



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:50 PM UTC

PDB ID : 4DKM / pdb_00004dkm
Title : Crystal Structure of Amphioxus GFPc1a
Authors : Deheyn, D.D.; Bomati, E.K.
Deposited on : 2012-02-03
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

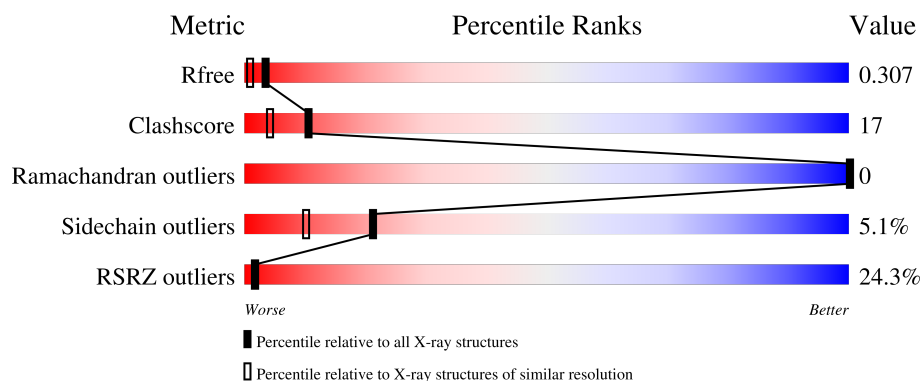
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



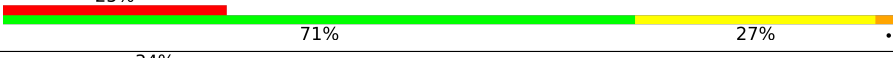
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	214	17% 70% 28% .
1	B	214	27% 70% 28% .
1	C	214	24% 71% 26% .
1	D	214	19% 70% 28% .
1	E	214	25% 70% 28% .

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Mol	Chain	Length	Quality of chain
1	F	214	 21% 69% 28% .
1	G	214	 25% 71% 27% .
1	H	214	 34% 71% 26% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13957 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 Amphioxus Green Fluorescent Protein, GFPc1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1672	1072	277	318	5			
1	B	214	Total	C	N	O	S	0	0	0
			1672	1072	277	318	5			
1	C	214	Total	C	N	O	S	0	0	0
			1672	1072	277	318	5			
1	D	214	Total	C	N	O	S	0	0	0
			1672	1072	277	318	5			
1	E	214	Total	C	N	O	S	0	0	0
			1672	1072	277	318	5			
1	F	214	Total	C	N	O	S	0	0	0
			1672	1072	277	318	5			
1	G	214	Total	C	N	O	S	0	0	0
			1672	1072	277	318	5			
1	H	214	Total	C	N	O	S	0	0	0
			1672	1072	277	318	5			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	CR2	GLY	chromophore	UNP C3YRA3
A	60	CR2	TYR	chromophore	UNP C3YRA3
A	60	CR2	GLY	chromophore	UNP C3YRA3
A	123	PRO	LEU	conflict	UNP C3YRA3
A	124	ALA	GLY	conflict	UNP C3YRA3
A	171	LEU	VAL	conflict	UNP C3YRA3
A	184	THR	SER	conflict	UNP C3YRA3
B	58	CR2	GLY	chromophore	UNP C3YRA3
B	58	CR2	TYR	chromophore	UNP C3YRA3
B	58	CR2	GLY	chromophore	UNP C3YRA3
B	123	PRO	LEU	conflict	UNP C3YRA3
B	124	ALA	GLY	conflict	UNP C3YRA3
B	171	LEU	VAL	conflict	UNP C3YRA3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	184	THR	SER	conflict	UNP C3YRA3
C	60	CR2	GLY	chromophore	UNP C3YRA3
C	60	CR2	TYR	chromophore	UNP C3YRA3
C	60	CR2	GLY	chromophore	UNP C3YRA3
C	123	PRO	LEU	conflict	UNP C3YRA3
C	124	ALA	GLY	conflict	UNP C3YRA3
C	171	LEU	VAL	conflict	UNP C3YRA3
C	184	THR	SER	conflict	UNP C3YRA3
D	60	CR2	GLY	chromophore	UNP C3YRA3
D	60	CR2	TYR	chromophore	UNP C3YRA3
D	60	CR2	GLY	chromophore	UNP C3YRA3
D	123	PRO	LEU	conflict	UNP C3YRA3
D	124	ALA	GLY	conflict	UNP C3YRA3
D	171	LEU	VAL	conflict	UNP C3YRA3
D	184	THR	SER	conflict	UNP C3YRA3
E	60	CR2	GLY	chromophore	UNP C3YRA3
E	60	CR2	TYR	chromophore	UNP C3YRA3
E	60	CR2	GLY	chromophore	UNP C3YRA3
E	123	PRO	LEU	conflict	UNP C3YRA3
E	124	ALA	GLY	conflict	UNP C3YRA3
E	171	LEU	VAL	conflict	UNP C3YRA3
E	184	THR	SER	conflict	UNP C3YRA3
F	60	CR2	GLY	chromophore	UNP C3YRA3
F	60	CR2	TYR	chromophore	UNP C3YRA3
F	60	CR2	GLY	chromophore	UNP C3YRA3
F	123	PRO	LEU	conflict	UNP C3YRA3
F	124	ALA	GLY	conflict	UNP C3YRA3
F	171	LEU	VAL	conflict	UNP C3YRA3
F	184	THR	SER	conflict	UNP C3YRA3
G	60	CR2	GLY	chromophore	UNP C3YRA3
G	60	CR2	TYR	chromophore	UNP C3YRA3
G	60	CR2	GLY	chromophore	UNP C3YRA3
G	123	PRO	LEU	conflict	UNP C3YRA3
G	124	ALA	GLY	conflict	UNP C3YRA3
G	171	LEU	VAL	conflict	UNP C3YRA3
G	184	THR	SER	conflict	UNP C3YRA3
H	60	CR2	GLY	chromophore	UNP C3YRA3
H	60	CR2	TYR	chromophore	UNP C3YRA3
H	60	CR2	GLY	chromophore	UNP C3YRA3
H	123	PRO	LEU	conflict	UNP C3YRA3
H	124	ALA	GLY	conflict	UNP C3YRA3
H	171	LEU	VAL	conflict	UNP C3YRA3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	184	THR	SER	conflict	UNP C3YRA3

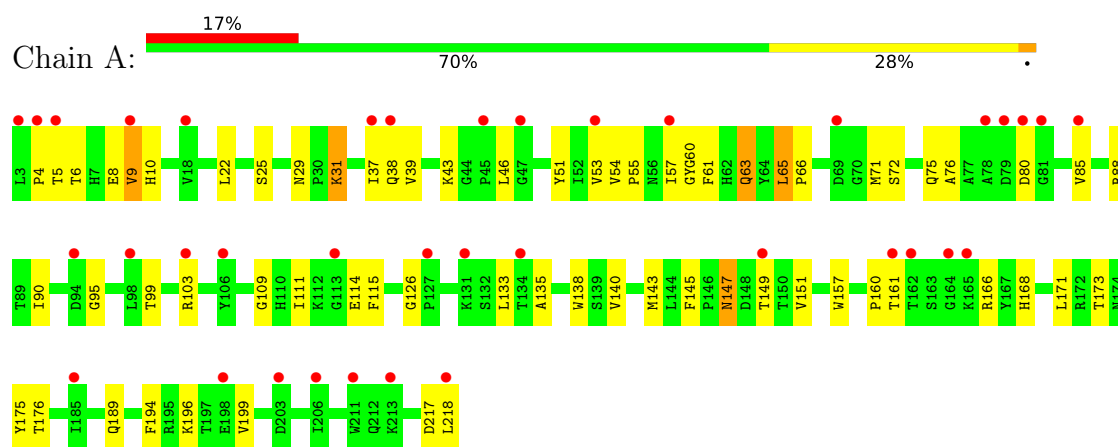
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	99	Total 99	O 99	0	0
2	B	101	Total 101	O 101	0	0
2	C	82	Total 82	O 82	0	0
2	D	52	Total 52	O 52	0	0
2	E	52	Total 52	O 52	0	0
2	F	88	Total 88	O 88	0	0
2	G	60	Total 60	O 60	0	0
2	H	47	Total 47	O 47	0	0

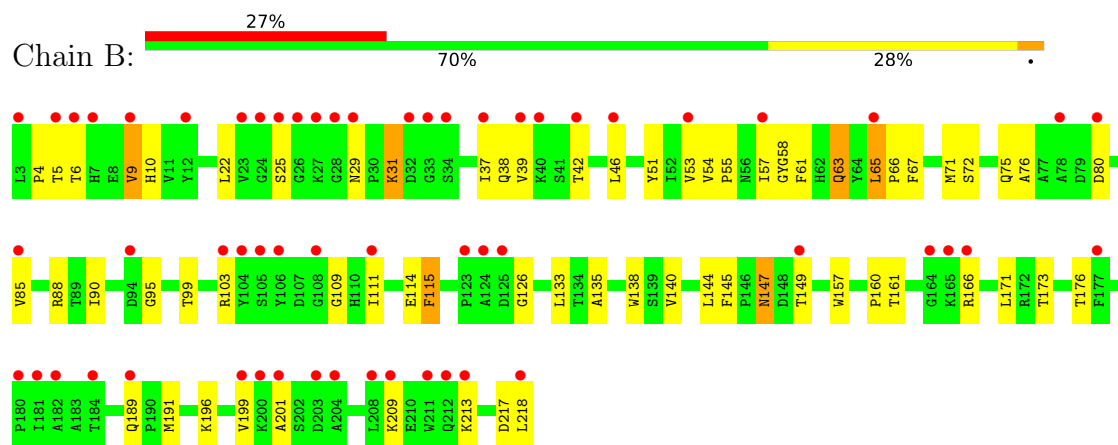
3 Residue-property plots [i](#)

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.

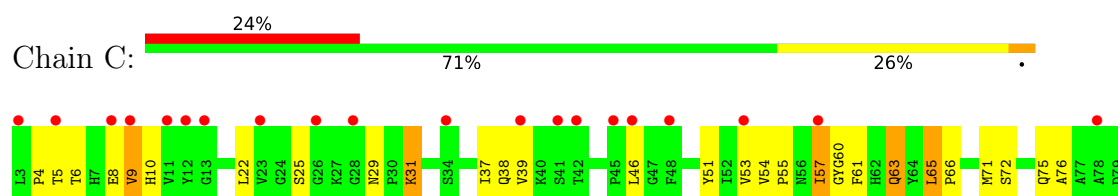
- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a

