



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:18 AM UTC

PDB ID : 6HP3 / pdb_00006hp3
Title : ARBITRIUM PEPTIDE RECEPTOR FROM SPBETA PHAGE
Authors : Marina, A.; Gallego del Sol, F.
Deposited on : 2018-09-19
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
Mogul : 2022.3.0, CSD as543be (2022)
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

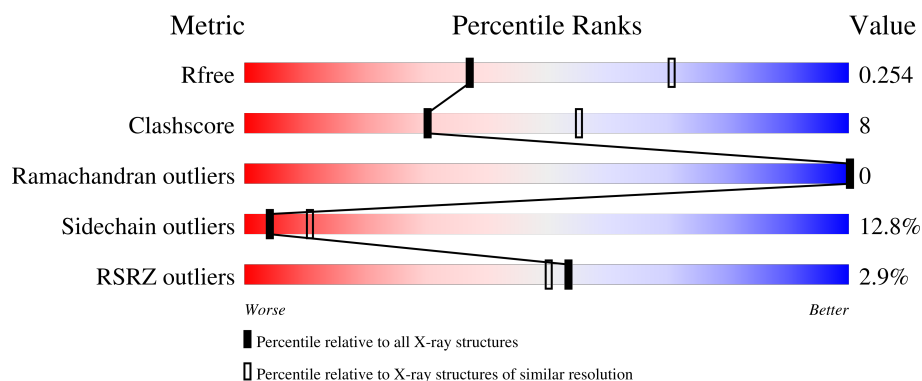
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

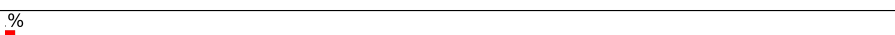
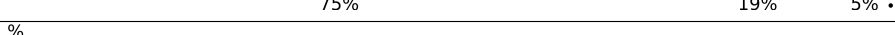
The reported resolution of this entry is 2.70 Å.

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	386	 79% 16% 5%
1	B	386	 2% 76% 18% 5%
1	C	386	 1% 78% 15% 6%
1	D	386	 1% 75% 19% 5%
1	E	386	 1% 75% 18% 6%

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Mol	Chain	Length	Quality of chain
1	F	386	75% 19% 5%
1	G	386	% 77% 17% 5%
1	H	386	17% 69% 22% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25680 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 SPBc2 prophage-derived uncharacterized protein YopK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	B	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	C	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	D	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	E	386	Total	C	N	O	S	Se	0	1	0
			3188	2035	528	603	6	16			
1	F	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	G	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			
1	H	386	Total	C	N	O	S	Se	0	0	0
			3183	2031	528	603	6	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	27	Total	O	0	0
			27	27		
2	C	36	Total	O	0	0
			36	36		
2	D	29	Total	O	0	0
			29	29		
2	E	20	Total	O	0	0
			20	20		
2	F	21	Total	O	0	0
			21	21		

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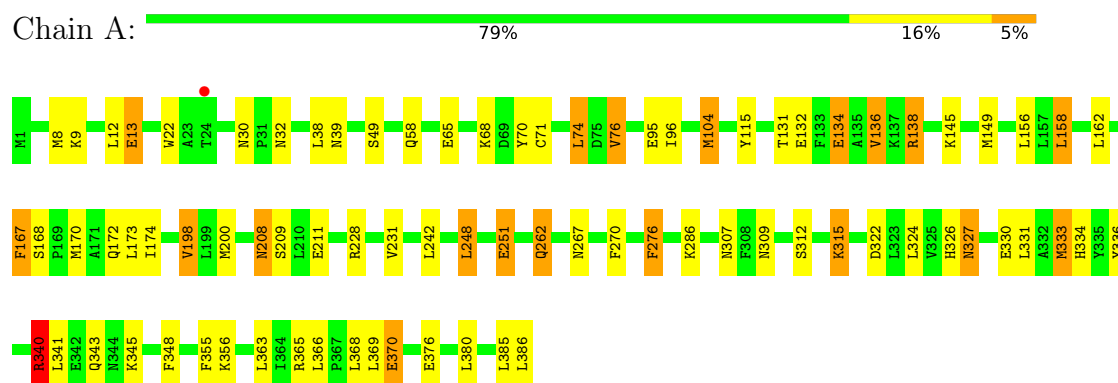
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	28	Total 28	O 28	0	0
2	H	6	Total 6	O 6	0	0

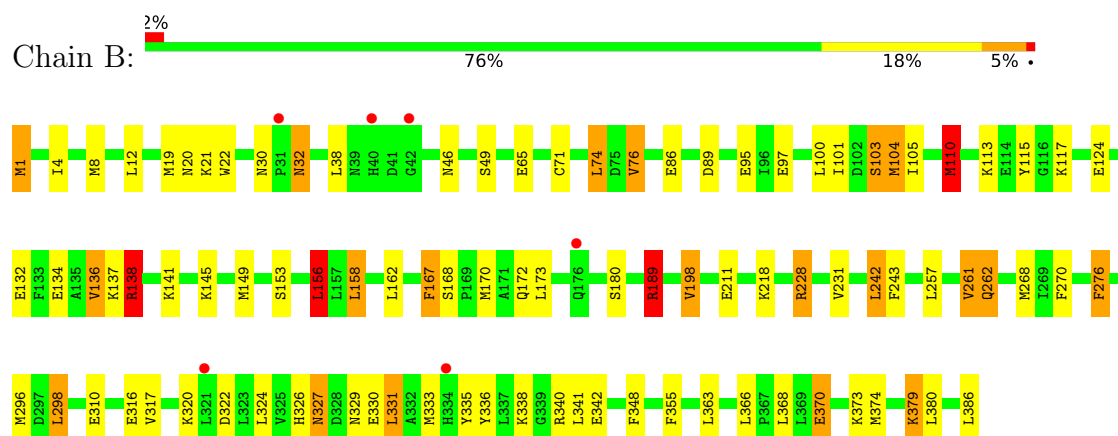
3 Residue-property plots

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.

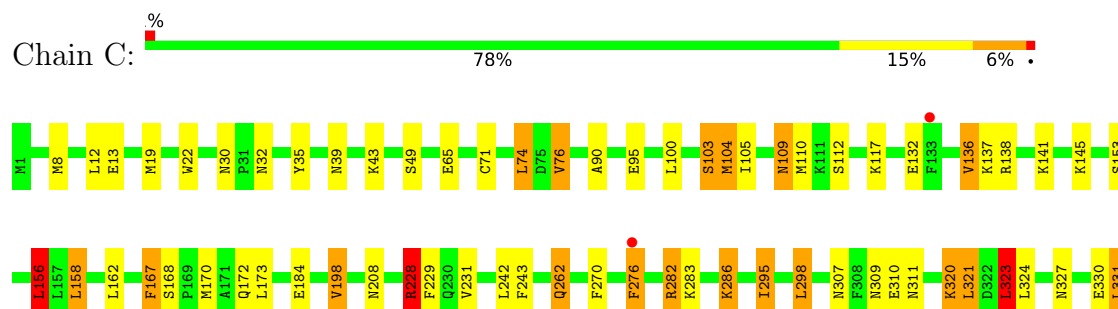
- Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK



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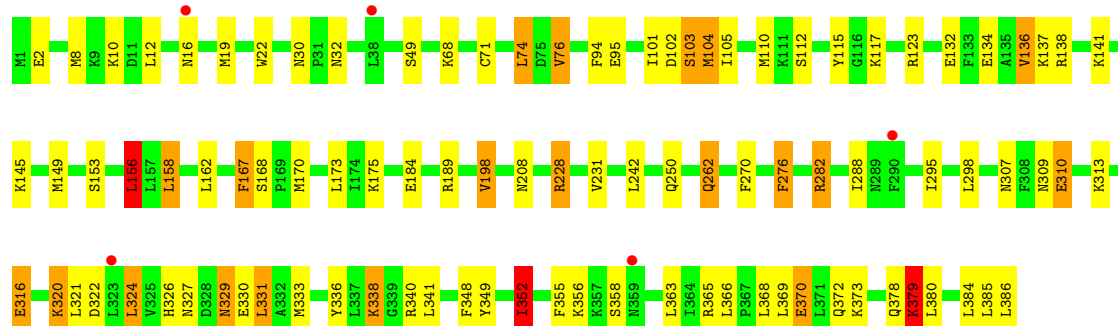
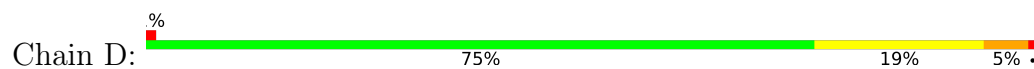


- Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK

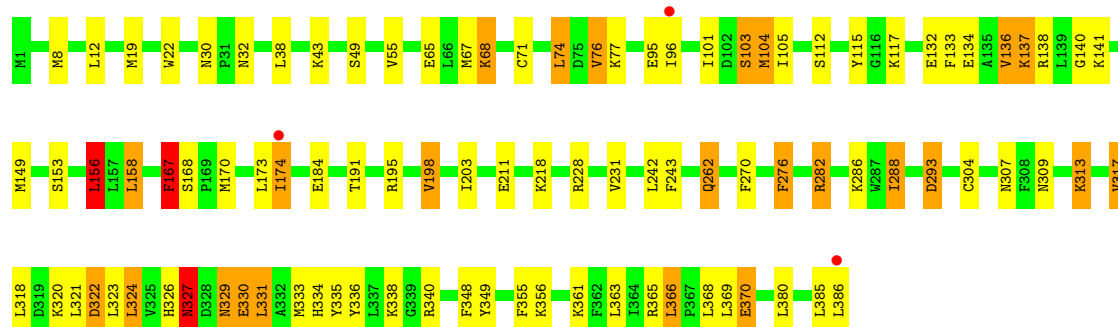
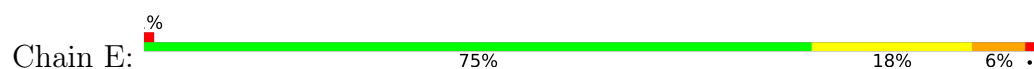




