



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:06 PM GMT

PDB ID : 4DKM
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

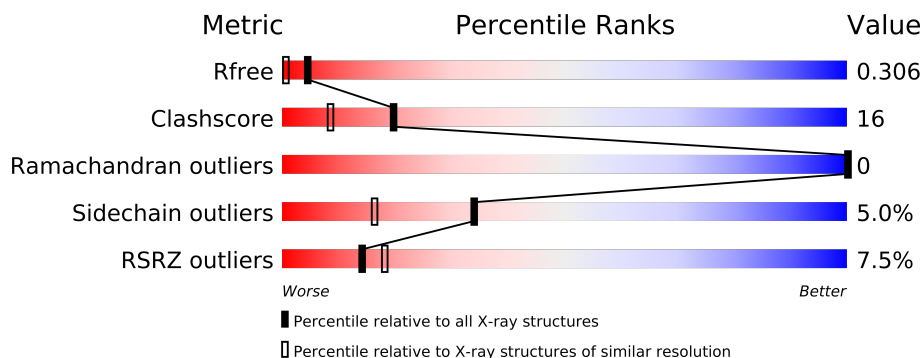
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	214	
1	B	214	
1	C	214	
1	D	214	
1	E	214	
1	F	214	
1	G	214	
1	H	214	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13957 atoms, of which 0 are hydrogen and 0 are deuterium.

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

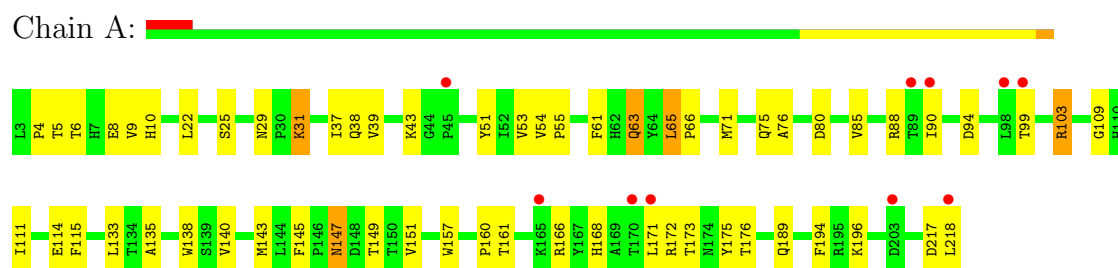
- Molecule 2 is water.

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

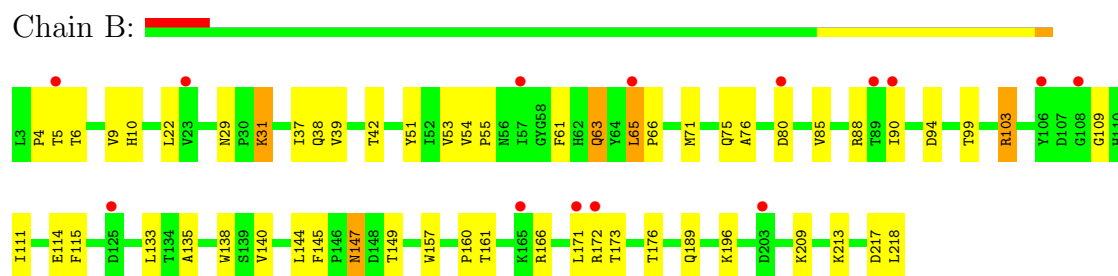
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