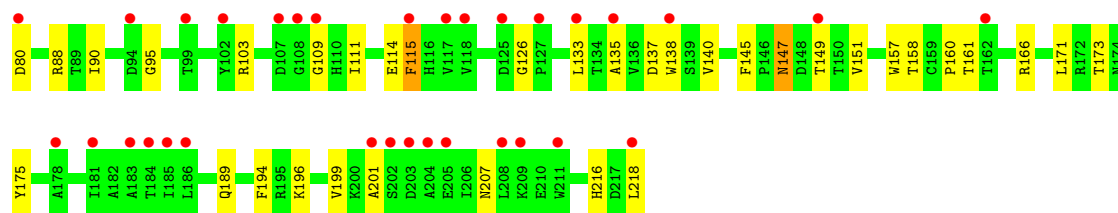


- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a

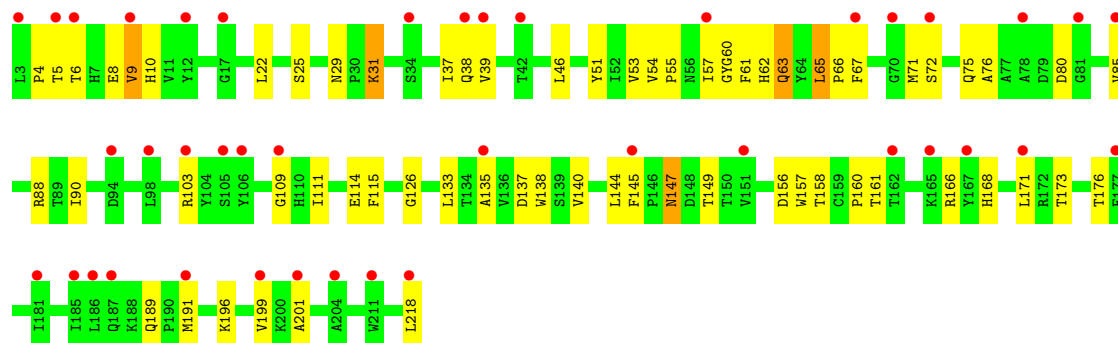


- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a

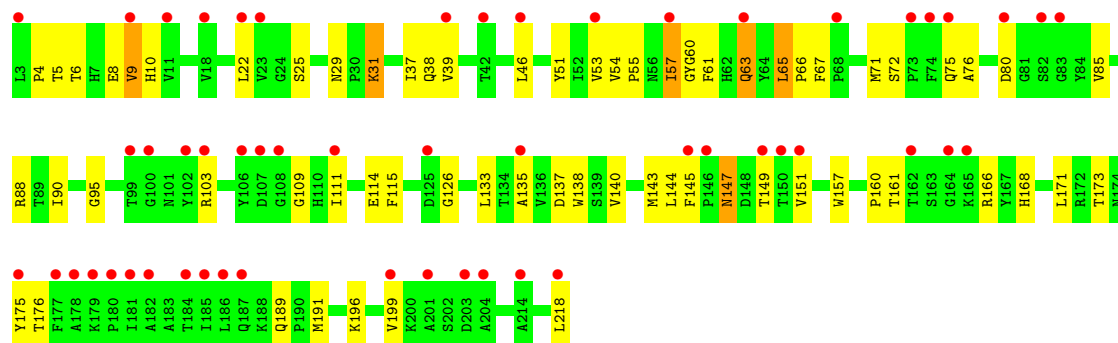




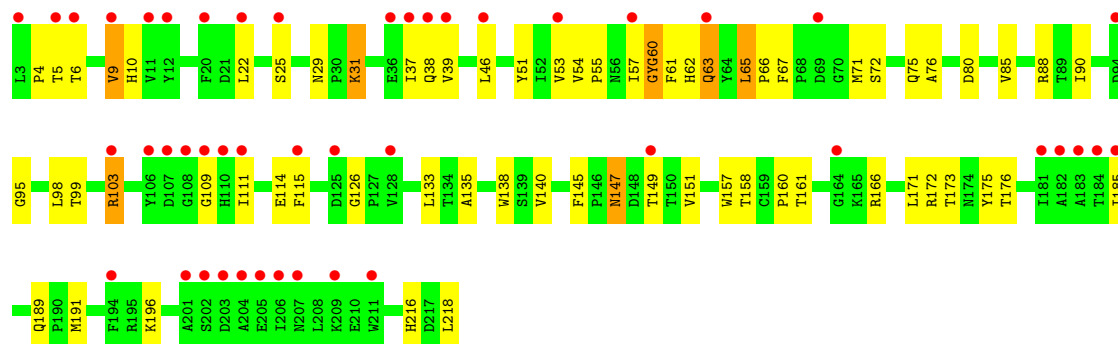
• Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a



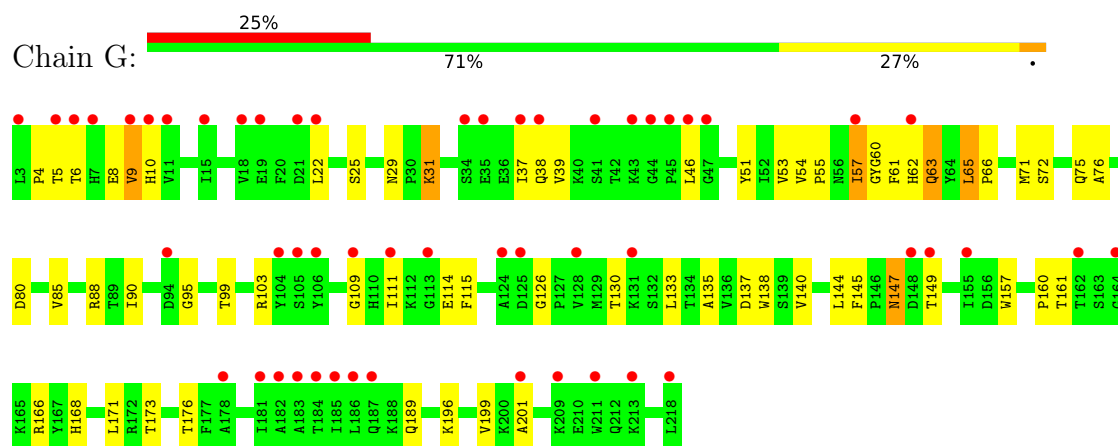
• Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a



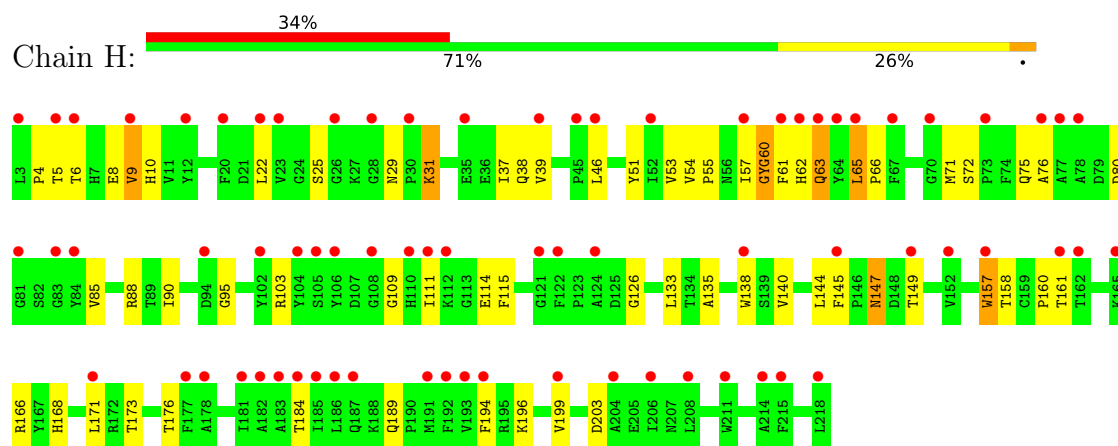
• Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a



• Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a



• Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.76Å 130.46Å 106.33Å 90.00° 128.39° 90.00°	Depositor
Resolution (Å)	45.02 – 1.95 45.02 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.02-1.95) 97.3 (45.02-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.293 , 0.320 0.297 , 0.307	Depositor DCC
R_{free} test set	6014 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13957	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: CR2

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	0.46	0/1701	0.94	5/2313 (0.2%)
1	B	0.45	0/1701	0.94	7/2313 (0.3%)
1	C	0.44	0/1701	0.94	7/2313 (0.3%)
1	D	0.41	0/1701	0.93	7/2313 (0.3%)
1	E	0.42	0/1701	0.94	6/2313 (0.3%)
1	F	0.46	0/1701	0.94	5/2313 (0.2%)
1	G	0.41	0/1701	0.94	7/2313 (0.3%)
1	H	0.42	0/1701	0.95	7/2313 (0.3%)
All	All	0.43	0/13608	0.94	51/18504 (0.3%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	GLY	CA-C-N	7.10	127.09	119.28
1	B	126	GLY	C-N-CA	7.10	127.09	119.28
1	H	72	SER	N-CA-C	-6.86	101.16	110.36
1	A	126	GLY	CA-C-N	6.49	126.99	119.47
1	A	126	GLY	C-N-CA	6.49	126.99	119.47
1	G	126	GLY	CA-C-N	6.39	126.31	119.28
1	G	126	GLY	C-N-CA	6.39	126.31	119.28
1	C	126	GLY	CA-C-N	6.06	126.50	119.47
1	C	126	GLY	C-N-CA	6.06	126.50	119.47
1	H	126	GLY	CA-C-N	5.89	126.30	119.47
1	H	126	GLY	C-N-CA	5.89	126.30	119.47
1	C	199	VAL	N-CA-C	5.67	116.05	108.11
1	D	126	GLY	CA-C-N	5.66	126.04	119.47
1	D	126	GLY	C-N-CA	5.66	126.04	119.47
1	C	72	SER	N-CA-C	-5.61	101.97	110.39
1	F	126	GLY	CA-C-N	5.61	125.72	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	126	GLY	C-N-CA	5.61	125.72	119.32
1	D	72	SER	N-CA-C	-5.59	102.00	110.39
1	B	72	SER	N-CA-C	-5.59	102.01	110.39
1	G	199	VAL	N-CA-C	5.52	115.84	108.11
1	E	199	VAL	N-CA-C	5.49	115.80	108.11
1	E	72	SER	N-CA-C	-5.48	102.17	110.39
1	H	199	VAL	N-CA-C	5.46	115.98	108.12
1	G	95	GLY	N-CA-C	-5.41	107.07	114.64
1	E	95	GLY	N-CA-C	-5.40	107.08	114.64
1	G	72	SER	N-CA-C	-5.39	102.30	110.39
1	F	72	SER	N-CA-C	-5.36	102.35	110.39
1	D	199	VAL	N-CA-C	5.34	115.81	108.12
1	B	95	GLY	N-CA-C	-5.32	107.19	114.64
1	A	72	SER	N-CA-C	-5.29	102.46	110.39
1	C	95	GLY	N-CA-C	-5.27	107.26	114.64
1	A	199	VAL	N-CA-C	5.26	115.47	108.11
1	C	115	PHE	N-CA-C	5.25	117.08	108.52
1	A	95	GLY	N-CA-C	-5.21	107.34	114.64
1	E	126	GLY	CA-C-N	5.21	125.52	119.47
1	E	126	GLY	C-N-CA	5.21	125.52	119.47
1	F	95	GLY	N-CA-C	-5.18	107.39	114.64
1	D	201	ALA	N-CA-C	5.11	117.02	108.99
1	H	95	GLY	N-CA-C	-5.11	107.48	114.64
1	D	168	HIS	N-CA-C	5.09	118.41	110.32
1	G	201	ALA	N-CA-C	5.08	116.96	108.99
1	B	199	VAL	N-CA-C	5.06	115.41	108.12
1	H	157	TRP	N-CA-C	5.06	117.74	109.59
1	F	216	HIS	N-CA-C	-5.06	107.66	113.88
1	D	156	ASP	N-CA-C	-5.04	100.30	108.41
1	B	115	PHE	N-CA-C	5.04	116.73	108.52
1	H	168	HIS	N-CA-C	5.03	118.32	110.32
1	E	168	HIS	N-CA-C	5.02	118.30	110.32
1	B	201	ALA	N-CA-C	5.01	116.86	108.99
1	G	168	HIS	N-CA-C	5.01	118.28	110.32
1	C	201	ALA	N-CA-C	5.01	116.85	108.99

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	1672	0	1599	56	0
1	B	1672	0	1599	61	0
1	C	1672	0	1599	55	0
1	D	1672	0	1599	58	0
1	E	1672	0	1599	57	0
1	F	1672	0	1599	58	0
1	G	1672	0	1599	54	0
1	H	1672	0	1599	54	3
2	A	99	0	0	4	0
2	B	101	0	0	8	0
2	C	82	0	0	2	0
2	D	52	0	0	1	0
2	E	52	0	0	1	0
2	F	88	0	0	3	0
2	G	60	0	0	1	0
2	H	47	0	0	1	0
All	All	13957	0	12792	439	3

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 17.

