



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:43 AM UTC

PDB ID : 1URZ / pdb_00001urz
Title : Low pH induced, membrane fusion conformation of the envelope protein of tick-borne encephalitis virus
Authors : Bressanelli, S.; Rey, F.A.
Deposited on : 2003-11-16
Resolution : 2.70 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:

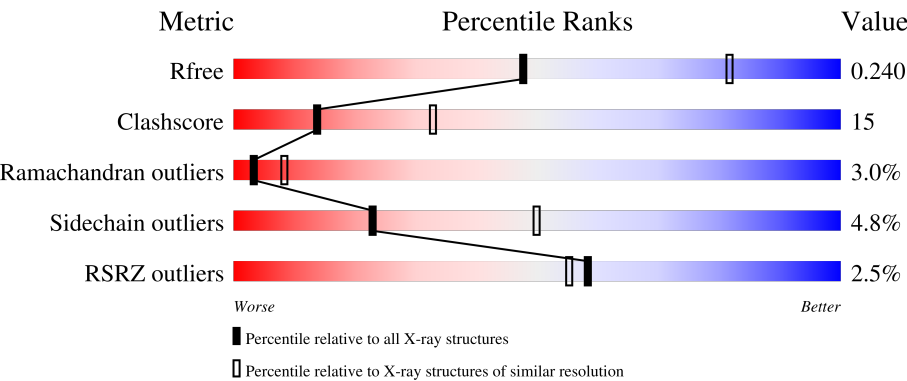
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	401	0% 65%25%5%
1	B	401	2% 67%26%5%
1	C	401	2% 65%27%5%
1	D	401	3% 69%22%5%
1	E	401	2% 70%21%5%

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Mol	Chain	Length	Quality of chain
1	F	401	4% 66% 24% 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17986 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 ENVELOPE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2921	1836	514	550	21			
1	B	387	Total	C	N	O	S	0	0	0
			2946	1851	519	555	21			
1	C	385	Total	C	N	O	S	0	0	0
			2936	1845	517	553	21			
1	D	386	Total	C	N	O	S	0	0	0
			2941	1848	518	554	21			
1	E	382	Total	C	N	O	S	0	0	0
			2921	1836	514	550	21			
1	F	388	Total	C	N	O	S	0	0	0
			2951	1854	520	556	21			

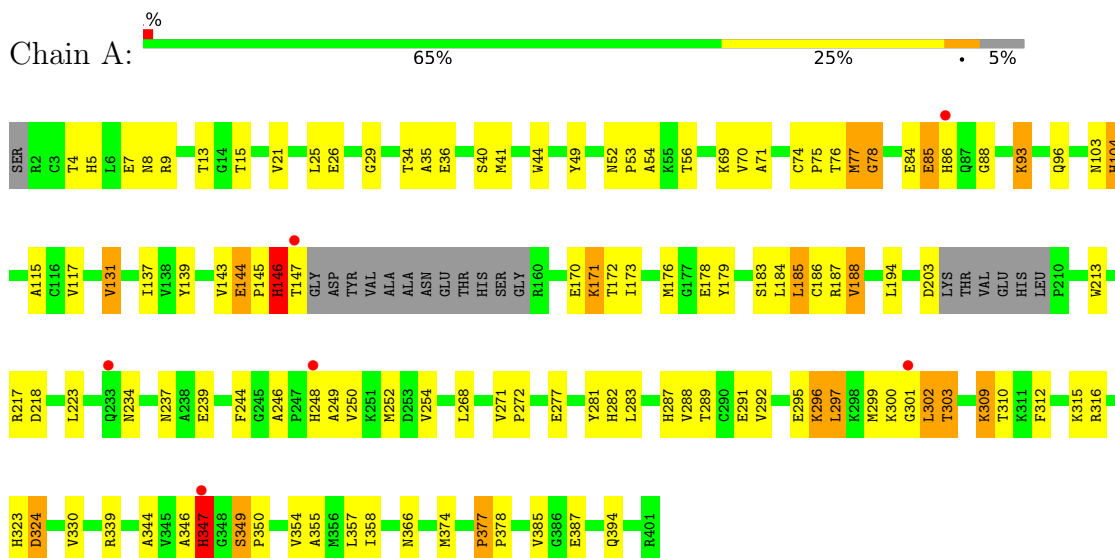
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	77	Total	O	0	0
			77	77		
2	C	64	Total	O	0	0
			64	64		
2	D	50	Total	O	0	0
			50	50		
2	E	49	Total	O	0	0
			49	49		
2	F	57	Total	O	0	0
			57	57		

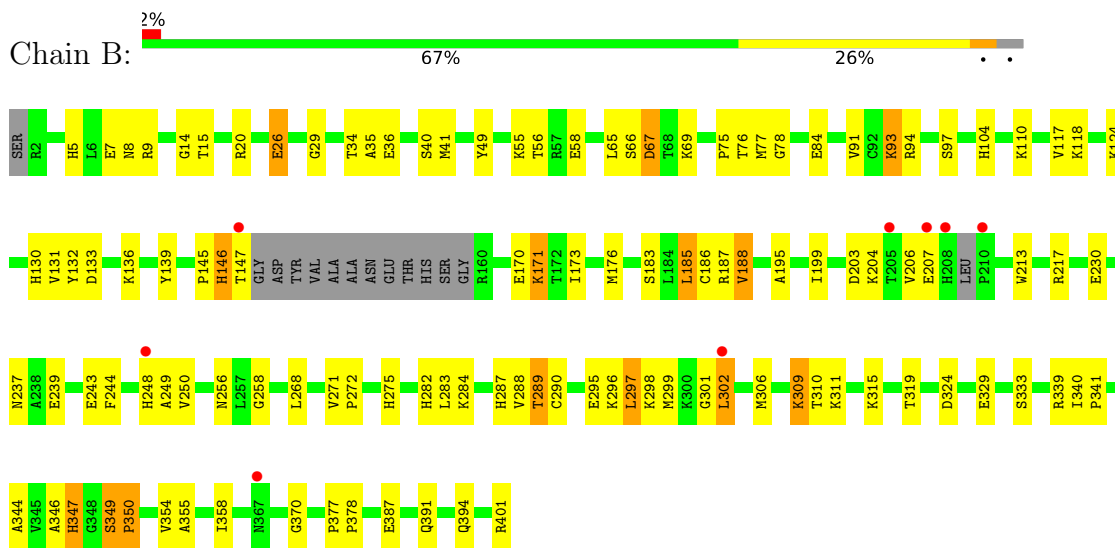
3 Residue-property plots [i](#)

