



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:13 PM UTC

PDB ID : 4CBH / pdb_00004cbh
Title : Pestivirus NS3 helicase
Authors : Tortorici, M.A.; Duquerroy, S.; Kwok, J.; Vonnrhein, C.; Perez, J.; Lamp, B.;
Bricogne, G.; Rumenapf, T.; Vachette, P.; Rey, F.A.
Deposited on : 2013-10-14
Resolution : 2.51 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

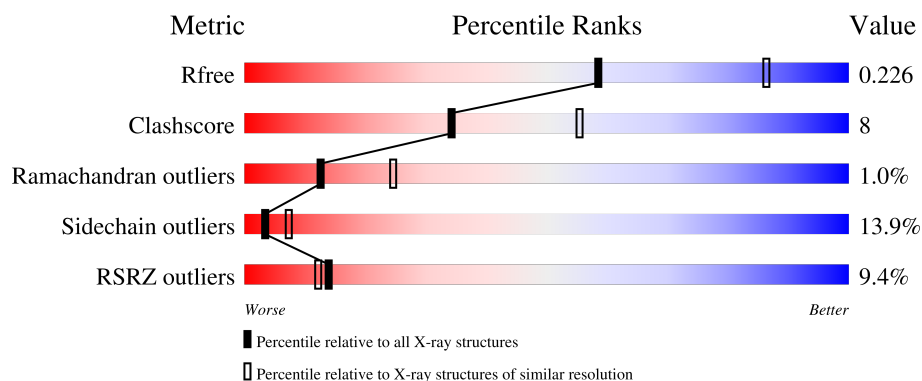
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	516	5% 46% 14% • • 35%
1	B	516	6% 47% 14% • 36%
1	C	516	5% 45% 14% • • 36%
1	D	516	9% 53% 16% • • 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11813 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 SERINE PROTEASE NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2664	1693	451	502	18			
1	B	330	Total	C	N	O	S	0	0	0
			2652	1688	448	498	18			
1	C	330	Total	C	N	O	S	0	1	1
			2654	1687	452	497	18			
1	D	385	Total	C	N	O	S	0	1	1
			3075	1948	530	579	18			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	MET	-	expression tag	UNP P19712
A	177	ALA	-	expression tag	UNP P19712
A	178	SER	-	expression tag	UNP P19712
A	179	HIS	-	expression tag	UNP P19712
A	180	HIS	-	expression tag	UNP P19712
A	181	HIS	-	expression tag	UNP P19712
A	182	HIS	-	expression tag	UNP P19712
A	183	HIS	-	expression tag	UNP P19712
A	184	HIS	-	expression tag	UNP P19712
A	185	HIS	-	expression tag	UNP P19712
A	186	GLU	-	expression tag	UNP P19712
A	187	ASN	-	expression tag	UNP P19712
A	188	LEU	-	expression tag	UNP P19712
A	189	TYR	-	expression tag	UNP P19712
A	190	PHE	-	expression tag	UNP P19712
A	191	GLN	-	expression tag	UNP P19712
A	192	GLY	-	expression tag	UNP P19712
B	176	MET	-	expression tag	UNP P19712
B	177	ALA	-	expression tag	UNP P19712
B	178	SER	-	expression tag	UNP P19712
B	179	HIS	-	expression tag	UNP P19712

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Chain	Residue	Modelled	Actual	Comment	Reference
B	180	HIS	-	expression tag	UNP P19712
B	181	HIS	-	expression tag	UNP P19712
B	182	HIS	-	expression tag	UNP P19712
B	183	HIS	-	expression tag	UNP P19712
B	184	HIS	-	expression tag	UNP P19712
B	185	HIS	-	expression tag	UNP P19712
B	186	GLU	-	expression tag	UNP P19712
B	187	ASN	-	expression tag	UNP P19712
B	188	LEU	-	expression tag	UNP P19712
B	189	TYR	-	expression tag	UNP P19712
B	190	PHE	-	expression tag	UNP P19712
B	191	GLN	-	expression tag	UNP P19712
B	192	GLY	-	expression tag	UNP P19712
C	176	MET	-	expression tag	UNP P19712
C	177	ALA	-	expression tag	UNP P19712
C	178	SER	-	expression tag	UNP P19712
C	179	HIS	-	expression tag	UNP P19712
C	180	HIS	-	expression tag	UNP P19712
C	181	HIS	-	expression tag	UNP P19712
C	182	HIS	-	expression tag	UNP P19712
C	183	HIS	-	expression tag	UNP P19712
C	184	HIS	-	expression tag	UNP P19712
C	185	HIS	-	expression tag	UNP P19712
C	186	GLU	-	expression tag	UNP P19712
C	187	ASN	-	expression tag	UNP P19712
C	188	LEU	-	expression tag	UNP P19712
C	189	TYR	-	expression tag	UNP P19712
C	190	PHE	-	expression tag	UNP P19712
C	191	GLN	-	expression tag	UNP P19712
C	192	GLY	-	expression tag	UNP P19712
D	176	MET	-	expression tag	UNP P19712
D	177	ALA	-	expression tag	UNP P19712
D	178	SER	-	expression tag	UNP P19712
D	179	HIS	-	expression tag	UNP P19712
D	180	HIS	-	expression tag	UNP P19712
D	181	HIS	-	expression tag	UNP P19712
D	182	HIS	-	expression tag	UNP P19712
D	183	HIS	-	expression tag	UNP P19712
D	184	HIS	-	expression tag	UNP P19712
D	185	HIS	-	expression tag	UNP P19712
D	186	GLU	-	expression tag	UNP P19712
D	187	ASN	-	expression tag	UNP P19712

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Chain	Residue	Modelled	Actual	Comment	Reference
D	188	LEU	-	expression tag	UNP P19712
D	189	TYR	-	expression tag	UNP P19712
D	190	PHE	-	expression tag	UNP P19712
D	191	GLN	-	expression tag	UNP P19712
D	192	GLY	-	expression tag	UNP P19712

