



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:39 PM UTC

PDB ID : 9RVT / pdb_00009rvt
Title : ACE2 extracellular domain in complex with the macrocyclic peptide GR1.4
Authors : Brear, P.; Hyvonen, M.
Deposited on : 2025-07-08
Resolution : 2.39 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

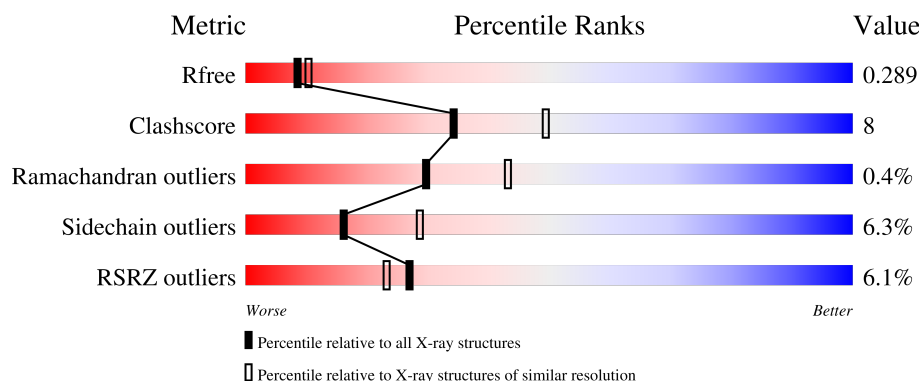
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	609	<div> <div>4%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
1	B	609	<div> <div>3%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	D	609	<div> <div>9%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	G	609	<div> <div>7%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>
2	C	14	<div> <div>21%</div> <div>86%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	14	<div><div></div><div>14%</div><div>86%</div><div>7%</div><div>7%</div></div>
2	F	14	<div><div></div><div>14%</div><div>64%</div><div>21%</div><div>14%</div></div>
2	H	14	<div><div></div><div>14%</div><div>64%</div><div>36%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20476 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	2	0
			4881	3122	810	920	29			
1	B	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			
1	D	595	Total	C	N	O	S	0	0	0
			4856	3108	804	915	29			
1	G	595	Total	C	N	O	S	0	1	0
			4866	3114	807	916	29			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP Q9BYF1
A	616	SER	-	expression tag	UNP Q9BYF1
A	617	SER	-	expression tag	UNP Q9BYF1
A	618	PRO	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
A	622	HIS	-	expression tag	UNP Q9BYF1
A	623	HIS	-	expression tag	UNP Q9BYF1
A	624	HIS	-	expression tag	UNP Q9BYF1
A	625	HIS	-	expression tag	UNP Q9BYF1
A	626	HIS	-	expression tag	UNP Q9BYF1
B	18	GLY	-	expression tag	UNP Q9BYF1
B	616	SER	-	expression tag	UNP Q9BYF1
B	617	SER	-	expression tag	UNP Q9BYF1
B	618	PRO	-	expression tag	UNP Q9BYF1
B	619	HIS	-	expression tag	UNP Q9BYF1
B	620	HIS	-	expression tag	UNP Q9BYF1
B	621	HIS	-	expression tag	UNP Q9BYF1
B	622	HIS	-	expression tag	UNP Q9BYF1
B	623	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	624	HIS	-	expression tag	UNP Q9BYF1
B	625	HIS	-	expression tag	UNP Q9BYF1
B	626	HIS	-	expression tag	UNP Q9BYF1
D	18	GLY	-	expression tag	UNP Q9BYF1
D	616	SER	-	expression tag	UNP Q9BYF1
D	617	SER	-	expression tag	UNP Q9BYF1
D	618	PRO	-	expression tag	UNP Q9BYF1
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1
D	622	HIS	-	expression tag	UNP Q9BYF1
D	623	HIS	-	expression tag	UNP Q9BYF1
D	624	HIS	-	expression tag	UNP Q9BYF1
D	625	HIS	-	expression tag	UNP Q9BYF1
D	626	HIS	-	expression tag	UNP Q9BYF1
G	18	GLY	-	expression tag	UNP Q9BYF1
G	616	SER	-	expression tag	UNP Q9BYF1
G	617	SER	-	expression tag	UNP Q9BYF1
G	618	PRO	-	expression tag	UNP Q9BYF1
G	619	HIS	-	expression tag	UNP Q9BYF1
G	620	HIS	-	expression tag	UNP Q9BYF1
G	621	HIS	-	expression tag	UNP Q9BYF1
G	622	HIS	-	expression tag	UNP Q9BYF1
G	623	HIS	-	expression tag	UNP Q9BYF1
G	624	HIS	-	expression tag	UNP Q9BYF1
G	625	HIS	-	expression tag	UNP Q9BYF1
G	626	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called macrocyclic peptide GR1.4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	14	Total 103	C 66	N 15	O 20	S 2	0	0	0
2	E	14	Total 103	C 66	N 15	O 20	S 2	0	0	0
2	F	14	Total 103	C 66	N 15	O 20	S 2	0	0	0
2	H	14	Total 103	C 66	N 15	O 20	S 2	0	0	0

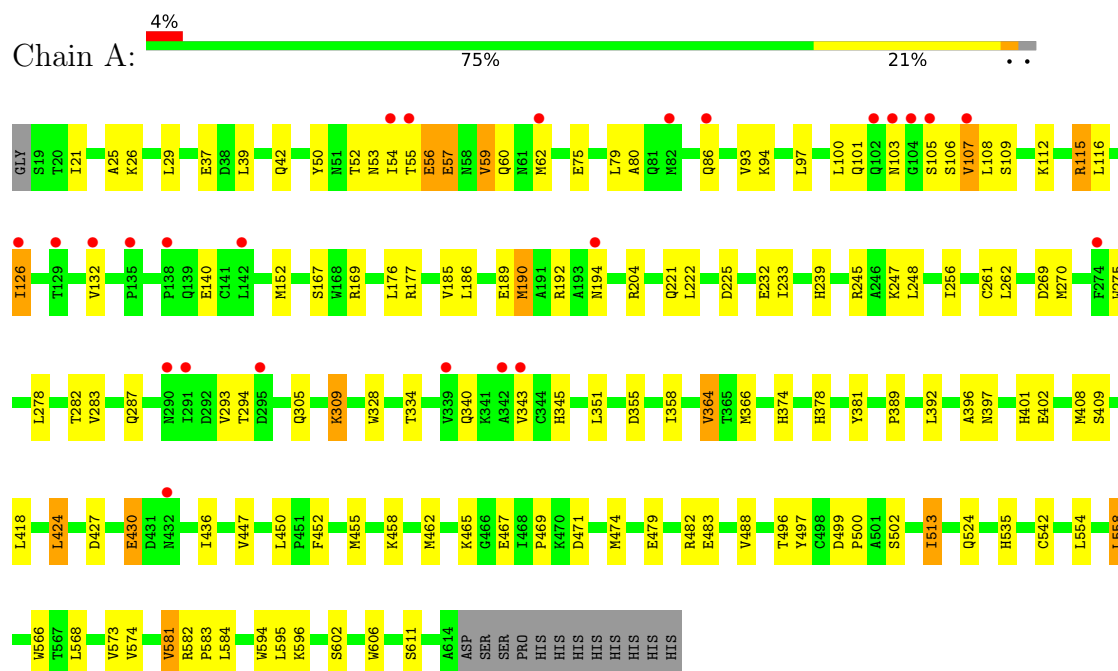
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	180	Total 180	O 180	0	0
3	B	161	Total 161	O 161	0	0
3	C	6	Total 6	O 6	0	0
3	D	102	Total 102	O 102	0	0
3	E	3	Total 3	O 3	0	0
3	F	3	Total 3	O 3	0	0
3	G	142	Total 142	O 142	0	0
3	H	2	Total 2	O 2	0	0

