



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:41 PM UTC

PDB ID : 3V93 / pdb_00003v93
Title : unliganded structure of TcrPDEC1 catalytic domain
Authors : Wang, H.; Kunz, S.; Chen, G.; Seebeck, T.; Wan, Y.; Robinson, H.; Martinelli, S.; Ke, H.
Deposited on : 2011-12-23
Resolution : 2.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

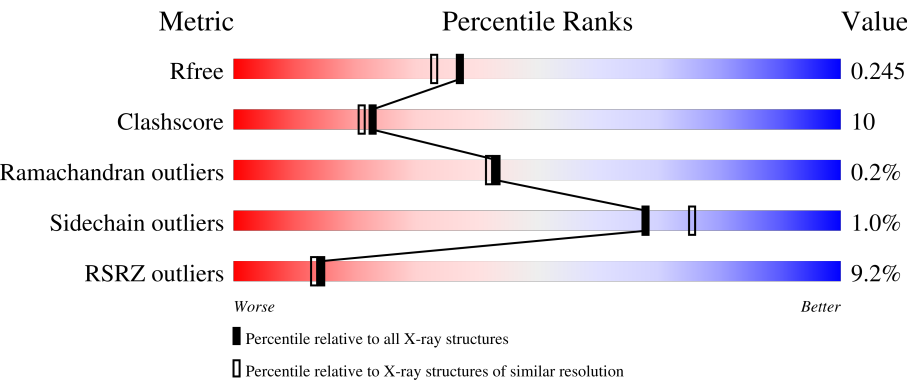
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	345	3% 80% 14% • 5%
1	B	345	6% 80% 16% • •
1	C	345	6% 77% 19% • •
1	D	345	25% 65% 28% • 6%
1	E	345	11% 77% 18% • 5%

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Mol	Chain	Length	Quality of chain
1	F	345	5% 76% 19% • •
1	G	345	6% 80% 16% • •
1	H	345	10% 75% 19% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21499 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 Cyclic nucleotide specific phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2553	1635	437	472	9			
1	B	333	Total	C	N	O	S	0	0	0
			2579	1650	441	479	9			
1	C	333	Total	C	N	O	S	0	0	0
			2579	1650	441	479	9			
1	D	324	Total	C	N	O	S	0	0	0
			2525	1618	432	467	8			
1	E	329	Total	C	N	O	S	0	0	0
			2555	1634	437	475	9			
1	F	334	Total	C	N	O	S	0	0	0
			2586	1654	442	481	9			
1	G	334	Total	C	N	O	S	0	0	0
			2586	1654	442	481	9			
1	H	328	Total	C	N	O	S	0	0	0
			2545	1629	436	471	9			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total 178	O 178	0	0
4	B	140	Total 140	O 140	0	0
4	C	136	Total 136	O 136	0	0
4	D	35	Total 35	O 35	0	0
4	E	90	Total 90	O 90	0	0
4	F	168	Total 168	O 168	0	0
4	G	147	Total 147	O 147	0	0

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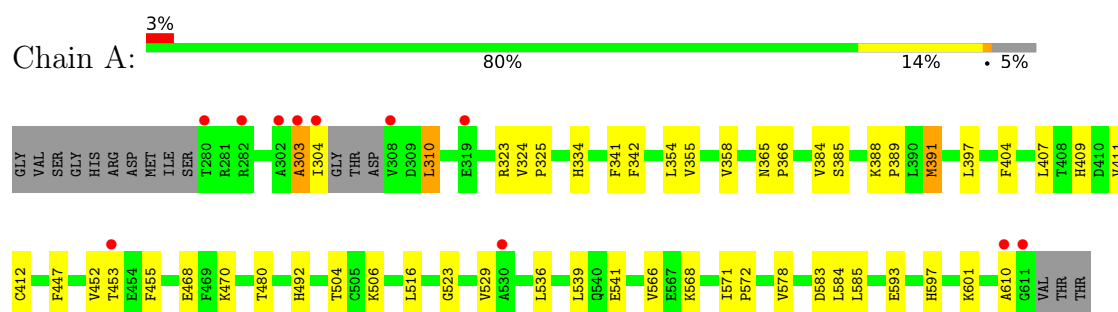
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	81	Total	O	0	0
			81	81		

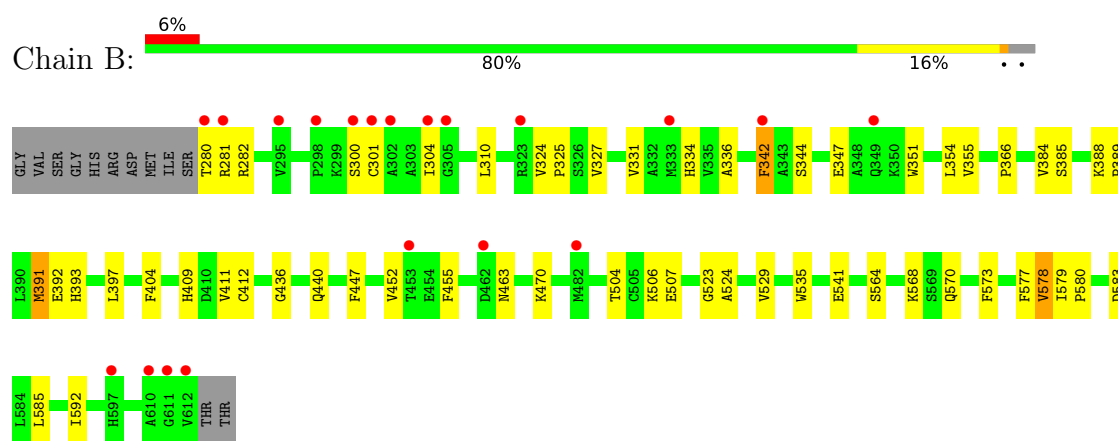
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

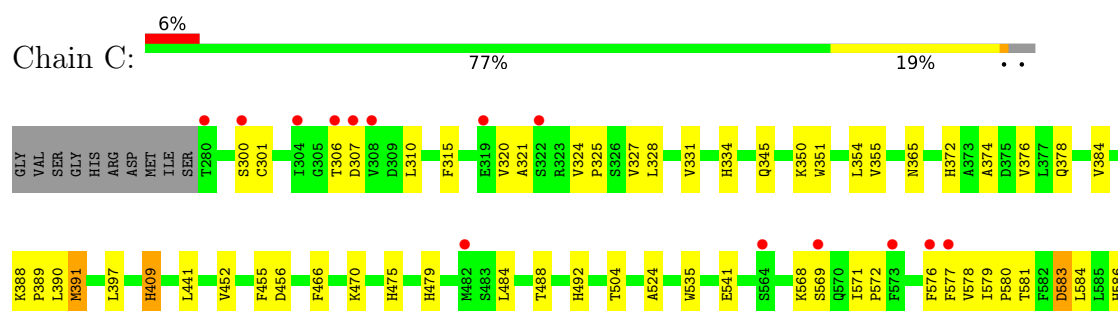
- Molecule 1: Cyclic nucleotide specific phosphodiesterase



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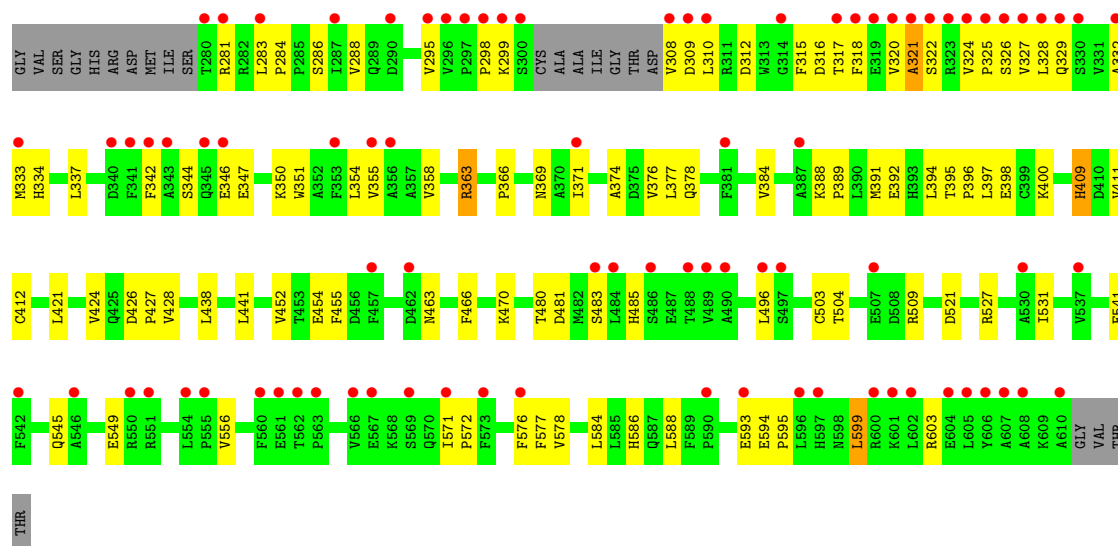