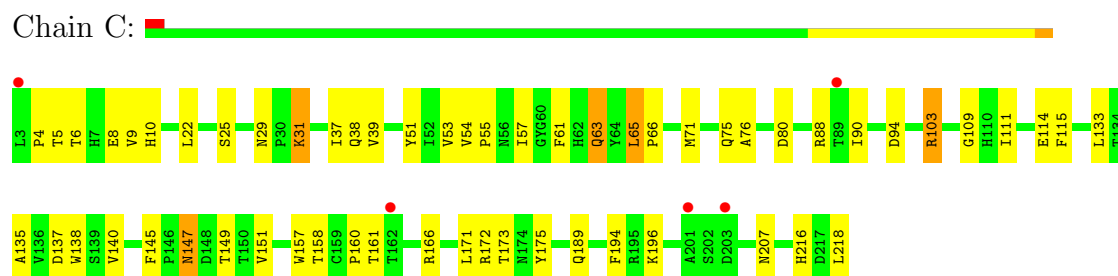
- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a



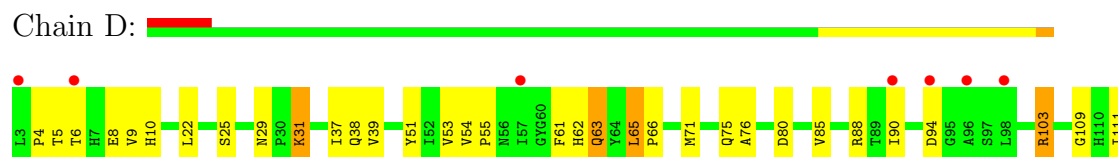
- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a



- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a



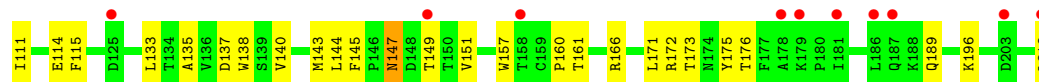
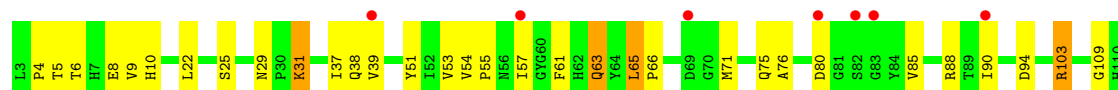
- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a





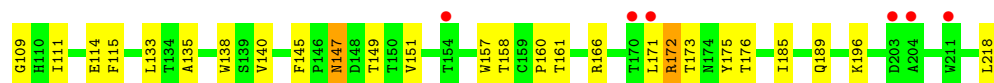
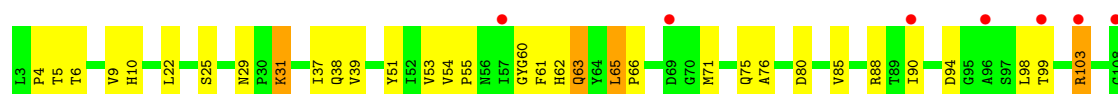
- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a

Chain E:



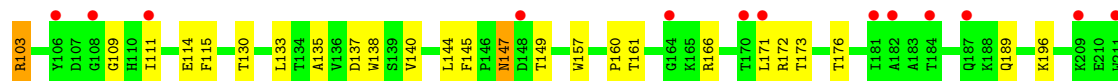
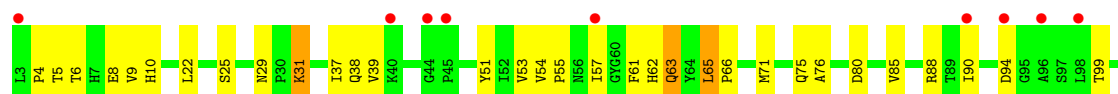
- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a

Chain F:



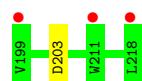
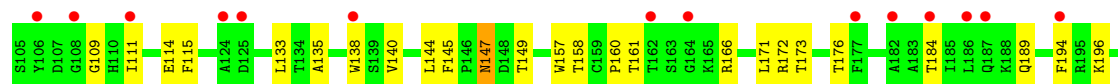
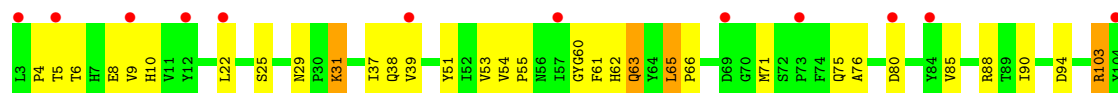
- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a

Chain G:



- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a

Chain H:



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 , 0.306	Depositor DCC
R_{free} test set	6014 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 120001 reflections	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.