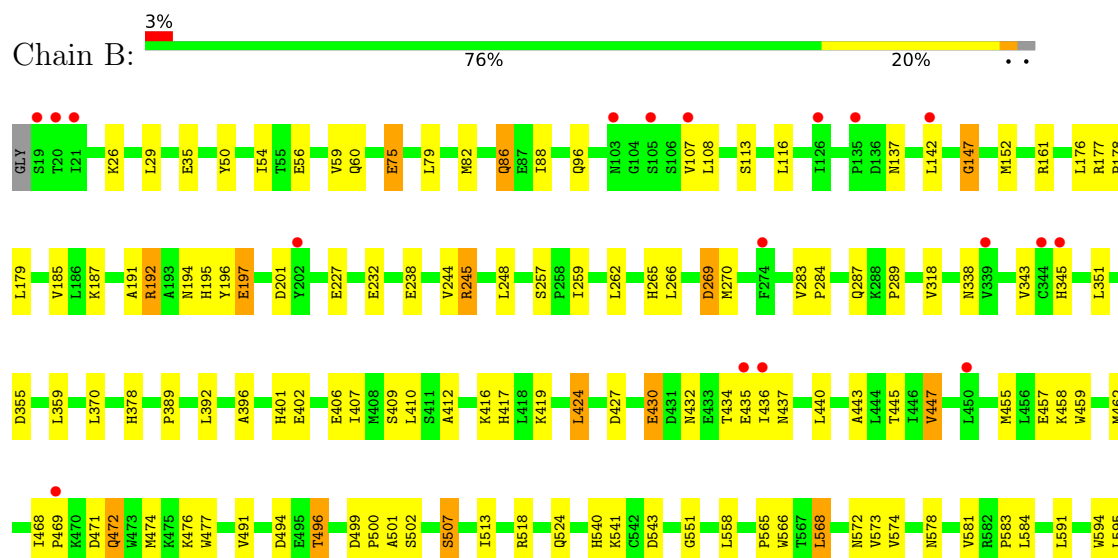
3 Residue-property plots [i](#)

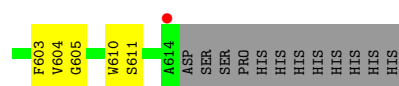
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Processed angiotensin-converting enzyme 2

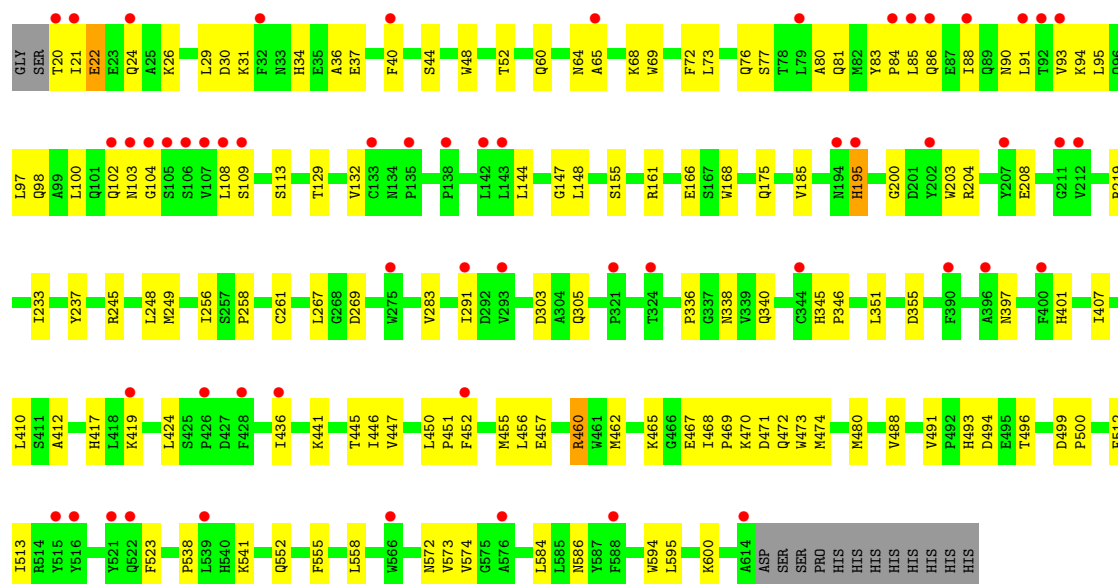
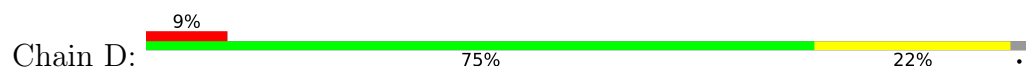


- Molecule 1: Processed angiotensin-converting enzyme 2

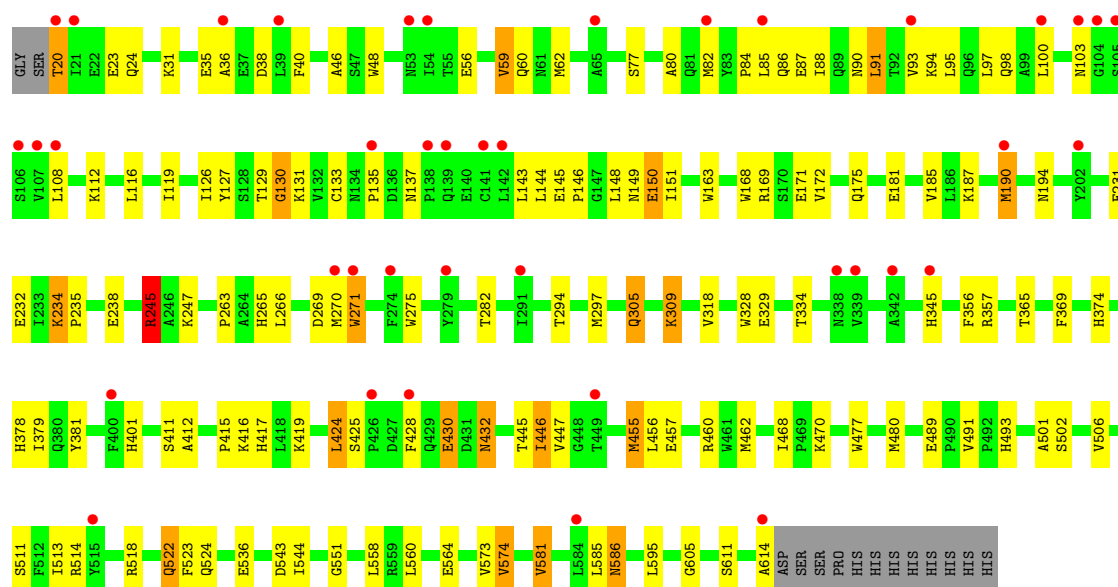
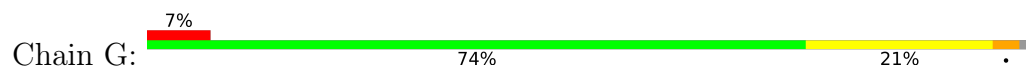