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: ENVELOPE PROTEIN

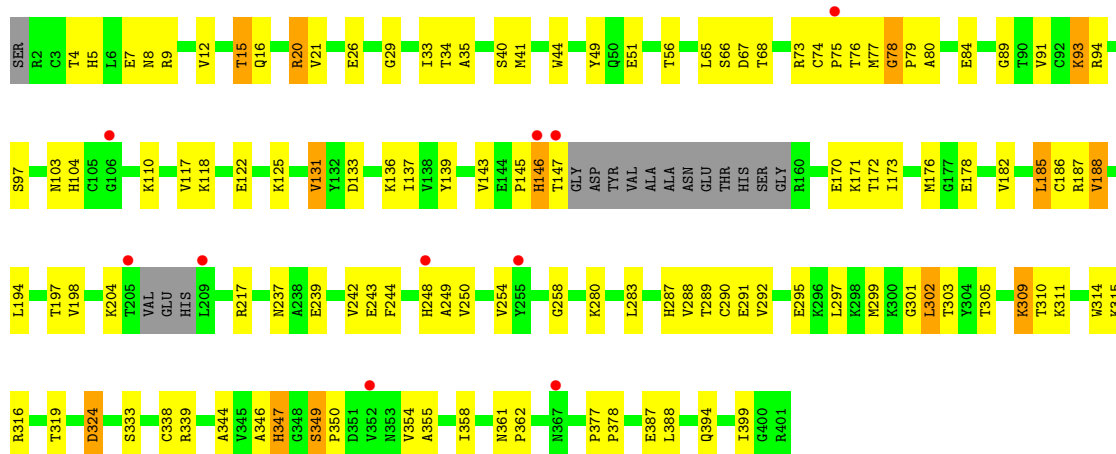


• Molecule 1: ENVELOPE PROTEIN

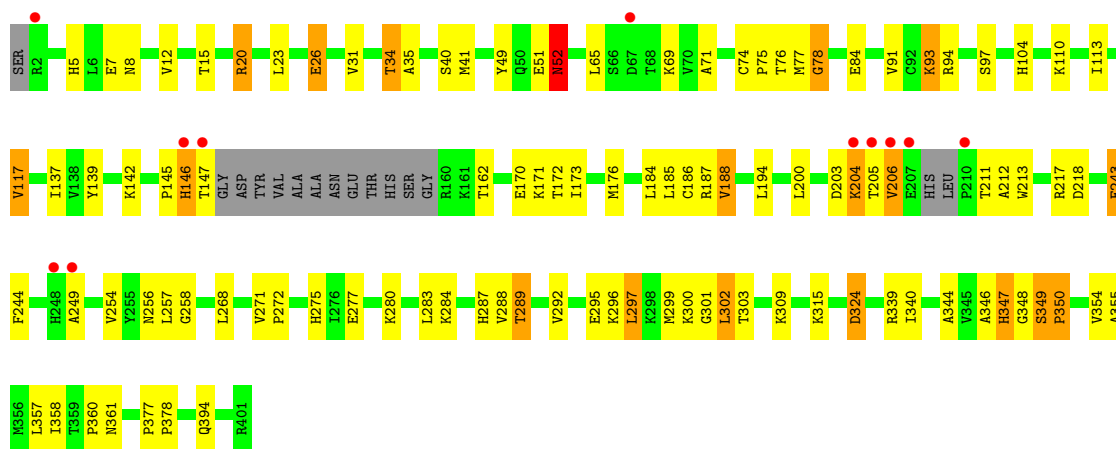


• Molecule 1: ENVELOPE PROTEIN

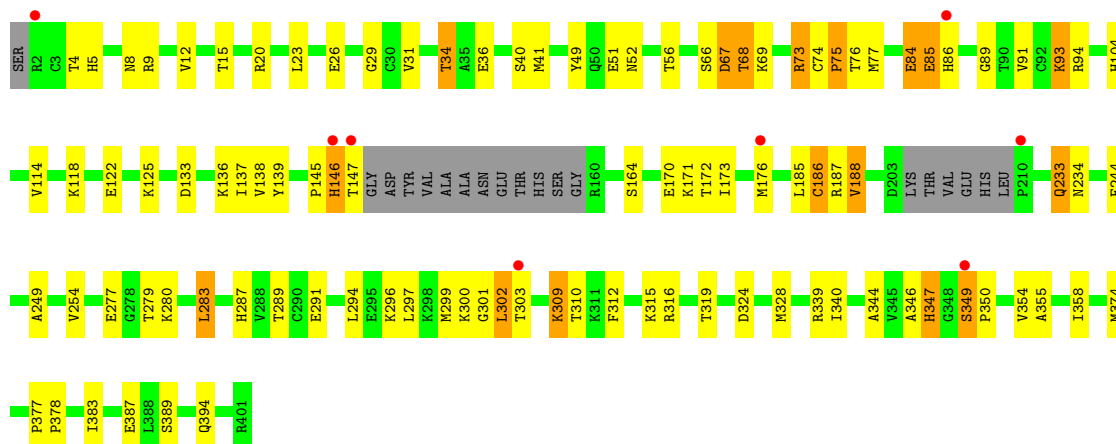




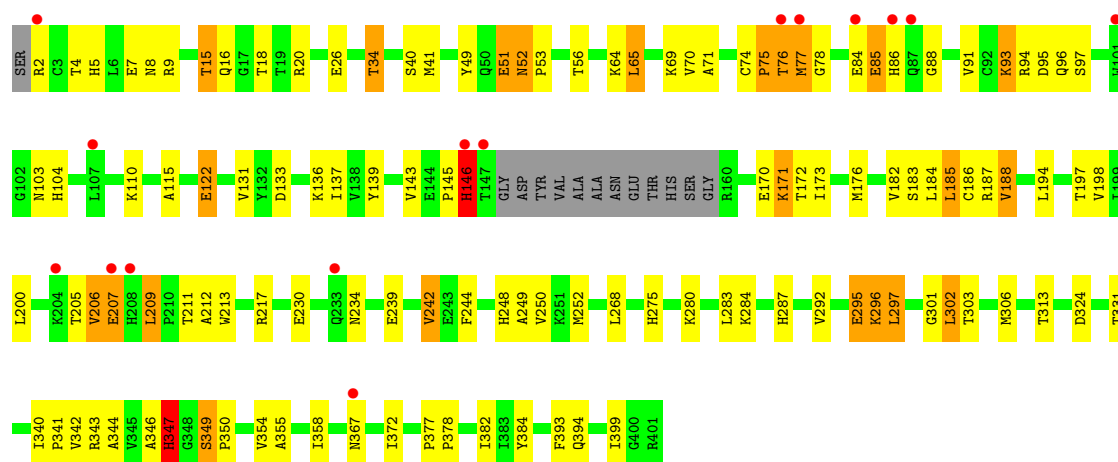
• Molecule 1: ENVELOPE PROTEIN



• Molecule 1: ENVELOPE PROTEIN



• Molecule 1: ENVELOPE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.50Å 142.90Å 173.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (40.00-2.70) 96.8 (40.00-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.242 0.206 , 0.240	Depositor DCC
R_{free} test set	4090 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17986	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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	0.48	0/2984	0.97	13/4046 (0.3%)
1	B	0.46	0/3009	0.96	8/4081 (0.2%)
1	C	0.45	0/2999	0.96	5/4068 (0.1%)
1	D	0.43	0/3004	0.96	12/4074 (0.3%)
1	E	0.43	0/2984	0.95	7/4046 (0.2%)
1	F	0.44	0/3015	0.97	7/4092 (0.2%)
All	All	0.45	0/17995	0.96	52/24407 (0.2%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	85	GLU	N-CA-C	-9.31	97.37	110.50
1	E	85	GLU	N-CA-C	-7.85	98.85	110.23
1	D	205	THR	N-CA-C	-7.84	102.20	112.24
1	A	85	GLU	N-CA-C	-7.67	98.93	110.28
1	C	358	ILE	N-CA-C	-6.81	102.75	112.35
1	F	242	VAL	N-CA-C	6.76	118.87	107.18
1	E	283	LEU	N-CA-C	-6.61	98.94	109.59
1	D	283	LEU	N-CA-C	-6.58	99.00	109.59
1	F	358	ILE	N-CA-C	-6.43	103.28	112.35
1	A	291	GLU	N-CA-C	-6.42	98.05	108.52
1	C	315	LYS	N-CA-C	-6.42	103.79	111.69
1	A	358	ILE	N-CA-C	-6.38	103.35	112.35
1	B	358	ILE	N-CA-C	-6.22	103.10	111.44
1	D	203	ASP	N-CA-C	6.13	118.23	110.33
1	D	315	LYS	N-CA-C	-6.08	104.56	112.23
1	E	358	ILE	N-CA-C	-6.08	103.78	112.35
1	F	283	LEU	N-CA-C	-6.02	99.89	109.59
1	F	324	ASP	N-CA-C	5.83	119.70	112.24
1	C	283	LEU	N-CA-C	-5.81	100.23	109.59
1	E	104	HIS	N-CA-C	5.80	119.66	112.58
1	E	186	CYS	N-CA-C	5.70	117.81	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	ILE	N-CA-C	5.68	113.51	108.63
1	A	377	PRO	CA-C-N	-5.66	114.14	119.85
1	A	377	PRO	C-N-CA	-5.66	114.14	119.85
1	D	324	ASP	N-CA-C	5.66	119.37	111.90
1	B	26	GLU	N-CA-C	-5.62	102.96	110.55
1	B	283	LEU	N-CA-C	-5.61	100.56	109.59
1	B	315	LYS	N-CA-C	-5.55	105.63	112.90
1	F	242	VAL	CB-CA-C	-5.54	104.09	110.41
1	A	283	LEU	N-CA-C	-5.49	100.75	109.59
1	C	324	ASP	N-CA-C	5.48	119.13	111.90
1	B	58	GLU	N-CA-C	-5.43	100.05	108.90
1	C	258	GLY	N-CA-C	5.38	121.22	112.61
1	E	340	ILE	N-CA-C	5.33	113.21	108.63
1	A	54	ALA	N-CA-C	5.32	117.74	110.24
1	B	104	HIS	N-CA-C	5.29	119.04	112.58
1	E	315	LYS	N-CA-C	-5.21	105.67	112.23
1	A	315	LYS	N-CA-C	-5.20	105.22	112.45
1	A	324	ASP	N-CA-C	5.19	118.75	111.90
1	A	77	MET	N-CA-C	-5.17	102.63	110.28
1	D	104	HIS	N-CA-C	5.13	118.80	111.92
1	A	144	GLU	CA-C-N	5.12	125.40	119.92
1	A	144	GLU	C-N-CA	5.12	125.40	119.92
1	D	357	LEU	N-CA-C	5.10	117.61	109.96
1	D	358	ILE	N-CA-C	-5.10	105.16	112.35
1	D	26	GLU	N-CA-C	-5.08	103.69	110.55
1	D	52	ASN	CA-C-N	5.08	124.98	119.85
1	D	52	ASN	C-N-CA	5.08	124.98	119.85
1	D	340	ILE	CB-CA-C	-5.05	105.44	110.89
1	A	104	HIS	N-CA-C	5.04	118.68	111.92
1	B	324	ASP	N-CA-C	5.03	118.68	112.24
1	F	340	ILE	CB-CA-C	-5.03	105.46	110.89

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	2921	0	2881	94	0
1	B	2946	0	2891	90	0
1	C	2936	0	2886	96	0
1	D	2941	0	2889	90	0
1	E	2921	0	2881	83	0
1	F	2951	0	2893	92	0
2	A	73	0	0	6	0
2	B	77	0	0	5	0
2	C	64	0	0	0	0
2	D	50	0	0	0	0
2	E	49	0	0	2	0
2	F	57	0	0	2	0
All	All	17986	0	17321	508	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 15.