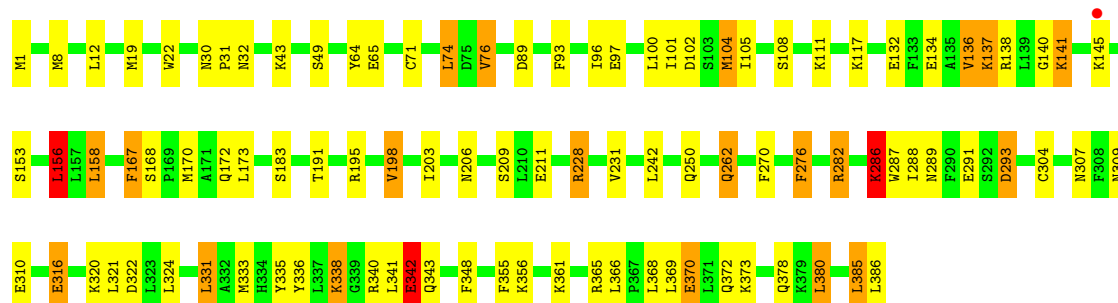
- Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK



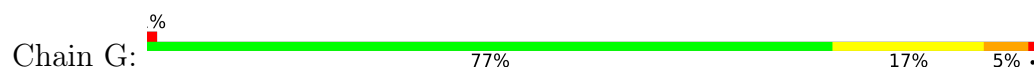
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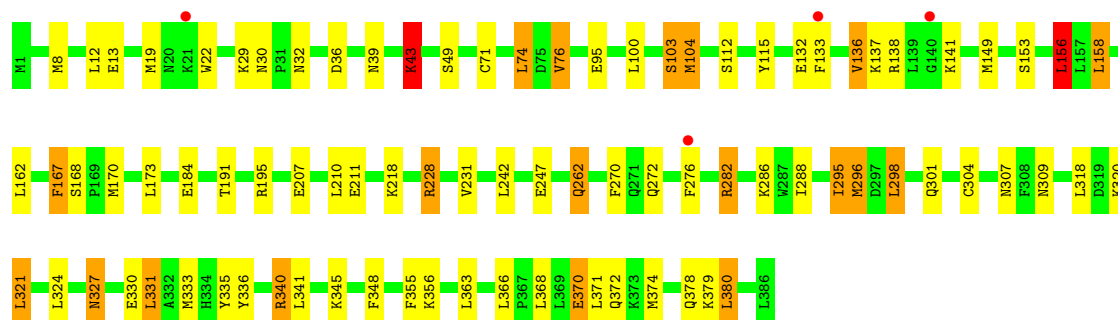


- Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK

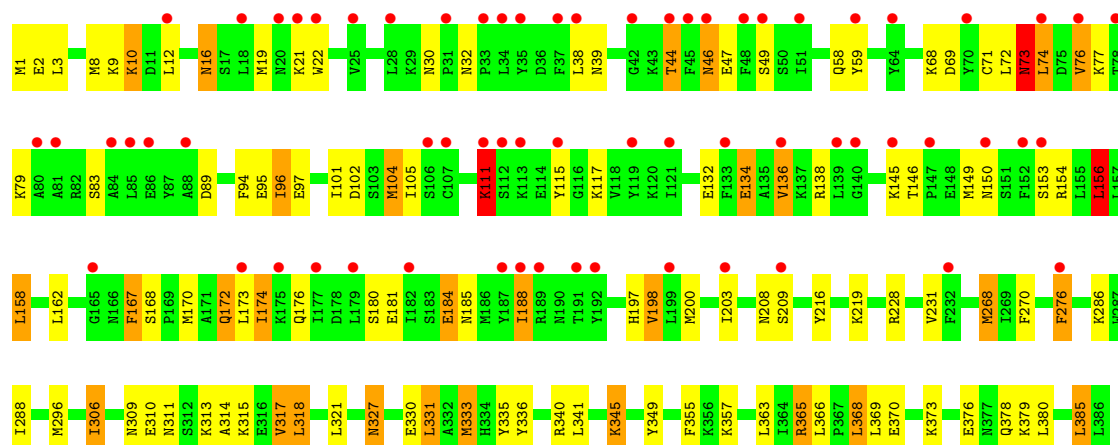


- Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK





- Molecule 1: SPBc2 prophage-derived uncharacterized protein YopK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.91Å 251.20Å 95.08Å 90.00° 90.89° 90.00°	Depositor
Resolution (Å)	125.60 – 2.70 125.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (125.60-2.70) 99.9 (125.60-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.219 , 0.250 0.226 , 0.254	Depositor DCC
R_{free} test set	4903 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25680	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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	1.03	0/3226	1.24	15/4315 (0.3%)
1	B	1.00	3/3226 (0.1%)	1.26	20/4315 (0.5%)
1	C	1.01	3/3226 (0.1%)	1.25	12/4315 (0.3%)
1	D	0.99	1/3226 (0.0%)	1.26	18/4315 (0.4%)
1	E	1.04	3/3234 (0.1%)	1.27	12/4325 (0.3%)
1	F	0.96	1/3226 (0.0%)	1.24	16/4315 (0.4%)
1	G	1.02	0/3226	1.26	10/4315 (0.2%)
1	H	1.11	4/3226 (0.1%)	1.30	17/4315 (0.4%)
All	All	1.02	15/25816 (0.1%)	1.26	120/34530 (0.3%)

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	E	0	1
1	H	0	1
All	All	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	16	ASN	CG-ND2	8.62	1.51	1.33
1	B	326	HIS	C-O	-6.94	1.15	1.23
1	F	1	MSE	SE-CE	-5.90	1.77	1.95
1	E	369	LEU	CB-CG	5.84	1.65	1.53
1	B	340	ARG	CZ-NH2	-5.80	1.25	1.33
1	C	379	LYS	CA-C	5.75	1.60	1.52
1	H	315	LYS	CE-NZ	5.45	1.65	1.49
1	E	276	PHE	CG-CD1	5.45	1.50	1.38
1	D	288	ILE	C-O	-5.33	1.18	1.24
1	C	35	TYR	CG-CD1	5.30	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	276	PHE	CG-CD1	5.17	1.49	1.38
1	E	288	ILE	C-O	-5.16	1.18	1.24
1	C	276	PHE	CG-CD1	5.15	1.49	1.38
1	B	276	PHE	CG-CD1	5.07	1.49	1.38
1	H	47	GLU	C-O	5.06	1.29	1.24