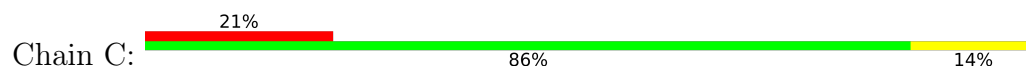
• Molecule 1: Processed angiotensin-converting enzyme 2

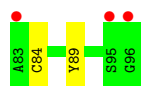


• Molecule 1: Processed angiotensin-converting enzyme 2

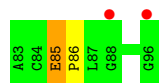
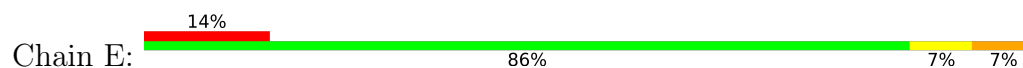


• Molecule 2: macrocyclic peptide GR1.4

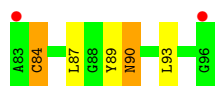




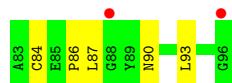
- Molecule 2: macrocyclic peptide GR1.4



- Molecule 2: macrocyclic peptide GR1.4



- Molecule 2: macrocyclic peptide GR1.4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.23Å 77.45Å 153.69Å 90.00° 101.22° 90.00°	Depositor
Resolution (Å)	69.07 – 2.39 69.07 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.4 (69.07-2.39) 99.3 (69.07-2.39)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.40Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (10-JUL-2024)	Depositor
R, R_{free}	0.249 , 0.298 0.246 , 0.289	Depositor DCC
R_{free} test set	2019 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20476	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9490e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.74	0/5019	1.16	6/6819 (0.1%)
1	B	0.74	0/4999	1.15	12/6792 (0.2%)
1	D	0.71	0/4993	1.13	11/6784 (0.2%)
1	G	0.74	1/5004 (0.0%)	1.18	19/6799 (0.3%)
2	C	0.81	0/105	1.28	1/140 (0.7%)
2	E	0.72	0/105	1.33	0/140
2	F	0.66	0/105	1.24	1/140 (0.7%)
2	H	0.77	0/105	1.32	1/140 (0.7%)
All	All	0.74	1/20435 (0.0%)	1.16	51/27754 (0.2%)