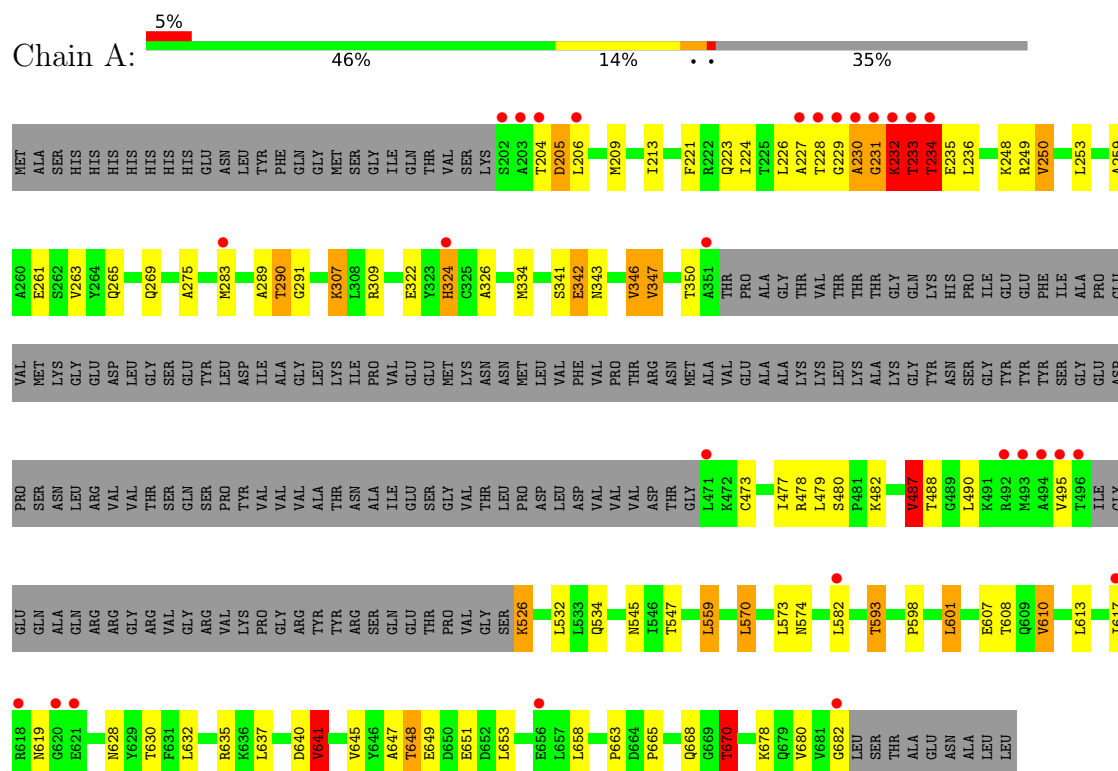
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	197	Total O 197 197	0	0
2	B	187	Total O 187 187	0	0
2	C	154	Total O 154 154	0	0
2	D	230	Total O 230 230	0	0

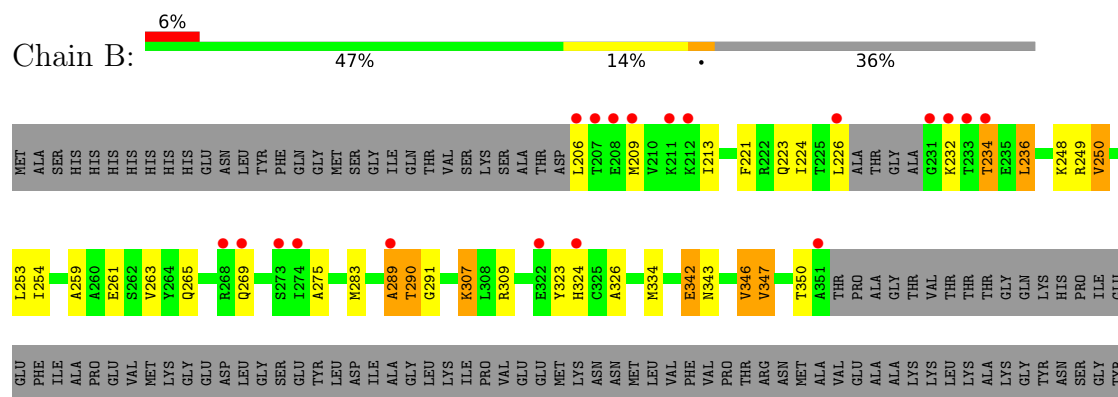
3 Residue-property plots

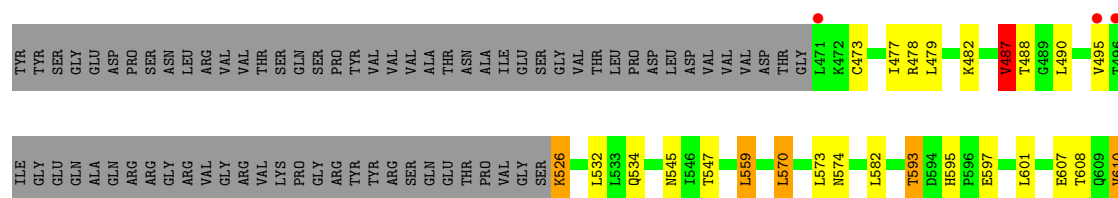
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SERINE PROTEASE NS3