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	LYS	CB-CA-C	9.49	126.55	110.79
1	G	301	GLN	CB-CA-C	9.35	126.31	110.79
1	B	110	MSE	CB-CA-C	-8.19	98.03	110.88
1	F	167	PHE	N-CA-C	7.80	120.68	111.71
1	E	326	HIS	N-CA-C	-7.75	102.87	113.18
1	G	340	ARG	NE-CZ-NH2	7.39	125.85	119.20
1	D	184	GLU	CB-CG-CD	-7.38	100.05	112.60
1	H	188	ILE	CB-CG1-CD1	7.31	129.16	113.80
1	B	327	ASN	N-CA-CB	-7.24	100.46	110.38
1	D	320	LYS	CA-CB-CG	7.20	128.51	114.10
1	H	73	ASN	N-CA-CB	7.10	122.28	110.92
1	G	286	LYS	CD-CE-NZ	-6.91	89.79	111.90
1	E	327	ASN	CB-CA-C	-6.85	96.86	109.46
1	E	167	PHE	N-CA-C	6.73	119.45	111.71
1	D	373	LYS	CG-CD-CE	6.72	126.76	111.30
1	C	167	PHE	N-CA-C	6.70	119.59	111.82
1	F	340	ARG	CA-CB-CG	-6.66	100.79	114.10
1	D	167	PHE	N-CA-C	6.61	119.31	111.71
1	B	113	LYS	CG-CD-CE	6.54	126.35	111.30
1	A	167	PHE	N-CA-C	6.53	119.40	111.82
1	B	340	ARG	CG-CD-NE	6.51	126.31	112.00
1	H	1	MSE	CG-SE-CE	6.46	113.14	98.92
1	B	167	PHE	N-CA-C	6.42	119.26	111.82
1	B	1	MSE	CG-SE-CE	6.41	113.03	98.92
1	H	156	LEU	CA-CB-CG	6.36	138.55	116.30
1	B	374	MSE	CG-SE-CE	6.35	112.90	98.92
1	C	156	LEU	CA-CB-CG	6.35	138.53	116.30
1	B	198	VAL	N-CA-CB	6.35	119.17	110.54
1	G	167	PHE	N-CA-C	6.33	119.17	111.82
1	D	156	LEU	CA-CB-CG	6.33	138.45	116.30
1	F	286	LYS	CG-CD-CE	6.33	125.85	111.30
1	A	340	ARG	CA-CB-CG	-6.30	101.51	114.10
1	F	156	LEU	CA-CB-CG	6.26	138.21	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	VAL	N-CA-CB	6.26	119.05	110.54
1	H	268	MSE	CG-SE-CE	6.25	112.68	98.92
1	G	156	LEU	CA-CB-CG	6.22	138.09	116.30
1	D	198	VAL	N-CA-CB	6.22	119.00	110.54
1	G	210	LEU	N-CA-C	6.22	118.06	111.28
1	B	156	LEU	CA-CB-CG	6.19	137.98	116.30
1	B	110	MSE	N-CA-CB	-6.18	101.04	110.01
1	A	340	ARG	NE-CZ-NH2	6.15	124.74	119.20
1	E	156	LEU	CA-CB-CG	6.14	137.80	116.30
1	H	134	GLU	CA-CB-CG	6.14	126.38	114.10
1	A	333	MSE	CG-SE-CE	-6.10	85.51	98.92
1	F	316	GLU	CA-CB-CG	6.10	126.29	114.10
1	C	295	ILE	CA-CB-CG1	6.02	120.63	110.40
1	H	198	VAL	N-CA-CB	6.00	118.71	110.54
1	F	293	ASP	N-CA-CB	5.94	119.93	110.73
1	F	322	ASP	N-CA-CB	5.88	120.32	110.32
1	B	268	MSE	CG-SE-CE	5.88	111.87	98.92
1	E	293	ASP	N-CA-CB	5.87	120.31	110.92
1	A	322	ASP	CB-CA-C	5.86	122.69	110.32
1	D	316	GLU	CA-CB-CG	5.86	125.83	114.10
1	A	228	ARG	NE-CZ-NH2	5.83	124.44	119.20
1	E	321	LEU	CB-CG-CD2	5.83	128.19	110.70
1	C	228	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	G	345	LYS	CG-CD-CE	5.78	124.60	111.30
1	B	189	ARG	CB-CG-CD	5.77	124.56	111.30
1	D	322	ASP	CB-CA-C	5.75	122.45	110.32
1	H	10	LYS	CB-CA-C	5.72	121.22	110.63
1	F	365	ARG	CD-NE-CZ	-5.68	116.45	124.40
1	D	379	LYS	CG-CD-CE	5.66	124.31	111.30
1	C	323	LEU	CB-CG-CD2	-5.58	93.95	110.70
1	G	295	ILE	CA-CB-CG1	5.58	119.88	110.40
1	F	198	VAL	N-CA-CB	5.56	118.92	110.58
1	H	167	PHE	N-CA-C	5.55	118.26	111.82
1	H	373	LYS	CD-CE-NZ	-5.54	94.16	111.90
1	D	338	LYS	CB-CG-CD	5.53	124.02	111.30
1	C	286	LYS	CD-CE-NZ	-5.52	94.24	111.90
1	H	111	LYS	CG-CD-CE	5.50	123.95	111.30
1	B	386	LEU	N-CA-CB	5.49	119.83	110.50
1	D	324	LEU	CA-CB-CG	5.49	135.51	116.30
1	H	311	ASN	N-CA-C	5.49	117.26	111.28
1	B	316	GLU	CA-CB-CG	5.47	125.05	114.10
1	F	276	PHE	N-CA-CB	5.47	117.94	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	ASP	CB-CA-C	5.46	121.83	110.32
1	F	385	LEU	CA-CB-CG	5.45	135.37	116.30
1	E	198	VAL	N-CA-CB	5.45	118.75	110.58
1	H	44	THR	OG1-CB-CG2	5.44	120.18	109.30
1	E	276	PHE	N-CA-CB	5.42	117.88	110.01
1	B	137	LYS	CG-CD-CE	-5.40	98.88	111.30
1	B	276	PHE	N-CA-CB	5.40	117.84	110.01
1	B	38	LEU	N-CA-C	5.40	117.24	111.36
1	A	276	PHE	N-CA-CB	5.38	117.81	110.01
1	A	198	VAL	N-CA-CB	5.37	118.64	110.58
1	F	373	LYS	CG-CD-CE	5.37	123.65	111.30
1	C	323	LEU	CA-CB-CG	5.37	135.09	116.30
1	G	228	ARG	NE-CZ-NH2	-5.36	114.37	119.20
1	E	174	ILE	CB-CA-C	-5.32	104.96	112.14
1	H	340	ARG	CA-CB-CG	-5.31	103.48	114.10
1	H	296	MSE	N-CA-CB	-5.31	102.03	109.94
1	E	322	ASP	CB-CA-C	-5.29	100.20	110.46
1	A	267	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	C	276	PHE	N-CA-CB	5.28	117.67	110.01
1	C	333	MSE	CG-SE-CE	-5.28	87.31	98.92
1	A	13	GLU	CA-CB-CG	5.27	124.64	114.10
1	H	333	MSE	CG-SE-CE	-5.27	87.33	98.92
1	H	94	PHE	N-CA-C	5.27	117.03	111.28
1	A	138	ARG	CD-NE-CZ	5.24	131.74	124.40
1	F	340	ARG	CB-CG-CD	5.22	123.31	111.30
1	B	138	ARG	CG-CD-NE	5.21	123.47	112.00
1	A	38	LEU	N-CA-C	5.21	117.03	111.36
1	B	322	ASP	N-CA-CB	5.18	119.14	110.32
1	D	352	ILE	CA-CB-CG2	5.18	119.31	110.50
1	G	43	LYS	CA-CB-CG	5.17	124.45	114.10
1	F	322	ASP	CB-CA-C	5.17	121.23	110.32
1	A	138	ARG	CG-CD-NE	5.16	123.35	112.00
1	A	200	MSE	CG-SE-CE	5.16	110.28	98.92
1	D	175	LYS	CA-CB-CG	5.16	124.41	114.10
1	F	108	SER	CA-CB-OG	-5.15	100.80	111.10
1	A	251	GLU	CG-CD-OE1	-5.13	106.59	118.40
1	D	94	PHE	N-CA-C	5.13	116.87	111.28
1	C	295	ILE	N-CA-CB	-5.11	104.03	110.57
1	D	276	PHE	N-CA-CB	5.11	117.41	110.01
1	E	38	LEU	N-CA-C	5.11	116.92	111.36
1	F	342	GLU	CA-CB-CG	5.09	124.29	114.10
1	E	365	ARG	NE-CZ-NH1	-5.09	116.41	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	322	ASP	N-CA-CB	5.07	118.94	110.32
1	D	123	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	C	311	ASN	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	167	PHE	Sidechain
1	H	16	ASN	Sidechain

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	3183	0	3179	52	0
1	B	3183	0	3179	45	1
1	C	3183	0	3179	42	0
1	D	3183	0	3179	50	0
1	E	3188	0	3188	62	0
1	F	3183	0	3179	55	0
1	G	3183	0	3179	51	0
1	H	3183	0	3179	91	1
2	A	44	0	0	3	0
2	B	27	0	0	2	0
2	C	36	0	0	1	0
2	D	29	0	0	2	0
2	E	20	0	0	1	0
2	F	21	0	0	2	0
2	G	28	0	0	0	0
2	H	6	0	0	0	0
All	All	25680	0	25441	427	1