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	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	194	ASN	C-N	6.69	1.43	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	ASP	CA-CB-CG	9.98	122.58	112.60
1	G	194	ASN	O-C-N	9.33	133.21	122.20
1	A	269	ASP	CA-CB-CG	7.74	120.34	112.60
1	G	585	LEU	CA-C-N	6.88	129.38	120.44
1	G	585	LEU	C-N-CA	6.88	129.38	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	446	ILE	N-CA-C	6.72	116.85	110.53
1	A	496	THR	N-CA-C	-6.71	105.09	113.28
1	D	269	ASP	CA-CB-CG	6.65	119.25	112.60
1	B	445	THR	CA-C-N	6.59	128.76	120.72
1	B	445	THR	C-N-CA	6.59	128.76	120.72
1	D	445	THR	CA-C-N	6.25	129.29	120.42
1	D	445	THR	C-N-CA	6.25	129.29	120.42
1	G	269	ASP	CA-CB-CG	6.22	118.82	112.60
1	G	263	PRO	CA-C-N	6.19	129.42	120.38
1	G	263	PRO	C-N-CA	6.19	129.42	120.38
1	D	303	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	397	ASN	CA-CB-CG	6.05	118.65	112.60
1	D	523	PHE	CA-CB-CG	-5.88	107.92	113.80
1	D	446	ILE	N-CA-C	5.81	116.58	110.72
1	G	586	ASN	CA-C-N	5.67	127.88	120.28
1	G	586	ASN	C-N-CA	5.67	127.88	120.28
1	D	267	LEU	N-CA-C	5.60	119.65	112.26
1	G	432	ASN	CA-CB-CG	5.53	118.13	112.60
1	G	275	TRP	CA-C-N	5.43	127.88	120.54
1	G	275	TRP	C-N-CA	5.43	127.88	120.54
1	D	397	ASN	CA-CB-CG	5.41	118.01	112.60
1	B	578	ASN	CA-C-N	5.41	128.52	120.90
1	B	578	ASN	C-N-CA	5.41	128.52	120.90
1	G	59	VAL	N-CA-CB	5.40	118.68	110.58
2	F	90	ASN	CB-CA-C	5.39	120.12	111.66
1	G	445	THR	CA-C-N	5.33	127.38	120.56
1	G	445	THR	C-N-CA	5.33	127.38	120.56
1	D	586	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	606	TRP	N-CA-C	5.25	117.36	109.23
1	B	201	ASP	CA-C-N	5.16	127.20	120.28
1	B	201	ASP	C-N-CA	5.16	127.20	120.28
1	G	181	GLU	CA-C-N	5.15	127.19	120.28
1	G	181	GLU	C-N-CA	5.15	127.19	120.28
2	H	90	ASN	N-CA-C	-5.15	106.94	113.23
1	B	338	ASN	CA-C-N	5.15	127.15	120.56
1	B	338	ASN	C-N-CA	5.15	127.15	120.56
1	B	289	PRO	CA-C-N	5.15	128.02	120.71
1	B	289	PRO	C-N-CA	5.15	128.02	120.71
1	D	452	PHE	CA-C-N	5.13	127.11	120.44
1	D	452	PHE	C-N-CA	5.13	127.11	120.44
2	C	89	TYR	CB-CA-C	5.10	118.98	111.73
1	B	496	THR	N-CA-C	-5.04	107.30	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	PHE	CA-C-N	5.02	127.27	120.44
1	A	452	PHE	C-N-CA	5.02	127.27	120.44
1	G	245	ARG	CA-C-N	5.00	126.99	120.28
1	G	245	ARG	C-N-CA	5.00	126.99	120.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Sidechain
1	A	169	ARG	Sidechain
1	B	245	ARG	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	4881	0	4652	70	0
1	B	4862	0	4639	62	1
1	D	4856	0	4634	79	1
1	G	4866	0	4640	79	0
2	C	103	0	93	1	0
2	E	103	0	93	2	0
2	F	103	0	93	5	0
2	H	103	0	93	3	0
3	A	180	0	0	3	0
3	B	161	0	0	0	0
3	C	6	0	0	0	0
3	D	102	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	142	0	0	1	0
3	H	2	0	0	0	0
All	All	20476	0	18937	293	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 (293) 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:D:24:GLN:HG2	1:D:83:TYR:CE1	2.02	0.94
1:D:21:ILE:HG21	1:D:84:PRO:HD2	1.50	0.92
1:D:24:GLN:HG2	1:D:83:TYR:HE1	1.40	0.83
1:A:105:SER:HA	1:A:194:ASN:HD21	1.46	0.79
1:A:56:GLU:HB3	3:A:866:HOH:O	1.85	0.76
1:D:88:ILE:HG21	1:D:94:LYS:HB2	1.68	0.75
1:A:50:TYR:CE2	1:A:54:ILE:HG23	2.24	0.71
1:A:345:HIS:HB3	2:C:84:CYS:SG	2.32	0.70
1:G:144:LEU:HB3	3:G:751:HOH:O	1.89	0.70
1:D:469:PRO:HB2	1:D:471:ASP:OD1	1.92	0.69
1:G:294:THR:HG23	1:G:365:THR:HA	1.73	0.69
1:D:65:ALA:HA	1:D:68:LYS:HD2	1.74	0.68
2:F:87:LEU:HD21	2:F:93:LEU:HB2	1.76	0.67
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.74	0.67
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.78	0.66
1:G:455:MET:HE3	1:G:480:MET:HB2	1.77	0.66
1:B:177:ARG:HH22	1:B:474:MET:HG2	1.61	0.66
1:G:144:LEU:HA	1:G:148:LEU:HB2	1.78	0.65
1:A:56:GLU:O	1:A:59:VAL:HG22	1.99	0.63
1:A:80:ALA:HB2	1:A:100:LEU:HD23	1.80	0.63
1:G:245:ARG:NH1	1:G:605:GLY:O	2.32	0.63
1:G:131:LYS:HG3	1:G:143:LEU:HG	1.81	0.62
1:G:491:VAL:HG23	1:G:493:HIS:CD2	2.34	0.62
1:A:56:GLU:O	1:A:60:GLN:HG3	1.99	0.62
1:D:245:ARG:O	1:D:249:MET:HG3	2.00	0.62
1:A:56:GLU:HA	1:A:59:VAL:HG13	1.82	0.62
1:D:31:LYS:HD3	1:D:31:LYS:C	2.25	0.61
1:G:85:LEU:HD21	1:G:97:LEU:HB2	1.82	0.61
1:G:85:LEU:HD22	1:G:94:LYS:HG3	1.83	0.61
1:A:479:GLU:O	1:A:483:GLU:HG3	2.02	0.59
1:G:381:TYR:CD1	1:G:558:LEU:HG	2.38	0.59
1:G:131:LYS:HE3	1:G:143:LEU:HD11	1.85	0.58
1:A:100:LEU:O	1:A:103:ASN:ND2	2.36	0.58
1:D:457:GLU:HG2	1:D:513:ILE:HB	1.85	0.58
1:G:412:ALA:HA	1:G:417:HIS:CD2	2.38	0.58
1:G:297:MET:HE1	1:G:369:PHE:HB2	1.86	0.58
1:D:470:LYS:HA	1:D:473:TRP:CD1	2.39	0.58
1:D:21:ILE:O	1:D:22:GLU:C	2.47	0.57
1:B:389:PRO:HD2	1:B:392:LEU:HD12	1.86	0.57
1:G:150:GLU:HG3	1:G:151:ILE:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:ALA:HB2	1:G:100:LEU:HD23	1.86	0.57
1:G:501:ALA:HA	1:G:506:VAL:HB	1.85	0.57
1:G:560:LEU:HD13	1:G:564:GLU:HG3	1.86	0.56
1:D:351:LEU:HB2	1:D:355:ASP:HB3	1.86	0.56
1:G:168:TRP:CZ3	1:G:172:VAL:HG21	2.40	0.56
1:D:91:LEU:HG	1:D:95:LEU:HG	1.87	0.56
1:G:345:HIS:HB3	2:H:84:CYS:SG	2.46	0.56
1:G:415:PRO:HG2	1:G:430:GLU:HG2	1.88	0.56
1:B:469:PRO:HG2	1:B:472:GLN:HB2	1.89	0.55
1:D:31:LYS:HA	1:D:34:HIS:HD2	1.72	0.55
1:G:415:PRO:HB3	1:G:428:PHE:HE2	1.71	0.55
1:D:85:LEU:HA	1:D:88:ILE:HD12	1.88	0.55
1:B:177:ARG:N	1:B:178:PRO:HD2	2.22	0.54
1:D:233:ILE:HD13	1:D:450:LEU:HD13	1.89	0.54
1:G:378:HIS:ND1	2:H:86:PRO:HG3	2.22	0.54
1:B:265:HIS:NE2	1:B:266:LEU:HD21	2.22	0.54
1:B:245:ARG:NH1	1:B:605:GLY:O	2.38	0.54
1:A:106:SER:C	1:A:108:LEU:H	2.16	0.54
1:A:109:SER:HB3	1:A:112:LYS:HG3	1.90	0.54
1:A:221:GLN:NE2	1:A:225:ASP:OD1	2.40	0.54
1:A:436:ILE:HD13	1:A:594:TRP:CD1	2.42	0.54
1:A:105:SER:HA	1:A:194:ASN:ND2	2.21	0.54
1:A:177:ARG:HD3	1:A:497:TYR:O	2.09	0.53
1:G:271:TRP:HE1	1:G:502:SER:C	2.15	0.53
1:A:465:LYS:HD3	1:A:467:GLU:HG3	1.90	0.53
1:D:40:PHE:CE1	2:F:89:TYR:HB3	2.44	0.53
1:G:524:GLN:HB3	1:G:574:VAL:HG11	1.90	0.53
1:B:343:VAL:HG12	1:B:345:HIS:CD2	2.44	0.53
1:G:144:LEU:HG	1:G:149:ASN:ND2	2.24	0.53
1:A:389:PRO:HD2	1:A:392:LEU:HD12	1.90	0.53
1:D:345:HIS:HB3	2:F:84:CYS:SG	2.49	0.53
1:D:474:MET:HE3	1:D:474:MET:HA	1.91	0.53
1:B:56:GLU:HA	1:B:59:VAL:HG12	1.91	0.52
1:D:77:SER:HB2	1:D:103:ASN:HB2	1.91	0.52
1:G:48:TRP:CD1	1:G:357:ARG:NH2	2.77	0.52
1:A:343:VAL:CG1	1:A:345:HIS:CD2	2.92	0.52
1:D:456:LEU:HD22	1:D:512:PHE:CD2	2.45	0.52
1:G:611:SER:HB2	1:G:614:ALA:HB2	1.91	0.52
1:D:203:TRP:CH2	1:D:460:ARG:NH2	2.78	0.52
1:A:204:ARG:HG2	1:A:222:LEU:HD23	1.92	0.52
1:G:247:LYS:HB2	1:G:282:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:HA	1:A:60:GLN:HE21	1.75	0.52
1:D:245:ARG:HD3	1:D:258:PRO:HA	1.91	0.52
1:D:291:ILE:HD12	1:D:424:LEU:HD11	1.91	0.52
1:G:108:LEU:HG	1:G:112:LYS:HB3	1.91	0.52
1:D:20:THR:HG23	1:D:22:GLU:HB3	1.90	0.51
1:G:48:TRP:CD1	1:G:357:ARG:HH21	2.28	0.51
1:G:232:GLU:HB2	1:G:581:VAL:HG11	1.90	0.51
1:A:396:ALA:HB1	1:A:566:TRP:HA	1.92	0.51
1:B:244:VAL:HG12	1:B:248:LEU:HD12	1.93	0.51
1:B:192:ARG:HD3	1:B:197:GLU:O	2.10	0.51
1:G:231:GLU:HA	1:G:234:LYS:HG3	1.93	0.51
1:G:94:LYS:O	1:G:98:GLN:HG3	2.11	0.51
1:G:143:LEU:O	1:G:144:LEU:C	2.54	0.51
1:A:239:HIS:CD2	1:A:596:LYS:HA	2.46	0.51
1:B:50:TYR:CE2	1:B:54:ILE:HG23	2.46	0.51
1:B:284:PRO:HB2	1:B:437:ASN:OD1	2.11	0.50
1:B:407:ILE:HA	1:B:410:LEU:HB2	1.92	0.50
1:G:374:HIS:CD2	1:G:378:HIS:NE2	2.79	0.50
1:D:80:ALA:HB2	1:D:100:LEU:HD23	1.92	0.50
1:D:538:PRO:HD2	1:D:541:LYS:HD3	1.93	0.50
1:B:565:PRO:HG2	1:B:568:LEU:HB2	1.93	0.50
1:G:456:LEU:HD12	1:G:477:TRP:HH2	1.77	0.50
1:B:318:VAL:O	1:B:551:GLY:HA3	2.11	0.50
1:D:21:ILE:HA	1:D:24:GLN:HB3	1.93	0.50
1:B:351:LEU:HB2	1:B:355:ASP:HB3	1.94	0.50
1:G:116:LEU:HA	1:G:119:ILE:HD12	1.94	0.49
1:B:259:ILE:HA	1:B:603:PHE:CD2	2.47	0.49
1:B:457:GLU:HG2	1:B:513:ILE:HB	1.94	0.49
1:D:455:MET:HE3	1:D:480:MET:HB2	1.94	0.49
1:D:462:MET:HB3	1:D:468:ILE:HG13	1.94	0.49
1:G:85:LEU:HB3	1:G:94:LYS:HE3	1.94	0.49
2:H:87:LEU:HD21	2:H:93:LEU:HB2	1.93	0.49
1:A:126:ILE:HD11	1:A:176:LEU:HD23	1.93	0.49