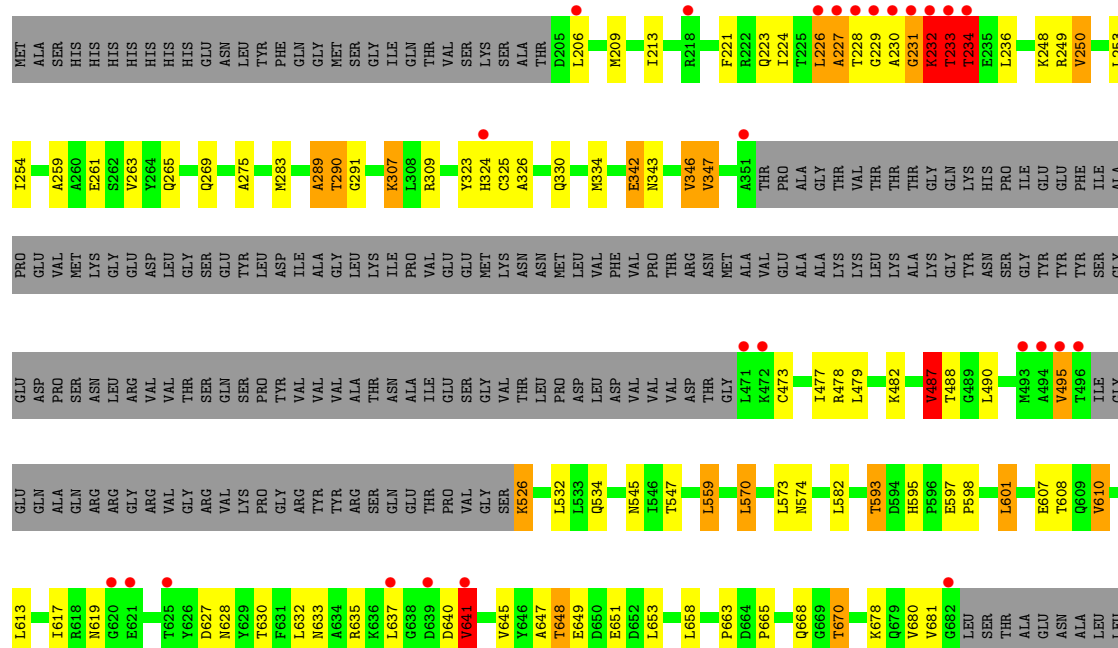


• Molecule 1: SERINE PROTEASE NS3

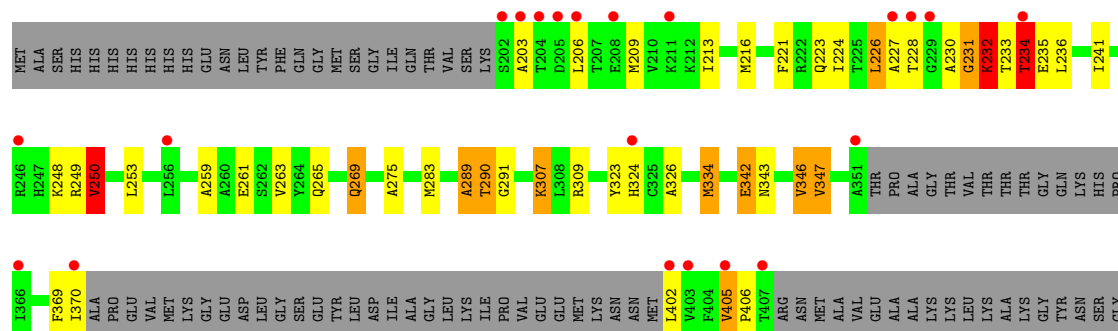


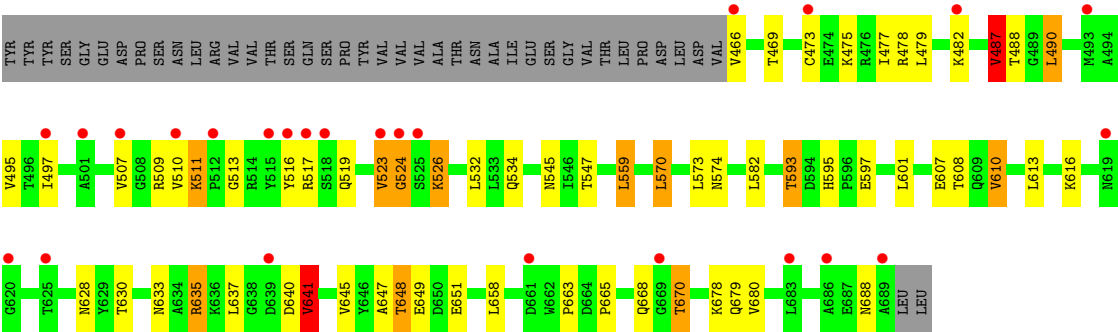


• Molecule 1: SERINE PROTEASE NS3



• Molecule 1: SERINE PROTEASE NS3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.07Å 144.44Å 118.69Å 90.00° 92.94° 90.00°	Depositor
Resolution (Å)	72.22 – 2.51 72.22 – 2.51	Depositor EDS
% Data completeness (in resolution range)	88.6 (72.22-2.51) 88.6 (72.22-2.51)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.13.0	Depositor
R, R_{free}	0.203 , 0.232 (Not available) , 0.226	Depositor DCC
R_{free} test set	3572 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 79.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11813	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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

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	0.85	0/2715	1.50	26/3671 (0.7%)
1	B	0.84	1/2702 (0.0%)	1.43	17/3651 (0.5%)
1	C	0.85	3/2705 (0.1%)	1.48	26/3657 (0.7%)
1	D	0.89	4/3132 (0.1%)	1.45	25/4234 (0.6%)
All	All	0.86	8/11254 (0.1%)	1.47	94/15213 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	254	ILE	CA-C	6.91	1.57	1.52
1	D	688	ASN	C-N	-6.05	1.24	1.33
1	C	254	ILE	CA-C	5.65	1.56	1.52
1	C	681	VAL	C-N	-5.56	1.25	1.33
1	C	231	GLY	C-N	5.31	1.41	1.33
1	D	216	MET	SD-CE	-5.24	1.66	1.79
1	D	234	THR	N-CA	-5.03	1.39	1.46
1	D	334	MET	SD-CE	-5.00	1.67	1.79