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	0.39	0/1701	0.66	0/2313
1	B	0.39	0/1701	0.65	0/2313
1	C	0.39	0/1701	0.66	0/2313
1	D	0.38	0/1701	0.65	0/2313
1	E	0.38	0/1701	0.65	0/2313
1	F	0.41	0/1701	0.66	0/2313
1	G	0.38	0/1701	0.65	0/2313
1	H	0.39	0/1701	0.65	0/2313
All	All	0.39	0/13608	0.65	0/18504

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1672	0	1599	54	0
1	B	1672	0	1599	59	0
1	C	1672	0	1599	54	0
1	D	1672	0	1599	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1672	0	1599	53	0
1	F	1672	0	1599	55	0
1	G	1672	0	1599	53	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	422	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (422) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:H:63:GLN:HG3	1:H:111:ILE:HD13	1.55	0.87
1:D:63:GLN:HG3	1:D:111:ILE:HD13	1.57	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:H:160:PRO:HG3	1:H:166:ARG:NH1	1.90	0.86
1:D:160:PRO:HG3	1:D:166:ARG:NH1	1.91	0.86
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:G:160:PRO:HG3	1:G:166:ARG:HH12	1.42	0.85
1:F:63:GLN:HG3	1:F:111:ILE:HD13	1.58	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:C:160:PRO:HG3	1:C:166:ARG:HH12	1.40	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: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:H:160:PRO:HG3	1:H:166:ARG:HH12	1.42	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:160:PRO:HG3	1:E:166:ARG:HH12	1.41	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:F:160:PRO:HG3	1:F:166:ARG:HH12	1.41	0.82
1:A:147:ASN:HD22	1:A:149:THR:H	1.24	0.82
1:G:147:ASN:HD22	1:G:149:THR:H	1.24	0.81
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:H:63:GLN:H	1:H:63:GLN:NE2	1.85	0.74
1:D:88:ARG:HD3	1:D:173:THR:OG1	1.85	0.74
1:B:99:THR:HG21	1:G:99:THR:HG21	1.69	0.74
1:A:63:GLN:NE2	1:A:63:GLN:H	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:E:63:GLN:H	1:E:63:GLN:NE2	1.88	0.72
1:C:90:ILE:HG12	1:C:171:LEU:HG	1.71	0.72
1:H:63:GLN:HG3	1:H:111:ILE:CD1	2.19	0.72
1:E:143:MET:HE3	2:E:352:HOH:O	1.89	0.72
1:G:63:GLN:HG3	1:G:111:ILE:CD1	2.20	0.72
1:F:63:GLN:NE2	1:F:63:GLN:H	1.87	0.72
1:E:88:ARG:HD3	1:E:173:THR:OG1	1.90	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
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:E:63:GLN:HG3	1:E:111:ILE:CD1	2.20	0.71
1:B:63:GLN:NE2	1:B:63:GLN:H	1.88	0.71
1:C:88:ARG:HD3	1:C:173:THR:OG1	1.89	0.71
