



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:26 AM UTC

PDB ID : 2W2W / pdb_00002w2w
Title : PLCg2 Split Pleckstrin Homology (PH) Domain
Authors : Opaleye, O.; Bunney, T.D.; Roe, S.M.; Pearl, L.H.
Deposited on : 2008-11-04
Resolution : 2.80 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

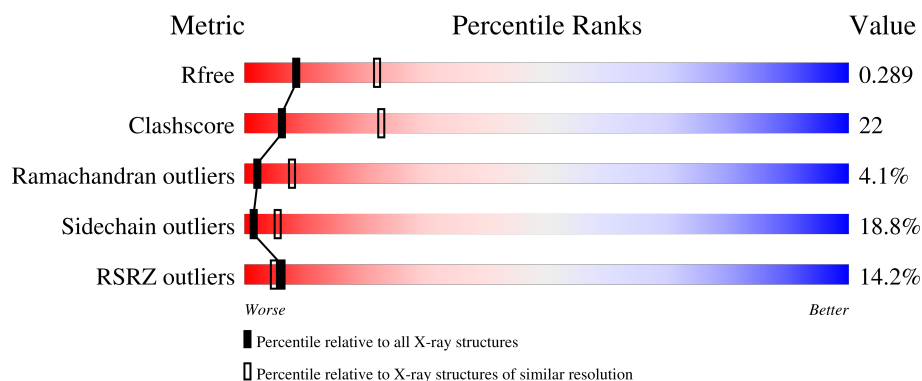
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	124	15% 48% 29% 8% 13%
1	B	124	6% 50% 22% 15% 13%
1	C	124	7% 54% 24% 6% 15%
1	D	124	6% 44% 26% 10% 20%
1	E	124	10% 52% 22% 8% 19%

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Mol	Chain	Length	Quality of chain
1	F	124	8% 48% 24% 12% • 14%
1	G	124	12% 47% 23% 11% • 19%
1	H	124	10% 49% 21% 6% 24%
1	I	124	10% 46% 24% 7% • 22%
1	J	124	8% 44% 25% 6% 24%
1	K	124	11% 50% 21% 8% 21%
1	L	124	30% 36% 19% • • 40%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9249 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 1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODIESTERASE GAMMA-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			858	548	138	168	4			
1	B	108	Total	C	N	O	S	0	0	0
			828	529	133	162	4			
1	C	105	Total	C	N	O	S	0	0	0
			817	525	131	158	3			
1	D	99	Total	C	N	O	S	0	0	0
			776	498	126	149	3			
1	E	101	Total	C	N	O	S	0	0	0
			785	506	125	151	3			
1	F	107	Total	C	N	O	S	0	0	0
			819	527	131	157	4			
1	G	101	Total	C	N	O	S	0	0	0
			786	507	125	151	3			
1	H	94	Total	C	N	O	S	0	0	0
			735	474	116	142	3			
1	I	97	Total	C	N	O	S	0	0	0
			757	486	119	149	3			
1	J	94	Total	C	N	O	S	0	0	0
			740	477	117	143	3			
1	K	98	Total	C	N	O	S	0	0	0
			763	492	121	147	3			
1	L	74	Total	C	N	O	S	0	0	0
			585	379	95	109	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	PHE	TYR	engineered mutation	UNP P16885
B	26	PHE	TYR	engineered mutation	UNP P16885
C	26	PHE	TYR	engineered mutation	UNP P16885
D	26	PHE	TYR	engineered mutation	UNP P16885

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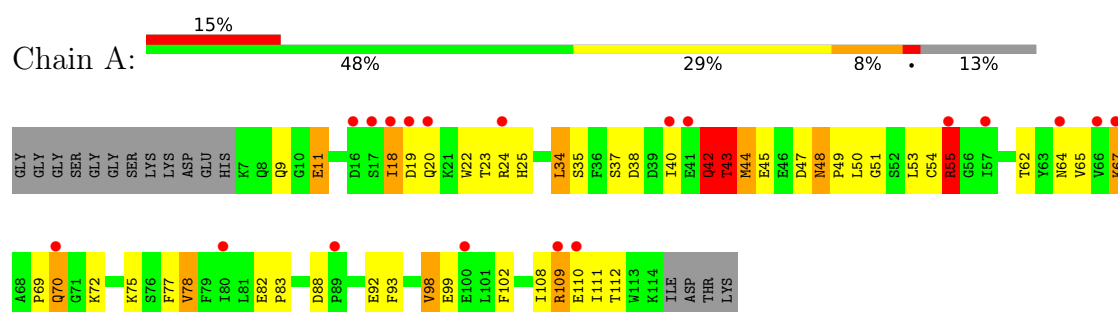
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Chain	Residue	Modelled	Actual	Comment	Reference
E	26	PHE	TYR	engineered mutation	UNP P16885
F	26	PHE	TYR	engineered mutation	UNP P16885
G	26	PHE	TYR	engineered mutation	UNP P16885
H	26	PHE	TYR	engineered mutation	UNP P16885
I	26	PHE	TYR	engineered mutation	UNP P16885
J	26	PHE	TYR	engineered mutation	UNP P16885
K	26	PHE	TYR	engineered mutation	UNP P16885
L	26	PHE	TYR	engineered mutation	UNP P16885
A	88	ASP	TYR	conflict	UNP P16885
B	88	ASP	TYR	conflict	UNP P16885
C	88	ASP	TYR	conflict	UNP P16885
D	88	ASP	TYR	conflict	UNP P16885
E	88	ASP	TYR	conflict	UNP P16885
F	88	ASP	TYR	conflict	UNP P16885
G	88	ASP	TYR	conflict	UNP P16885
H	88	ASP	TYR	conflict	UNP P16885
I	88	ASP	TYR	conflict	UNP P16885
J	88	ASP	TYR	conflict	UNP P16885
K	88	ASP	TYR	conflict	UNP P16885
L	88	ASP	TYR	conflict	UNP P16885
A	97	LYS	ARG	conflict	UNP P16885
B	97	LYS	ARG	conflict	UNP P16885
C	97	LYS	ARG	conflict	UNP P16885
D	97	LYS	ARG	conflict	UNP P16885
E	97	LYS	ARG	conflict	UNP P16885
F	97	LYS	ARG	conflict	UNP P16885
G	97	LYS	ARG	conflict	UNP P16885
H	97	LYS	ARG	conflict	UNP P16885
I	97	LYS	ARG	conflict	UNP P16885
J	97	LYS	ARG	conflict	UNP P16885
K	97	LYS	ARG	conflict	UNP P16885
L	97	LYS	ARG	conflict	UNP P16885

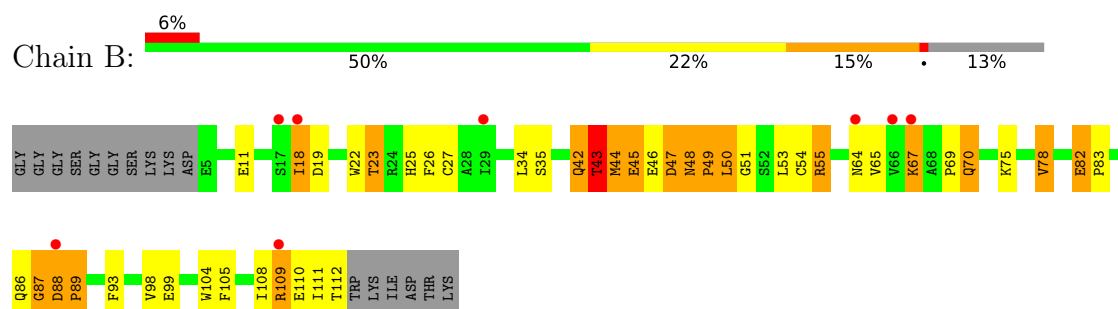
3 Residue-property plots [i](#)

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.