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	THR	N-CA-C	12.81	126.67	111.82
1	A	233	THR	CA-C-N	12.79	145.98	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	THR	C-N-CA	12.79	145.98	121.54
1	C	233	THR	CA-C-N	12.49	145.40	121.54
1	C	233	THR	C-N-CA	12.49	145.40	121.54
1	D	290	THR	N-CA-C	12.46	126.28	111.82
1	C	290	THR	N-CA-C	12.42	126.23	111.82
1	B	290	THR	N-CA-C	12.21	125.98	111.82
1	B	234	THR	CB-CA-C	9.45	125.97	109.15
1	D	233	THR	N-CA-C	-9.08	101.64	112.89
1	A	231	GLY	CA-C-N	8.90	137.72	121.70
1	A	231	GLY	C-N-CA	8.90	137.72	121.70
1	C	229	GLY	CA-C-N	8.25	136.56	121.70
1	C	229	GLY	C-N-CA	8.25	136.56	121.70
1	B	487	VAL	N-CA-CB	7.34	121.80	111.82
1	B	641	VAL	N-CA-CB	7.26	117.99	110.23
1	C	487	VAL	N-CA-CB	7.21	121.62	111.82
1	D	487	VAL	N-CA-CB	7.17	121.57	111.82
1	B	250	VAL	N-CA-CB	7.08	121.18	111.41
1	C	250	VAL	N-CA-CB	6.99	121.06	111.41
1	A	229	GLY	CA-C-N	6.94	134.19	121.70
1	A	229	GLY	C-N-CA	6.94	134.19	121.70
1	D	231	GLY	CA-C-N	6.86	134.04	121.70
1	D	231	GLY	C-N-CA	6.86	134.04	121.70
1	A	610	VAL	N-CA-C	6.86	114.34	107.55
1	D	641	VAL	N-CA-CB	6.85	117.56	110.23
1	A	250	VAL	N-CA-CB	6.84	121.51	111.52
1	A	641	VAL	N-CA-CB	6.80	117.51	110.23
1	A	641	VAL	CB-CA-C	6.70	117.17	110.94
1	C	641	VAL	N-CA-CB	6.69	117.39	110.23
1	B	610	VAL	N-CA-C	6.68	114.16	107.55
1	D	250	VAL	N-CA-CB	6.64	121.21	111.52
1	A	205	ASP	CA-CB-CG	6.62	119.22	112.60
1	C	641	VAL	CB-CA-C	6.49	116.97	110.94
1	A	487	VAL	N-CA-CB	6.45	121.54	111.99
1	D	641	VAL	CB-CA-C	6.42	116.91	110.94
1	C	610	VAL	N-CA-C	6.33	113.82	107.55
1	B	641	VAL	CB-CA-C	6.29	116.79	110.94
1	D	203	ALA	CA-C-N	6.28	128.60	120.44
1	D	203	ALA	C-N-CA	6.28	128.60	120.44
1	B	487	VAL	CB-CA-C	6.27	118.88	110.42
1	A	487	VAL	CB-CA-C	6.24	118.60	110.12
1	D	610	VAL	N-CA-C	6.12	113.61	107.55
1	C	487	VAL	CB-CA-C	6.12	118.68	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	THR	N-CA-CB	5.96	120.56	110.49
1	C	347	VAL	CB-CA-C	5.87	118.34	110.42
1	B	347	VAL	CB-CA-C	5.81	118.26	110.42
1	A	632	LEU	N-CA-C	5.80	117.60	111.28
1	D	487	VAL	CB-CA-C	5.78	118.22	110.42
1	D	234	THR	CB-CA-C	5.75	121.86	110.42
1	D	347	VAL	CB-CA-C	5.67	118.07	110.42
1	D	289	ALA	CA-C-N	5.62	128.85	120.31
1	D	289	ALA	C-N-CA	5.62	128.85	120.31
1	C	227	ALA	N-CA-C	5.55	117.00	109.11
1	C	495	VAL	N-CA-C	5.53	120.85	109.34
1	D	679	GLN	CA-C-N	5.52	128.02	120.46
1	D	679	GLN	C-N-CA	5.52	128.02	120.46
1	C	232	LYS	CA-C-N	5.50	131.60	121.70
1	C	232	LYS	C-N-CA	5.50	131.60	121.70
1	A	645	VAL	N-CA-C	-5.50	104.60	112.35
1	C	227	ALA	CA-C-N	5.48	131.57	121.70
1	C	227	ALA	C-N-CA	5.48	131.57	121.70
1	C	632	LEU	N-CA-C	5.45	117.22	111.28
1	C	641	VAL	N-CA-C	5.44	113.31	108.63
1	B	645	VAL	N-CA-C	-5.43	104.70	112.35
1	D	645	VAL	N-CA-C	-5.39	104.74	112.35
1	A	641	VAL	N-CA-C	5.34	113.22	108.63
1	C	325	CYS	N-CA-C	-5.33	106.28	112.89
1	A	341	SER	CA-C-N	5.33	127.95	120.28
1	A	341	SER	C-N-CA	5.33	127.95	120.28
1	C	645	VAL	N-CA-C	-5.31	104.86	112.35
1	C	289	ALA	CA-C-N	5.30	128.37	120.31
1	C	289	ALA	C-N-CA	5.30	128.37	120.31
1	A	347	VAL	CB-CA-C	5.25	118.22	110.77
1	C	627	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	534	GLN	CA-C-N	5.21	127.79	120.28
1	B	534	GLN	C-N-CA	5.21	127.79	120.28
1	A	227	ALA	CA-C-N	5.20	131.48	121.54
1	A	227	ALA	C-N-CA	5.20	131.48	121.54
1	D	497	ILE	CA-C-N	5.20	125.72	120.00
1	D	497	ILE	C-N-CA	5.20	125.72	120.00
1	D	641	VAL	N-CA-C	5.16	113.06	108.63
1	A	232	LYS	CA-C-N	5.15	130.98	121.70
1	A	232	LYS	C-N-CA	5.15	130.98	121.70
1	B	641	VAL	N-CA-C	5.08	113.00	108.63
1	A	670	THR	CB-CA-C	5.08	120.00	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	ALA	CA-C-N	5.08	128.03	120.31
1	B	289	ALA	C-N-CA	5.08	128.03	120.31
1	D	534	GLN	CA-C-N	5.05	127.55	120.28
1	D	534	GLN	C-N-CA	5.05	127.55	120.28
1	D	269	GLN	CB-CG-CD	5.05	121.18	112.60
1	B	679	GLN	CA-C-N	5.03	127.36	120.46
1	B	679	GLN	C-N-CA	5.03	127.36	120.46
1	A	480	SER	N-CA-C	5.03	114.08	108.25

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	THR	Mainchain,Peptide
1	C	233	THR	Mainchain,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	2664	0	2666	44	0
1	B	2652	0	2658	42	0
1	C	2654	0	2658	47	0
1	D	3075	0	3078	48	0
2	A	197	0	0	3	0
2	B	187	0	0	1	0
2	C	154	0	0	3	0
2	D	230	0	0	2	0
All	All	11813	0	11060	169	0

