



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:28 AM UTC

PDB ID : 1VLN / pdb_00001vln
Title : A TRICLINIC CRYSTAL FORM OF THE LECTIN CONCAVALIN A
Authors : Kanellopoulos, P.N.; Tucker, P.A.; Hamodrakas, S.J.
Deposited on : 1996-04-03
Resolution : 2.40 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

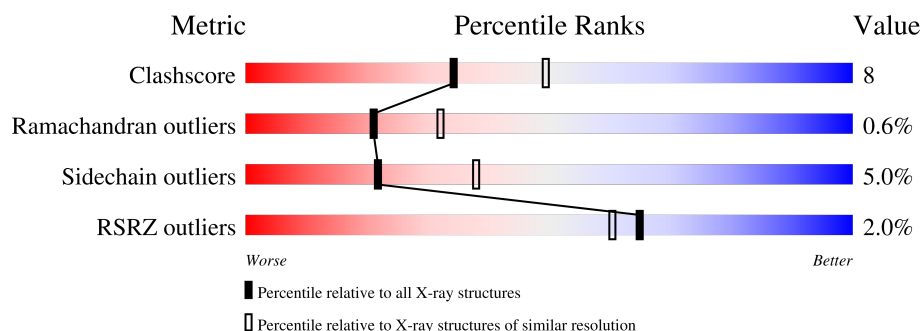
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
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	237	% 77% 18% • •
1	B	237	% 79% 18% •
1	C	237	3% 78% 21% •
1	D	237	3% 75% 20% •
1	E	237	2% 77% 21% •
1	F	237	% 82% 14% •

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Mol	Chain	Length	Quality of chain
1	G	237	2% 81% 16%
1	H	237	2% 75% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14520 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 CONCANAVALIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	B	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	C	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	D	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	E	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	F	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	G	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	H	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ASP	GLU	conflict	UNP P08902
A	155	GLU	ARG	conflict	UNP P08902
B	151	ASP	GLU	conflict	UNP P08902
B	155	GLU	ARG	conflict	UNP P08902
C	151	ASP	GLU	conflict	UNP P08902
C	155	GLU	ARG	conflict	UNP P08902
D	151	ASP	GLU	conflict	UNP P08902
D	155	GLU	ARG	conflict	UNP P08902
E	151	ASP	GLU	conflict	UNP P08902
E	155	GLU	ARG	conflict	UNP P08902
F	151	ASP	GLU	conflict	UNP P08902
F	155	GLU	ARG	conflict	UNP P08902
G	151	ASP	GLU	conflict	UNP P08902

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Chain	Residue	Modelled	Actual	Comment	Reference
G	155	GLU	ARG	conflict	UNP P08902
H	151	ASP	GLU	conflict	UNP P08902
H	155	GLU	ARG	conflict	UNP P08902

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0
2	G	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

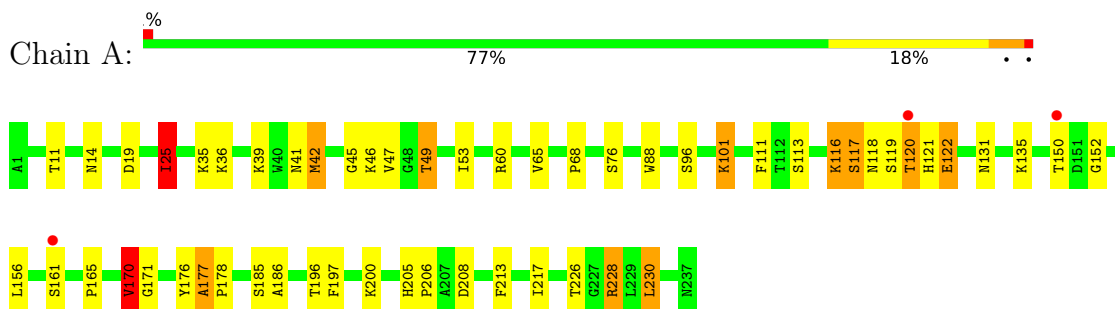
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	4	Total O 4 4	0	0
4	C	4	Total O 4 4	0	0
4	D	4	Total O 4 4	0	0
4	E	4	Total O 4 4	0	0
4	F	4	Total O 4 4	0	0
4	G	4	Total O 4 4	0	0
4	H	4	Total O 4 4	0	0

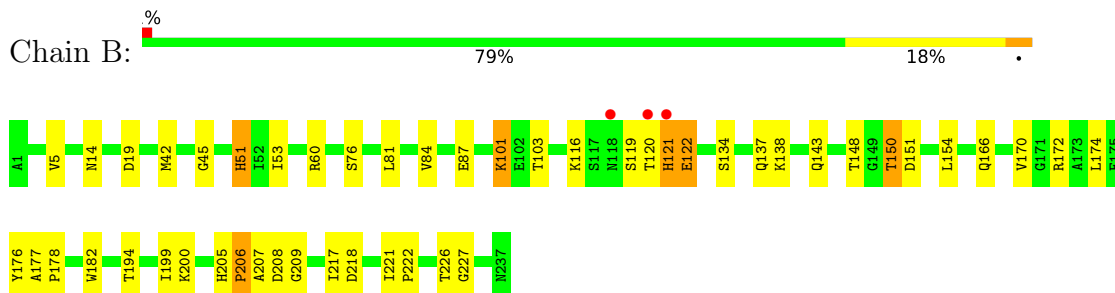
3 Residue-property plots

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.