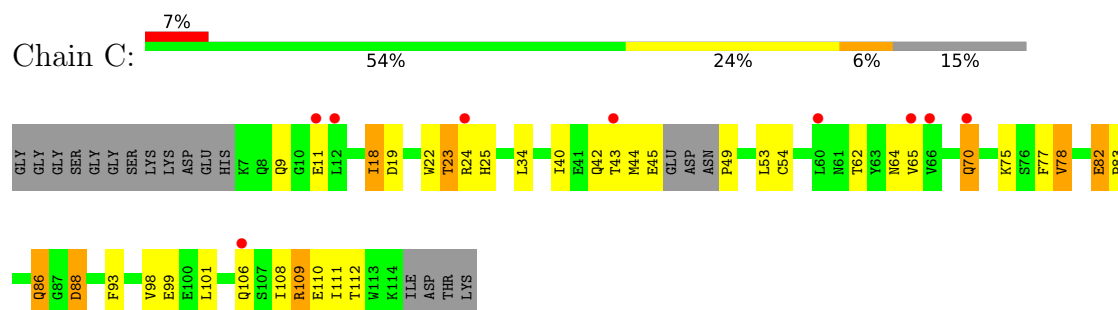
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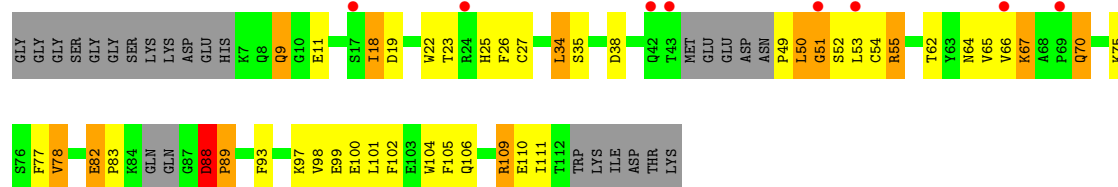
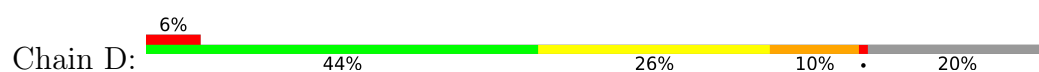
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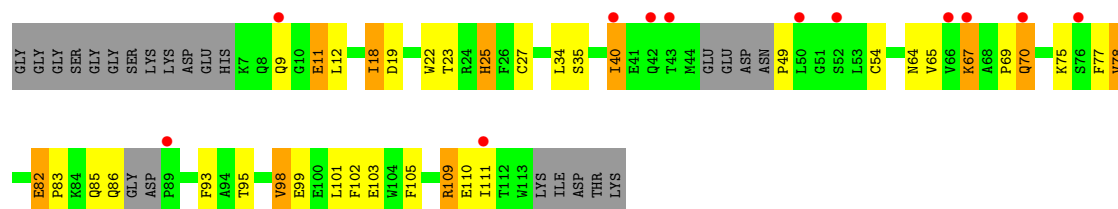
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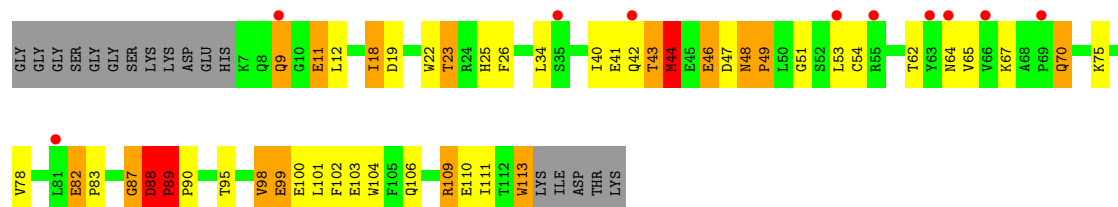
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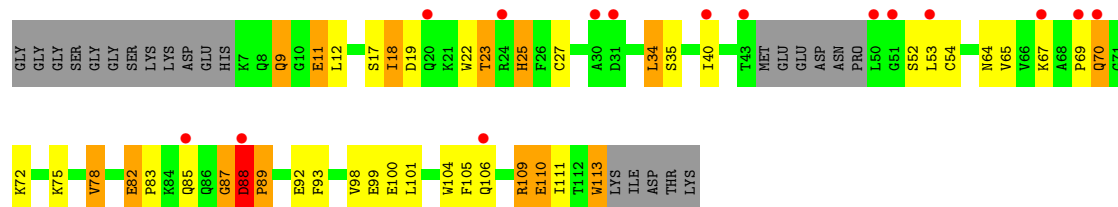
- Molecule 1: 1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODIESTERASE GAMMA-2



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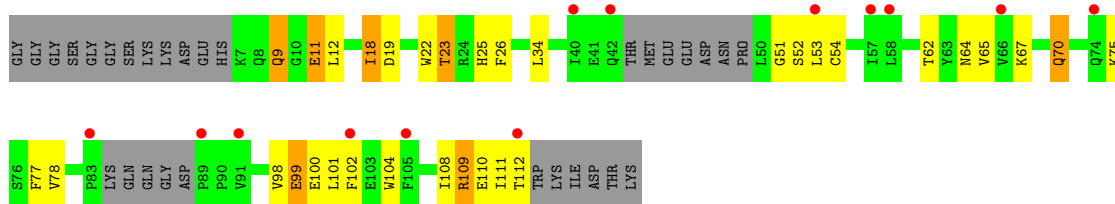


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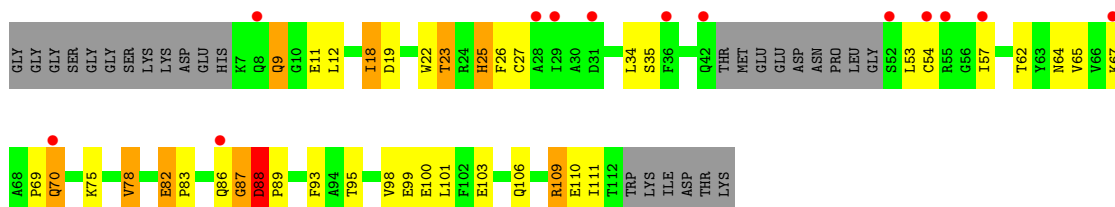


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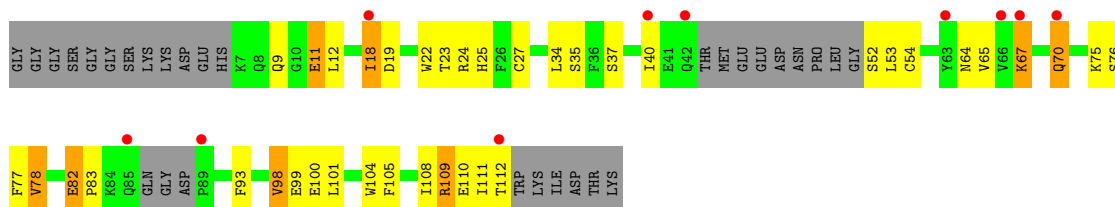




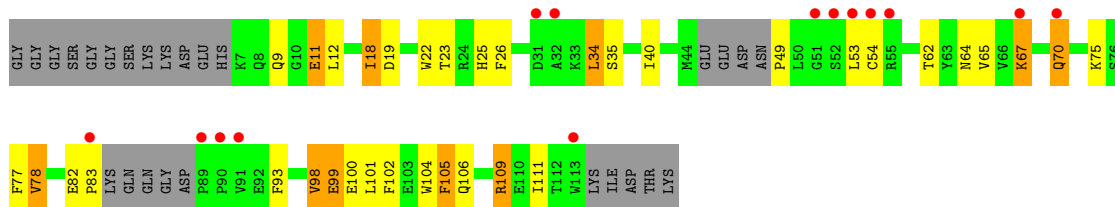
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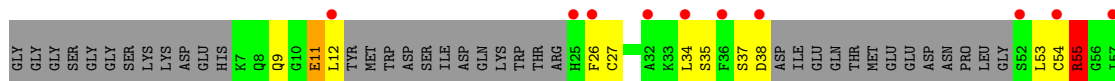
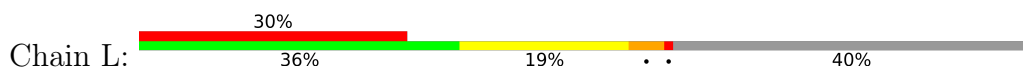
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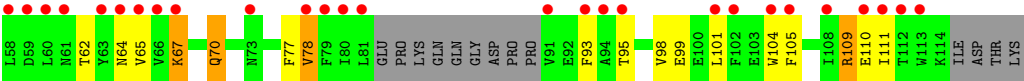


• Molecule 1: 1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODIESTERASE GAMMA-2



• Molecule 1: 1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODIESTERASE GAMMA-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.22Å 106.02Å 194.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.05 – 2.80 97.05 – 3.30	Depositor EDS
% Data completeness (in resolution range)	88.9 (97.05-2.80) 98.0 (97.05-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.303 , 0.352 (Not available) , 0.289	Depositor DCC
R_{free} test set	1462 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	91.4	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9249	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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	0.79	0/880	1.12	10/1198 (0.8%)
1	B	0.64	0/848	0.98	6/1155 (0.5%)
1	C	0.64	0/838	0.95	4/1141 (0.4%)
1	D	0.63	0/793	1.07	7/1074 (0.7%)
1	E	0.55	0/804	0.88	3/1094 (0.3%)
1	F	0.68	0/841	1.23	6/1149 (0.5%)
1	G	0.61	0/806	1.26	4/1097 (0.4%)
1	H	0.48	0/752	0.78	0/1021
1	I	0.52	0/775	0.82	4/1055 (0.4%)
1	J	0.49	0/757	0.82	2/1028 (0.2%)
1	K	0.53	0/781	0.85	0/1060
1	L	0.57	0/595	0.91	3/802 (0.4%)
All	All	0.60	0/9470	0.99	49/12874 (0.4%)