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

All (169) 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:A:682:GLY:O	1:B:685:THR:CG2	1.75	1.35
1:A:324:HIS:CD2	1:A:350:THR:OG1	2.02	1.11
1:A:682:GLY:O	1:B:685:THR:HG22	0.93	1.09
1:A:324:HIS:HD2	1:A:350:THR:OG1	1.53	0.91
1:B:234:THR:HG21	1:B:263:VAL:HG11	1.55	0.88
1:C:227:ALA:HA	1:C:228:THR:CG2	2.03	0.87
1:D:607:GLU:OE2	1:D:670:THR:HG21	1.74	0.87
1:B:607:GLU:OE2	1:B:670:THR:HG21	1.76	0.85
1:A:665:PRO:HB3	1:A:670:THR:HG23	1.59	0.84
1:D:665:PRO:HB3	1:D:670:THR:HG23	1.60	0.84
1:B:665:PRO:HB3	1:B:670:THR:HG23	1.60	0.82
1:A:607:GLU:OE2	1:A:670:THR:HG21	1.80	0.81
1:C:665:PRO:HB3	1:C:670:THR:HG23	1.61	0.81
1:C:607:GLU:OE2	1:C:670:THR:HG21	1.79	0.80
1:D:226:LEU:HG	1:D:231:GLY:HA3	1.66	0.77
1:B:593:THR:HG23	1:B:630:THR:O	1.86	0.75
1:C:593:THR:HG23	1:C:630:THR:O	1.86	0.75
1:C:227:ALA:HA	1:C:228:THR:HG23	1.68	0.74
1:A:593:THR:HG23	1:A:630:THR:O	1.88	0.74
1:D:593:THR:HG23	1:D:630:THR:O	1.87	0.74
1:C:227:ALA:HA	1:C:228:THR:HG22	1.69	0.73
1:C:226:LEU:O	1:C:228:THR:HG22	1.89	0.72
1:B:213:ILE:HD11	1:B:224:ILE:HD11	1.76	0.68
1:C:309:ARG:HH21	1:C:343:ASN:HD21	1.43	0.67
1:C:213:ILE:HD11	1:C:224:ILE:HD11	1.76	0.67
1:A:309:ARG:HH21	1:A:343:ASN:HD21	1.43	0.67
2:A:2180:HOH:O	1:B:686:ALA:O	2.12	0.66
1:A:648:THR:HG21	2:A:2134:HOH:O	1.95	0.66
1:B:309:ARG:HH21	1:B:343:ASN:HD21	1.44	0.66
1:A:213:ILE:HD11	1:A:224:ILE:HD11	1.79	0.65
1:D:213:ILE:HD11	1:D:224:ILE:HD11	1.79	0.64
1:B:547:THR:HG21	1:B:570:LEU:HB3	1.81	0.63
1:D:309:ARG:HH21	1:D:343:ASN:HD21	1.47	0.62
1:C:231:GLY:O	1:C:232:LYS:HB3	1.99	0.62
1:D:547:THR:HG21	1:D:570:LEU:HB3	1.81	0.62
1:D:275:ALA:O	1:D:291:GLY:HA3	2.00	0.62
1:C:595:HIS:HD2	1:C:597:GLU:H	1.48	0.61
1:D:641:VAL:HG22	1:D:663:PRO:HD3	1.81	0.61
1:B:635:ARG:NH2	1:B:640:ASP:O	2.30	0.61
1:C:259:ALA:O	1:C:263:VAL:HG23	2.01	0.61
1:B:641:VAL:HG22	1:B:663:PRO:HD3	1.83	0.61
1:C:547:THR:HG21	1:C:570:LEU:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:ARG:NH2	1:C:640:ASP:O	2.32	0.60
1:C:326:ALA:HB3	1:C:526:LYS:HE2	1.82	0.60
1:D:259:ALA:O	1:D:263:VAL:HG23	2.02	0.60
1:D:595:HIS:HD2	1:D:597:GLU:H	1.49	0.60
1:B:275:ALA:O	1:B:291:GLY:HA3	2.01	0.60
1:C:641:VAL:HG22	1:C:663:PRO:HD3	1.84	0.60
1:A:547:THR:HG21	1:A:570:LEU:HB3	1.84	0.60
1:B:259:ALA:O	1:B:263:VAL:HG23	2.02	0.59
1:B:595:HIS:HD2	1:B:597:GLU:H	1.51	0.59
1:A:259:ALA:O	1:A:263:VAL:HG23	2.03	0.59
1:A:641:VAL:HG22	1:A:663:PRO:HD3	1.84	0.59
1:D:265:GLN:O	1:D:269:GLN:HG2	2.02	0.59
1:A:232:LYS:HA	1:A:233:THR:C	2.28	0.59
1:D:466:VAL:HG23	1:D:507:VAL:HG13	1.86	0.57
1:B:234:THR:HG21	1:B:263:VAL:CG1	2.32	0.57
1:A:249:ARG:HD2	1:A:289:ALA:O	2.05	0.56
1:A:322:GLU:HA	1:A:324:HIS:NE2	2.19	0.56
1:C:275:ALA:O	1:C:291:GLY:HA3	2.04	0.56
1:A:275:ALA:O	1:A:291:GLY:HA3	2.05	0.56
1:A:334:MET:CE	1:A:559:LEU:HD23	2.36	0.56
1:B:265:GLN:O	1:B:269:GLN:HG3	2.06	0.55
1:C:648:THR:HG22	1:C:651:GLU:H	1.71	0.55
1:D:249:ARG:HD2	1:D:289:ALA:O	2.07	0.54
1:A:648:THR:HG22	1:A:651:GLU:H	1.72	0.54
1:B:648:THR:HG22	1:B:651:GLU:H	1.73	0.54
1:D:648:THR:HG22	1:D:651:GLU:H	1.73	0.54
1:B:249:ARG:HD2	1:B:289:ALA:O	2.07	0.54
1:C:334:MET:CE	1:C:559:LEU:HD23	2.38	0.54
1:A:635:ARG:NH2	1:A:640:ASP:O	2.33	0.53
1:D:510:VAL:HG13	1:D:511:LYS:HD2	1.90	0.53
1:C:249:ARG:HD2	1:C:289:ALA:O	2.08	0.53
1:C:265:GLN:O	1:C:269:GLN:HG3	2.07	0.53
1:A:265:GLN:O	1:A:269:GLN:HG3	2.09	0.53
1:C:232:LYS:HA	1:C:233:THR:C	2.34	0.52
1:D:334:MET:CE	1:D:559:LEU:HD23	2.39	0.52
1:B:487:VAL:HA	1:B:647:ALA:O	2.10	0.52
1:B:545:ASN:CB	1:C:342:GLU:HG2	2.40	0.52
1:D:487:VAL:HA	1:D:647:ALA:O	2.09	0.52
1:C:324:HIS:HB2	2:C:2052:HOH:O	2.10	0.52
1:A:234:THR:HG22	1:A:235:GLU:N	2.25	0.51
1:D:221:PHE:HD1	1:D:346:VAL:HG22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLU:HG2	1:C:545:ASN:CB	2.40	0.51
1:D:241:ILE:HD12	1:D:250:VAL:HG13	1.92	0.51
1:A:545:ASN:CB	1:D:342:GLU:HG2	2.40	0.51
1:B:334:MET:CE	1:B:559:LEU:HD23	2.41	0.51
