



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:47 am BST

PDB ID : 4PEM  
Title : Crystal Structure of S1G mutant of Penicillin G Acylase from *Kluyvera citrophila*  
Authors : Ramasamy, S.; Varshney, N.K.; Brannigan, J.A.; Wilkinson, A.J.; Suresh, C.G.  
Deposited on : 2014-04-24  
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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

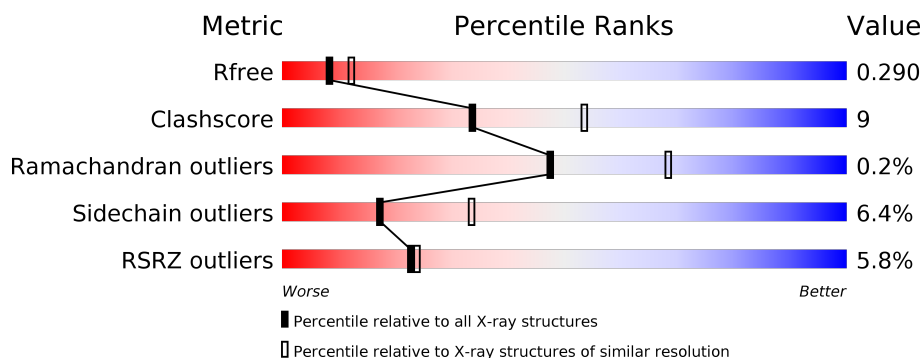
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 respectively. 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	286	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>13%</div> <div>•</div> <div>18%</div> </div> </div>
1	C	286	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>
1	E	286	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>10%</div> </div> </div>
1	G	286	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>10%</div> </div> </div>
2	B	568	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>••</div> </div> </div>
2	D	568	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	568	<div><div>6%</div><div><div></div><div>79%</div><div>17%</div><div></div></div><div>..</div></div>
2	H	568	<div><div>7%</div><div><div></div><div>79%</div><div>17%</div><div></div></div><div>..</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25838 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 Penicillin G acylase Alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1831	1171	308	344	8			
1	C	258	Total	C	N	O	S	0	0	0
			2026	1290	343	385	8			
1	E	258	Total	C	N	O	S	0	0	0
			2026	1290	343	385	8			
1	G	258	Total	C	N	O	S	0	0	0
			2026	1290	343	385	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP A0A068F6N5
A	-24	LYS	-	expression tag	UNP A0A068F6N5
A	-23	ASN	-	expression tag	UNP A0A068F6N5
A	-22	ARG	-	expression tag	UNP A0A068F6N5
A	-21	ASN	-	expression tag	UNP A0A068F6N5
A	-20	ARG	-	expression tag	UNP A0A068F6N5
C	-25	MET	-	initiating methionine	UNP A0A068F6N5
C	-24	LYS	-	expression tag	UNP A0A068F6N5
C	-23	ASN	-	expression tag	UNP A0A068F6N5
C	-22	ARG	-	expression tag	UNP A0A068F6N5
C	-21	ASN	-	expression tag	UNP A0A068F6N5
C	-20	ARG	-	expression tag	UNP A0A068F6N5
E	-25	MET	-	initiating methionine	UNP A0A068F6N5
E	-24	LYS	-	expression tag	UNP A0A068F6N5
E	-23	ASN	-	expression tag	UNP A0A068F6N5
E	-22	ARG	-	expression tag	UNP A0A068F6N5
E	-21	ASN	-	expression tag	UNP A0A068F6N5
E	-20	ARG	-	expression tag	UNP A0A068F6N5
G	-25	MET	-	initiating methionine	UNP A0A068F6N5
G	-24	LYS	-	expression tag	UNP A0A068F6N5
G	-23	ASN	-	expression tag	UNP A0A068F6N5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-22	ARG	-	expression tag	UNP A0A068F6N5
G	-21	ASN	-	expression tag	UNP A0A068F6N5
G	-20	ARG	-	expression tag	UNP A0A068F6N5

- Molecule 2 is a protein called Penicillin G acylase Beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	549	Total	C	N	O	S	0	0	0
			4304	2743	744	809	8			
2	D	560	Total	C	N	O	S	0	0	0
			4399	2800	762	829	8			
2	F	560	Total	C	N	O	S	0	0	0
			4398	2800	762	828	8			
2	H	560	Total	C	N	O	S	0	0	0
			4399	2800	762	829	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	GLY	SER	engineered mutation	UNP A0A068F6N5
D	264	GLY	SER	engineered mutation	UNP A0A068F6N5
F	264	GLY	SER	engineered mutation	UNP A0A068F6N5
H	264	GLY	SER	engineered mutation	UNP A0A068F6N5

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	81	Total	O	0	0
			81	81		
4	C	42	Total	O	0	0
			42	42		
4	D	69	Total	O	0	0
			69	69		

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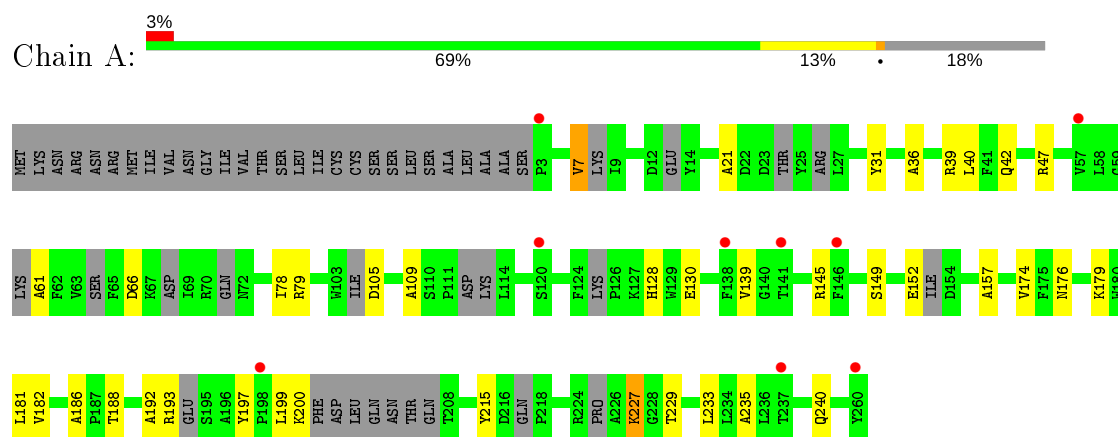
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	38	Total 38	O 38	0	0
4	F	63	Total 63	O 63	0	0
4	G	31	Total 31	O 31	0	0
4	H	74	Total 74	O 74	0	0

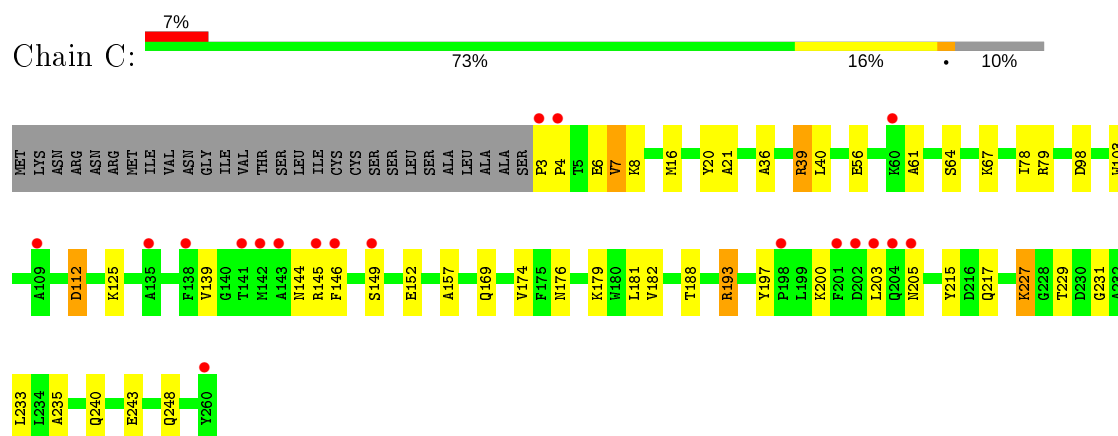
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

