD2	1:B:25:LEU:H	1.07	0.97
1:F:23:HIS:HD2	1:F:25:LEU:H	1.07	0.95
1:D:23:HIS:HD2	1:D:25:LEU:H	1.07	0.94
1:E:546:THR:HG21	1:F:546:THR:HG21	0.98	0.91
1:C:23:HIS:HD2	1:C:25:LEU:H	1.07	0.91
1:F:211:ARG:CD	1:F:211:ARG:H	1.86	0.88
1:D:211:ARG:H	1:D:211:ARG:CD	1.86	0.88
1:B:211:ARG:H	1:B:211:ARG:CD	1.86	0.87
1:E:546:THR:HG23	1:F:546:THR:HG21	1.55	0.87
1:E:211:ARG:CD	1:E:211:ARG:H	1.86	0.87
1:A:211:ARG:H	1:A:211:ARG:CD	1.86	0.86
1:F:664:THR:HG22	1:F:667:GLU:H	1.40	0.86
1:C:664:THR:HG22	1:C:667:GLU:H	1.40	0.86
1:A:664:THR:HG22	1:A:667:GLU:H	1.40	0.86
1:E:664:THR:HG22	1:E:667:GLU:H	1.40	0.85
1:B:664:THR:HG22	1:B:667:GLU:H	1.40	0.85
1:C:211:ARG:H	1:C:211:ARG:CD	1.86	0.85
1:D:664:THR:HG22	1:D:667:GLU:H	1.40	0.85
1:C:546:THR:HG21	1:D:546:THR:HG23	1.57	0.84
1:C:546:THR:HG23	1:D:546:THR:HG21	1.56	0.84
1:D:507:THR:HG21	3:D:1235:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:THR:HG21	3:C:1235:HOH:O	1.80	0.82
1:C:137:GLN:OE1	1:C:212:ARG:NH2	2.13	0.81
1:F:211:ARG:N	1:F:211:ARG:HD3	1.93	0.81
1:E:137:GLN:OE1	1:E:212:ARG:NH2	2.13	0.81
1:B:507:THR:HG21	3:B:1235:HOH:O	1.80	0.81
1:F:507:THR:HG21	3:F:1235:HOH:O	1.80	0.81
1:A:137:GLN:OE1	1:A:212:ARG:NH2	2.13	0.80
1:E:507:THR:HG21	3:E:1235:HOH:O	1.80	0.80
1:E:311:PRO:HA	1:E:313:GLN:NE2	1.96	0.80
1:A:311:PRO:HA	1:A:313:GLN:NE2	1.96	0.80
1:B:311:PRO:HA	1:B:313:GLN:NE2	1.96	0.80
1:C:211:ARG:N	1:C:211:ARG:HD3	1.93	0.80
1:D:137:GLN:OE1	1:D:212:ARG:NH2	2.13	0.80
1:F:137:GLN:OE1	1:F:212:ARG:NH2	2.13	0.80
1:B:137:GLN:OE1	1:B:212:ARG:NH2	2.13	0.80
1:B:211:ARG:HD3	1:B:211:ARG:N	1.93	0.80
1:E:211:ARG:N	1:E:211:ARG:HD3	1.93	0.80
1:A:507:THR:HG21	3:A:1235:HOH:O	1.80	0.80
1:D:311:PRO:HA	1:D:313:GLN:NE2	1.96	0.79
1:C:546:THR:HG21	1:D:546:THR:HG21	0.97	0.79
1:A:546:THR:HG21	1:B:546:THR:HG23	1.59	0.79
1:F:311:PRO:HA	1:F:313:GLN:NE2	1.96	0.79
1:E:546:THR:HG21	1:F:546:THR:HG23	1.58	0.79
1:A:546:THR:HG23	1:B:546:THR:HG21	1.57	0.79
1:A:211:ARG:HD3	1:A:211:ARG:N	1.93	0.79
1:C:311:PRO:HA	1:C:313:GLN:NE2	1.96	0.79
1:A:546:THR:HG21	1:B:546:THR:HG21	0.97	0.77
1:E:338:CYS:HG	1:E:364:CYS:HG	0.78	0.76
1:B:328[B]:MET:HE2	3:B:1510:HOH:O	1.85	0.76
1:F:328[B]:MET:HE2	3:F:1510:HOH:O	1.85	0.76
1:D:527:ASN:HD22	1:D:529:ASN:H	1.34	0.76
1:A:546:THR:HG23	1:B:546:THR:CG2	2.14	0.76
1:E:527:ASN:HD22	1:E:529:ASN:H	1.34	0.76
1:B:527:ASN:HD22	1:B:529:ASN:H	1.34	0.76
1:E:546:THR:CG2	1:F:546:THR:HG23	2.13	0.76
1:D:211:ARG:HD3	1:D:211:ARG:N	1.93	0.75
1:C:157:THR:HB	1:C:159:GLY:H	1.51	0.75
1:A:527:ASN:HD22	1:A:529:ASN:H	1.34	0.75
1:C:546:THR:CG2	1:D:546:THR:HG23	2.13	0.75
1:F:527:ASN:HD22	1:F:529:ASN:H	1.34	0.75
1:A:546:THR:CG2	1:B:546:THR:HG23	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:THR:HB	1:B:159:GLY:H	1.51	0.75
1:E:157:THR:HB	1:E:159:GLY:H	1.51	0.75
1:E:546:THR:HG23	1:F:546:THR:CG2	2.11	0.75
1:F:157:THR:HB	1:F:159:GLY:H	1.51	0.75
1:D:23:HIS:CD2	1:D:25:LEU:H	2.00	0.75
1:A:157:THR:HB	1:A:159:GLY:H	1.51	0.74
1:D:157:THR:HB	1:D:159:GLY:H	1.51	0.74
1:F:468:ILE:H	1:F:473:ASN:HD21	1.36	0.74
1:A:468:ILE:H	1:A:473:ASN:HD21	1.36	0.74
1:B:23:HIS:CD2	1:B:25:LEU:H	2.00	0.73
1:D:468:ILE:H	1:D:473:ASN:HD21	1.36	0.73
1:C:527:ASN:HD22	1:C:529:ASN:H	1.34	0.73
1:F:23:HIS:CD2	1:F:25:LEU:H	2.00	0.73
1:E:23:HIS:CD2	1:E:25:LEU:H	2.00	0.73
1:C:23:HIS:CD2	1:C:25:LEU:H	2.00	0.73
1:B:468:ILE:H	1:B:473:ASN:HD21	1.36	0.72
1:E:468:ILE:H	1:E:473:ASN:HD21	1.36	0.72
1:A:328[B]:MET:HE2	3:A:1510:HOH:O	1.91	0.71
1:E:328[B]:MET:HE2	3:E:1510:HOH:O	1.91	0.71
1:C:546:THR:HG23	1:D:546:THR:CG2	2.12	0.70
1:E:527:ASN:ND2	1:E:529:ASN:H	1.89	0.70
1:B:527:ASN:ND2	1:B:529:ASN:H	1.89	0.70
1:D:70:GLN:HG3	3:D:1501:HOH:O	1.92	0.70
1:F:70:GLN:HG3	3:F:1501:HOH:O	1.92	0.70
1:C:527:ASN:ND2	1:C:529:ASN:H	1.89	0.69
1:B:70:GLN:HG3	3:B:1501:HOH:O	1.92	0.69
1:C:70:GLN:HG3	3:C:1501:HOH:O	1.92	0.69
1:C:468:ILE:H	1:C:473:ASN:HD21	1.36	0.69
1:F:21:PRO:HG3	1:F:77:ARG:CZ	2.23	0.69
1:E:21:PRO:HG3	1:E:77:ARG:CZ	2.23	0.69
1:F:527:ASN:ND2	1:F:529:ASN:H	1.89	0.69
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.23	0.69
1:D:21:PRO:HG3	1:D:77:ARG:CZ	2.23	0.69
1:A:527:ASN:ND2	1:A:529:ASN:H	1.89	0.69
1:D:527:ASN:ND2	1:D:529:ASN:H	1.89	0.68
1:A:21:PRO:HG3	1:A:77:ARG:CZ	2.23	0.68
1:A:70:GLN:HG3	3:A:1501:HOH:O	1.92	0.68
1:A:406:GLU:OE2	1:B:376:HIS:ND1	2.27	0.68
1:D:439:GLU:HG3	1:D:441:GLY:H	1.59	0.68
1:E:70:GLN:HG3	3:E:1501:HOH:O	1.92	0.68
1:C:21:PRO:HG3	1:C:77:ARG:CZ	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:GLU:HG3	1:E:441:GLY:H	1.59	0.68
1:A:439:GLU:HG3	1:A:441:GLY:H	1.59	0.68
1:E:494:TYR:CE1	1:F:313:GLN:HG2	2.28	0.68
1:B:439:GLU:HG3	1:B:441:GLY:H	1.59	0.68
1:F:439:GLU:HG3	1:F:441:GLY:H	1.59	0.67
1:A:23:HIS:CD2	1:A:25:LEU:H	2.00	0.66
1:E:286:HIS:HD2	3:F:1371:HOH:O	1.77	0.66
1:C:328[B]:MET:HE2	3:C:1510:HOH:O	1.94	0.66
1:A:457:GLN:HE22	1:A:552:LEU:H	1.43	0.66
1:A:286:HIS:HD2	3:B:1371:HOH:O	1.77	0.66
1:C:439:GLU:HG3	1:C:441:GLY:H	1.59	0.66
1:A:507:THR:HG23	1:A:605:GLY:O	1.96	0.66
1:E:507:THR:HG23	1:E:605:GLY:O	1.96	0.66
1:C:439:GLU:C	1:C:441:GLY:H	1.99	0.66
1:A:246:GLN:HB2	1:A:341:VAL:HG21	1.78	0.66
1:C:457:GLN:HE22	1:C:552:LEU:H	1.43	0.66
1:B:507:THR:HG23	1:B:605:GLY:O	1.96	0.65
1:A:494:TYR:CE1	1:B:313:GLN:HG2	2.31	0.65
1:D:507:THR:HG23	1:D:605:GLY:O	1.96	0.65
1:E:457:GLN:HE22	1:E:552:LEU:H	1.43	0.65
1:F:246:GLN:HB2	1:F:341:VAL:HG21	1.78	0.65
1:F:457:GLN:HE22	1:F:552:LEU:H	1.43	0.65
1:B:457:GLN:HE22	1:B:552:LEU:H	1.43	0.65
1:A:439:GLU:C	1:A:441:GLY:H	1.99	0.65