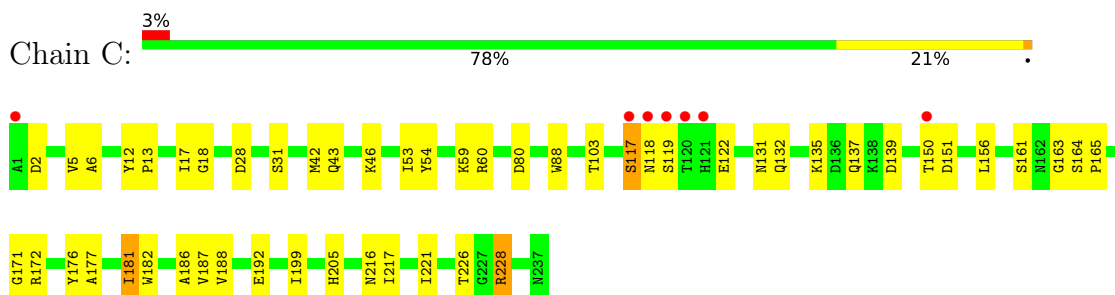
• Molecule 1: CONCANAVALIN A



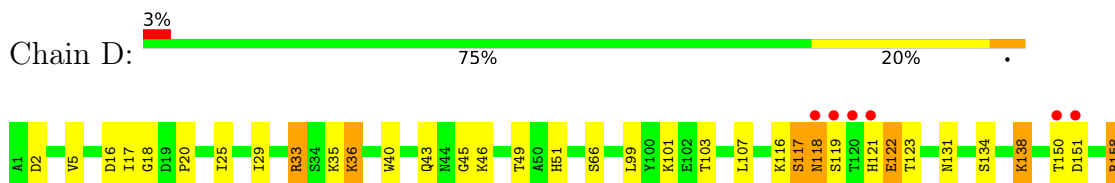
• Molecule 1: CONCANAVALIN A



• Molecule 1: CONCANAVALIN A

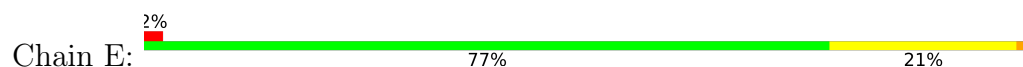


• Molecule 1: CONCANAVALIN A

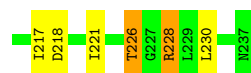
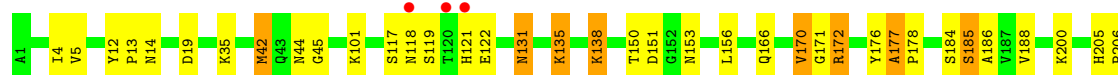
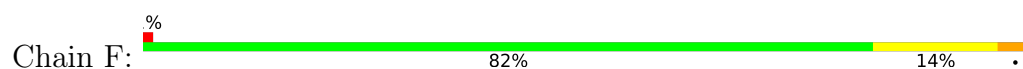




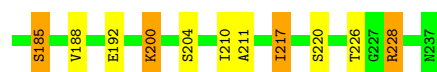
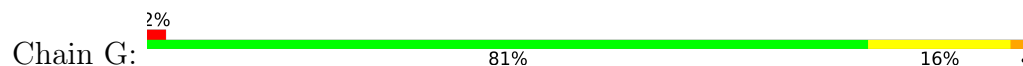
• Molecule 1: CONCANAVALIN A



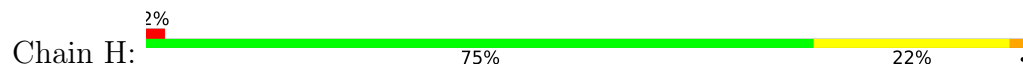
• Molecule 1: CONCANAVALIN A



• Molecule 1: CONCANAVALIN A



• Molecule 1: CONCANAVALIN A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.80Å 79.30Å 133.30Å 97.10° 90.20° 97.50°	Depositor
Resolution (Å)	6.00 – 2.40 6.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.4 (6.00-2.40) 78.6 (6.00-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.205 , 0.265 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.2	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	0.95	EDS
Total number of atoms	14520	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN, CA