All (439) 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:E:147:ASN:HD22	1:E:149:THR:H	1.22	0.88
1:G:63:GLN:HG3	1:G:111:ILE:HD13	1.56	0.88
1:H:147:ASN:HD22	1:H:149:THR:H	1.23	0.87
1:E:63:GLN:HG3	1:E:111:ILE:HD13	1.56	0.87
1:D:63:GLN:HG3	1:D:111:ILE:HD13	1.57	0.87
1:H:63:GLN:HG3	1:H:111:ILE:HD13	1.55	0.87
1:C:160:PRO:HG3	1:C:166:ARG:NH1	1.90	0.86
1:A:63:GLN:HG3	1:A:111:ILE:HD13	1.56	0.86
1:G:160:PRO:HG3	1:G:166:ARG:NH1	1.90	0.86
1:D:160:PRO:HG3	1:D:166:ARG:NH1	1.91	0.86
1:H:160:PRO:HG3	1:H:166:ARG:NH1	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:PRO:HG3	1:F:166:ARG:NH1	1.91	0.86
1:A:160:PRO:HG3	1:A:166:ARG:NH1	1.91	0.85
1:B:63:GLN:HG3	1:B:111:ILE:HD13	1.58	0.85
1:E:160:PRO:HG3	1:E:166:ARG:NH1	1.89	0.85
1:F:63:GLN:HG3	1:F:111:ILE:HD13	1.58	0.85
1:G:160:PRO:HG3	1:G:166:ARG:HH12	1.42	0.85
1:B:160:PRO:HG3	1:B:166:ARG:HH12	1.42	0.85
1:C:63:GLN:HG3	1:C:111:ILE:HD13	1.58	0.85
1:C:160:PRO:HG3	1:C:166:ARG:HH12	1.40	0.85
1:B:147:ASN:HD22	1:B:149:THR:H	1.25	0.85
1:D:160:PRO:HG3	1:D:166:ARG:HH12	1.41	0.85
1:E:160:PRO:HG3	1:E:166:ARG:HH12	1.41	0.84
1:H:160:PRO:HG3	1:H:166:ARG:HH12	1.42	0.84
1:A:99:THR:HG21	1:F:99:THR:HG21	1.60	0.84
1:B:160:PRO:HG3	1:B:166:ARG:NH1	1.92	0.83
1:D:147:ASN:HD22	1:D:149:THR:H	1.23	0.83
1:C:147:ASN:HD22	1:C:149:THR:H	1.23	0.83
1:A:160:PRO:HG3	1:A:166:ARG:HH12	1.40	0.83
1:F:147:ASN:HD22	1:F:149:THR:H	1.24	0.82
1:A:147:ASN:HD22	1:A:149:THR:H	1.24	0.82
1:F:160:PRO:HG3	1:F:166:ARG:HH12	1.41	0.82
1:G:147:ASN:HD22	1:G:149:THR:H	1.24	0.81
1:E:143:MET:HE3	2:E:352:HOH:O	1.81	0.79
1:A:88:ARG:HD3	1:A:173:THR:OG1	1.82	0.78
1:F:88:ARG:HD3	1:F:173:THR:OG1	1.84	0.78
1:C:207:ASN:HB3	2:C:319:HOH:O	1.84	0.76
1:B:88:ARG:HD3	1:B:173:THR:OG1	1.85	0.75
1:D:88:ARG:HD3	1:D:173:THR:OG1	1.85	0.74
1:H:63:GLN:H	1:H:63:GLN:NE2	1.85	0.74
1:B:99:THR:HG21	1:G:99:THR:HG21	1.69	0.74
1:A:63:GLN:H	1:A:63:GLN:NE2	1.86	0.73
1:D:31:LYS:HG2	1:G:130:THR:HB	1.69	0.72
1:D:140:VAL:HG11	1:H:140:VAL:HG11	1.72	0.72
1:C:90:ILE:HG12	1:C:171:LEU:HG	1.71	0.72
1:E:63:GLN:H	1:E:63:GLN:NE2	1.88	0.72
1:H:63:GLN:HG3	1:H:111:ILE:CD1	2.19	0.72
1:E:88:ARG:HD3	1:E:173:THR:OG1	1.90	0.72
1:F:63:GLN:H	1:F:63:GLN:NE2	1.87	0.72
1:G:63:GLN:HG3	1:G:111:ILE:CD1	2.20	0.72
1:A:63:GLN:HG3	1:A:111:ILE:CD1	2.20	0.72
1:G:149:THR:HG22	2:G:355:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:ARG:HD3	1:G:173:THR:OG1	1.88	0.71
1:D:63:GLN:HG3	1:D:111:ILE:CD1	2.21	0.71
1:F:90:ILE:HG12	1:F:171:LEU:HG	1.73	0.71
1:B:63:GLN:H	1:B:63:GLN:NE2	1.88	0.71
1:B:90:ILE:HG12	1:B:171:LEU:HG	1.73	0.71
1:C:88:ARG:HD3	1:C:173:THR:OG1	1.89	0.71
1:E:63:GLN:HG3	1:E:111:ILE:CD1	2.20	0.71
1:C:22:LEU:HB3	1:C:39:VAL:CG2	2.21	0.70
1:F:63:GLN:HG3	1:F:111:ILE:CD1	2.21	0.70
1:G:63:GLN:H	1:G:63:GLN:NE2	1.88	0.70
1:H:22:LEU:HB3	1:H:39:VAL:CG2	2.22	0.70
1:G:90:ILE:HG12	1:G:171:LEU:HG	1.73	0.70
1:D:63:GLN:H	1:D:63:GLN:NE2	1.89	0.70
1:C:63:GLN:HG3	1:C:111:ILE:CD1	2.22	0.69
1:D:22:LEU:HB3	1:D:39:VAL:CG2	2.22	0.69
1:A:90:ILE:HG12	1:A:171:LEU:HG	1.73	0.69
1:F:22:LEU:HB3	1:F:39:VAL:CG2	2.22	0.69
1:D:90:ILE:HG12	1:D:171:LEU:HG	1.74	0.69
1:A:22:LEU:HB3	1:A:39:VAL:HG21	1.75	0.69
1:B:63:GLN:HG3	1:B:111:ILE:CD1	2.22	0.69
1:G:4:PRO:HB3	1:G:111:ILE:HD11	1.74	0.69
1:G:22:LEU:HB3	1:G:39:VAL:CG2	2.21	0.69
1:H:90:ILE:HG12	1:H:171:LEU:HG	1.75	0.69
1:A:22:LEU:HB3	1:A:39:VAL:CG2	2.22	0.69
1:A:143:MET:HE3	2:A:313:HOH:O	1.92	0.69
1:B:22:LEU:HB3	1:B:39:VAL:CG2	2.23	0.68
1:H:4:PRO:HB3	1:H:111:ILE:HD11	1.75	0.68
1:F:29:ASN:OD1	1:F:31:LYS:HB2	1.93	0.68
1:C:22:LEU:HB3	1:C:39:VAL:HG21	1.76	0.68
1:F:22:LEU:HB3	1:F:39:VAL:HG21	1.76	0.68
1:C:63:GLN:H	1:C:63:GLN:NE2	1.92	0.68
1:H:29:ASN:OD1	1:H:31:LYS:HB2	1.93	0.68
1:H:88:ARG:HD3	1:H:173:THR:OG1	1.93	0.68
1:E:22:LEU:HB3	1:E:39:VAL:CG2	2.23	0.68
1:B:4:PRO:HB3	1:B:111:ILE:HD11	1.76	0.67
1:D:29:ASN:OD1	1:D:31:LYS:HB2	1.93	0.67
1:G:22:LEU:HB3	1:G:39:VAL:HG21	1.76	0.67
1:H:22:LEU:HB3	1:H:39:VAL:HG21	1.76	0.67
1:B:22:LEU:HB3	1:B:39:VAL:HG21	1.77	0.67
1:B:29:ASN:OD1	1:B:31:LYS:HB2	1.95	0.67
1:A:4:PRO:HB3	1:A:111:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LYS:HE2	2:B:389:HOH:O	1.93	0.67
1:D:4:PRO:HB3	1:D:111:ILE:HD11	1.77	0.67
1:G:29:ASN:OD1	1:G:31:LYS:HB2	1.95	0.66
1:C:29:ASN:OD1	1:C:31:LYS:HB2	1.96	0.66
1:E:22:LEU:HB3	1:E:39:VAL:HG21	1.76	0.66
1:B:213:LYS:HD2	2:B:310:HOH:O	1.94	0.66
1:E:4:PRO:HB3	1:E:111:ILE:HD11	1.76	0.66
1:B:9:VAL:HG22	1:B:61:PHE:CZ	2.31	0.65
1:E:90:ILE:HG12	1:E:171:LEU:HG	1.78	0.65
1:A:29:ASN:OD1	1:A:31:LYS:HB2	1.95	0.65
1:D:9:VAL:HG22	1:D:61:PHE:CZ	2.31	0.65
1:C:4:PRO:HB3	1:C:111:ILE:HD11	1.77	0.65
1:F:4:PRO:HB3	1:F:111:ILE:HD11	1.77	0.65
1:G:9:VAL:HG22	1:G:61:PHE:CZ	2.32	0.65
1:A:63:GLN:H	1:A:63:GLN:HE21	1.44	0.65
1:G:51:TYR:CE2	1:G:135:ALA:HA	2.32	0.65
1:H:63:GLN:H	1:H:63:GLN:HE21	1.43	0.65
1:H:51:TYR:CE2	1:H:135:ALA:HA	2.32	0.65
1:E:29:ASN:OD1	1:E:31:LYS:HB2	1.96	0.65
1:B:51:TYR:CE2	1:B:135:ALA:HA	2.32	0.65
1:E:51:TYR:CE2	1:E:135:ALA:HA	2.32	0.65
1:D:22:LEU:HB3	1:D:39:VAL:HG21	1.76	0.64
1:H:9:VAL:HG22	1:H:61:PHE:CZ	2.33	0.64
1:E:61:PHE:HA	1:E:63:GLN:NE2	2.13	0.64
1:A:9:VAL:HG22	1:A:61:PHE:CZ	2.32	0.64
1:E:9:VAL:HG22	1:E:61:PHE:CZ	2.33	0.64
1:F:63:GLN:H	1:F:63:GLN:HE21	1.43	0.63
1:C:51:TYR:CE2	1:C:135:ALA:HA	2.33	0.63
1:A:51:TYR:CE2	1:A:135:ALA:HA	2.34	0.62
1:E:61:PHE:C	1:E:63:GLN:HE21	2.06	0.62
1:D:51:TYR:CE2	1:D:135:ALA:HA	2.32	0.62
1:C:61:PHE:HA	1:C:63:GLN:NE2	2.14	0.62
1:G:147:ASN:ND2	1:G:149:THR:H	1.97	0.62
1:H:61:PHE:HA	1:H:63:GLN:NE2	2.15	0.62
1:H:61:PHE:C	1:H:63:GLN:HE21	2.07	0.62
1:G:54:VAL:HB	1:G:55:PRO:HD3	1.82	0.62
1:G:76:ALA:O	1:G:80:ASP:HB2	2.00	0.62
1:D:61:PHE:C	1:D:63:GLN:HE21	2.08	0.62
1:E:147:ASN:ND2	1:E:149:THR:H	1.96	0.61
1:H:54:VAL:HB	1:H:55:PRO:HD3	1.82	0.61
1:B:54:VAL:HB	1:B:55:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:GLN:H	1:D:63:GLN:HE21	1.48	0.61
1:D:54:VAL:HB	1:D:55:PRO:HD3	1.83	0.61
1:F:51:TYR:CE2	1:F:135:ALA:HA	2.35	0.61
1:A:76:ALA:O	1:A:80:ASP:HB2	2.01	0.61
1:G:61:PHE:C	1:G:63:GLN:HE21	2.09	0.61
1:A:147:ASN:ND2	1:A:149:THR:H	1.98	0.61
1:B:63:GLN:H	1:B:63:GLN:HE21	1.46	0.61
1:C:61:PHE:C	1:C:63:GLN:HE21	2.09	0.61
1:F:76:ALA:O	1:F:80:ASP:HB2	2.01	0.61
1:D:61:PHE:HA	1:D:63:GLN:NE2	2.16	0.60
1:F:61:PHE:C	1:F:63:GLN:HE21	2.09	0.60
1:G:61:PHE:HA	1:G:63:GLN:NE2	2.15	0.60
1:F:9:VAL:HG22	1:F:61:PHE:CZ	2.36	0.60
1:B:147:ASN:ND2	1:B:149:THR:H	1.99	0.60
1:G:63:GLN:H	1:G:63:GLN:HE21	1.47	0.60
1:B:76:ALA:O	1:B:80:ASP:HB2	2.01	0.60
1:E:54:VAL:HB	1:E:55:PRO:HD3	1.84	0.60
1:C:54:VAL:HB	1:C:55:PRO:HD3	1.84	0.60
1:F:54:VAL:HB	1:F:55:PRO:HD3	1.84	0.60
1:A:61:PHE:HA	1:A:63:GLN:NE2	2.16	0.60
1:D:147:ASN:ND2	1:D:149:THR:H	1.96	0.60
1:C:9:VAL:HG22	1:C:61:PHE:CZ	2.36	0.59
1:H:76:ALA:O	1:H:80:ASP:HB2	2.02	0.59
1:E:76:ALA:O	1:E:80:ASP:HB2	2.02	0.59
1:B:61:PHE:HA	1:B:63:GLN:NE2	2.16	0.59
1:B:61:PHE:C	1:B:63:GLN:HE21	2.11	0.59
1:C:76:ALA:O	1:C:80:ASP:HB2	2.01	0.59
1:F:61:PHE:HA	1:F:63:GLN:NE2	2.17	0.59
1:A:61:PHE:C	1:A:63:GLN:HE21	2.09	0.59
1:A:43:LYS:HE2	2:A:355:HOH:O	2.03	0.59
1:E:63:GLN:H	1:E:63:GLN:HE21	1.48	0.59
1:B:5:THR:HG23	1:B:6:THR:HG23	1.83	0.59
1:C:147:ASN:ND2	1:C:149:THR:H	1.97	0.59
1:F:166:ARG:HH11	1:F:166:ARG:HG2	1.68	0.58
1:D:76:ALA:O	1:D:80:ASP:HB2	2.02	0.58
1:H:147:ASN:ND2	1:H:149:THR:H	1.96	0.58
1:D:166:ARG:HH11	1:D:166:ARG:HG2	1.69	0.58
1:A:54:VAL:HB	1:A:55:PRO:HD3	1.86	0.58
1:D:5:THR:HG23	1:D:6:THR:HG23	1.86	0.57
1:C:5:THR:HG23	1:C:6:THR:HG23	1.86	0.57
1:H:184:THR:HG21	2:H:338:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:166:ARG:HG2	1:H:166:ARG:HH11	1.68	0.57
1:C:166:ARG:HG2	1:C:166:ARG:HH11	1.69	0.57
1:A:166:ARG:HG2	1:A:166:ARG:HH11	1.67	0.57
1:C:140:VAL:HG11	1:E:140:VAL:HG11	1.87	0.56
1:E:5:THR:HG23	1:E:6:THR:HG23	1.86	0.56
1:C:63:GLN:H	1:C:63:GLN:HE21	1.52	0.56
1:H:5:THR:HG23	1:H:6:THR:HG23	1.86	0.56
1:A:5:THR:HG23	1:A:6:THR:HG23	1.87	0.56
1:F:5:THR:HG23	1:F:6:THR:HG23	1.88	0.56
1:F:103:ARG:HD2	2:F:320:HOH:O	2.05	0.55
1:G:5:THR:HG23	1:G:6:THR:HG23	1.88	0.55
1:C:158:THR:HG21	1:E:144:LEU:HD11	1.88	0.55
1:H:103:ARG:HG3	1:H:114:GLU:HB3	1.89	0.54
1:A:65:LEU:HD22	1:A:66:PRO:O	2.08	0.54
1:F:103:ARG:HG3	1:F:114:GLU:HB3	1.90	0.54
1:B:166:ARG:HG2	1:B:166:ARG:HH11	1.72	0.54
1:E:145:PHE:H	1:E:189:GLN:NE2	2.06	0.53
1:D:103:ARG:HG3	1:D:114:GLU:HB3	1.90	0.53
1:F:140:VAL:HG11	1:G:140:VAL:HG11	1.89	0.53
1:E:65:LEU:HD22	1:E:66:PRO:O	2.09	0.53
1:E:166:ARG:HG2	1:E:166:ARG:HH11	1.73	0.53
1:A:145:PHE:H	1:A:189:GLN:NE2	2.05	0.53
1:G:166:ARG:HG2	1:G:166:ARG:HH11	1.72	0.53
1:A:194:PHE:CD2	1:B:218:LEU:HB2	2.44	0.53
1:D:144:LEU:HD11	1:H:158:THR:HG21	1.91	0.53
1:B:103:ARG:HG3	1:B:114:GLU:HB3	1.91	0.52
1:A:140:VAL:HG11	1:B:140:VAL:HG11	1.91	0.52
1:F:138:TRP:CZ2	1:F:196:LYS:HE3	2.44	0.52
1:B:138:TRP:CZ2	1:B:196:LYS:HE3	2.44	0.52
1:C:103:ARG:HG3	1:C:114:GLU:HB3	1.91	0.52
1:H:65:LEU:HD22	1:H:66:PRO:O	2.10	0.51
1:C:4:PRO:CB	1:C:111:ILE:HD11	2.41	0.51
1:H:4:PRO:CB	1:H:111:ILE:HD11	2.40	0.51
1:H:145:PHE:H	1:H:189:GLN:NE2	2.07	0.51
1:A:103:ARG:HG3	1:A:114:GLU:HB3	1.92	0.51
1:B:103:ARG:HB3	2:B:303:HOH:O	2.10	0.51
1:C:133:LEU:HD23	1:C:161:THR:HG22	1.93	0.51
1:D:147:ASN:ND2	1:D:149:THR:HG22	2.24	0.51
1:G:103:ARG:HG3	1:G:114:GLU:HB3	1.91	0.51
1:F:185:ILE:HD12	2:F:359:HOH:O	2.09	0.51
1:G:65:LEU:HD22	1:G:66:PRO:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASP:OD1	1:A:218:LEU:N	2.44	0.51
1:B:149:THR:HG22	2:B:317:HOH:O	2.10	0.51
1:C:103:ARG:NH1	1:C:114:GLU:HG2	2.26	0.51