All (508) 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:F:15:THR:HG22	1:F:16:GLN:HE21	1.31	0.92
1:E:233:GLN:HE21	1:E:234:ASN:H	1.14	0.91
1:C:15:THR:HG22	1:C:16:GLN:OE1	1.75	0.87
1:F:8:ASN:OD1	1:F:301:GLY:HA3	1.78	0.84
1:A:170:GLU:HG2	1:A:185:LEU:HD23	1.60	0.84
1:B:170:GLU:HG2	1:B:185:LEU:HD23	1.58	0.83
1:B:69:LYS:HE3	1:E:316:ARG:NH2	1.94	0.83
1:A:277:GLU:HG3	1:A:277:GLU:O	1.77	0.82
1:C:170:GLU:HG2	1:C:185:LEU:HD23	1.61	0.82
1:A:295:GLU:HG2	1:B:9:ARG:HG2	1.61	0.82
1:A:309:LYS:HG2	1:A:387:GLU:HG3	1.62	0.80
1:B:295:GLU:HG2	1:C:9:ARG:HG2	1.64	0.79
1:D:5:HIS:HB2	1:D:302:LEU:HD23	1.64	0.78
1:F:170:GLU:HG2	1:F:185:LEU:HD23	1.64	0.78
1:D:170:GLU:HG2	1:D:185:LEU:HD23	1.65	0.78
1:E:309:LYS:HG2	1:E:387:GLU:HG3	1.64	0.77
1:F:15:THR:HG22	1:F:16:GLN:NE2	2.01	0.74
1:E:316:ARG:HH12	1:E:319:THR:HG21	1.52	0.74
1:D:93:LYS:HB2	1:D:244:PHE:CD2	2.23	0.73
1:B:41:MET:HG3	1:B:176:MET:CE	2.20	0.72
1:E:93:LYS:HD3	1:E:94:ARG:N	2.03	0.72
1:D:206:VAL:CB	1:D:211:THR:HG21	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:CYS:HB3	1:A:288:VAL:CG1	2.20	0.72
1:B:309:LYS:HG2	1:B:387:GLU:HG3	1.72	0.71
1:A:25:LEU:HB3	2:A:2007:HOH:O	1.90	0.71
1:D:295:GLU:HG2	1:E:9:ARG:HG2	1.72	0.70
1:A:139:TYR:CZ	1:A:188:VAL:HG13	2.26	0.70
1:A:277:GLU:HG2	1:A:282:HIS:NE2	2.07	0.70
1:E:66:SER:OG	1:E:118:LYS:HB2	1.92	0.69
1:D:302:LEU:HD12	1:D:303:THR:H	1.57	0.68
1:D:302:LEU:HD12	1:D:303:THR:N	2.08	0.68
1:B:5:HIS:HB2	1:B:302:LEU:HD23	1.75	0.68
1:A:301:GLY:O	1:A:302:LEU:HB2	1.92	0.67
1:D:76:THR:OG1	1:D:77:MET:HE2	1.94	0.67
1:E:74:CYS:HB2	1:E:77:MET:HG2	1.76	0.67
1:F:139:TYR:CZ	1:F:188:VAL:HG13	2.29	0.67
1:A:88:GLY:HA3	1:A:234:ASN:ND2	2.10	0.67
1:A:8:ASN:OD1	1:A:301:GLY:HA3	1.93	0.67
1:B:20:ARG:HD3	1:C:12:VAL:HG23	1.77	0.67
1:E:170:GLU:HG2	1:E:185:LEU:HD23	1.75	0.67
1:D:12:VAL:HG23	1:F:20:ARG:HD3	1.76	0.66
1:E:56:THR:HA	1:F:399:ILE:HD13	1.78	0.66
1:D:8:ASN:OD1	1:D:301:GLY:HA3	1.95	0.66
1:E:233:GLN:NE2	1:E:234:ASN:H	1.90	0.66
1:D:41:MET:HG3	1:D:176:MET:CE	2.27	0.65
1:E:233:GLN:CD	1:E:233:GLN:H	2.05	0.65
1:A:93:LYS:HB2	1:A:244:PHE:CD2	2.32	0.64
1:F:64:LYS:HB2	1:F:122:GLU:OE1	1.98	0.64
1:B:9:ARG:HD3	2:B:2001:HOH:O	1.96	0.64
1:B:8:ASN:OD1	1:B:301:GLY:HA3	1.97	0.64
1:A:170:GLU:HG2	1:A:185:LEU:CD2	2.27	0.64
1:C:8:ASN:OD1	1:C:301:GLY:HA3	1.98	0.64
1:A:76:THR:OG1	1:A:77:MET:HE2	1.98	0.64
1:B:173:ILE:HD12	1:C:9:ARG:HH21	1.61	0.64
1:E:378:PRO:HA	1:E:394:GLN:HB3	1.79	0.63
1:D:339:ARG:NH1	1:D:361:ASN:OD1	2.31	0.63
1:B:20:ARG:HG2	2:B:2063:HOH:O	1.97	0.63
1:A:36:GLU:OE2	1:A:300:LYS:HE2	1.98	0.63
1:F:344:ALA:HB3	1:F:355:ALA:HB2	1.81	0.62
1:D:20:ARG:HG3	1:D:20:ARG:HH11	1.64	0.62
1:D:20:ARG:HG3	1:D:20:ARG:NH1	2.13	0.62
1:B:170:GLU:HG2	1:B:185:LEU:CD2	2.28	0.62
1:E:8:ASN:OD1	1:E:301:GLY:HA3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:THR:OG1	1:C:77:MET:HE2	1.99	0.62
1:C:41:MET:CE	1:C:145:PRO:HA	2.30	0.62
1:F:91:VAL:HG12	1:F:244:PHE:HE2	1.63	0.62
1:A:302:LEU:HD13	1:A:303:THR:N	2.15	0.61
1:E:170:GLU:OE1	1:F:187:ARG:NH2	2.32	0.61
1:A:277:GLU:HG2	1:A:282:HIS:CD2	2.34	0.61
1:D:5:HIS:CB	1:D:302:LEU:HD23	2.28	0.61
1:D:139:TYR:CZ	1:D:188:VAL:HG13	2.35	0.61
1:F:170:GLU:HG2	1:F:185:LEU:CD2	2.30	0.61
1:F:176:MET:HE2	1:F:182:VAL:HG21	1.80	0.61
1:A:349:SER:H	1:A:350:PRO:CD	2.12	0.61
1:D:5:HIS:HB2	1:D:302:LEU:CD2	2.30	0.61
1:D:186:CYS:HB3	1:D:288:VAL:CG1	2.31	0.61
1:C:74:CYS:HB2	1:C:77:MET:HG2	1.82	0.61
1:F:2:ARG:N	1:F:367:ASN:HD21	1.99	0.61
1:C:5:HIS:HB2	1:C:302:LEU:HD23	1.82	0.61
1:B:186:CYS:HB3	1:B:288:VAL:HG13	1.82	0.60
1:D:344:ALA:HB3	1:D:355:ALA:HB2	1.83	0.60
1:D:217:ARG:HG3	1:D:217:ARG:HH11	1.66	0.59
1:D:51:GLU:HG2	1:E:378:PRO:HG2	1.83	0.59
1:B:271:VAL:HG13	1:B:272:PRO:HD2	1.83	0.59
1:A:56:THR:HG23	1:A:131:VAL:HG22	1.84	0.59
1:B:69:LYS:HG3	1:B:84:GLU:OE2	2.02	0.59
1:B:36:GLU:HG3	1:B:298:LYS:HD3	1.83	0.59
1:D:40:SER:O	1:D:41:MET:HE2	2.03	0.59
1:D:187:ARG:NH2	1:F:170:GLU:OE1	2.35	0.59
1:C:176:MET:HE2	1:C:182:VAL:HG11	1.85	0.58
1:E:316:ARG:HH11	1:E:316:ARG:HG2	1.68	0.58
1:B:5:HIS:HB2	1:B:302:LEU:CD2	2.34	0.58
1:E:91:VAL:HG12	1:E:244:PHE:HE2	1.68	0.58
1:B:217:ARG:HB2	1:B:217:ARG:NH1	2.18	0.58
1:B:344:ALA:HB3	1:B:355:ALA:HB2	1.84	0.58
1:C:84:GLU:N	1:C:84:GLU:OE1	2.36	0.58
1:C:349:SER:H	1:C:350:PRO:CD	2.17	0.58
1:F:378:PRO:HA	1:F:394:GLN:HB3	1.84	0.58
1:C:170:GLU:HG3	1:C:186:CYS:O	2.04	0.58
1:C:244:PHE:CE1	1:C:254:VAL:HG22	2.39	0.58
1:D:69:LYS:HG3	1:D:84:GLU:OE2	2.04	0.58
1:F:115:ALA:HB3	1:F:252:MET:HE3	1.86	0.58
1:A:84:GLU:N	1:A:84:GLU:OE1	2.36	0.58
1:F:209:LEU:H	1:F:211:THR:HG23	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HG12	1:A:71:ALA:N	2.19	0.57
1:A:143:VAL:HG11	1:A:176:MET:SD	2.44	0.57
1:C:309:LYS:HG3	1:C:310:THR:HG23	1.86	0.57
1:F:93:LYS:HB2	1:F:244:PHE:CD2	2.40	0.57
1:B:69:LYS:HE3	1:E:316:ARG:HH21	1.70	0.57
1:C:139:TYR:CZ	1:C:188:VAL:HG13	2.39	0.57
1:B:309:LYS:CG	1:B:387:GLU:HG3	2.34	0.57
1:F:84:GLU:N	1:F:84:GLU:OE1	2.38	0.57
1:C:93:LYS:HB2	1:C:244:PHE:CD2	2.40	0.57
1:E:52:ASN:OD1	1:E:279:THR:HB	2.04	0.56
1:E:36:GLU:OE2	1:E:300:LYS:HE2	2.05	0.56
1:F:145:PRO:O	1:F:146:HIS:HB3	2.04	0.56
1:A:170:GLU:OE1	1:B:187:ARG:NH2	2.38	0.56
1:B:170:GLU:OE1	1:C:187:ARG:NH2	2.39	0.56
1:F:349:SER:H	1:F:350:PRO:CD	2.19	0.56
1:C:68:THR:HA	1:C:117:VAL:HG12	1.88	0.56
1:E:76:THR:OG1	1:E:77:MET:HE2	2.05	0.56
1:D:145:PRO:O	1:D:146:HIS:HB3	2.05	0.56
1:E:349:SER:H	1:E:350:PRO:CD	2.19	0.55
1:F:143:VAL:HG11	1:F:176:MET:SD	2.46	0.55