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

All (427) 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:H:170:MSE:O	1:H:174:ILE:HD11	1.40	1.21
1:A:167:PHE:HA	1:A:170:MSE:HE3	1.31	1.12
1:F:372:GLN:HE21	1:F:378:GLN:HG2	1.10	1.11
1:H:170:MSE:O	1:H:174:ILE:CD1	2.00	1.08
1:H:167:PHE:HA	1:H:170:MSE:HE3	1.34	1.06
1:B:167:PHE:HA	1:B:170:MSE:HE3	1.33	1.06
1:D:167:PHE:HA	1:D:170:MSE:HE3	1.33	1.06
1:C:167:PHE:HA	1:C:170:MSE:HE3	1.33	1.05
1:G:167:PHE:HA	1:G:170:MSE:HE3	1.32	1.05
1:H:172:GLN:HA	1:H:172:GLN:OE1	1.54	1.05
1:A:68:LYS:HG3	1:A:96:ILE:HD11	1.07	1.04
1:G:298:LEU:HB3	1:G:321:LEU:HD11	1.51	0.93
1:A:68:LYS:HG3	1:A:96:ILE:CD1	1.99	0.90
1:E:68:LYS:CG	1:E:96:ILE:HD11	2.00	0.90
1:A:68:LYS:CG	1:A:96:ILE:HD11	2.00	0.90
1:H:174:ILE:HD13	1:H:174:ILE:H	1.34	0.89
1:D:310:GLU:HG2	1:D:313:LYS:HD3	1.52	0.88
1:A:251:GLU:OE1	1:D:250:GLN:NE2	2.07	0.88
1:H:174:ILE:HG13	1:H:203:ILE:HD13	1.55	0.88
1:E:68:LYS:HG3	1:E:96:ILE:HD11	1.53	0.88
1:A:172:GLN:NE2	1:B:132:GLU:OE1	2.07	0.88
1:H:174:ILE:HD13	1:H:174:ILE:N	1.87	0.87
1:H:306:ILE:HD11	1:H:314:ALA:HB1	1.57	0.87
1:D:327:ASN:OD1	1:D:330:GLU:HG3	1.76	0.84
1:G:371:LEU:HD23	1:G:374:MSE:HE3	1.59	0.84
1:F:372:GLN:NE2	1:F:378:GLN:HG2	1.92	0.84
1:F:93:PHE:HB3	1:F:96:ILE:CD1	2.10	0.81
1:B:257:LEU:O	1:B:261:VAL:HG22	1.81	0.81
1:E:67:MSE:HA	1:E:67:MSE:HE2	1.61	0.81
1:F:93:PHE:HB3	1:F:96:ILE:HD13	1.61	0.81
1:H:174:ILE:HG13	1:H:203:ILE:CD1	2.11	0.81
1:D:282:ARG:NH2	1:D:340:ARG:NH2	2.28	0.80
1:F:372:GLN:HE21	1:F:378:GLN:CG	1.94	0.80
1:A:333:MSE:HE1	1:A:366:LEU:HD12	1.64	0.79
1:H:3:LEU:HG	1:H:69:ASP:OD2	1.82	0.79
1:H:158:LEU:HD13	1:H:173:LEU:HD23	1.65	0.79
1:A:307:ASN:OD1	1:A:340:ARG:NH2	2.16	0.78
1:F:333:MSE:HE1	1:F:366:LEU:HD12	1.65	0.78
1:H:306:ILE:HD11	1:H:314:ALA:CB	2.14	0.78
1:H:306:ILE:CD1	1:H:314:ALA:CB	2.63	0.77
1:H:200:MSE:HB3	1:H:216:TYR:CD2	2.19	0.77
1:C:383:LEU:HD13	1:D:352:ILE:HG12	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:ILE:HD12	1:H:96:ILE:N	2.00	0.76
1:E:55:VAL:HG21	1:E:67:MSE:HE3	1.68	0.76
1:G:298:LEU:CB	1:G:321:LEU:HD11	2.16	0.76
1:E:137:LYS:HG2	1:F:140:GLY:HA2	1.68	0.76
1:G:307:ASN:OD1	1:G:340:ARG:NH2	2.19	0.76
1:G:371:LEU:HD23	1:G:374:MSE:CE	2.16	0.76
1:H:170:MSE:C	1:H:174:ILE:HD11	2.11	0.75
1:C:333:MSE:HE1	1:C:366:LEU:HD23	1.69	0.74
1:B:298:LEU:HD23	1:B:317:VAL:HG13	1.70	0.74
1:G:333:MSE:HE1	1:G:366:LEU:HD12	1.68	0.73
1:H:2:GLU:CG	1:H:73:ASN:HD21	2.02	0.73
1:B:333:MSE:HE1	1:B:366:LEU:HD12	1.71	0.73
1:H:158:LEU:HD11	1:H:174:ILE:CD1	2.19	0.73
1:G:348:PHE:HD2	1:G:374:MSE:HE1	1.53	0.73
1:A:208:ASN:HD21	1:A:365:ARG:HH22	1.37	0.72
1:A:13:GLU:HB2	1:E:324:LEU:HG	1.69	0.72
1:H:83:SER:HA	1:H:188:ILE:HD11	1.70	0.72
1:C:172:GLN:NE2	1:D:132:GLU:OE1	2.23	0.71
1:A:208:ASN:HD21	1:A:365:ARG:NH2	1.89	0.71
1:B:327:ASN:CB	1:B:330:GLU:HG3	2.21	0.71
1:C:90:ALA:O	1:C:228:ARG:HG2	1.91	0.71
1:G:348:PHE:CD2	1:G:374:MSE:HE1	2.25	0.70
1:C:298:LEU:HB3	1:C:321:LEU:HD21	1.74	0.69
1:F:158:LEU:HD13	1:F:173:LEU:HD23	1.74	0.69
1:G:158:LEU:HD13	1:G:173:LEU:HD23	1.75	0.69
1:H:96:ILE:H	1:H:96:ILE:CD1	2.05	0.69
1:B:158:LEU:HD13	1:B:173:LEU:HD23	1.75	0.69
1:D:282:ARG:CZ	1:D:340:ARG:NH2	2.55	0.69
1:E:333:MSE:HE1	1:E:366:LEU:HD23	1.74	0.69
1:C:158:LEU:HD13	1:C:173:LEU:HD23	1.75	0.69
1:E:167:PHE:HD2	1:E:170:MSE:HE2	1.57	0.69
1:H:96:ILE:N	1:H:96:ILE:CD1	2.55	0.69
1:E:158:LEU:HD13	1:E:173:LEU:HD23	1.75	0.68
1:E:327:ASN:HB2	1:E:330:GLU:HG3	1.74	0.68
1:H:333:MSE:HE1	1:H:366:LEU:HD12	1.73	0.68
1:A:158:LEU:HD13	1:A:173:LEU:HD23	1.74	0.68
1:F:167:PHE:HD2	1:F:170:MSE:HE2	1.58	0.67
1:D:282:ARG:NH2	1:D:340:ARG:HH22	1.89	0.67
1:D:158:LEU:HD13	1:D:173:LEU:HD23	1.75	0.67
1:H:306:ILE:HD13	1:H:314:ALA:HB2	1.76	0.67
1:B:257:LEU:O	1:B:261:VAL:CG2	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ASN:OD1	1:D:340:ARG:NH1	2.27	0.67
1:G:298:LEU:HB3	1:G:321:LEU:CD1	2.25	0.67
1:H:83:SER:HA	1:H:188:ILE:CD1	2.25	0.66
1:B:327:ASN:HB2	1:B:330:GLU:HG3	1.76	0.66
1:D:333:MSE:HE1	1:D:366:LEU:HD12	1.76	0.66
1:H:200:MSE:CB	1:H:216:TYR:CD2	2.79	0.66
1:D:228:ARG:NH1	2:D:401:HOH:O	2.28	0.66
1:A:326:HIS:CB	1:A:331:LEU:HD12	2.26	0.65
1:F:361:LYS:HD3	1:F:386:LEU:HD22	1.78	0.65
1:C:307:ASN:OD1	1:C:340:ARG:NH1	2.29	0.65
1:E:327:ASN:CB	1:E:330:GLU:HG3	2.27	0.65
1:E:170:MSE:HE3	1:E:203:ILE:HG12	1.79	0.65
1:D:329:ASN:ND2	1:D:358:SER:OG	2.30	0.64
1:A:340:ARG:NH1	1:A:340:ARG:HG2	2.11	0.64
1:H:12:LEU:HD11	1:H:19:MSE:HG2	1.80	0.64
1:H:46:ASN:ND2	1:H:46:ASN:H	1.96	0.64
1:A:326:HIS:HB2	1:A:331:LEU:CD1	2.27	0.64
1:H:174:ILE:CD1	1:H:174:ILE:H	1.95	0.63
1:A:30:ASN:OD1	1:A:32:ASN:HB2	1.98	0.63
1:E:243:PHE:HE1	1:E:366:LEU:HD13	1.63	0.63
1:F:289:ASN:OD1	1:F:291:GLU:HG2	1.98	0.63
1:A:340:ARG:HG2	1:A:340:ARG:HH11	1.64	0.63
1:H:306:ILE:CD1	1:H:314:ALA:HB1	2.27	0.62
1:F:167:PHE:HD2	1:F:170:MSE:CE	2.12	0.62
1:H:208:ASN:OD1	1:H:365:ARG:NH2	2.33	0.62
1:A:326:HIS:CB	1:A:331:LEU:CD1	2.77	0.62
1:E:167:PHE:HD2	1:E:170:MSE:CE	2.13	0.62
1:F:19:MSE:CE	1:F:31:PRO:HB3	2.29	0.62
1:F:338:LYS:O	1:F:342:GLU:HG2	1.99	0.62
1:A:39:ASN:ND2	1:E:322:ASP:O	2.33	0.62
1:D:282:ARG:CZ	1:D:340:ARG:HH22	2.10	0.61
1:E:12:LEU:HD11	1:E:19:MSE:HG2	1.82	0.61
1:C:30:ASN:OD1	1:C:32:ASN:HB2	2.00	0.61
1:G:30:ASN:OD1	1:G:32:ASN:HB2	2.01	0.61
1:H:153:SER:HA	1:H:156:LEU:HD13	1.83	0.61
1:D:326:HIS:CB	1:D:331:LEU:HD13	2.30	0.61
1:G:298:LEU:HD23	1:G:321:LEU:HD12	1.81	0.61
1:G:298:LEU:HD23	1:G:321:LEU:CD1	2.30	0.61
1:F:12:LEU:HD11	1:F:19:MSE:HG2	1.82	0.61
1:F:30:ASN:OD1	1:F:32:ASN:HB2	2.01	0.61
1:H:71:CYS:HA	1:H:74:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:PHE:CD2	1:E:170:MSE:HE2	2.36	0.61
1:C:377:ASN:C	1:C:377:ASN:HD22	2.07	0.60
1:D:30:ASN:OD1	1:D:32:ASN:HB2	2.00	0.60
1:F:153:SER:HA	1:F:156:LEU:HD13	1.83	0.60
1:H:167:PHE:HD1	1:H:170:MSE:CE	2.14	0.60
1:D:12:LEU:HD11	1:D:19:MSE:HG2	1.82	0.60
1:E:30:ASN:OD1	1:E:32:ASN:HB2	2.01	0.60
1:H:333:MSE:HE3	1:H:363:LEU:HD13	1.83	0.60
1:E:153:SER:HA	1:E:156:LEU:HD13	1.82	0.60
1:E:68:LYS:HG2	1:E:96:ILE:HD11	1.83	0.60
1:C:8:MSE:HG2	1:C:22:TRP:CH2	2.36	0.60
1:D:153:SER:HA	1:D:156:LEU:HD13	1.83	0.60
1:A:167:PHE:HD1	1:A:170:MSE:CE	2.15	0.60
1:H:8:MSE:HG2	1:H:22:TRP:CH2	2.37	0.60
1:C:109:ASN:ND2	1:C:112:SER:H	2.00	0.60
1:F:167:PHE:CD2	1:F:170:MSE:HE2	2.36	0.60
1:G:12:LEU:HD11	1:G:19:MSE:HG2	1.84	0.59
1:H:345:LYS:HE3	1:H:376:GLU:OE1	2.02	0.59
1:A:8:MSE:HG2	1:A:22:TRP:CH2	2.37	0.59
1:F:8:MSE:HG2	1:F:22:TRP:CH2	2.37	0.59
1:F:64:TYR:CE1	1:F:96:ILE:HD11	2.37	0.59
1:C:298:LEU:HB3	1:C:321:LEU:CD2	2.32	0.59
1:G:133:PHE:CZ	1:H:181:GLU:OE1	2.55	0.59
1:F:170:MSE:HE3	1:F:203:ILE:HG12	1.83	0.59
1:A:131:THR:OG1	1:A:134:GLU:HG2	2.02	0.59
1:F:333:MSE:HE2	1:F:355:PHE:HZ	1.68	0.59
1:D:333:MSE:HE2	1:D:355:PHE:HZ	1.67	0.59
1:C:167:PHE:HD1	1:C:170:MSE:CE	2.16	0.59
1:G:153:SER:HA	1:G:156:LEU:HD13	1.84	0.59
1:E:327:ASN:HB2	1:E:330:GLU:CG	2.33	0.58
1:B:167:PHE:HD1	1:B:170:MSE:CE	2.16	0.58
1:B:153:SER:HA	1:B:156:LEU:HD13	1.85	0.58
1:G:167:PHE:HD1	1:G:170:MSE:CE	2.16	0.58
1:B:180:SER:HA	1:B:189:ARG:NH2	2.18	0.58
1:C:320:LYS:O	1:C:323:LEU:HG	2.03	0.58
1:H:306:ILE:HD13	1:H:314:ALA:CB	2.32	0.58
1:A:333:MSE:HE1	1:A:366:LEU:CD1	2.32	0.58
1:G:133:PHE:HZ	1:H:181:GLU:OE1	1.87	0.58
1:A:132:GLU:OE1	1:B:172:GLN:NE2	2.37	0.58
1:E:140:GLY:HA2	1:F:137:LYS:HG2	1.86	0.58
1:A:345:LYS:HE2	1:A:376:GLU:OE1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:MSE:HE2	1:B:355:PHE:HZ	1.69	0.57
1:C:153:SER:HA	1:C:156:LEU:HD13	1.86	0.57
1:G:333:MSE:HE2	1:G:355:PHE:HZ	1.69	0.57
1:A:334:HIS:HD2	2:A:408:HOH:O	1.86	0.57
1:H:200:MSE:HB3	1:H:216:TYR:CE2	2.38	0.57
1:B:8:MSE:HG2	1:B:22:TRP:CH2	2.39	0.57
1:B:327:ASN:HB3	1:B:330:GLU:HG3	1.86	0.57
1:E:136:VAL:HG22	1:F:136:VAL:HG22	1.86	0.57
1:C:109:ASN:HD22	1:C:112:SER:H	1.50	0.57
1:D:8:MSE:HG2	1:D:22:TRP:CH2	2.38	0.57
1:E:333:MSE:HE2	1:E:355:PHE:HZ	1.70	0.57
1:D:352:ILE:HD11	1:D:384:LEU:HD22	1.86	0.57
1:B:30:ASN:OD1	1:B:32:ASN:HB3	2.05	0.57
1:E:329:ASN:HD22	1:E:330:GLU:N	2.03	0.57
1:E:327:ASN:HB2	1:E:330:GLU:CD	2.30	0.56
1:B:379:LYS:HE2	1:B:379:LYS:H	1.71	0.56
1:C:331:LEU:HD22	1:C:335:TYR:CE2	2.40	0.56
1:A:333:MSE:HE2	1:A:355:PHE:HZ	1.70	0.56
1:C:228:ARG:HG3	1:C:229:PHE:N	2.20	0.56
1:E:313:LYS:O	1:E:317:VAL:HG12	2.06	0.56
1:H:306:ILE:HD11	1:H:341:LEU:HD13	1.87	0.56
1:B:228:ARG:NH1	2:B:401:HOH:O	2.38	0.55
1:C:208:ASN:OD1	1:C:365:ARG:NH2	2.38	0.55
1:B:12:LEU:HD11	1:B:19:MSE:HG2	1.88	0.55
1:H:306:ILE:CD1	1:H:341:LEU:HD13	2.36	0.55
1:H:58:GLN:CG	1:H:59:TYR:CE1	2.90	0.55
1:B:110:MSE:HA	1:B:110:MSE:HE3	1.88	0.55
1:C:12:LEU:HD11	1:C:19:MSE:HG2	1.88	0.55
1:F:93:PHE:HB3	1:F:96:ILE:HD12	1.86	0.55
1:C:243:PHE:HE1	1:C:366:LEU:HD13	1.72	0.54
1:B:124:GLU:OE1	1:B:138:ARG:NH1	2.39	0.54
1:C:105:ILE:HD12	1:C:117:LYS:HG2	1.90	0.54
1:H:158:LEU:HD11	1:H:174:ILE:HD13	1.89	0.54
1:E:105:ILE:HD12	1:E:117:LYS:HG2	1.89	0.54
1:G:272:GLN:HE21	1:G:296:MSE:HE1	1.73	0.54
1:G:331:LEU:HD22	1:G:335:TYR:CE2	2.42	0.54
1:C:167:PHE:CA	1:C:170:MSE:HE3	2.23	0.54
1:A:167:PHE:HD1	1:A:170:MSE:HE1	1.73	0.53
1:H:162:LEU:HA	1:H:170:MSE:HE1	1.90	0.53
1:E:361:LYS:NZ	1:E:386:LEU:HD22	2.23	0.53
1:D:352:ILE:HD13	1:D:384:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:ASN:HB2	1:E:330:GLU:OE1	2.09	0.53
1:F:105:ILE:HD12	1:F:117:LYS:HG2	1.90	0.53
1:E:137:LYS:O	1:F:140:GLY:HA3	2.09	0.53
1:H:58:GLN:HG3	1:H:59:TYR:CE1	2.43	0.53
1:C:162:LEU:HA	1:C:170:MSE:HE1	1.91	0.53
1:C:333:MSE:HE2	1:C:355:PHE:HZ	1.73	0.53