1:C:507:THR:HG23	1:C:605:GLY:O	1.96	0.65
1:E:308:PRO:HB3	1:F:497:ALA:HB2	1.77	0.65
1:D:328[B]:MET:HE2	3:D:1510:HOH:O	1.97	0.65
1:F:507:THR:HG23	1:F:605:GLY:O	1.96	0.64
1:E:406:GLU:OE2	1:F:376:HIS:ND1	2.29	0.64
1:E:527:ASN:C	1:E:527:ASN:HD22	2.01	0.64
1:C:246:GLN:HB2	1:C:341:VAL:HG21	1.78	0.64
1:E:313:GLN:HG2	1:F:494:TYR:CE1	2.33	0.64
1:A:527:ASN:HD22	1:A:527:ASN:C	2.01	0.64
1:E:439:GLU:C	1:E:441:GLY:H	1.99	0.64
1:F:439:GLU:C	1:F:441:GLY:H	1.99	0.64
1:B:246:GLN:HB2	1:B:341:VAL:HG21	1.78	0.64
1:D:457:GLN:HE22	1:D:552:LEU:H	1.43	0.64
1:F:338:CYS:HG	1:F:364:CYS:HG	0.77	0.64
1:D:439:GLU:C	1:D:441:GLY:H	1.99	0.64
1:D:338:CYS:HG	1:D:364:CYS:CB	2.11	0.63
1:E:246:GLN:HB2	1:E:341:VAL:HG21	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:GLN:HB2	1:D:341:VAL:HG21	1.78	0.63
1:D:527:ASN:C	1:D:527:ASN:HD22	2.01	0.63
1:B:527:ASN:C	1:B:527:ASN:HD22	2.01	0.63
1:C:313:GLN:HG2	1:D:494:TYR:CE1	2.33	0.63
1:C:527:ASN:HD22	1:C:527:ASN:C	2.01	0.63
1:A:308:PRO:HB3	1:B:497:ALA:HB2	1.81	0.63
1:F:527:ASN:HD22	1:F:527:ASN:C	2.01	0.63
1:B:439:GLU:C	1:B:441:GLY:H	1.99	0.63
1:E:546:THR:HG21	1:F:546:THR:HG22	1.71	0.62
1:F:504:THR:HG21	3:F:1434:HOH:O	2.00	0.62
1:A:338:CYS:CB	1:A:364:CYS:HG	2.12	0.62
1:C:504:THR:HG21	3:C:1434:HOH:O	2.00	0.62
1:C:494:TYR:CE1	1:D:313:GLN:HG2	2.33	0.62
1:E:504:THR:HG21	3:E:1434:HOH:O	2.00	0.62
1:A:313:GLN:HG2	1:B:494:TYR:CE1	2.35	0.62
3:C:1371:HOH:O	1:D:286:HIS:HD2	1.83	0.62
1:B:664:THR:CG2	1:B:667:GLU:HG3	2.31	0.61
1:C:497:ALA:HB2	1:D:308:PRO:HB3	1.82	0.61
1:F:664:THR:CG2	1:F:667:GLU:HG3	2.31	0.61
1:E:664:THR:CG2	1:E:667:GLU:HG3	2.31	0.61
1:B:504:THR:HG21	3:B:1434:HOH:O	2.00	0.61
1:D:664:THR:CG2	1:D:667:GLU:HG3	2.31	0.61
1:E:497:ALA:HB2	1:F:308:PRO:HB3	1.82	0.61
1:C:664:THR:CG2	1:C:667:GLU:HG3	2.31	0.61
1:D:504:THR:HG21	3:D:1434:HOH:O	2.00	0.61
1:C:308:PRO:HB3	1:D:497:ALA:HB2	1.83	0.60
1:E:338:CYS:CB	1:E:364:CYS:HG	2.15	0.60
1:A:504:THR:HG21	3:A:1434:HOH:O	2.00	0.60
1:A:664:THR:CG2	1:A:667:GLU:HG3	2.31	0.60
1:F:211:ARG:CD	1:F:211:ARG:N	2.60	0.59
1:C:376:HIS:ND1	1:D:406:GLU:OE2	2.33	0.59
1:B:338:CYS:HG	1:B:364:CYS:CB	2.13	0.59
1:C:527:ASN:HD21	1:C:529:ASN:HB2	1.68	0.59
1:E:527:ASN:HD21	1:E:529:ASN:HB2	1.68	0.59
1:F:338:CYS:CB	1:F:364:CYS:HG	2.15	0.59
1:C:286:HIS:HD2	3:D:1371:HOH:O	1.85	0.58
1:F:631:PHE:CG	1:F:632:PRO:HA	2.39	0.58
1:B:527:ASN:HD21	1:B:529:ASN:HB2	1.68	0.58
1:B:631:PHE:CG	1:B:632:PRO:HA	2.39	0.58
1:F:527:ASN:HD21	1:F:529:ASN:HB2	1.68	0.58
3:E:1371:HOH:O	1:F:286:HIS:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:PHE:CG	1:C:632:PRO:HA	2.39	0.58
1:E:631:PHE:CG	1:E:632:PRO:HA	2.39	0.58
1:A:527:ASN:HD21	1:A:529:ASN:HB2	1.68	0.58
1:A:631:PHE:CG	1:A:632:PRO:HA	2.39	0.58
1:B:392:THR:HG22	3:B:1004:HOH:O	2.03	0.58
1:D:631:PHE:CG	1:D:632:PRO:HA	2.39	0.58
1:B:467:ARG:HD2	1:B:471:ASP:OD1	2.05	0.57
1:C:392:THR:HG22	3:C:1004:HOH:O	2.04	0.57
1:F:467:ARG:HD2	1:F:471:ASP:OD1	2.05	0.57
1:D:527:ASN:HD21	1:D:529:ASN:HB2	1.68	0.57
1:A:664:THR:HG22	1:A:667:GLU:HG3	1.87	0.57
1:E:664:THR:HG22	1:E:667:GLU:HG3	1.87	0.57
1:C:546:THR:HG22	1:D:546:THR:HG21	1.71	0.57
1:D:62:LYS:HE2	1:D:66[A]:GLN:OE1	2.05	0.57
1:E:467:ARG:HD2	1:E:471:ASP:OD1	2.04	0.56
1:A:467:ARG:HD2	1:A:471:ASP:OD1	2.04	0.56
1:B:62:LYS:HE2	1:B:66[A]:GLN:OE1	2.05	0.56
1:C:338:CYS:HG	1:C:364:CYS:CB	2.14	0.56
1:F:62:LYS:HE2	1:F:66[A]:GLN:OE1	2.05	0.56
1:C:467:ARG:HD2	1:C:471:ASP:OD1	2.05	0.56
1:F:664:THR:HG22	1:F:667:GLU:HG3	1.87	0.56
1:B:664:THR:HG22	1:B:667:GLU:HG3	1.87	0.56
1:F:392:THR:HG22	3:F:1004:HOH:O	2.06	0.56
1:A:62:LYS:HE2	1:A:66[A]:GLN:OE1	2.05	0.56
1:C:375:LYS:HG3	1:C:388:VAL:HG22	1.88	0.56
1:E:211:ARG:N	1:E:211:ARG:CD	2.60	0.56
1:D:392:THR:HG22	3:D:1004:HOH:O	2.06	0.56
1:D:467:ARG:HD2	1:D:471:ASP:OD1	2.05	0.56
1:C:182:ASP:OD1	1:D:664:THR:HG23	2.05	0.56
1:E:375:LYS:HG3	1:E:388:VAL:HG22	1.88	0.56
1:E:62:LYS:HE2	1:E:66[A]:GLN:OE1	2.05	0.56
1:A:546:THR:HG21	1:B:546:THR:HG22	1.72	0.56
1:C:62:LYS:HE2	1:C:66[A]:GLN:OE1	2.05	0.55
1:C:664:THR:HG22	1:C:667:GLU:HG3	1.87	0.55
1:D:375:LYS:HG3	1:D:388:VAL:HG22	1.88	0.55
1:A:497:ALA:HB2	1:B:308:PRO:HB3	1.87	0.55
1:D:664:THR:HG22	1:D:667:GLU:HG3	1.87	0.55
1:E:157:THR:HB	1:E:159:GLY:N	2.21	0.55
1:C:664:THR:HG23	1:D:182:ASP:OD1	2.06	0.55
1:A:182:ASP:OD1	1:B:664:THR:HG23	2.06	0.55
1:F:375:LYS:HG3	1:F:388:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1371:HOH:O	1:B:286:HIS:HD2	1.89	0.55
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.42	0.55
1:F:631:PHE:CD1	1:F:632:PRO:HA	2.42	0.54
1:C:631:PHE:CD1	1:C:632:PRO:HA	2.42	0.54
1:D:631:PHE:CD1	1:D:632:PRO:HA	2.42	0.54
1:E:631:PHE:CD1	1:E:632:PRO:HA	2.42	0.54
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.42	0.54
1:A:375:LYS:HG3	1:A:388:VAL:HG22	1.88	0.54
1:A:310:PHE:HA	1:A:313:GLN:NE2	2.23	0.54
1:F:479:ASP:HB3	1:F:519:THR:HB	1.90	0.54
1:D:310:PHE:HA	1:D:313:GLN:NE2	2.23	0.54
1:B:310:PHE:HA	1:B:313:GLN:NE2	2.23	0.54
1:B:157:THR:HB	1:B:159:GLY:N	2.21	0.54
1:E:479:ASP:HB3	1:E:519:THR:HB	1.90	0.54
1:B:479:ASP:HB3	1:B:519:THR:HB	1.90	0.54
1:E:310:PHE:HA	1:E:313:GLN:NE2	2.23	0.54
1:F:157:THR:HB	1:F:159:GLY:N	2.21	0.54
1:A:468:ILE:N	1:A:473:ASN:HD21	2.05	0.54
1:D:479:ASP:HB3	1:D:519:THR:HB	1.90	0.54
1:C:211:ARG:N	1:C:211:ARG:CD	2.60	0.54
1:C:310:PHE:HA	1:C:313:GLN:NE2	2.23	0.53
1:E:439:GLU:C	1:E:441:GLY:N	2.62	0.53
1:A:439:GLU:C	1:A:441:GLY:N	2.62	0.53
1:E:376:HIS:ND1	1:F:406:GLU:OE2	2.40	0.53
1:A:211:ARG:CD	1:A:211:ARG:N	2.60	0.53
1:C:330:ASN:O	1:C:332:LEU:HD13	2.08	0.53