1:F:65:LEU:HD22	1:F:66:PRO:O	2.11	0.51
1:E:103:ARG:HG3	1:E:114:GLU:HB3	1.92	0.51
1:H:103:ARG:NH1	1:H:114:GLU:HG2	2.26	0.51
1:A:71:MET:HG2	1:A:75:GLN:HE21	1.76	0.50
1:E:138:TRP:CZ2	1:E:196:LYS:HE3	2.47	0.50
1:H:138:TRP:CZ2	1:H:196:LYS:HE3	2.46	0.50
1:A:4:PRO:CB	1:A:111:ILE:HD11	2.41	0.50
1:B:65:LEU:HD22	1:B:66:PRO:O	2.11	0.50
1:F:145:PHE:H	1:F:189:GLN:NE2	2.09	0.50
1:D:71:MET:HG2	1:D:75:GLN:HE21	1.76	0.50
1:F:71:MET:HG2	1:F:75:GLN:HE21	1.76	0.50
1:F:9:VAL:HG23	1:F:37:ILE:HD11	1.93	0.50
1:G:138:TRP:CZ2	1:G:196:LYS:HE3	2.46	0.50
1:B:4:PRO:CB	1:B:111:ILE:HD11	2.40	0.50
1:D:133:LEU:HD23	1:D:161:THR:HG22	1.93	0.50
1:B:103:ARG:NH1	1:B:114:GLU:HG2	2.27	0.50
1:C:65:LEU:HD22	1:C:66:PRO:O	2.11	0.50
1:D:145:PHE:H	1:D:189:GLN:NE2	2.10	0.50
1:C:71:MET:HG2	1:C:75:GLN:HE21	1.76	0.49
1:D:138:TRP:CZ2	1:D:196:LYS:HE3	2.46	0.49
1:E:71:MET:HG2	1:E:75:GLN:HE21	1.77	0.49
1:F:4:PRO:CB	1:F:111:ILE:HD11	2.41	0.49
1:B:38:GLN:HB2	2:B:372:HOH:O	2.13	0.49
1:D:4:PRO:CB	1:D:111:ILE:HD11	2.42	0.49
1:D:218:LEU:HB2	1:H:194:PHE:CD2	2.47	0.49
1:D:65:LEU:HD22	1:D:66:PRO:O	2.12	0.49
1:F:25:SER:C	1:F:37:ILE:HG13	2.38	0.49
1:G:145:PHE:H	1:G:189:GLN:NE2	2.11	0.49
1:H:133:LEU:HD23	1:H:161:THR:HG22	1.95	0.49
1:C:145:PHE:H	1:C:189:GLN:NE2	2.11	0.49
1:D:66:PRO:HG2	2:D:331:HOH:O	2.12	0.49
1:D:103:ARG:NH1	1:D:114:GLU:HG2	2.28	0.49
1:A:103:ARG:NH1	1:A:114:GLU:HG2	2.27	0.48
1:A:133:LEU:HD23	1:A:161:THR:HG22	1.95	0.48
1:A:138:TRP:CZ2	1:A:196:LYS:HE3	2.47	0.48
1:F:133:LEU:HD23	1:F:161:THR:HG22	1.95	0.48
1:F:147:ASN:ND2	1:F:149:THR:H	2.00	0.48
1:E:4:PRO:CB	1:E:111:ILE:HD11	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:PRO:CB	1:G:111:ILE:HD11	2.40	0.48
1:B:88:ARG:CD	1:B:173:THR:OG1	2.59	0.48
1:B:103:ARG:HD3	2:B:335:HOH:O	2.13	0.48
1:E:133:LEU:HD23	1:E:161:THR:HG22	1.94	0.48
1:F:103:ARG:NH1	1:F:114:GLU:HG2	2.28	0.48
1:C:147:ASN:ND2	1:C:149:THR:HG22	2.28	0.48
1:B:145:PHE:H	1:B:189:GLN:NE2	2.11	0.48
1:H:71:MET:HG2	1:H:75:GLN:HE21	1.78	0.48
1:A:168:HIS:HD2	2:A:397:HOH:O	1.97	0.47
1:B:133:LEU:HD23	1:B:161:THR:HG22	1.96	0.47
1:E:103:ARG:NH1	1:E:114:GLU:HG2	2.29	0.47
1:G:9:VAL:HG23	1:G:37:ILE:HD11	1.96	0.47
1:B:147:ASN:ND2	1:B:149:THR:HG22	2.29	0.47
1:D:10:HIS:ND1	1:D:114:GLU:OE2	2.46	0.47
1:H:22:LEU:HB3	1:H:39:VAL:HG22	1.97	0.47
1:C:22:LEU:HB3	1:C:39:VAL:HG22	1.96	0.47
1:C:138:TRP:CZ2	1:C:196:LYS:HE3	2.50	0.47
1:G:71:MET:HG2	1:G:75:GLN:HE21	1.80	0.47
1:B:10:HIS:ND1	1:B:114:GLU:OE2	2.47	0.47
1:G:133:LEU:HD23	1:G:161:THR:HG22	1.95	0.47
1:A:37:ILE:HG12	1:A:38:GLN:N	2.30	0.47
1:C:37:ILE:HG12	1:C:38:GLN:N	2.29	0.47
1:C:115:PHE:CD1	1:C:115:PHE:N	2.83	0.47
1:F:9:VAL:HG23	1:F:37:ILE:CD1	2.45	0.47
1:G:10:HIS:ND1	1:G:114:GLU:OE2	2.47	0.47
1:G:25:SER:C	1:G:37:ILE:HG13	2.39	0.47
1:A:63:GLN:CG	1:A:111:ILE:HD13	2.38	0.47
1:B:37:ILE:HG12	1:B:38:GLN:N	2.30	0.47
1:H:147:ASN:ND2	1:H:149:THR:HG22	2.29	0.47
1:E:10:HIS:ND1	1:E:114:GLU:OE2	2.48	0.47
1:F:10:HIS:ND1	1:F:114:GLU:OE2	2.46	0.47
1:G:103:ARG:NH1	1:G:114:GLU:HG2	2.29	0.47
1:G:147:ASN:HD22	1:G:147:ASN:C	2.22	0.47
1:H:37:ILE:HG12	1:H:38:GLN:N	2.29	0.47
1:B:71:MET:HG2	1:B:75:GLN:HE21	1.80	0.46
1:E:37:ILE:HG12	1:E:38:GLN:N	2.30	0.46
1:H:9:VAL:HG23	1:H:37:ILE:HD11	1.97	0.46
1:D:158:THR:HG21	1:H:144:LEU:HD11	1.97	0.46
1:E:147:ASN:ND2	1:E:149:THR:HG22	2.30	0.46
1:G:37:ILE:HG12	1:G:38:GLN:N	2.29	0.46
1:B:147:ASN:HD22	1:B:147:ASN:C	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:SER:C	1:C:37:ILE:HG13	2.40	0.46
1:D:9:VAL:HG22	1:D:61:PHE:HZ	1.78	0.46
1:F:37:ILE:HG12	1:F:38:GLN:N	2.30	0.46
1:A:88:ARG:CD	1:A:173:THR:OG1	2.58	0.46
1:A:147:ASN:HD22	1:A:147:ASN:C	2.23	0.46
1:C:9:VAL:HG23	1:C:37:ILE:HD11	1.96	0.46
1:H:147:ASN:HD22	1:H:147:ASN:C	2.23	0.46
1:A:147:ASN:ND2	1:A:149:THR:HG22	2.30	0.46
1:H:25:SER:C	1:H:37:ILE:HG13	2.41	0.46
1:F:115:PHE:N	1:F:115:PHE:CD1	2.84	0.46
1:D:22:LEU:HB3	1:D:39:VAL:HG22	1.97	0.46
1:F:63:GLN:CG	1:F:111:ILE:HD13	2.40	0.45
1:F:158:THR:HG21	1:G:144:LEU:HD11	1.98	0.45
1:D:37:ILE:HG12	1:D:38:GLN:N	2.31	0.45
1:E:9:VAL:HG23	1:E:37:ILE:HD11	1.98	0.45
1:G:22:LEU:HB3	1:G:39:VAL:HG22	1.97	0.45
1:A:166:ARG:NH1	1:A:166:ARG:HG2	2.31	0.45
1:C:147:ASN:HD22	1:C:147:ASN:C	2.25	0.45
1:D:25:SER:C	1:D:37:ILE:HG13	2.42	0.45
1:H:10:HIS:ND1	1:H:114:GLU:OE2	2.49	0.45
1:B:9:VAL:HG22	1:B:61:PHE:HZ	1.78	0.45
1:B:217:ASP:OD1	1:B:218:LEU:N	2.47	0.45
1:C:166:ARG:NH1	1:C:166:ARG:HG2	2.32	0.45
1:D:9:VAL:HG23	1:D:37:ILE:HD11	1.98	0.45
1:E:9:VAL:HG22	1:E:61:PHE:HZ	1.81	0.45
1:B:5:THR:HG22	1:B:109:GLY:O	2.17	0.45
1:E:115:PHE:N	1:E:115:PHE:CD1	2.84	0.45
1:B:22:LEU:HB3	1:B:39:VAL:HG22	1.98	0.45
1:B:115:PHE:N	1:B:115:PHE:CD1	2.85	0.45
1:E:114:GLU:C	1:E:115:PHE:HD1	2.26	0.45
1:G:5:THR:HG22	1:G:109:GLY:O	2.17	0.45
1:G:51:TYR:CD2	1:G:135:ALA:HA	2.52	0.45
2:A:349:HOH:O	1:B:144:LEU:HD12	2.17	0.44
1:C:194:PHE:CD2	1:E:218:LEU:HB2	2.52	0.44
1:A:9:VAL:HG23	1:A:37:ILE:HD11	1.99	0.44
1:D:115:PHE:N	1:D:115:PHE:CD1	2.85	0.44
1:D:147:ASN:HD22	1:D:147:ASN:C	2.26	0.44
1:F:166:ARG:NH1	1:F:166:ARG:HG2	2.32	0.44
1:G:147:ASN:ND2	1:G:149:THR:HG22	2.32	0.44
1:C:5:THR:HG22	1:C:109:GLY:O	2.18	0.44
1:G:137:ASP:OD2	1:G:166:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG22	1:A:61:PHE:HZ	1.80	0.44
1:A:10:HIS:ND1	1:A:114:GLU:OE2	2.49	0.44
1:B:25:SER:C	1:B:37:ILE:HG13	2.42	0.44
1:C:216:HIS:HD2	2:C:359:HOH:O	2.00	0.44
1:G:9:VAL:HG23	1:G:37:ILE:CD1	2.47	0.44
1:F:5:THR:HG22	1:F:109:GLY:O	2.18	0.44
1:C:114:GLU:C	1:C:115:PHE:HD1	2.26	0.44
1:G:115:PHE:N	1:G:115:PHE:CD1	2.84	0.44
1:H:5:THR:HG22	1:H:109:GLY:O	2.17	0.44
1:A:22:LEU:HB3	1:A:39:VAL:HG22	1.99	0.44
1:H:9:VAL:HG22	1:H:61:PHE:HZ	1.80	0.44
1:C:9:VAL:HG23	1:C:37:ILE:CD1	2.48	0.44
1:B:42:THR:HA	2:B:324:HOH:O	2.17	0.43
1:B:51:TYR:CD2	1:B:135:ALA:HA	2.53	0.43
1:H:60:CR2:HA12	1:H:60:CR2:HA31	1.87	0.43
1:A:25:SER:C	1:A:37:ILE:HG13	2.42	0.43
1:E:151:VAL:HB	1:E:175:TYR:HB2	2.00	0.43
1:C:10:HIS:ND1	1:C:114:GLU:OE2	2.50	0.43
1:E:88:ARG:CD	1:E:173:THR:OG1	2.64	0.43
1:F:22:LEU:HB3	1:F:39:VAL:HG22	1.96	0.43
1:G:88:ARG:CD	1:G:173:THR:OG1	2.63	0.43
1:H:51:TYR:CD2	1:H:135:ALA:HA	2.53	0.43
1:H:115:PHE:CD1	1:H:115:PHE:N	2.86	0.43
1:F:172:ARG:NH2	2:F:345:HOH:O	2.52	0.43
1:H:166:ARG:NH1	1:H:166:ARG:HG2	2.32	0.43
1:E:5:THR:HG22	1:E:109:GLY:O	2.18	0.43
1:C:63:GLN:CG	1:C:111:ILE:HD13	2.41	0.43
1:D:8:GLU:HA	1:D:25:SER:HA	2.01	0.43
1:E:9:VAL:HG23	1:E:37:ILE:CD1	2.49	0.43
1:E:22:LEU:HB3	1:E:39:VAL:HG22	1.99	0.43
1:E:85:VAL:HG12	1:E:176:THR:HB	2.01	0.43
1:E:147:ASN:HD22	1:E:147:ASN:C	2.26	0.43
1:A:115:PHE:CD1	1:A:115:PHE:N	2.86	0.43
1:D:9:VAL:HG23	1:D:37:ILE:CD1	2.48	0.43
1:D:135:ALA:O	1:D:160:PRO:HD2	2.19	0.43
1:A:151:VAL:HB	1:A:175:TYR:HB2	2.00	0.43
1:B:9:VAL:HG23	1:B:37:ILE:HD11	2.00	0.43
1:B:103:ARG:HD2	2:B:303:HOH:O	2.18	0.43
1:C:88:ARG:CD	1:C:173:THR:OG1	2.63	0.43
1:D:114:GLU:C	1:D:115:PHE:HD1	2.27	0.43
1:E:25:SER:C	1:E:37:ILE:HG13	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:GLU:C	1:G:115:PHE:HD1	2.26	0.43
1:D:51:TYR:CD2	1:D:135:ALA:HA	2.53	0.42
1:F:60:CR2:HA12	1:F:60:CR2:HA31	1.85	0.42
1:C:137:ASP:OD2	1:C:166:ARG:NH1	2.52	0.42
1:D:5:THR:HG22	1:D:109:GLY:O	2.19	0.42
1:F:147:ASN:ND2	1:F:149:THR:HG22	2.33	0.42
1:A:5:THR:HG22	1:A:109:GLY:O	2.18	0.42
1:B:85:VAL:HG12	1:B:176:THR:HB	2.02	0.42
1:D:88:ARG:CD	1:D:173:THR:OG1	2.61	0.42
1:F:62:HIS:N	1:F:63:GLN:HE21	2.18	0.42
1:D:166:ARG:NH1	1:D:166:ARG:HG2	2.32	0.42
1:H:85:VAL:HG12	1:H:176:THR:HB	2.00	0.42
1:F:114:GLU:C	1:F:115:PHE:HD1	2.28	0.42
1:C:8:GLU:HA	1:C:25:SER:HA	2.02	0.42
1:F:151:VAL:HB	1:F:175:TYR:HB2	2.02	0.42
1:H:9:VAL:HG23	1:H:37:ILE:CD1	2.49	0.42
1:B:67:PHE:CD2	1:B:191:MET:HE2	2.55	0.42
1:D:31:LYS:HE2	1:D:31:LYS:HA	2.01	0.42
1:D:85:VAL:HG12	1:D:176:THR:HB	2.02	0.42
1:E:51:TYR:CD2	1:E:135:ALA:HA	2.55	0.42
1:E:63:GLN:CG	1:E:111:ILE:HD13	2.39	0.42
1:F:51:TYR:CD2	1:F:135:ALA:HA	2.55	0.42
1:F:147:ASN:HD22	1:F:147:ASN:C	2.28	0.42
1:G:85:VAL:HG12	1:G:176:THR:HB	2.02	0.42
1:C:57:ILE:HD12	1:C:57:ILE:HA	1.92	0.41
1:D:137:ASP:OD2	1:D:166:ARG:NH1	2.53	0.41
1:F:90:ILE:HB	1:F:98:LEU:HB3	2.02	0.41
1:G:8:GLU:HA	1:G:25:SER:HA	2.03	0.41
1:B:31:LYS:HA	1:B:31:LYS:HE2	2.02	0.41
1:A:51:TYR:CD2	1:A:135:ALA:HA	2.54	0.41
1:E:57:ILE:HD12	1:E:57:ILE:HA	1.93	0.41
1:E:166:ARG:NH1	1:E:166:ARG:HG2	2.35	0.41
1:B:9:VAL:HG23	1:B:37:ILE:CD1	2.50	0.41
1:G:9:VAL:HG22	1:G:61:PHE:HZ	1.80	0.41
1:A:9:VAL:HG23	1:A:37:ILE:CD1	2.51	0.41
1:C:61:PHE:CA	1:C:63:GLN:HE21	2.34	0.41
1:G:57:ILE:HD12	1:G:57:ILE:HA	1.92	0.41
1:B:63:GLN:CG	1:B:111:ILE:HD13	2.40	0.41
1:F:85:VAL:HG12	1:F:176:THR:HB	2.02	0.41
1:E:67:PHE:CD2	1:E:191:MET:HE2	2.56	0.41
1:H:62:HIS:N	1:H:63:GLN:HE21	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:GLN:CG	1:H:111:ILE:HD13	2.38	0.41
1:A:8:GLU:HA	1:A:25:SER:HA	2.02	0.41
1:B:166:ARG:NH1	1:B:166:ARG:HG2	2.35	0.41
1:F:218:LEU:HD23	1:F:218:LEU:HA	1.92	0.41
1:D:62:HIS:N	1:D:63:GLN:HE21	2.18	0.41
1:E:61:PHE:CA	1:E:63:GLN:HE21	2.34	0.41
1:F:31:LYS:HA	1:F:31:LYS:HE2	2.03	0.41
1:H:31:LYS:HA	1:H:31:LYS:HE2	2.02	0.41
1:E:137:ASP:OD2	1:E:166:ARG:NH1	2.54	0.40
1:A:85:VAL:HG12	1:A:176:THR:HB	2.02	0.40
1:C:218:LEU:HD23	1:C:218:LEU:HA	1.92	0.40
1:H:8:GLU:HA	1:H:25:SER:HA	2.02	0.40
1:F:67:PHE:CD2	1:F:191:MET:HE2	2.56	0.40
1:G:62:HIS:N	1:G:63:GLN:HE21	2.20	0.40
1:E:8:GLU:HA	1:E:25:SER:HA	2.03	0.40
1:A:114:GLU:C	1:A:115:PHE:HD1	2.30	0.40
1:C:151:VAL:HB	1:C:175:TYR:HB2	2.02	0.40
1:D:67:PHE:CD2	1:D:191:MET:HE2	2.56	0.40