1:A:25:ALA:HB1	1:A:97:LEU:HD11	1.94	0.49
1:G:90:ASN:HB3	1:G:93:VAL:HG22	1.93	0.49
1:D:98:GLN:O	1:D:102:GLN:HG3	2.12	0.49
1:G:457:GLU:HG2	1:G:513:ILE:HB	1.94	0.49
1:D:491:VAL:HG23	1:D:493:HIS:CD2	2.48	0.49
1:G:305:GLN:O	1:G:309:LYS:HB2	2.13	0.48
1:B:402:GLU:HB3	1:B:518:ARG:HD3	1.96	0.48
1:D:36:ALA:HA	1:D:69:TRP:HZ3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LEU:O	1:D:95:LEU:N	2.42	0.48
1:D:85:LEU:HA	1:D:88:ILE:CD1	2.44	0.48
1:G:82:MET:O	1:G:84:PRO:HD3	2.13	0.48
1:A:418:LEU:HB2	1:A:424:LEU:HD22	1.94	0.48
1:B:419:LYS:HG3	1:B:424:LEU:HB3	1.95	0.48
1:G:309:LYS:HD2	1:G:328:TRP:CH2	2.48	0.48
1:B:359:LEU:C	1:B:359:LEU:HD23	2.38	0.48
1:D:237:TYR:CE1	1:D:451:PRO:HG2	2.49	0.48
1:D:48:TRP:O	1:D:52:THR:HG23	2.14	0.47
1:D:72:PHE:O	1:D:76:GLN:HG2	2.14	0.47
1:G:489:GLU:O	1:G:489:GLU:HG2	2.12	0.47
1:A:105:SER:HB2	3:A:863:HOH:O	2.14	0.47
1:D:436:ILE:HD13	1:D:594:TRP:CD1	2.48	0.47
1:G:518:ARG:O	1:G:522:GLN:HB3	2.14	0.47
1:D:465:LYS:HZ2	1:D:467:GLU:CD	2.23	0.47
1:A:116:LEU:HD13	1:A:186:LEU:HB2	1.96	0.47
1:D:499:ASP:N	1:D:500:PRO:HD2	2.29	0.47
1:A:233:ILE:HD13	1:A:450:LEU:HD13	1.96	0.47
1:B:116:LEU:HD21	1:B:187:LYS:HD3	1.97	0.47
1:G:168:TRP:NE1	1:G:502:SER:HB2	2.30	0.47
1:G:425:SER:HB3	1:G:428:PHE:HB2	1.97	0.47
1:D:419:LYS:HG3	1:D:424:LEU:HB3	1.97	0.47
1:D:491:VAL:HG23	1:D:493:HIS:NE2	2.30	0.47
1:G:419:LYS:HG3	1:G:424:LEU:HB3	1.97	0.46
1:B:416:LYS:HD3	1:B:543:ASP:HB3	1.96	0.46
1:B:265:HIS:CD2	1:B:266:LEU:CD2	2.99	0.46
1:G:56:GLU:O	1:G:60:GLN:HG2	2.16	0.46
1:B:378:HIS:CG	2:E:86:PRO:HG2	2.51	0.46
1:B:432:ASN:N	1:B:432:ASN:OD1	2.48	0.46
1:B:458:LYS:HG2	1:B:462:MET:HE3	1.97	0.46
1:D:419:LYS:CG	1:D:424:LEU:HB3	2.46	0.46
1:G:247:LYS:CB	1:G:282:THR:HG22	2.45	0.46
1:G:511:SER:OG	1:G:514:ARG:NH2	2.48	0.46
1:D:494:ASP:OD1	1:D:496:THR:OG1	2.34	0.46
1:D:20:THR:CG2	1:D:22:GLU:HB3	2.45	0.46
1:D:346:PRO:O	2:F:84:CYS:HB2	2.15	0.46
1:A:351:LEU:HB2	1:A:355:ASP:HB3	1.98	0.45
1:D:155:SER:O	1:D:161:ARG:HD2	2.16	0.45
1:G:265:HIS:NE2	1:G:266:LEU:HD21	2.31	0.45
1:A:53:ASN:ND2	1:A:55:THR:HG23	2.32	0.45
1:B:430:GLU:CD	1:B:430:GLU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:270:MET:HB3	1:G:271:TRP:CE3	2.51	0.45
1:G:144:LEU:HG	1:G:149:ASN:HD21	1.79	0.45
1:A:535:HIS:CD2	1:A:542:CYS:HB2	2.51	0.45
1:B:436:ILE:HD13	1:B:594:TRP:CD1	2.52	0.45
1:B:524:GLN:HB3	1:B:574:VAL:HG11	1.99	0.45
1:G:356:PHE:HB3	1:G:379:ILE:HD12	1.97	0.45
1:B:459:TRP:CG	1:B:477:TRP:HE3	2.35	0.45
1:D:469:PRO:HG2	1:D:472:GLN:HB2	1.97	0.45
1:A:247:LYS:HB2	1:A:282:THR:HG22	1.98	0.45
1:A:513:ILE:HG22	3:A:765:HOH:O	2.16	0.45
1:B:469:PRO:HB2	1:B:471:ASP:OD1	2.17	0.45
1:B:501:ALA:O	1:B:507:SER:OG	2.28	0.45
1:B:513:ILE:HD12	1:B:513:ILE:HA	1.92	0.45
1:G:46:ALA:HB1	1:G:62:MET:HA	1.98	0.45
1:A:499:ASP:N	1:A:500:PRO:HD2	2.31	0.45
1:B:29:LEU:HD11	1:B:96:GLN:HB2	1.98	0.45
1:A:105:SER:C	1:A:107:VAL:H	2.24	0.44
1:A:261:CYS:HB2	1:A:488:VAL:HB	1.99	0.44
1:D:30:ASP:O	1:D:34:HIS:CD2	2.70	0.44
1:D:88:ILE:CG2	1:D:94:LYS:HB2	2.41	0.44
1:D:555:PHE:HA	1:D:558:LEU:HB2	1.99	0.44
1:A:26:LYS:HE2	1:A:93:VAL:HG21	1.99	0.44
1:A:458:LYS:HG2	1:A:462:MET:HE3	1.99	0.44
1:G:135:PRO:HD2	1:G:163:TRP:NE1	2.32	0.44
1:D:237:TYR:CZ	1:D:451:PRO:HG2	2.52	0.44
1:B:238:GLU:HG2	1:B:604:VAL:HG12	1.99	0.44
1:D:21:ILE:CG2	1:D:84:PRO:HD2	2.35	0.44
1:A:275:TRP:HB3	1:A:278:LEU:HD12	2.00	0.44
1:G:77:SER:HB2	1:G:103:ASN:ND2	2.32	0.44
1:G:446:ILE:HD13	1:G:523:PHE:HZ	1.83	0.44
1:A:132:VAL:HB	1:A:167:SER:HB3	2.00	0.44
1:G:318:VAL:HG11	1:G:544:ILE:HD12	1.99	0.44
1:A:106:SER:C	1:A:108:LEU:N	2.74	0.43
1:A:185:VAL:O	1:A:189:GLU:HG3	2.17	0.43
1:A:248:LEU:HB3	1:A:256:ILE:HD13	2.00	0.43
1:A:474:MET:HE3	1:A:474:MET:HA	1.99	0.43
1:B:86:GLN:HE21	1:B:86:GLN:HB2	1.67	0.43
1:B:232:GLU:HB2	1:B:581:VAL:HG11	1.99	0.43
1:B:412:ALA:HA	1:B:417:HIS:CD2	2.53	0.43
1:B:540:HIS:CD2	1:B:541:LYS:HG3	2.52	0.43
1:A:293:VAL:HG22	1:A:366:MET:SD	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ARG:HB2	1:B:262:LEU:HD21	2.00	0.43
1:D:60:GLN:HE21	1:D:64:ASN:HD21	1.66	0.43
1:D:208:GLU:HB2	1:D:219:ARG:HG2	2.00	0.43
1:G:169:ARG:HH12	1:G:270:MET:HG3	1.83	0.43
1:G:190:MET:HE3	1:G:190:MET:HB3	1.79	0.43
1:A:381:TYR:HA	1:A:558:LEU:HG	1.99	0.43
1:B:477:TRP:CE3	1:B:500:PRO:HG3	2.52	0.43
1:D:470:LYS:C	1:D:472:GLN:H	2.26	0.43
1:G:20:THR:HG23	1:G:23:GLU:HB2	2.00	0.43
1:D:132:VAL:HG22	1:D:148:LEU:HD11	1.99	0.43
1:A:499:ASP:O	1:A:502:SER:OG	2.28	0.43
1:G:234:LYS:HB2	1:G:235:PRO:HD3	2.00	0.43
1:A:115:ARG:HA	1:A:115:ARG:HD2	1.79	0.43
1:D:412:ALA:HA	1:D:417:HIS:CD2	2.52	0.43
1:G:318:VAL:O	1:G:551:GLY:HA3	2.19	0.43
1:A:75:GLU:O	1:A:79:LEU:HG	2.18	0.43
1:D:513:ILE:HD12	1:D:513:ILE:HA	1.94	0.43
1:G:145:GLU:HA	1:G:146:PRO:HA	1.65	0.43
1:D:31:LYS:HA	1:D:34:HIS:CD2	2.52	0.43
1:A:39:LEU:HA	1:A:42[B]:GLN:HG2	2.01	0.43
1:A:232:GLU:HB2	1:A:581:VAL:HG11	2.00	0.43
1:A:378:HIS:NE2	1:A:402:GLU:OE2	2.52	0.43
1:B:142:LEU:HB3	1:B:147:GLY:HA3	2.01	0.43
1:B:396:ALA:HB1	1:B:566:TRP:HA	2.01	0.43
1:A:309:LYS:HD2	1:A:328:TRP:CH2	2.54	0.42
1:G:416:LYS:HD3	1:G:543:ASP:HB3	2.01	0.42
1:B:75:GLU:O	1:B:79:LEU:HG	2.19	0.42
1:B:161:ARG:HE	1:B:266:LEU:HA	1.84	0.42
1:B:257:SER:HB2	1:B:610:TRP:CE2	2.54	0.42
1:B:499:ASP:O	1:B:502:SER:OG	2.30	0.42
1:A:524:GLN:HB3	1:A:574:VAL:HG11	2.01	0.42
1:B:402:GLU:O	1:B:406:GLU:HG2	2.19	0.42
1:B:435:GLU:OE1	1:B:541:LYS:NZ	2.53	0.42
1:D:336:PRO:HG2	1:D:340:GLN:O	2.19	0.42
1:G:20:THR:OG1	1:G:23:GLU:HG2	2.18	0.42
1:G:491:VAL:HG23	1:G:493:HIS:HD2	1.82	0.42
1:A:152:MET:HG3	1:A:270:MET:HA	2.01	0.42
1:A:245:ARG:HA	1:A:262:LEU:HD21	2.02	0.42
1:B:440:LEU:HD23	1:B:591:LEU:HD11	2.01	0.42
1:G:126:ILE:HG22	1:G:172:VAL:HG13	2.02	0.42
1:A:105:SER:O	1:A:190:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:LEU:HD23	1:D:113:SER:HA	2.01	0.42
1:G:462:MET:HB3	1:G:468:ILE:HG13	2.01	0.42
1:B:259:ILE:HA	1:B:603:PHE:HD2	1.83	0.42
1:G:91:LEU:HD23	1:G:95:LEU:HG	2.02	0.42
1:B:474:MET:HE3	1:B:474:MET:HA	2.02	0.41
1:G:90:ASN:O	1:G:93:VAL:HG22	2.19	0.41
1:A:469:PRO:HB2	1:A:471:ASP:OD1	2.20	0.41
1:B:370:LEU:HB3	1:B:409:SER:HB2	2.02	0.41
1:B:176:LEU:HA	1:B:179:LEU:HD12	2.02	0.41
1:D:91:LEU:O	1:D:95:LEU:HG	2.20	0.41
1:A:52:THR:O	1:A:340:GLN:NE2	2.54	0.41
1:A:55:THR:O	1:A:59:VAL:HG13	2.20	0.41
1:A:408:MET:HE1	1:A:554:LEU:HD21	2.02	0.41
1:D:48:TRP:NE1	1:D:52:THR:HG21	2.35	0.41
1:G:187:LYS:O	1:G:190:MET:HE3	2.21	0.41
1:B:191:ALA:O	1:B:196:TYR:HB2	2.21	0.41
1:D:21:ILE:HG23	1:D:83:TYR:CD1	2.55	0.41
1:G:129:THR:O	1:G:130:GLY:C	2.63	0.41
1:G:135:PRO:HD2	1:G:163:TRP:HE1	1.85	0.41
1:B:86:GLN:H	1:B:86:GLN:HG3	1.57	0.41
1:D:29:LEU:HD21	1:D:97:LEU:HD23	2.01	0.41
1:D:248:LEU:HB3	1:D:256:ILE:CD1	2.49	0.41
1:D:407:ILE:HA	1:D:410:LEU:HD12	2.02	0.41
1:D:81:GLN:H	1:D:81:GLN:HG2	1.72	0.41
1:B:462:MET:HB3	1:B:468:ILE:HG13	2.02	0.41
1:D:77:SER:OG	1:D:104:GLY:N	2.52	0.41
1:D:144:LEU:HD13	1:D:168:TRP:CE2	2.54	0.41
1:A:50:TYR:CD2	1:A:59:VAL:HG12	2.56	0.41
1:A:56:GLU:HA	1:A:59:VAL:CG1	2.50	0.41
1:B:443:ALA:HA	1:B:447:VAL:HG13	2.03	0.41
1:D:44:SER:HB2	2:F:90:ASN:ND2	2.36	0.41
1:D:200:GLY:O	1:D:204:ARG:HG3	2.21	0.41
1:G:20:THR:O	1:G:24:GLN:HG3	2.21	0.41
1:D:203:TRP:HH2	1:D:460:ARG:NH2	2.17	0.41
1:D:261:CYS:HB2	1:D:488:VAL:HB	2.03	0.41
1:A:53:ASN:OD1	1:A:340:GLN:HG3	2.21	0.40
1:A:294:THR:HG23	1:A:364:VAL:O	2.21	0.40
1:B:494:ASP:OD1	1:B:496:THR:OG1	2.38	0.40
1:D:166:GLU:OE1	1:D:491:VAL:HG21	2.21	0.40
2:E:85:GLU:HA	2:E:86:PRO:HD3	1.83	0.40
1:A:374:HIS:HE2	1:A:402:GLU:CD	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:MET:HG3	1:B:270:MET:HA	2.03	0.40
1:D:90:ASN:HB2	1:D:93:VAL:HG22	2.03	0.40
1:A:430:GLU:CD	1:A:430:GLU:H	2.30	0.40
1:G:36:ALA:O	1:G:40:PHE:HB3	2.22	0.40
1:G:127:TYR:CE2	1:G:168:TRP:HZ2	2.40	0.40
1:A:97:LEU:O	1:A:101:GLN:HG3	2.21	0.40
1:D:60:GLN:HE21	1:D:64:ASN:ND2	2.19	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:195:HIS:O	1:D:195:HIS:O[2_445]	1.64	0.56