1:B:90:ILE:HG12	1:B:171:LEU:HG	1.73	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:NE2	1:G:63:GLN:H	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:G:4:PRO:HB3	1:G:111:ILE:HD11	1.74	0.69
1:B:63:GLN:HG3	1:B:111:ILE:CD1	2.22	0.69
1:A:22:LEU:HB3	1:A:39:VAL:HG21	1.75	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:H:4:PRO:HB3	1:H:111:ILE:HD11	1.75	0.68
1:B:22:LEU:HB3	1:B:39:VAL:CG2	2.23	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
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:D:9:VAL:HG22	1:D:61:PHE:CZ	2.31	0.65
1:A:29:ASN:OD1	1:A:31:LYS:HB2	1.95	0.65
1:F:4:PRO:HB3	1:F:111:ILE:HD11	1.77	0.65
1:C:4:PRO:HB3	1:C:111:ILE:HD11	1.77	0.65
1:G:9:VAL:HG22	1:G:61:PHE:CZ	2.32	0.65
1:H:63:GLN:H	1:H:63:GLN:HE21	1.43	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:GLN:HE21	1:A:63:GLN:H	1.44	0.65
1:G:51:TYR:CE2	1:G:135:ALA:HA	2.32	0.65
1:A:143:MET:HE3	2:A:313:HOH:O	1.96	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:E:51:TYR:CE2	1:E:135:ALA:HA	2.32	0.65
1:B:51:TYR:CE2	1:B: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:HE21	1:F:63:GLN:H	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:D:51:TYR:CE2	1:D:135:ALA:HA	2.32	0.62
1:H:61:PHE:HA	1:H:63:GLN:NE2	2.15	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: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: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
1:D:63:GLN:H	1:D:63:GLN:HE21	1.48	0.61
1:F:51:TYR:CE2	1:F:135:ALA:HA	2.35	0.61
1:D:54:VAL:HB	1:D:55:PRO:HD3	1.83	0.61
1:A:76:ALA:O	1:A:80:ASP:HB2	2.01	0.61
1:A:147:ASN:ND2	1:A:149:THR:H	1.98	0.61
1:B:63:GLN:HE21	1:B:63:GLN:H	1.46	0.61
1:F:76:ALA:O	1:F:80:ASP:HB2	2.01	0.61
1:G:61:PHE:HA	1:G:63:GLN:NE2	2.15	0.60
1:D:61:PHE:HA	1:D:63:GLN:NE2	2.16	0.60
1:F:9:VAL:HG22	1:F:61:PHE:CZ	2.36	0.60
1:G:63:GLN:HE21	1:G:63:GLN:H	1.47	0.60
1:B:147:ASN:ND2	1:B:149:THR:H	1.99	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:F:54:VAL:HB	1:F:55:PRO:HD3	1.84	0.60
1:C:54:VAL:HB	1:C: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:43:LYS:HE2	2:A:355:HOH:O	2.03	0.59
1:E:63:GLN:HE21	1:E:63:GLN:H	1.48	0.59
1:C:147:ASN:ND2	1:C:149:THR:H	1.97	0.59
1:B:5:THR:HG23	1:B:6:THR:HG23	1.83	0.59
1:F:166:ARG:HG2	1:F:166:ARG:HH11	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:HG2	1:D:166:ARG:HH11	1.69	0.58
1:E:61:PHE:C	1:E:63:GLN:HE21	2.06	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:H:184:THR:HG21	2:H:338:HOH:O	2.03	0.57
1:C:5:THR:HG23	1:C:6:THR:HG23	1.86	0.57
1:H:166:ARG:HH11	1:H:166:ARG:HG2	1.68	0.57