1:H:21:LYS:NZ	1:H:21:LYS:HB3	2.24	0.53
1:B:180:SER:HA	1:B:189:ARG:HH21	1.74	0.52
1:G:167:PHE:HD1	1:G:170:MSE:HE1	1.75	0.52
1:H:9:LYS:HZ3	1:H:38:LEU:HB3	1.74	0.52
1:H:172:GLN:OE1	1:H:172:GLN:CA	2.43	0.52
1:H:200:MSE:CB	1:H:216:TYR:CE2	2.93	0.52
1:D:105:ILE:HD12	1:D:117:LYS:HG2	1.92	0.52
1:A:162:LEU:HA	1:A:170:MSE:HE1	1.91	0.52
1:F:132:GLU:O	1:F:136:VAL:HG12	2.10	0.52
1:H:167:PHE:CA	1:H:170:MSE:HE3	2.25	0.52
1:B:162:LEU:HA	1:B:170:MSE:HE1	1.92	0.52
1:H:21:LYS:HB3	1:H:21:LYS:HZ3	1.75	0.52
1:H:331:LEU:HD22	1:H:335:TYR:CE2	2.45	0.52
1:H:333:MSE:HE2	1:H:355:PHE:HZ	1.75	0.51
1:E:8:MSE:HG2	1:E:22:TRP:CH2	2.44	0.51
1:H:9:LYS:NZ	1:H:38:LEU:HB3	2.25	0.51
1:G:8:MSE:HG2	1:G:22:TRP:CH2	2.45	0.51
1:G:71:CYS:HA	1:G:74:LEU:HD22	1.93	0.51
1:A:208:ASN:ND2	1:A:365:ARG:HH22	2.06	0.51
1:H:30:ASN:OD1	1:H:32:ASN:HB2	2.11	0.51
1:B:71:CYS:HA	1:B:74:LEU:HD22	1.93	0.51
1:F:141:LYS:HG3	1:F:141:LYS:O	2.10	0.51
1:B:167:PHE:HD1	1:B:170:MSE:HE1	1.75	0.51
1:H:2:GLU:HG2	1:H:73:ASN:HD21	1.73	0.51
1:D:162:LEU:HA	1:D:170:MSE:HE1	1.92	0.51
1:G:132:GLU:O	1:G:136:VAL:HG12	2.11	0.51
1:C:377:ASN:HD22	1:C:378:GLN:N	2.08	0.51
1:H:170:MSE:O	1:H:174:ILE:CG1	2.57	0.51
1:C:71:CYS:HA	1:C:74:LEU:HD22	1.93	0.51
1:H:2:GLU:HG3	1:H:73:ASN:HD21	1.75	0.51
1:H:167:PHE:HD1	1:H:170:MSE:HE1	1.75	0.50
1:G:167:PHE:CA	1:G:170:MSE:HE3	2.23	0.50
1:F:71:CYS:HA	1:F:74:LEU:HD22	1.92	0.50
1:C:167:PHE:HD1	1:C:170:MSE:HE1	1.76	0.50
1:D:326:HIS:HB2	1:D:331:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:LEU:HA	1:G:170:MSE:HE1	1.93	0.50
1:H:368:LEU:HD23	1:H:385:LEU:HD13	1.94	0.50
1:E:67:MSE:HA	1:E:67:MSE:CE	2.35	0.50
1:D:348:PHE:O	1:D:352:ILE:HG23	2.12	0.50
1:H:111:LYS:HD2	1:H:146:THR:CG2	2.42	0.50
1:E:132:GLU:O	1:E:136:VAL:HG12	2.12	0.49
1:E:331:LEU:HD23	1:E:335:TYR:CE2	2.47	0.49
1:C:132:GLU:O	1:C:136:VAL:HG12	2.12	0.49
1:H:333:MSE:HE1	1:H:366:LEU:CD1	2.43	0.49
1:B:105:ILE:HD12	1:B:117:LYS:HG2	1.93	0.49
1:E:71:CYS:HA	1:E:74:LEU:HD22	1.93	0.49
1:H:105:ILE:HD12	1:H:117:LYS:HG2	1.94	0.49
1:B:132:GLU:O	1:B:136:VAL:HG12	2.12	0.49
1:H:132:GLU:O	1:H:136:VAL:HG12	2.13	0.49
1:A:71:CYS:HA	1:A:74:LEU:HD22	1.94	0.49
1:H:208:ASN:CG	1:H:365:ARG:HH22	2.21	0.49
1:D:71:CYS:HA	1:D:74:LEU:HD22	1.93	0.48
1:D:132:GLU:O	1:D:136:VAL:HG12	2.12	0.48
1:A:132:GLU:O	1:A:136:VAL:HG12	2.13	0.48
1:B:167:PHE:CA	1:B:170:MSE:HE3	2.24	0.48
1:G:36:ASP:HB3	1:G:43:LYS:HG3	1.96	0.48
1:H:96:ILE:H	1:H:96:ILE:HD13	1.79	0.48
1:H:313:LYS:O	1:H:317:VAL:HG12	2.13	0.48
1:C:377:ASN:C	1:C:377:ASN:ND2	2.72	0.47
1:D:295:ILE:HD13	1:D:330:GLU:OE2	2.14	0.47
1:F:76:VAL:HG13	1:F:104:MSE:HG3	1.95	0.47
1:H:184:GLU:OE2	1:H:185:ASN:HB2	2.14	0.47
1:B:333:MSE:HE1	1:B:366:LEU:CD1	2.41	0.47
1:D:310:GLU:HG2	1:D:313:LYS:CD	2.36	0.47
1:H:174:ILE:CD1	1:H:203:ILE:HD11	2.44	0.47
1:H:76:VAL:HG13	1:H:104:MSE:HG3	1.95	0.47
1:A:167:PHE:CA	1:A:170:MSE:HE3	2.22	0.47
1:B:89:ASP:OD2	1:B:97:GLU:OE2	2.32	0.47
1:B:242:LEU:HD23	1:B:243:PHE:CE1	2.49	0.47
1:C:167:PHE:HA	1:C:170:MSE:CE	2.24	0.47
1:F:170:MSE:HE3	1:F:203:ILE:CG1	2.43	0.47
1:E:348:PHE:CZ	1:E:370:GLU:HG3	2.49	0.47
1:H:318:LEU:CD2	1:H:341:LEU:HD22	2.45	0.47
1:C:282:ARG:HG3	1:C:307:ASN:CG	2.40	0.46
1:D:348:PHE:CZ	1:D:370:GLU:HG3	2.51	0.46
1:D:333:MSE:HE1	1:D:366:LEU:CD1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:ILE:HD12	2:F:410:HOH:O	2.16	0.46
1:F:282:ARG:HG3	1:F:307:ASN:CG	2.40	0.46
1:G:133:PHE:HB2	1:H:176:GLN:OE1	2.15	0.46
1:G:336:TYR:CE1	1:G:366:LEU:HB3	2.51	0.46
1:D:329:ASN:HD22	1:D:329:ASN:HA	1.52	0.46
1:H:89:ASP:OD2	1:H:97:GLU:OE2	2.34	0.46
1:A:9:LYS:HG2	1:E:323:LEU:O	2.15	0.46
1:B:76:VAL:HG21	1:B:103:SER:HB2	1.97	0.46
1:E:282:ARG:HG3	1:E:307:ASN:CG	2.41	0.46
1:F:228:ARG:NH1	2:F:401:HOH:O	2.48	0.46
1:A:76:VAL:HG13	1:A:104:MSE:HG3	1.98	0.46
1:A:326:HIS:HB3	1:A:331:LEU:CD1	2.46	0.46
1:G:272:GLN:NE2	1:G:296:MSE:HE1	2.30	0.46
1:H:167:PHE:HD1	1:H:170:MSE:HE3	1.80	0.46
1:A:327:ASN:ND2	1:A:330:GLU:H	2.14	0.46
1:E:76:VAL:HG13	1:E:104:MSE:HG3	1.98	0.46
1:E:167:PHE:CD2	1:E:170:MSE:CE	2.96	0.46
1:H:336:TYR:CE1	1:H:366:LEU:HB3	2.50	0.46
1:C:39:ASN:HB3	2:C:408:HOH:O	2.15	0.46
1:D:76:VAL:HG13	1:D:104:MSE:HG3	1.97	0.46
1:E:43:LYS:HE2	2:E:402:HOH:O	2.15	0.46
1:B:4:ILE:HG22	2:B:408:HOH:O	2.16	0.45
1:B:336:TYR:CE1	1:B:366:LEU:HB3	2.51	0.45
1:E:55:VAL:HG21	1:E:67:MSE:CE	2.41	0.45
1:D:336:TYR:CE1	1:D:366:LEU:HB3	2.51	0.45
1:A:70:TYR:HE1	2:A:419:HOH:O	1.98	0.45
1:A:348:PHE:CZ	1:A:370:GLU:HG3	2.51	0.45
1:D:352:ILE:CD1	1:D:384:LEU:HD13	2.47	0.45
1:E:137:LYS:HG2	1:F:140:GLY:CA	2.43	0.45
1:E:336:TYR:CE1	1:E:366:LEU:HB3	2.52	0.45
1:H:167:PHE:HA	1:H:170:MSE:CE	2.25	0.45
1:B:76:VAL:HG13	1:B:104:MSE:HG3	1.98	0.45
1:F:336:TYR:CE1	1:F:366:LEU:HB3	2.52	0.45
1:F:262:GLN:H	1:F:262:GLN:NE2	2.15	0.45
1:D:282:ARG:HG3	1:D:307:ASN:CG	2.42	0.45
1:H:79:LYS:HE3	1:H:184:GLU:HG2	1.99	0.45
1:E:262:GLN:H	1:E:262:GLN:NE2	2.16	0.44
1:E:334:HIS:HE1	1:E:338:LYS:HE3	1.82	0.44
1:F:361:LYS:CD	1:F:386:LEU:HD22	2.46	0.44
1:H:318:LEU:HD22	1:H:341:LEU:HD22	1.99	0.44
1:A:336:TYR:CE1	1:A:366:LEU:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ARG:HH11	1:A:340:ARG:CG	2.28	0.44
1:E:170:MSE:HE3	1:E:203:ILE:CG1	2.46	0.44
1:F:89:ASP:OD2	1:F:97:GLU:OE2	2.36	0.44
1:G:282:ARG:HG3	1:G:307:ASN:CG	2.42	0.44
1:F:93:PHE:CB	1:F:96:ILE:HD13	2.40	0.44
1:C:76:VAL:HG21	1:C:103:SER:HB2	2.00	0.44
1:F:167:PHE:CD2	1:F:170:MSE:CE	2.95	0.44
1:G:333:MSE:HE1	1:G:366:LEU:CD1	2.40	0.44
1:C:336:TYR:CE1	1:C:366:LEU:HB3	2.51	0.44
1:H:197:HIS:CE1	1:H:219:LYS:HD2	2.51	0.44
1:D:76:VAL:HG21	1:D:103:SER:HB2	2.00	0.44
1:A:326:HIS:CB	1:A:331:LEU:HD13	2.48	0.44
1:G:262:GLN:H	1:G:262:GLN:NE2	2.15	0.44
1:E:76:VAL:HG21	1:E:103:SER:HB2	2.00	0.43
1:A:167:PHE:HD1	1:A:170:MSE:HE3	1.83	0.43
1:B:167:PHE:HA	1:B:170:MSE:CE	2.24	0.43
1:F:348:PHE:CZ	1:F:370:GLU:HG3	2.53	0.43
1:H:68:LYS:O	1:H:72:LEU:HD23	2.18	0.43
1:A:262:GLN:H	1:A:262:GLN:NE2	2.16	0.43
1:B:262:GLN:H	1:B:262:GLN:NE2	2.16	0.43
1:G:76:VAL:HG21	1:G:103:SER:HB2	2.00	0.43
1:G:104:MSE:HG2	1:G:112:SER:HB3	2.01	0.43
1:C:348:PHE:CZ	1:C:370:GLU:HG3	2.53	0.43
1:E:136:VAL:HG13	1:F:136:VAL:HG21	2.01	0.43
1:A:115:TYR:HA	1:A:149:MSE:SE	2.69	0.43
1:B:231:VAL:HG13	1:B:270:PHE:CE2	2.53	0.43
1:G:296:MSE:HE2	1:G:296:MSE:HB3	1.91	0.43
1:D:167:PHE:CA	1:D:170:MSE:HE3	2.24	0.43
1:F:191:THR:O	1:F:195:ARG:HG3	2.19	0.43
1:H:174:ILE:CD1	1:H:174:ILE:N	2.58	0.43
1:F:333:MSE:HE1	1:F:366:LEU:CD1	2.41	0.43
1:D:262:GLN:H	1:D:262:GLN:NE2	2.16	0.42
1:G:348:PHE:CD2	1:G:374:MSE:CE	3.01	0.42
1:H:331:LEU:HD22	1:H:335:TYR:HE2	1.84	0.42
1:E:349:TYR:CE1	1:F:380:LEU:HD13	2.54	0.42
1:D:16:ASN:OD1	1:G:247:GLU:OE2	2.36	0.42
1:F:167:PHE:CE2	1:F:206:ASN:HB2	2.54	0.42
1:G:327:ASN:CG	1:G:330:GLU:HG3	2.44	0.42
1:D:231:VAL:HG13	1:D:270:PHE:CE2	2.54	0.42
1:G:191:THR:O	1:G:195:ARG:HG3	2.19	0.42
1:A:315:LYS:HE3	1:A:315:LYS:HB2	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASN:HD21	1:D:365:ARG:HH12	1.68	0.42
1:E:133:PHE:CZ	1:E:137:LYS:HD2	2.55	0.42
1:E:231:VAL:HG13	1:E:270:PHE:CE2	2.55	0.42
1:E:288:ILE:HD11	1:E:304:CYS:HB2	2.02	0.42
1:F:231:VAL:HG13	1:F:270:PHE:CE2	2.55	0.42
1:H:327:ASN:CG	1:H:330:GLU:HG3	2.45	0.42
1:E:243:PHE:CE1	1:E:366:LEU:HD13	2.48	0.42
1:F:288:ILE:HD11	1:F:304:CYS:HB2	2.01	0.42
1:A:262:GLN:H	1:A:262:GLN:CD	2.28	0.42
1:C:379:LYS:HG2	1:D:349:TYR:CE2	2.55	0.42
1:F:286:LYS:HD3	1:F:287:TRP:CE2	2.55	0.42
1:G:76:VAL:HG13	1:G:104:MSE:HG3	2.02	0.42
1:H:115:TYR:HA	1:H:149:MSE:SE	2.69	0.42
1:H:231:VAL:HG13	1:H:270:PHE:CE2	2.55	0.42
1:A:334:HIS:CD2	2:A:408:HOH:O	2.67	0.42
1:C:76:VAL:HG13	1:C:104:MSE:HG3	2.01	0.42
1:C:231:VAL:HG13	1:C:270:PHE:CE2	2.55	0.42
1:C:262:GLN:H	1:C:262:GLN:NE2	2.17	0.42
1:H:200:MSE:HB2	1:H:216:TYR:CD2	2.55	0.42
1:A:231:VAL:HG13	1:A:270:PHE:CE2	2.55	0.41
1:D:104:MSE:HG2	1:D:112:SER:HB3	2.02	0.41
1:B:115:TYR:HA	1:B:149:MSE:SE	2.70	0.41
1:B:262:GLN:H	1:B:262:GLN:CD	2.29	0.41
1:B:331:LEU:HD22	1:B:335:TYR:CE2	2.55	0.41
1:E:385:LEU:O	1:E:386:LEU:HB2	2.20	0.41
1:E:191:THR:O	1:E:195:ARG:HG3	2.19	0.41
1:F:262:GLN:H	1:F:262:GLN:CD	2.28	0.41
1:G:115:TYR:HA	1:G:149:MSE:SE	2.70	0.41
1:G:167:PHE:HD1	1:G:170:MSE:HE3	1.84	0.41
1:E:101:ILE:O	1:E:105:ILE:HG12	2.20	0.41
1:F:101:ILE:O	1:F:105:ILE:HG12	2.21	0.41
1:G:348:PHE:CZ	1:G:370:GLU:HG3	2.56	0.41
1:H:174:ILE:CG1	1:H:203:ILE:CD1	2.92	0.41
1:B:348:PHE:CZ	1:B:370:GLU:HG3	2.56	0.41
1:G:231:VAL:HG13	1:G:270:PHE:CE2	2.56	0.41
1:B:101:ILE:O	1:B:105:ILE:HG12	2.21	0.41
1:E:115:TYR:HA	1:E:149:MSE:SE	2.71	0.41
1:E:104:MSE:HG2	1:E:112:SER:HB3	2.03	0.41
1:F:331:LEU:HD22	1:F:335:TYR:CE2	2.56	0.41
1:H:145:LYS:HB3	1:H:145:LYS:HE3	1.87	0.41
1:D:115:TYR:HA	1:D:149:MSE:SE	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:HIS:HB3	1:A:331:LEU:HD12	2.02	0.40
1:G:288:ILE:HD11	1:G:304:CYS:HB2	2.02	0.40
1:G:262:GLN:H	1:G:262:GLN:CD	2.29	0.40
1:G:380:LEU:HD13	1:H:349:TYR:CE1	2.57	0.40
1:H:101:ILE:O	1:H:105:ILE:HG12	2.20	0.40
1:A:248:LEU:HD22	2:D:405:HOH:O	2.22	0.40
1:C:327:ASN:CG	1:C:330:GLU:HG3	2.46	0.40
1:E:71:CYS:O	1:E:74:LEU:HB2	2.21	0.40
1:E:329:ASN:ND2	1:E:330:GLU:N	2.68	0.40
1:A:22:TRP:CZ2	1:A:58:GLN:HG2	2.57	0.40
1:G:372:GLN:CD	1:G:378:GLN:OE1	2.64	0.40
1:B:86:GLU:OE1	1:B:86:GLU:HA	2.22	0.40
1:D:101:ILE:O	1:D:105:ILE:HG12	2.20	0.40
1:D:372:GLN:CD	1:D:378:GLN:OE1	2.65	0.40
1:D:379:LYS:HA	1:D:379:LYS:HD2	1.91	0.40
1:F:71:CYS:O	1:F:74:LEU:HB2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ASN:ND2	1:H:378:GLN:OE1[1_455]	1.97	0.23