1:D:439:GLU:C	1:D:441:GLY:N	2.62	0.53
1:C:439:GLU:C	1:C:441:GLY:N	2.62	0.53
1:B:375:LYS:HG3	1:B:388:VAL:HG22	1.88	0.53
1:E:146:ASN:C	1:E:146:ASN:HD22	2.12	0.53
1:D:557:SER:O	1:D:561:LYS:HG3	2.09	0.53
1:F:155:PRO:HB2	1:F:171:GLN:OE1	2.09	0.53
1:E:330:ASN:O	1:E:332:LEU:HD13	2.08	0.53
1:A:376:HIS:ND1	1:B:406:GLU:OE2	2.42	0.53
1:F:310:PHE:HA	1:F:313:GLN:NE2	2.23	0.53
1:A:330:ASN:O	1:A:332:LEU:HD13	2.08	0.53
1:A:664:THR:HG23	1:B:182:ASP:OD1	2.08	0.53
1:F:330:ASN:O	1:F:332:LEU:HD13	2.08	0.53
1:D:468:ILE:N	1:D:473:ASN:HD21	2.05	0.53
1:C:406:GLU:OE2	1:D:376:HIS:ND1	2.36	0.53
1:B:146:ASN:HD22	1:B:146:ASN:C	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:ASP:HB3	1:C:519:THR:HB	1.90	0.53
1:C:155:PRO:HB2	1:C:171:GLN:OE1	2.09	0.53
1:A:392:THR:HG22	3:A:1004:HOH:O	2.08	0.53
1:E:155:PRO:HB2	1:E:171:GLN:OE1	2.09	0.53
1:A:406:GLU:HG3	1:B:375:LYS:O	2.09	0.53
1:B:330:ASN:O	1:B:332:LEU:HD13	2.08	0.53
1:F:439:GLU:C	1:F:441:GLY:N	2.62	0.53
1:C:557:SER:O	1:C:561:LYS:HG3	2.09	0.53
1:F:557:SER:O	1:F:561:LYS:HG3	2.09	0.53
1:A:557:SER:O	1:A:561:LYS:HG3	2.09	0.53
1:D:155:PRO:HB2	1:D:171:GLN:OE1	2.09	0.53
1:B:439:GLU:C	1:B:441:GLY:N	2.62	0.53
1:E:457:GLN:NE2	1:E:552:LEU:H	2.07	0.53
1:A:155:PRO:HB2	1:A:171:GLN:OE1	2.09	0.53
1:A:554:LYS:NZ	1:B:483:SER:O	2.38	0.53
1:C:483:SER:O	1:D:554:LYS:NZ	2.42	0.53
1:B:557:SER:O	1:B:561:LYS:HG3	2.09	0.52
1:E:392:THR:HG22	3:E:1004:HOH:O	2.09	0.52
1:C:157:THR:HB	1:C:159:GLY:N	2.21	0.52
1:C:468:ILE:N	1:C:473:ASN:HD21	2.05	0.52
1:C:146:ASN:C	1:C:146:ASN:HD22	2.11	0.52
1:A:338:CYS:HG	1:A:364:CYS:HG	0.83	0.52
1:D:157:THR:HB	1:D:159:GLY:N	2.21	0.52
1:F:439:GLU:HG3	1:F:441:GLY:N	2.25	0.52
1:A:457:GLN:NE2	1:A:552:LEU:H	2.07	0.52
1:A:479:ASP:HB3	1:A:519:THR:HB	1.90	0.52
1:E:557:SER:O	1:E:561:LYS:HG3	2.09	0.52
1:B:155:PRO:HB2	1:B:171:GLN:OE1	2.09	0.52
1:F:146:ASN:C	1:F:146:ASN:HD22	2.11	0.52
1:E:439:GLU:HG3	1:E:441:GLY:N	2.25	0.52
1:D:457:GLN:NE2	1:D:552:LEU:H	2.07	0.52
1:C:312:HIS:HD2	3:C:1289:HOH:O	1.93	0.52
1:B:468:ILE:N	1:B:473:ASN:HD21	2.05	0.52
1:A:312:HIS:HD2	3:A:1289:HOH:O	1.93	0.52
1:E:312:HIS:HD2	3:E:1289:HOH:O	1.93	0.52
1:E:444:GLY:HA3	1:E:452:ASN:HD21	1.75	0.52
1:E:182:ASP:OD1	1:F:664:THR:HG23	2.10	0.52
1:D:330:ASN:O	1:D:332:LEU:HD13	2.08	0.52
1:B:312:HIS:HD2	3:B:1289:HOH:O	1.93	0.52
1:D:146:ASN:C	1:D:146:ASN:HD22	2.11	0.52
1:D:547:GLN:NE2	1:D:640:THR:H	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:554:LYS:NZ	1:F:483:SER:O	2.41	0.52
1:A:146:ASN:C	1:A:146:ASN:HD22	2.11	0.52
1:E:468:ILE:H	1:E:473:ASN:ND2	2.08	0.51
1:A:573:VAL:HG11	1:A:598:MET:HE1	1.92	0.51
1:E:547:GLN:NE2	1:E:640:THR:H	2.08	0.51
1:F:444:GLY:HA3	1:F:452:ASN:HD21	1.75	0.51
1:F:547:GLN:NE2	1:F:640:THR:H	2.08	0.51
1:D:335:GLY:O	1:D:336:CYS:HB2	2.11	0.51
1:E:546:THR:HG22	1:F:546:THR:HG21	1.71	0.51
1:E:468:ILE:N	1:E:473:ASN:HD21	2.05	0.51
1:B:444:GLY:HA3	1:B:452:ASN:HD21	1.75	0.51
1:B:547:GLN:NE2	1:B:640:THR:H	2.08	0.51
1:D:439:GLU:HG3	1:D:441:GLY:N	2.25	0.51
1:B:457:GLN:NE2	1:B:552:LEU:H	2.07	0.51
1:A:157:THR:HB	1:A:159:GLY:N	2.21	0.51
1:A:439:GLU:HG3	1:A:441:GLY:N	2.25	0.51
1:C:457:GLN:NE2	1:C:552:LEU:H	2.07	0.51
1:A:547:GLN:NE2	1:A:640:THR:H	2.08	0.51
1:D:312:HIS:HD2	3:D:1289:HOH:O	1.93	0.51
3:A:1008:HOH:O	1:B:375:LYS:HE2	2.11	0.51
1:C:335:GLY:O	1:C:336:CYS:HB2	2.11	0.51
1:C:444:GLY:HA3	1:C:452:ASN:HD21	1.75	0.51
1:E:335:GLY:O	1:E:336:CYS:HB2	2.11	0.51
1:D:444:GLY:HA3	1:D:452:ASN:HD21	1.75	0.51
1:A:335:GLY:O	1:A:336:CYS:HB2	2.11	0.51
1:B:335:GLY:O	1:B:336:CYS:HB2	2.11	0.51
1:C:332:LEU:HD23	1:C:364:CYS:HB3	1.93	0.51
1:A:444:GLY:HA3	1:A:452:ASN:HD21	1.75	0.51
1:F:332:LEU:HD23	1:F:364:CYS:HB3	1.93	0.51
1:F:312:HIS:HD2	3:F:1289:HOH:O	1.93	0.51
1:E:332:LEU:HD23	1:E:364:CYS:HB3	1.93	0.51
1:D:468:ILE:H	1:D:473:ASN:ND2	2.08	0.51
1:C:439:GLU:HG3	1:C:441:GLY:N	2.25	0.51
1:B:598:MET:HE3	1:B:602:ILE:HG13	1.93	0.51
1:A:176:TYR:HB3	1:A:185:GLN:HB2	1.93	0.50
1:C:23:HIS:HD2	1:C:25:LEU:N	1.92	0.50
1:F:468:ILE:N	1:F:473:ASN:HD21	2.05	0.50
1:E:176:TYR:HB3	1:E:185:GLN:HB2	1.93	0.50
1:C:547:GLN:NE2	1:C:640:THR:H	2.08	0.50
1:F:335:GLY:O	1:F:336:CYS:HB2	2.10	0.50
1:A:330:ASN:HD22	1:B:375:LYS:HZ3	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:HD23	1:B:364:CYS:HB3	1.93	0.50
1:B:439:GLU:HG3	1:B:441:GLY:N	2.25	0.50
1:A:332:LEU:HD23	1:A:364:CYS:HB3	1.93	0.50
1:D:328[B]:MET:CE	3:D:1510:HOH:O	2.56	0.50
1:D:332:LEU:HD23	1:D:364:CYS:HB3	1.93	0.50
1:C:176:TYR:HB3	1:C:185:GLN:HB2	1.93	0.50
3:C:1008:HOH:O	1:D:375:LYS:HE2	2.11	0.49
1:E:494:TYR:CG	1:F:313:GLN:HG2	2.42	0.49
1:B:23:HIS:HD2	1:B:25:LEU:N	1.92	0.49
1:F:176:TYR:HB3	1:F:185:GLN:HB2	1.93	0.49
1:D:176:TYR:HB3	1:D:185:GLN:HB2	1.93	0.49
1:A:414:MET:HE2	1:A:420:ARG:HB2	1.93	0.49
1:F:262:SER:O	1:F:263:ASN:HB2	2.13	0.49
1:E:406:GLU:HG3	1:F:375:LYS:O	2.12	0.49
1:F:457:GLN:NE2	1:F:552:LEU:H	2.07	0.49
1:C:414:MET:HE2	1:C:420:ARG:HB2	1.94	0.49
1:C:468:ILE:H	1:C:473:ASN:ND2	2.08	0.49
1:B:176:TYR:HB3	1:B:185:GLN:HB2	1.93	0.49
1:B:211:ARG:CD	1:B:211:ARG:N	2.60	0.49
1:C:375:LYS:HE2	3:D:1008:HOH:O	2.12	0.49
1:A:449:PRO:HD3	1:B:534:TYR:CE1	2.48	0.49
1:E:23:HIS:HD2	1:E:25:LEU:N	1.92	0.49
1:B:262:SER:O	1:B:263:ASN:HB2	2.13	0.49
1:E:664:THR:HG23	1:F:182:ASP:OD1	2.13	0.48
1:D:405:TPQ:H3	3:D:1053:HOH:O	2.13	0.48
1:D:262:SER:O	1:D:263:ASN:HB2	2.13	0.48
1:E:262:SER:O	1:E:263:ASN:HB2	2.13	0.48
1:F:468:ILE:H	1:F:473:ASN:ND2	2.08	0.48
1:C:262:SER:O	1:C:263:ASN:HB2	2.13	0.48
1:F:405:TPQ:H3	3:F:1053:HOH:O	2.13	0.48
1:D:23:HIS:HD2	1:D:25:LEU:N	1.92	0.48