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	0.66	1/1851 (0.1%)	1.10	10/2522 (0.4%)
1	B	0.62	0/1851	1.11	9/2522 (0.4%)
1	C	0.63	0/1851	1.05	12/2522 (0.5%)
1	D	0.66	0/1851	1.09	12/2522 (0.5%)
1	E	0.61	0/1851	1.04	11/2522 (0.4%)
1	F	0.65	0/1851	1.09	16/2522 (0.6%)
1	G	0.66	0/1851	1.10	8/2522 (0.3%)
1	H	0.64	0/1851	1.07	9/2522 (0.4%)
All	All	0.64	1/14808 (0.0%)	1.08	87/20176 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	ILE	CA-CB	5.10	1.60	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	HIS	CA-C-N	9.97	129.92	119.85
1	B	205	HIS	C-N-CA	9.97	129.92	119.85
1	A	117	SER	N-CA-C	7.69	120.94	110.55
1	H	205	HIS	CA-C-N	7.66	127.62	120.03
1	H	205	HIS	C-N-CA	7.66	127.62	120.03
1	C	205	HIS	CA-C-N	7.62	127.57	120.03
1	C	205	HIS	C-N-CA	7.62	127.57	120.03
1	H	5	VAL	N-CA-C	-7.40	96.76	107.78
1	G	176	TYR	N-CA-C	7.38	119.32	111.28
1	D	176	TYR	N-CA-C	7.11	119.93	111.33
1	B	176	TYR	N-CA-C	7.03	118.59	111.07
1	D	117	SER	N-CA-C	7.03	120.10	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	99	LEU	N-CA-C	-6.96	103.69	111.28
1	C	176	TYR	N-CA-C	6.86	119.34	111.11
1	D	187	VAL	N-CA-C	-6.82	104.21	110.82
1	B	5	VAL	N-CA-C	-6.79	97.83	107.75
1	B	217	ILE	N-CA-C	6.76	118.32	110.62
1	D	18	GLY	N-CA-C	6.72	122.84	114.37
1	G	6	ALA	N-CA-C	6.72	119.65	109.23
1	F	226	THR	N-CA-C	-6.53	101.34	110.35
1	A	213	PHE	N-CA-C	6.51	119.61	109.52
1	E	228	ARG	N-CA-C	6.41	120.19	112.38
1	A	176	TYR	N-CA-C	6.29	118.13	111.28
1	D	228	ARG	N-CA-C	6.24	119.99	112.38
1	A	228	ARG	N-CA-C	6.19	120.30	112.87
1	E	85	LEU	N-CA-C	6.11	118.41	110.40
1	F	230	LEU	N-CA-C	6.08	119.93	111.90
1	C	6	ALA	N-CA-C	6.01	118.32	109.24
1	C	117	SER	N-CA-C	5.94	118.53	109.62
1	D	5	VAL	N-CA-C	-5.93	99.09	107.75
1	E	24	HIS	N-CA-C	5.92	117.96	109.14
1	F	228	ARG	N-CA-C	5.88	120.06	113.01
1	H	177	ALA	N-CA-C	5.85	117.04	109.72
1	A	152	GLY	N-CA-C	-5.83	107.21	115.43
1	F	177	ALA	CA-C-N	5.79	125.70	119.85
1	F	177	ALA	C-N-CA	5.79	125.70	119.85
1	E	5	VAL	N-CA-C	-5.79	99.21	107.77
1	F	5	VAL	N-CA-C	-5.76	99.25	107.77
1	B	101	LYS	N-CA-C	5.74	117.69	109.14
1	C	181	ILE	N-CA-C	5.70	116.47	110.72
1	F	138	LYS	N-CA-C	5.68	119.69	112.87
1	H	124	ASN	N-CA-C	-5.65	99.98	109.07
1	A	131	ASN	N-CA-C	-5.63	105.75	113.30
1	G	101	LYS	N-CA-C	5.53	116.37	108.74
1	G	131	ASN	N-CA-C	-5.53	105.89	113.30
1	G	85	LEU	N-CA-C	5.52	118.90	110.50
1	E	213	PHE	N-CA-C	5.50	118.05	109.52
1	F	4	ILE	N-CA-C	5.49	115.80	108.11
1	B	209	GLY	N-CA-C	5.47	117.47	110.96
1	E	176	TYR	N-CA-C	5.47	116.92	111.07
1	E	219	SER	N-CA-C	5.45	118.14	110.23
1	D	131	ASN	N-CA-C	-5.45	105.85	112.88
1	B	206	PRO	N-CA-C	5.45	120.05	111.38
1	F	206	PRO	N-CA-C	5.42	119.54	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	66	SER	N-CA-C	5.42	117.04	108.96
1	D	20	PRO	N-CA-C	-5.42	103.63	111.22
1	C	18	GLY	N-CA-C	5.41	121.95	114.92
1	F	176	TYR	N-CA-C	5.40	117.59	111.11
1	A	230	LEU	N-CA-C	5.38	119.00	111.90
1	F	131	ASN	N-CA-C	-5.36	106.12	113.30
1	C	177	ALA	N-CA-C	5.35	116.56	109.93
1	G	138	LYS	N-CA-C	5.34	119.28	112.87
1	C	5	VAL	N-CA-C	-5.33	99.87	107.77
1	D	158	ARG	N-CA-C	5.32	118.03	110.10
1	E	230	LEU	N-CA-C	5.30	119.05	112.47
1	E	73	ALA	N-CA-C	-5.28	101.10	109.59
1	G	204	SER	N-CA-C	5.25	117.69	111.33
1	E	124	ASN	N-CA-C	-5.24	100.36	108.90
1	F	218	ASP	N-CA-C	5.21	118.46	112.57
1	D	66	SER	N-CA-C	5.20	116.71	108.96
1	E	66	SER	N-CA-C	5.19	116.70	108.96
1	A	119	SER	N-CA-C	-5.18	99.50	108.52
1	G	124	ASN	N-CA-C	-5.17	100.98	109.40
1	A	170	VAL	CB-CA-C	-5.16	101.78	110.71
1	A	177	ALA	N-CA-C	5.15	116.56	110.07
1	F	118	ASN	N-CA-C	5.12	116.94	109.71
1	D	138	LYS	N-CA-C	5.11	117.59	111.71
1	C	217	ILE	N-CA-C	5.10	116.43	110.62
1	H	176	TYR	N-CA-C	5.07	116.81	111.28
1	D	151	ASP	N-CA-C	-5.06	107.06	113.23
1	C	164	SER	CA-C-N	5.05	124.95	119.85
1	C	164	SER	C-N-CA	5.05	124.95	119.85
1	F	205	HIS	CA-C-N	5.03	125.01	120.03
1	F	205	HIS	C-N-CA	5.03	125.01	120.03
1	F	172	ARG	CB-CG-CD	-5.03	99.73	111.30
1	B	138	LYS	N-CA-C	5.03	118.90	112.87
1	H	222	PRO	N-CA-C	5.00	118.59	111.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1809	0	1755	32	0
1	B	1809	0	1755	29	0
1	C	1809	0	1755	28	0
1	D	1809	0	1755	33	0
1	E	1809	0	1755	34	0
1	F	1809	0	1755	20	0
1	G	1809	0	1755	28	0
1	H	1809	0	1755	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	4	0	0	0	0
4	H	4	0	0	0	0
All	All	14520	0	14040	216	0