- Molecule 1: Cyclic nucleotide specific phosphodiesterase

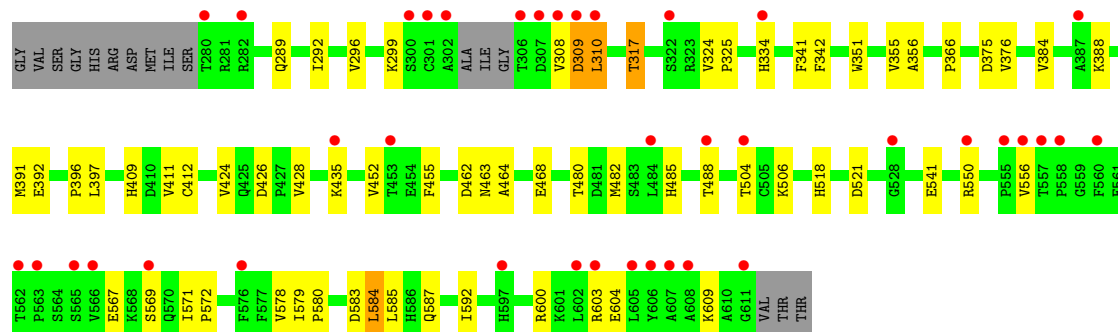
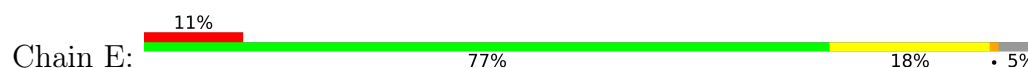




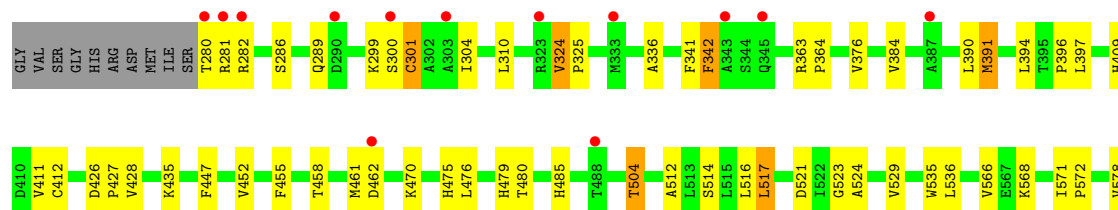
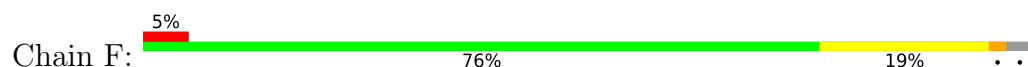
- Molecule 1: Cyclic nucleotide specific phosphodiesterase



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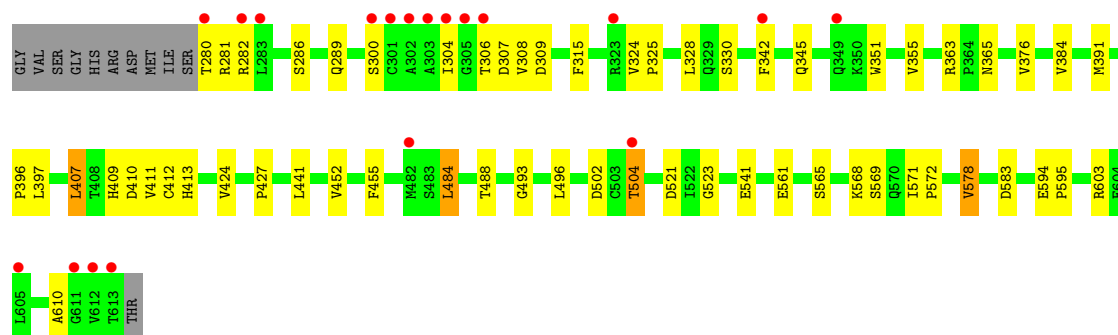
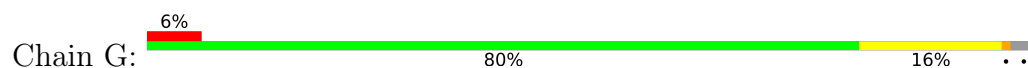


- Molecule 1: Cyclic nucleotide specific phosphodiesterase

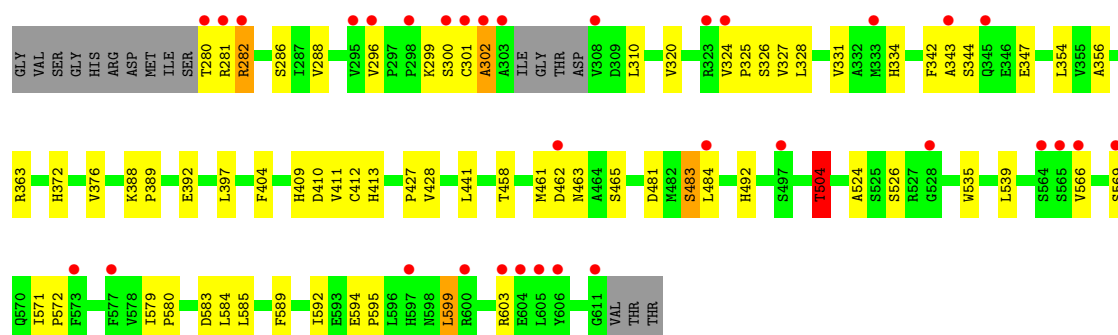
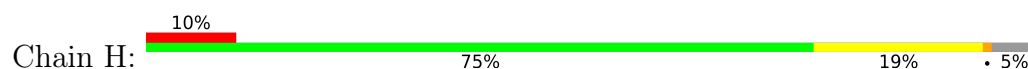




- Molecule 1: Cyclic nucleotide specific phosphodiesterase



- Molecule 1: Cyclic nucleotide specific phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	130.34Å 130.34Å 388.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 91.1 (30.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.97Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.226 0.215 , 0.245	Depositor DCC
R_{free} test set	21151 reflections (9.66%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21499	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, ZN

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	0.42	0/2617	0.84	9/3560 (0.3%)
1	B	0.40	0/2644	0.85	8/3599 (0.2%)
1	C	0.39	0/2644	0.82	4/3599 (0.1%)
1	D	0.33	0/2589	0.81	7/3522 (0.2%)
1	E	0.38	0/2619	0.85	8/3563 (0.2%)
1	F	0.41	0/2651	0.86	10/3609 (0.3%)
1	G	0.40	0/2651	0.84	6/3609 (0.2%)
1	H	0.36	0/2609	0.82	7/3549 (0.2%)
All	All	0.39	0/21024	0.83	59/28610 (0.2%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	435	LYS	N-CA-C	11.63	123.64	110.97
1	B	578	VAL	N-CA-C	9.48	119.52	110.42
1	F	578	VAL	N-CA-C	9.28	119.33	110.42
1	G	578	VAL	N-CA-C	7.93	118.00	110.30
1	A	578	VAL	N-CA-C	7.65	117.76	110.42
1	G	583	ASP	N-CA-C	-7.57	102.17	111.40
1	B	342	PHE	N-CA-C	7.13	121.07	109.59
1	A	583	ASP	N-CA-C	-7.09	103.48	111.14
1	F	583	ASP	N-CA-C	-7.07	102.77	111.40
1	A	504	THR	N-CA-C	-6.95	104.78	113.18
1	B	583	ASP	N-CA-C	-6.83	103.76	111.14
1	F	409	HIS	N-CA-C	6.81	120.47	111.75
1	G	504	THR	N-CA-C	-6.69	105.09	113.18
1	F	342	PHE	N-CA-C	6.64	120.22	109.40
1	E	342	PHE	N-CA-C	6.56	120.09	109.40
1	E	578	VAL	N-CA-C	6.45	116.61	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	504	THR	N-CA-C	-6.42	104.94	112.89
1	G	409	HIS	N-CA-C	6.36	119.89	111.75
1	A	342	PHE	N-CA-C	6.31	119.75	109.59
1	G	342	PHE	N-CA-C	6.31	119.81	109.72
1	H	589	PHE	CA-C-N	6.17	126.63	119.47
1	H	589	PHE	C-N-CA	6.17	126.63	119.47
1	B	523	GLY	N-CA-C	6.15	125.49	115.46
1	E	504	THR	N-CA-C	-6.12	105.64	113.23
1	E	341	PHE	N-CA-C	6.11	117.94	111.28
1	B	529	VAL	N-CA-C	6.10	116.28	110.42
1	E	409	HIS	N-CA-C	6.03	119.46	111.75
1	D	480	THR	N-CA-C	-6.01	105.71	113.16
1	F	529	VAL	N-CA-C	5.90	116.56	110.36
1	C	504	THR	N-CA-C	-5.87	105.61	112.89
1	H	583	ASP	N-CA-C	-5.83	104.84	111.14
1	D	578	VAL	N-CA-C	5.74	115.87	110.30
1	A	529	VAL	N-CA-C	5.73	116.38	110.36
1	C	583	ASP	N-CA-C	-5.72	105.12	111.36
1	H	409	HIS	N-CA-C	5.68	119.02	111.75
1	C	409	HIS	N-CA-C	5.61	119.64	112.34
1	E	480	THR	N-CA-C	-5.58	106.25	113.16
1	A	409	HIS	N-CA-C	5.57	119.17	112.38
1	D	409	HIS	N-CA-C	5.56	118.87	111.75
1	B	409	HIS	N-CA-C	5.53	118.82	111.75
1	B	504	THR	N-CA-C	-5.50	106.34	113.16
1	F	523	GLY	N-CA-C	5.46	124.36	115.46
1	C	578	VAL	N-CA-C	5.38	115.59	110.42
1	E	310	LEU	N-CA-C	-5.31	106.77	113.20
1	F	341	PHE	N-CA-C	5.29	117.13	111.36
1	H	343	ALA	N-CA-C	-5.27	107.22	113.97
1	A	341	PHE	N-CA-C	5.24	116.67	111.07
1	D	342	PHE	N-CA-C	5.22	118.58	110.17
1	F	324	VAL	N-CA-C	5.22	113.63	107.84
1	D	504	THR	N-CA-C	-5.21	106.88	113.18
1	A	523	GLY	N-CA-C	5.20	123.93	115.46
1	F	480	THR	N-CA-C	-5.14	106.79	113.16
1	H	342	PHE	N-CA-C	5.14	118.44	110.17
1	G	523	GLY	N-CA-C	5.12	123.81	115.46
1	D	577	PHE	N-CA-C	5.12	118.98	112.12
1	D	503	CYS	N-CA-C	5.10	118.99	112.87
1	A	480	THR	N-CA-C	-5.07	107.09	113.28
1	B	577	PHE	N-CA-C	5.03	118.67	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	504	THR	N-CA-C	-5.03	106.65	112.89