1:E:144:PRO:HB2	1:E:146:ASN:ND2	2.29	0.48
1:A:144:PRO:HB2	1:A:146:ASN:ND2	2.29	0.48
1:E:405:TPQ:H3	3:E:1053:HOH:O	2.13	0.48
1:C:144:PRO:HB2	1:C:146:ASN:ND2	2.29	0.48
1:C:554:LYS:NZ	1:D:483:SER:O	2.45	0.48
1:E:301:MET:O	1:E:318:LEU:HA	2.14	0.48
1:E:414:MET:HE2	1:E:420:ARG:HB2	1.95	0.48
1:F:144:PRO:HB2	1:F:146:ASN:ND2	2.29	0.48
1:D:301:MET:O	1:D:318:LEU:HA	2.14	0.48
1:F:301:MET:O	1:F:318:LEU:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ARG:N	1:D:211:ARG:CD	2.60	0.48
1:A:330:ASN:HD22	1:B:375:LYS:NZ	2.11	0.48
1:A:262:SER:O	1:A:263:ASN:HB2	2.13	0.48
1:A:405:TPQ:H3	3:A:1053:HOH:O	2.13	0.48
1:F:23:HIS:HD2	1:F:25:LEU:N	1.92	0.47
1:A:598:MET:CE	1:A:602:ILE:HG13	2.44	0.47
1:B:405:TPQ:H3	3:B:1053:HOH:O	2.13	0.47
1:C:598:MET:CE	1:C:602:ILE:HG13	2.44	0.47
1:C:405:TPQ:H3	3:C:1053:HOH:O	2.13	0.47
1:F:598:MET:CE	1:F:602:ILE:HG13	2.45	0.47
1:A:656:ASP:O	1:B:236:ARG:HG3	2.14	0.47
1:D:69:GLU:CD	1:D:467:ARG:HH22	2.18	0.47
1:B:69:GLU:CD	1:B:467:ARG:HH22	2.18	0.47
1:C:69:GLU:CD	1:C:467:ARG:HH22	2.18	0.47
1:A:633:LEU:HD13	1:B:374:PHE:CD1	2.49	0.47
1:E:598:MET:CE	1:E:602:ILE:HG13	2.44	0.47
1:A:664:THR:HG23	1:B:182:ASP:CG	2.34	0.47
1:A:328[B]:MET:CE	3:A:1510:HOH:O	2.56	0.47
1:E:581:TYR:HA	1:E:582:PRO:HD2	1.77	0.47
3:E:1008:HOH:O	1:F:375:LYS:HE2	2.14	0.47
1:C:328[B]:MET:CE	3:C:1510:HOH:O	2.56	0.47
1:D:144:PRO:HB2	1:D:146:ASN:ND2	2.29	0.47
1:B:301:MET:O	1:B:318:LEU:HA	2.14	0.47
1:C:301:MET:O	1:C:318:LEU:HA	2.14	0.47
1:B:468:ILE:H	1:B:473:ASN:ND2	2.08	0.47
1:A:69:GLU:CD	1:A:467:ARG:HH22	2.18	0.47
1:B:598:MET:CE	1:B:602:ILE:HG13	2.44	0.47
1:D:598:MET:CE	1:D:602:ILE:HG13	2.45	0.47
1:E:69:GLU:CD	1:E:467:ARG:HH22	2.18	0.47
1:C:546:THR:HG21	1:D:546:THR:HG22	1.71	0.47
1:B:144:PRO:HB2	1:B:146:ASN:ND2	2.29	0.47
1:C:244:VAL:HG22	1:D:244:VAL:HG22	1.96	0.47
1:A:301:MET:O	1:A:318:LEU:HA	2.14	0.46
1:D:527:ASN:HD21	1:D:529:ASN:HD22	1.64	0.46
1:E:527:ASN:HD21	1:E:529:ASN:HD22	1.64	0.46
1:B:527:ASN:HD21	1:B:529:ASN:HD22	1.63	0.46
1:A:527:ASN:HD21	1:A:529:ASN:HD22	1.64	0.46
1:F:527:ASN:HD21	1:F:529:ASN:HD22	1.64	0.46
1:F:69:GLU:CD	1:F:467:ARG:HH22	2.18	0.46
1:C:581:TYR:HA	1:C:582:PRO:HD2	1.77	0.46
1:A:468:ILE:H	1:A:473:ASN:ND2	2.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:GLU:HG3	1:F:441:GLY:HA2	1.98	0.46
1:C:439:GLU:HG3	1:C:441:GLY:HA2	1.98	0.46
1:C:573:VAL:HG11	1:C:598:MET:HE1	1.98	0.46
1:F:573:VAL:HG11	1:F:598:MET:HE1	1.97	0.46
1:B:439:GLU:HG3	1:B:441:GLY:HA2	1.98	0.46
1:B:185:GLN:HG2	3:B:1266:HOH:O	2.16	0.46
1:E:656:ASP:O	1:F:236:ARG:HG3	2.16	0.46
1:F:68:LYS:HE2	1:F:280:ASP:OD2	2.16	0.46
1:A:375:LYS:HE2	3:B:1008:HOH:O	2.14	0.46
1:F:414:MET:HE2	1:F:420:ARG:HB2	1.96	0.46
1:C:375:LYS:O	1:D:406:GLU:HG3	2.15	0.46
1:A:244:VAL:HG22	1:B:244:VAL:HG22	1.97	0.46
1:C:344:TYR:CD1	1:C:361:ASN:HB3	2.51	0.46
1:C:374:PHE:CD1	1:D:633:LEU:HD13	2.51	0.46
1:A:185:GLN:HG2	3:A:1266:HOH:O	2.16	0.46
1:D:185:GLN:HG2	3:D:1266:HOH:O	2.16	0.46
1:E:449:PRO:HD3	1:F:534:TYR:CE1	2.52	0.46
1:C:68:LYS:HE2	1:C:280:ASP:OD2	2.16	0.46
1:F:344:TYR:CD1	1:F:361:ASN:HB3	2.51	0.46
1:B:344:TYR:CD1	1:B:361:ASN:HB3	2.51	0.46
1:C:185:GLN:HG2	3:C:1266:HOH:O	2.16	0.45
1:D:598:MET:HE3	1:D:602:ILE:HG13	1.97	0.45
1:C:633:LEU:HD13	1:D:374:PHE:CD1	2.51	0.45
1:A:23:HIS:HD2	1:A:25:LEU:N	1.92	0.45
1:F:185:GLN:HG2	3:F:1266:HOH:O	2.16	0.45
1:A:344:TYR:CD1	1:A:361:ASN:HB3	2.51	0.45
1:A:598:MET:HE2	1:A:602:ILE:HG13	1.98	0.45
1:E:68:LYS:HE2	1:E:280:ASP:OD2	2.16	0.45
1:E:633:LEU:HD13	1:F:374:PHE:CD1	2.51	0.45
1:B:414:MET:HE2	1:B:420:ARG:HB2	1.97	0.45
1:D:218:HIS:CE1	1:D:450:ASN:ND2	2.85	0.45
1:D:344:TYR:CD1	1:D:361:ASN:HB3	2.51	0.45
1:E:344:TYR:CD1	1:E:361:ASN:HB3	2.51	0.45
1:C:218:HIS:CE1	1:C:450:ASN:ND2	2.85	0.45
1:C:527:ASN:HD21	1:C:529:ASN:HD22	1.64	0.45
1:E:328[B]:MET:CE	3:E:1510:HOH:O	2.56	0.45
1:F:218:HIS:CE1	1:F:450:ASN:ND2	2.85	0.45
1:B:50:SER:HB2	1:B:352:ARG:CG	2.47	0.45
1:E:439:GLU:HG3	1:E:441:GLY:HA2	1.98	0.45
1:C:146:ASN:C	1:C:146:ASN:ND2	2.71	0.45
1:A:146:ASN:C	1:A:146:ASN:ND2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:573:VAL:HG11	1:E:598:MET:HE1	1.98	0.45
1:B:218:HIS:CE1	1:B:450:ASN:ND2	2.85	0.45
1:F:50:SER:HB2	1:F:352:ARG:CG	2.47	0.45
1:B:68:LYS:HE2	1:B:280:ASP:OD2	2.16	0.45
1:B:392:THR:CG2	3:B:1004:HOH:O	2.61	0.45
1:E:146:ASN:C	1:E:146:ASN:ND2	2.71	0.45
1:D:146:ASN:ND2	1:D:146:ASN:C	2.70	0.45
1:E:573:VAL:HG11	1:E:598:MET:CE	2.47	0.45
1:D:50:SER:HB2	1:D:352:ARG:CG	2.47	0.45
1:A:494:TYR:CG	1:B:313:GLN:HG2	2.46	0.44
1:A:573:VAL:HG11	1:A:598:MET:CE	2.47	0.44
1:E:218:HIS:CE1	1:E:450:ASN:ND2	2.85	0.44
1:A:68:LYS:HE2	1:A:280:ASP:OD2	2.16	0.44
1:E:330:ASN:HD22	1:F:375:LYS:NZ	2.14	0.44
1:D:439:GLU:HG3	1:D:441:GLY:HA2	1.98	0.44
1:F:392:THR:CG2	3:F:1004:HOH:O	2.64	0.44
1:B:146:ASN:C	1:B:146:ASN:ND2	2.70	0.44
1:E:669:LYS:NZ	1:F:181:GLU:OE1	2.39	0.44
1:D:414:MET:HE2	1:D:420:ARG:HB2	1.99	0.44
1:C:330:ASN:HD22	1:D:375:LYS:HZ3	1.64	0.44
1:C:50:SER:HB2	1:C:352:ARG:CG	2.47	0.44
1:C:330:ASN:HD22	1:D:375:LYS:NZ	2.16	0.44
1:D:68:LYS:HE2	1:D:280:ASP:OD2	2.16	0.44
1:A:439:GLU:HG3	1:A:441:GLY:HA2	1.98	0.44
1:C:146:ASN:HD22	1:C:147:GLU:N	2.16	0.44
1:B:573:VAL:HG11	1:B:598:MET:CE	2.47	0.44
1:E:565:TRP:CD1	1:E:582:PRO:HB2	2.53	0.44
1:D:581:TYR:HA	1:D:582:PRO:HD2	1.77	0.44
1:F:458:HIS:O	1:F:621:GLY:HA3	2.18	0.44
1:E:50:SER:HB2	1:E:352:ARG:CG	2.47	0.44
1:A:218:HIS:CE1	1:A:450:ASN:ND2	2.85	0.44
1:F:146:ASN:ND2	1:F:146:ASN:C	2.70	0.44
1:D:146:ASN:HD22	1:D:147:GLU:N	2.16	0.44