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

All (216) 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:119:SER:HB2	1:B:122:GLU:HB2	1.45	0.98
1:D:119:SER:HB2	1:D:122:GLU:HB2	1.59	0.83
1:E:119:SER:HB2	1:E:122:GLU:HB2	1.63	0.81
1:F:170:VAL:HG22	1:F:226:THR:HG22	1.63	0.79
1:H:119:SER:HB2	1:H:122:GLU:HB2	1.65	0.76
1:G:58:ASP:HB3	1:G:60:ARG:NH1	2.01	0.76
1:B:42:MET:HE1	1:B:206:PRO:HG3	1.68	0.76
1:G:29:ILE:H	1:G:35:LYS:HE3	1.53	0.73
1:E:122:GLU:HG3	1:F:131:ASN:HB3	1.71	0.72
1:C:117:SER:HA	1:C:186:ALA:HA	1.73	0.70
1:E:170:VAL:HG23	1:E:226:THR:HG22	1.76	0.68
1:F:119:SER:HB2	1:F:122:GLU:HB2	1.75	0.68
1:H:94:SER:OG	1:H:172:ARG:HG2	1.94	0.67
1:B:14:ASN:O	1:B:19:ASP:HB2	1.95	0.66
1:G:170:VAL:HG22	1:G:226:THR:HG22	1.78	0.65
1:A:39:LYS:NZ	1:A:41:ASN:HD21	1.95	0.65
1:A:45:GLY:HA2	1:A:200:LYS:HG2	1.77	0.65
1:H:117:SER:HA	1:H:186:ALA:HA	1.77	0.64
1:A:39:LYS:HZ2	1:A:41:ASN:HD21	1.44	0.64
1:B:119:SER:HB2	1:B:122:GLU:CB	2.26	0.62
1:E:119:SER:HB2	1:E:122:GLU:CB	2.30	0.61
1:G:60:ARG:NH1	1:G:60:ARG:HB2	2.14	0.61
1:A:60:ARG:NH2	1:C:60:ARG:HD2	2.16	0.61
1:A:36:LYS:HD3	1:A:76:SER:O	2.02	0.60
1:E:172:ARG:HD2	1:E:221:ILE:HG12	1.82	0.60
1:D:45:GLY:HA2	1:D:200:LYS:HG2	1.83	0.60
1:G:131:ASN:HB3	1:H:122:GLU:HG3	1.82	0.60
1:F:151:ASP:HB2	1:F:153:ASN:HD22	1.67	0.60
1:C:59:LYS:HD2	1:C:80:ASP:HA	1.83	0.59
1:E:11:THR:O	1:E:205:HIS:HE1	1.84	0.59
1:E:42:MET:HE1	1:E:206:PRO:HG3	1.84	0.59
1:C:181:ILE:HG23	1:C:182:TRP:CD1	2.38	0.59
1:D:170:VAL:HG22	1:D:226:THR:HG22	1.83	0.59
1:F:156:LEU:O	1:F:171:GLY:HA3	2.03	0.59
1:E:36:LYS:NZ	1:E:36:LYS:HB2	2.18	0.59
1:A:156:LEU:O	1:A:171:GLY:HA3	2.03	0.58
1:C:181:ILE:HG23	1:C:182:TRP:HD1	1.68	0.58
1:D:178:PRO:HB3	1:D:217:ILE:HD11	1.85	0.58
1:G:53:ILE:HG22	1:G:192:GLU:HG3	1.86	0.58
1:A:68:PRO:HA	1:C:118:ASN:OD1	2.03	0.57
1:B:120:THR:HG23	1:D:196:THR:HG21	1.85	0.57
1:G:58:ASP:HB3	1:G:60:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:SER:HB3	1:A:122:GLU:HB2	1.85	0.57
1:B:121:HIS:ND1	1:B:121:HIS:O	2.37	0.57
1:B:116:LYS:HZ3	1:D:51:HIS:HB2	1.69	0.56
1:A:42:MET:HE1	1:A:206:PRO:HG2	1.86	0.56
1:A:170:VAL:HG22	1:A:226:THR:HG22	1.87	0.56
1:E:25:ILE:HG12	1:E:65:VAL:HG21	1.88	0.56
1:E:156:LEU:O	1:E:171:GLY:HA3	2.04	0.56
1:H:101:LYS:HD2	1:H:165:PRO:O	2.05	0.55
1:E:170:VAL:CG2	1:E:226:THR:HG22	2.36	0.55
1:E:4:ILE:HD13	1:E:215:SER:HB3	1.89	0.55
1:A:25:ILE:HD12	1:A:65:VAL:HG23	1.88	0.54
1:A:39:LYS:HZ2	1:A:41:ASN:ND2	2.05	0.54
1:C:156:LEU:O	1:C:171:GLY:HA3	2.07	0.54
1:B:120:THR:O	1:B:121:HIS:HB3	2.07	0.54
1:G:115:LEU:O	1:G:123:THR:HA	2.08	0.54
1:H:100:TYR:HB2	1:H:207:ALA:HB3	1.89	0.54
1:E:36:LYS:HB2	1:E:36:LYS:HZ3	1.73	0.53
1:G:35:LYS:N	1:G:35:LYS:HE2	2.23	0.53
1:C:172:ARG:HD2	1:C:221:ILE:CG1	2.38	0.53
1:A:39:LYS:NZ	1:A:41:ASN:ND2	2.56	0.53
1:B:194:THR:HG21	1:D:121:HIS:CD2	2.43	0.53
1:B:87:GLU:HG3	1:B:182:TRP:O	2.09	0.53
1:C:172:ARG:HD2	1:C:221:ILE:HG12	1.90	0.53
1:E:117:SER:HA	1:E:186:ALA:HA	1.90	0.53
1:A:116:LYS:O	1:A:186:ALA:HA	2.09	0.52
1:C:103:THR:HG23	1:C:165:PRO:HG3	1.91	0.52
1:B:42:MET:CE	1:B:206:PRO:HG3	2.39	0.52
1:H:110:SER:OG	1:H:129:MET:HG3	2.10	0.52
1:E:172:ARG:HD2	1:E:221:ILE:CG1	2.40	0.52
1:C:103:THR:O	1:C:199:ILE:HA	2.10	0.51
1:B:81:LEU:HA	1:B:84:VAL:HG22	1.91	0.51
1:E:177:ALA:HB2	1:F:177:ALA:HB2	1.93	0.51