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	1
1	B	0	1
1	F	0	2
All	All	0	4

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	88	ASP	CA-C-N	-20.77	98.99	120.38
1	G	88	ASP	C-N-CA	-20.77	98.99	120.38
1	F	88	ASP	CA-C-N	-18.73	101.08	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	88	ASP	C-N-CA	-18.73	101.08	120.38
1	D	88	ASP	CA-C-N	11.69	132.42	120.38
1	D	88	ASP	C-N-CA	11.69	132.42	120.38
1	C	88	ASP	CA-C-N	-10.50	109.57	120.38
1	C	88	ASP	C-N-CA	-10.50	109.57	120.38
1	A	50	LEU	N-CA-C	-10.45	100.53	113.28
1	A	88	ASP	CA-C-N	8.96	129.61	120.38
1	A	88	ASP	C-N-CA	8.96	129.61	120.38
1	D	49	PRO	N-CA-CB	7.99	111.79	103.00
1	L	55	ARG	NE-CZ-NH2	7.64	126.08	119.20
1	A	42	GLN	CB-CA-C	-7.10	97.75	111.03
1	L	55	ARG	NE-CZ-NH1	-7.10	114.40	121.50
1	A	55	ARG	NE-CZ-NH2	6.97	125.47	119.20
1	A	55	ARG	NE-CZ-NH1	-6.91	114.59	121.50
1	E	49	PRO	N-CA-CB	6.39	110.03	103.00
1	F	44	MET	N-CA-C	6.15	123.89	110.80
1	B	50	LEU	N-CA-C	-6.14	103.13	111.55
1	A	43	THR	N-CA-C	-5.92	98.19	110.80
1	A	44	MET	N-CA-C	5.88	117.49	111.14
1	D	82	GLU	CA-C-N	5.81	126.00	120.31
1	D	82	GLU	C-N-CA	5.81	126.00	120.31
1	G	82	GLU	CA-C-N	5.79	126.25	120.52
1	G	82	GLU	C-N-CA	5.79	126.25	120.52
1	D	88	ASP	C-N-CD	-5.72	101.55	125.00
1	F	89	PRO	N-CA-C	5.64	117.58	110.70
1	B	82	GLU	CA-C-N	5.52	125.98	120.52
1	B	82	GLU	C-N-CA	5.52	125.98	120.52
1	F	82	GLU	CA-C-N	5.50	125.70	120.31
1	F	82	GLU	C-N-CA	5.50	125.70	120.31
1	L	55	ARG	CD-NE-CZ	5.50	132.10	124.40
1	A	48	ASN	CA-C-N	5.47	127.35	121.00
1	A	48	ASN	C-N-CA	5.47	127.35	121.00
1	B	55	ARG	NE-CZ-NH2	-5.36	114.37	119.20
1	C	82	GLU	CA-C-N	5.36	125.56	120.31
1	C	82	GLU	C-N-CA	5.36	125.56	120.31
1	E	82	GLU	CA-C-N	5.31	125.77	120.14
1	E	82	GLU	C-N-CA	5.31	125.77	120.14
1	J	82	GLU	CA-C-N	5.28	126.44	119.84
1	J	82	GLU	C-N-CA	5.28	126.44	119.84
1	I	88	ASP	CA-C-N	5.28	125.82	120.38
1	I	88	ASP	C-N-CA	5.28	125.82	120.38
1	B	87	GLY	N-CA-C	-5.17	105.14	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	82	GLU	CA-C-N	5.14	125.34	120.31
1	I	82	GLU	C-N-CA	5.14	125.34	120.31
1	D	55	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	B	43	THR	N-CA-C	5.01	121.47	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	GLN	Mainchain
1	B	42	GLN	Peptide
1	F	42	GLN	Peptide
1	F	88	ASP	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	858	0	782	52	1
1	B	828	0	741	44	0
1	C	817	0	735	25	1
1	D	776	0	713	67	0
1	E	785	0	701	29	0
1	F	819	0	727	57	0
1	G	786	0	706	51	1
1	H	735	0	668	26	0
1	I	757	0	680	25	1
1	J	740	0	673	56	0
1	K	763	0	698	46	0
1	L	585	0	548	26	0
All	All	9249	0	8372	395	2

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 22.