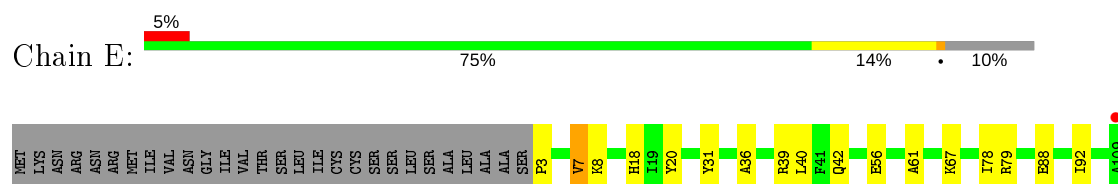
#### • Molecule 1: Penicillin G acylase Alpha



#### • Molecule 1: Penicillin G acylase Alpha

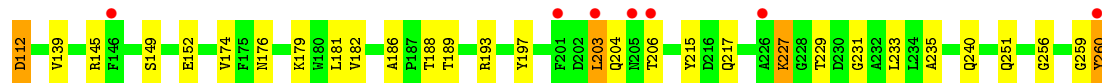
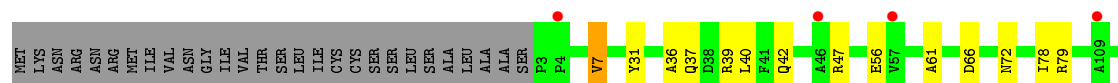
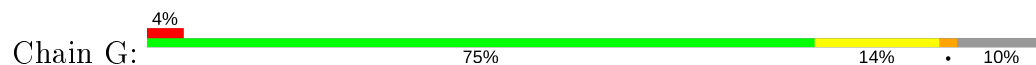


#### • Molecule 1: Penicillin G acylase Alpha

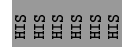
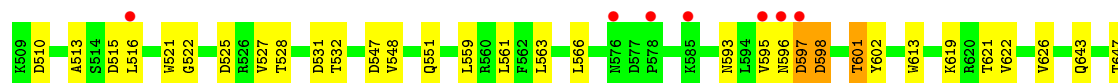
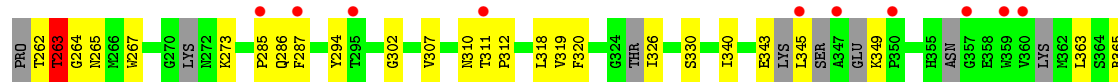
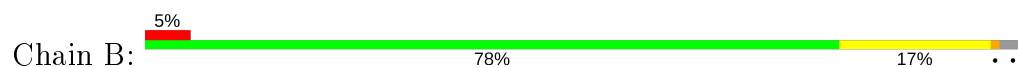




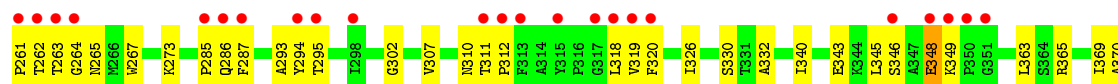
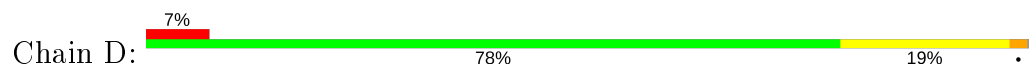
• Molecule 1: Penicillin G acylase Alpha



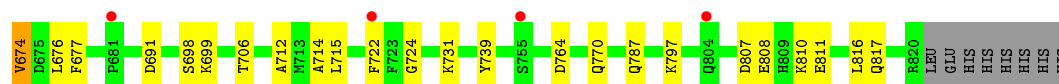
• Molecule 2: Penicillin G acylase Beta



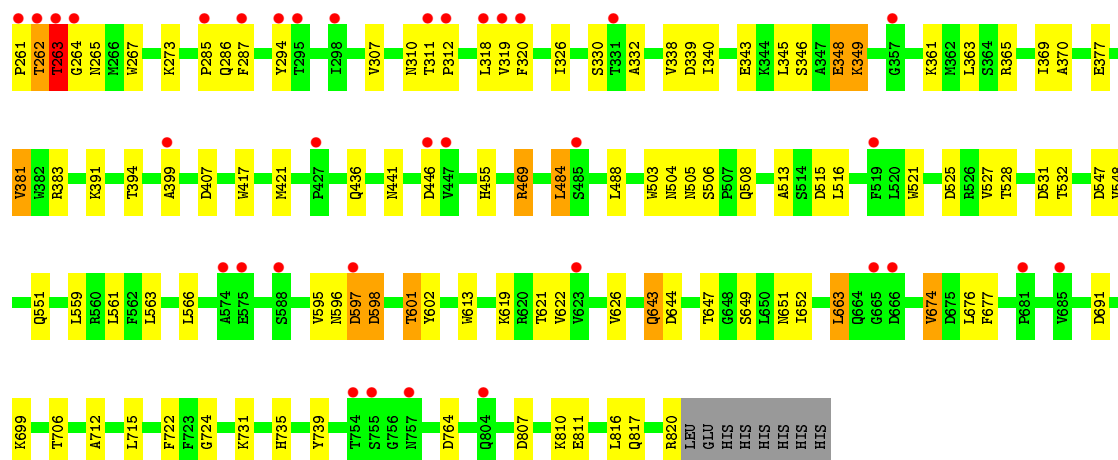
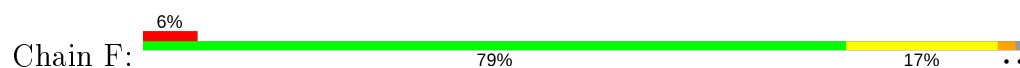
• Molecule 2: Penicillin G acylase Beta



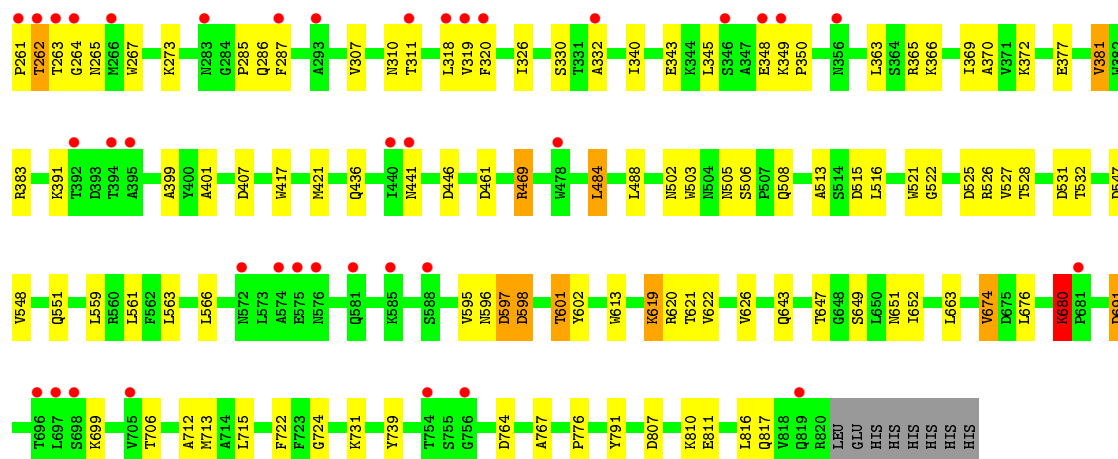
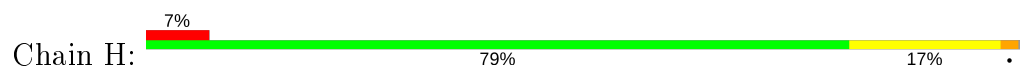




• Molecule 2: Penicillin G acylase Beta



• Molecule 2: Penicillin G acylase Beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.00Å 124.56Å 135.14Å 104.05° 101.37° 96.51°	Depositor
Resolution (Å)	38.00 – 2.50 37.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	76.3 (38.00-2.50) 76.4 (37.85-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.248 , 0.292 0.251 , 0.290	Depositor DCC
$R_{free}$ test set	4354 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.9	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	25838	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.49% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.57	0/1862	0.64	0/2503
1	C	0.57	0/2075	0.66	1/2816 (0.0%)
1	E	0.53	0/2075	0.62	0/2816
1	G	0.54	0/2075	0.63	0/2816
2	B	0.54	0/4422	0.63	1/6019 (0.0%)
2	D	0.54	0/4528	0.62	0/6175
2	F	0.52	0/4527	0.62	1/6174 (0.0%)
2	H	0.53	0/4528	0.62	0/6175
All	All	0.54	0/26092	0.63	3/35494 (0.0%)

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
2	F	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	469	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	F	263	THR	CA-CB-CG2	-5.12	105.23	112.40
1	C	39	ARG	NE-CZ-NH2	5.10	122.85	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	263	THR	Peptide
2	H	680	LYS	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	1831	0	1769	39	0
1	C	2026	0	1978	48	1
1	E	2026	0	1978	38	0
1	G	2026	0	1978	33	0
2	B	4304	0	4108	69	0
2	D	4399	0	4221	83	0
2	F	4398	0	4218	106	1
2	H	4399	0	4221	93	0
3	A	1	0	0	0	0
4	A	30	0	0	3	0
4	B	81	0	0	7	0
4	C	42	0	0	11	0
4	D	69	0	0	12	0
4	E	38	0	0	10	0
4	F	63	0	0	9	0
4	G	31	0	0	6	0
4	H	74	0	0	8	0
All	All	25838	0	24471	426	1

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 9.