1:H:103:THR:O	1:H:199:ILE:HA	2.09	0.51
1:E:88:TRP:CG	1:F:138:LYS:HD2	2.46	0.50
1:B:134:SER:H	1:B:137:GLN:NE2	2.10	0.50
1:D:49:THR:OG1	1:D:196:THR:HG22	2.12	0.50
1:B:148:THR:HG22	1:B:154:LEU:HD13	1.93	0.49
1:G:156:LEU:O	1:G:171:GLY:HA3	2.12	0.49
1:B:143:GLN:HB2	1:B:172:ARG:HB2	1.94	0.49
1:H:27:ILE:HG22	1:H:29:ILE:CD1	2.43	0.49
1:D:17:ILE:HD13	1:D:228:ARG:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ILE:HG22	1:C:192:GLU:HG3	1.95	0.49
1:E:87:GLU:HG2	1:E:180:HIS:CD2	2.48	0.49
1:H:222:PRO:HG2	1:H:225:SER:HB3	1.95	0.48
1:C:28:ASP:HB3	1:C:31:SER:O	2.14	0.48
1:E:210:ILE:HG22	1:E:211:ALA:N	2.27	0.48
1:H:150:THR:O	1:H:151:ASP:HB2	2.13	0.48
1:D:117:SER:HA	1:D:186:ALA:HA	1.95	0.48
1:E:45:GLY:HA2	1:E:200:LYS:HG2	1.94	0.48
1:C:88:TRP:CD2	1:D:138:LYS:HB2	2.49	0.48
1:G:119:SER:HB2	1:G:122:GLU:HG3	1.96	0.48
1:A:14:ASN:C	1:A:19:ASP:HB2	2.39	0.48
1:B:150:THR:O	1:B:151:ASP:HB2	2.14	0.48
1:C:54:TYR:OH	1:C:59:LYS:HD3	2.14	0.48
1:C:119:SER:HB2	1:C:122:GLU:HB2	1.96	0.47
1:D:43:GLN:NE2	1:D:46:LYS:HD2	2.29	0.47
1:D:158:ARG:HG3	1:D:158:ARG:HH11	1.78	0.47
1:F:184:SER:O	1:F:185:SER:HB3	2.15	0.47
1:E:9:LEU:HG	1:E:25:ILE:HD11	1.97	0.47
1:B:81:LEU:HA	1:B:84:VAL:CG2	2.45	0.47
1:F:117:SER:HA	1:F:186:ALA:HA	1.96	0.47
1:D:174:LEU:N	1:D:174:LEU:HD12	2.29	0.47
1:F:45:GLY:HA2	1:F:200:LYS:HG2	1.96	0.47
1:F:135:LYS:HE3	1:F:135:LYS:H	1.80	0.47
1:D:116:LYS:HD2	1:D:121:HIS:HA	1.96	0.47
1:G:210:ILE:HG22	1:G:211:ALA:N	2.30	0.47
1:C:42:MET:HG2	1:C:43:GLN:N	2.30	0.47
1:F:12:TYR:HA	1:F:13:PRO:HD3	1.76	0.46
1:F:177:ALA:HA	1:F:178:PRO:HD3	1.79	0.46
1:G:29:ILE:H	1:G:35:LYS:CE	2.23	0.46
1:E:178:PRO:HB3	1:E:217:ILE:HD11	1.96	0.46
1:H:210:ILE:HG22	1:H:211:ALA:N	2.30	0.46
1:C:2:ASP:HB3	1:C:216:ASN:OD1	2.16	0.46
1:A:96:SER:OG	1:A:230:LEU:HA	2.15	0.46
1:B:51:HIS:CE1	1:D:116:LYS:HZ2	2.33	0.46
1:C:131:ASN:HB3	1:D:122:GLU:HG3	1.98	0.46
1:A:120:THR:O	1:A:121:HIS:HB2	2.16	0.46
1:A:170:VAL:HG22	1:A:226:THR:CG2	2.46	0.46
1:G:60:ARG:HB2	1:G:60:ARG:CZ	2.46	0.45
1:H:181:ILE:HG23	1:H:182:TRP:HD1	1.81	0.45
1:A:11:THR:O	1:A:205:HIS:HE1	1.98	0.45
1:C:43:GLN:HE21	1:C:46:LYS:HG3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:SER:HB2	1:H:122:GLU:CB	2.40	0.45
1:H:198:LEU:HD13	1:H:200:LYS:HE3	1.99	0.45
1:B:60:ARG:HE	1:B:76:SER:HB3	1.81	0.45
1:B:103:THR:O	1:B:199:ILE:HA	2.17	0.45
1:F:172:ARG:HD2	1:F:221:ILE:HG12	1.99	0.45
1:G:119:SER:O	1:G:121:HIS:N	2.50	0.45
1:H:121:HIS:O	1:H:121:HIS:CG	2.69	0.45
1:H:207:ALA:HA	1:H:208:ASP:HA	1.79	0.45
1:D:117:SER:HB3	1:D:118:ASN:H	1.64	0.45
1:E:201:SER:HB2	1:E:206:PRO:HB3	1.99	0.44
1:G:14:ASN:C	1:G:19:ASP:HB2	2.41	0.44
1:H:14:ASN:C	1:H:19:ASP:HB2	2.42	0.44
1:A:111:PHE:CE2	1:A:113:SER:HB2	2.51	0.44
1:F:178:PRO:HB3	1:F:217:ILE:HD11	1.98	0.44
1:C:12:TYR:HA	1:C:13:PRO:HD3	1.81	0.44
1:G:200:LYS:HB2	1:G:200:LYS:NZ	2.33	0.44
1:H:117:SER:O	1:H:187:VAL:HG23	2.17	0.44
1:A:42:MET:HE3	1:A:42:MET:HB3	1.83	0.44
1:B:174:LEU:HD12	1:B:174:LEU:N	2.32	0.44
1:B:221:ILE:HA	1:B:222:PRO:HD3	1.90	0.44
1:B:120:THR:CG2	1:D:196:THR:HG21	2.46	0.44
1:F:119:SER:HB2	1:F:122:GLU:CB	2.47	0.44
1:H:53:ILE:HG22	1:H:192:GLU:HG3	2.00	0.44
1:A:88:TRP:HB3	1:A:217:ILE:HD11	2.00	0.43
1:C:135:LYS:HD2	1:C:135:LYS:O	2.18	0.43
1:E:32:VAL:HG22	1:E:32:VAL:O	2.18	0.43
1:H:120:THR:O	1:H:121:HIS:HB3	2.17	0.43