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	2553	0	2514	35	0
1	B	2579	0	2538	50	0
1	C	2579	0	2538	58	0
1	D	2525	0	2485	78	0
1	E	2555	0	2509	51	0
1	F	2586	0	2545	50	0
1	G	2586	0	2545	55	0
1	H	2545	0	2503	59	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	178	0	0	2	0
4	B	140	0	0	1	0
4	C	136	0	0	2	0
4	D	35	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	90	0	0	5	0
4	F	168	0	0	5	0
4	G	147	0	0	10	0
4	H	81	0	0	1	0
All	All	21499	0	20177	422	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (422) 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:G:571:ILE:HG23	1:G:603:ARG:HH12	0.99	1.12
1:G:571:ILE:HG23	1:G:603:ARG:NH1	1.66	1.10
1:C:571:ILE:HG23	1:C:603:ARG:HH12	1.19	1.08
1:E:299:LYS:HD3	1:E:325:PRO:HB2	1.44	1.00
1:D:571:ILE:HG23	1:D:603:ARG:HH12	1.31	0.96
1:C:571:ILE:HG23	1:C:603:ARG:NH1	1.83	0.93
1:F:289:GLN:HB3	1:F:363:ARG:NH2	1.81	0.93
1:C:391:MET:HE2	1:C:391:MET:HA	1.52	0.92
1:G:571:ILE:CG2	1:G:603:ARG:HH12	1.83	0.91
1:F:289:GLN:HB3	1:F:363:ARG:HH21	1.30	0.91
1:B:388:LYS:H	1:B:388:LYS:HD2	1.34	0.90
1:H:286:SER:HB2	1:H:427:PRO:HG2	1.54	0.89
1:G:391:MET:HE2	1:G:391:MET:HA	1.53	0.89
1:B:300:SER:HB3	1:B:325:PRO:HG3	1.51	0.88
1:G:568:LYS:HG3	1:G:610:ALA:HB1	1.56	0.86
1:E:391:MET:HE2	1:E:391:MET:HA	1.57	0.86
1:E:571:ILE:HG23	1:E:603:ARG:HH12	1.41	0.84
1:B:564:SER:HB3	1:C:600:ARG:HH21	1.46	0.80
1:D:586:HIS:CD2	1:D:593:GLU:HG2	2.16	0.80
1:G:488:THR:HG21	4:G:883:HOH:O	1.80	0.80
1:D:286:SER:HB2	1:D:427:PRO:HG2	1.64	0.80
1:F:391:MET:HA	1:F:391:MET:HE2	1.64	0.79
1:B:393:HIS:NE2	1:F:504:THR:HG21	1.97	0.79
1:G:286:SER:HB2	1:G:427:PRO:HG2	1.65	0.78
1:F:281:ARG:HH21	1:H:463:ASN:HD22	1.32	0.78
1:D:363:ARG:HH11	1:D:363:ARG:HA	1.49	0.77
1:C:568:LYS:HG2	1:C:610:ALA:HB1	1.64	0.77
1:G:502:ASP:OD2	1:G:504:THR:HG22	1.84	0.76
1:C:603:ARG:HG3	1:C:603:ARG:HH11	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:VAL:HG12	1:D:391:MET:HE3	1.68	0.76
1:D:571:ILE:HG23	1:D:603:ARG:NH1	2.01	0.76
1:E:384:VAL:HG12	1:E:391:MET:HE3	1.67	0.76
1:D:310:LEU:HG	1:D:334:HIS:CD2	2.21	0.75
1:F:384:VAL:HG12	1:F:391:MET:HE3	1.68	0.75
1:E:571:ILE:HG23	1:E:603:ARG:NH1	2.03	0.74
1:E:567:GLU:HG2	1:E:609:LYS:HG2	1.69	0.74
1:A:355:VAL:HG22	1:A:407:LEU:HD11	1.69	0.74
1:G:304:ILE:HG21	1:G:315:PHE:HE1	1.54	0.73
1:B:281:ARG:HH11	1:D:463:ASN:HD22	1.38	0.71
1:E:485:HIS:O	1:E:488:THR:HG22	1.90	0.71
1:H:428:VAL:HG11	1:H:441:LEU:HD12	1.72	0.71
1:F:300:SER:O	1:F:301:CYS:HB2	1.91	0.71
1:H:571:ILE:HG23	1:H:603:ARG:NH1	2.07	0.70
1:G:384:VAL:HG12	1:G:391:MET:HE3	1.73	0.70
1:H:458:THR:O	1:H:461:MET:HB2	1.91	0.70
1:F:286:SER:HB2	1:F:427:PRO:HG2	1.74	0.69
1:C:569:SER:O	1:C:572:PRO:HD2	1.92	0.69
1:B:280:THR:HB	1:B:282:ARG:CZ	2.23	0.68
1:E:585:LEU:HD21	1:E:592:ILE:HD12	1.76	0.68
1:E:603:ARG:HG3	1:E:603:ARG:HH11	1.58	0.68
1:G:289:GLN:HB2	1:G:363:ARG:HH21	1.56	0.68
1:H:603:ARG:HG3	1:H:603:ARG:HH11	1.58	0.68
1:C:571:ILE:CG2	1:C:603:ARG:HH12	2.01	0.67
1:D:391:MET:HA	1:D:391:MET:HE2	1.76	0.66
1:H:324:VAL:CG2	1:H:325:PRO:HD2	2.24	0.66
1:E:324:VAL:HG22	1:E:325:PRO:HD2	1.76	0.66
1:H:324:VAL:HG23	1:H:325:PRO:HD2	1.78	0.66
1:B:463:ASN:HD22	1:D:281:ARG:HH11	1.43	0.66
4:E:847:HOH:O	1:H:504:THR:HG21	1.96	0.66
1:H:282:ARG:HG2	1:H:282:ARG:O	1.96	0.66
1:C:571:ILE:HB	1:C:572:PRO:HD3	1.77	0.66
1:E:324:VAL:CG2	1:E:325:PRO:HD2	2.26	0.65
1:C:607:ALA:HB1	1:C:612:VAL:HB	1.79	0.65
1:G:595:PRO:HG2	4:G:832:HOH:O	1.94	0.65
1:H:288:VAL:HG11	1:H:441:LEU:HD11	1.78	0.65
1:C:391:MET:HA	1:C:391:MET:CE	2.26	0.65
1:B:463:ASN:ND2	1:D:281:ARG:HH11	1.95	0.65
1:C:320:VAL:HG12	1:C:327:VAL:HG22	1.78	0.65
1:F:447:PHE:CZ	1:F:470:LYS:HG3	2.33	0.64
1:F:300:SER:HB3	1:F:325:PRO:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:481:ASP:OD2	1:H:483:SER:HB3	1.97	0.64
1:D:354:LEU:C	1:D:354:LEU:HD23	2.23	0.64
1:C:586:HIS:CE1	1:C:593:GLU:HG2	2.33	0.63
1:D:298:PRO:HA	1:D:329:GLN:OE1	1.97	0.63
1:D:324:VAL:CG2	1:D:325:PRO:HD2	2.28	0.63
1:D:324:VAL:HG23	1:D:325:PRO:HD2	1.81	0.62
1:D:571:ILE:HB	1:D:572:PRO:HD3	1.79	0.62
1:B:300:SER:O	1:B:301:CYS:HB2	1.99	0.62
1:B:585:LEU:HD21	1:B:592:ILE:HD12	1.80	0.62
1:D:603:ARG:HG3	1:D:603:ARG:HH11	1.64	0.62
1:H:441:LEU:C	1:H:441:LEU:HD23	2.24	0.62
1:A:358:VAL:HG11	1:A:407:LEU:HD23	1.81	0.62
1:D:395:THR:OG1	1:D:398:GLU:HG3	2.00	0.62
1:F:282:ARG:HD3	1:F:282:ARG:C	2.25	0.62
1:H:492:HIS:HB2	1:H:584:LEU:HD21	1.80	0.62
1:B:281:ARG:HH11	1:D:463:ASN:ND2	1.97	0.62
1:G:363:ARG:NH2	4:G:921:HOH:O	2.26	0.61
1:E:388:LYS:HE3	1:E:392:GLU:OE2	2.01	0.61
1:B:280:THR:HG23	4:D:828:HOH:O	2.00	0.61
1:C:300:SER:O	1:C:301:CYS:HB2	2.00	0.61
1:F:516:LEU:CD2	1:F:585:LEU:HD11	2.31	0.61
1:C:300:SER:HB3	1:C:325:PRO:HG3	1.83	0.61
1:C:321:ALA:HA	1:C:327:VAL:CG2	2.31	0.60
1:G:328:LEU:HD11	1:G:407:LEU:HD12	1.83	0.60
1:B:388:LYS:O	1:B:392:GLU:HG3	2.01	0.60
1:D:424:VAL:HG12	1:D:424:VAL:O	2.00	0.60
1:D:309:ASP:OD1	1:D:309:ASP:O	2.20	0.60
1:B:388:LYS:N	1:B:389:PRO:HD2	2.16	0.60