1:D:378:PRO:HA	1:D:394:GLN:HB3	1.89	0.55
1:C:170:GLU:HG2	1:C:185:LEU:CD2	2.33	0.55
1:B:93:LYS:HB2	1:B:244:PHE:CD2	2.41	0.55
1:C:339:ARG:HH11	1:C:339:ARG:HG2	1.71	0.55
1:D:77:MET:O	1:D:78:GLY:O	2.23	0.55
1:F:2:ARG:N	1:F:367:ASN:ND2	2.55	0.55
1:D:349:SER:H	1:D:350:PRO:CD	2.18	0.55
1:A:349:SER:H	1:A:350:PRO:HD3	1.71	0.55
1:B:41:MET:CE	1:B:145:PRO:HA	2.36	0.55
1:E:328:MET:HE1	1:E:374:MET:HE3	1.89	0.55
1:A:69:LYS:HG3	1:A:84:GLU:OE2	2.08	0.55
1:B:20:ARG:HD3	1:C:12:VAL:CG2	2.37	0.55
1:C:349:SER:H	1:C:350:PRO:HD3	1.72	0.55
1:D:170:GLU:HG2	1:D:185:LEU:CD2	2.36	0.55
1:B:378:PRO:HA	1:B:394:GLN:HB3	1.90	0.54
1:A:96:GLN:HE22	1:B:110:LYS:HG3	1.70	0.54
1:A:344:ALA:HB3	1:A:355:ALA:HB2	1.90	0.54
1:D:65:LEU:HB3	1:D:117:VAL:HG21	1.89	0.54
1:E:339:ARG:HH11	1:E:339:ARG:HG2	1.72	0.54
1:A:13:THR:HG22	2:A:2004:HOH:O	2.08	0.54
1:E:74:CYS:C	1:E:76:THR:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:GLU:O	1:E:86:HIS:HB2	2.07	0.54
1:A:246:ALA:HB1	1:C:79:PRO:HG3	1.89	0.54
1:A:297:LEU:HD23	1:A:297:LEU:O	2.08	0.54
1:B:40:SER:O	1:B:41:MET:HE2	2.08	0.54
1:C:74:CYS:C	1:C:76:THR:H	2.15	0.54
1:E:139:TYR:CZ	1:E:188:VAL:HG13	2.42	0.54
1:E:93:LYS:HD3	1:E:94:ARG:H	1.73	0.54
1:B:84:GLU:OE1	1:B:84:GLU:N	2.40	0.54
1:C:186:CYS:HB3	1:C:288:VAL:HG13	1.89	0.54
1:D:41:MET:CE	1:D:145:PRO:HA	2.38	0.54
1:E:170:GLU:HG3	1:E:186:CYS:O	2.07	0.54
1:A:346:ALA:O	1:A:347:HIS:C	2.51	0.53
1:F:217:ARG:HG3	1:F:217:ARG:HH11	1.73	0.53
1:A:115:ALA:HB3	1:A:252:MET:HE3	1.89	0.53
1:A:330:VAL:HG11	1:A:385:VAL:HG11	1.90	0.53
1:C:176:MET:HE2	1:C:182:VAL:HG21	1.90	0.53
1:D:339:ARG:HG3	1:D:339:ARG:HH11	1.72	0.53
1:D:74:CYS:HB2	1:D:77:MET:HG2	1.90	0.53
1:A:223:LEU:HA	2:A:2040:HOH:O	2.08	0.53
1:B:55:LYS:HG2	1:B:130:HIS:CE1	2.44	0.53
1:B:139:TYR:CZ	1:B:188:VAL:HG13	2.44	0.53
1:E:233:GLN:NE2	1:E:233:GLN:H	2.05	0.53
1:E:344:ALA:HB3	1:E:355:ALA:HB2	1.91	0.53
1:F:93:LYS:HD3	1:F:94:ARG:N	2.24	0.53
1:A:244:PHE:CE1	1:A:254:VAL:HG22	2.44	0.53
1:F:15:THR:CG2	1:F:16:GLN:HE21	2.14	0.53
1:A:145:PRO:O	1:A:146:HIS:HB3	2.08	0.53
1:E:20:ARG:HD3	1:E:291:GLU:OE2	2.08	0.53
1:F:301:GLY:O	1:F:302:LEU:HB2	2.09	0.53
1:B:130:HIS:HB2	1:B:199:ILE:HB	1.90	0.53
1:C:344:ALA:HB3	1:C:355:ALA:HB2	1.91	0.53
1:D:35:ALA:HB2	1:D:299:MET:CE	2.38	0.53
1:E:310:THR:HG22	1:E:387:GLU:OE1	2.09	0.53
1:A:85:GLU:O	1:A:86:HIS:HB2	2.08	0.52
1:C:137:ILE:HD12	1:C:194:LEU:HD11	1.90	0.52
1:F:41:MET:CE	1:F:145:PRO:HA	2.39	0.52
1:A:378:PRO:HA	1:A:394:GLN:HB3	1.90	0.52
1:B:97:SER:O	1:B:110:LYS:HA	2.09	0.52
1:D:349:SER:H	1:D:350:PRO:HD3	1.74	0.52
1:E:74:CYS:O	1:E:76:THR:N	2.35	0.52
1:F:5:HIS:HB2	1:F:302:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:SER:H	1:B:350:PRO:CD	2.21	0.52
1:D:97:SER:O	1:D:110:LYS:HA	2.10	0.52
1:C:93:LYS:HD3	1:C:94:ARG:N	2.24	0.52
1:D:35:ALA:HB2	1:D:299:MET:HE1	1.91	0.52
1:C:145:PRO:O	1:C:146:HIS:HB3	2.10	0.52
1:D:297:LEU:HD23	1:D:297:LEU:O	2.10	0.52
1:C:137:ILE:HD12	1:C:194:LEU:CD1	2.41	0.51
1:D:344:ALA:CB	1:D:355:ALA:HB2	2.39	0.51
1:C:56:THR:HG23	1:C:131:VAL:HG22	1.92	0.51
1:F:74:CYS:O	1:F:76:THR:N	2.41	0.51
1:C:301:GLY:O	1:C:302:LEU:HB2	2.09	0.51
1:D:170:GLU:OE1	1:E:187:ARG:NH2	2.44	0.51
1:C:35:ALA:HB2	1:C:299:MET:CE	2.41	0.51
1:E:244:PHE:CE1	1:E:254:VAL:HG22	2.45	0.51
1:E:301:GLY:O	1:E:302:LEU:HB2	2.09	0.51
1:B:55:LYS:HD2	1:B:230:GLU:OE1	2.09	0.51
1:C:378:PRO:HA	1:C:394:GLN:HB3	1.92	0.51
1:E:349:SER:H	1:E:350:PRO:HD3	1.76	0.51
1:E:5:HIS:HB2	1:E:302:LEU:HD23	1.93	0.50
1:C:316:ARG:HH21	1:D:69:LYS:HE3	1.75	0.50
2:B:2038:HOH:O	1:C:9:ARG:HD3	2.10	0.50
1:B:93:LYS:HD3	1:B:94:ARG:N	2.27	0.50
1:B:349:SER:H	1:B:350:PRO:HD3	1.76	0.50
1:C:172:THR:HG22	1:C:173:ILE:N	2.27	0.50
1:A:271:VAL:HG13	1:A:272:PRO:HD2	1.94	0.50
1:E:93:LYS:O	1:E:114:VAL:HG23	2.11	0.50
1:E:145:PRO:O	1:E:146:HIS:HB3	2.12	0.50
1:C:139:TYR:CG	1:C:188:VAL:HG22	2.47	0.49
1:A:244:PHE:CD1	1:A:254:VAL:HG22	2.47	0.49
1:A:349:SER:N	1:A:350:PRO:CD	2.73	0.49
1:C:91:VAL:HG12	1:C:244:PHE:HE2	1.77	0.49
1:A:187:ARG:NH2	1:C:170:GLU:OE1	2.45	0.49
1:A:248:HIS:O	1:A:250:VAL:N	2.45	0.49
1:D:354:VAL:HB	1:D:377:PRO:HG2	1.94	0.49
1:A:35:ALA:HB2	1:A:299:MET:CE	2.42	0.49
1:B:344:ALA:CB	1:B:355:ALA:HB2	2.42	0.49
1:F:70:VAL:HG12	1:F:71:ALA:N	2.26	0.49
1:D:271:VAL:HG13	1:D:272:PRO:HD2	1.93	0.49
1:F:7:GLU:HA	1:F:302:LEU:O	2.12	0.49
1:D:348:GLY:O	1:D:349:SER:OG	2.26	0.49
1:A:74:CYS:O	1:A:76:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:ARG:HG3	1:E:77:MET:HB2	1.95	0.49
1:F:26:GLU:HA	1:F:287:HIS:HB3	1.94	0.49
1:B:401:ARG:NE	2:B:2077:HOH:O	2.46	0.49
1:D:7:GLU:HA	1:D:302:LEU:O	2.12	0.49
1:C:77:MET:O	1:C:78:GLY:O	2.31	0.49
1:C:346:ALA:O	1:C:347:HIS:C	2.55	0.49
1:F:349:SER:H	1:F:350:PRO:HD3	1.77	0.49
1:C:74:CYS:O	1:C:76:THR:N	2.45	0.48
1:B:275:HIS:CD2	1:B:284:LYS:HG3	2.48	0.48
1:C:73:ARG:HG2	1:C:80:ALA:HB2	1.95	0.48
1:D:12:VAL:HG21	1:F:20:ARG:HB2	1.95	0.48
1:D:256:ASN:C	1:D:258:GLY:H	2.20	0.48
1:E:41:MET:CE	1:E:145:PRO:HA	2.43	0.48
1:E:49:TYR:CZ	1:E:280:LYS:HE3	2.48	0.48
1:E:316:ARG:NH1	1:E:319:THR:HG21	2.25	0.48
1:F:213:TRP:CD2	1:F:268:LEU:HD13	2.47	0.48
1:F:349:SER:N	1:F:350:PRO:CD	2.76	0.48
1:B:49:TYR:HB3	1:B:282:HIS:ND1	2.28	0.48
1:C:349:SER:N	1:C:350:PRO:CD	2.76	0.48
1:D:93:LYS:HD3	1:D:94:ARG:N	2.28	0.48
1:B:310:THR:HG22	1:B:387:GLU:OE1	2.13	0.48
1:C:26:GLU:HA	1:C:287:HIS:CB	2.43	0.48
1:A:184:LEU:HD23	1:A:292:VAL:HG22	1.95	0.48
1:B:256:ASN:OD1	1:B:258:GLY:N	2.40	0.48
1:C:288:VAL:HG12	1:C:290:CYS:SG	2.53	0.48
1:D:26:GLU:HA	1:D:287:HIS:CB	2.43	0.48