1:A:146:ASN:HD22	1:A:147:GLU:N	2.16	0.44
1:E:185:GLN:HG2	3:E:1266:HOH:O	2.16	0.44
1:F:573:VAL:HG11	1:F:598:MET:CE	2.47	0.44
1:D:565:TRP:CD1	1:D:582:PRO:HB2	2.53	0.44
1:B:452:ASN:HD22	1:B:453:ALA:N	2.16	0.44
1:A:565:TRP:CD1	1:A:582:PRO:HB2	2.53	0.44
1:A:50:SER:HB2	1:A:352:ARG:CG	2.47	0.44
1:C:311:PRO:CA	1:C:313:GLN:NE2	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:ASN:ND2	1:F:147:GLU:HG3	2.33	0.44
1:C:573:VAL:HG11	1:C:598:MET:CE	2.47	0.44
1:F:565:TRP:CD1	1:F:582:PRO:HB2	2.53	0.44
1:D:458:HIS:O	1:D:621:GLY:HA3	2.18	0.44
1:A:546:THR:HG22	1:B:546:THR:HG21	1.73	0.44
1:E:452:ASN:HD22	1:E:453:ALA:N	2.16	0.44
1:F:452:ASN:HD22	1:F:453:ALA:N	2.16	0.44
1:D:120:ASP:OD2	1:D:352:ARG:NH2	2.43	0.44
1:C:182:ASP:CG	1:D:664:THR:HG23	2.38	0.43
1:E:157:THR:CB	1:E:159:GLY:H	2.27	0.43
1:E:375:LYS:HE2	3:F:1008:HOH:O	2.18	0.43
1:A:392:THR:HG23	1:A:415:GLN:OE1	2.18	0.43
1:A:146:ASN:ND2	1:A:147:GLU:HG3	2.33	0.43
1:D:452:ASN:HD22	1:D:453:ALA:N	2.16	0.43
1:A:452:ASN:HD22	1:A:453:ALA:N	2.16	0.43
1:B:234:ALA:HB1	3:B:1231:HOH:O	2.17	0.43
1:C:458:HIS:O	1:C:621:GLY:HA3	2.18	0.43
1:C:375:LYS:NZ	1:D:330:ASN:HD22	2.15	0.43
1:F:392:THR:HG23	1:F:415:GLN:OE1	2.18	0.43
1:E:146:ASN:ND2	1:E:147:GLU:HG3	2.33	0.43
1:C:146:ASN:ND2	1:C:147:GLU:HG3	2.33	0.43
1:D:573:VAL:HG11	1:D:598:MET:HE1	2.00	0.43
1:B:294:HIS:HD2	3:B:1287:HOH:O	2.01	0.43
1:E:392:THR:HG23	1:E:415:GLN:OE1	2.18	0.43
1:F:146:ASN:HD22	1:F:147:GLU:N	2.16	0.43
1:F:581:TYR:HA	1:F:582:PRO:HD2	1.77	0.43
1:D:369:ASP:OD1	1:D:390:ARG:NH1	2.52	0.43
1:F:382:ASN:ND2	3:F:1071:HOH:O	2.50	0.43
1:A:669:LYS:NZ	1:B:181:GLU:OE1	2.35	0.43
1:A:23:HIS:HA	1:A:24:PRO:HD3	1.91	0.43
1:C:303:VAL:HA	1:C:457:GLN:O	2.19	0.43
1:E:303:VAL:HA	1:E:457:GLN:O	2.19	0.43
1:B:146:ASN:ND2	1:B:147:GLU:HG3	2.33	0.43
1:A:369:ASP:OD1	1:A:390:ARG:NH1	2.52	0.43
1:B:458:HIS:O	1:B:621:GLY:HA3	2.18	0.43
1:B:290:ARG:HA	1:B:291:PRO:HD3	1.90	0.43
1:C:369:ASP:OD1	1:C:390:ARG:NH1	2.52	0.43
1:C:406:GLU:HG3	1:D:375:LYS:O	2.18	0.43
1:A:303:VAL:HA	1:A:457:GLN:O	2.19	0.43
1:E:146:ASN:HD22	1:E:147:GLU:N	2.16	0.43
1:D:573:VAL:HG11	1:D:598:MET:CE	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:634:MET:HA	1:F:635:PRO:HD3	1.83	0.43
1:F:221:ALA:HA	3:F:1210:HOH:O	2.19	0.43
1:B:303:VAL:HA	1:B:457:GLN:O	2.19	0.43
1:C:392:THR:CG2	3:C:1004:HOH:O	2.63	0.43
1:D:392:THR:HG23	1:D:415:GLN:OE1	2.18	0.43
1:C:66[B]:GLN:HE21	1:C:72:GLY:HA3	1.84	0.43
1:B:146:ASN:HD22	1:B:147:GLU:N	2.16	0.43
1:D:146:ASN:ND2	1:D:147:GLU:HG3	2.33	0.43
1:A:458:HIS:O	1:A:621:GLY:HA3	2.18	0.43
1:F:369:ASP:OD1	1:F:390:ARG:NH1	2.52	0.43
1:F:66[B]:GLN:HE21	1:F:72:GLY:HA3	1.84	0.43
1:C:452:ASN:HD22	1:C:453:ALA:N	2.16	0.43
1:E:294:HIS:HD2	3:E:1287:HOH:O	2.01	0.43
1:D:221:ALA:HA	3:D:1210:HOH:O	2.19	0.43
1:E:244:VAL:HG22	1:F:244:VAL:HG22	2.00	0.43
1:E:66[B]:GLN:HE21	1:E:72:GLY:HA3	1.84	0.43
1:D:373:LEU:HD12	1:D:373:LEU:HA	1.88	0.43
1:E:140:LEU:HD12	1:E:140:LEU:HA	1.86	0.43
1:A:176:TYR:CE1	1:A:189:PRO:HB3	2.54	0.43
1:E:458:HIS:O	1:E:621:GLY:HA3	2.18	0.43
1:B:565:TRP:CD1	1:B:582:PRO:HB2	2.53	0.43
1:F:303:VAL:HA	1:F:457:GLN:O	2.19	0.43
1:D:66[B]:GLN:HE21	1:D:72:GLY:HA3	1.84	0.43
1:B:66[B]:GLN:HE21	1:B:72:GLY:HA3	1.84	0.43
1:B:581:TYR:HA	1:B:582:PRO:HD2	1.77	0.43
1:D:294:HIS:HD2	3:D:1287:HOH:O	2.01	0.43
1:A:294:HIS:HD2	3:A:1287:HOH:O	2.01	0.43
1:C:385:THR:OG1	1:C:665:THR:HA	2.19	0.43
1:F:311:PRO:CA	1:F:313:GLN:NE2	2.75	0.42
1:C:23:HIS:HA	1:C:24:PRO:HD3	1.91	0.42
1:C:221:ALA:HA	3:C:1210:HOH:O	2.19	0.42
1:F:294:HIS:HD2	3:F:1287:HOH:O	2.01	0.42
1:A:385:THR:OG1	1:A:665:THR:HA	2.19	0.42
1:B:439:GLU:HG3	1:B:441:GLY:CA	2.50	0.42
1:C:646:ARG:O	1:C:647:HIS:HB2	2.20	0.42
1:E:310:PHE:HA	1:E:313:GLN:HE21	1.85	0.42
1:A:311:PRO:CA	1:A:313:GLN:NE2	2.75	0.42
1:C:310:PHE:HA	1:C:313:GLN:HE21	1.85	0.42
1:C:439:GLU:HG3	1:C:441:GLY:CA	2.50	0.42
1:B:392:THR:HG23	1:B:415:GLN:OE1	2.18	0.42
1:A:270:PHE:HA	1:A:275:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:THR:CB	1:C:159:GLY:H	2.27	0.42
1:A:439:GLU:HG3	1:A:441:GLY:CA	2.50	0.42
1:C:176:TYR:CE1	1:C:189:PRO:HB3	2.54	0.42
1:D:176:TYR:CE1	1:D:189:PRO:HB3	2.54	0.42
1:C:565:TRP:CD1	1:C:582:PRO:HB2	2.53	0.42
1:E:53:THR:O	1:E:81:TYR:HA	2.20	0.42
1:F:53:THR:O	1:F:81:TYR:HA	2.20	0.42
1:D:303:VAL:HA	1:D:457:GLN:O	2.19	0.42
1:C:392:THR:HG23	1:C:415:GLN:OE1	2.18	0.42
1:E:176:TYR:CE1	1:E:189:PRO:HB3	2.54	0.42
1:F:176:TYR:CE1	1:F:189:PRO:HB3	2.54	0.42
1:E:369:ASP:OD1	1:E:390:ARG:NH1	2.52	0.42
1:D:128:ILE:HG13	1:D:129:ARG:N	2.35	0.42
1:E:221:ALA:HA	3:E:1210:HOH:O	2.19	0.42
1:B:646:ARG:O	1:B:647:HIS:HB2	2.20	0.42
1:D:53:THR:O	1:D:81:TYR:HA	2.20	0.42
1:E:646:ARG:O	1:E:647:HIS:HB2	2.20	0.42
1:A:374:PHE:CD1	1:B:633:LEU:HD13	2.54	0.42
1:D:270:PHE:HA	1:D:275:GLY:O	2.20	0.42
1:D:439:GLU:HG3	1:D:441:GLY:CA	2.49	0.42
1:C:598:MET:HE3	1:C:602:ILE:HG13	2.01	0.42
1:D:385:THR:OG1	1:D:665:THR:HA	2.19	0.42
1:B:385:THR:OG1	1:B:665:THR:HA	2.19	0.42
1:E:385:THR:OG1	1:E:665:THR:HA	2.19	0.42
1:F:124:THR:O	1:F:127:VAL:HG13	2.20	0.42
1:B:128:ILE:HG13	1:B:129:ARG:N	2.35	0.42
1:A:66[B]:GLN:HE21	1:A:72:GLY:HA3	1.84	0.42
1:E:598:MET:O	1:E:598:MET:HE3	2.20	0.42
1:E:120:ASP:OD2	1:E:352:ARG:NH2	2.43	0.42
1:A:581:TYR:HA	1:A:582:PRO:HD2	1.77	0.42
1:B:645:PRO:O	1:B:646:ARG:HD2	2.20	0.42
1:E:345:LEU:HB2	1:E:363:VAL:HB	2.02	0.42
1:A:425:LEU:HB3	3:A:1499:HOH:O	2.20	0.42
1:E:197:ASP:CG	1:E:200:GLU:HB2	2.40	0.42
1:A:345:LEU:HB2	1:A:363:VAL:HB	2.02	0.42
1:B:369:ASP:OD1	1:B:390:ARG:NH1	2.52	0.42
1:A:175:VAL:HG11	1:A:190:LEU:HD12	2.02	0.42