All (395) 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:B:89:PRO:HG2	1:D:70:GLN:O	1.37	1.21
1:G:18:ILE:HD11	1:K:101:LEU:HD23	1.28	1.15
1:D:18:ILE:HG12	1:J:67:LYS:HZ2	1.13	1.12
1:D:18:ILE:HD13	1:J:67:LYS:HE3	1.35	1.08
1:D:18:ILE:HD11	1:J:67:LYS:HD3	1.37	1.06
1:D:18:ILE:CD1	1:J:67:LYS:HD3	1.86	1.05
1:B:44:MET:HA	1:B:45:GLU:HB2	1.38	1.02
1:B:18:ILE:HG21	1:D:67:LYS:HE3	1.36	1.02
1:A:70:GLN:HE21	1:A:70:GLN:H	1.01	1.00
1:D:18:ILE:HD13	1:J:67:LYS:CE	1.92	0.99
1:L:70:GLN:H	1:L:70:GLN:HE21	1.05	0.98
1:D:18:ILE:CD1	1:J:67:LYS:CD	2.43	0.97
1:H:70:GLN:H	1:H:70:GLN:HE21	0.97	0.96
1:G:18:ILE:HG12	1:K:67:LYS:HD2	1.47	0.96
1:I:70:GLN:H	1:I:70:GLN:HE21	0.99	0.96
1:D:70:GLN:H	1:D:70:GLN:HE21	0.99	0.95
1:F:70:GLN:H	1:F:70:GLN:HE21	1.00	0.95
1:D:18:ILE:HG12	1:J:67:LYS:NZ	1.83	0.93
1:B:44:MET:SD	1:C:53:LEU:HD21	2.09	0.93
1:B:70:GLN:H	1:B:70:GLN:HE21	0.94	0.93
1:C:70:GLN:H	1:C:70:GLN:HE21	0.93	0.92
1:G:18:ILE:HB	1:K:67:LYS:HE3	1.50	0.92
1:J:70:GLN:H	1:J:70:GLN:HE21	1.06	0.92
1:D:18:ILE:HD11	1:J:67:LYS:CD	2.01	0.91
1:E:70:GLN:H	1:E:70:GLN:HE21	1.05	0.91
1:G:53:LEU:HD13	1:L:37:SER:OG	1.72	0.90
1:K:70:GLN:H	1:K:70:GLN:HE21	0.93	0.90
1:C:70:GLN:H	1:C:70:GLN:NE2	1.71	0.89
1:G:70:GLN:H	1:G:70:GLN:HE21	0.94	0.88
1:D:18:ILE:CG1	1:J:67:LYS:NZ	2.37	0.87
1:D:18:ILE:HB	1:J:67:LYS:HZ1	1.39	0.87
1:D:18:ILE:CD1	1:J:67:LYS:CE	2.52	0.87
1:K:70:GLN:H	1:K:70:GLN:NE2	1.73	0.87
1:A:11:GLU:OE2	1:F:9:GLN:OE1	1.93	0.86
1:G:70:GLN:H	1:G:70:GLN:NE2	1.73	0.84
1:C:70:GLN:HE21	1:C:70:GLN:N	1.75	0.84
1:L:12:LEU:HD21	1:L:104:TRP:NE1	1.91	0.84
1:K:70:GLN:HE21	1:K:70:GLN:N	1.76	0.84
1:D:18:ILE:CG1	1:J:67:LYS:HZ2	1.87	0.84
1:G:52:SER:C	1:L:53:LEU:HB2	2.03	0.83
1:B:70:GLN:H	1:B:70:GLN:NE2	1.75	0.83
1:B:48:ASN:CB	1:B:49:PRO:HA	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:GLN:H	1:H:70:GLN:NE2	1.76	0.82
1:H:53:LEU:HD11	1:J:40:ILE:HG22	1.61	0.82
1:D:70:GLN:H	1:D:70:GLN:NE2	1.77	0.81
1:D:97:LYS:HD3	1:D:100:GLU:OE2	1.80	0.81
1:B:70:GLN:HE21	1:B:70:GLN:N	1.78	0.80
1:D:18:ILE:CG1	1:J:67:LYS:HD3	2.10	0.80
1:I:70:GLN:H	1:I:70:GLN:NE2	1.78	0.80
1:A:53:LEU:HD21	1:F:44:MET:SD	2.22	0.80
1:A:70:GLN:H	1:A:70:GLN:NE2	1.80	0.80
1:G:18:ILE:CB	1:K:67:LYS:HE3	2.12	0.79
1:B:89:PRO:CG	1:D:70:GLN:O	2.28	0.79
1:J:105:PHE:HE2	1:J:109:ARG:HD3	1.47	0.79
1:A:42:GLN:C	1:A:44:MET:N	2.35	0.79
1:F:70:GLN:H	1:F:70:GLN:NE2	1.79	0.78
1:F:44:MET:HE2	1:F:44:MET:H	1.48	0.78
1:H:70:GLN:HE21	1:H:70:GLN:N	1.79	0.78
1:B:18:ILE:CG2	1:D:67:LYS:HE3	2.13	0.77
1:D:50:LEU:HA	1:D:51:GLY:O	1.85	0.77
1:G:70:GLN:HE21	1:G:70:GLN:N	1.77	0.76
1:F:70:GLN:HE21	1:F:70:GLN:N	1.82	0.75
1:I:70:GLN:HE21	1:I:70:GLN:N	1.82	0.75
1:K:67:LYS:HD3	1:K:105:PHE:HD1	1.51	0.75
1:K:105:PHE:HE2	1:K:109:ARG:HD3	1.51	0.74
1:A:69:PRO:O	1:D:106:GLN:CD	2.30	0.74
1:A:43:THR:HG23	1:A:51:GLY:HA3	1.70	0.73
1:D:70:GLN:HE21	1:D:70:GLN:N	1.81	0.73
1:G:18:ILE:CD1	1:K:101:LEU:HD23	2.13	0.73
1:D:18:ILE:HB	1:J:67:LYS:NZ	2.02	0.73
1:E:70:GLN:H	1:E:70:GLN:NE2	1.85	0.73
1:B:43:THR:O	1:B:44:MET:HG2	1.88	0.72
1:L:70:GLN:H	1:L:70:GLN:NE2	1.84	0.71
1:A:42:GLN:O	1:A:43:THR:C	2.30	0.71
1:C:18:ILE:HG22	1:C:19:ASP:N	2.06	0.71
1:D:18:ILE:CB	1:J:67:LYS:HZ1	2.03	0.70
1:I:57:ILE:HD12	1:K:49:PRO:HG3	1.73	0.70
1:B:44:MET:CA	1:B:45:GLU:HB2	2.17	0.70
1:D:18:ILE:CB	1:J:67:LYS:NZ	2.53	0.70
1:J:70:GLN:HE21	1:J:70:GLN:N	1.87	0.70
1:D:18:ILE:HG22	1:D:19:ASP:N	2.05	0.69
1:K:67:LYS:HD3	1:K:105:PHE:CD1	2.27	0.69
1:F:43:THR:HG23	1:F:43:THR:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:ILE:HG22	1:G:19:ASP:N	2.07	0.69
1:F:41:GLU:O	1:F:43:THR:HB	1.92	0.69
1:B:44:MET:SD	1:C:53:LEU:CD2	2.81	0.68
1:D:88:ASP:O	1:D:89:PRO:O	2.11	0.68
1:F:109:ARG:NE	1:F:113:TRP:CH2	2.61	0.68
1:L:70:GLN:HE21	1:L:70:GLN:N	1.87	0.68
1:A:55:ARG:HG3	1:A:55:ARG:O	1.94	0.68
1:J:70:GLN:H	1:J:70:GLN:NE2	1.87	0.67
1:A:18:ILE:HG22	1:A:19:ASP:N	2.09	0.67
1:B:18:ILE:HG22	1:B:19:ASP:N	2.10	0.67
1:F:103:GLU:O	1:F:104:TRP:C	2.38	0.67
1:D:109:ARG:C	1:D:111:ILE:H	2.02	0.67
1:G:87:GLY:HA3	1:G:88:ASP:CB	2.26	0.66
1:D:88:ASP:N	1:J:76:SER:OG	2.28	0.66
1:E:18:ILE:HG22	1:E:19:ASP:N	2.10	0.66
1:D:18:ILE:HG12	1:J:67:LYS:HD3	1.78	0.65
1:K:18:ILE:HG22	1:K:19:ASP:N	2.10	0.65
1:I:18:ILE:HG22	1:I:19:ASP:N	2.10	0.65
1:A:70:GLN:HE21	1:A:70:GLN:N	1.83	0.65
1:A:109:ARG:C	1:A:111:ILE:H	2.05	0.65
1:G:18:ILE:HG12	1:K:67:LYS:CD	2.24	0.64
1:A:53:LEU:HD21	1:F:44:MET:HE1	1.79	0.64
1:F:109:ARG:HE	1:F:113:TRP:HH2	1.45	0.64
1:H:18:ILE:HG22	1:H:19:ASP:N	2.12	0.64
1:A:37:SER:HB2	1:F:53:LEU:HD13	1.79	0.64
1:F:109:ARG:C	1:F:111:ILE:H	2.05	0.64
1:J:18:ILE:HG22	1:J:19:ASP:N	2.13	0.64
1:L:55:ARG:O	1:L:55:ARG:HG3	1.97	0.63
1:E:70:GLN:HE21	1:E:70:GLN:N	1.88	0.63
1:F:18:ILE:HG22	1:F:19:ASP:N	2.12	0.63
1:G:53:LEU:CD1	1:L:37:SER:OG	2.46	0.63
1:H:109:ARG:C	1:H:111:ILE:H	2.06	0.63
1:I:109:ARG:C	1:I:111:ILE:H	2.06	0.63
1:K:109:ARG:C	1:K:111:ILE:H	2.07	0.63
1:B:109:ARG:C	1:B:111:ILE:H	2.08	0.62
1:G:53:LEU:N	1:L:53:LEU:HB2	2.15	0.62
1:D:9:GLN:OE1	1:E:11:GLU:OE2	2.17	0.61
1:J:109:ARG:C	1:J:111:ILE:H	2.07	0.61
1:H:99:GLU:O	1:H:102:PHE:HB3	2.00	0.61
1:L:12:LEU:HD21	1:L:104:TRP:CD1	2.34	0.61
1:C:45:GLU:C	1:C:49:PRO:HG2	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:ARG:C	1:E:111:ILE:H	2.08	0.61
1:G:109:ARG:C	1:G:111:ILE:H	2.06	0.61
1:A:11:GLU:CG	1:F:9:GLN:HE22	2.14	0.60
1:A:43:THR:CG2	1:A:51:GLY:HA3	2.30	0.60
1:A:40:ILE:HD12	1:F:26:PHE:CZ	2.36	0.60
1:G:53:LEU:HD13	1:L:37:SER:CB	2.31	0.60
1:A:67:LYS:HE3	1:A:102:PHE:CZ	2.35	0.60
1:C:109:ARG:C	1:C:111:ILE:H	2.08	0.60
1:A:48:ASN:OD1	1:A:48:ASN:C	2.43	0.60
1:D:18:ILE:HG12	1:J:67:LYS:CD	2.32	0.60
1:A:40:ILE:HD12	1:F:26:PHE:HZ	1.66	0.60
1:B:44:MET:CE	1:C:53:LEU:HD21	2.31	0.60
1:A:53:LEU:HD21	1:F:44:MET:CE	2.31	0.59
1:A:11:GLU:OE2	1:F:9:GLN:CD	2.44	0.59
1:L:67:LYS:HB2	1:L:105:PHE:CE1	2.38	0.59
1:L:109:ARG:C	1:L:111:ILE:H	2.10	0.59
1:L:67:LYS:HB2	1:L:105:PHE:HE1	1.66	0.59
1:F:44:MET:HE2	1:F:44:MET:N	2.18	0.59
1:D:18:ILE:CG1	1:J:67:LYS:CE	2.81	0.58
1:F:44:MET:H	1:F:44:MET:CE	2.16	0.58
1:A:24:ARG:NH2	1:F:9:GLN:OE1	2.26	0.58
1:A:69:PRO:C	1:D:106:GLN:NE2	2.62	0.58
1:F:12:LEU:HD21	1:F:104:TRP:NE1	2.18	0.58
1:D:18:ILE:CG1	1:J:67:LYS:CD	2.80	0.57
1:G:85:GLN:C	1:G:87:GLY:H	2.13	0.57
1:B:26:PHE:CZ	1:C:40:ILE:HD12	2.39	0.57
1:B:69:PRO:O	1:K:106:GLN:CD	2.48	0.56
1:B:26:PHE:HZ	1:C:40:ILE:HD12	1.69	0.56
1:B:49:PRO:HD2	1:B:51:GLY:N	2.20	0.56
1:A:70:GLN:HA	1:D:106:GLN:OE1	2.05	0.56
1:A:11:GLU:CD	1:F:9:GLN:HE22	2.14	0.56
1:H:53:LEU:CD1	1:J:40:ILE:HG22	2.34	0.55
1:D:18:ILE:HG12	1:J:67:LYS:CE	2.37	0.55
1:F:48:ASN:N	1:F:49:PRO:HD3	2.21	0.55
1:K:99:GLU:O	1:K:102:PHE:HB3	2.07	0.55
1:G:69:PRO:HD2	1:G:70:GLN:HE22	1.71	0.54
1:I:22:TRP:NE1	1:I:75:LYS:HG2	2.22	0.54
1:A:67:LYS:HE2	1:D:102:PHE:CE1	2.43	0.54
1:B:55:ARG:HD2	1:D:66:VAL:HG11	1.88	0.54
1:G:110:GLU:O	1:G:110:GLU:HG2	2.08	0.54
1:G:12:LEU:HD21	1:G:104:TRP:NE1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLN:O	1:A:45:GLU:N	2.41	0.54
1:J:22:TRP:NE1	1:J:75:LYS:HG2	2.23	0.54
1:K:67:LYS:HB2	1:K:105:PHE:CE1	2.42	0.54
1:J:23:THR:O	1:J:25:HIS:HD2	1.92	0.53
1:B:48:ASN:CB	1:B:49:PRO:CA	2.84	0.53
1:H:22:TRP:NE1	1:H:75:LYS:HG2	2.24	0.53
1:A:37:SER:CB	1:F:53:LEU:HD13	2.37	0.53
1:F:102:PHE:C	1:F:102:PHE:CD2	2.87	0.53
1:A:38:ASP:OD1	1:A:55:ARG:HD2	2.08	0.53
1:B:67:LYS:HE2	1:K:102:PHE:CE1	2.44	0.53
1:C:42:GLN:C	1:C:44:MET:H	2.18	0.52
1:I:87:GLY:O	1:I:88:ASP:C	2.51	0.52
1:K:105:PHE:HD2	1:K:105:PHE:O	1.92	0.52
1:J:11:GLU:O	1:J:12:LEU:HD23	2.09	0.52
1:B:46:GLU:O	1:B:47:ASP:C	2.51	0.52
1:F:109:ARG:HG2	1:F:113:TRP:CZ3	2.44	0.52
1:D:83:PRO:CG	1:D:88:ASP:O	2.58	0.52
1:A:40:ILE:CD1	1:F:26:PHE:HZ	2.22	0.52
1:A:53:LEU:HA	1:F:53:LEU:HB2	1.92	0.52
1:A:42:GLN:HA	1:A:45:GLU:HB2	1.91	0.51
1:C:106:GLN:CD	1:I:69:PRO:O	2.53	0.51
1:A:22:TRP:NE1	1:A:75:LYS:HG2	2.26	0.51
1:G:53:LEU:HD13	1:L:37:SER:HG	1.72	0.51
1:C:22:TRP:NE1	1:C:75:LYS:HG2	2.25	0.51
1:D:9:GLN:HE22	1:E:11:GLU:CG	2.24	0.51
1:A:47:ASP:O	1:A:49:PRO:HD3	2.11	0.50
1:B:44:MET:HA	1:B:45:GLU:CB	2.18	0.50
1:B:88:ASP:CB	1:B:89:PRO:HD3	2.41	0.50
1:D:26:PHE:CZ	1:E:40:ILE:HD12	2.46	0.50
1:D:53:LEU:HD11	1:E:40:ILE:HG22	1.92	0.50
1:D:89:PRO:HG3	1:J:76:SER:O	2.12	0.50
1:A:34:LEU:HD23	1:A:35:SER:N	2.27	0.50