1:D:346:ALA:O	1:D:347:HIS:C	2.56	0.48
1:A:147:THR:HG23	1:A:147:THR:O	2.14	0.48
1:A:297:LEU:HD23	1:A:297:LEU:C	2.39	0.48
1:D:217:ARG:HG3	1:D:217:ARG:NH1	2.28	0.48
1:A:366:ASN:N	1:A:366:ASN:HD22	2.11	0.48
1:B:349:SER:N	1:B:350:PRO:CD	2.77	0.48
1:C:314:TRP:CD1	1:C:388:LEU:HD11	2.49	0.48
1:F:306:MET:CE	1:F:341:PRO:HB3	2.44	0.48
1:F:344:ALA:CB	1:F:355:ALA:HB2	2.44	0.48
1:C:93:LYS:HD3	1:C:93:LYS:C	2.39	0.47
1:D:256:ASN:C	1:D:258:GLY:N	2.72	0.47
1:D:349:SER:N	1:D:350:PRO:CD	2.76	0.47
1:F:393:PHE:HB3	2:F:2054:HOH:O	2.13	0.47
1:B:306:MET:HE3	1:B:339:ARG:O	2.15	0.47
1:D:204:LYS:C	1:D:206:VAL:N	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:PHE:HB2	2:E:2037:HOH:O	2.15	0.47
1:F:342:VAL:HG21	1:F:372:ILE:HD13	1.96	0.47
1:D:93:LYS:HD3	1:D:93:LYS:C	2.39	0.47
1:E:172:THR:HG22	1:E:173:ILE:N	2.28	0.47
1:A:357:LEU:HD23	1:A:374:MET:HB3	1.96	0.47
1:B:311:LYS:HB3	1:B:333:SER:OG	2.15	0.47
1:E:137:ILE:HG22	1:E:139:TYR:CE1	2.50	0.47
1:E:346:ALA:O	1:E:347:HIS:C	2.57	0.47
1:A:316:ARG:NE	2:A:2053:HOH:O	2.48	0.47
1:A:323:HIS:ND1	2:A:2054:HOH:O	2.35	0.47
1:B:346:ALA:O	1:B:347:HIS:C	2.58	0.47
1:E:26:GLU:HA	1:E:287:HIS:CB	2.44	0.47
1:F:18:THR:HA	1:F:295:GLU:OE1	2.15	0.47
1:F:26:GLU:HA	1:F:287:HIS:CB	2.44	0.47
1:F:172:THR:HG22	1:F:173:ILE:N	2.29	0.47
1:A:176:MET:HB2	1:A:179:TYR:HB2	1.97	0.47
1:D:91:VAL:HG12	1:D:244:PHE:HE2	1.79	0.47
1:A:74:CYS:C	1:A:76:THR:H	2.22	0.47
1:C:7:GLU:HA	1:C:302:LEU:O	2.14	0.47
1:B:306:MET:HE2	1:B:341:PRO:HB3	1.96	0.47
1:C:40:SER:O	1:C:41:MET:HE2	2.15	0.47
1:D:142:LYS:NZ	1:D:162:THR:OG1	2.46	0.47
1:E:84:GLU:OE1	1:E:84:GLU:N	2.48	0.47
1:E:349:SER:N	1:E:350:PRO:CD	2.77	0.47
1:F:354:VAL:HB	1:F:377:PRO:HG2	1.97	0.47
1:A:41:MET:CE	1:A:145:PRO:HA	2.44	0.46
1:B:145:PRO:O	1:B:146:HIS:HB3	2.13	0.46
1:C:354:VAL:HB	1:C:377:PRO:HG2	1.97	0.46
1:D:147:THR:O	1:D:147:THR:HG23	2.15	0.46
1:A:295:GLU:HG2	1:B:9:ARG:CG	2.37	0.46
1:B:35:ALA:HB2	1:B:299:MET:CE	2.46	0.46
1:B:91:VAL:HG12	1:B:244:PHE:HE2	1.80	0.46
1:C:103:ASN:O	1:C:104:HIS:HB2	2.16	0.46
1:E:176:MET:HB2	1:E:176:MET:HE3	1.77	0.46
1:F:85:GLU:O	1:F:86:HIS:HB2	2.15	0.46
1:A:36:GLU:CD	1:A:300:LYS:HE2	2.41	0.46
1:A:172:THR:HG22	1:A:173:ILE:N	2.31	0.46
1:D:200:LEU:HD23	1:D:268:LEU:HD11	1.97	0.46
1:F:75:PRO:O	1:F:76:THR:HG23	2.16	0.46
1:F:97:SER:O	1:F:110:LYS:HA	2.14	0.46
1:E:91:VAL:HG12	1:E:244:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LEU:HD23	1:B:297:LEU:O	2.15	0.46
1:F:347:HIS:CE1	1:F:382:ILE:HD11	2.50	0.46
1:D:12:VAL:CG2	1:F:20:ARG:HD3	2.43	0.46
1:D:23:LEU:HD22	1:D:31:VAL:HG21	1.97	0.46
1:A:354:VAL:HB	1:A:377:PRO:HG2	1.98	0.46
1:B:213:TRP:CD2	1:B:268:LEU:HD13	2.51	0.46
1:F:239:GLU:HA	1:F:242:VAL:O	2.16	0.46
1:A:186:CYS:HB3	1:A:288:VAL:HG11	1.98	0.46
1:E:133:ASP:HB3	1:E:136:LYS:HB2	1.97	0.46
1:E:244:PHE:CD1	1:E:254:VAL:HG22	2.51	0.46
1:C:29:GLY:O	1:C:44:TRP:HB2	2.15	0.45
1:C:311:LYS:HB3	1:C:333:SER:OG	2.16	0.45
1:E:67:ASP:O	1:E:68:THR:CB	2.64	0.45
1:E:23:LEU:HD22	1:E:31:VAL:HG11	1.99	0.45
1:E:173:ILE:HD12	1:F:9:ARG:HH21	1.81	0.45
1:F:40:SER:O	1:F:41:MET:HE2	2.16	0.45
1:F:65:LEU:HD11	1:F:242:VAL:HG21	1.99	0.45
1:F:170:GLU:HG3	1:F:186:CYS:O	2.16	0.45
1:A:139:TYR:CE1	1:A:188:VAL:CG1	3.00	0.45
1:A:309:LYS:HG2	1:A:309:LYS:O	2.15	0.45
1:D:275:HIS:CD2	1:D:284:LYS:HG3	2.50	0.45
1:F:206:VAL:O	1:F:207:GLU:C	2.59	0.45
1:F:217:ARG:HG3	1:F:217:ARG:NH1	2.31	0.45
1:B:66:SER:OG	1:B:118:LYS:HB2	2.16	0.45
1:C:20:ARG:NE	1:C:291:GLU:CD	2.75	0.45
1:F:95:ASP:OD1	1:F:96:GLN:N	2.39	0.45
1:A:29:GLY:O	1:A:44:TRP:HB2	2.16	0.45
1:C:186:CYS:HB3	1:C:288:VAL:CG1	2.46	0.45
1:C:310:THR:HG22	1:C:387:GLU:OE1	2.16	0.45
1:E:26:GLU:HA	1:E:287:HIS:HB3	1.99	0.45
1:B:7:GLU:HA	1:B:302:LEU:O	2.17	0.45
1:E:89:GLY:HA2	2:E:2030:HOH:O	2.16	0.45
1:F:34:THR:HB	1:F:40:SER:OG	2.16	0.45
1:F:53:PRO:HB2	1:F:131:VAL:O	2.16	0.45
1:C:33:ILE:O	1:C:33:ILE:HG13	2.17	0.45
1:D:31:VAL:O	1:D:31:VAL:HG23	2.16	0.45
1:E:49:TYR:CE2	1:E:280:LYS:HE3	2.50	0.45
1:F:346:ALA:O	1:F:347:HIS:C	2.60	0.45
1:C:122:GLU:O	1:C:125:LYS:HB2	2.17	0.45
1:C:239:GLU:CD	1:C:239:GLU:H	2.25	0.45
1:E:75:PRO:O	1:E:76:THR:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:THR:HG23	1:B:147:THR:O	2.17	0.45
1:C:133:ASP:HB3	1:C:136:LYS:HB2	1.99	0.45
1:A:170:GLU:HG3	1:A:186:CYS:O	2.17	0.44
1:E:316:ARG:HG2	1:E:316:ARG:NH1	2.31	0.44
1:A:213:TRP:CD2	1:A:268:LEU:HD13	2.53	0.44
1:A:366:ASN:N	1:A:366:ASN:ND2	2.64	0.44
1:C:339:ARG:HG2	1:C:339:ARG:NH1	2.32	0.44
1:F:133:ASP:HB3	1:F:136:LYS:HB2	2.00	0.44
1:F:275:HIS:CD2	1:F:284:LYS:HG3	2.53	0.44
1:B:139:TYR:CE1	1:B:188:VAL:HG13	2.53	0.44
1:C:197:THR:HG22	1:C:198:VAL:N	2.33	0.44
1:E:34:THR:HB	1:E:40:SER:OG	2.18	0.44
1:A:137:ILE:HD12	1:A:194:LEU:HD11	2.00	0.44
1:C:41:MET:HE1	1:C:145:PRO:CB	2.47	0.44
1:C:143:VAL:HG11	1:C:176:MET:SD	2.58	0.44
1:D:51:GLU:HG2	1:E:378:PRO:CG	2.45	0.44
1:F:49:TYR:CZ	1:F:280:LYS:HE3	2.52	0.44
1:A:339:ARG:HG3	1:A:339:ARG:HH11	1.82	0.44
1:B:186:CYS:HB3	1:B:288:VAL:CG1	2.48	0.44
1:E:40:SER:O	1:E:41:MET:HE2	2.18	0.44
1:B:26:GLU:HA	1:B:287:HIS:CB	2.48	0.44
1:B:237:ASN:HA	1:B:239:GLU:OE2	2.18	0.44
1:C:237:ASN:HA	1:C:239:GLU:OE2	2.18	0.44
1:A:344:ALA:CB	1:A:355:ALA:HB2	2.48	0.43
1:B:76:THR:OG1	1:B:77:MET:HE2	2.18	0.43
1:C:248:HIS:O	1:C:250:VAL:N	2.51	0.43
1:D:20:ARG:HD2	1:E:12:VAL:HG23	1.99	0.43
1:F:306:MET:HE1	1:F:341:PRO:HB3	1.99	0.43
1:A:9:ARG:HD3	1:C:295:GLU:OE2	2.18	0.43
1:D:170:GLU:HG3	1:D:186:CYS:O	2.18	0.43
1:E:301:GLY:O	1:E:302:LEU:CB	2.66	0.43