All (426) 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)
2:F:263:THR:HG21	2:F:504:ASN:ND2	1.59	1.14
2:D:263:THR:HB	2:D:264:GLY:HA3	1.31	1.11
2:F:263:THR:CG2	2:F:504:ASN:ND2	2.13	1.11
2:F:262:THR:HG21	2:F:649:SER:HB3	1.28	1.07
2:F:820:ARG:NH2	4:F:907:HOH:O	1.85	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:263:THR:HG23	2:F:504:ASN:OD1	1.56	1.05
2:F:262:THR:HB	2:F:263:THR:HA	1.39	1.04
2:F:262:THR:HG22	2:F:263:THR:O	1.57	1.02
2:D:797:LYS:NZ	4:D:946:HOH:O	1.92	1.00
2:F:262:THR:CG2	2:F:649:SER:HB3	1.91	0.99
2:F:263:THR:HG23	2:F:264:GLY:H	1.24	0.98
2:B:796:ARG:NH1	4:B:1027:HOH:O	1.92	0.97
2:F:263:THR:HG21	2:F:504:ASN:HD21	1.23	0.96
2:H:263:THR:CG2	2:H:526:ARG:HH22	1.80	0.95
1:E:92:ILE:HG13	4:E:336:HOH:O	1.67	0.94
1:A:128:HIS:HB2	2:H:366:LYS:HE3	1.51	0.93
2:H:340:ILE:HG23	4:H:964:HOH:O	1.69	0.93
2:F:262:THR:CB	2:F:263:THR:HA	2.00	0.92
2:H:263:THR:CB	2:H:526:ARG:HH22	1.83	0.92
1:C:146:PHE:CE1	2:D:261:PRO:CD	2.44	0.92
2:F:263:THR:CG2	2:F:504:ASN:CG	2.37	0.91
2:B:264:GLY:HA2	2:B:286:GLN:HG3	1.53	0.91
2:F:263:THR:HG23	2:F:504:ASN:CG	1.90	0.90
2:F:262:THR:CG2	2:F:649:SER:CB	2.50	0.90
1:C:146:PHE:CB	2:D:261:PRO:HG2	1.99	0.89
2:H:263:THR:HB	2:H:526:ARG:HH22	1.39	0.88
2:F:338:VAL:O	4:F:956:HOH:O	1.91	0.87
1:E:88:GLU:O	4:E:336:HOH:O	1.93	0.86
2:F:263:THR:HG23	2:F:264:GLY:N	1.89	0.86
1:A:128:HIS:HB2	2:H:366:LYS:CE	2.07	0.85
2:F:261:PRO:O	2:F:286:GLN:O	1.94	0.85
2:F:735:HIS:ND1	4:F:908:HOH:O	2.08	0.84
2:F:262:THR:CG2	2:F:263:THR:O	2.24	0.84
2:H:263:THR:HG21	2:H:526:ARG:HH12	1.41	0.84
2:H:263:THR:HB	2:H:526:ARG:NH2	1.91	0.84
2:H:263:THR:HG21	2:H:649:SER:OG	1.78	0.83
2:F:262:THR:HG23	2:F:649:SER:OG	1.79	0.83
2:F:262:THR:HG23	2:F:649:SER:CB	2.11	0.81
2:F:263:THR:CG2	2:F:504:ASN:HD21	1.86	0.81
1:C:215:TYR:O	4:C:336:HOH:O	1.97	0.80
1:E:218:PRO:O	4:E:323:HOH:O	1.99	0.79
4:E:323:HOH:O	2:F:391:LYS:NZ	2.15	0.79
2:F:339:ASP:OD1	4:F:956:HOH:O	2.00	0.78
2:F:262:THR:HG22	2:F:263:THR:C	2.03	0.77
2:F:262:THR:HG22	2:F:263:THR:CA	2.14	0.77
2:D:261:PRO:HA	2:D:287:PHE:CD1	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:HIS:O	2:H:366:LYS:NZ	2.19	0.76
2:F:264:GLY:HA2	2:F:286:GLN:HG3	1.66	0.76
2:D:261:PRO:HA	2:D:287:PHE:HD1	1.49	0.76
2:F:264:GLY:O	2:F:503:TRP:HD1	1.69	0.75
1:E:146:PHE:CE1	2:F:261:PRO:HD3	2.21	0.74
2:D:610:LEU:HB3	4:D:964:HOH:O	1.89	0.73
2:D:263:THR:CB	2:D:264:GLY:HA3	2.11	0.73
1:E:152:GLU:OE2	4:F:956:HOH:O	2.07	0.72
2:H:401:ALA:N	4:H:964:HOH:O	2.21	0.72
1:E:18:HIS:NE2	4:E:320:HOH:O	2.23	0.71
2:F:264:GLY:O	2:F:503:TRP:CD1	2.44	0.71
2:F:262:THR:HG23	2:F:649:SER:HG	1.56	0.70
1:C:243:GLU:OE2	4:C:329:HOH:O	2.09	0.70
2:F:349:LYS:O	4:F:909:HOH:O	2.09	0.69
2:H:503:TRP:HB3	2:H:527:VAL:HG22	1.74	0.69
1:G:251:GLN:HA	4:G:320:HOH:O	1.92	0.69
2:F:503:TRP:HB3	2:F:527:VAL:HG22	1.75	0.69
2:H:263:THR:CG2	2:H:649:SER:OG	2.40	0.69
1:G:188:THR:HA	2:H:506:SER:O	1.94	0.68
2:D:558:ASN:HB2	4:D:964:HOH:O	1.93	0.68
1:C:125:LYS:HB3	4:C:337:HOH:O	1.91	0.68
2:D:503:TRP:HB3	2:D:527:VAL:HG22	1.76	0.68
2:F:262:THR:CG2	2:F:649:SER:OG	2.42	0.68
2:B:503:TRP:HB3	2:B:527:VAL:HG22	1.76	0.67
2:B:478:TRP:O	4:B:1066:HOH:O	2.13	0.67
2:D:263:THR:OG1	2:D:504:ASN:ND2	2.28	0.66
2:D:714:ALA:HB3	4:D:941:HOH:O	1.95	0.66
1:E:217:GLN:NE2	4:E:332:HOH:O	2.27	0.66
2:H:691:ASP:OD1	4:H:901:HOH:O	2.14	0.66
1:A:152:GLU:HB2	2:B:340:ILE:HD12	1.77	0.66
1:A:188:THR:HA	2:B:506:SER:O	1.97	0.65
1:G:37:GLN:OE1	4:G:301:HOH:O	2.15	0.64
1:C:193:ARG:HB3	4:C:328:HOH:O	1.96	0.64
1:A:176:ASN:OD1	2:B:469:ARG:NH2	2.30	0.64
1:E:188:THR:HA	2:F:506:SER:O	1.97	0.64
1:G:259:GLY:O	1:G:260:TYR:C	2.37	0.64
1:E:176:ASN:OD1	2:F:469:ARG:NH2	2.31	0.63
2:F:263:THR:OG1	2:F:264:GLY:N	2.31	0.63
2:B:263:THR:OG1	2:B:264:GLY:N	2.30	0.63
1:G:256:GLY:O	4:G:325:HOH:O	2.16	0.63
1:E:145:ARG:NH1	4:E:338:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:GLU:HB2	2:H:340:ILE:HD12	1.81	0.62
2:B:262:THR:O	2:B:263:THR:HG22	2.00	0.62
1:C:188:THR:HA	2:D:506:SER:O	1.99	0.62
2:D:262:THR:C	2:D:286:GLN:O	2.38	0.62
2:F:596:ASN:ND2	2:F:601:THR:OG1	2.30	0.61
1:G:47:ARG:NE	4:G:309:HOH:O	2.31	0.61
2:H:713:MET:HA	4:H:937:HOH:O	1.99	0.61
2:H:263:THR:HG22	2:H:526:ARG:HH22	1.60	0.61
2:F:262:THR:CB	2:F:263:THR:CA	2.78	0.61
2:D:345:LEU:HD11	2:D:399:ALA:HB2	1.82	0.60
2:F:261:PRO:O	2:F:262:THR:CB	2.49	0.60
2:F:263:THR:HG23	2:F:504:ASN:ND2	2.05	0.60
2:D:596:ASN:ND2	2:D:601:THR:OG1	2.31	0.60
2:B:262:THR:N	2:B:287:PHE:CD1	2.71	0.59
1:C:152:GLU:HB2	2:D:340:ILE:HD12	1.83	0.59
2:D:787:GLN:NE2	4:D:905:HOH:O	2.17	0.59
2:B:345:LEU:HD11	2:B:399:ALA:HB2	1.84	0.59
2:B:561:LEU:HD11	2:B:652:ILE:HD13	1.84	0.59
2:D:263:THR:HB	2:D:264:GLY:CA	2.21	0.59
1:C:146:PHE:HB3	2:D:261:PRO:HG2	1.84	0.59
2:H:345:LEU:HD11	2:H:399:ALA:HB2	1.84	0.59
1:C:146:PHE:CB	2:D:261:PRO:CG	2.74	0.59
1:G:179:LYS:HG3	2:H:469:ARG:HD2	1.85	0.59
2:H:263:THR:CG2	2:H:526:ARG:NH2	2.60	0.58
2:F:262:THR:CG2	2:F:263:THR:CA	2.80	0.58
2:H:503:TRP:CB	2:H:527:VAL:HG22	2.34	0.58
2:F:345:LEU:HD11	2:F:399:ALA:HB2	1.84	0.58
2:B:820:ARG:NH1	4:B:1047:HOH:O	2.34	0.58
2:H:263:THR:OG1	2:H:649:SER:HB3	2.04	0.58
2:H:561:LEU:HD11	2:H:652:ILE:HD13	1.86	0.58
1:E:145:ARG:NH1	4:E:330:HOH:O	2.30	0.57
2:B:503:TRP:CB	2:B:527:VAL:HG22	2.34	0.57
2:F:503:TRP:CB	2:F:527:VAL:HG22	2.33	0.57
2:D:484:LEU:HG	2:D:488:LEU:HD13	1.86	0.57
1:E:152:GLU:HB2	2:F:340:ILE:HD12	1.85	0.57
1:E:3:PRO:N	4:E:310:HOH:O	2.37	0.57
2:D:561:LEU:HD11	2:D:652:ILE:HD13	1.87	0.57
2:B:285:PRO:HB2	2:B:287:PHE:CE2	2.39	0.57
1:C:193:ARG:N	4:C:328:HOH:O	2.37	0.57
2:D:285:PRO:HB2	2:D:287:PHE:CE2	2.40	0.56
1:A:145:ARG:HG3	2:B:722:PHE:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:VAL:HG11	2:B:421:MET:HB3	1.88	0.56
2:F:285:PRO:HB2	2:F:287:PHE:CE2	2.40	0.56
1:C:16:MET:CB	4:D:946:HOH:O	2.54	0.56
2:H:285:PRO:HB2	2:H:287:PHE:CE2	2.40	0.56
2:H:307:VAL:HG11	2:H:421:MET:HB3	1.88	0.56
2:D:503:TRP:CB	2:D:527:VAL:HG22	2.35	0.56
1:C:227:LYS:HG3	1:C:233:LEU:HD23	1.87	0.56
1:G:227:LYS:HG3	1:G:233:LEU:HD23	1.87	0.56
2:B:264:GLY:HA2	2:B:286:GLN:CG	2.31	0.55
2:B:505:ASN:OD1	2:B:527:VAL:HG21	2.07	0.55
1:E:197:TYR:CA	2:F:508:GLN:HE21	2.19	0.55
1:G:176:ASN:OD1	2:H:469:ARG:NH2	2.39	0.55
2:H:598:ASP:N	2:H:598:ASP:OD1	2.36	0.55