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	384/386 (100%)	378 (98%)	6 (2%)	0	100	100
1	B	384/386 (100%)	378 (98%)	6 (2%)	0	100	100
1	C	384/386 (100%)	376 (98%)	8 (2%)	0	100	100
1	D	384/386 (100%)	378 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	385/386 (100%)	377 (98%)	8 (2%)	0	100	100
1	F	384/386 (100%)	378 (98%)	6 (2%)	0	100	100
1	G	384/386 (100%)	377 (98%)	7 (2%)	0	100	100
1	H	384/386 (100%)	377 (98%)	7 (2%)	0	100	100
All	All	3073/3088 (100%)	3019 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	360/345 (104%)	320 (89%)	40 (11%)	6	15
1	B	360/345 (104%)	314 (87%)	46 (13%)	4	11
1	C	360/345 (104%)	313 (87%)	47 (13%)	4	10
1	D	360/345 (104%)	312 (87%)	48 (13%)	4	10
1	E	361/345 (105%)	315 (87%)	46 (13%)	4	11
1	F	360/345 (104%)	312 (87%)	48 (13%)	4	10
1	G	360/345 (104%)	316 (88%)	44 (12%)	5	12
1	H	360/345 (104%)	310 (86%)	50 (14%)	3	9
All	All	2881/2760 (104%)	2512 (87%)	369 (13%)	4	11