1:E:328:MET:CE	1:E:374:MET:HE3	2.48	0.43
1:D:139:TYR:CG	1:D:188:VAL:HG22	2.53	0.43
1:A:310:THR:HG22	1:A:387:GLU:OE1	2.18	0.43
1:C:49:TYR:CZ	1:C:280:LYS:HE3	2.53	0.43
1:C:89:GLY:O	1:C:118:LYS:HA	2.19	0.43
1:A:7:GLU:HA	1:A:302:LEU:O	2.18	0.43
1:B:56:THR:HA	1:C:399:ILE:HD13	2.01	0.43
1:E:122:GLU:O	1:E:125:LYS:HB2	2.18	0.43
1:F:171:LYS:HE2	1:F:183:SER:HB2	1.99	0.43
1:B:26:GLU:HA	1:B:287:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:GLU:OE2	1:D:360:PRO:HD2	2.18	0.43
1:C:288:VAL:CG1	1:C:290:CYS:SG	3.07	0.43
1:C:305:THR:O	1:C:338:CYS:HB2	2.19	0.43
1:B:41:MET:HG3	1:B:176:MET:HE2	2.00	0.43
1:D:173:ILE:HD12	1:E:9:ARG:HH21	1.83	0.43
1:F:137:ILE:HD12	1:F:194:LEU:HD11	1.99	0.43
1:B:65:LEU:HB3	1:B:117:VAL:HG21	2.00	0.43
1:F:172:THR:HG22	1:F:173:ILE:H	1.84	0.43
1:F:197:THR:HG22	1:F:198:VAL:N	2.33	0.43
1:F:301:GLY:O	1:F:302:LEU:CB	2.67	0.43
1:B:124:LYS:C	1:B:203:ASP:OD2	2.62	0.43
1:D:184:LEU:HD23	1:D:292:VAL:HG22	2.00	0.43
1:F:139:TYR:CE1	1:F:188:VAL:CG1	3.01	0.43
1:C:5:HIS:CB	1:C:302:LEU:HD23	2.47	0.42
1:E:294:LEU:HD22	1:E:299:MET:HE3	2.00	0.42
1:B:295:GLU:HG3	2:B:2038:HOH:O	2.18	0.42
1:D:243:GLU:OE1	1:D:257:LEU:HD11	2.19	0.42
1:F:297:LEU:HD23	2:F:2003:HOH:O	2.19	0.42
1:A:49:TYR:HB3	1:A:282:HIS:ND1	2.35	0.42
1:B:20:ARG:HB2	1:C:12:VAL:HG21	2.01	0.42
1:B:41:MET:HG3	1:B:176:MET:HE1	1.99	0.42
1:B:217:ARG:HH11	1:B:217:ARG:CB	2.32	0.42
1:B:354:VAL:HB	1:B:377:PRO:HG2	2.01	0.42
1:A:217:ARG:HH21	1:C:217:ARG:HH21	1.66	0.42
1:D:74:CYS:O	1:D:76:THR:N	2.53	0.42
1:B:288:VAL:HG12	1:B:290:CYS:SG	2.59	0.42
1:C:344:ALA:CB	1:C:355:ALA:HB2	2.49	0.42
1:D:41:MET:HG3	1:D:176:MET:HE3	2.01	0.42
1:C:172:THR:HG22	1:C:173:ILE:H	1.84	0.42
1:A:53:PRO:HD2	1:A:281:TYR:CD1	2.54	0.42
1:A:137:ILE:HG22	1:A:139:TYR:CE1	2.54	0.42
1:B:26:GLU:CD	1:B:29:GLY:HA3	2.44	0.42
1:B:170:GLU:CD	1:C:187:ARG:NH2	2.78	0.42
1:B:217:ARG:HB2	1:B:217:ARG:CZ	2.50	0.42
1:B:354:VAL:HB	1:B:377:PRO:CG	2.50	0.42
1:E:354:VAL:HB	1:E:377:PRO:HG2	2.01	0.42
1:C:26:GLU:HA	1:C:287:HIS:HB3	2.01	0.42
1:C:65:LEU:HD21	1:C:242:VAL:CG2	2.50	0.42
1:C:301:GLY:O	1:C:302:LEU:CB	2.68	0.42
1:D:51:GLU:O	1:D:52:ASN:C	2.62	0.42
1:D:137:ILE:HD12	1:D:194:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:THR:HG21	1:F:170:GLU:OE2	2.19	0.42
1:E:93:LYS:HB2	1:E:244:PHE:CD2	2.55	0.42
1:F:146:HIS:ND1	1:F:146:HIS:C	2.78	0.42
1:F:313:THR:OG1	1:F:331:THR:HB	2.19	0.42
1:B:171:LYS:HE2	1:B:183:SER:HB2	2.01	0.42
1:C:74:CYS:C	1:C:76:THR:N	2.78	0.42
1:E:69:LYS:HG3	1:E:84:GLU:OE2	2.20	0.42
1:F:51:GLU:O	1:F:52:ASN:C	2.63	0.42
1:A:26:GLU:HA	1:A:287:HIS:CB	2.50	0.41
1:A:40:SER:O	1:A:41:MET:HE2	2.19	0.41
1:C:147:THR:HG23	1:C:147:THR:O	2.20	0.41
1:A:77:MET:O	1:A:78:GLY:O	2.37	0.41
1:B:217:ARG:NH1	1:B:217:ARG:CB	2.81	0.41
1:D:26:GLU:HA	1:D:287:HIS:HB3	2.02	0.41
1:E:147:THR:HG23	1:E:147:THR:O	2.20	0.41
1:F:74:CYS:C	1:F:76:THR:H	2.26	0.41
1:D:91:VAL:HG12	1:D:244:PHE:CE2	2.56	0.41
1:D:244:PHE:CD1	1:D:254:VAL:HG22	2.55	0.41
1:F:69:LYS:HG3	1:F:84:GLU:OE2	2.20	0.41
1:B:288:VAL:CG1	1:B:290:CYS:SG	3.09	0.41
1:C:97:SER:O	1:C:110:LYS:HA	2.20	0.41
1:F:5:HIS:CB	1:F:302:LEU:HD23	2.50	0.41
1:F:213:TRP:CE3	1:F:268:LEU:HD13	2.56	0.41
1:A:312:PHE:HB2	2:A:2051:HOH:O	2.21	0.41
1:E:4:THR:CG2	1:E:5:HIS:N	2.84	0.41
1:A:171:LYS:HE2	1:A:183:SER:HB2	2.03	0.41
1:A:295:GLU:O	1:A:296:LYS:C	2.63	0.41
1:C:35:ALA:HB2	1:C:299:MET:HE1	2.01	0.41
1:C:41:MET:HE1	1:C:145:PRO:HA	2.00	0.41
1:D:49:TYR:CD2	1:D:49:TYR:C	2.98	0.41
1:F:295:GLU:OE1	1:F:295:GLU:HA	2.21	0.41
1:D:200:LEU:O	1:D:212:ALA:HA	2.20	0.41
1:F:76:THR:OG1	1:F:77:MET:HE3	2.21	0.41
1:A:26:GLU:HA	1:A:287:HIS:HB3	2.03	0.41
1:C:66:SER:OG	1:C:67:ASP:N	2.50	0.41
1:A:4:THR:CG2	1:A:5:HIS:N	2.84	0.41
1:A:139:TYR:CZ	1:A:188:VAL:CG1	3.02	0.41
1:A:139:TYR:CE1	1:A:188:VAL:HG13	2.56	0.41
1:D:213:TRP:CD2	1:D:268:LEU:HD13	2.56	0.41
1:D:244:PHE:CE1	1:D:254:VAL:HG22	2.55	0.41
1:F:88:GLY:HA3	1:F:234:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:ARG:HG2	1:F:384:TYR:HB2	2.01	0.41
1:A:21:VAL:HB	1:A:292:VAL:HB	2.04	0.41
1:B:195:ALA:O	1:B:217:ARG:HD2	2.21	0.41
1:B:297:LEU:HD23	1:B:297:LEU:C	2.45	0.41
1:D:34:THR:O	1:D:300:LYS:HB2	2.20	0.41
1:B:133:ASP:HB3	1:B:136:LYS:HB2	2.03	0.40
1:D:287:HIS:CD2	1:D:289:THR:HG22	2.56	0.40
1:E:26:GLU:CD	1:E:29:GLY:HA3	2.46	0.40
1:F:248:HIS:O	1:F:250:VAL:N	2.54	0.40
1:B:329:GLU:HA	1:B:370:GLY:O	2.21	0.40
1:D:172:THR:HG22	1:D:173:ILE:N	2.36	0.40
1:F:184:LEU:HD23	1:F:292:VAL:HG22	2.02	0.40
1:A:144:GLU:HA	1:A:145:PRO:HD3	1.82	0.40
1:A:218:ASP:OD1	1:C:217:ARG:NH2	2.54	0.40
1:C:21:VAL:HB	1:C:292:VAL:HB	2.03	0.40
1:D:71:ALA:O	1:D:113:ILE:HA	2.21	0.40
1:D:93:LYS:HB2	1:D:244:PHE:CE2	2.56	0.40
1:D:277:GLU:OE2	1:D:280:LYS:HD2	2.22	0.40
1:E:137:ILE:HD13	1:E:283:LEU:HD11	2.03	0.40
1:F:103:ASN:O	1:F:104:HIS:HB2	2.21	0.40
1:F:200:LEU:O	1:F:212:ALA:HA	2.21	0.40
1:F:296:LYS:O	1:F:296:LYS:HG3	2.21	0.40
1:A:35:ALA:HB2	1:A:299:MET:HE1	2.04	0.40
1:A:139:TYR:CE1	1:A:188:VAL:HG11	2.57	0.40
1:A:170:GLU:OE2	1:B:289:THR:HG21	2.21	0.40
1:B:14:GLY:HA3	1:C:12:VAL:HG13	2.04	0.40
1:C:361:ASN:HA	1:C:362:PRO:HD2	1.95	0.40
1:D:218:ASP:OD2	1:F:56:THR:HG21	2.22	0.40
1:E:138:VAL:HG13	1:E:164:SER:HB3	2.02	0.40
1:E:383:ILE:O	1:E:389:SER:HA	2.21	0.40
1:F:139:TYR:CE1	1:F:188:VAL:HG13	2.55	0.40
1:A:103:ASN:O	1:A:104:HIS:HB2	2.20	0.40
1:A:237:ASN:HA	1:A:239:GLU:OE2	2.21	0.40
1:B:132:TYR:CE2	1:B:199:ILE:HD11	2.57	0.40
1:B:248:HIS:O	1:B:250:VAL:N	2.55	0.40