1:C:321:ALA:HA	1:C:327:VAL:HG23	1.84	0.60
1:E:324:VAL:HG22	4:E:869:HOH:O	2.02	0.60
1:C:484:LEU:O	1:C:488:THR:HG23	2.02	0.59
1:A:324:VAL:CG2	1:A:325:PRO:HD2	2.32	0.59
1:D:496:LEU:HD13	1:D:588:LEU:HD23	1.84	0.59
1:E:317:THR:HG21	1:E:375:ASP:HA	1.85	0.59
1:B:388:LYS:HD2	1:B:388:LYS:N	2.13	0.59
1:C:345:GLN:HE21	1:C:345:GLN:HA	1.67	0.59
1:F:462:ASP:HB2	4:F:889:HOH:O	2.00	0.59
1:D:309:ASP:CG	1:D:312:ASP:HB3	2.28	0.59
1:D:595:PRO:O	1:D:599:LEU:HD22	2.02	0.59
1:G:603:ARG:CZ	4:G:847:HOH:O	2.50	0.59
1:A:304:ILE:HG12	1:A:334:HIS:CE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:584:LEU:HD23	1:F:584:LEU:C	2.28	0.58
1:F:384:VAL:CG1	1:F:391:MET:HE3	2.33	0.58
1:A:304:ILE:H	1:A:334:HIS:HE1	1.50	0.58
1:E:384:VAL:CG1	1:E:391:MET:HE3	2.30	0.58
1:E:463:ASN:HD22	1:G:281:ARG:HH11	1.52	0.58
1:G:289:GLN:HB2	1:G:363:ARG:NH2	2.19	0.58
1:H:310:LEU:HG	1:H:334:HIS:CD2	2.39	0.58
1:G:384:VAL:CG1	1:G:391:MET:HE3	2.33	0.58
1:D:426:ASP:OD1	1:D:428:VAL:HG22	2.04	0.57
1:D:397:LEU:C	1:D:397:LEU:HD23	2.28	0.57
1:H:388:LYS:HE3	1:H:392:GLU:CD	2.29	0.57
1:D:320:VAL:C	1:D:322:SER:H	2.13	0.57
1:C:492:HIS:HB2	1:C:584:LEU:HD21	1.85	0.57
1:D:308:VAL:HG22	1:D:308:VAL:O	2.02	0.57
1:E:583:ASP:O	1:E:587:GLN:HG3	2.04	0.57
1:H:585:LEU:HD21	1:H:592:ILE:HD12	1.85	0.57
1:G:345:GLN:HA	1:G:345:GLN:NE2	2.19	0.56
1:G:282:ARG:O	1:G:282:ARG:HD3	2.06	0.56
1:D:366:PRO:HD2	1:D:541:GLU:HG2	1.88	0.56
1:F:516:LEU:HD23	1:F:585:LEU:HD11	1.86	0.56
1:D:286:SER:HB2	1:D:427:PRO:CG	2.36	0.56
1:D:317:THR:HG23	1:D:327:VAL:HG11	1.88	0.56
1:H:282:ARG:H	1:H:282:ARG:HD2	1.70	0.56
1:B:568:LYS:NZ	1:C:580:PRO:HB3	2.21	0.55
1:E:308:VAL:O	1:E:309:ASP:HB2	2.04	0.55
1:H:579:ILE:HB	1:H:580:PRO:HD3	1.88	0.55
1:G:561:GLU:HG3	4:G:894:HOH:O	2.05	0.55
1:D:384:VAL:CG1	1:D:391:MET:HE3	2.37	0.55
1:B:281:ARG:NH1	1:D:463:ASN:HD22	2.03	0.54
1:B:447:PHE:CE1	1:B:470:LYS:HG3	2.43	0.54
1:C:397:LEU:C	1:C:397:LEU:HD23	2.33	0.54
1:G:424:VAL:HG12	1:G:424:VAL:O	2.06	0.54
1:D:308:VAL:O	1:D:309:ASP:HB3	2.05	0.54
1:A:324:VAL:HG22	1:A:325:PRO:HD2	1.89	0.54
1:E:376:VAL:HG22	1:E:521:ASP:HA	1.89	0.54
1:G:397:LEU:HD23	1:G:397:LEU:C	2.33	0.54
1:B:280:THR:HG22	1:B:281:ARG:N	2.21	0.54
1:C:306:THR:HG22	1:C:307:ASP:N	2.23	0.54
1:D:333:MET:O	1:D:337:LEU:HG	2.08	0.54
1:C:376:VAL:HG21	1:C:409:HIS:CE1	2.43	0.54
1:C:603:ARG:NH1	1:C:603:ARG:HG3	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:584:LEU:CD2	1:F:588:LEU:HD12	2.38	0.53
1:H:397:LEU:C	1:H:397:LEU:HD23	2.33	0.53
1:F:325:PRO:HG2	4:F:892:HOH:O	2.08	0.53
1:G:300:SER:HB2	1:G:325:PRO:HG3	1.90	0.53
1:D:421:LEU:HD11	1:D:438:LEU:HD21	1.91	0.52
1:E:463:ASN:ND2	1:G:281:ARG:HH11	2.07	0.52
1:A:453:THR:HG23	4:A:963:HOH:O	2.08	0.52
1:D:549:GLU:OE2	1:D:556:VAL:HA	2.08	0.52
1:G:391:MET:HA	1:G:391:MET:CE	2.32	0.52
1:H:280:THR:HG22	1:H:281:ARG:N	2.24	0.52
1:B:463:ASN:HD22	1:D:281:ARG:NH1	2.07	0.52
1:D:363:ARG:HH11	1:D:363:ARG:CA	2.20	0.52
1:G:282:ARG:HD3	1:G:282:ARG:C	2.34	0.52
1:D:584:LEU:C	1:D:584:LEU:HD13	2.34	0.52
1:E:585:LEU:CD2	1:E:592:ILE:HD12	2.38	0.52
1:G:484:LEU:O	1:G:488:THR:HG23	2.10	0.52
1:E:424:VAL:HG12	1:E:424:VAL:O	2.09	0.52
1:E:600:ARG:O	1:E:604:GLU:HG3	2.10	0.52
1:B:280:THR:HB	1:B:282:ARG:NH1	2.24	0.51
1:E:309:ASP:HA	4:E:879:HOH:O	2.09	0.51
1:H:526:SER:HB2	1:H:599:LEU:HD22	1.90	0.51
1:H:539:LEU:HD11	1:H:566:VAL:HG13	1.92	0.51
1:G:304:ILE:HG21	1:G:315:PHE:CE1	2.41	0.51
1:G:376:VAL:HG22	1:G:521:ASP:HA	1.91	0.51
1:B:568:LYS:HZ3	1:C:580:PRO:HB3	1.75	0.51
1:F:476:LEU:HB3	1:F:517:LEU:HD12	1.93	0.51
1:F:584:LEU:HD23	1:F:588:LEU:HD12	1.93	0.51
1:H:299:LYS:HD3	1:H:325:PRO:HB2	1.92	0.51
1:B:388:LYS:H	1:B:388:LYS:CD	2.14	0.51
1:H:571:ILE:HB	1:H:572:PRO:HD3	1.92	0.51
1:B:384:VAL:CG1	1:B:391:MET:HE3	2.41	0.50
1:H:594:GLU:N	1:H:595:PRO:HD2	2.26	0.50
1:A:303:ALA:HA	1:A:334:HIS:CE1	2.47	0.50
1:B:447:PHE:CZ	1:B:470:LYS:HG3	2.47	0.50
1:E:603:ARG:NH1	1:E:603:ARG:HG3	2.25	0.50
1:E:351:TRP:O	1:E:355:VAL:HG23	2.11	0.50
1:E:571:ILE:CG2	1:E:603:ARG:HH12	2.20	0.50
1:H:327:VAL:O	1:H:331:VAL:HG23	2.11	0.50
1:A:468:GLU:OE2	1:A:506:LYS:HD2	2.11	0.50
1:E:468:GLU:OE2	1:E:506:LYS:HD2	2.11	0.50
1:E:482:MET:SD	1:E:518:HIS:HE1	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:THR:HG22	1:G:308:VAL:H	1.76	0.50
1:D:321:ALA:HA	1:D:327:VAL:CG2	2.41	0.50
1:F:324:VAL:HB	1:F:325:PRO:HD2	1.94	0.50
1:F:397:LEU:C	1:F:397:LEU:HD23	2.36	0.50
1:H:302:ALA:HB3	1:H:324:VAL:HG23	1.93	0.50
1:C:345:GLN:HA	1:C:345:GLN:NE2	2.26	0.49
1:D:369:ASN:OD1	1:D:371:ILE:HB	2.11	0.49
1:G:325:PRO:HG2	4:G:885:HOH:O	2.12	0.49
1:A:388:LYS:HB3	1:A:389:PRO:HD3	1.95	0.49
1:G:569:SER:HB2	4:G:922:HOH:O	2.10	0.49
1:D:316:ASP:O	1:D:320:VAL:HG23	2.12	0.49
1:E:567:GLU:HG2	1:E:609:LYS:CG	2.40	0.49
1:F:524:ALA:HB1	1:F:535:TRP:CD1	2.47	0.49
1:A:536:LEU:HD13	1:A:566:VAL:HG11	1.94	0.49
1:B:397:LEU:HD23	1:B:397:LEU:C	2.37	0.49
1:G:365:ASN:HB3	1:G:541:GLU:OE1	2.12	0.49
1:B:452:VAL:HB	1:B:455:PHE:CD2	2.48	0.49