1:A:128:HIS:N	2:H:366:LYS:HZ1	2.04	0.55
1:A:227:LYS:HG3	1:A:233:LEU:HD23	1.88	0.55
1:E:227:LYS:HG3	1:E:233:LEU:HD23	1.87	0.55
2:H:484:LEU:HG	2:H:488:LEU:HD13	1.88	0.55
2:B:484:LEU:HG	2:B:488:LEU:HD13	1.87	0.55
2:F:561:LEU:HD11	2:F:652:ILE:HD13	1.88	0.55
2:H:505:ASN:OD1	2:H:527:VAL:HG21	2.07	0.55
1:A:130:GLU:OE2	2:H:366:LYS:O	2.25	0.55
2:F:484:LEU:HG	2:F:488:LEU:HD13	1.88	0.55
1:G:259:GLY:O	1:G:260:TYR:O	2.23	0.55
2:B:598:ASP:N	2:B:598:ASP:OD1	2.37	0.55
2:F:307:VAL:HG11	2:F:421:MET:HB3	1.88	0.54
2:B:649:SER:O	4:B:1018:HOH:O	2.18	0.54
1:C:145:ARG:HG3	2:D:722:PHE:HE2	1.72	0.54
2:F:262:THR:HG22	2:F:263:THR:N	2.22	0.54
2:F:365:ARG:HG2	2:F:381:VAL:HG13	1.89	0.54
2:D:365:ARG:HG2	2:D:381:VAL:HG13	1.89	0.54
2:H:596:ASN:ND2	2:H:601:THR:OG1	2.30	0.54
2:F:505:ASN:OD1	2:F:527:VAL:HG21	2.07	0.54
2:F:263:THR:CG2	2:F:264:GLY:N	2.55	0.53
2:D:307:VAL:HG11	2:D:421:MET:HB3	1.89	0.53
2:D:505:ASN:OD1	2:D:527:VAL:HG21	2.07	0.53
2:F:264:GLY:HA2	2:F:286:GLN:CG	2.38	0.53
1:E:145:ARG:HG3	2:F:722:PHE:HE2	1.73	0.53
2:H:365:ARG:HG2	2:H:381:VAL:HG13	1.90	0.53
2:B:365:ARG:HG2	2:B:381:VAL:HG13	1.90	0.53
2:H:265:ASN:HB3	2:H:503:TRP:CD1	2.44	0.53
1:G:260:TYR:CD2	2:H:262:THR:HB	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:598:ASP:N	2:D:598:ASP:OD1	2.36	0.52
1:C:197:TYR:CA	2:D:508:GLN:HE21	2.22	0.52
1:C:193:ARG:NH2	4:C:339:HOH:O	2.42	0.52
1:E:112:ASP:OD1	1:E:112:ASP:N	2.42	0.52
1:C:176:ASN:OD1	2:D:469:ARG:NH2	2.43	0.52
1:C:16:MET:HB3	4:D:946:HOH:O	2.09	0.52
2:B:596:ASN:ND2	2:B:601:THR:OG1	2.32	0.52
1:C:39:ARG:NH1	2:D:295:THR:O	2.40	0.52
2:D:580:ARG:NH2	4:D:904:HOH:O	2.42	0.52
2:D:262:THR:HG22	2:D:262:THR:O	2.09	0.51
1:C:3:PRO:HG2	1:C:6:GLU:OE1	2.09	0.51
2:H:566:LEU:HD21	2:H:613:TRP:CE2	2.46	0.51
1:A:197:TYR:CA	2:B:508:GLN:HE21	2.24	0.51
2:F:265:ASN:HB3	2:F:503:TRP:CD1	2.45	0.51
2:H:263:THR:HG21	2:H:526:ARG:NH1	2.18	0.51
2:F:598:ASP:OD1	2:F:598:ASP:N	2.38	0.51
1:A:47:ARG:NE	4:A:1024:HOH:O	2.43	0.51
1:A:179:LYS:HG3	2:B:469:ARG:HD2	1.93	0.50
2:D:621:THR:HB	2:D:676:LEU:HB3	1.93	0.50
1:A:128:HIS:CA	2:H:366:LYS:HZ1	2.25	0.50
2:D:265:ASN:HB3	2:D:503:TRP:CD1	2.46	0.50
1:E:240:GLN:OE1	1:E:240:GLN:HA	2.12	0.50
2:F:262:THR:CG2	2:F:263:THR:HA	2.41	0.50
1:A:128:HIS:C	2:H:366:LYS:NZ	2.66	0.50
1:C:144:ASN:HB3	4:C:338:HOH:O	2.12	0.49
2:F:262:THR:HB	2:F:286:GLN:O	2.12	0.49
2:F:263:THR:HG21	2:F:332:ALA:HB3	1.94	0.49
1:A:130:GLU:OE2	2:H:366:LYS:C	2.50	0.49
1:G:240:GLN:OE1	1:G:240:GLN:HA	2.13	0.49
1:E:7:VAL:HG13	2:F:816:LEU:HB2	1.94	0.49
2:H:263:THR:OG1	2:H:649:SER:CB	2.61	0.49
2:B:621:THR:HB	2:B:676:LEU:HB3	1.94	0.49
1:G:197:TYR:CA	2:H:508:GLN:HE21	2.25	0.49
2:H:559:LEU:HD11	2:H:563:LEU:HD22	1.95	0.49
1:G:66:ASP:HB3	2:H:369:ILE:HD13	1.94	0.49
2:B:559:LEU:HD11	2:B:563:LEU:HD22	1.95	0.49
2:F:285:PRO:HG3	2:F:320:PHE:CZ	2.48	0.49
1:C:240:GLN:OE1	1:C:240:GLN:HA	2.13	0.49
1:E:195:SER:HB3	4:E:321:HOH:O	2.13	0.49
2:H:621:THR:HB	2:H:676:LEU:HB3	1.94	0.49
1:G:7:VAL:HG13	2:H:816:LEU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:ASN:HB3	2:B:503:TRP:CD1	2.47	0.49
2:H:649:SER:O	4:H:942:HOH:O	2.20	0.49
2:D:285:PRO:HG3	2:D:320:PHE:CZ	2.48	0.48
2:F:621:THR:HB	2:F:676:LEU:HB3	1.94	0.48
1:E:215:TYR:CE2	1:E:217:GLN:HB2	2.47	0.48
2:F:262:THR:CG2	2:F:263:THR:C	2.75	0.48
2:B:285:PRO:HG3	2:B:320:PHE:CZ	2.49	0.48
1:G:231:GLY:O	2:H:724:GLY:HA2	2.13	0.48
2:D:566:LEU:HD21	2:D:613:TRP:CE2	2.49	0.48
1:E:146:PHE:CD1	2:F:261:PRO:HD3	2.48	0.48
1:G:215:TYR:CE2	1:G:217:GLN:HB2	2.48	0.48
2:H:285:PRO:HG3	2:H:320:PHE:CZ	2.49	0.48
2:D:559:LEU:HD11	2:D:563:LEU:HD22	1.95	0.47
2:F:261:PRO:O	2:F:287:PHE:HA	2.14	0.47
1:A:105:ASP:OD2	4:A:1015:HOH:O	2.20	0.47
2:D:263:THR:OG1	2:D:332:ALA:HB3	2.14	0.47
1:C:7:VAL:HG13	2:D:816:LEU:HB2	1.95	0.47
1:G:188:THR:HG22	2:H:506:SER:OG	2.14	0.47
1:A:240:GLN:HA	1:A:240:GLN:OE1	2.15	0.47
2:D:596:ASN:HD22	2:D:601:THR:HG1	1.55	0.47
1:A:174:VAL:HG22	2:B:674:VAL:HG12	1.95	0.47
1:A:7:VAL:HG13	2:B:816:LEU:HB2	1.96	0.47
1:C:174:VAL:HG22	2:D:674:VAL:HG12	1.97	0.47
1:A:109:ALA:HB2	2:H:350:PRO:HG2	1.97	0.47
2:F:261:PRO:O	2:F:262:THR:HB	2.15	0.47
1:G:145:ARG:HG3	2:H:722:PHE:HE2	1.80	0.47
1:C:16:MET:HB2	4:D:946:HOH:O	2.13	0.46
2:F:559:LEU:HD11	2:F:563:LEU:HD22	1.96	0.46
2:H:596:ASN:HD22	2:H:601:THR:HG1	1.57	0.46
1:A:128:HIS:HB2	2:H:366:LYS:NZ	2.30	0.46
2:B:525:ASP:OD1	2:B:527:VAL:HG23	2.15	0.46
1:C:179:LYS:HE2	2:D:515:ASP:O	2.16	0.46
2:F:381:VAL:HA	4:F:904:HOH:O	2.15	0.46
2:H:525:ASP:OD1	2:H:527:VAL:HG23	2.15	0.46
2:B:547:ASP:O	2:B:551:GLN:HG3	2.15	0.46
1:C:215:TYR:CE2	1:C:217:GLN:HB2	2.50	0.46
2:B:267:TRP:CZ2	2:B:548:VAL:HB	2.51	0.46
2:F:263:THR:CG2	2:F:264:GLY:H	2.07	0.46
2:F:330:SER:HA	2:F:441:ASN:O	2.16	0.46
1:C:39:ARG:NH2	2:D:770:GLN:O	2.47	0.46
1:G:72:ASN:HB3	4:G:306:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:566:LEU:HD21	2:F:613:TRP:CE2	2.51	0.45
2:H:326:ILE:HG22	2:H:446:ASP:HB3	1.98	0.45
2:H:547:ASP:O	2:H:551:GLN:HG3	2.16	0.45
2:B:593:ASN:HB2	4:B:1043:HOH:O	2.16	0.45
2:F:547:ASP:O	2:F:551:GLN:HG3	2.16	0.45
1:E:174:VAL:HG22	2:F:674:VAL:HG12	1.98	0.45
2:B:566:LEU:HD21	2:B:613:TRP:CE2	2.51	0.45
2:F:262:THR:HG23	2:F:649:SER:H	1.81	0.45
2:F:596:ASN:HD22	2:F:601:THR:HG1	1.58	0.45
2:F:715:LEU:HB2	2:F:739:TYR:HA	1.98	0.45
1:C:21:ALA:O	2:D:302:GLY:HA3	2.17	0.45
2:D:602:TYR:CE2	2:D:712:ALA:HA	2.51	0.45
2:F:602:TYR:CE2	2:F:712:ALA:HA	2.51	0.45
1:A:128:HIS:C	2:H:366:LYS:HZ2	2.18	0.45
2:D:547:ASP:O	2:D:551:GLN:HG3	2.17	0.45
1:A:21:ALA:O	2:B:302:GLY:HA3	2.17	0.45
2:D:715:LEU:HB2	2:D:739:TYR:HA	1.98	0.45
2:H:602:TYR:CE2	2:H:712:ALA:HA	2.51	0.45
2:B:715:LEU:HB2	2:B:739:TYR:HA	1.97	0.45
2:D:525:ASP:OD1	2:D:527:VAL:HG23	2.17	0.45
2:D:267:TRP:CZ2	2:D:548:VAL:HB	2.52	0.44
2:F:263:THR:OG1	2:F:264:GLY:CA	2.65	0.44
2:F:263:THR:OG1	2:F:264:GLY:HA3	2.18	0.44
2:F:528:THR:O	2:F:532:THR:HG22	2.18	0.44
2:H:267:TRP:CZ2	2:H:548:VAL:HB	2.52	0.44
1:A:199:LEU:HD12	2:B:484:LEU:HD21	1.98	0.44
1:C:39:ARG:NH1	2:D:293:ALA:O	2.51	0.44
2:D:643:GLN:O	4:D:941:HOH:O	2.21	0.44
1:G:203:LEU:O	1:G:206:THR:HG22	2.17	0.44
2:B:450:ASN:ND2	4:B:1002:HOH:O	2.51	0.44
1:E:257:LEU:HD21	4:F:941:HOH:O	2.17	0.44
1:C:103:TRP:NE1	4:C:306:HOH:O	2.36	0.44