1:G:22:TRP:NE1	1:G:75:LYS:HG2	2.26	0.50
1:G:85:GLN:C	1:G:87:GLY:N	2.68	0.50
1:C:77:PHE:HB3	1:C:101:LEU:HD22	1.94	0.49
1:E:67:LYS:HE2	1:F:102:PHE:CE1	2.47	0.49
1:F:99:GLU:O	1:F:102:PHE:HB3	2.12	0.49
1:B:49:PRO:HD2	1:B:51:GLY:H	1.76	0.49
1:G:18:ILE:CG1	1:K:67:LYS:HD2	2.33	0.49
1:B:55:ARG:NH1	1:D:82:GLU:OE1	2.46	0.49
1:J:104:TRP:O	1:J:105:PHE:C	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:C	1:A:111:ILE:N	2.70	0.49
1:F:109:ARG:C	1:F:111:ILE:N	2.70	0.48
1:L:78:VAL:HB	1:L:93:PHE:O	2.14	0.48
1:D:26:PHE:HZ	1:E:40:ILE:HD12	1.78	0.48
1:H:53:LEU:HD11	1:J:40:ILE:CG2	2.37	0.48
1:E:77:PHE:CE1	1:E:98:VAL:HB	2.48	0.48
1:G:109:ARG:C	1:G:111:ILE:N	2.72	0.48
1:F:46:GLU:O	1:F:49:PRO:HD3	2.14	0.48
1:D:38:ASP:OD2	1:D:51:GLY:HA2	2.14	0.48
1:K:22:TRP:NE1	1:K:75:LYS:HG2	2.28	0.47
1:J:23:THR:O	1:J:25:HIS:CD2	2.67	0.47
1:K:67:LYS:HB2	1:K:105:PHE:HE1	1.78	0.47
1:E:22:TRP:NE1	1:E:75:LYS:HG2	2.29	0.47
1:D:18:ILE:CG2	1:D:19:ASP:N	2.73	0.47
1:L:38:ASP:OD1	1:L:55:ARG:HD2	2.15	0.47
1:B:78:VAL:HB	1:B:93:PHE:O	2.14	0.47
1:E:102:PHE:HE1	1:F:98:VAL:HG22	1.80	0.47
1:D:104:TRP:O	1:D:105:PHE:C	2.57	0.47
1:G:18:ILE:HD12	1:K:98:VAL:HG23	1.97	0.47
1:F:100:GLU:O	1:F:101:LEU:C	2.56	0.47
1:I:109:ARG:C	1:I:111:ILE:N	2.71	0.47
1:A:69:PRO:O	1:D:106:GLN:NE2	2.47	0.47
1:B:46:GLU:O	1:B:47:ASP:O	2.33	0.47
1:B:109:ARG:C	1:B:111:ILE:N	2.73	0.47
1:D:27:CYS:HA	1:D:35:SER:O	2.15	0.47
1:E:67:LYS:HE2	1:F:102:PHE:HE1	1.80	0.46
1:J:109:ARG:C	1:J:111:ILE:N	2.72	0.46
1:K:105:PHE:C	1:K:105:PHE:CD2	2.93	0.46
1:B:22:TRP:NE1	1:B:75:LYS:HG2	2.30	0.46
1:I:23:THR:O	1:I:25:HIS:HD2	1.97	0.46
1:I:25:HIS:N	1:I:25:HIS:CD2	2.82	0.46
1:E:78:VAL:HB	1:E:93:PHE:O	2.16	0.46
1:J:18:ILE:HA	1:J:18:ILE:HD12	1.67	0.46
1:B:18:ILE:HD12	1:B:18:ILE:HA	1.68	0.46
1:D:22:TRP:NE1	1:D:75:LYS:HG2	2.30	0.46
1:E:109:ARG:C	1:E:111:ILE:N	2.73	0.46
1:K:11:GLU:O	1:K:12:LEU:HD23	2.16	0.46
1:K:25:HIS:N	1:K:25:HIS:CD2	2.84	0.46
1:K:105:PHE:HD2	1:K:105:PHE:C	2.23	0.46
1:F:22:TRP:NE1	1:F:75:LYS:HG2	2.31	0.46
1:G:23:THR:O	1:G:25:HIS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:PHE:O	1:G:106:GLN:C	2.59	0.46
1:C:25:HIS:N	1:C:25:HIS:CD2	2.83	0.46
1:D:18:ILE:HD12	1:D:18:ILE:HA	1.41	0.46
1:H:25:HIS:N	1:H:25:HIS:CD2	2.83	0.46
1:J:25:HIS:CD2	1:J:25:HIS:N	2.84	0.46
1:G:52:SER:HA	1:L:53:LEU:H	1.81	0.45
1:J:82:GLU:HA	1:J:83:PRO:HD3	1.70	0.45
1:A:18:ILE:HD12	1:A:18:ILE:HA	1.70	0.45
1:E:69:PRO:O	1:F:106:GLN:CD	2.59	0.45
1:F:109:ARG:NH1	1:F:113:TRP:CZ2	2.85	0.45
1:G:11:GLU:O	1:G:12:LEU:HD23	2.17	0.45
1:I:53:LEU:O	1:I:53:LEU:HD23	2.16	0.45
1:B:70:GLN:HA	1:K:106:GLN:OE1	2.16	0.45
1:D:100:GLU:O	1:D:101:LEU:C	2.59	0.45
1:I:9:GLN:OE1	1:K:11:GLU:OE2	2.34	0.45
1:D:109:ARG:C	1:D:111:ILE:N	2.68	0.45
1:J:67:LYS:HD2	1:J:101:LEU:HD21	1.98	0.45
1:D:9:GLN:HE22	1:E:11:GLU:HG2	1.82	0.45
1:D:78:VAL:HB	1:D:93:PHE:O	2.17	0.45
1:H:100:GLU:O	1:H:101:LEU:C	2.59	0.45
1:A:53:LEU:CD2	1:F:44:MET:SD	2.99	0.45
1:A:77:PHE:CE1	1:A:98:VAL:HB	2.52	0.45
1:B:88:ASP:CB	1:B:89:PRO:CD	2.95	0.45
1:K:23:THR:O	1:K:25:HIS:HD2	2.00	0.45
1:C:82:GLU:HA	1:C:83:PRO:HD3	1.76	0.45
1:H:11:GLU:O	1:H:12:LEU:HD23	2.17	0.45
1:H:51:GLY:O	1:J:53:LEU:HB3	2.17	0.45
1:D:105:PHE:O	1:D:106:GLN:C	2.59	0.45
1:C:18:ILE:HA	1:C:18:ILE:HD12	1.69	0.44
1:A:40:ILE:HG22	1:F:53:LEU:HD11	1.99	0.44
1:D:83:PRO:HG3	1:D:88:ASP:O	2.16	0.44
1:G:53:LEU:HB2	1:L:53:LEU:HA	1.98	0.44
1:I:88:ASP:HA	1:I:89:PRO:HD3	1.68	0.44
1:A:23:THR:O	1:A:25:HIS:HD2	1.99	0.44
1:G:52:SER:C	1:L:53:LEU:CB	2.84	0.44
1:G:69:PRO:HD2	1:G:70:GLN:NE2	2.33	0.44
1:K:109:ARG:C	1:K:111:ILE:N	2.73	0.44
1:F:18:ILE:CG2	1:F:19:ASP:N	2.80	0.44
1:F:53:LEU:CG	1:F:53:LEU:O	2.65	0.44
1:I:83:PRO:HG2	1:I:88:ASP:O	2.18	0.44
1:K:18:ILE:HD12	1:K:18:ILE:HA	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:LEU:HD22	1:E:95:THR:HG22	1.99	0.44
1:E:23:THR:O	1:E:25:HIS:HD2	2.01	0.44
1:G:89:PRO:HG2	1:K:70:GLN:O	2.17	0.44
1:G:105:PHE:CE2	1:G:109:ARG:HD3	2.53	0.44
1:H:108:ILE:O	1:H:112:THR:HG23	2.17	0.44
1:F:53:LEU:O	1:F:53:LEU:HG	2.16	0.44
1:G:105:PHE:C	1:G:105:PHE:CD2	2.96	0.44
1:H:18:ILE:HA	1:H:18:ILE:HD12	1.77	0.44
1:A:34:LEU:C	1:A:34:LEU:CD2	2.91	0.43
1:E:18:ILE:HD12	1:E:18:ILE:HA	1.74	0.43
1:F:23:THR:O	1:F:25:HIS:HD2	2.01	0.43
1:H:109:ARG:C	1:H:111:ILE:N	2.73	0.43
1:I:78:VAL:HB	1:I:93:PHE:O	2.17	0.43
1:A:53:LEU:HD23	1:A:53:LEU:O	2.18	0.43
1:J:27:CYS:HA	1:J:35:SER:O	2.18	0.43
1:J:77:PHE:CE1	1:J:98:VAL:HB	2.53	0.43
1:K:100:GLU:O	1:K:101:LEU:C	2.61	0.43
1:B:104:TRP:O	1:B:105:PHE:C	2.60	0.43
1:G:82:GLU:HA	1:G:83:PRO:HD3	1.73	0.43
1:B:53:LEU:HD11	1:C:40:ILE:HG22	2.00	0.43
1:G:17:SER:O	1:K:98:VAL:HG21	2.18	0.43
1:H:77:PHE:HB3	1:H:101:LEU:HD22	2.00	0.43
1:I:87:GLY:O	1:I:88:ASP:O	2.37	0.43
1:G:12:LEU:HD21	1:G:104:TRP:CD1	2.53	0.43
1:G:100:GLU:O	1:G:101:LEU:C	2.61	0.43
1:A:82:GLU:HA	1:A:83:PRO:HD3	1.72	0.43
1:H:23:THR:O	1:H:25:HIS:HD2	2.01	0.43
1:H:26:PHE:CZ	1:J:40:ILE:HD12	2.53	0.43
1:B:67:LYS:HE2	1:K:102:PHE:HE1	1.83	0.43
1:E:82:GLU:HA	1:E:83:PRO:HD3	1.72	0.43
1:B:23:THR:O	1:B:25:HIS:HD2	2.02	0.43
1:C:109:ARG:C	1:C:111:ILE:N	2.74	0.43
1:D:83:PRO:HG2	1:D:88:ASP:O	2.18	0.43
1:F:82:GLU:HA	1:F:83:PRO:HD3	1.73	0.43
1:G:34:LEU:HD23	1:G:35:SER:N	2.34	0.43
1:K:82:GLU:HA	1:K:83:PRO:HD3	1.70	0.43
1:G:25:HIS:N	1:G:25:HIS:CD2	2.86	0.42
1:J:67:LYS:HB2	1:J:105:PHE:CE1	2.54	0.42
1:D:23:THR:O	1:D:25:HIS:HD2	2.02	0.42
1:G:9:GLN:HE22	1:L:11:GLU:HG2	1.84	0.42
1:L:77:PHE:HB3	1:L:101:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:LEU:HD23	1:D:35:SER:N	2.34	0.42
1:G:27:CYS:HA	1:G:35:SER:O	2.20	0.42
1:H:53:LEU:HD13	1:J:37:SER:OG	2.19	0.42
1:F:87:GLY:HA2	1:F:88:ASP:HA	1.27	0.42
1:E:77:PHE:HB3	1:E:101:LEU:HD22	2.02	0.42
1:I:12:LEU:HD22	1:I:95:THR:HG22	2.01	0.42
1:L:12:LEU:HD22	1:L:95:THR:HG22	2.02	0.42
1:G:53:LEU:HD12	1:L:26:PHE:HB3	2.00	0.42
1:A:78:VAL:HB	1:A:93:PHE:O	2.20	0.42
1:F:12:LEU:HD22	1:F:95:THR:HG22	2.01	0.42
1:F:43:THR:O	1:F:43:THR:CG2	2.63	0.42
1:G:72:LYS:HE2	1:G:92:GLU:OE2	2.20	0.42
1:F:11:GLU:O	1:F:12:LEU:HD23	2.19	0.41
1:I:53:LEU:HD11	1:K:40:ILE:HG22	2.02	0.41
1:B:49:PRO:HB2	1:B:50:LEU:H	1.30	0.41
1:C:23:THR:O	1:C:25:HIS:HD2	2.02	0.41
1:E:27:CYS:HA	1:E:35:SER:O	2.20	0.41
1:F:25:HIS:CD2	1:F:25:HIS:N	2.88	0.41
1:H:9:GLN:OE1	1:J:24:ARG:NH2	2.44	0.41
1:H:53:LEU:HD21	1:J:40:ILE:HA	2.01	0.41
1:K:78:VAL:HB	1:K:93:PHE:O	2.20	0.41
1:L:27:CYS:HA	1:L:35:SER:O	2.20	0.41
1:C:108:ILE:O	1:C:112:THR:HG23	2.21	0.41
1:F:49:PRO:HB2	1:F:51:GLY:H	1.86	0.41
1:D:77:PHE:HB3	1:D:101:LEU:HD22	2.03	0.41
1:B:27:CYS:HA	1:B:35:SER:O	2.19	0.41
1:C:78:VAL:HB	1:C:93:PHE:O	2.21	0.41
1:D:55:ARG:O	1:D:55:ARG:HG3	2.20	0.41
1:H:12:LEU:HD21	1:H:104:TRP:NE1	2.36	0.41
1:K:12:LEU:HD21	1:K:104:TRP:NE1	2.35	0.41
1:A:108:ILE:O	1:A:112:THR:HG23	2.21	0.41
1:F:89:PRO:HA	1:F:90:PRO:HD3	1.86	0.41
1:G:78:VAL:HB	1:G:93:PHE:O	2.20	0.41
1:I:26:PHE:CD2	1:I:26:PHE:C	2.98	0.41
1:I:82:GLU:HA	1:I:83:PRO:HD3	1.73	0.41
1:J:67:LYS:NZ	1:J:67:LYS:HB3	2.35	0.41
1:K:53:LEU:HD23	1:K:53:LEU:O	2.21	0.41
1:K:77:PHE:HB3	1:K:101:LEU:HD22	2.02	0.41
1:E:85:GLN:O	1:E:86:GLN:C	2.64	0.41
1:G:18:ILE:HG12	1:K:67:LYS:CE	2.51	0.41
1:H:52:SER:HA	1:J:52:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:23:THR:O	1:I:25:HIS:CD2	2.72	0.41
1:B:87:GLY:HA3	1:B:88:ASP:HA	1.91	0.40
1:D:82:GLU:HA	1:D:83:PRO:HD3	1.72	0.40
1:G:18:ILE:HD12	1:G:18:ILE:HA	1.68	0.40
1:A:11:GLU:HG2	1:F:9:GLN:HE22	1.84	0.40
1:C:24:ARG:C	1:C:25:HIS:CD2	2.99	0.40
1:G:53:LEU:O	1:G:53:LEU:HG	2.21	0.40
1:H:52:SER:HA	1:J:53:LEU:H	1.86	0.40
1:A:72:LYS:HE2	1:A:92:GLU:OE2	2.21	0.40
1:B:82:GLU:HA	1:B:83:PRO:HD3	1.70	0.40
1:E:25:HIS:CD2	1:E:25:HIS:N	2.88	0.40
1:I:27:CYS:HA	1:I:35:SER:O	2.21	0.40
1:L:105:PHE:C	1:L:105:PHE:CD2	2.99	0.40
1:A:34:LEU:HD23	1:A:34:LEU:C	2.46	0.40
1:E:103:GLU:C	1:E:105:PHE:N	2.79	0.40
1:J:78:VAL:HB	1:J:93:PHE:O	2.22	0.40
1:J:100:GLU:O	1:J:101:LEU:C	2.64	0.40
1:K:26:PHE:CD2	1:K:26:PHE:C	2.99	0.40
1:K:34:LEU:HD23	1:K:35:SER:N	2.36	0.40
1:A:11:GLU:HB3	1:F:9:GLN:NE2	2.37	0.40
1:B:108:ILE:O	1:B:112:THR:HG23	2.22	0.40
1:C:53:LEU:HD23	1:C:53:LEU:O	2.21	0.40
1:D:9:GLN:HE22	1:E:11:GLU:CD	2.29	0.40
1:I:100:GLU:O	1:I:101:LEU:C	2.62	0.40
1:J:108:ILE:O	1:J:112:THR:HG23	2.20	0.40