1:D:198:LEU:HD13	1:D:200:LYS:HE3	2.01	0.43
1:E:42:MET:HE3	1:E:42:MET:HB3	1.88	0.43
1:G:90:ARG:NH1	1:G:217:ILE:HG23	2.34	0.43
1:F:151:ASP:HB2	1:F:153:ASN:ND2	2.31	0.43
1:G:17:ILE:HD13	1:G:228:ARG:HD3	2.00	0.43
1:G:117:SER:HA	1:G:185:SER:O	2.17	0.43
1:B:207:ALA:HA	1:B:208:ASP:HA	1.88	0.43
1:B:194:THR:HG21	1:D:121:HIS:NE2	2.34	0.43
1:D:208:ASP:OD2	1:D:227:GLY:HA2	2.18	0.43
1:A:14:ASN:O	1:A:19:ASP:HB2	2.19	0.43
1:D:207:ALA:HA	1:D:208:ASP:HA	1.85	0.43
1:A:118:ASN:CB	1:A:185:SER:HB2	2.49	0.43
1:B:45:GLY:HA2	1:B:200:LYS:HB3	2.01	0.43
1:A:46:LYS:HA	1:A:46:LYS:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HA	1:A:197:PHE:O	2.19	0.42
1:B:226:THR:HG22	1:B:227:GLY:N	2.35	0.42
1:F:42:MET:HE2	1:F:44:ASN:HA	2.01	0.42
1:H:48:GLY:O	1:H:196:THR:HA	2.20	0.42
1:A:116:LYS:N	1:A:116:LYS:CD	2.82	0.42
1:A:177:ALA:HA	1:A:178:PRO:HD3	1.88	0.42
1:E:170:VAL:CG2	1:E:226:THR:HA	2.50	0.42
1:G:177:ALA:HB2	1:H:177:ALA:HB2	2.01	0.42
1:G:178:PRO:HB3	1:G:217:ILE:CD1	2.49	0.42
1:H:148:THR:HG22	1:H:154:LEU:HD13	2.02	0.42
1:C:132:GLN:HE21	1:C:132:GLN:HB2	1.72	0.42
1:C:137:GLN:HG3	1:C:139:ASP:OD1	2.20	0.42
1:B:177:ALA:HA	1:B:178:PRO:HD3	1.89	0.42
1:D:2:ASP:HB3	1:D:216:ASN:OD1	2.20	0.42
1:E:25:ILE:O	1:E:37:THR:HA	2.20	0.41
1:H:100:TYR:HB2	1:H:207:ALA:CB	2.49	0.41
1:E:143:GLN:OE1	1:E:172:ARG:HD3	2.19	0.41
1:C:42:MET:HE2	1:C:42:MET:HB3	1.78	0.41
1:G:42:MET:HE3	1:G:42:MET:HB3	1.89	0.41
1:E:25:ILE:HG22	1:E:38:ALA:HB3	2.02	0.41
1:G:117:SER:O	1:G:119:SER:N	2.54	0.41
1:E:25:ILE:HG12	1:E:65:VAL:CG2	2.49	0.41
1:H:156:LEU:O	1:H:171:GLY:HA3	2.20	0.41
1:D:103:THR:O	1:D:199:ILE:HA	2.21	0.41
1:D:181:ILE:HG23	1:D:182:TRP:HD1	1.85	0.41
1:G:36:LYS:HD2	1:G:36:LYS:HA	1.93	0.41
1:G:58:ASP:HB3	1:G:60:ARG:HH12	1.80	0.41
1:A:101:LYS:HG3	1:A:165:PRO:HB2	2.03	0.41
1:B:14:ASN:C	1:B:19:ASP:HB2	2.44	0.41
1:D:16:ASP:OD2	1:D:228:ARG:NH2	2.54	0.41
1:D:33:ARG:HD3	1:D:236:ALA:O	2.20	0.41
1:D:43:GLN:HE21	1:D:46:LYS:HD2	1.85	0.41
1:A:116:LYS:N	1:A:116:LYS:HD3	2.36	0.41
1:E:124:ASN:ND2	1:F:131:ASN:H	2.18	0.41
1:H:177:ALA:HA	1:H:178:PRO:HD3	1.98	0.41
1:C:161:SER:C	1:C:163:GLY:H	2.29	0.40
1:D:107:LEU:N	1:D:107:LEU:HD12	2.35	0.40
1:G:118:ASN:H	1:G:118:ASN:HD22	1.68	0.40
1:G:177:ALA:HA	1:G:178:PRO:HD3	1.88	0.40
1:D:25:ILE:HG23	1:D:40:TRP:HB2	2.04	0.40
1:E:42:MET:HE1	1:E:206:PRO:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:ASN:C	1:F:19:ASP:HB2	2.45	0.40
1:C:17:ILE:CD1	1:C:228:ARG:HD3	2.52	0.40
1:D:35:LYS:HA	1:D:35:LYS:HD3	1.73	0.40
1:E:14:ASN:C	1:E:19:ASP:HB2	2.46	0.40
1:E:36:LYS:HD2	1:E:76:SER:O	2.22	0.40
1:H:20:PRO:HD2	1:H:24:HIS:CE1	2.57	0.40
1:A:35:LYS:HD3	1:A:35:LYS:HA	1.92	0.40
1:A:49:THR:OG1	1:A:196:THR:HG22	2.22	0.40
1:C:187:VAL:HG13	1:C:188:VAL:HG23	2.04	0.40
1:D:36:LYS:HE3	1:D:36:LYS:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/237 (99%)	220 (94%)	14 (6%)	1 (0%)	30	43
1	B	235/237 (99%)	221 (94%)	14 (6%)	0	100	100
1	C	235/237 (99%)	219 (93%)	15 (6%)	1 (0%)	30	43
1	D	235/237 (99%)	218 (93%)	15 (6%)	2 (1%)	14	22
1	E	235/237 (99%)	219 (93%)	14 (6%)	2 (1%)	14	22
1	F	235/237 (99%)	217 (92%)	17 (7%)	1 (0%)	30	43
1	G	235/237 (99%)	215 (92%)	17 (7%)	3 (1%)	9	14
1	H	235/237 (99%)	214 (91%)	20 (8%)	1 (0%)	30	43
All	All	1880/1896 (99%)	1743 (93%)	126 (7%)	11 (1%)	21	32