1:C:175:VAL:HG11	1:C:190:LEU:HD12	2.02	0.42
1:A:197:ASP:CG	1:A:200:GLU:HB2	2.40	0.42
1:E:664:THR:HG23	1:F:182:ASP:CG	2.40	0.42
1:E:330:ASN:HD22	1:F:375:LYS:HZ3	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:TYR:CE1	1:B:189:PRO:HB3	2.54	0.42
1:D:598:MET:HE3	1:D:598:MET:O	2.20	0.42
1:B:221:ALA:HA	3:B:1210:HOH:O	2.19	0.42
1:D:124:THR:O	1:D:127:VAL:HG13	2.20	0.42
1:F:385:THR:OG1	1:F:665:THR:HA	2.19	0.42
1:A:128:ILE:HG13	1:A:129:ARG:N	2.35	0.42
1:B:270:PHE:HA	1:B:275:GLY:O	2.20	0.42
1:C:558:LEU:HA	1:C:558:LEU:HD23	1.88	0.42
1:D:646:ARG:O	1:D:647:HIS:HB2	2.20	0.42
1:F:439:GLU:HG3	1:F:441:GLY:CA	2.50	0.41
1:E:312:HIS:HE1	3:E:1060:HOH:O	2.03	0.41
1:F:598:MET:HE3	1:F:602:ILE:HG13	2.02	0.41
1:B:53:THR:O	1:B:81:TYR:HA	2.20	0.41
1:A:221:ALA:HA	3:A:1210:HOH:O	2.19	0.41
1:E:375:LYS:HG2	1:E:376:HIS:N	2.35	0.41
1:B:573:VAL:HG11	1:B:598:MET:HE1	2.03	0.41
1:C:598:MET:HE3	1:C:598:MET:O	2.20	0.41
1:E:598:MET:HE3	1:E:602:ILE:HG13	2.01	0.41
1:D:645:PRO:O	1:D:646:ARG:HD2	2.20	0.41
1:A:475:ALA:HA	1:A:524:ASP:O	2.21	0.41
1:B:425:LEU:HB3	3:B:1499:HOH:O	2.20	0.41
1:E:483:SER:O	1:F:554:LYS:NZ	2.51	0.41
1:A:53:THR:O	1:A:81:TYR:HA	2.20	0.41
1:A:483:SER:O	1:B:554:LYS:NZ	2.53	0.41
1:D:475:ALA:HA	1:D:524:ASP:O	2.21	0.41
1:C:290:ARG:HA	1:C:291:PRO:HD3	1.90	0.41
1:B:310:PHE:HA	1:B:313:GLN:HE21	1.85	0.41
1:F:375:LYS:HG2	1:F:376:HIS:N	2.35	0.41
1:E:645:PRO:O	1:E:646:ARG:HD2	2.20	0.41
1:C:124:THR:O	1:C:127:VAL:HG13	2.20	0.41
1:A:124:THR:O	1:A:127:VAL:HG13	2.20	0.41
1:A:646:ARG:O	1:A:647:HIS:HB2	2.20	0.41
1:E:475:ALA:HA	1:E:524:ASP:O	2.21	0.41
1:C:294:HIS:HD2	3:C:1287:HOH:O	2.01	0.41
1:F:425:LEU:HB3	3:F:1499:HOH:O	2.20	0.41
1:E:439:GLU:HG3	1:E:441:GLY:CA	2.50	0.41
1:F:598:MET:O	1:F:598:MET:HE3	2.20	0.41
1:D:290:ARG:HA	1:D:291:PRO:HD3	1.90	0.41
1:D:345:LEU:HB2	1:D:363:VAL:HB	2.02	0.41
1:C:346:ASP:OD2	1:C:360:LYS:HE3	2.21	0.41
1:A:558:LEU:HD23	1:A:558:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:ALA:HA	1:C:524:ASP:O	2.21	0.41
1:E:311:PRO:CA	1:E:313:GLN:NE2	2.75	0.41
1:C:312:HIS:HE1	3:C:1060:HOH:O	2.03	0.41
1:F:120:ASP:OD2	1:F:352:ARG:NH2	2.43	0.41
1:E:270:PHE:HA	1:E:275:GLY:O	2.20	0.41
1:F:270:PHE:HA	1:F:275:GLY:O	2.20	0.41
1:D:197:ASP:CG	1:D:200:GLU:HB2	2.40	0.41
1:C:345:LEU:HB2	1:C:363:VAL:HB	2.02	0.41
1:C:270:PHE:HA	1:C:275:GLY:O	2.20	0.41
1:C:375:LYS:HG2	1:C:376:HIS:N	2.35	0.41
1:A:645:PRO:O	1:A:646:ARG:HD2	2.20	0.41
1:B:382:ASN:ND2	3:B:1071:HOH:O	2.48	0.41
1:B:197:ASP:CG	1:B:200:GLU:HB2	2.40	0.41
1:F:345:LEU:HB2	1:F:363:VAL:HB	2.02	0.41
1:F:157:THR:CB	1:F:159:GLY:H	2.27	0.41
1:C:527:ASN:ND2	1:C:527:ASN:C	2.73	0.41
1:B:598:MET:O	1:B:598:MET:HE3	2.20	0.41
1:C:197:ASP:CG	1:C:200:GLU:HB2	2.40	0.41
1:E:124:THR:O	1:E:127:VAL:HG13	2.20	0.41
1:D:375:LYS:HG2	1:D:376:HIS:N	2.35	0.41
1:B:312:HIS:HE1	3:B:1060:HOH:O	2.03	0.41
1:F:645:PRO:O	1:F:646:ARG:HD2	2.20	0.41
1:F:175:VAL:HG11	1:F:190:LEU:HD12	2.02	0.41
1:F:475:ALA:HA	1:F:524:ASP:O	2.20	0.41
1:C:348:HIS:HD2	3:C:1460:HOH:O	2.04	0.41
1:B:124:THR:O	1:B:127:VAL:HG13	2.20	0.41
1:D:310:PHE:HA	1:D:313:GLN:HE21	1.85	0.41
1:A:406:GLU:CD	1:B:376:HIS:HA	2.40	0.41
1:B:157:THR:CB	1:B:159:GLY:H	2.27	0.41
1:A:598:MET:O	1:A:598:MET:HE3	2.21	0.41
1:F:312:HIS:HE1	3:F:1060:HOH:O	2.03	0.41
1:F:646:ARG:O	1:F:647:HIS:HB2	2.20	0.41
1:C:128:ILE:HG13	1:C:129:ARG:N	2.35	0.41
1:C:53:THR:O	1:C:81:TYR:HA	2.20	0.41
1:A:346:ASP:OD2	1:A:360:LYS:HE3	2.21	0.41
1:E:374:PHE:CD1	1:F:633:LEU:HD13	2.55	0.41
1:F:197:ASP:CG	1:F:200:GLU:HB2	2.40	0.41
1:B:175:VAL:HG11	1:B:190:LEU:HD12	2.02	0.41
1:C:375:LYS:HZ3	1:D:330:ASN:HD22	1.69	0.41
1:A:312:HIS:HE1	3:A:1060:HOH:O	2.03	0.41
1:C:645:PRO:O	1:C:646:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:HB2	1:B:363:VAL:HB	2.02	0.41
1:F:131:ASP:HA	1:F:132:PRO:HD3	1.97	0.41
1:B:475:ALA:HA	1:B:524:ASP:O	2.20	0.41
1:F:23:HIS:HA	1:F:24:PRO:HD3	1.91	0.40
1:E:406:GLU:HG2	1:E:427:GLY:CA	2.51	0.40
1:B:70:GLN:HA	1:B:70:GLN:NE2	2.36	0.40
1:D:392:THR:CG2	3:D:1004:HOH:O	2.65	0.40
1:E:50:SER:HB2	1:E:352:ARG:HG3	2.03	0.40
1:F:234:ALA:HB1	3:F:1231:HOH:O	2.21	0.40
1:E:175:VAL:HG11	1:E:190:LEU:HD12	2.02	0.40
1:D:23:HIS:CD2	1:D:24:PRO:HD2	2.57	0.40
1:B:375:LYS:HG2	1:B:376:HIS:N	2.35	0.40
1:C:406:GLU:HG2	1:C:427:GLY:CA	2.51	0.40
1:D:121:LEU:HD12	1:D:328[B]:MET:HE1	2.03	0.40
1:B:406:GLU:HG2	1:B:427:GLY:CA	2.52	0.40
1:F:348:HIS:HD2	3:F:1460:HOH:O	2.04	0.40
1:A:23:HIS:CD2	1:A:24:PRO:HD2	2.57	0.40
1:D:312:HIS:HE1	3:D:1060:HOH:O	2.03	0.40
1:B:23:HIS:CD2	1:B:24:PRO:HD2	2.57	0.40
1:D:23:HIS:HA	1:D:24:PRO:HD3	1.91	0.40
1:C:664:THR:HG23	1:D:182:ASP:CG	2.41	0.40
1:E:191:ASP:OD1	1:E:212:ARG:NH1	2.55	0.40
1:D:50:SER:HB2	1:D:352:ARG:HG3	2.03	0.40
1:B:346:ASP:OD2	1:B:360:LYS:HE3	2.21	0.40
1:D:425:LEU:HB3	3:D:1499:HOH:O	2.20	0.40
1:F:75:PRO:HA	1:F:76:PRO:HD3	1.97	0.40
1:D:346:ASP:OD2	1:D:360:LYS:HE3	2.21	0.40
1:D:175:VAL:HG11	1:D:190:LEU:HD12	2.02	0.40
1:F:346:ASP:OD2	1:F:360:LYS:HE3	2.21	0.40
1:C:313:GLN:HG2	1:D:494:TYR:CG	2.52	0.40
1:C:70:GLN:HA	1:C:70:GLN:NE2	2.36	0.40
1:B:348:HIS:HD2	3:B:1460:HOH:O	2.04	0.40
1:E:128:ILE:HG13	1:E:129:ARG:N	2.35	0.40
1:A:290:ARG:HA	1:A:291:PRO:HD3	1.90	0.40
1:E:348:HIS:HD2	3:E:1460:HOH:O	2.04	0.40

All (4) 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:B:20:ARG:CZ	1:E:70:GLN:OE1[4_455]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:CZ	1:D:70:GLN:OE1[4_555]	2.10	0.10
1:A:66[B]:GLN:OE1	3:D:1255:HOH:O[4_555]	2.18	0.02
1:A:20:ARG:NH1	1:D:70:GLN:OE1[4_555]	2.19	0.01