There are no symmetry-related clashes.

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	376/401 (94%)	349 (93%)	18 (5%)	9 (2%)	4	12
1	B	381/401 (95%)	344 (90%)	23 (6%)	14 (4%)	2	6
1	C	379/401 (94%)	348 (92%)	22 (6%)	9 (2%)	4	12
1	D	380/401 (95%)	350 (92%)	17 (4%)	13 (3%)	3	7
1	E	376/401 (94%)	344 (92%)	22 (6%)	10 (3%)	4	10
1	F	384/401 (96%)	352 (92%)	19 (5%)	13 (3%)	3	7
All	All	2276/2406 (95%)	2087 (92%)	121 (5%)	68 (3%)	3	8

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	GLY
1	A	302	LEU
1	A	349	SER
1	B	206	VAL
1	B	302	LEU
1	B	349	SER
1	C	204	LYS
1	C	302	LEU
1	C	349	SER
1	D	78	GLY
1	D	204	LYS
1	D	302	LEU
1	D	349	SER
1	E	68	THR
1	E	302	LEU
1	E	349	SER
1	F	78	GLY
1	F	302	LEU
1	F	349	SER
1	A	75	PRO

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Mol	Chain	Res	Type
1	A	249	ALA
1	A	296	LYS
1	B	78	GLY
1	B	296	LYS
1	C	78	GLY
1	D	206	VAL
1	F	209	LEU
1	A	309	LYS
1	A	347	HIS
1	B	67	ASP
1	B	204	LYS
1	B	207	GLU
1	B	249	ALA
1	B	309	LYS
1	B	347	HIS
1	C	75	PRO
1	C	249	ALA
1	C	309	LYS
1	C	347	HIS
1	D	75	PRO
1	D	296	LYS
1	D	309	LYS
1	D	347	HIS
1	E	75	PRO
1	E	296	LYS
1	E	309	LYS
1	E	347	HIS
1	F	75	PRO
1	F	205	THR
1	F	207	GLU
1	F	249	ALA
1	F	296	LYS
1	A	146	HIS
1	B	146	HIS
1	C	146	HIS
1	D	249	ALA
1	E	67	ASP
1	E	146	HIS
1	E	249	ALA
1	F	347	HIS
1	B	75	PRO
1	D	146	HIS