All (2) 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:A:20:GLN:OE1	1:I:106:GLN:NE2[4_455]	1.99	0.21
1:C:86:GLN:O	1:G:113:TRP:NE1[4_455]	2.11	0.09

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	106/124 (86%)	94 (89%)	10 (9%)	2 (2%)	6	22
1	B	106/124 (86%)	86 (81%)	9 (8%)	11 (10%)	0	1
1	C	101/124 (82%)	85 (84%)	12 (12%)	4 (4%)	2	8
1	D	93/124 (75%)	78 (84%)	9 (10%)	6 (6%)	1	3
1	E	95/124 (77%)	85 (90%)	9 (10%)	1 (1%)	11	36
1	F	105/124 (85%)	84 (80%)	11 (10%)	10 (10%)	0	1
1	G	97/124 (78%)	82 (84%)	11 (11%)	4 (4%)	2	8
1	H	88/124 (71%)	81 (92%)	6 (7%)	1 (1%)	11	36
1	I	93/124 (75%)	79 (85%)	9 (10%)	5 (5%)	1	4
1	J	88/124 (71%)	79 (90%)	8 (9%)	1 (1%)	11	36
1	K	92/124 (74%)	84 (91%)	8 (9%)	0	100	100
1	L	66/124 (53%)	61 (92%)	4 (6%)	1 (2%)	8	28
All	All	1130/1488 (76%)	978 (86%)	106 (9%)	46 (4%)	2	8