1:D:329:GLN:HA	1:D:355:VAL:HG11	1.95	0.49
1:E:571:ILE:HB	1:E:572:PRO:HD3	1.95	0.49
1:G:603:ARG:HG3	1:G:603:ARG:HH11	1.76	0.49
1:G:603:ARG:NH2	4:G:847:HOH:O	2.46	0.49
1:B:324:VAL:HB	1:B:325:PRO:HD2	1.95	0.49
1:A:397:LEU:C	1:A:397:LEU:HD23	2.38	0.49
1:E:550:ARG:HG3	1:E:556:VAL:HG22	1.94	0.49
1:E:366:PRO:HD2	1:E:541:GLU:HG2	1.94	0.48
1:E:452:VAL:HB	1:E:455:PHE:CD2	2.48	0.48
1:F:304:ILE:HG13	1:F:310:LEU:HD21	1.95	0.48
1:A:516:LEU:HD23	1:A:585:LEU:HD21	1.94	0.48
1:B:344:SER:OG	1:B:347:GLU:HG3	2.13	0.48
1:E:289:GLN:NE2	1:E:292:ILE:HD11	2.28	0.48
1:F:299:LYS:HG3	4:F:876:HOH:O	2.12	0.48
1:F:391:MET:HA	1:F:391:MET:CE	2.39	0.48
1:C:310:LEU:HG	1:C:334:HIS:CD2	2.48	0.48
1:D:299:LYS:HD2	1:D:326:SER:OG	2.14	0.48
1:E:584:LEU:HA	1:E:587:GLN:NE2	2.28	0.48
1:E:296:VAL:HG23	1:E:356:ALA:HB1	1.94	0.48
1:F:485:HIS:HE1	1:F:581:THR:OG1	1.97	0.48
1:H:484:LEU:N	1:H:484:LEU:HD12	2.29	0.48
1:C:466:PHE:CE2	1:C:470:LYS:HD2	2.49	0.48
1:F:458:THR:O	1:F:461:MET:HB2	2.13	0.48
1:A:571:ILE:HB	1:A:572:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:LYS:HB3	1:D:389:PRO:CD	2.44	0.48
1:G:452:VAL:HB	1:G:455:PHE:CD2	2.49	0.48
1:E:317:THR:CG2	1:E:375:ASP:OD1	2.62	0.47
1:D:481:ASP:CG	1:D:483:SER:HB3	2.39	0.47
1:B:391:MET:HE2	1:B:391:MET:HA	1.97	0.47
1:H:524:ALA:HB1	1:H:535:TRP:CD1	2.49	0.47
1:A:365:ASN:HB3	1:A:541:GLU:OE1	2.14	0.47
1:A:452:VAL:HB	1:A:455:PHE:CD2	2.49	0.47
1:A:568:LYS:CG	1:A:610:ALA:HB1	2.45	0.47
1:B:304:ILE:HG13	1:B:310:LEU:HD21	1.96	0.47
1:C:327:VAL:O	1:C:331:VAL:HG23	2.15	0.47
1:E:325:PRO:HG2	4:E:869:HOH:O	2.12	0.47
1:E:569:SER:O	1:E:572:PRO:HD2	2.15	0.47
1:E:584:LEU:HA	1:E:587:GLN:HE21	1.79	0.47
1:H:492:HIS:CB	1:H:584:LEU:HD21	2.45	0.47
1:H:569:SER:O	1:H:572:PRO:HD2	2.15	0.47
1:C:384:VAL:HG12	1:C:391:MET:HE3	1.96	0.47
1:D:454:GLU:N	1:D:454:GLU:OE1	2.48	0.47
1:H:280:THR:HG22	1:H:281:ARG:H	1.79	0.47
1:C:577:PHE:O	1:C:580:PRO:HG2	2.15	0.46
1:G:603:ARG:NE	4:G:847:HOH:O	2.46	0.46
1:A:366:PRO:HD2	1:A:541:GLU:CG	2.46	0.46
1:B:351:TRP:O	1:B:355:VAL:HG23	2.15	0.46
1:D:320:VAL:O	1:D:324:VAL:HG12	2.14	0.46
1:C:372:HIS:O	1:C:376:VAL:HG23	2.16	0.46
1:G:363:ARG:HA	1:G:363:ARG:HD3	1.79	0.46
1:G:411:VAL:O	1:G:412:CYS:HB2	2.14	0.46
1:E:411:VAL:O	1:E:412:CYS:HB2	2.16	0.46
1:F:452:VAL:HB	1:F:455:PHE:CD2	2.49	0.46
1:B:325:PRO:HG2	4:B:911:HOH:O	2.16	0.46
1:G:502:ASP:CG	1:G:504:THR:HG22	2.41	0.46
1:F:475:HIS:CD2	1:F:514:SER:OG	2.69	0.46
1:B:354:LEU:HD21	1:B:404:PHE:HE2	1.81	0.46
1:D:318:PHE:O	1:D:321:ALA:HB3	2.16	0.46
1:E:324:VAL:HG22	1:E:325:PRO:CD	2.44	0.46
1:D:324:VAL:HG22	1:D:326:SER:H	1.81	0.46
1:B:327:VAL:O	1:B:331:VAL:HG23	2.17	0.45
1:H:441:LEU:HD23	1:H:441:LEU:O	2.15	0.45
1:C:345:GLN:HE21	1:C:345:GLN:CA	2.28	0.45
1:A:324:VAL:HG22	4:A:903:HOH:O	2.15	0.45
1:C:492:HIS:CB	1:C:584:LEU:HD21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:LYS:HE3	1:D:392:GLU:CD	2.42	0.45
1:D:603:ARG:NH1	1:D:603:ARG:HG3	2.30	0.45
1:F:536:LEU:HD13	1:F:566:VAL:HG11	1.98	0.45
1:H:344:SER:OG	1:H:347:GLU:HG3	2.16	0.45
1:B:436:GLY:O	1:B:440:GLN:HG3	2.16	0.45
1:C:324:VAL:HB	1:C:325:PRO:HD2	1.99	0.45
1:D:376:VAL:HG22	1:D:521:ASP:HA	1.97	0.45
1:E:388:LYS:O	1:E:392:GLU:HG3	2.16	0.45
1:A:385:SER:HA	1:A:391:MET:HG3	1.99	0.45
1:C:576:PHE:O	1:C:576:PHE:CD2	2.69	0.45
1:B:366:PRO:HD2	1:B:541:GLU:HG2	1.97	0.45
1:A:354:LEU:HD21	1:A:404:PHE:CE2	2.52	0.45
1:A:539:LEU:HD11	1:A:566:VAL:HG13	1.99	0.45
1:F:475:HIS:O	1:F:479:HIS:HD2	2.00	0.45
1:D:328:LEU:HA	1:D:374:ALA:HB2	1.98	0.45
1:C:603:ARG:NH1	1:C:603:ARG:CG	2.80	0.44
1:D:283:LEU:HB3	1:D:284:PRO:HD2	2.00	0.44
1:G:306:THR:HG22	1:G:307:ASP:N	2.32	0.44
1:A:447:PHE:CZ	1:A:470:LYS:HG3	2.51	0.44
1:A:597:HIS:O	1:A:601:LYS:HG3	2.18	0.44
1:C:321:ALA:N	1:C:327:VAL:HG21	2.32	0.44
1:D:309:ASP:OD1	1:D:312:ASP:HB3	2.16	0.44
1:F:568:LYS:HG2	1:F:610:ALA:HB1	2.00	0.44
1:H:585:LEU:HD23	1:H:585:LEU:O	2.17	0.44
1:A:568:LYS:HG2	1:A:610:ALA:HB1	1.99	0.44
1:C:325:PRO:HG2	4:C:861:HOH:O	2.16	0.44
1:D:584:LEU:HD13	1:D:584:LEU:O	2.17	0.44
1:H:595:PRO:O	1:H:599:LEU:HD22	2.17	0.44
1:H:354:LEU:HD21	1:H:404:PHE:CE2	2.53	0.44
1:A:358:VAL:HG11	1:A:407:LEU:CD2	2.48	0.44
1:B:336:ALA:HB1	1:B:342:PHE:CE2	2.52	0.44
1:D:351:TRP:O	1:D:355:VAL:HG23	2.17	0.44
1:D:376:VAL:HG21	1:D:409:HIS:CE1	2.52	0.44
1:F:582:PHE:CD2	1:F:595:PRO:HB2	2.53	0.44
1:G:324:VAL:HB	1:G:325:PRO:HD2	2.00	0.44
1:B:354:LEU:HD21	1:B:404:PHE:CE2	2.52	0.44
1:A:411:VAL:O	1:A:412:CYS:HB2	2.17	0.44
1:G:280:THR:HG22	1:G:280:THR:O	2.18	0.44
1:G:565:SER:OG	1:G:568:LYS:HB2	2.16	0.44
1:H:354:LEU:HD21	1:H:404:PHE:HE2	1.83	0.44
1:C:354:LEU:HB2	1:C:455:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:396:PRO:HG2	4:E:863:HOH:O	2.18	0.43
1:H:282:ARG:O	1:H:282:ARG:CG	2.65	0.43
1:D:411:VAL:O	1:D:412:CYS:HB2	2.18	0.43
1:G:594:GLU:N	1:G:595:PRO:HD2	2.34	0.43
1:H:481:ASP:CG	1:H:483:SER:HB3	2.42	0.43
1:B:411:VAL:O	1:B:412:CYS:HB2	2.18	0.43
1:C:388:LYS:N	1:C:389:PRO:HD2	2.33	0.43
1:D:441:LEU:HD23	1:D:441:LEU:C	2.42	0.43