1:B:221:PHE:HD1	1:B:346:VAL:HG22	1.75	0.51
1:A:487:VAL:HA	1:A:647:ALA:O	2.11	0.51
1:A:545:ASN:HB3	1:D:342:GLU:HG2	1.93	0.50
1:C:648:THR:HG21	2:C:2088:HOH:O	2.10	0.50
1:A:234:THR:HG22	1:A:235:GLU:HG2	1.94	0.50
1:C:477:ILE:HG22	1:C:488:THR:HG22	1.93	0.50
1:C:487:VAL:HA	1:C:647:ALA:O	2.12	0.50
1:A:477:ILE:HG22	1:A:488:THR:HG22	1.94	0.50
1:B:477:ILE:HG22	1:B:488:THR:HG22	1.93	0.49
1:B:648:THR:HG21	2:B:2116:HOH:O	2.12	0.49
1:C:221:PHE:HD1	1:C:346:VAL:HG22	1.76	0.49
1:C:228:THR:H	1:C:230:ALA:HB3	1.77	0.49
1:C:595:HIS:CD2	1:C:597:GLU:H	2.28	0.49
1:A:221:PHE:HD1	1:A:346:VAL:HG22	1.76	0.49
1:D:547:THR:H	1:D:574:ASN:ND2	2.10	0.49
1:A:547:THR:H	1:A:574:ASN:ND2	2.10	0.48
1:D:477:ILE:HG22	1:D:488:THR:HG22	1.94	0.48
1:D:635:ARG:NH2	1:D:640:ASP:O	2.33	0.48
1:C:283:MET:HE1	1:C:307:LYS:HE3	1.95	0.48
1:D:595:HIS:CD2	1:D:597:GLU:H	2.28	0.48
1:C:547:THR:H	1:C:574:ASN:ND2	2.10	0.48
1:B:593:THR:CG2	1:B:630:THR:O	2.60	0.48
1:A:593:THR:CG2	1:A:630:THR:O	2.60	0.48
1:D:234:THR:HG22	1:D:235:GLU:HG2	1.96	0.48
1:B:323:TYR:CE2	1:B:350:THR:HB	2.49	0.47
1:B:342:GLU:HG2	1:C:545:ASN:HB3	1.95	0.47
1:B:595:HIS:CD2	1:B:597:GLU:H	2.29	0.47
1:D:234:THR:HG22	1:D:235:GLU:N	2.29	0.47
1:B:547:THR:H	1:B:574:ASN:ND2	2.12	0.47
1:A:230:ALA:HA	1:A:231:GLY:HA3	1.64	0.47
1:B:283:MET:HE1	1:B:307:LYS:HE3	1.97	0.47
1:D:249:ARG:NH2	2:D:2020:HOH:O	2.37	0.46
1:A:342:GLU:HG2	1:D:545:ASN:CB	2.44	0.46
1:B:326:ALA:HB3	1:B:526:LYS:HE2	1.97	0.46
1:B:545:ASN:HB3	1:C:342:GLU:HG2	1.98	0.46
1:A:283:MET:HE1	1:A:307:LYS:HE3	1.98	0.46
1:A:326:ALA:HB3	1:A:526:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:VAL:HG13	1:D:524:GLY:H	1.81	0.46
1:B:545:ASN:HB2	1:C:342:GLU:HG2	1.98	0.46
1:D:507:VAL:HB	1:D:513:GLY:HA3	1.98	0.46
1:A:248:LYS:O	1:A:290:THR:O	2.35	0.45
1:C:479:LEU:HD11	1:C:570:LEU:HD13	1.98	0.45
1:D:326:ALA:HB3	1:D:526:LYS:HE2	1.99	0.45
1:D:593:THR:CG2	1:D:630:THR:O	2.60	0.45
1:A:342:GLU:HG2	1:D:545:ASN:HB3	1.98	0.45
1:C:248:LYS:O	1:C:290:THR:O	2.34	0.44
1:A:209:MET:O	1:A:213:ILE:HG12	2.17	0.44
1:D:209:MET:O	1:D:213:ILE:HG12	2.17	0.44
1:D:248:LYS:O	1:D:290:THR:O	2.35	0.44
1:C:209:MET:O	1:C:213:ILE:HG12	2.17	0.44
1:D:283:MET:HE1	1:D:307:LYS:HE3	1.99	0.44
1:A:479:LEU:HD11	1:A:570:LEU:HD13	1.99	0.44
1:B:209:MET:O	1:B:213:ILE:HG12	2.18	0.44
1:D:405:VAL:HG22	1:D:406:PRO:HD2	2.00	0.44
1:B:479:LEU:HD11	1:B:570:LEU:HD13	1.99	0.44
1:D:478:ARG:HD3	1:D:649:GLU:OE2	2.19	0.43
1:A:322:GLU:HA	1:A:324:HIS:CE1	2.53	0.43
1:B:478:ARG:HD3	1:B:649:GLU:OE2	2.18	0.43
1:C:593:THR:CG2	1:C:630:THR:O	2.60	0.43
1:D:323:TYR:C	1:D:323:TYR:CD1	2.97	0.43
1:A:478:ARG:HD3	1:A:649:GLU:OE2	2.18	0.42
1:C:478:ARG:HD3	1:C:649:GLU:OE2	2.18	0.42
1:B:342:GLU:HG2	1:C:545:ASN:HB2	2.01	0.42
1:D:479:LEU:HD11	1:D:570:LEU:HD13	2.02	0.42
1:A:598:PRO:O	1:A:601:LEU:HB2	2.19	0.42
1:A:534:GLN:NE2	2:A:2101:HOH:O	2.52	0.42
1:B:248:LYS:O	1:B:290:THR:O	2.37	0.42
1:D:369:PHE:HB2	1:D:516:TYR:HA	2.02	0.41
1:C:309:ARG:HH21	1:C:343:ASN:ND2	2.13	0.41
1:C:617:ILE:HD13	1:C:653:LEU:HD23	2.02	0.41
1:D:616:LYS:HG2	2:D:2175:HOH:O	2.20	0.41
1:C:534:GLN:NE2	2:C:2080:HOH:O	2.52	0.41
1:A:617:ILE:HD13	1:A:653:LEU:HD23	2.03	0.41
1:D:227:ALA:HB3	1:D:230:ALA:HB3	2.02	0.41
1:A:324:HIS:HD2	1:A:350:THR:CB	2.29	0.41
1:C:323:TYR:HA	1:C:330:GLN:NE2	2.35	0.41
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.96	0.41
1:D:232:LYS:H	1:D:234:THR:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:LYS:HG2	1:D:490:LEU:HD13	2.03	0.41
1:B:617:ILE:HD13	1:B:653:LEU:HD23	2.04	0.40
1:C:598:PRO:O	1:C:601:LEU:HB2	2.21	0.40
1:D:477:ILE:HD12	1:D:479:LEU:HD21	2.04	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	327/516 (63%)	315 (96%)	7 (2%)	5 (2%)	8	16
1	B	322/516 (62%)	316 (98%)	4 (1%)	2 (1%)	21	38
1	C	325/516 (63%)	314 (97%)	7 (2%)	4 (1%)	10	20
1	D	378/516 (73%)	364 (96%)	11 (3%)	3 (1%)	16	31
All	All	1352/2064 (66%)	1309 (97%)	29 (2%)	14 (1%)	12	24