## 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	654/692 (94%)	619 (95%)	34 (5%)	1 (0%)	52	75
1	B	654/692 (94%)	619 (95%)	34 (5%)	1 (0%)	52	75
1	C	654/692 (94%)	619 (95%)	34 (5%)	1 (0%)	52	75
1	D	654/692 (94%)	619 (95%)	34 (5%)	1 (0%)	52	75
1	E	654/692 (94%)	619 (95%)	34 (5%)	1 (0%)	52	75
1	F	654/692 (94%)	619 (95%)	34 (5%)	1 (0%)	52	75
All	All	3924/4152 (94%)	3714 (95%)	204 (5%)	6 (0%)	52	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	GLU
1	B	200	GLU
1	C	200	GLU
1	D	200	GLU
1	E	200	GLU
1	F	200	GLU

### 5.3.2 Protein sidechains [i](#)

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	566/592 (96%)	533 (94%)	33 (6%)	25	45
1	B	566/592 (96%)	533 (94%)	33 (6%)	25	45
1	C	566/592 (96%)	533 (94%)	33 (6%)	25	45
1	D	566/592 (96%)	533 (94%)	33 (6%)	25	45
1	E	566/592 (96%)	533 (94%)	33 (6%)	25	45
1	F	566/592 (96%)	533 (94%)	33 (6%)	25	45
All	All	3396/3552 (96%)	3198 (94%)	198 (6%)	24	45

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	68	LYS
1	A	69	GLU
1	A	109	LEU
1	A	112	VAL
1	A	114	PRO
1	A	127	VAL
1	A	140	LEU
1	A	146	ASN
1	A	157	THR
1	A	170	LEU
1	A	211	ARG
1	A	215	VAL
1	A	311	PRO
1	A	313	GLN
1	A	329	THR
1	A	332	LEU
1	A	359	VAL
1	A	364	CYS
1	A	392	THR
1	A	394	LEU
1	A	421	LEU
1	A	452	ASN
1	A	462	LEU
1	A	466	PRO
1	A	487	LEU
1	A	504	THR

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Mol	Chain	Res	Type
1	A	507	THR
1	A	527	ASN
1	A	546	THR
1	A	633	LEU
1	A	641	LEU
1	A	664	THR
1	B	48	LYS
1	B	68	LYS
1	B	69	GLU
1	B	109	LEU
1	B	112	VAL
1	B	114	PRO
1	B	127	VAL
1	B	140	LEU
1	B	146	ASN
1	B	157	THR
1	B	170	LEU
1	B	211	ARG
1	B	215	VAL
1	B	311	PRO
1	B	313	GLN
1	B	329	THR
1	B	332	LEU
1	B	359	VAL
1	B	364	CYS
1	B	392	THR
1	B	394	LEU
1	B	421	LEU
1	B	452	ASN
1	B	462	LEU
1	B	466	PRO
1	B	487	LEU
1	B	504	THR
1	B	507	THR
1	B	527	ASN
1	B	546	THR
1	B	633	LEU
1	B	641	LEU
1	B	664	THR
1	C	48	LYS
1	C	68	LYS
1	C	69	GLU

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Mol	Chain	Res	Type
1	C	109	LEU
1	C	112	VAL
1	C	114	PRO
1	C	127	VAL
1	C	140	LEU
1	C	146	ASN
1	C	157	THR
1	C	170	LEU
1	C	211	ARG
1	C	215	VAL
1	C	311	PRO
1	C	313	GLN
1	C	329	THR
1	C	332	LEU
1	C	359	VAL
1	C	364	CYS
1	C	392	THR
1	C	394	LEU
1	C	421	LEU
1	C	452	ASN
1	C	462	LEU
1	C	466	PRO
1	C	487	LEU
1	C	504	THR
1	C	507	THR
1	C	527	ASN
1	C	546	THR
1	C	633	LEU
1	C	641	LEU
1	C	664	THR
1	D	48	LYS
1	D	68	LYS
1	D	69	GLU
1	D	109	LEU
1	D	112	VAL
1	D	114	PRO
1	D	127	VAL
1	D	140	LEU
1	D	146	ASN
1	D	157	THR
1	D	170	LEU
1	D	211	ARG

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Mol	Chain	Res	Type
1	D	215	VAL
1	D	311	PRO
1	D	313	GLN
1	D	329	THR
1	D	332	LEU
1	D	359	VAL
1	D	364	CYS
1	D	392	THR
1	D	394	LEU
1	D	421	LEU
1	D	452	ASN
1	D	462	LEU
1	D	466	PRO
1	D	487	LEU
1	D	504	THR
1	D	507	THR
1	D	527	ASN
1	D	546	THR
1	D	633	LEU
1	D	641	LEU
1	D	664	THR
1	E	48	LYS
1	E	68	LYS
1	E	69	GLU
1	E	109	LEU
1	E	112	VAL
1	E	114	PRO
1	E	127	VAL
1	E	140	LEU
1	E	146	ASN
1	E	157	THR
1	E	170	LEU
1	E	211	ARG
1	E	215	VAL
1	E	311	PRO
1	E	313	GLN
1	E	329	THR
1	E	332	LEU
1	E	359	VAL
1	E	364	CYS
1	E	392	THR
1	E	394	LEU

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Mol	Chain	Res	Type
1	E	421	LEU
1	E	452	ASN
1	E	462	LEU
1	E	466	PRO
1	E	487	LEU
1	E	504	THR
1	E	507	THR
1	E	527	ASN
1	E	546	THR
1	E	633	LEU
1	E	641	LEU
1	E	664	THR
1	F	48	LYS
1	F	68	LYS
1	F	69	GLU
1	F	109	LEU
1	F	112	VAL
1	F	114	PRO
1	F	127	VAL
1	F	140	LEU
1	F	146	ASN
1	F	157	THR
1	F	170	LEU
1	F	211	ARG
1	F	215	VAL
1	F	311	PRO
1	F	313	GLN
1	F	329	THR
1	F	332	LEU
1	F	359	VAL
1	F	364	CYS
1	F	392	THR
1	F	394	LEU
1	F	421	LEU
1	F	452	ASN
1	F	462	LEU
1	F	466	PRO
1	F	487	LEU
1	F	504	THR
1	F	507	THR
1	F	527	ASN
1	F	546	THR

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Mol	Chain	Res	Type
1	F	633	LEU
1	F	641	LEU
1	F	664	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	70	GLN
1	A	146	ASN
1	A	218	HIS
1	A	288	ASN
1	A	294	HIS
1	A	312	HIS
1	A	313	GLN
1	A	330	ASN
1	A	361	ASN
1	A	450	ASN
1	A	452	ASN
1	A	457	GLN
1	A	473	ASN
1	A	527	ASN
1	A	547	GLN
1	B	23	HIS
1	B	70	GLN
1	B	146	ASN
1	B	218	HIS
1	B	288	ASN
1	B	294	HIS
1	B	312	HIS
1	B	313	GLN
1	B	330	ASN
1	B	361	ASN
1	B	450	ASN
1	B	452	ASN
1	B	457	GLN
1	B	473	ASN
1	B	527	ASN
1	B	547	GLN
1	C	23	HIS
1	C	70	GLN
1	C	146	ASN

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Mol	Chain	Res	Type
1	C	218	HIS
1	C	288	ASN
1	C	294	HIS
1	C	312	HIS
1	C	313	GLN
1	C	330	ASN
1	C	361	ASN
1	C	450	ASN
1	C	452	ASN
1	C	457	GLN
1	C	473	ASN
1	C	527	ASN
1	C	547	GLN
1	D	23	HIS
1	D	70	GLN
1	D	146	ASN
1	D	218	HIS
1	D	288	ASN
1	D	294	HIS
1	D	312	HIS
1	D	313	GLN
1	D	330	ASN
1	D	361	ASN
1	D	450	ASN
1	D	452	ASN
1	D	457	GLN
1	D	473	ASN
1	D	527	ASN
1	D	547	GLN
1	E	23	HIS
1	E	70	GLN
1	E	146	ASN
1	E	218	HIS
1	E	288	ASN
1	E	294	HIS
1	E	312	HIS
1	E	313	GLN
1	E	330	ASN
1	E	361	ASN
1	E	450	ASN
1	E	452	ASN
1	E	457	GLN

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Mol	Chain	Res	Type
1	E	473	ASN
1	E	527	ASN
1	E	547	GLN
1	F	23	HIS
1	F	70	GLN
1	F	146	ASN
1	F	218	HIS
1	F	288	ASN
1	F	294	HIS
1	F	312	HIS
1	F	313	GLN
1	F	330	ASN
1	F	361	ASN
1	F	450	ASN
1	F	452	ASN
1	F	457	GLN
1	F	473	ASN
1	F	527	ASN
1	F	547	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	TPQ	A	405	1	13,14,15	2.36	5 (38%)	15,19,21	1.88	5 (33%)
1	TPQ	B	405	1	13,14,15	2.37	5 (38%)	15,19,21	1.88	5 (33%)
1	TPQ	C	405	1	13,14,15	2.37	5 (38%)	15,19,21	1.88	5 (33%)
1	TPQ	D	405	1	13,14,15	2.36	5 (38%)	15,19,21	1.89	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPQ	E	405	1	13,14,15	2.36	5 (38%)	15,19,21	1.90	5 (33%)