2:D:513:ALA:HB2	2:D:521:TRP:CE3	2.52	0.44
2:F:267:TRP:CZ2	2:F:548:VAL:HB	2.52	0.44
2:H:261:PRO:HB2	2:H:332:ALA:HB2	1.99	0.44
2:H:715:LEU:HB2	2:H:739:TYR:HA	1.98	0.44
1:A:61:ALA:HB1	1:A:235:ALA:HB2	1.98	0.44
2:D:330:SER:HA	2:D:441:ASN:O	2.18	0.44
2:D:499:TYR:OH	2:D:531:ASP:OD1	2.31	0.44
2:F:294:TYR:CE2	2:F:312:PRO:HB3	2.52	0.44
2:F:525:ASP:OD1	2:F:527:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:ASP:OD1	1:G:112:ASP:N	2.43	0.44
1:G:189:THR:HG21	2:H:502:ASN:HB2	1.99	0.44
2:H:620:ARG:NE	4:H:973:HOH:O	2.51	0.44
2:B:326:ILE:HG22	2:B:446:ASP:HB3	2.00	0.43
2:B:820:ARG:HG2	4:B:1011:HOH:O	2.17	0.43
1:C:36:ALA:O	1:C:40:LEU:HB2	2.18	0.43
2:D:326:ILE:HG22	2:D:446:ASP:HB3	2.00	0.43
1:E:78:ILE:HD11	1:E:139:VAL:HG11	1.99	0.43
1:E:215:TYR:OH	2:F:391:LYS:HD3	2.18	0.43
1:E:36:ALA:O	1:E:40:LEU:HB2	2.18	0.43
1:E:56:GLU:CG	2:F:370:ALA:HB3	2.48	0.43
2:F:663:LEU:HD13	2:F:677:PHE:HZ	1.83	0.43
1:C:56:GLU:CG	2:D:370:ALA:HB3	2.49	0.43
2:D:528:THR:O	2:D:532:THR:HG22	2.19	0.43
2:H:619:LYS:HD3	4:H:973:HOH:O	2.17	0.43
2:B:330:SER:HA	2:B:441:ASN:O	2.18	0.43
2:D:651:ASN:OD1	2:D:652:ILE:N	2.51	0.43
2:B:596:ASN:HD22	2:B:601:THR:HG1	1.59	0.43
2:F:643:GLN:HG2	2:F:644:ASP:N	2.34	0.43
2:B:602:TYR:CE2	2:B:712:ALA:HA	2.53	0.43
1:C:78:ILE:HD11	1:C:139:VAL:HG11	2.00	0.43
1:G:78:ILE:HD11	1:G:139:VAL:HG11	2.01	0.43
2:D:597:ASP:N	2:D:597:ASP:OD1	2.52	0.43
2:H:807:ASP:O	2:H:810:LYS:HD2	2.19	0.43
1:A:36:ALA:O	1:A:40:LEU:HB2	2.18	0.43
1:A:78:ILE:HD11	1:A:139:VAL:HG11	2.01	0.43
2:B:680:LYS:HG2	2:B:684:GLU:CD	2.39	0.43
1:E:231:GLY:O	2:F:724:GLY:HA2	2.18	0.43
1:C:157:ALA:HB2	1:C:215:TYR:HD2	1.84	0.43
1:C:188:THR:HG22	2:D:506:SER:OG	2.18	0.43
2:D:698:SER:OG	4:D:967:HOH:O	2.22	0.43
1:G:36:ALA:O	1:G:40:LEU:HB2	2.18	0.43
2:H:372:LYS:NZ	4:H:944:HOH:O	2.40	0.43
1:E:179:LYS:HG3	2:F:469:ARG:HD2	2.00	0.43
2:D:310:ASN:ND2	2:D:764:ASP:OD2	2.52	0.42
2:D:319:VAL:HG12	2:D:320:PHE:CE1	2.54	0.42
2:D:643:GLN:HG2	2:D:644:ASP:N	2.34	0.42
2:H:330:SER:HA	2:H:441:ASN:O	2.18	0.42
2:D:318:LEU:HB2	2:D:421:MET:SD	2.59	0.42
2:D:580:ARG:CZ	4:D:904:HOH:O	2.67	0.42
2:F:651:ASN:OD1	2:F:652:ILE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:263:THR:CB	2:H:526:ARG:NH2	2.58	0.42
2:B:528:THR:O	2:B:532:THR:HG22	2.19	0.42
2:B:319:VAL:HG12	2:B:320:PHE:CE1	2.55	0.42
1:A:200:LYS:NZ	2:B:510:ASP:OD2	2.48	0.42
2:D:294:TYR:CE2	2:D:312:PRO:HB3	2.54	0.42
1:A:179:LYS:HE2	2:B:515:ASP:O	2.20	0.42
2:B:597:ASP:N	2:B:597:ASP:OD1	2.53	0.42
2:B:286:GLN:HG2	2:B:743:GLY:HA2	2.01	0.42
1:C:67:LYS:HG3	2:D:369:ILE:CD1	2.49	0.42
1:C:215:TYR:OH	2:D:391:LYS:HD3	2.19	0.42
2:F:318:LEU:HB2	2:F:421:MET:SD	2.59	0.42
4:G:302:HOH:O	2:H:776:PRO:O	2.22	0.42
1:C:112:ASP:N	1:C:112:ASP:OD1	2.43	0.42
1:E:188:THR:HG22	2:F:506:SER:OG	2.19	0.42
2:F:513:ALA:HB2	2:F:521:TRP:CE3	2.54	0.42
2:H:513:ALA:HB2	2:H:521:TRP:CE3	2.55	0.42
1:A:66:ASP:HB3	2:B:369:ILE:HD13	2.02	0.42
1:C:169:GLN:HG3	4:C:333:HOH:O	2.18	0.42
2:D:622:VAL:O	2:D:626:VAL:HG23	2.20	0.42
2:F:326:ILE:HG22	2:F:446:ASP:HB3	2.01	0.42
1:G:56:GLU:CG	2:H:370:ALA:HB3	2.50	0.42
2:H:310:ASN:ND2	2:H:764:ASP:OD2	2.52	0.42
2:B:663:LEU:HD13	2:B:677:PHE:HZ	1.84	0.42
1:C:200:LYS:NZ	2:D:510:ASP:OD2	2.44	0.42
1:E:61:ALA:HB1	1:E:235:ALA:HB2	2.02	0.42
1:G:174:VAL:HG22	2:H:674:VAL:HG12	2.01	0.42
2:H:265:ASN:HB3	2:H:503:TRP:CG	2.55	0.42
2:H:622:VAL:O	2:H:626:VAL:HG23	2.20	0.42
2:B:651:ASN:OD1	2:B:652:ILE:N	2.52	0.42
1:C:64:SER:HB2	4:C:340:HOH:O	2.19	0.42
1:E:78:ILE:CD1	1:E:139:VAL:HG11	2.50	0.42
2:F:807:ASP:O	2:F:810:LYS:HD2	2.19	0.42
1:G:215:TYR:OH	2:H:391:LYS:HD3	2.19	0.42
2:H:461:ASP:HA	2:H:484:LEU:HD13	2.02	0.42
2:H:651:ASN:OD1	2:H:652:ILE:N	2.52	0.42
1:A:197:TYR:N	2:B:508:GLN:HE21	2.18	0.41
2:B:513:ALA:HB2	2:B:521:TRP:CE3	2.55	0.41
1:C:61:ALA:HB1	1:C:235:ALA:HB2	2.03	0.41
2:D:346:SER:OG	2:D:348:GLU:HG3	2.20	0.41
2:D:663:LEU:HD13	2:D:677:PHE:HZ	1.85	0.41
2:H:528:THR:O	2:H:532:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:ASP:HA	2:B:484:LEU:HD13	2.02	0.41
2:B:807:ASP:O	2:B:810:LYS:HD2	2.21	0.41
1:C:231:GLY:O	2:D:724:GLY:HA2	2.20	0.41
1:E:39:ARG:HD2	1:E:42:GLN:OE1	2.21	0.41
1:E:8:LYS:HB3	1:E:20:TYR:HB2	2.02	0.41
2:F:319:VAL:HG12	2:F:320:PHE:CE1	2.56	0.41
2:D:262:THR:O	2:D:263:THR:O	2.37	0.41
2:F:597:ASP:N	2:F:597:ASP:OD1	2.54	0.41
1:A:157:ALA:HB2	1:A:215:TYR:HD2	1.86	0.41
1:E:67:LYS:HG3	2:F:369:ILE:CD1	2.50	0.41
1:C:248:GLN:NE2	4:C:307:HOH:O	2.53	0.41
2:D:426:TRP:HB3	2:D:427:PRO:HD3	2.03	0.41
1:A:192:ALA:HA	4:A:1020:HOH:O	2.19	0.41
2:B:622:VAL:O	2:B:626:VAL:HG23	2.20	0.41
2:D:265:ASN:HB3	2:D:503:TRP:CG	2.56	0.41
1:G:39:ARG:HD2	1:G:42:GLN:OE1	2.21	0.41
2:H:261:PRO:HA	2:H:286:GLN:O	2.20	0.41
2:H:319:VAL:HG12	2:H:320:PHE:CE1	2.56	0.41
2:H:383:ARG:NH2	2:H:407:ASP:OD2	2.53	0.41
2:F:310:ASN:ND2	2:F:764:ASP:OD2	2.53	0.41
2:H:264:GLY:HA2	2:H:286:GLN:HG3	2.02	0.41
2:F:622:VAL:O	2:F:626:VAL:HG23	2.21	0.41
1:G:186:ALA:HA	2:H:522:GLY:O	2.21	0.41
2:H:596:ASN:ND2	2:H:601:THR:HG1	2.17	0.41
2:B:264:GLY:CA	2:B:286:GLN:HG3	2.38	0.41
2:D:461:ASP:HA	2:D:484:LEU:HD13	2.02	0.41
2:H:484:LEU:HA	2:H:484:LEU:HD12	1.91	0.41
1:A:188:THR:HG22	2:B:506:SER:OG	2.21	0.41
1:E:197:TYR:HA	2:F:508:GLN:HE21	1.86	0.41
1:G:61:ALA:HB1	1:G:235:ALA:HB2	2.02	0.41
2:H:263:THR:HG22	2:H:526:ARG:NH2	2.32	0.41
2:H:767:ALA:HB2	2:H:791:TYR:HB2	2.03	0.41
1:A:215:TYR:OH	2:B:391:LYS:HD3	2.20	0.40
2:D:807:ASP:O	2:D:810:LYS:HD2	2.21	0.40
2:F:515:ASP:OD2	4:F:956:HOH:O	2.22	0.40
2:B:310:ASN:ND2	2:B:764:ASP:OD2	2.54	0.40
2:D:262:THR:O	2:D:286:GLN:O	2.39	0.40
1:E:157:ALA:HB2	1:E:215:TYR:HD2	1.87	0.40
2:H:318:LEU:HB2	2:H:421:MET:SD	2.61	0.40
2:H:597:ASP:OD1	2:H:597:ASP:N	2.55	0.40
1:A:39:ARG:HD2	1:A:42:GLN:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:TYR:CE2	2:B:312:PRO:HB3	2.56	0.40
2:B:383:ARG:NH2	2:B:407:ASP:OD2	2.53	0.40
1:C:78:ILE:CD1	1:C:139:VAL:HG11	2.52	0.40
1:C:8:LYS:HB3	1:C:20:TYR:HB2	2.03	0.40
1:C:157:ALA:HB2	1:C:215:TYR:CD2	2.55	0.40
2:F:383:ARG:NH2	2:F:407:ASP:OD2	2.54	0.40
1:G:179:LYS:HE2	2:H:515:ASP:O	2.21	0.40
1:A:157:ALA:HB2	1:A:215:TYR:CD2	2.56	0.40
2:B:318:LEU:HB2	2:B:421:MET:SD	2.62	0.40
1:A:186:ALA:HA	2:B:522:GLY:O	2.21	0.40
2:F:346:SER:OG	2:F:348:GLU:HG3	2.22	0.40