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	LYS
1	C	495	VAL
1	D	523	VAL
1	C	234	THR
1	D	524	GLY
1	A	228	THR
1	A	234	THR
1	D	232	LYS
1	A	230	ALA
1	A	619	ASN
1	B	232	LYS

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Mol	Chain	Res	Type
1	C	232	LYS
1	C	619	ASN
1	B	619	ASN

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	289/442 (65%)	249 (86%)	40 (14%)	3	7
1	B	289/442 (65%)	250 (86%)	39 (14%)	4	8
1	C	288/442 (65%)	251 (87%)	37 (13%)	4	9
1	D	333/442 (75%)	283 (85%)	50 (15%)	3	6
All	All	1199/1768 (68%)	1033 (86%)	166 (14%)	3	7

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	THR
1	A	205	ASP
1	A	206	LEU
1	A	223	GLN
1	A	226	LEU
1	A	234	THR
1	A	236	LEU
1	A	250	VAL
1	A	253	LEU
1	A	261	GLU
1	A	307	LYS
1	A	324	HIS
1	A	342	GLU
1	A	346	VAL
1	A	347	VAL
1	A	473	CYS
1	A	482	LYS
1	A	487	VAL

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Mol	Chain	Res	Type
1	A	490	LEU
1	A	495	VAL
1	A	526	LYS
1	A	532	LEU
1	A	559	LEU
1	A	570	LEU
1	A	573	LEU
1	A	582	LEU
1	A	593	THR
1	A	601	LEU
1	A	608	THR
1	A	610	VAL
1	A	613	LEU
1	A	628	ASN
1	A	637	LEU
1	A	641	VAL
1	A	648	THR
1	A	658	LEU
1	A	668	GLN
1	A	670	THR
1	A	678	LYS
1	A	680	VAL
1	B	206	LEU
1	B	223	GLN
1	B	226	LEU
1	B	236	LEU
1	B	250	VAL
1	B	253	LEU
1	B	261	GLU
1	B	307	LYS
1	B	324	HIS
1	B	342	GLU
1	B	346	VAL
1	B	347	VAL
1	B	473	CYS
1	B	482	LYS
1	B	487	VAL
1	B	490	LEU
1	B	495	VAL
1	B	526	LYS
1	B	532	LEU
1	B	559	LEU

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Mol	Chain	Res	Type
1	B	570	LEU
1	B	573	LEU
1	B	582	LEU
1	B	593	THR
1	B	601	LEU
1	B	608	THR
1	B	610	VAL
1	B	613	LEU
1	B	628	ASN
1	B	633	ASN
1	B	637	LEU
1	B	641	VAL
1	B	648	THR
1	B	658	LEU
1	B	668	GLN
1	B	670	THR
1	B	678	LYS
1	B	680	VAL
1	B	683	LEU
1	C	206	LEU
1	C	223	GLN
1	C	226	LEU
1	C	234	THR
1	C	236	LEU
1	C	250	VAL
1	C	253	LEU
1	C	261	GLU
1	C	307	LYS
1	C	342	GLU
1	C	346	VAL
1	C	347	VAL
1	C	473	CYS
1	C	482	LYS
1	C	487	VAL
1	C	490	LEU
1	C	526	LYS
1	C	532	LEU
1	C	559	LEU
1	C	570	LEU
1	C	573	LEU
1	C	582	LEU
1	C	593	THR

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Mol	Chain	Res	Type
1	C	601	LEU
1	C	608	THR
1	C	610	VAL
1	C	613	LEU
1	C	628	ASN
1	C	633	ASN
1	C	637	LEU
1	C	641	VAL
1	C	648	THR
1	C	658	LEU
1	C	668	GLN
1	C	670	THR
1	C	678	LYS
1	C	680	VAL
1	D	206	LEU
1	D	223	GLN
1	D	226	LEU
1	D	228	THR
1	D	232	LYS
1	D	234	THR
1	D	236	LEU
1	D	250	VAL
1	D	253	LEU
1	D	261	GLU
1	D	307	LYS
1	D	324	HIS
1	D	342	GLU
1	D	346	VAL
1	D	347	VAL
1	D	370	ILE
1	D	402	LEU
1	D	405	VAL
1	D	469	THR
1	D	473	CYS
1	D	482	LYS
1	D	487	VAL
1	D	490	LEU
1	D	495	VAL
1	D	509	ARG
1	D	511	LYS
1	D	517	ARG
1	D	519	GLN