1:F:281:ARG:HH21	1:H:463:ASN:ND2	2.10	0.43
1:A:593:GLU:HG2	1:A:597:HIS:CD2	2.53	0.43
1:C:475:HIS:O	1:C:479:HIS:HD2	2.00	0.43
1:D:452:VAL:HB	1:D:455:PHE:CD2	2.54	0.43
1:F:426:ASP:OD1	1:F:428:VAL:HG12	2.19	0.43
1:H:372:HIS:O	1:H:376:VAL:HG23	2.18	0.43
1:H:441:LEU:C	1:H:441:LEU:CD2	2.91	0.43
1:D:332:ALA:HA	1:D:377:LEU:HD21	1.99	0.43
1:H:411:VAL:O	1:H:412:CYS:HB2	2.19	0.43
1:G:410:ASP:O	1:G:413:HIS:HB2	2.19	0.43
1:E:391:MET:HA	1:E:391:MET:CE	2.37	0.43
1:G:351:TRP:O	1:G:355:VAL:HG23	2.19	0.43
1:B:385:SER:HA	1:B:391:MET:HG3	2.00	0.43
1:C:384:VAL:CG1	1:C:391:MET:HE3	2.49	0.43
1:C:579:ILE:N	1:C:580:PRO:HD2	2.34	0.43
1:E:397:LEU:C	1:E:397:LEU:HD23	2.43	0.43
1:G:571:ILE:HB	1:G:572:PRO:HD3	2.01	0.43
1:B:585:LEU:CD2	1:B:592:ILE:HD12	2.47	0.43
1:C:365:ASN:HB3	1:C:541:GLU:OE1	2.19	0.43
1:F:411:VAL:O	1:F:412:CYS:HB2	2.18	0.43
1:A:324:VAL:HG22	1:A:325:PRO:CD	2.48	0.42
1:A:447:PHE:CE1	1:A:470:LYS:HG3	2.54	0.42
1:E:426:ASP:OD1	1:E:428:VAL:HG22	2.19	0.42
1:A:354:LEU:HD21	1:A:404:PHE:HE2	1.84	0.42
1:A:384:VAL:O	1:A:391:MET:HG2	2.18	0.42
1:F:376:VAL:HG22	1:F:521:ASP:HA	1.99	0.42
1:H:296:VAL:HG23	1:H:356:ALA:HB1	2.00	0.42
1:H:299:LYS:HD2	1:H:326:SER:HB2	2.01	0.42
1:H:300:SER:O	1:H:301:CYS:HB2	2.17	0.42
1:C:595:PRO:HG2	4:C:834:HOH:O	2.19	0.42
1:D:288:VAL:HG11	1:D:441:LEU:HD11	2.02	0.42
1:F:447:PHE:CE1	1:F:470:LYS:HG3	2.53	0.42
1:G:345:GLN:HA	1:G:345:GLN:HE21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:324:VAL:HG22	1:H:325:PRO:HD2	2.01	0.42
1:B:524:ALA:HB1	1:B:535:TRP:CD1	2.54	0.42
1:C:315:PHE:CD2	1:C:378:GLN:HG3	2.55	0.42
1:D:396:PRO:O	1:D:400:LYS:HG3	2.19	0.42
1:H:302:ALA:CB	1:H:324:VAL:HG23	2.50	0.42
1:B:570:GLN:O	1:B:573:PHE:HB3	2.20	0.42
1:D:466:PHE:CE2	1:D:470:LYS:HD2	2.55	0.42
1:D:594:GLU:N	1:D:595:PRO:HD2	2.34	0.42
1:F:396:PRO:HG2	4:F:965:HOH:O	2.19	0.42
1:F:610:ALA:HB3	1:F:612:VAL:HG23	2.02	0.42
1:B:579:ILE:HB	1:B:580:PRO:HD3	2.02	0.42
1:D:317:THR:HG22	1:D:371:ILE:HG23	2.01	0.42
1:D:545:GLN:O	1:D:549:GLU:HG3	2.20	0.42
1:F:571:ILE:HB	1:F:572:PRO:HD3	2.01	0.42
1:H:320:VAL:O	1:H:324:VAL:HG12	2.20	0.42
1:H:595:PRO:HG2	4:H:853:HOH:O	2.19	0.42
1:B:384:VAL:HG12	1:B:391:MET:HG2	2.02	0.41
1:D:527:ARG:HB3	1:D:531:ILE:HD12	2.02	0.41
1:E:579:ILE:HB	1:E:580:PRO:HD3	2.02	0.41
1:F:336:ALA:HB1	1:F:342:PHE:CE2	2.55	0.41
1:C:351:TRP:O	1:C:355:VAL:HG23	2.20	0.41
1:C:524:ALA:HB1	1:C:535:TRP:CD1	2.55	0.41
1:B:506:LYS:HE3	1:B:507:GLU:OE2	2.21	0.41
1:C:452:VAL:HB	1:C:455:PHE:CD2	2.55	0.41
1:D:346:GLU:HG2	1:D:350:LYS:HE3	2.03	0.41
1:D:354:LEU:O	1:D:358:VAL:HG23	2.21	0.41
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.91	0.41
1:B:310:LEU:HG	1:B:334:HIS:CD2	2.55	0.41
1:D:394:LEU:HD23	1:D:509:ARG:HD2	2.03	0.41
1:F:280:THR:HG22	1:F:280:THR:O	2.19	0.41
1:G:441:LEU:C	1:G:441:LEU:HD23	2.45	0.41
1:H:388:LYS:HB3	1:H:389:PRO:CD	2.50	0.41
1:B:585:LEU:O	1:B:585:LEU:HD23	2.21	0.41
1:F:435:LYS:HD3	4:F:947:HOH:O	2.19	0.41
1:D:344:SER:OG	1:D:347:GLU:HG3	2.21	0.41
1:F:579:ILE:HB	1:F:580:PRO:HD3	2.01	0.41
1:G:396:PRO:HG2	4:G:877:HOH:O	2.21	0.41
1:H:410:ASP:O	1:H:413:HIS:HB2	2.21	0.41
1:H:324:VAL:CG2	1:H:325:PRO:CD	2.98	0.41
1:A:323:ARG:HE	1:A:323:ARG:HB2	1.62	0.41
1:B:585:LEU:HD21	1:B:592:ILE:CD1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:LEU:HA	1:C:374:ALA:HB2	2.03	0.41
1:C:583:ASP:O	1:C:587:GLN:HG2	2.21	0.41
1:D:576:PHE:CD2	1:D:576:PHE:O	2.74	0.41
1:F:390:LEU:HG	1:F:394:LEU:HD11	2.03	0.41
1:H:363:ARG:HA	1:H:363:ARG:HD3	1.95	0.41
1:C:350:LYS:HD3	1:C:456:ASP:O	2.21	0.41
1:A:492:HIS:HB2	1:A:584:LEU:HD21	2.03	0.40
1:F:363:ARG:HB3	1:F:364:PRO:HD2	2.03	0.40
1:G:304:ILE:CG2	1:G:315:PHE:HE1	2.30	0.40
1:C:390:LEU:HD23	1:C:390:LEU:HA	1.92	0.40
1:H:397:LEU:HD23	1:H:397:LEU:O	2.21	0.40
1:C:441:LEU:C	1:C:441:LEU:HD23	2.46	0.40
1:C:586:HIS:HE1	1:C:593:GLU:HG2	1.79	0.40
1:D:315:PHE:CD2	1:D:378:GLN:HG3	2.57	0.40
1:E:310:LEU:CD1	1:E:334:HIS:HB3	2.51	0.40
1:E:462:ASP:OD2	1:E:464:ALA:HB3	2.21	0.40
1:F:512:ALA:O	1:F:516:LEU:HG	2.22	0.40
1:F:596:LEU:HD21	1:F:600:ARG:NH2	2.37	0.40
1:G:493:GLY:O	1:G:496:LEU:HB3	2.21	0.40
1:C:321:ALA:CA	1:C:327:VAL:CG2	2.99	0.40
1:D:295:VAL:HA	1:D:455:PHE:HZ	1.87	0.40
1:G:304:ILE:CD1	1:G:330:SER:HB3	2.51	0.40
1:H:462:ASP:HB3	1:H:465:SER:H	1.86	0.40
1:H:603:ARG:NH1	1:H:603:ARG:CG	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	325/345 (94%)	321 (99%)	3 (1%)	1 (0%)	36 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	331/345 (96%)	322 (97%)	9 (3%)	0	100	100
1	C	331/345 (96%)	324 (98%)	7 (2%)	0	100	100
1	D	320/345 (93%)	307 (96%)	11 (3%)	2 (1%)	21	17
1	E	325/345 (94%)	314 (97%)	11 (3%)	0	100	100
1	F	332/345 (96%)	325 (98%)	6 (2%)	1 (0%)	36	35
1	G	332/345 (96%)	328 (99%)	4 (1%)	0	100	100
1	H	324/345 (94%)	311 (96%)	12 (4%)	1 (0%)	36	35
All	All	2620/2760 (95%)	2552 (97%)	63 (2%)	5 (0%)	43	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	ALA
1	H	302	ALA
1	D	485	HIS
1	F	301	CYS
1	D	321	ALA