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	596/609 (98%)	577 (97%)	17 (3%)	2 (0%)	36	50
1	B	594/609 (98%)	570 (96%)	22 (4%)	2 (0%)	36	50
1	D	593/609 (97%)	573 (97%)	17 (3%)	3 (0%)	24	37
1	G	594/609 (98%)	569 (96%)	23 (4%)	2 (0%)	36	50
2	C	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	E	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	F	12/14 (86%)	7 (58%)	4 (33%)	1 (8%)	0	0
2	H	12/14 (86%)	9 (75%)	3 (25%)	0	100	100
All	All	2425/2492 (97%)	2327 (96%)	88 (4%)	10 (0%)	30	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	137	ASN
1	A	107	VAL
2	F	84	CYS
1	G	130	GLY
1	D	147	GLY
1	B	147	GLY
1	D	22	GLU
1	D	195	HIS
1	A	364	VAL
1	B	107	VAL

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	528/538 (98%)	491 (93%)	37 (7%)	14	24
1	B	526/538 (98%)	490 (93%)	36 (7%)	14	25
1	D	525/538 (98%)	503 (96%)	22 (4%)	26	45
1	G	526/538 (98%)	487 (93%)	39 (7%)	13	22
2	C	11/11 (100%)	11 (100%)	0	100	100
2	E	11/11 (100%)	10 (91%)	1 (9%)	9	14
2	F	11/11 (100%)	11 (100%)	0	100	100
2	H	11/11 (100%)	11 (100%)	0	100	100
All	All	2149/2196 (98%)	2014 (94%)	135 (6%)	16	29