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Mol	Chain	Res	Type
1	D	526	LYS
1	D	532	LEU
1	D	559	LEU
1	D	570	LEU
1	D	573	LEU
1	D	582	LEU
1	D	593	THR
1	D	601	LEU
1	D	608	THR
1	D	610	VAL
1	D	613	LEU
1	D	628	ASN
1	D	633	ASN
1	D	635	ARG
1	D	637	LEU
1	D	641	VAL
1	D	648	THR
1	D	658	LEU
1	D	668	GLN
1	D	670	THR
1	D	678	LYS
1	D	680	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	302	GLN
1	A	324	HIS
1	A	343	ASN
1	A	529	HIS
1	A	534	GLN
1	A	536	GLN
1	A	574	ASN
1	A	588	ASN
1	A	667	ASN
1	A	668	GLN
1	B	302	GLN
1	B	343	ASN
1	B	529	HIS
1	B	536	GLN
1	B	574	ASN

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Mol	Chain	Res	Type
1	B	588	ASN
1	B	595	HIS
1	B	667	ASN
1	C	223	GLN
1	C	302	GLN
1	C	343	ASN
1	C	529	HIS
1	C	574	ASN
1	C	595	HIS
1	C	600	GLN
1	C	667	ASN
1	C	668	GLN
1	D	223	GLN
1	D	302	GLN
1	D	305	GLN
1	D	343	ASN
1	D	519	GLN
1	D	529	HIS
1	D	574	ASN
1	D	595	HIS
1	D	600	GLN
1	D	667	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	333/516 (64%)	0.48	28 (8%) 17 15	33, 53, 112, 149	0
1	B	330/516 (63%)	0.44	30 (9%) 15 13	30, 54, 105, 125	0
1	C	330/516 (63%)	0.51	26 (7%) 18 16	22, 56, 101, 129	1 (0%)
1	D	385/516 (74%)	0.59	46 (11%) 9 7	20, 54, 117, 146	1 (0%)
All	All	1378/2064 (66%)	0.51	130 (9%) 14 12	20, 54, 111, 149	2 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	THR	7.7
1	D	227	ALA	6.9
1	A	682	GLY	6.6
1	A	351	ALA	6.3
1	A	230	ALA	5.8
1	C	495	VAL	5.8
1	A	495	VAL	5.8
1	C	351	ALA	5.6
1	A	496	THR	5.3
1	D	523	VAL	5.3
1	A	233	THR	5.1
1	D	407	THR	4.8
1	C	496	THR	4.7
1	C	231	GLY	4.7
1	C	233	THR	4.6
1	D	370	ILE	4.6
1	D	351	ALA	4.2
1	A	471	LEU	4.1
1	B	234	THR	4.0
1	D	366	ILE	4.0
1	C	324	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	231	GLY	4.0
1	A	234	THR	4.0
1	D	228	THR	4.0
1	B	687	GLU	3.9
1	D	203	ALA	3.9
1	B	233	THR	3.9
1	B	496	THR	3.9
1	B	685	THR	3.9
1	B	351	ALA	3.9
1	A	232	LYS	3.9
1	A	324	HIS	3.8
1	D	206	LEU	3.8
1	D	204	THR	3.7
1	D	324	HIS	3.7
1	B	495	VAL	3.7
1	A	227	ALA	3.7
1	B	231	GLY	3.6
1	B	206	LEU	3.6
1	D	510	VAL	3.6
1	B	628	ASN	3.5
1	D	202	SER	3.5
1	B	324	HIS	3.5
1	A	494	ALA	3.4
1	D	501	ALA	3.4
1	C	471	LEU	3.4
1	C	620	GLY	3.3
1	C	226	LEU	3.3
1	C	227	ALA	3.3
1	D	405	VAL	3.2
1	D	639	ASP	3.1
1	D	402	LEU	3.1
1	A	228	THR	3.1
1	C	229	GLY	3.1
1	C	682	GLY	3.1
1	C	232	LYS	3.0
1	D	234	THR	3.0
1	D	619	ASN	3.0
1	B	209	MET	2.9
1	C	494	ALA	2.9
1	B	684	SER	2.9
1	C	230	ALA	2.9
1	A	617	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	403	VAL	2.9
1	A	229	GLY	2.9
1	C	621	GLU	2.8
1	B	620	GLY	2.8
1	A	202	SER	2.8
1	D	497	ILE	2.8
1	C	641	VAL	2.7
1	B	471	LEU	2.7
1	B	269	GLN	2.7
1	B	627	ASP	2.6
1	C	625	THR	2.6
1	D	525	SER	2.6
1	D	512	PRO	2.6
1	A	582	LEU	2.6
1	C	206	LEU	2.6
1	A	283	MET	2.5
1	D	229	GLY	2.5
1	B	207	THR	2.5
1	C	493	MET	2.5
1	D	524	GLY	2.5
1	A	493	MET	2.5
1	D	516	TYR	2.4
1	D	689	ALA	2.4
1	B	232	LYS	2.4
1	C	637	LEU	2.4
1	D	482	LYS	2.4
1	C	218[A]	ARG	2.4
1	D	517	ARG	2.4
1	C	234	THR	2.3
1	A	203	ALA	2.3
1	D	620	GLY	2.3
1	D	493	MET	2.3
1	D	208	GLU	2.3
1	B	274	ILE	2.2
1	D	211	LYS	2.2
1	B	208	GLU	2.2
1	B	619	ASN	2.2
1	C	472	LYS	2.2
1	A	206	LEU	2.2
1	D	256	LEU	2.2
1	B	211	LYS	2.2
1	B	226	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	682	GLY	2.2
1	B	322	GLU	2.2
1	B	289	ALA	2.2
1	D	205	ASP	2.2
1	A	492	ARG	2.2
1	A	618	ARG	2.2
1	D	466	VAL	2.1
1	D	686	ALA	2.1
1	A	204	THR	2.1
1	A	620	GLY	2.1
1	D	669	GLY	2.1
1	A	656	GLU	2.1
1	A	621	GLU	2.1
1	D	515	TYR	2.1
1	B	273	SER	2.1
1	D	246	ARG	2.1
1	D	518	SER	2.1
1	D	507	VAL	2.1
1	B	268	ARG	2.1
1	D	683	LEU	2.1
1	D	625	THR	2.1
1	B	212	LYS	2.1
1	D	661	ASP	2.1
1	D	473	CYS	2.1
1	C	639	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.