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Mol	Chain	Res	Type
1	F	146	HIS
1	D	52	ASN
1	F	206	VAL
1	F	52	ASN
1	B	350	PRO
1	D	350	PRO

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	315/331 (95%)	298 (95%)	17 (5%)	20	45
1	B	315/331 (95%)	302 (96%)	13 (4%)	27	56
1	C	315/331 (95%)	298 (95%)	17 (5%)	20	45
1	D	315/331 (95%)	304 (96%)	11 (4%)	32	61
1	E	315/331 (95%)	301 (96%)	14 (4%)	25	53
1	F	315/331 (95%)	297 (94%)	18 (6%)	18	43
All	All	1890/1986 (95%)	1800 (95%)	90 (5%)	23	50

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	34	THR
1	A	52	ASN
1	A	93	LYS
1	A	117	VAL
1	A	131	VAL
1	A	146	HIS
1	A	171	LYS
1	A	178	GLU
1	A	185	LEU
1	A	188	VAL
1	A	203	ASP

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Mol	Chain	Res	Type
1	A	289	THR
1	A	297	LEU
1	A	303	THR
1	A	324	ASP
1	A	347	HIS
1	B	15	THR
1	B	34	THR
1	B	67	ASP
1	B	93	LYS
1	B	131	VAL
1	B	171	LYS
1	B	185	LEU
1	B	188	VAL
1	B	243	GLU
1	B	289	THR
1	B	297	LEU
1	B	319	THR
1	B	391	GLN
1	C	4	THR
1	C	15	THR
1	C	20	ARG
1	C	34	THR
1	C	51	GLU
1	C	93	LYS
1	C	131	VAL
1	C	171	LYS
1	C	178	GLU
1	C	185	LEU
1	C	188	VAL
1	C	243	GLU
1	C	289	THR
1	C	297	LEU
1	C	303	THR
1	C	319	THR
1	C	324	ASP
1	D	15	THR
1	D	20	ARG
1	D	34	THR
1	D	93	LYS
1	D	117	VAL
1	D	171	LYS
1	D	188	VAL

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Mol	Chain	Res	Type
1	D	243	GLU
1	D	289	THR
1	D	297	LEU
1	D	324	ASP
1	E	15	THR
1	E	34	THR
1	E	51	GLU
1	E	73	ARG
1	E	84	GLU
1	E	93	LYS
1	E	171	LYS
1	E	188	VAL
1	E	233	GLN
1	E	277	GLU
1	E	289	THR
1	E	297	LEU
1	E	303	THR
1	E	324	ASP
1	F	4	THR
1	F	15	THR
1	F	34	THR
1	F	51	GLU
1	F	65	LEU
1	F	76	THR
1	F	77	MET
1	F	93	LYS
1	F	122	GLU
1	F	146	HIS
1	F	171	LYS
1	F	185	LEU
1	F	188	VAL
1	F	230	GLU
1	F	295	GLU
1	F	297	LEU
1	F	303	THR
1	F	347	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	96	GLN

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Mol	Chain	Res	Type
1	A	214	GLN
1	A	221	ASN
1	A	234	ASN
1	A	248	HIS
1	A	275	HIS
1	A	366	ASN
1	B	16	GLN
1	B	96	GLN
1	B	104	HIS
1	B	130	HIS
1	B	221	ASN
1	B	234	ASN
1	B	275	HIS
1	B	366	ASN
1	B	391	GLN
1	C	96	GLN
1	C	221	ASN
1	C	233	GLN
1	C	234	ASN
1	C	237	ASN
1	C	275	HIS
1	C	366	ASN
1	D	62	HIS
1	D	96	GLN
1	D	234	ASN
1	D	248	HIS
1	D	275	HIS
1	D	366	ASN
1	E	16	GLN
1	E	96	GLN
1	E	221	ASN
1	E	233	GLN
1	E	237	ASN
1	E	366	ASN
1	F	16	GLN
1	F	52	ASN
1	F	96	GLN
1	F	104	HIS
1	F	221	ASN
1	F	233	GLN
1	F	234	ASN
1	F	237	ASN

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Mol	Chain	Res	Type
1	F	275	HIS
1	F	323	HIS
1	F	347	HIS
1	F	366	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 ⓘ

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	382/401 (95%)	-0.20	6 (1%) 70 68	13, 33, 67, 89	0
1	B	387/401 (96%)	-0.15	8 (2%) 63 61	12, 35, 70, 94	0
1	C	385/401 (96%)	-0.11	10 (2%) 57 54	12, 37, 71, 94	0
1	D	386/401 (96%)	-0.06	11 (2%) 55 51	16, 41, 74, 98	0
1	E	382/401 (95%)	-0.02	8 (2%) 63 61	13, 41, 75, 95	0
1	F	388/401 (96%)	-0.03	15 (3%) 43 39	13, 37, 76, 99	0
All	All	2310/2406 (96%)	-0.09	58 (2%) 58 55	12, 37, 74, 99	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	147	THR	4.4
1	E	147	THR	4.1
1	D	207	GLU	3.8
1	B	205	THR	3.8
1	C	147	THR	3.6
1	A	347	HIS	3.5
1	A	147	THR	3.4
1	E	86	HIS	3.4
1	E	146	HIS	3.2
1	A	86	HIS	3.1
1	B	147	THR	3.0
1	C	248	HIS	2.9
1	A	248	HIS	2.9
1	D	146	HIS	2.9
1	D	204	LYS	2.9
1	C	367	ASN	2.8
1	C	352	VAL	2.8
1	B	210	PRO	2.7
1	F	207	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	146	HIS	2.6
1	E	210	PRO	2.6
1	F	147	THR	2.5
1	C	209	LEU	2.5
1	F	208	HIS	2.5
1	A	301	GLY	2.5
1	E	176	MET	2.5
1	F	87	GLN	2.4
1	C	205	THR	2.4
1	B	302	LEU	2.4
1	F	107	LEU	2.4
1	B	208	HIS	2.3
1	F	76	THR	2.3
1	D	210	PRO	2.3
1	D	248	HIS	2.3
1	F	146	HIS	2.3
1	F	77	MET	2.3
1	F	233	GLN	2.3
1	B	248	HIS	2.3
1	C	255	TYR	2.3
1	F	84	GLU	2.3
1	B	367	ASN	2.2
1	D	249	ALA	2.2
1	F	367	ASN	2.2
1	A	233	GLN	2.2
1	F	101	TRP	2.2
1	D	205	THR	2.2
1	D	2	ARG	2.2
1	F	2	ARG	2.2
1	D	67	ASP	2.2
1	C	75	PRO	2.1
1	E	349	SER	2.1
1	B	207	GLU	2.1
1	F	204	LYS	2.1
1	C	106	GLY	2.1
1	D	206	VAL	2.1
1	E	2	ARG	2.0
1	F	86	HIS	2.0
1	E	303	THR	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.