1:H:61:PHE:C	1:H:63:GLN:HE21	2.07	0.57
1:C:166:ARG:HH11	1:C:166:ARG:HG2	1.69	0.57
1:D:61:PHE:C	1:D:63:GLN:HE21	2.08	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:G:61:PHE:C	1:G:63:GLN:HE21	2.09	0.56
1:H:5:THR:HG23	1:H:6:THR:HG23	1.86	0.56
1:C:61:PHE:C	1:C:63:GLN:HE21	2.09	0.56
1:F:5:THR:HG23	1:F:6:THR:HG23	1.88	0.56
1:A:5:THR:HG23	1:A:6:THR:HG23	1.87	0.56
1:F:61:PHE:C	1:F:63:GLN:HE21	2.09	0.55
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:B:61:PHE:C	1:B:63:GLN:HE21	2.11	0.54
1:H:103:ARG:HG3	1:H:114:GLU:HB3	1.89	0.54
1:A:61:PHE:C	1:A:63:GLN:HE21	2.09	0.54
1:F:103:ARG:HG3	1:F:114:GLU:HB3	1.90	0.54
1:A:65:LEU:HD22	1:A:66:PRO:O	2.08	0.54
1:B:166:ARG:HG2	1:B:166:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:145:PHE:H	1:E:189:GLN:NE2	2.06	0.53
1:F:140:VAL:HG11	1:G:140:VAL:HG11	1.89	0.53
1:D:103:ARG:HG3	1:D:114:GLU:HB3	1.90	0.53
1:E:166:ARG:HG2	1:E:166:ARG:HH11	1.73	0.53
1:E:65:LEU:HD22	1:E:66:PRO:O	2.09	0.53
1:G:166:ARG:HG2	1:G:166:ARG:HH11	1.72	0.53
1:A:145:PHE:H	1:A:189:GLN:NE2	2.05	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:F:138:TRP:CZ2	1:F:196:LYS:HE3	2.44	0.52
1:A:140:VAL:HG11	1:B:140:VAL:HG11	1.91	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:H:4:PRO:CB	1:H:111:ILE:HD11	2.40	0.51
1:C:4:PRO:CB	1:C:111:ILE:HD11	2.41	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:D:147:ASN:ND2	1:D:149:THR:HG22	2.24	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:G:103:ARG:HG3	1:G:114:GLU:HB3	1.91	0.51
1:G:65:LEU:HD22	1:G:66:PRO:O	2.11	0.51
1:F:185:ILE:HD12	2:F:359:HOH:O	2.09	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:A:217:ASP:OD1	1:A:218:LEU:N	2.44	0.51
1:F:65:LEU:HD22	1:F:66:PRO:O	2.11	0.51
1:H:103:ARG:NH1	1:H:114:GLU:HG2	2.26	0.51
1:E:103:ARG:HG3	1:E:114:GLU:HB3	1.92	0.51
1:A:71:MET:HG2	1:A:75:GLN:HE21	1.76	0.50
1:H:138:TRP:CZ2	1:H:196:LYS:HE3	2.46	0.50
1:E:138:TRP:CZ2	1:E:196:LYS:HE3	2.47	0.50
1:A:4:PRO:CB	1:A:111:ILE:HD11	2.41	0.50
1:F:145:PHE:H	1:F:189:GLN:NE2	2.09	0.50
1:B:65:LEU:HD22	1:B:66:PRO:O	2.11	0.50
1:F:71:MET:HG2	1:F:75:GLN:HE21	1.76	0.50
1:D:71:MET:HG2	1:D: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:145:PHE:H	1:D:189:GLN:NE2	2.10	0.50
1:C:65:LEU:HD22	1:C:66:PRO:O	2.11	0.50
1:E:71:MET:HG2	1:E:75:GLN:HE21	1.77	0.49
1:D:138:TRP:CZ2	1:D:196:LYS:HE3	2.46	0.49
1:C:71:MET:HG2	1:C:75:GLN:HE21	1.76	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:G:145:PHE:H	1:G:189:GLN:NE2	2.11	0.49
1:D:65:LEU:HD22	1:D:66:PRO:O	2.12	0.49