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	THR
1	E	120	THR
1	F	185	SER
1	G	118	ASN
1	G	120	THR
1	H	117	SER
1	C	150	THR
1	E	118	ASN
1	D	118	ASN
1	D	234	PRO
1	G	217	ILE

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	203/203 (100%)	190 (94%)	13 (6%)	16	28
1	B	203/203 (100%)	194 (96%)	9 (4%)	25	43
1	C	203/203 (100%)	200 (98%)	3 (2%)	57	77
1	D	203/203 (100%)	187 (92%)	16 (8%)	11	19
1	E	203/203 (100%)	197 (97%)	6 (3%)	36	58
1	F	203/203 (100%)	193 (95%)	10 (5%)	22	39
1	G	203/203 (100%)	191 (94%)	12 (6%)	18	31
1	H	203/203 (100%)	191 (94%)	12 (6%)	18	31
All	All	1624/1624 (100%)	1543 (95%)	81 (5%)	22	38

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	42	MET
1	A	49	THR
1	A	53	ILE
1	A	101	LYS

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Mol	Chain	Res	Type
1	A	116	LYS
1	A	122	GLU
1	A	135	LYS
1	A	150	THR
1	A	161	SER
1	A	170	VAL
1	A	208	ASP
1	A	228	ARG
1	B	51	HIS
1	B	53	ILE
1	B	101	LYS
1	B	121	HIS
1	B	122	GLU
1	B	150	THR
1	B	166	GLN
1	B	170	VAL
1	B	218	ASP
1	C	151	ASP
1	C	226	THR
1	C	228	ARG
1	D	29	ILE
1	D	33	ARG
1	D	36	LYS
1	D	99	LEU
1	D	101	LYS
1	D	122	GLU
1	D	123	THR
1	D	134	SER
1	D	150	THR
1	D	170	VAL
1	D	183	GLU
1	D	188	VAL
1	D	198	LEU
1	D	217	ILE
1	D	228	ARG
1	D	235	ASP
1	E	25	ILE
1	E	36	LYS
1	E	53	ILE
1	E	122	GLU
1	E	132	GLN
1	E	147	THR