All (3) 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:H:203:ASP:CG	1:H:203:ASP:OD2[2_453]	2.09	0.11
1:H:203:ASP:OD1	1:H:203:ASP:OD1[2_453]	2.12	0.08
1:H:203:ASP:OD1	1:H:203:ASP:OD2[2_453]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	209/214 (98%)	204 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
1	C	209/214 (98%)	204 (98%)	5 (2%)	0	100	100
1	D	209/214 (98%)	205 (98%)	4 (2%)	0	100	100
1	E	209/214 (98%)	205 (98%)	4 (2%)	0	100	100
1	F	209/214 (98%)	205 (98%)	4 (2%)	0	100	100
1	G	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
1	H	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
All	All	1672/1712 (98%)	1632 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/179 (100%)	170 (95%)	9 (5%)	22	11
1	B	179/179 (100%)	170 (95%)	9 (5%)	22	11
1	C	179/179 (100%)	170 (95%)	9 (5%)	22	11
1	D	179/179 (100%)	170 (95%)	9 (5%)	22	11
1	E	179/179 (100%)	170 (95%)	9 (5%)	22	11
1	F	179/179 (100%)	169 (94%)	10 (6%)	19	8
1	G	179/179 (100%)	170 (95%)	9 (5%)	22	11
1	H	179/179 (100%)	170 (95%)	9 (5%)	22	11
All	All	1432/1432 (100%)	1359 (95%)	73 (5%)	21	10