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	43	THR
1	B	47	ASP
1	B	49	PRO
1	D	89	PRO
1	F	43	THR
1	F	44	MET
1	F	46	GLU
1	B	45	GLU
1	B	86	GLN
1	B	89	PRO
1	C	86	GLN
1	D	51	GLY
1	D	52	SER
1	F	87	GLY
1	F	88	ASP
1	G	87	GLY
1	G	88	ASP
1	G	89	PRO
1	I	86	GLN

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Mol	Chain	Res	Type
1	I	87	GLY
1	I	88	ASP
1	A	110	GLU
1	B	48	ASN
1	B	110	GLU
1	C	43	THR
1	D	50	LEU
1	D	110	GLU
1	A	43	THR
1	E	110	GLU
1	F	48	ASN
1	I	110	GLU
1	J	110	GLU
1	B	42	GLN
1	B	44	MET
1	B	88	ASP
1	C	110	GLU
1	D	88	ASP
1	F	47	ASP
1	F	89	PRO
1	F	110	GLU
1	H	110	GLU
1	I	103	GLU
1	L	110	GLU
1	G	110	GLU
1	C	88	ASP
1	F	49	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	90/109 (83%)	75 (83%)	15 (17%)	2	8
1	B	83/109 (76%)	70 (84%)	13 (16%)	2	9
1	C	83/109 (76%)	69 (83%)	14 (17%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	80/109 (73%)	66 (82%)	14 (18%)	2	7
1	E	79/109 (72%)	64 (81%)	15 (19%)	1	5
1	F	81/109 (74%)	64 (79%)	17 (21%)	1	4
1	G	79/109 (72%)	62 (78%)	17 (22%)	1	4
1	H	76/109 (70%)	61 (80%)	15 (20%)	1	5
1	I	78/109 (72%)	62 (80%)	16 (20%)	1	4
1	J	77/109 (71%)	64 (83%)	13 (17%)	2	7
1	K	79/109 (72%)	64 (81%)	15 (19%)	1	5
1	L	61/109 (56%)	47 (77%)	14 (23%)	1	3
All	All	946/1308 (72%)	768 (81%)	178 (19%)	1	5

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	11	GLU
1	A	18	ILE
1	A	34	LEU
1	A	54	CYS
1	A	55	ARG
1	A	62	THR
1	A	64	ASN
1	A	65	VAL
1	A	67	LYS
1	A	70	GLN
1	A	78	VAL
1	A	98	VAL
1	A	99	GLU
1	A	109	ARG
1	B	11	GLU
1	B	18	ILE
1	B	23	THR
1	B	34	LEU
1	B	54	CYS
1	B	64	ASN
1	B	65	VAL
1	B	67	LYS
1	B	70	GLN
1	B	78	VAL

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Mol	Chain	Res	Type
1	B	98	VAL
1	B	99	GLU
1	B	109	ARG
1	C	9	GLN
1	C	11	GLU
1	C	18	ILE
1	C	23	THR
1	C	34	LEU
1	C	54	CYS
1	C	62	THR
1	C	64	ASN
1	C	65	VAL
1	C	70	GLN
1	C	78	VAL
1	C	98	VAL
1	C	99	GLU
1	C	109	ARG
1	D	9	GLN
1	D	11	GLU
1	D	18	ILE
1	D	34	LEU
1	D	54	CYS
1	D	62	THR
1	D	64	ASN
1	D	65	VAL
1	D	67	LYS
1	D	70	GLN
1	D	78	VAL
1	D	98	VAL
1	D	99	GLU
1	D	109	ARG
1	E	9	GLN
1	E	11	GLU
1	E	18	ILE
1	E	25	HIS
1	E	34	LEU
1	E	40	ILE
1	E	54	CYS
1	E	64	ASN
1	E	65	VAL
1	E	67	LYS
1	E	70	GLN

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Mol	Chain	Res	Type
1	E	78	VAL
1	E	98	VAL
1	E	99	GLU
1	E	109	ARG
1	F	9	GLN
1	F	11	GLU
1	F	18	ILE
1	F	23	THR
1	F	34	LEU
1	F	40	ILE
1	F	54	CYS
1	F	62	THR
1	F	64	ASN
1	F	65	VAL
1	F	67	LYS
1	F	70	GLN
1	F	78	VAL
1	F	98	VAL
1	F	99	GLU
1	F	109	ARG
1	F	113	TRP
1	G	9	GLN
1	G	11	GLU
1	G	18	ILE
1	G	23	THR
1	G	25	HIS
1	G	34	LEU
1	G	40	ILE
1	G	54	CYS
1	G	64	ASN
1	G	65	VAL
1	G	67	LYS
1	G	70	GLN
1	G	78	VAL
1	G	98	VAL
1	G	99	GLU
1	G	109	ARG
1	G	113	TRP
1	H	9	GLN
1	H	11	GLU
1	H	18	ILE
1	H	23	THR

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Mol	Chain	Res	Type
1	H	34	LEU
1	H	54	CYS
1	H	62	THR
1	H	64	ASN
1	H	65	VAL
1	H	67	LYS
1	H	70	GLN
1	H	78	VAL
1	H	98	VAL
1	H	99	GLU
1	H	109	ARG
1	I	9	GLN
1	I	11	GLU
1	I	18	ILE
1	I	23	THR
1	I	25	HIS
1	I	34	LEU
1	I	54	CYS
1	I	62	THR
1	I	64	ASN
1	I	65	VAL
1	I	67	LYS
1	I	70	GLN
1	I	78	VAL
1	I	98	VAL
1	I	99	GLU
1	I	109	ARG
1	J	9	GLN
1	J	11	GLU
1	J	18	ILE
1	J	34	LEU
1	J	54	CYS
1	J	64	ASN
1	J	65	VAL
1	J	67	LYS
1	J	70	GLN
1	J	78	VAL
1	J	98	VAL
1	J	99	GLU
1	J	109	ARG
1	K	9	GLN
1	K	11	GLU