All (369) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	49	SER
1	A	65	GLU
1	A	74	LEU
1	A	76	VAL
1	A	95	GLU

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Mol	Chain	Res	Type
1	A	104	MSE
1	A	134	GLU
1	A	136	VAL
1	A	138	ARG
1	A	145	LYS
1	A	156	LEU
1	A	158	LEU
1	A	168	SER
1	A	174	ILE
1	A	198	VAL
1	A	208	ASN
1	A	209	SER
1	A	211	GLU
1	A	242	LEU
1	A	248	LEU
1	A	262	GLN
1	A	276	PHE
1	A	286	LYS
1	A	309	ASN
1	A	312	SER
1	A	315	LYS
1	A	324	LEU
1	A	327	ASN
1	A	340	ARG
1	A	341	LEU
1	A	343	GLN
1	A	356	LYS
1	A	363	LEU
1	A	368	LEU
1	A	369	LEU
1	A	370	GLU
1	A	380	LEU
1	A	385	LEU
1	A	386	LEU
1	B	1	MSE
1	B	20	ASN
1	B	21	LYS
1	B	32	ASN
1	B	49	SER
1	B	65	GLU
1	B	74	LEU
1	B	76	VAL

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Mol	Chain	Res	Type
1	B	95	GLU
1	B	100	LEU
1	B	103	SER
1	B	104	MSE
1	B	110	MSE
1	B	134	GLU
1	B	136	VAL
1	B	138	ARG
1	B	141	LYS
1	B	145	LYS
1	B	156	LEU
1	B	158	LEU
1	B	168	SER
1	B	189	ARG
1	B	198	VAL
1	B	211	GLU
1	B	218	LYS
1	B	228	ARG
1	B	242	LEU
1	B	261	VAL
1	B	262	GLN
1	B	276	PHE
1	B	296	MSE
1	B	298	LEU
1	B	310	GLU
1	B	320	LYS
1	B	324	LEU
1	B	329	ASN
1	B	331	LEU
1	B	338	LYS
1	B	341	LEU
1	B	342	GLU
1	B	363	LEU
1	B	368	LEU
1	B	370	GLU
1	B	373	LYS
1	B	379	LYS
1	B	380	LEU
1	C	13	GLU
1	C	43	LYS
1	C	49	SER
1	C	65	GLU

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Mol	Chain	Res	Type
1	C	74	LEU
1	C	76	VAL
1	C	95	GLU
1	C	100	LEU
1	C	103	SER
1	C	104	MSE
1	C	109	ASN
1	C	110	MSE
1	C	136	VAL
1	C	137	LYS
1	C	138	ARG
1	C	141	LYS
1	C	145	LYS
1	C	156	LEU
1	C	158	LEU
1	C	168	SER
1	C	184	GLU
1	C	198	VAL
1	C	228	ARG
1	C	242	LEU
1	C	262	GLN
1	C	276	PHE
1	C	282	ARG
1	C	283	LYS
1	C	286	LYS
1	C	295	ILE
1	C	298	LEU
1	C	309	ASN
1	C	310	GLU
1	C	320	LYS
1	C	321	LEU
1	C	323	LEU
1	C	324	LEU
1	C	331	LEU
1	C	341	LEU
1	C	363	LEU
1	C	365	ARG
1	C	366	LEU
1	C	368	LEU
1	C	369	LEU
1	C	370	GLU
1	C	379	LYS

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Mol	Chain	Res	Type
1	C	380	LEU
1	D	2	GLU
1	D	10	LYS
1	D	49	SER
1	D	68	LYS
1	D	74	LEU
1	D	76	VAL
1	D	95	GLU
1	D	102	ASP
1	D	103	SER
1	D	104	MSE
1	D	110	MSE
1	D	134	GLU
1	D	136	VAL
1	D	137	LYS
1	D	138	ARG
1	D	141	LYS
1	D	145	LYS
1	D	156	LEU
1	D	158	LEU
1	D	168	SER
1	D	189	ARG
1	D	198	VAL
1	D	228	ARG
1	D	242	LEU
1	D	262	GLN
1	D	276	PHE
1	D	282	ARG
1	D	298	LEU
1	D	309	ASN
1	D	310	GLU
1	D	316	GLU
1	D	320	LYS
1	D	321	LEU
1	D	324	LEU
1	D	329	ASN
1	D	331	LEU
1	D	338	LYS
1	D	341	LEU
1	D	352	ILE
1	D	356	LYS
1	D	363	LEU

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Mol	Chain	Res	Type
1	D	368	LEU
1	D	369	LEU
1	D	370	GLU
1	D	379	LYS
1	D	380	LEU
1	D	385	LEU
1	D	386	LEU
1	E	49	SER
1	E	65	GLU
1	E	68	LYS
1	E	74	LEU
1	E	76	VAL
1	E	77	LYS
1	E	95	GLU
1	E	103	SER
1	E	104	MSE
1	E	134	GLU
1	E	136	VAL
1	E	137	LYS
1	E	138	ARG
1	E	141	LYS
1	E	156	LEU
1	E	158	LEU
1	E	168	SER
1	E	174	ILE
1	E	184	GLU
1	E	198	VAL
1	E	211	GLU
1	E	218	LYS
1	E	228	ARG
1	E	242	LEU
1	E	262	GLN
1	E	276	PHE
1	E	282	ARG
1	E	286	LYS
1	E	293	ASP
1	E	309	ASN
1	E	313	LYS
1	E	317	VAL
1	E	318	LEU
1	E	320	LYS
1	E	324	LEU