All (1) 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:C:98:ASP:OD2	2:F:361:LYS:NZ[1_565]	2.11	0.09

## 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	202/286 (71%)	196 (97%)	6 (3%)	0	100	100
1	C	256/286 (90%)	249 (97%)	6 (2%)	1 (0%)	34	54
1	E	256/286 (90%)	252 (98%)	4 (2%)	0	100	100
1	G	256/286 (90%)	249 (97%)	7 (3%)	0	100	100
2	B	529/568 (93%)	509 (96%)	18 (3%)	2 (0%)	34	54
2	D	558/568 (98%)	533 (96%)	24 (4%)	1 (0%)	47	68
2	F	558/568 (98%)	537 (96%)	19 (3%)	2 (0%)	34	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	558/568 (98%)	534 (96%)	23 (4%)	1 (0%)	47	68
All	All	3173/3416 (93%)	3059 (96%)	107 (3%)	7 (0%)	47	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	262	THR
1	C	4	PRO
2	B	263	THR
2	D	455	HIS
2	F	455	HIS
2	B	455	HIS
2	H	680	LYS

### 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	188/235 (80%)	179 (95%)	9 (5%)	25	48
1	C	211/235 (90%)	200 (95%)	11 (5%)	23	44
1	E	211/235 (90%)	200 (95%)	11 (5%)	23	44
1	G	211/235 (90%)	198 (94%)	13 (6%)	18	35
2	B	439/459 (96%)	409 (93%)	30 (7%)	16	30
2	D	451/459 (98%)	419 (93%)	32 (7%)	14	28
2	F	450/459 (98%)	420 (93%)	30 (7%)	16	31
2	H	451/459 (98%)	420 (93%)	31 (7%)	15	30
All	All	2612/2776 (94%)	2445 (94%)	167 (6%)	17	33