1:H:133:LEU:HD23	1:H:161:THR:HG22	1.95	0.49
1:D:103:ARG:NH1	1:D:114:GLU:HG2	2.28	0.49
1:D:66:PRO:HG2	2:D:331:HOH:O	2.12	0.49
1:C:145:PHE:H	1:C:189:GLN:NE2	2.11	0.49
1:A:103:ARG:NH1	1:A:114:GLU:HG2	2.27	0.48
1:F:147:ASN:ND2	1:F:149:THR:H	2.00	0.48
1:A:138:TRP:CZ2	1:A:196:LYS:HE3	2.47	0.48
1:A:133:LEU:HD23	1:A:161:THR:HG22	1.95	0.48
1:F:133:LEU:HD23	1:F:161:THR:HG22	1.95	0.48
1:G:4:PRO:CB	1:G:111:ILE:HD11	2.40	0.48
1:E:4:PRO:CB	1:E:111:ILE:HD11	2.42	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:H:71:MET:HG2	1:H:75:GLN:HE21	1.78	0.48
1:B:145:PHE:H	1:B:189:GLN:NE2	2.11	0.48
1:A:168:HIS:HD2	2:A:397:HOH:O	1.97	0.47
1:G:9:VAL:HG23	1:G:37:ILE:HD11	1.96	0.47
1:E:103:ARG:NH1	1:E:114:GLU:HG2	2.29	0.47
1:B:133:LEU:HD23	1:B:161:THR:HG22	1.96	0.47
1:B:147:ASN:ND2	1:B:149:THR:HG22	2.29	0.47
1:H:22:LEU:HB3	1:H:39:VAL:HG22	1.97	0.47
1:D:10:HIS:ND1	1:D:114:GLU:OE2	2.46	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:F:9:VAL:HG23	1:F:37:ILE:CD1	2.45	0.47
1:C:37:ILE:HG12	1:C:38:GLN:N	2.29	0.47
1:G:10:HIS:ND1	1:G:114:GLU:OE2	2.47	0.47
1:C:115:PHE:CD1	1:C:115:PHE:N	2.83	0.47
1:A:63:GLN:CG	1:A:111:ILE:HD13	2.38	0.47
1:H:147:ASN:ND2	1:H:149:THR:HG22	2.29	0.47
1:B:37:ILE:HG12	1:B:38:GLN:N	2.30	0.47
1:H:37:ILE:HG12	1:H:38:GLN:N	2.29	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:E:10:HIS:ND1	1:E:114:GLU:OE2	2.48	0.47
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:B:71:MET:HG2	1:B:75:GLN:HE21	1.80	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:D:158:THR:HG21	1:H:144:LEU:HD11	1.97	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:C:9:VAL:HG23	1:C:37:ILE:HD11	1.96	0.46
1:A:147:ASN:ND2	1:A:149:THR:HG22	2.30	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: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:E:9:VAL:HG22	1:E:61:PHE:HZ	1.81	0.45
1:D:9:VAL:HG23	1:D:37:ILE:HD11	1.98	0.45
1:C:166:ARG:NH1	1:C:166:ARG:HG2	2.32	0.45
1:B:217:ASP:OD1	1:B:218:LEU:N	2.47	0.45
1:B:5:THR:HG22	1:B:109:GLY:O	2.17	0.45
1:E:115:PHE:CD1	1:E:115:PHE:N	2.84	0.45
1:B:22:LEU:HB3	1:B:39:VAL:HG22	1.98	0.45
1:G:51:TYR:CD2	1:G:135:ALA:HA	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:5:THR:HG22	1:G:109:GLY:O	2.17	0.45
1:B:115:PHE:CD1	1:B:115:PHE:N	2.85	0.45
1:C:194:PHE:CD2	1:E:218:LEU:HB2	2.52	0.44
2:A:349:HOH:O	1:B:144:LEU:HD12	2.17	0.44
1:A:9:VAL:HG23	1:A:37:ILE:HD11	1.99	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:D:115:PHE:CD1	1:D:115:PHE:N	2.85	0.44