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	273/286 (96%)	271 (99%)	2 (1%)	76	82
1	B	276/286 (96%)	274 (99%)	2 (1%)	76	82
1	C	276/286 (96%)	274 (99%)	2 (1%)	76	82
1	D	271/286 (95%)	269 (99%)	2 (1%)	76	82
1	E	274/286 (96%)	271 (99%)	3 (1%)	65	73
1	F	277/286 (97%)	274 (99%)	3 (1%)	65	73
1	G	277/286 (97%)	273 (99%)	4 (1%)	59	66
1	H	272/286 (95%)	267 (98%)	5 (2%)	51	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2196/2288 (96%)	2173 (99%)	23 (1%)	68 75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LEU
1	A	391	MET
1	B	391	MET
1	B	578	VAL
1	C	391	MET
1	C	581	THR
1	D	363	ARG
1	D	599	LEU
1	E	309	ASP
1	E	317	THR
1	E	584	LEU
1	F	391	MET
1	F	517	LEU
1	F	603	ARG
1	G	309	ASP
1	G	407	LEU
1	G	484	LEU
1	G	578	VAL
1	H	282	ARG
1	H	328	LEU
1	H	483	SER
1	H	504	THR
1	H	599	LEU

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

Mol	Chain	Res	Type
1	A	334	HIS
1	A	345	GLN
1	A	360	ASN
1	A	425	GLN
1	A	492	HIS
1	B	345	GLN
1	B	360	ASN
1	B	365	ASN
1	B	463	ASN