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	29	LEU
1	A	37	GLU
1	A	56	GLU
1	A	57	GLU
1	A	59	VAL

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Mol	Chain	Res	Type
1	A	62	MET
1	A	86	GLN
1	A	94	LYS
1	A	126	ILE
1	A	140	GLU
1	A	190	MET
1	A	192	ARG
1	A	283	VAL
1	A	287	GLN
1	A	305	GLN
1	A	309	LYS
1	A	334	THR
1	A	358	ILE
1	A	401	HIS
1	A	409	SER
1	A	424	LEU
1	A	427	ASP
1	A	430	GLU
1	A	447	VAL
1	A	455	MET
1	A	482	ARG
1	A	513	ILE
1	A	558	LEU
1	A	568	LEU
1	A	573	VAL
1	A	581	VAL
1	A	582	ARG
1	A	584	LEU
1	A	595	LEU
1	A	602	SER
1	A	611	SER
1	B	26	LYS
1	B	35	GLU
1	B	60	GLN
1	B	75	GLU
1	B	82	MET
1	B	86	GLN
1	B	88	ILE
1	B	108	LEU
1	B	113	SER
1	B	137	ASN
1	B	185	VAL

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Mol	Chain	Res	Type
1	B	192	ARG
1	B	194	ASN
1	B	197	GLU
1	B	227	GLU
1	B	269	ASP
1	B	283	VAL
1	B	287	GLN
1	B	401	HIS
1	B	424	LEU
1	B	427	ASP
1	B	430	GLU
1	B	434	THR
1	B	447	VAL
1	B	455	MET
1	B	472	GLN
1	B	476	LYS
1	B	491	VAL
1	B	507	SER
1	B	558	LEU
1	B	568	LEU
1	B	572	ASN
1	B	573	VAL
1	B	584	LEU
1	B	595	LEU
1	B	611	SER
1	D	26	LYS
1	D	37	GLU
1	D	73	LEU
1	D	86	GLN
1	D	109	SER
1	D	129	THR
1	D	175	GLN
1	D	185	VAL
1	D	283	VAL
1	D	305	GLN
1	D	338	ASN
1	D	401	HIS
1	D	441	LYS
1	D	447	VAL
1	D	460	ARG
1	D	552	GLN
1	D	572	ASN

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Mol	Chain	Res	Type
1	D	573	VAL
1	D	574	VAL
1	D	584	LEU
1	D	595	LEU
1	D	600	LYS
2	E	85	GLU
1	G	20	THR
1	G	31	LYS
1	G	35	GLU
1	G	38	ASP
1	G	59	VAL
1	G	86	GLN
1	G	87	GLU
1	G	88	ILE
1	G	91	LEU
1	G	133	CYS
1	G	150	GLU
1	G	171	GLU
1	G	175	GLN
1	G	185	VAL
1	G	190	MET
1	G	234	LYS
1	G	238	GLU
1	G	245	ARG
1	G	271	TRP
1	G	305	GLN
1	G	309	LYS
1	G	329	GLU
1	G	334	THR
1	G	401	HIS
1	G	411	SER
1	G	424	LEU
1	G	430	GLU
1	G	432	ASN
1	G	447	VAL
1	G	455	MET
1	G	460	ARG
1	G	470	LYS
1	G	522	GLN
1	G	536	GLU
1	G	573	VAL
1	G	574	VAL