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Mol	Chain	Res	Type
1	F	35	LYS
1	F	42	MET
1	F	101	LYS
1	F	121	HIS
1	F	135	LYS
1	F	150	THR
1	F	166	GLN
1	F	170	VAL
1	F	188	VAL
1	F	228	ARG
1	G	42	MET
1	G	64	VAL
1	G	72	SER
1	G	116	LYS
1	G	118	ASN
1	G	150	THR
1	G	170	VAL
1	G	185	SER
1	G	188	VAL
1	G	200	LYS
1	G	220	SER
1	G	228	ARG
1	H	36	LYS
1	H	39	LYS
1	H	42	MET
1	H	64	VAL
1	H	69	ASN
1	H	116	LYS
1	H	122	GLU
1	H	135	LYS
1	H	150	THR
1	H	158	ARG
1	H	198	LEU
1	H	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	166	GLN
1	A	237	ASN
1	B	43	GLN

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Mol	Chain	Res	Type
1	B	51	HIS
1	B	132	GLN
1	B	137	GLN
1	C	43	GLN
1	C	69	ASN
1	C	83	ASN
1	D	43	GLN
1	D	131	ASN
1	D	162	ASN
1	D	166	GLN
1	E	41	ASN
1	E	51	HIS
1	E	118	ASN
1	E	124	ASN
1	E	132	GLN
1	E	205	HIS
1	E	237	ASN
1	F	43	GLN
1	F	51	HIS
1	F	153	ASN
1	F	237	ASN
1	G	69	ASN
1	G	153	ASN
1	G	237	ASN
1	H	43	GLN

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

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	237/237 (100%)	-0.70	3 (1%) 75 71	16, 27, 58, 89	0
1	B	237/237 (100%)	-0.65	3 (1%) 75 71	15, 30, 60, 89	0
1	C	237/237 (100%)	-0.58	7 (2%) 52 48	17, 31, 63, 99	0
1	D	237/237 (100%)	-0.70	7 (2%) 52 48	15, 27, 55, 100	0
1	E	237/237 (100%)	-0.60	5 (2%) 63 59	18, 32, 62, 96	0
1	F	237/237 (100%)	-0.73	3 (1%) 75 71	13, 27, 57, 84	0
1	G	237/237 (100%)	-0.67	5 (2%) 63 59	17, 27, 61, 99	0
1	H	237/237 (100%)	-0.64	5 (2%) 63 59	18, 31, 60, 101	0
All	All	1896/1896 (100%)	-0.66	38 (2%) 65 60	13, 29, 60, 101	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	ASN	6.1
1	G	119	SER	5.4
1	H	121	HIS	5.3
1	B	121	HIS	5.1
1	C	120	THR	5.1
1	E	121	HIS	5.1
1	G	118	ASN	4.9
1	F	121	HIS	4.6
1	G	120	THR	4.3
1	D	119	SER	4.1
1	B	120	THR	3.7
1	H	120	THR	3.7
1	H	119	SER	3.5
1	B	118	ASN	3.5
1	C	119	SER	3.4
1	E	1	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	118	ASN	3.3
1	E	119	SER	3.3
1	F	120	THR	3.2
1	C	117	SER	3.0
1	A	120	THR	3.0
1	D	120	THR	3.0
1	G	121	HIS	3.0
1	H	118	ASN	2.9
1	D	121	HIS	2.8
1	E	118	ASN	2.8
1	C	121	HIS	2.7
1	A	150	THR	2.5
1	A	161	SER	2.5
1	D	150	THR	2.3
1	C	1	ALA	2.3
1	F	118	ASN	2.3
1	C	150	THR	2.2
1	G	162	ASN	2.2
1	D	151	ASP	2.1
1	H	185	SER	2.1
1	D	185	SER	2.1
1	E	120	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	B	238	1/1	0.93	0.04	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	E	238	1/1	0.94	0.04	30,30,30,30	0
3	CA	D	239	1/1	0.94	0.02	25,25,25,25	0
2	MN	G	238	1/1	0.95	0.02	38,38,38,38	0
2	MN	D	238	1/1	0.96	0.04	38,38,38,38	0
3	CA	E	239	1/1	0.97	0.05	26,26,26,26	0
3	CA	G	239	1/1	0.97	0.02	26,26,26,26	0
3	CA	H	239	1/1	0.97	0.02	29,29,29,29	0
3	CA	B	239	1/1	0.98	0.02	28,28,28,28	0
3	CA	C	239	1/1	0.98	0.03	24,24,24,24	0
2	MN	F	238	1/1	0.98	0.02	34,34,34,34	0
2	MN	A	238	1/1	0.98	0.02	33,33,33,33	0
2	MN	H	238	1/1	0.98	0.02	40,40,40,40	0
3	CA	A	239	1/1	0.98	0.03	21,21,21,21	0
2	MN	C	238	1/1	0.99	0.02	41,41,41,41	0
3	CA	F	239	1/1	0.99	0.01	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.