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Mol	Chain	Res	Type
1	K	18	ILE
1	K	34	LEU
1	K	54	CYS
1	K	62	THR
1	K	64	ASN
1	K	65	VAL
1	K	67	LYS
1	K	70	GLN
1	K	78	VAL
1	K	98	VAL
1	K	99	GLU
1	K	105	PHE
1	K	109	ARG
1	L	9	GLN
1	L	11	GLU
1	L	34	LEU
1	L	54	CYS
1	L	55	ARG
1	L	62	THR
1	L	64	ASN
1	L	65	VAL
1	L	67	LYS
1	L	70	GLN
1	L	78	VAL
1	L	98	VAL
1	L	99	GLU
1	L	109	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	70	GLN
1	A	73	ASN
1	B	8	GLN
1	B	70	GLN
1	B	73	ASN
1	B	106	GLN
1	C	8	GLN
1	C	64	ASN
1	C	70	GLN
1	C	73	ASN

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Mol	Chain	Res	Type
1	D	8	GLN
1	D	70	GLN
1	E	8	GLN
1	E	64	ASN
1	E	70	GLN
1	E	73	ASN
1	F	8	GLN
1	F	64	ASN
1	F	70	GLN
1	F	73	ASN
1	G	8	GLN
1	G	64	ASN
1	G	70	GLN
1	H	8	GLN
1	H	64	ASN
1	H	70	GLN
1	H	73	ASN
1	I	8	GLN
1	I	64	ASN
1	I	70	GLN
1	I	73	ASN
1	J	8	GLN
1	J	70	GLN
1	K	8	GLN
1	K	64	ASN
1	K	70	GLN
1	K	73	ASN
1	L	8	GLN
1	L	9	GLN
1	L	64	ASN
1	L	70	GLN
1	L	73	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	108/124 (87%)	1.31	19 (17%) 4 3	56, 85, 106, 116	0
1	B	108/124 (87%)	0.90	8 (7%) 20 15	69, 94, 115, 148	0
1	C	105/124 (84%)	1.09	9 (8%) 16 12	68, 90, 107, 120	0
1	D	99/124 (79%)	0.91	8 (8%) 18 13	66, 93, 112, 120	0
1	E	101/124 (81%)	0.95	12 (11%) 9 7	76, 96, 112, 120	0
1	F	107/124 (86%)	1.05	10 (9%) 14 10	68, 92, 111, 120	0
1	G	101/124 (81%)	1.03	15 (14%) 5 4	68, 94, 115, 134	0
1	H	94/124 (75%)	1.21	13 (13%) 6 5	80, 98, 115, 123	0
1	I	97/124 (78%)	0.98	13 (13%) 7 5	73, 94, 114, 122	0
1	J	94/124 (75%)	0.85	10 (10%) 11 8	75, 97, 113, 121	0
1	K	98/124 (79%)	1.12	14 (14%) 6 5	76, 98, 114, 121	0
1	L	74/124 (59%)	2.03	37 (50%) 0 0	82, 100, 120, 142	0
All	All	1186/1488 (79%)	1.10	168 (14%) 6 5	56, 94, 114, 148	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	GLN	5.7
1	F	66	VAL	5.4
1	A	40	ILE	5.0
1	A	18	ILE	4.9
1	L	66	VAL	4.7
1	E	43	THR	4.3
1	L	105	PHE	4.2
1	L	65	VAL	4.2
1	D	43	THR	4.1
1	A	17	SER	4.1
1	I	29	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	102	PHE	3.8
1	L	67	LYS	3.7
1	J	40	ILE	3.7
1	L	81	LEU	3.7
1	L	79	PHE	3.7
1	C	66	VAL	3.7
1	D	42	GLN	3.6
1	K	89	PRO	3.6
1	J	67	LYS	3.6
1	A	109	ARG	3.5
1	A	66	VAL	3.5
1	L	58	LEU	3.5
1	L	94	ALA	3.5
1	H	66	VAL	3.5
1	H	89	PRO	3.5
1	C	70	GLN	3.4
1	I	42	GLN	3.4
1	K	55	ARG	3.4
1	E	70	GLN	3.4
1	L	60	LEU	3.3
1	H	105	PHE	3.3
1	L	95	THR	3.3
1	L	112	THR	3.3
1	J	42	GLN	3.3
1	D	17	SER	3.2
1	A	67	LYS	3.2
1	G	31	ASP	3.2
1	A	89	PRO	3.2
1	L	80	ILE	3.2
1	D	51	GLY	3.2
1	E	40	ILE	3.2
1	A	64	ASN	3.1
1	L	91	VAL	3.1
1	H	83	PRO	3.1
1	I	55	ARG	3.1
1	L	101	LEU	3.1
1	B	88	ASP	3.1
1	D	53	LEU	3.1
1	L	38	ASP	3.0
1	G	53	LEU	3.0
1	G	69	PRO	3.0
1	B	18	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	43	THR	3.0
1	A	57	ILE	3.0
1	L	110	GLU	2.9
1	A	24	ARG	2.9
1	E	76	SER	2.9
1	K	113	TRP	2.9
1	G	106	GLN	2.9
1	J	85	GLN	2.9
1	L	63	TYR	2.9
1	J	66	VAL	2.9
1	L	78	VAL	2.9
1	K	90	PRO	2.9
1	G	67	LYS	2.9
1	K	31	ASP	2.8
1	L	12	LEU	2.8
1	L	108	ILE	2.8
1	F	9	GLN	2.8
1	G	70	GLN	2.8
1	H	42	GLN	2.7
1	H	40	ILE	2.7
1	A	100	GLU	2.7
1	A	41	GLU	2.7
1	I	67	LYS	2.7
1	K	67	LYS	2.7
1	J	63	TYR	2.7
1	B	17	SER	2.7
1	B	66	VAL	2.7
1	L	104	TRP	2.7
1	C	43	THR	2.6
1	H	91	VAL	2.6
1	G	40	ILE	2.6
1	A	80	ILE	2.6
1	I	70	GLN	2.6
1	I	36	PHE	2.6
1	L	113	TRP	2.6
1	C	60	LEU	2.6
1	L	34	LEU	2.6
1	E	9	GLN	2.6
1	K	51	GLY	2.6
1	A	110	GLU	2.6
1	G	85	GLN	2.6
1	L	73	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	109	ARG	2.5
1	F	55	ARG	2.5
1	L	52	SER	2.5
1	K	53	LEU	2.5
1	K	91	VAL	2.5
1	E	50	LEU	2.4
1	G	88	ASP	2.4
1	L	111	ILE	2.4
1	H	112	THR	2.4
1	F	53	LEU	2.4
1	K	83	PRO	2.4
1	G	30	ALA	2.4
1	E	42	GLN	2.4
1	E	67	LYS	2.4
1	L	93	PHE	2.4
1	K	52	SER	2.4
1	C	24	ARG	2.3
1	L	54	CYS	2.3
1	L	32	ALA	2.3
1	F	42	GLN	2.3
1	B	64	ASN	2.3
1	G	51	GLY	2.3
1	F	35	SER	2.3
1	J	18	ILE	2.3
1	G	20	GLN	2.3
1	H	53	LEU	2.3
1	J	70	GLN	2.3
1	A	55	ARG	2.3
1	L	64	ASN	2.3
1	A	20	GLN	2.3
1	J	112	THR	2.3
1	D	66	VAL	2.3
1	L	102	PHE	2.2
1	H	74	GLN	2.2
1	I	8	GLN	2.2
1	K	54	CYS	2.2
1	I	52	SER	2.2
1	L	26	PHE	2.2
1	B	29	ILE	2.2
1	I	57	ILE	2.2
1	K	32	ALA	2.2
1	G	24	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	24	ARG	2.2
1	C	65	VAL	2.2
1	J	89	PRO	2.2
1	C	12	LEU	2.2
1	L	59	ASP	2.1
1	B	67	LYS	2.1
1	F	81	LEU	2.1
1	G	50	LEU	2.1
1	F	64	ASN	2.1
1	A	19	ASP	2.1
1	H	57	ILE	2.1
1	L	57	ILE	2.1
1	C	106	GLN	2.1
1	L	25	HIS	2.1
1	F	69	PRO	2.1
1	L	36	PHE	2.1
1	E	111	ILE	2.1
1	I	28	ALA	2.1
1	K	70	GLN	2.1
1	E	89	PRO	2.1
1	E	52	SER	2.0
1	D	69	PRO	2.0
1	L	61	ASN	2.0
1	I	31	ASP	2.0
1	F	63	TYR	2.0
1	I	86	GLN	2.0
1	I	54	CYS	2.0
1	H	58	LEU	2.0
1	A	16	ASP	2.0
1	C	11	GLU	2.0
1	E	66	VAL	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.