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	31	LYS

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Mol	Chain	Res	Type
1	A	46	LEU
1	A	53	VAL
1	A	57	ILE
1	A	63	GLN
1	A	65	LEU
1	A	147	ASN
1	A	157	TRP
1	B	9	VAL
1	B	31	LYS
1	B	46	LEU
1	B	53	VAL
1	B	57	ILE
1	B	63	GLN
1	B	65	LEU
1	B	147	ASN
1	B	157	TRP
1	C	9	VAL
1	C	31	LYS
1	C	46	LEU
1	C	53	VAL
1	C	57	ILE
1	C	63	GLN
1	C	65	LEU
1	C	147	ASN
1	C	157	TRP
1	D	9	VAL
1	D	31	LYS
1	D	46	LEU
1	D	53	VAL
1	D	57	ILE
1	D	63	GLN
1	D	65	LEU
1	D	147	ASN
1	D	157	TRP
1	E	9	VAL
1	E	31	LYS
1	E	46	LEU
1	E	53	VAL
1	E	57	ILE
1	E	63	GLN
1	E	65	LEU
1	E	147	ASN

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Mol	Chain	Res	Type
1	E	157	TRP
1	F	9	VAL
1	F	31	LYS
1	F	46	LEU
1	F	53	VAL
1	F	57	ILE
1	F	63	GLN
1	F	65	LEU
1	F	103	ARG
1	F	147	ASN
1	F	157	TRP
1	G	9	VAL
1	G	31	LYS
1	G	46	LEU
1	G	53	VAL
1	G	57	ILE
1	G	63	GLN
1	G	65	LEU
1	G	147	ASN
1	G	157	TRP
1	H	9	VAL
1	H	31	LYS
1	H	46	LEU
1	H	53	VAL
1	H	57	ILE
1	H	63	GLN
1	H	65	LEU
1	H	147	ASN
1	H	157	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	75	GLN
1	A	101	ASN
1	A	147	ASN
1	A	168	HIS
1	A	174	ASN
1	A	187	GLN
1	A	189	GLN
1	B	63	GLN

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Mol	Chain	Res	Type
1	B	75	GLN
1	B	101	ASN
1	B	147	ASN
1	B	174	ASN
1	B	189	GLN
1	C	63	GLN
1	C	75	GLN
1	C	101	ASN
1	C	147	ASN
1	C	189	GLN
1	C	216	HIS
1	D	38	GLN
1	D	63	GLN
1	D	75	GLN
1	D	101	ASN
1	D	147	ASN
1	D	189	GLN
1	E	63	GLN
1	E	75	GLN
1	E	101	ASN
1	E	147	ASN
1	E	189	GLN
1	F	63	GLN
1	F	75	GLN
1	F	101	ASN
1	F	147	ASN
1	F	174	ASN
1	F	189	GLN
1	G	63	GLN
1	G	75	GLN
1	G	101	ASN
1	G	147	ASN
1	G	174	ASN
1	G	189	GLN
1	H	63	GLN
1	H	75	GLN
1	H	101	ASN
1	H	147	ASN
1	H	174	ASN
1	H	189	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CR2	A	60	1	20,20,21	3.64	7 (35%)	25,27,29	4.39	11 (44%)
1	CR2	G	60	1	20,20,21	3.67	7 (35%)	25,27,29	4.31	9 (36%)
1	CR2	B	58	1	20,20,21	3.62	8 (40%)	25,27,29	4.13	12 (48%)
1	CR2	D	60	1	20,20,21	3.68	7 (35%)	25,27,29	4.31	11 (44%)
1	CR2	C	60	1	20,20,21	3.66	6 (30%)	25,27,29	4.44	10 (40%)
1	CR2	H	60	1	20,20,21	3.70	7 (35%)	25,27,29	4.30	11 (44%)
1	CR2	F	60	1	20,20,21	3.73	7 (35%)	25,27,29	4.32	11 (44%)
1	CR2	E	60	1	20,20,21	3.80	8 (40%)	25,27,29	4.34	9 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR2	A	60	1	-	1/6/25/26	0/2/2/2
1	CR2	G	60	1	-	1/6/25/26	0/2/2/2
1	CR2	B	58	1	-	1/6/25/26	0/2/2/2
1	CR2	D	60	1	-	1/6/25/26	0/2/2/2
1	CR2	C	60	1	-	1/6/25/26	0/2/2/2
1	CR2	H	60	1	-	1/6/25/26	0/2/2/2
1	CR2	F	60	1	-	1/6/25/26	0/2/2/2
1	CR2	E	60	1	-	1/6/25/26	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	60	CR2	CB2-CA2	11.34	1.46	1.35
1	H	60	CR2	CB2-CA2	11.17	1.45	1.35
1	D	60	CR2	CB2-CA2	10.90	1.45	1.35
1	G	60	CR2	CB2-CA2	10.62	1.45	1.35
1	F	60	CR2	CB2-CA2	10.48	1.45	1.35
1	B	58	CR2	CB2-CA2	10.40	1.45	1.35
1	A	60	CR2	CB2-CA2	10.39	1.45	1.35
1	C	60	CR2	CB2-CA2	10.27	1.45	1.35
1	F	60	CR2	CA2-N2	-8.71	1.20	1.38
1	C	60	CR2	CA2-N2	-8.50	1.20	1.38
1	A	60	CR2	CA2-N2	-8.42	1.20	1.38
1	G	60	CR2	CA2-N2	-8.34	1.20	1.38
1	D	60	CR2	CA2-N2	-8.28	1.20	1.38
1	E	60	CR2	CA2-N2	-8.20	1.21	1.38
1	B	58	CR2	CA2-N2	-8.16	1.21	1.38
1	H	60	CR2	CA2-N2	-8.02	1.21	1.38
1	F	60	CR2	C2-N3	-5.58	1.27	1.40
1	E	60	CR2	C2-N3	-5.36	1.27	1.40
1	D	60	CR2	C2-N3	-5.32	1.27	1.40
1	H	60	CR2	C2-N3	-5.25	1.27	1.40
1	A	60	CR2	C2-N3	-5.20	1.28	1.40
1	B	58	CR2	C2-N3	-5.20	1.28	1.40
1	C	60	CR2	C2-N3	-5.17	1.28	1.40
1	G	60	CR2	C2-N3	-5.13	1.28	1.40
1	A	60	CR2	OH-CZ	-5.08	1.25	1.37
1	F	60	CR2	OH-CZ	-5.06	1.25	1.37
1	H	60	CR2	OH-CZ	-4.96	1.25	1.37
1	B	58	CR2	OH-CZ	-4.92	1.25	1.37
1	D	60	CR2	OH-CZ	-4.81	1.26	1.37
1	C	60	CR2	OH-CZ	-4.81	1.26	1.37
1	G	60	CR2	OH-CZ	-4.75	1.26	1.37
1	E	60	CR2	OH-CZ	-4.56	1.26	1.37
1	C	60	CR2	C1-N3	-3.91	1.30	1.37
1	E	60	CR2	C1-N3	-3.60	1.31	1.37
1	G	60	CR2	C1-N3	-3.53	1.31	1.37
1	F	60	CR2	C1-N3	-3.51	1.31	1.37
1	G	60	CR2	CE2-CZ	-3.23	1.32	1.39
1	H	60	CR2	CE2-CZ	-3.18	1.33	1.39
1	A	60	CR2	C1-N3	-3.17	1.32	1.37
1	E	60	CR2	CE2-CZ	-3.16	1.33	1.39
1	H	60	CR2	C1-N3	-3.09	1.32	1.37
1	A	60	CR2	CE2-CZ	-3.07	1.33	1.39
1	D	60	CR2	CE2-CZ	-3.03	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	58	CR2	CE2-CZ	-2.99	1.33	1.39
1	F	60	CR2	CE2-CZ	-2.86	1.33	1.39
1	B	58	CR2	CA1-C1	2.84	1.52	1.49
1	D	60	CR2	C1-N3	-2.83	1.32	1.37
1	C	60	CR2	CE2-CZ	-2.65	1.34	1.39
1	E	60	CR2	CA3-N3	-2.57	1.42	1.47
1	B	58	CR2	C1-N3	-2.55	1.33	1.37
1	F	60	CR2	CA3-N3	-2.22	1.43	1.47
1	D	60	CR2	CA3-N3	-2.19	1.43	1.47
1	G	60	CR2	CA3-N3	-2.18	1.43	1.47
1	E	60	CR2	CA2-C2	-2.12	1.46	1.48
1	B	58	CR2	CA3-N3	-2.06	1.43	1.47
1	A	60	CR2	CA3-N3	-2.02	1.43	1.47
1	H	60	CR2	CA3-N3	-2.00	1.43	1.47