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL

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Mol	Chain	Res	Type
1	A	31	TYR
1	A	79	ARG
1	A	149	SER
1	A	181	LEU
1	A	182	VAL
1	A	193	ARG
1	A	227	LYS
1	A	229	THR
2	B	263	THR
2	B	273	LYS
2	B	311	THR
2	B	343	GLU
2	B	349	LYS
2	B	363	LEU
2	B	381	VAL
2	B	417	TRP
2	B	436	GLN
2	B	469	ARG
2	B	484	LEU
2	B	516	LEU
2	B	531	ASP
2	B	595	VAL
2	B	597	ASP
2	B	598	ASP
2	B	601	THR
2	B	619	LYS
2	B	643	GLN
2	B	647	THR
2	B	663	LEU
2	B	674	VAL
2	B	680	LYS
2	B	691	ASP
2	B	699	LYS
2	B	706	THR
2	B	731	LYS
2	B	808	GLU
2	B	811	GLU
2	B	817	GLN
1	C	7	VAL
1	C	79	ARG
1	C	112	ASP
1	C	149	SER

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Mol	Chain	Res	Type
1	C	181	LEU
1	C	182	VAL
1	C	193	ARG
1	C	203	LEU
1	C	205	ASN
1	C	227	LYS
1	C	229	THR
2	D	273	LYS
2	D	311	THR
2	D	343	GLU
2	D	348	GLU
2	D	349	LYS
2	D	363	LEU
2	D	377	GLU
2	D	381	VAL
2	D	394	THR
2	D	417	TRP
2	D	436	GLN
2	D	439	THR
2	D	469	ARG
2	D	484	LEU
2	D	516	LEU
2	D	531	ASP
2	D	595	VAL
2	D	597	ASP
2	D	598	ASP
2	D	601	THR
2	D	619	LYS
2	D	643	GLN
2	D	647	THR
2	D	663	LEU
2	D	674	VAL
2	D	691	ASP
2	D	699	LYS
2	D	706	THR
2	D	731	LYS
2	D	808	GLU
2	D	811	GLU
2	D	817	GLN
1	E	7	VAL
1	E	31	TYR
1	E	79	ARG

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Mol	Chain	Res	Type
1	E	112	ASP
1	E	149	SER
1	E	181	LEU
1	E	182	VAL
1	E	193	ARG
1	E	217	GLN
1	E	227	LYS
1	E	229	THR
2	F	273	LYS
2	F	311	THR
2	F	343	GLU
2	F	348	GLU
2	F	349	LYS
2	F	363	LEU
2	F	377	GLU
2	F	381	VAL
2	F	394	THR
2	F	417	TRP
2	F	436	GLN
2	F	469	ARG
2	F	484	LEU
2	F	516	LEU
2	F	531	ASP
2	F	595	VAL
2	F	597	ASP
2	F	598	ASP
2	F	601	THR
2	F	619	LYS
2	F	643	GLN
2	F	647	THR
2	F	663	LEU
2	F	674	VAL
2	F	691	ASP
2	F	699	LYS
2	F	706	THR
2	F	731	LYS
2	F	811	GLU
2	F	817	GLN
1	G	7	VAL
1	G	31	TYR
1	G	79	ARG
1	G	112	ASP