1	TPQ	F	405	1	13,14,15	2.37	5 (38%)	15,19,21	1.90	5 (33%)

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
1	TPQ	A	405	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	405	1	-	0/4/22/24	0/1/1/1
1	TPQ	C	405	1	-	0/4/22/24	0/1/1/1
1	TPQ	D	405	1	-	0/4/22/24	0/1/1/1
1	TPQ	E	405	1	-	0/4/22/24	0/1/1/1
1	TPQ	F	405	1	-	0/4/22/24	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	405	TPQ	C1-C2	-5.04	1.42	1.49
1	C	405	TPQ	C1-C2	-5.01	1.42	1.49
1	D	405	TPQ	C1-C2	-4.98	1.42	1.49
1	A	405	TPQ	C1-C2	-4.98	1.42	1.49
1	E	405	TPQ	C1-C2	-4.96	1.42	1.49
1	B	405	TPQ	C1-C2	-4.96	1.42	1.49
1	F	405	TPQ	O4-C4	2.05	1.39	1.34
1	C	405	TPQ	O4-C4	2.07	1.39	1.34
1	B	405	TPQ	O4-C4	2.08	1.39	1.34
1	D	405	TPQ	O4-C4	2.08	1.39	1.34
1	A	405	TPQ	O4-C4	2.08	1.39	1.34
1	E	405	TPQ	O4-C4	2.09	1.39	1.34
1	D	405	TPQ	C6-C1	2.89	1.42	1.34
1	A	405	TPQ	C6-C1	2.90	1.42	1.34
1	C	405	TPQ	C6-C1	2.90	1.42	1.34
1	F	405	TPQ	C6-C1	2.90	1.42	1.34
1	B	405	TPQ	C6-C1	2.91	1.42	1.34
1	E	405	TPQ	C6-C1	2.91	1.42	1.34
1	D	405	TPQ	O5-C5	2.97	1.32	1.24
1	F	405	TPQ	O5-C5	2.97	1.32	1.24
1	A	405	TPQ	O5-C5	2.98	1.32	1.24
1	E	405	TPQ	O5-C5	2.98	1.32	1.24
1	B	405	TPQ	O5-C5	2.98	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	405	TPQ	O5-C5	3.00	1.32	1.24
1	C	405	TPQ	C3-C4	4.70	1.43	1.35
1	A	405	TPQ	C3-C4	4.71	1.43	1.35
1	D	405	TPQ	C3-C4	4.72	1.43	1.35
1	F	405	TPQ	C3-C4	4.73	1.43	1.35
1	E	405	TPQ	C3-C4	4.74	1.43	1.35
1	B	405	TPQ	C3-C4	4.74	1.43	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	405	TPQ	C1-C6-C5	-3.70	120.72	122.97
1	F	405	TPQ	C1-C6-C5	-3.65	120.75	122.97
1	D	405	TPQ	C1-C6-C5	-3.63	120.76	122.97
1	A	405	TPQ	C1-C6-C5	-3.60	120.78	122.97
1	C	405	TPQ	C1-C6-C5	-3.57	120.80	122.97
1	B	405	TPQ	C1-C6-C5	-3.56	120.80	122.97
1	B	405	TPQ	O2-C2-C1	-2.37	118.79	120.85
1	E	405	TPQ	O2-C2-C1	-2.35	118.80	120.85
1	A	405	TPQ	O2-C2-C1	-2.34	118.80	120.85
1	D	405	TPQ	O2-C2-C1	-2.34	118.81	120.85
1	F	405	TPQ	O2-C2-C1	-2.33	118.81	120.85
1	C	405	TPQ	O2-C2-C1	-2.32	118.83	120.85
1	A	405	TPQ	C3-C2-C1	2.51	120.18	118.30
1	B	405	TPQ	C3-C2-C1	2.51	120.18	118.30
1	E	405	TPQ	C3-C2-C1	2.52	120.18	118.30
1	C	405	TPQ	C3-C2-C1	2.53	120.19	118.30
1	D	405	TPQ	C3-C2-C1	2.54	120.20	118.30
1	F	405	TPQ	C3-C2-C1	2.58	120.23	118.30
1	B	405	TPQ	C6-C1-C2	2.63	120.30	118.44
1	F	405	TPQ	CA-CB-C1	2.64	118.92	113.63
1	D	405	TPQ	C6-C1-C2	2.65	120.31	118.44
1	C	405	TPQ	C6-C1-C2	2.65	120.31	118.44
1	C	405	TPQ	CA-CB-C1	2.65	118.93	113.63
1	A	405	TPQ	CA-CB-C1	2.65	118.94	113.63
1	A	405	TPQ	C6-C1-C2	2.66	120.31	118.44
1	E	405	TPQ	CA-CB-C1	2.66	118.95	113.63
1	D	405	TPQ	CA-CB-C1	2.66	118.96	113.63
1	B	405	TPQ	CA-CB-C1	2.66	118.97	113.63
1	F	405	TPQ	C6-C1-C2	2.68	120.33	118.44
1	E	405	TPQ	C6-C1-C2	2.68	120.33	118.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	405	TPQ	1	0
1	B	405	TPQ	1	0
1	C	405	TPQ	1	0
1	D	405	TPQ	1	0
1	E	405	TPQ	1	0
1	F	405	TPQ	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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	654/692 (94%)	-0.50	6 (0%) 85 88	16, 26, 46, 81	0
1	B	654/692 (94%)	-0.49	9 (1%) 78 80	16, 26, 46, 81	0
1	C	654/692 (94%)	-0.34	27 (4%) 41 46	16, 26, 46, 81	0
1	D	654/692 (94%)	-0.41	18 (2%) 56 61	16, 26, 46, 81	0
1	E	654/692 (94%)	-0.47	2 (0%) 94 95	16, 26, 46, 81	0
1	F	654/692 (94%)	-0.47	11 (1%) 73 76	16, 26, 46, 81	0
All	All	3924/4152 (94%)	-0.45	73 (1%) 70 73	16, 26, 46, 81	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	PRO	9.6
1	D	20	ARG	8.2
1	D	19	ALA	7.8
1	D	21	PRO	6.2
1	D	334	LEU	6.0
1	B	672	VAL	5.8
1	D	130	ASN	5.6
1	E	672	VAL	5.5
1	D	46	GLY	5.3
1	F	18	PRO	5.1
1	C	18	PRO	5.0
1	C	340	GLY	4.9
1	D	335	GLY	4.7
1	A	671	ALA	4.4
1	B	46	GLY	4.3
1	F	19	ALA	4.3
1	A	672	VAL	4.3
1	C	672	VAL	4.1
1	F	672	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	46	GLY	3.9
1	B	48	LYS	3.9
1	C	20	ARG	3.7
1	D	333	SER	3.6
1	C	46	GLY	3.6
1	C	70	GLN	3.6
1	F	48	LYS	3.5
1	E	671	ALA	3.5
1	A	334	LEU	3.4
1	C	48	LYS	3.4
1	A	670	ARG	3.3
1	D	336	CYS	3.3
1	D	672	VAL	3.2
1	F	334	LEU	3.2
1	D	22	ALA	3.1
1	B	340	GLY	3.1
1	B	334	LEU	3.1
1	C	45	ALA	3.1
1	B	671	ALA	2.9
1	A	335	GLY	2.9
1	C	335	GLY	2.9
1	C	71	GLY	2.9
1	C	19	ALA	2.8
1	C	671	ALA	2.8
1	F	86	ALA	2.8
1	C	334	LEU	2.8
1	C	341	VAL	2.8
1	C	44	PHE	2.6
1	C	101	LEU	2.6
1	F	335	GLY	2.6
1	F	20	ARG	2.5
1	F	130	ASN	2.5
1	A	668	ALA	2.4
1	C	333	SER	2.4
1	D	48	LYS	2.3
1	C	200	GLU	2.3
1	C	130	ASN	2.3
1	B	670	ARG	2.3
1	D	671	ALA	2.2
1	B	179	SER	2.2
1	C	21	PRO	2.2
1	C	339	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	146	ASN	2.2
1	B	45	ALA	2.1
1	D	45	ALA	2.1
1	D	87	GLY	2.1
1	C	42	SER	2.1
1	C	47	LYS	2.1
1	F	671	ALA	2.1
1	C	201	LYS	2.1
1	C	437	ASP	2.1
1	C	328[A]	MET	2.0
1	D	241	PRO	2.0
1	C	670	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	TPQ	A	405	14/15	0.91	0.21	-	32,47,55,57	0
1	TPQ	C	405	14/15	0.91	0.16	-	32,47,55,57	0
1	TPQ	E	405	14/15	0.92	0.21	-	32,47,55,57	0
1	TPQ	D	405	14/15	0.92	0.20	-	32,47,55,57	0
1	TPQ	F	405	14/15	0.92	0.19	-	32,47,55,57	0
1	TPQ	B	405	14/15	0.89	0.24	-	32,47,55,57	0

## 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	CU	E	701	1/1	0.99	0.08	-1.31	31,31,31,31	0
2	CU	A	701	1/1	0.99	0.03	-2.13	31,31,31,31	0
2	CU	D	701	1/1	1.00	0.03	-2.27	31,31,31,31	0
2	CU	B	701	1/1	0.99	0.02	-2.42	31,31,31,31	0
2	CU	F	701	1/1	1.00	0.04	-2.61	31,31,31,31	0
2	CU	C	701	1/1	0.99	0.02	-6.20	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.