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Mol	Chain	Res	Type
1	E	327	ASN
1	E	329	ASN
1	E	330	GLU
1	E	331	LEU
1	E	340	ARG
1	E	356	LYS
1	E	363	LEU
1	E	366	LEU
1	E	368	LEU
1	E	370	GLU
1	E	380	LEU
1	F	43	LYS
1	F	49	SER
1	F	65	GLU
1	F	74	LEU
1	F	76	VAL
1	F	100	LEU
1	F	102	ASP
1	F	104	MSE
1	F	111	LYS
1	F	134	GLU
1	F	136	VAL
1	F	137	LYS
1	F	138	ARG
1	F	141	LYS
1	F	145	LYS
1	F	156	LEU
1	F	158	LEU
1	F	168	SER
1	F	172	GLN
1	F	183	SER
1	F	198	VAL
1	F	209	SER
1	F	211	GLU
1	F	228	ARG
1	F	242	LEU
1	F	250	GLN
1	F	262	GLN
1	F	276	PHE
1	F	282	ARG
1	F	286	LYS
1	F	293	ASP

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Mol	Chain	Res	Type
1	F	309	ASN
1	F	310	GLU
1	F	316	GLU
1	F	320	LYS
1	F	321	LEU
1	F	324	LEU
1	F	331	LEU
1	F	338	LYS
1	F	341	LEU
1	F	342	GLU
1	F	343	GLN
1	F	356	LYS
1	F	368	LEU
1	F	369	LEU
1	F	370	GLU
1	F	380	LEU
1	F	385	LEU
1	G	13	GLU
1	G	29	LYS
1	G	39	ASN
1	G	43	LYS
1	G	49	SER
1	G	74	LEU
1	G	76	VAL
1	G	95	GLU
1	G	100	LEU
1	G	103	SER
1	G	104	MSE
1	G	136	VAL
1	G	137	LYS
1	G	138	ARG
1	G	141	LYS
1	G	156	LEU
1	G	158	LEU
1	G	168	SER
1	G	184	GLU
1	G	207	GLU
1	G	211	GLU
1	G	218	LYS
1	G	228	ARG
1	G	242	LEU
1	G	262	GLN

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Mol	Chain	Res	Type
1	G	276	PHE
1	G	282	ARG
1	G	295	ILE
1	G	296	MSE
1	G	298	LEU
1	G	309	ASN
1	G	318	LEU
1	G	320	LYS
1	G	321	LEU
1	G	324	LEU
1	G	327	ASN
1	G	331	LEU
1	G	341	LEU
1	G	356	LYS
1	G	363	LEU
1	G	368	LEU
1	G	370	GLU
1	G	379	LYS
1	G	380	LEU
1	H	10	LYS
1	H	39	ASN
1	H	44	THR
1	H	46	ASN
1	H	49	SER
1	H	73	ASN
1	H	74	LEU
1	H	76	VAL
1	H	77	LYS
1	H	95	GLU
1	H	96	ILE
1	H	102	ASP
1	H	104	MSE
1	H	111	LYS
1	H	134	GLU
1	H	136	VAL
1	H	138	ARG
1	H	150	ASN
1	H	154	ARG
1	H	156	LEU
1	H	158	LEU
1	H	168	SER
1	H	172	GLN

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Mol	Chain	Res	Type
1	H	174	ILE
1	H	180	SER
1	H	184	GLU
1	H	198	VAL
1	H	209	SER
1	H	228	ARG
1	H	268	MSE
1	H	276	PHE
1	H	286	LYS
1	H	288	ILE
1	H	306	ILE
1	H	309	ASN
1	H	310	GLU
1	H	317	VAL
1	H	318	LEU
1	H	321	LEU
1	H	327	ASN
1	H	331	LEU
1	H	345	LYS
1	H	357	LYS
1	H	365	ARG
1	H	368	LEU
1	H	369	LEU
1	H	370	GLU
1	H	379	LYS
1	H	380	LEU
1	H	385	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	190	ASN
1	A	208	ASN
1	A	250	GLN
1	A	265	ASN
1	A	278	ASN
1	A	311	ASN
1	A	327	ASN
1	A	359	ASN
1	B	32	ASN
1	B	39	ASN

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Mol	Chain	Res	Type
1	B	160	HIS
1	B	176	GLN
1	B	193	GLN
1	B	208	ASN
1	B	250	GLN
1	B	265	ASN
1	B	278	ASN
1	B	311	ASN
1	B	359	ASN
1	B	372	GLN
1	C	39	ASN
1	C	109	ASN
1	C	190	ASN
1	C	250	GLN
1	C	265	ASN
1	C	278	ASN
1	C	334	HIS
1	C	359	ASN
1	C	377	ASN
1	D	14	ASN
1	D	39	ASN
1	D	46	ASN
1	D	143	ASN
1	D	190	ASN
1	D	206	ASN
1	D	208	ASN
1	D	265	ASN
1	D	278	ASN
1	D	329	ASN
1	D	359	ASN
1	D	372	GLN
1	E	32	ASN
1	E	39	ASN
1	E	190	ASN
1	E	206	ASN
1	E	250	GLN
1	E	265	ASN
1	E	278	ASN
1	E	329	ASN
1	E	334	HIS
1	E	359	ASN
1	E	372	GLN

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Mol	Chain	Res	Type
1	F	73	ASN
1	F	160	HIS
1	F	172	GLN
1	F	190	ASN
1	F	250	GLN
1	F	265	ASN
1	F	278	ASN
1	F	301	GLN
1	F	334	HIS
1	F	359	ASN
1	F	372	GLN
1	G	14	ASN
1	G	46	ASN
1	G	190	ASN
1	G	250	GLN
1	G	265	ASN
1	G	271	GLN
1	G	272	GLN
1	G	278	ASN
1	G	327	ASN
1	G	334	HIS
1	G	359	ASN
1	G	372	GLN
1	H	46	ASN
1	H	73	ASN
1	H	190	ASN
1	H	250	GLN
1	H	265	ASN
1	H	278	ASN
1	H	311	ASN
1	H	327	ASN
1	H	334	HIS
1	H	359	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	371/386 (96%)	-0.21	1 (0%) 90 89	33, 51, 81, 100	0
1	B	371/386 (96%)	0.13	6 (1%) 70 68	26, 62, 106, 142	0
1	C	371/386 (96%)	-0.11	2 (0%) 87 86	34, 57, 91, 117	0
1	D	371/386 (96%)	-0.05	5 (1%) 75 73	34, 58, 99, 144	0
1	E	371/386 (96%)	0.07	3 (0%) 82 81	39, 65, 90, 108	0
1	F	371/386 (96%)	0.09	1 (0%) 90 89	37, 69, 109, 131	0
1	G	371/386 (96%)	-0.04	4 (1%) 78 76	31, 57, 95, 114	0
1	H	371/386 (96%)	0.88	65 (17%) 4 3	41, 79, 135, 183	0
All	All	2968/3088 (96%)	0.09	87 (2%) 53 50	26, 61, 106, 183	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	37	PHE	4.5
1	H	78	THR	4.4
1	H	85	LEU	4.1
1	H	46	ASN	3.9
1	H	31	PRO	3.9
1	H	177	ILE	3.6
1	H	81	ALA	3.6
1	H	192	TYR	3.6
1	H	150	ASN	3.4
1	H	45	PHE	3.4
1	G	133	PHE	3.3
1	C	133	PHE	3.2
1	G	276	PHE	3.2
1	B	42	GLY	3.0
1	H	84	ALA	3.0
1	H	21	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	22	TRP	2.9
1	H	34	LEU	2.9
1	H	33	PRO	2.9
1	H	44	THR	2.8
1	H	48	PHE	2.8
1	B	40	HIS	2.8
1	H	153	SER	2.8
1	H	28	LEU	2.8
1	H	147	PRO	2.8
1	H	38	LEU	2.8
1	H	188	ILE	2.7
1	H	191	THR	2.6
1	H	20	ASN	2.6
1	H	64	TYR	2.6
1	E	386	LEU	2.5
1	H	119	TYR	2.5
1	H	189	ARG	2.5
1	H	182	ILE	2.5
1	H	139	LEU	2.5
1	H	179	LEU	2.5
1	H	12	LEU	2.5
1	H	121	ILE	2.5
1	B	334	HIS	2.4
1	H	115	TYR	2.4
1	H	133	PHE	2.4
1	H	18	LEU	2.4
1	H	199	LEU	2.4
1	H	175	LYS	2.4
1	C	276	PHE	2.4
1	H	70	TYR	2.4
1	E	96	ILE	2.4
1	D	359	ASN	2.4
1	B	31	PRO	2.4
1	H	49	SER	2.3
1	G	21	LYS	2.3
1	H	106	SER	2.3
1	H	111	LYS	2.2
1	H	59	TYR	2.2
1	H	107	CYS	2.2
1	B	321	LEU	2.2
1	H	203	ILE	2.2
1	D	323	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	76	VAL	2.2
1	D	290	PHE	2.2
1	F	145	LYS	2.1
1	H	136	VAL	2.1
1	H	232	PHE	2.1
1	H	113	LYS	2.1
1	H	25	VAL	2.1
1	H	152	PHE	2.1
1	H	88	ALA	2.1
1	H	276	PHE	2.1
1	H	80	ALA	2.1
1	H	209	SER	2.1
1	H	86	GLU	2.1
1	H	145	LYS	2.1
1	A	24	THR	2.1
1	B	176	GLN	2.1
1	H	173	LEU	2.1
1	H	42	GLY	2.1
1	H	165	GLY	2.1
1	H	35	TYR	2.1
1	H	112	SER	2.0
1	D	16	ASN	2.0
1	H	51	ILE	2.0
1	D	38	LEU	2.0
1	H	74	LEU	2.0
1	E	174	ILE	2.0
1	G	140	GLY	2.0
1	H	140	GLY	2.0
1	H	187	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.