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Mol	Chain	Res	Type
1	G	149	SER
1	G	181	LEU
1	G	182	VAL
1	G	193	ARG
1	G	203	LEU
1	G	204	GLN
1	G	227	LYS
1	G	229	THR
1	G	260	TYR
2	H	262	THR
2	H	273	LYS
2	H	311	THR
2	H	343	GLU
2	H	348	GLU
2	H	349	LYS
2	H	363	LEU
2	H	377	GLU
2	H	381	VAL
2	H	417	TRP
2	H	436	GLN
2	H	469	ARG
2	H	484	LEU
2	H	516	LEU
2	H	531	ASP
2	H	595	VAL
2	H	597	ASP
2	H	598	ASP
2	H	601	THR
2	H	619	LYS
2	H	643	GLN
2	H	647	THR
2	H	663	LEU
2	H	674	VAL
2	H	680	LYS
2	H	691	ASP
2	H	699	LYS
2	H	706	THR
2	H	731	LYS
2	H	811	GLU
2	H	817	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	508	GLN
1	C	205	ASN
1	C	217	GLN
2	D	508	GLN
1	E	217	GLN
1	G	217	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 1 ligands modelled in this entry, 1 is 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	235/286 (82%)	0.34	9 (3%)	40 43	29, 39, 52, 75	0
1	C	258/286 (90%)	0.60	19 (7%)	14 15	27, 42, 63, 110	0
1	E	258/286 (90%)	0.53	13 (5%)	28 30	31, 44, 65, 105	0
1	G	258/286 (90%)	0.41	11 (4%)	35 38	27, 43, 63, 103	0
2	B	549/568 (96%)	0.51	27 (4%)	29 31	25, 40, 62, 80	0
2	D	560/568 (98%)	0.53	37 (6%)	18 19	27, 42, 64, 99	0
2	F	560/568 (98%)	0.56	35 (6%)	20 21	29, 45, 67, 94	0
2	H	560/568 (98%)	0.58	38 (6%)	17 17	29, 43, 65, 106	0
All	All	3238/3416 (94%)	0.52	189 (5%)	23 24	25, 43, 64, 110	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	261	PRO	10.3
2	D	262	THR	10.1
2	D	261	PRO	6.3
1	G	201	PHE	5.3
1	C	205	ASN	5.1
1	E	203	LEU	5.0
2	D	348	GLU	4.8
2	D	263	THR	4.8
1	C	198	PRO	4.4
1	E	202	ASP	4.3
2	H	394	THR	4.3
1	C	203	LEU	4.2
2	F	399	ALA	4.2
1	G	206	THR	4.1
2	F	262	THR	4.0
1	G	57	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	320	PHE	3.8
1	E	205	ASN	3.8
2	H	588	SER	3.8
2	F	294	TYR	3.8
2	B	350	PRO	3.7
1	A	198	PRO	3.7
2	D	311	THR	3.7
1	E	201	PHE	3.7
2	D	287	PHE	3.6
2	D	575	GLU	3.6
2	F	287	PHE	3.6
2	B	347	ALA	3.6
2	F	447	VAL	3.6
2	F	263	THR	3.6
2	D	681	PRO	3.5
2	F	754	THR	3.5
2	F	295	THR	3.4
2	D	264	GLY	3.4
2	D	298	ILE	3.4
1	C	4	PRO	3.4
2	H	705	VAL	3.4
2	F	357	GLY	3.3
2	F	311	THR	3.3
1	E	196	ALA	3.3
2	B	287	PHE	3.3
1	C	143	ALA	3.3
2	H	287	PHE	3.3
2	H	320	PHE	3.3
1	G	260	TYR	3.2
1	G	203	LEU	3.2
2	D	320	PHE	3.2
1	C	260	TYR	3.1
1	C	204	GLN	3.1
2	H	349	LYS	3.1
2	D	755	SER	3.1
2	H	264	GLY	3.1
2	H	575	GLU	3.1
1	E	198	PRO	3.0
1	E	193	ARG	3.0
2	F	755	SER	3.0
1	C	141	THR	3.0
2	D	319	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	298	ILE	2.9
2	D	294	TYR	2.9
2	D	568	ASP	2.9
2	H	348	GLU	2.9
2	D	375	GLN	2.9
2	B	477	LYS	2.9
2	D	313	PHE	2.9
2	F	757	ASN	2.9
2	B	345	LEU	2.9
2	H	262	THR	2.9
1	A	120	SER	2.8
2	B	597	ASP	2.8
1	C	142	MET	2.8
2	F	597	ASP	2.8
2	B	595	VAL	2.8
2	D	673	ALA	2.8
2	H	585	LYS	2.8
2	D	439	THR	2.8
2	H	697	LEU	2.8
2	B	755	SER	2.8
1	E	146	PHE	2.7
2	D	318	LEU	2.7
2	F	685	VAL	2.7
2	D	346	SER	2.7
2	B	757	ASN	2.7
2	B	705	VAL	2.7
2	H	572	ASN	2.7
1	C	138	PHE	2.7
2	F	331	THR	2.7
2	H	440	ILE	2.7
2	D	572	ASN	2.7
2	D	350	PRO	2.7
2	B	585	LYS	2.6
1	A	146	PHE	2.6
2	D	373	ASP	2.6
2	F	485	SER	2.6
1	E	109	ALA	2.6
1	G	205	ASN	2.6
2	H	311	THR	2.6
2	F	575	GLU	2.6
2	H	576	ASN	2.6
1	C	146	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	4	PRO	2.6
2	B	596	ASN	2.6
2	B	697	LEU	2.6
2	D	349	LYS	2.6
2	B	706	THR	2.5
2	F	681	PRO	2.5
2	D	722	PHE	2.5
2	B	686	ILE	2.5
2	H	478	TRP	2.5
2	H	754	THR	2.5
1	C	149	SER	2.5
2	B	394	THR	2.5
2	F	574	ALA	2.5
2	H	266	MET	2.5
2	F	318	LEU	2.4
2	F	446	ASP	2.4
1	G	109	ALA	2.4
2	D	317	GLY	2.4
2	F	312	PRO	2.4
2	B	311	THR	2.4
2	H	574	ALA	2.4
1	E	235	ALA	2.4
1	C	201	PHE	2.4
2	F	319	VAL	2.4
2	H	696	THR	2.4
2	H	319	VAL	2.4
2	H	819	GLN	2.4
1	E	138	PHE	2.3
2	B	359	TRP	2.3
2	D	378	THR	2.3
2	H	681	PRO	2.3
2	B	285	PRO	2.3
2	D	312	PRO	2.3
2	H	756	GLY	2.3
1	C	202	ASP	2.3
2	F	623	VAL	2.3
2	D	315	TYR	2.3
2	F	666	ASP	2.2
2	H	332	ALA	2.2
2	D	804	GLN	2.2
2	H	356	ASN	2.2
2	B	295	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	360	VAL	2.2
2	F	285	PRO	2.2
2	B	576	ASN	2.2
1	A	3	PRO	2.2
2	D	376	PRO	2.2
1	A	141	THR	2.2
1	C	3	PRO	2.2
2	B	375	GLN	2.1
2	D	286	GLN	2.1
2	D	285	PRO	2.1
2	H	261	PRO	2.1
1	A	237	THR	2.1
1	C	60	LYS	2.1
2	D	351	GLY	2.1
2	H	395	ALA	2.1
2	H	581	GLN	2.1
2	H	318	LEU	2.1
2	D	576	ASN	2.1
2	F	665	GLY	2.1
1	C	145	ARG	2.1
2	B	430	THR	2.1
2	F	427	PRO	2.1
1	E	236	LEU	2.1
2	F	264	GLY	2.1
1	C	135	ALA	2.1
1	G	226	ALA	2.1
1	A	138	PHE	2.1
2	B	516	LEU	2.1
2	F	519	PHE	2.1
2	F	588	SER	2.1
2	H	346	SER	2.1
2	H	698	SER	2.1
2	B	357	GLY	2.1
1	C	109	ALA	2.0
1	G	46	ALA	2.0
2	H	283	ASN	2.0
2	H	441	ASN	2.0
2	H	293	ALA	2.0
2	D	295	THR	2.0
2	H	263	THR	2.0
2	H	392	THR	2.0
1	E	260	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	804	GLN	2.0
1	A	57	VAL	2.0
1	A	260	TYR	2.0
1	G	146	PHE	2.0
2	B	578	PRO	2.0

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

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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	A	901	1/1	0.95	0.04	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.