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Mol	Chain	Res	Type
1	B	492	HIS
1	C	289	GLN
1	C	345	GLN
1	C	360	ASN
1	C	365	ASN
1	C	475	HIS
1	C	479	HIS
1	C	485	HIS
1	C	586	HIS
1	D	289	GLN
1	D	334	HIS
1	D	345	GLN
1	D	360	ASN
1	D	365	ASN
1	D	463	ASN
1	D	485	HIS
1	D	586	HIS
1	E	289	GLN
1	E	345	GLN
1	E	360	ASN
1	E	440	GLN
1	E	463	ASN
1	E	485	HIS
1	E	587	GLN
1	F	289	GLN
1	F	345	GLN
1	F	360	ASN
1	F	475	HIS
1	F	479	HIS
1	F	485	HIS
1	G	345	GLN
1	G	360	ASN
1	G	393	HIS
1	G	463	ASN
1	H	345	GLN
1	H	360	ASN
1	H	463	ASN
1	H	485	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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, 95th 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 ²)	Q<0.9
1	A	329/345 (95%)	-0.07	11 (3%)	49	48	12, 20, 38, 70	0
1	B	333/345 (96%)	0.31	20 (6%)	27	26	16, 25, 47, 72	0
1	C	333/345 (96%)	0.24	20 (6%)	27	26	13, 25, 50, 74	0
1	D	324/345 (93%)	1.36	85 (26%)	1	1	20, 45, 64, 69	0
1	E	329/345 (95%)	0.55	39 (11%)	9	8	17, 29, 61, 72	0
1	F	334/345 (96%)	0.07	17 (5%)	33	32	14, 22, 40, 68	0
1	G	334/345 (96%)	0.16	19 (5%)	29	28	15, 24, 46, 64	0
1	H	328/345 (95%)	0.48	33 (10%)	12	11	17, 32, 54, 73	0
All	All	2644/2760 (95%)	0.38	244 (9%)	14	13	12, 27, 55, 74	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	612	VAL	8.0
1	H	308	VAL	7.3
1	A	303	ALA	7.1
1	B	610	ALA	6.6
1	C	612	VAL	6.3
1	D	308	VAL	6.2
1	E	302	ALA	6.0
1	H	303	ALA	5.9
1	E	306	THR	5.7
1	H	280	THR	5.2
1	E	576	PHE	5.0
1	A	302	ALA	4.9
1	D	309	ASP	4.9
1	G	612	VAL	4.8
1	A	611	GLY	4.7
1	A	304	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	326	SER	4.5
1	F	612	VAL	4.5
1	G	304	ILE	4.5
1	E	611	GLY	4.5
1	E	308	VAL	4.4
1	D	610	ALA	4.3
1	D	300	SER	4.2
1	E	566	VAL	4.2
1	F	613	THR	4.1
1	D	576	PHE	4.1
1	D	343	ALA	4.0
1	D	280	THR	4.0
1	C	304	ILE	3.9
1	F	462	ASP	3.9
1	D	387	ALA	3.9
1	D	333	MET	3.9
1	F	611	GLY	3.8
1	D	296	VAL	3.8
1	D	566	VAL	3.8
1	C	576	PHE	3.8
1	H	611	GLY	3.7
1	D	324	VAL	3.7
1	A	280	THR	3.7
1	E	310	LEU	3.6
1	D	497	SER	3.6
1	B	280	THR	3.6
1	G	306	THR	3.6
1	H	282	ARG	3.6
1	C	573	PHE	3.6
1	C	307	ASP	3.5
1	E	322	SER	3.5
1	H	281	ARG	3.5
1	G	302	ALA	3.4
1	D	600	ARG	3.4
1	E	301	CYS	3.4
1	C	280	THR	3.4
1	D	323	ARG	3.4
1	B	302	ALA	3.3
1	B	611	GLY	3.3
1	D	484	LEU	3.3
1	B	349	GLN	3.3
1	E	280	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	280	THR	3.3
1	D	496	LEU	3.3
1	H	604	GLU	3.3
1	B	333	MET	3.3
1	D	330	SER	3.2
1	D	555	PRO	3.2
1	D	320	VAL	3.2
1	G	482	MET	3.2
1	B	300	SER	3.2
1	G	613	THR	3.2
1	C	611	GLY	3.1
1	H	298	PRO	3.1
1	E	309	ASP	3.1
1	D	328	LEU	3.1
1	A	610	ALA	3.1
1	G	303	ALA	3.1
1	C	322	SER	3.1
1	D	342	PHE	3.0
1	D	560	PHE	3.0
1	D	462	ASP	3.0
1	H	484	LEU	3.0
1	B	453	THR	3.0
1	C	577	PHE	3.0
1	C	608	ALA	3.0
1	F	300	SER	3.0
1	C	308	VAL	3.0
1	E	307	ASP	2.9
1	D	563	PRO	2.9
1	F	303	ALA	2.9
1	C	569	SER	2.9
1	G	300	SER	2.9
1	D	298	PRO	2.9
1	E	560	PHE	2.9
1	G	305	GLY	2.9
1	D	551	ARG	2.8
1	F	345	GLN	2.8
1	D	488	THR	2.8
1	E	300	SER	2.8
1	D	602	LEU	2.8
1	E	605	LEU	2.8
1	D	325	PRO	2.8
1	F	333	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	489	VAL	2.8
1	F	280	THR	2.8
1	B	298	PRO	2.8
1	H	333	MET	2.7
1	D	561	GLU	2.7
1	H	605	LEU	2.7
1	H	301	CYS	2.7
1	C	300	SER	2.7
1	C	597	HIS	2.7
1	H	462	ASP	2.7
1	D	327	VAL	2.7
1	D	607	ALA	2.6
1	D	318	PHE	2.6
1	G	283	LEU	2.6
1	G	301	CYS	2.6
1	D	281	ARG	2.6
1	E	562	THR	2.6
1	D	283	LEU	2.6
1	D	486	SER	2.6
1	F	282	ARG	2.6
1	H	324	VAL	2.6
1	B	597	HIS	2.6
1	E	435	LYS	2.6
1	B	462	ASP	2.6
1	E	563	PRO	2.6
1	F	323	ARG	2.6
1	D	310	LEU	2.6
1	G	605	LEU	2.6
1	H	577	PHE	2.5
1	H	345	GLN	2.5
1	D	319	GLU	2.5
1	D	295	VAL	2.5
1	G	611	GLY	2.5
1	D	601	LYS	2.5
1	B	323	ARG	2.5
1	E	282	ARG	2.5
1	D	530	ALA	2.5
1	F	343	ALA	2.5
1	D	604	GLU	2.5
1	E	606	TYR	2.5
1	G	504	THR	2.5
1	D	321	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	555	PRO	2.5
1	D	299	LYS	2.5
1	G	282	ARG	2.5
1	D	567	GLU	2.5
1	H	302	ALA	2.5
1	D	569	SER	2.4
1	E	608	ALA	2.4
1	D	571	ILE	2.4
1	D	562	THR	2.4
1	F	281	ARG	2.4
1	A	282	ARG	2.4
1	B	301	CYS	2.4
1	D	554	LEU	2.4
1	D	605	LEU	2.4
1	D	290	ASP	2.4
1	D	542	PHE	2.4
1	D	597	HIS	2.4
1	F	488	THR	2.4
1	D	356	ALA	2.3
1	D	546	ALA	2.3
1	D	608	ALA	2.3
1	D	590	PRO	2.3
1	C	610	ALA	2.3
1	B	342	PHE	2.3
1	D	381	PHE	2.3
1	H	573	PHE	2.3
1	E	569	SER	2.3
1	D	355	VAL	2.3
1	H	566	VAL	2.3
1	E	488	THR	2.3
1	E	484	LEU	2.3
1	H	600	ARG	2.3
1	C	609	LYS	2.3
1	E	565	SER	2.3
1	H	497	SER	2.3
1	D	345	GLN	2.3
1	G	323	ARG	2.3
1	D	322	SER	2.2
1	D	329	GLN	2.2
1	D	371	ILE	2.2
1	A	308	VAL	2.2
1	E	453	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	530	ALA	2.2
1	E	597	HIS	2.2
1	G	349	GLN	2.2
1	H	565	SER	2.2
1	C	306	THR	2.2
1	F	610	ALA	2.2
1	H	597	HIS	2.2
1	H	603	ARG	2.2
1	D	297	PRO	2.2
1	D	317	THR	2.2
1	E	387	ALA	2.2
1	C	564	SER	2.2
1	D	550	ARG	2.2
1	D	606	TYR	2.2
1	E	557	THR	2.2
1	D	287	ILE	2.1
1	D	457	PHE	2.1
1	B	295	VAL	2.1
1	H	528	GLY	2.1
1	D	332	ALA	2.1
1	D	490	ALA	2.1
1	C	319	GLU	2.1
1	B	304	ILE	2.1
1	D	573	PHE	2.1
1	B	281	ARG	2.1
1	E	603	ARG	2.1
1	F	387	ALA	2.1
1	D	596	LEU	2.1
1	H	300	SER	2.1
1	A	319	GLU	2.1
1	D	507	GLU	2.1
1	F	290	ASP	2.1
1	D	314	GLY	2.1
1	E	550	ARG	2.1
1	D	341	PHE	2.1
1	D	353	PHE	2.1
1	D	537	VAL	2.1
1	D	346	GLU	2.1
1	E	334	HIS	2.1
1	E	528	GLY	2.1
1	E	556	VAL	2.1
1	H	295	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	343	ALA	2.1
1	H	564	SER	2.1
1	C	482	MET	2.0
1	D	340	ASP	2.0
1	A	453	THR	2.0
1	D	593	GLU	2.0
1	G	342	PHE	2.0
1	H	296	VAL	2.0
1	B	482	MET	2.0
1	D	483	SER	2.0
1	H	569	SER	2.0
1	E	607	ALA	2.0
1	E	602	LEU	2.0
1	H	323	ARG	2.0
1	E	504	THR	2.0
1	E	558	PRO	2.0
1	B	305	GLY	2.0
1	H	606	TYR	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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
3	MG	E	702	1/1	0.94	0.06	26,26,26,26	0
3	MG	D	702	1/1	0.95	0.13	31,31,31,31	0
3	MG	B	702	1/1	0.95	0.07	21,21,21,21	0
3	MG	F	702	1/1	0.96	0.10	19,19,19,19	0
3	MG	G	702	1/1	0.96	0.07	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	702	1/1	0.97	0.08	18,18,18,18	0
2	ZN	D	701	1/1	0.97	0.04	34,34,34,34	0
3	MG	H	702	1/1	0.97	0.10	25,25,25,25	0
3	MG	C	702	1/1	0.98	0.05	15,15,15,15	0
2	ZN	C	701	1/1	0.99	0.02	19,19,19,19	0
2	ZN	A	701	1/1	0.99	0.02	18,18,18,18	0
2	ZN	E	701	1/1	0.99	0.03	25,25,25,25	0
2	ZN	F	701	1/1	0.99	0.01	20,20,20,20	0
2	ZN	G	701	1/1	0.99	0.02	22,22,22,22	0
2	ZN	H	701	1/1	0.99	0.02	25,25,25,25	0
2	ZN	B	701	1/1	0.99	0.03	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.