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Mol	Chain	Res	Type
1	G	581	VAL
1	G	586	ASN
1	G	595	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	60	GLN
1	A	63	ASN
1	A	76	GLN
1	A	86	GLN
1	A	96	GLN
1	A	98	GLN
1	A	103	ASN
1	A	117	ASN
1	A	149	ASN
1	A	194	ASN
1	A	345	HIS
1	A	442	GLN
1	A	540	HIS
1	A	572	ASN
1	A	586	ASN
1	B	61	ASN
1	B	86	GLN
1	B	117	ASN
1	B	134	ASN
1	B	149	ASN
1	B	194	ASN
1	B	287	GLN
1	B	322	ASN
1	B	345	HIS
1	B	417	HIS
1	B	442	GLN
1	B	552	GLN
1	B	556	ASN
1	B	601	ASN
1	D	33	ASN
1	D	34	HIS
1	D	51	ASN
1	D	60	GLN
1	D	64	ASN

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Mol	Chain	Res	Type
1	D	96	GLN
1	D	139	GLN
1	D	322	ASN
1	D	345	HIS
1	D	417	HIS
1	D	442	GLN
1	D	472	GLN
1	D	552	GLN
1	D	599	ASN
1	D	601	ASN
2	F	90	ASN
1	G	42	GLN
1	G	60	GLN
1	G	76	GLN
1	G	86	GLN
1	G	149	ASN
1	G	194	ASN
1	G	221	GLN
1	G	239	HIS
1	G	417	HIS
1	G	442	GLN
1	G	540	HIS
1	G	556	ASN
1	G	572	ASN
1	G	586	ASN
1	G	599	ASN
1	G	601	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	596/609 (97%)	0.54	25 (4%)	40	36	24, 51, 80, 96	2 (0%)
1	B	596/609 (97%)	0.54	19 (3%)	50	46	36, 52, 79, 101	0
1	D	595/609 (97%)	1.00	56 (9%)	14	11	41, 62, 102, 124	0
1	G	595/609 (97%)	0.77	40 (6%)	24	20	25, 56, 83, 100	1 (0%)
2	C	14/14 (100%)	0.99	3 (21%)	2	2	44, 53, 58, 65	0
2	E	14/14 (100%)	0.98	2 (14%)	6	5	45, 54, 58, 64	0
2	F	14/14 (100%)	0.62	2 (14%)	6	5	53, 57, 63, 68	0
2	H	14/14 (100%)	1.03	2 (14%)	6	5	51, 53, 61, 66	0
All	All	2438/2492 (97%)	0.72	149 (6%)	27	23	24, 54, 86, 124	3 (0%)

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	195	HIS	6.8
1	D	105	SER	6.6
1	D	107	VAL	6.1
1	A	105	SER	5.3
1	D	108	LEU	4.8
1	D	104	GLY	4.8
1	D	106	SER	4.5
1	D	194	ASN	4.2
1	D	92	THR	4.2
1	D	21	ILE	4.1
1	G	107	VAL	3.9
2	E	96	GLY	3.9
1	G	103	ASN	3.9
1	A	107	VAL	3.8
1	G	339	VAL	3.8
1	G	105	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	103	ASN	3.7
1	B	339	VAL	3.7
1	G	20	THR	3.6
1	B	107	VAL	3.6
1	D	426	PRO	3.6
1	D	202	TYR	3.5
2	C	96	GLY	3.5
1	D	207	TYR	3.4
1	D	109	SER	3.3
1	G	584	LEU	3.3
1	A	343	VAL	3.3
1	D	85	LEU	3.2
1	D	91	LEU	3.1
1	G	345	HIS	3.1
1	D	390	PHE	3.0
1	D	396	ALA	3.0
1	G	36	ALA	3.0
1	D	84	PRO	3.0
1	D	138	PRO	3.0
1	D	515	TYR	2.9
1	D	211	GLY	2.9
1	D	614	ALA	2.9
2	C	83	ALA	2.9
2	F	96	GLY	2.9
1	G	271	TRP	2.9
1	D	428	PHE	2.8
1	A	274	PHE	2.8
1	D	566	TRP	2.8
1	G	202	TYR	2.8
1	D	516	TYR	2.8
1	G	108	LEU	2.8
2	H	88	GLY	2.7
1	A	126	ILE	2.7
1	A	103	ASN	2.7
1	D	344	CYS	2.7
1	A	342	ALA	2.7
1	G	106	SER	2.7
1	A	339	VAL	2.6
1	D	93	VAL	2.6
1	G	21	ILE	2.6
1	G	190	MET	2.6
1	G	135	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	135	PRO	2.5
1	D	522	GLN	2.5
1	D	20	THR	2.5
1	G	291	ILE	2.5
1	G	142	LEU	2.5
1	A	290	ASN	2.5
1	G	65	ALA	2.5
1	B	345	HIS	2.5
1	A	102	GLN	2.5
1	G	54	ILE	2.5
1	A	55	THR	2.4
1	A	54	ILE	2.4
1	G	338	ASN	2.4
2	F	83	ALA	2.4
1	G	104	GLY	2.4
1	G	141	CYS	2.4
1	D	400	PHE	2.4
1	A	82	MET	2.4
1	A	295	ASP	2.4
1	G	138	PRO	2.4
1	B	344	CYS	2.4
1	D	275	TRP	2.4
2	H	96	GLY	2.4
1	B	19	SER	2.4
1	A	132	VAL	2.4
1	G	100	LEU	2.3
1	D	135	PRO	2.3
1	D	88	ILE	2.3
1	D	24	GLN	2.3
1	G	274	PHE	2.3
1	G	428	PHE	2.3
1	A	142	LEU	2.3
1	B	436	ILE	2.3
1	D	79	LEU	2.3
1	D	419	LYS	2.3
1	G	82	MET	2.3
1	D	293	VAL	2.3
1	B	103	ASN	2.2
1	A	135	PRO	2.2
1	A	104	GLY	2.2
1	A	86	GLN	2.2
1	A	291	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	324	THR	2.2
1	D	576	ALA	2.2
2	C	95	SER	2.2
1	D	142	LEU	2.2
1	G	85	LEU	2.2
1	G	53	ASN	2.2
2	E	88	GLY	2.2
1	D	102	GLN	2.2
1	G	342	ALA	2.2
1	D	521	TYR	2.2
1	B	126	ILE	2.2
1	D	291	ILE	2.2
1	D	212	VAL	2.2
1	A	62	MET	2.2
1	G	400	PHE	2.2
1	G	515	TYR	2.1
1	A	194	ASN	2.1
1	A	432	ASN	2.1
1	D	133	CYS	2.1
1	B	105	SER	2.1
1	B	21	ILE	2.1
1	D	143	LEU	2.1
1	D	436	ILE	2.1
1	D	539	LEU	2.1
1	B	435	GLU	2.1
1	A	138	PRO	2.1
1	B	274	PHE	2.1
1	B	469	PRO	2.1
1	D	65	ALA	2.1
1	G	39	LEU	2.1
1	D	321	PRO	2.1
1	D	452	PHE	2.1
1	D	86	GLN	2.1
1	G	93	VAL	2.1
1	D	40	PHE	2.1
1	A	129	THR	2.0
1	B	20	THR	2.0
1	G	426	PRO	2.0
1	B	202	TYR	2.0
1	G	279	TYR	2.0
1	D	32	PHE	2.0
1	D	588	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	270	MET	2.0
1	G	449	THR	2.0
1	B	614	ALA	2.0
1	G	614	ALA	2.0
1	G	139	GLN	2.0
1	B	142	LEU	2.0
1	B	450	LEU	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.