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	CR2	O2-C2-CA2	-15.74	120.98	131.02
1	E	60	CR2	O2-C2-CA2	-15.41	121.19	131.02
1	A	60	CR2	O2-C2-CA2	-15.08	121.40	131.02
1	G	60	CR2	O2-C2-CA2	-15.07	121.40	131.02
1	D	60	CR2	O2-C2-CA2	-15.06	121.41	131.02
1	F	60	CR2	O2-C2-CA2	-15.06	121.41	131.02
1	H	60	CR2	O2-C2-CA2	-14.87	121.53	131.02
1	B	58	CR2	O2-C2-CA2	-14.15	121.99	131.02
1	A	60	CR2	C3-CA3-N3	8.43	131.62	112.43
1	A	60	CR2	CG2-CB2-CA2	8.40	139.86	129.87
1	H	60	CR2	C3-CA3-N3	8.33	131.39	112.43
1	F	60	CR2	C3-CA3-N3	8.32	131.37	112.43
1	H	60	CR2	CG2-CB2-CA2	8.30	139.73	129.87
1	C	60	CR2	C3-CA3-N3	8.22	131.15	112.43
1	E	60	CR2	C3-CA3-N3	8.21	131.11	112.43
1	D	60	CR2	C3-CA3-N3	8.17	131.02	112.43
1	G	60	CR2	C3-CA3-N3	8.17	131.02	112.43
1	B	58	CR2	CG2-CB2-CA2	8.14	139.54	129.87
1	B	58	CR2	C3-CA3-N3	8.13	130.93	112.43
1	C	60	CR2	CG2-CB2-CA2	8.11	139.50	129.87
1	D	60	CR2	CG2-CB2-CA2	7.99	139.37	129.87
1	E	60	CR2	CG2-CB2-CA2	7.90	139.26	129.87
1	G	60	CR2	CG2-CB2-CA2	7.87	139.23	129.87
1	F	60	CR2	CG2-CB2-CA2	7.81	139.15	129.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	CR2	C2-N3-C1	-6.01	105.38	108.08
1	C	60	CR2	C2-N3-C1	-6.00	105.38	108.08
1	G	60	CR2	C2-N3-C1	-5.87	105.44	108.08
1	F	60	CR2	C2-N3-C1	-5.67	105.53	108.08
1	D	60	CR2	C2-N3-C1	-5.59	105.57	108.08
1	H	60	CR2	C2-N3-C1	-5.46	105.62	108.08
1	E	60	CR2	C2-N3-C1	-5.16	105.76	108.08
1	B	58	CR2	C2-N3-C1	-4.73	105.95	108.08
1	C	60	CR2	CA2-C2-N3	4.07	106.92	103.50
1	G	60	CR2	CA2-C2-N3	4.05	106.90	103.50
1	E	60	CR2	CA2-C2-N3	3.93	106.80	103.50
1	D	60	CR2	CA2-C2-N3	3.90	106.78	103.50
1	F	60	CR2	CA2-C2-N3	3.86	106.74	103.50
1	E	60	CR2	C2-CA2-N2	-3.81	106.22	108.95
1	A	60	CR2	CA2-C2-N3	3.79	106.68	103.50
1	H	60	CR2	CA2-C2-N3	3.74	106.64	103.50
1	C	60	CR2	O2-C2-N3	3.74	132.10	124.31
1	E	60	CR2	O2-C2-N3	3.69	132.01	124.31
1	A	60	CR2	O2-C2-N3	3.65	131.92	124.31
1	G	60	CR2	C2-CA2-N2	-3.64	106.34	108.95
1	C	60	CR2	C2-CA2-N2	-3.63	106.35	108.95
1	F	60	CR2	O2-C2-N3	3.61	131.85	124.31
1	H	60	CR2	O2-C2-N3	3.60	131.83	124.31
1	D	60	CR2	O2-C2-N3	3.60	131.81	124.31
1	G	60	CR2	O2-C2-N3	3.54	131.70	124.31
1	F	60	CR2	C2-CA2-N2	-3.51	106.43	108.95
1	H	60	CR2	C2-CA2-N2	-3.51	106.44	108.95
1	B	58	CR2	O2-C2-N3	3.49	131.59	124.31
1	B	58	CR2	CA2-C2-N3	3.47	106.42	103.50
1	A	60	CR2	CA3-N3-C2	3.46	131.28	123.67
1	B	58	CR2	C2-CA2-N2	-3.39	106.52	108.95
1	F	60	CR2	CA3-N3-C2	3.36	131.05	123.67
1	D	60	CR2	C2-CA2-N2	-3.36	106.55	108.95
1	E	60	CR2	CA3-N3-C2	3.34	131.02	123.67
1	G	60	CR2	CA3-N3-C2	3.31	130.94	123.67
1	D	60	CR2	CA3-N3-C2	3.31	130.93	123.67
1	A	60	CR2	C2-CA2-N2	-3.29	106.59	108.95
1	C	60	CR2	CA3-N3-C2	3.29	130.90	123.67
1	H	60	CR2	CA3-N3-C2	3.27	130.85	123.67
1	B	58	CR2	CA3-N3-C2	3.10	130.49	123.67
1	B	58	CR2	CB2-CA2-C2	2.39	125.25	122.36
1	E	60	CR2	CB2-CA2-C2	2.26	125.10	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	60	CR2	CB2-CA2-C2	2.25	125.08	122.36
1	F	60	CR2	CB2-CA2-C2	2.22	125.05	122.36
1	A	60	CR2	CE2-CZ-CE1	2.21	123.29	119.77
1	C	60	CR2	CB2-CA2-C2	2.19	125.01	122.36
1	H	60	CR2	CB2-CA2-C2	2.19	125.01	122.36
1	A	60	CR2	CB2-CA2-C2	2.17	124.99	122.36
1	G	60	CR2	CB2-CA2-C2	2.16	124.98	122.36
1	D	60	CR2	CD1-CE1-CZ	-2.13	117.62	119.88
1	F	60	CR2	CE2-CZ-CE1	2.11	123.12	119.77
1	B	58	CR2	CE2-CZ-CE1	2.11	123.12	119.77
1	B	58	CR2	C1-CA1-N1	-2.09	108.23	112.85
1	D	60	CR2	CE2-CZ-CE1	2.05	123.03	119.77
1	A	60	CR2	CD1-CE1-CZ	-2.05	117.71	119.88
1	C	60	CR2	CE2-CZ-CE1	2.05	123.03	119.77
1	H	60	CR2	CD1-CE1-CZ	-2.04	117.72	119.88
1	H	60	CR2	CE2-CZ-CE1	2.01	122.96	119.77
1	B	58	CR2	CD1-CE1-CZ	-2.01	117.75	119.88
1	F	60	CR2	CD1-CE1-CZ	-2.01	117.76	119.88

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	60	CR2	C3-CA3-N3-C2
1	B	58	CR2	C3-CA3-N3-C2
1	C	60	CR2	C3-CA3-N3-C2
1	D	60	CR2	C3-CA3-N3-C2
1	E	60	CR2	C3-CA3-N3-C2
1	F	60	CR2	C3-CA3-N3-C2
1	G	60	CR2	C3-CA3-N3-C2
1	H	60	CR2	C3-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	60	CR2	1	0
1	F	60	CR2	1	0

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	213/214 (99%)	1.29	37 (17%) 4 4	23, 40, 54, 65	0
1	B	213/214 (99%)	1.55	58 (27%) 1 1	26, 41, 54, 65	0
1	C	213/214 (99%)	1.50	52 (24%) 2 2	27, 42, 55, 65	0
1	D	213/214 (99%)	1.33	41 (19%) 3 3	30, 43, 56, 64	0
1	E	213/214 (99%)	1.56	54 (25%) 1 1	29, 43, 55, 64	0
1	F	213/214 (99%)	1.45	46 (21%) 2 2	27, 40, 55, 64	0
1	G	213/214 (99%)	1.54	53 (24%) 2 1	30, 43, 56, 65	0
1	H	213/214 (99%)	1.78	73 (34%) 1 0	33, 44, 56, 64	0
All	All	1704/1712 (99%)	1.50	414 (24%) 2 2	23, 42, 55, 65	0

All (414) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	LEU	4.7
1	F	204	ALA	4.6
1	E	149	THR	4.3
1	G	45	PRO	4.3
1	E	218	LEU	4.3
1	B	149	THR	4.3
1	E	39	VAL	4.3
1	C	9	VAL	4.2
1	B	108	GLY	4.2
1	B	164	GLY	4.2
1	G	44	GLY	4.2
1	A	218	LEU	4.2
1	G	3	LEU	4.2
1	B	80	ASP	4.2
1	F	53	VAL	4.0
1	F	211	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	3	LEU	4.0
1	B	39	VAL	4.0
1	G	5	THR	3.9
1	A	80	ASP	3.9
1	C	186	LEU	3.9
1	B	106	TYR	3.8
1	B	5	THR	3.8
1	F	108	GLY	3.8
1	H	183	ALA	3.8
1	B	125	ASP	3.8
1	B	165	LYS	3.8
1	F	9	VAL	3.7
1	H	78	ALA	3.7
1	E	186	LEU	3.7
1	C	3	LEU	3.6
1	E	80	ASP	3.6
1	F	203	ASP	3.6
1	E	83	GLY	3.6
1	C	5	THR	3.6
1	F	3	LEU	3.6
1	C	28	GLY	3.6
1	H	46	LEU	3.6
1	A	57	ILE	3.6
1	E	203	ASP	3.6
1	B	204	ALA	3.5
1	H	211	TRP	3.5
1	F	183	ALA	3.5
1	F	5	THR	3.5
1	E	57	ILE	3.5
1	B	199	VAL	3.5
1	H	184	THR	3.5
1	G	164	GLY	3.5
1	H	185	ILE	3.4
1	H	73	PRO	3.4
1	H	194	PHE	3.4
1	E	46	LEU	3.4
1	A	185	ILE	3.4
1	B	37	ILE	3.4
1	D	181	ILE	3.4
1	F	185	ILE	3.4
1	B	26	GLY	3.4
1	F	164	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	182	ALA	3.4
1	B	208	LEU	3.4
1	A	3	LEU	3.3
1	B	46	LEU	3.3
1	E	3	LEU	3.3
1	H	204	ALA	3.3
1	C	203	ASP	3.3
1	H	64	TYR	3.3
1	A	149	THR	3.3
1	D	186	LEU	3.3
1	H	218	LEU	3.3
1	H	62	HIS	3.2
1	H	182	ALA	3.2
1	B	34	SER	3.2
1	G	109	GLY	3.2
1	B	27	LYS	3.2
1	B	182	ALA	3.2
1	F	22	LEU	3.2
1	B	57	ILE	3.2
1	B	184	THR	3.2
1	D	5	THR	3.2
1	H	84	TYR	3.2
1	H	3	LEU	3.2
1	A	164	GLY	3.2
1	E	162	THR	3.1
1	A	4	PRO	3.1
1	D	94	ASP	3.1
1	A	203	ASP	3.1
1	E	179	LYS	3.1
1	H	5	THR	3.1
1	G	211	TRP	3.1
1	H	199	VAL	3.1
1	B	28	GLY	3.1
1	F	94	ASP	3.0
1	G	46	LEU	3.0
1	F	11	VAL	3.0
1	H	9	VAL	3.0
1	H	61	PHE	3.0
1	B	25	SER	3.0
1	D	135	ALA	3.0
1	F	111	ILE	3.0
1	D	3	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	33	GLY	3.0
1	E	214	ALA	3.0
1	F	57	ILE	3.0
1	A	53	VAL	3.0
1	F	39	VAL	3.0
1	G	213	LYS	3.0
1	F	109	GLY	3.0
1	H	106	TYR	2.9
1	A	45	PRO	2.9
1	B	211	TRP	2.9
1	H	165	LYS	2.9
1	E	125	ASP	2.9
1	F	69	ASP	2.9
1	H	121	GLY	2.9
1	H	149	THR	2.9
1	E	177	PHE	2.9
1	C	183	ALA	2.9
1	C	201	ALA	2.9
1	C	204	ALA	2.9
1	D	218	LEU	2.9
1	F	184	THR	2.9
1	G	22	LEU	2.9
1	C	23	VAL	2.8
1	G	184	THR	2.8
1	H	162	THR	2.8
1	C	78	ALA	2.8
1	A	94	ASP	2.8
1	G	94	ASP	2.8
1	C	133	LEU	2.8
1	H	65	LEU	2.8
1	H	181	ILE	2.8
1	E	106	TYR	2.8
1	D	105	SER	2.8
1	D	191	MET	2.8
1	H	177	PHE	2.8
1	D	187	GLN	2.8
1	H	81	GLY	2.8
1	H	187	GLN	2.8
1	A	37	ILE	2.8
1	G	57	ILE	2.8
1	G	62	HIS	2.8
1	B	85	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	203	ASP	2.8
1	C	135	ALA	2.8
1	B	103	ARG	2.8
1	G	43	LYS	2.8
1	D	6	THR	2.8
1	G	218	LEU	2.8
1	D	57	ILE	2.8
1	E	181	ILE	2.8
1	F	125	ASP	2.8
1	H	138	TRP	2.8
1	D	201	ALA	2.7
1	H	77	ALA	2.7
1	H	67	PHE	2.7
1	C	162	THR	2.7
1	H	94	ASP	2.7
1	B	23	VAL	2.7
1	H	23	VAL	2.7
1	A	106	TYR	2.7
1	H	104	TYR	2.7
1	E	42	THR	2.7
1	E	180	PRO	2.7
1	E	178	ALA	2.6
1	G	113	GLY	2.6
1	B	12	TYR	2.6
1	G	187	GLN	2.6
1	C	42	THR	2.6
1	D	162	THR	2.6
1	D	177	PHE	2.6
1	E	99	THR	2.6
1	F	149	THR	2.6
1	E	165	LYS	2.6
1	A	9	VAL	2.6
1	C	125	ASP	2.6
1	E	201	ALA	2.6
1	F	106	TYR	2.6
1	B	6	THR	2.6
1	C	202	SER	2.6
1	H	105	SER	2.6
1	B	180	PRO	2.6
1	C	46	LEU	2.6
1	B	24	GLY	2.6
1	C	205	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	205	GLU	2.6
1	B	124	ALA	2.6
1	F	201	ALA	2.6
1	A	131	LYS	2.6
1	D	72	SER	2.6
1	B	7	HIS	2.6
1	H	186	LEU	2.6
1	C	57	ILE	2.6
1	D	185	ILE	2.6
1	H	52	ILE	2.6
1	E	164	GLY	2.6
1	A	85	VAL	2.6
1	E	204	ALA	2.6
1	H	12	TYR	2.5
1	H	102	TYR	2.5
1	B	94	ASP	2.5
1	B	105	SER	2.5
1	D	85	VAL	2.5
1	E	23	VAL	2.5
1	H	192	PHE	2.5
1	H	215	PHE	2.5
1	C	26	GLY	2.5
1	H	111	ILE	2.5
1	B	166	ARG	2.5
1	C	8	GLU	2.5
1	D	9	VAL	2.5
1	E	11	VAL	2.5
1	G	149	THR	2.5
1	C	127	PRO	2.5
1	E	107	ASP	2.5
1	A	165	LYS	2.5
1	C	108	GLY	2.5
1	D	103	ARG	2.5
1	E	111	ILE	2.5
1	F	37	ILE	2.5
1	F	206	ILE	2.5
1	G	35	GLU	2.5
1	G	38	GLN	2.5
1	F	182	ALA	2.5
1	C	11	VAL	2.5
1	F	128	VAL	2.5
1	G	125	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	26	GLY	2.4
1	G	7	HIS	2.4
1	A	18	VAL	2.4
1	F	46	LEU	2.4
1	H	191	MET	2.4
1	G	155	ILE	2.4
1	G	181	ILE	2.4
1	C	99	THR	2.4
1	E	199	VAL	2.4
1	H	108	GLY	2.4
1	E	82	SER	2.4
1	F	202	SER	2.4
1	A	213	LYS	2.4
1	C	208	LEU	2.4
1	G	186	LEU	2.4
1	B	177	PHE	2.4
1	E	74	PHE	2.4
1	A	162	THR	2.4
1	G	15	ILE	2.4
1	G	185	ILE	2.4
1	H	124	ALA	2.4
1	F	38	GLN	2.4
1	C	117	VAL	2.4
1	D	199	VAL	2.4
1	E	53	VAL	2.4
1	F	25	SER	2.4
1	C	149	THR	2.3
1	C	185	ILE	2.3
1	F	181	ILE	2.3
1	B	40	LYS	2.3
1	B	209	LYS	2.3
1	E	151	VAL	2.3
1	F	63	GLN	2.3
1	D	106	TYR	2.3
1	G	104	TYR	2.3
1	C	178	ALA	2.3
1	H	45	PRO	2.3
1	G	209	LYS	2.3
1	H	28	GLY	2.3
1	H	83	GLY	2.3
1	F	107	ASP	2.3
1	H	39	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	152	VAL	2.3
1	A	211	TRP	2.3
1	D	211	TRP	2.3
1	F	194	PHE	2.3
1	H	112	LYS	2.3
1	E	68	PRO	2.3
1	E	73	PRO	2.3
1	H	76	ALA	2.3
1	A	113	GLY	2.3
1	E	100	GLY	2.3
1	E	103	ARG	2.3
1	H	206	ILE	2.3
1	C	34	SER	2.3
1	B	32	ASP	2.3
1	G	19	GLU	2.3
1	B	9	VAL	2.3
1	C	118	VAL	2.3
1	B	42	THR	2.3
1	C	209	LYS	2.3
1	H	22	LEU	2.3
1	C	48	PHE	2.2
1	E	175	TYR	2.2
1	H	145	PHE	2.2
1	B	111	ILE	2.2
1	E	63	GLN	2.2
1	C	39	VAL	2.2
1	B	29	ASN	2.2
1	F	207	ASN	2.2
1	F	6	THR	2.2
1	G	6	THR	2.2
1	G	162	THR	2.2
1	H	161	THR	2.2
1	D	81	GLY	2.2
1	C	107	ASP	2.2
1	C	115	PHE	2.2
1	C	138	TRP	2.2
1	H	20	PHE	2.2
1	A	103	ARG	2.2
1	C	53	VAL	2.2
1	D	39	VAL	2.2
1	E	187	GLN	2.2
1	G	21	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	78	ALA	2.2
1	B	78	ALA	2.2
1	H	214	ALA	2.2
1	B	104	TYR	2.2
1	F	115	PHE	2.2
1	H	122	PHE	2.2
1	A	206	ILE	2.2
1	D	38	GLN	2.2
1	H	63	GLN	2.2
1	A	134	THR	2.2
1	A	69	ASP	2.2
1	G	148	ASP	2.2
1	B	218	LEU	2.2
1	D	109	GLY	2.2
1	E	146	PRO	2.2
1	C	102	TYR	2.1
1	G	106	TYR	2.1
1	H	35	GLU	2.1
1	E	185	ILE	2.1
1	G	111	ILE	2.1
1	B	212	GLN	2.1
1	C	211	TRP	2.1
1	A	5	THR	2.1
1	C	80	ASP	2.1
1	D	151	VAL	2.1
1	E	150	THR	2.1
1	C	13	GLY	2.1
1	D	70	GLY	2.1
1	C	218	LEU	2.1
1	E	22	LEU	2.1
1	H	30	PRO	2.1
1	F	36	GLU	2.1
1	D	78	ALA	2.1
1	D	204	ALA	2.1
1	E	135	ALA	2.1
1	G	183	ALA	2.1
1	B	181	ILE	2.1
1	D	12	TYR	2.1
1	F	12	TYR	2.1
1	C	94	ASP	2.1
1	C	109	GLY	2.1
1	E	108	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	11	VAL	2.1
1	G	18	VAL	2.1
1	G	131	LYS	2.1
1	A	198	GLU	2.1
1	A	127	PRO	2.1
1	B	123	PRO	2.1
1	H	171	LEU	2.1
1	H	208	LEU	2.1
1	D	67	PHE	2.1
1	D	145	PHE	2.1
1	C	12	TYR	2.1
1	C	181	ILE	2.1
1	C	41	SER	2.1
1	G	105	SER	2.1
1	E	184	THR	2.1
1	F	209	LYS	2.1
1	H	6	THR	2.1
1	H	110	HIS	2.1
1	G	128	VAL	2.1
1	H	157	TRP	2.1
1	B	189	GLN	2.1
1	A	98	LEU	2.1
1	E	182	ALA	2.1
1	G	124	ALA	2.1
1	G	178	ALA	2.1
1	H	178	ALA	2.1
1	D	34	SER	2.0
1	D	165	LYS	2.0
1	F	20	PHE	2.0
1	G	37	ILE	2.0
1	E	102	TYR	2.0
1	A	161	THR	2.0
1	A	47	GLY	2.0
1	A	81	GLY	2.0
1	D	17	GLY	2.0
1	F	110	HIS	2.0
1	H	70	GLY	2.0
1	E	9	VAL	2.0
1	E	18	VAL	2.0
1	G	9	VAL	2.0
1	H	193	VAL	2.0
1	D	98	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	171	LEU	2.0
1	B	201	ALA	2.0
1	F	103	ARG	2.0
1	G	201	ALA	2.0
1	A	79	ASP	2.0
1	B	200	LYS	2.0
1	B	213	LYS	2.0
1	G	34	SER	2.0
1	G	41	SER	2.0
1	E	145	PHE	2.0
1	G	10	HIS	2.0
1	H	57	ILE	2.0
1	A	38	GLN	2.0
1	C	184	THR	2.0
1	D	42	THR	2.0
1	E	75	GLN	2.0
1	G	47	GLY	2.0
1	D	167	TYR	2.0
1	C	45	PRO	2.0
1	B	53	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CR2	H	60	19/20	0.77	0.14	43,45,46,47	0
1	CR2	G	60	19/20	0.78	0.13	43,45,47,47	0
1	CR2	E	60	19/20	0.83	0.12	42,44,46,47	0
1	CR2	D	60	19/20	0.86	0.10	41,43,45,45	0
1	CR2	C	60	19/20	0.86	0.13	40,42,43,44	0
1	CR2	B	58	19/20	0.89	0.09	36,39,41,42	0
1	CR2	F	60	19/20	0.89	0.10	39,41,43,44	0
1	CR2	A	60	19/20	0.90	0.10	35,41,42,43	0

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.