1:G:137:ASP:OD2	1:G:166:ARG:NH1	2.51	0.44
1:C:5:THR:HG22	1:C:109:GLY:O	2.18	0.44
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: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:H:5:THR:HG22	1:H:109:GLY:O	2.17	0.44
1:G:115:PHE:CD1	1:G:115:PHE:N	2.84	0.44
1:H:9:VAL:HG22	1:H:61:PHE:HZ	1.80	0.44
1:A:22:LEU:HB3	1:A:39:VAL:HG22	1.99	0.44
1:C:9:VAL:HG23	1:C:37:ILE:CD1	2.48	0.44
1:B:51:TYR:CD2	1:B:135:ALA:HA	2.53	0.43
1:B:42:THR:HA	2:B:324:HOH:O	2.17	0.43
1:H:60:CR2:HA12	1:H:60:CR2:HA31	1.87	0.43
1:E:151:VAL:HB	1:E:175:TYR:HB2	2.00	0.43
1:E:88:ARG:CD	1:E:173:THR:OG1	2.64	0.43
1:G:88:ARG:CD	1:G:173:THR:OG1	2.63	0.43
1:F:22:LEU:HB3	1:F:39:VAL:HG22	1.96	0.43
1:H:51:TYR:CD2	1:H:135:ALA:HA	2.53	0.43
1:C:10:HIS:ND1	1:C:114:GLU:OE2	2.50	0.43
1:H:115:PHE:CD1	1:H:115:PHE:N	2.86	0.43
1:H:166:ARG:HG2	1:H:166:ARG:NH1	2.32	0.43
1:F:172:ARG:NH2	2:F:345:HOH:O	2.52	0.43
1:E:5:THR:HG22	1:E:109:GLY:O	2.18	0.43
1:E:9:VAL:HG23	1:E:37:ILE:CD1	2.49	0.43
1:F:25:SER:C	1:F:37:ILE:HG13	2.38	0.43
1:C:63:GLN:CG	1:C:111:ILE:HD13	2.41	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:D:8:GLU:HA	1:D:25:SER:HA	2.01	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:115:PHE:CD1	1:A:115:PHE:N	2.86	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:9:VAL:HG23	1:B:37:ILE:HD11	2.00	0.43
1:C:88:ARG:CD	1:C:173:THR:OG1	2.63	0.43
1:B:103:ARG:HD2	2:B:303:HOH:O	2.18	0.43
1:A:151:VAL:HB	1:A:175:TYR:HB2	2.00	0.43
1:D:51:TYR:CD2	1:D:135:ALA:HA	2.53	0.42
1:F:60:CR2:HA31	1:F:60:CR2:HA12	1.85	0.42
1:C:137:ASP:OD2	1:C:166:ARG:NH1	2.52	0.42
1:F:147:ASN:ND2	1:F:149:THR:HG22	2.33	0.42
1:D:5:THR:HG22	1:D:109:GLY:O	2.19	0.42
1:D:88:ARG:CD	1:D:173:THR:OG1	2.61	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:G:25:SER:C	1:G:37:ILE:HG13	2.39	0.42
1:F:62:HIS:N	1:F:63:GLN:HE21	2.18	0.42
1:D:166:ARG:HG2	1:D:166:ARG:NH1	2.32	0.42
1:H:85:VAL:HG12	1:H:176:THR:HB	2.00	0.42
1:H:9:VAL:HG23	1:H:37:ILE:CD1	2.49	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:E:63:GLN:CG	1:E:111:ILE:HD13	2.39	0.42
1:G:147:ASN:HD22	1:G:147:ASN:C	2.22	0.42
1:D:31:LYS:HE2	1:D:31:LYS:HA	2.01	0.42
1:E:51:TYR:CD2	1:E:135:ALA:HA	2.55	0.42
1:F:51:TYR:CD2	1:F:135:ALA:HA	2.55	0.42
1:D:85:VAL:HG12	1:D:176:THR:HB	2.02	0.42
1:B:147:ASN:C	1:B:147:ASN:HD22	2.24	0.42
1:G:85:VAL:HG12	1:G:176:THR:HB	2.02	0.42
1:G:8:GLU:HA	1:G:25:SER:HA	2.03	0.41
1:D:137:ASP:OD2	1:D:166:ARG:NH1	2.53	0.41
1:A:147:ASN:C	1:A:147:ASN:HD22	2.23	0.41
1:F:90:ILE:HB	1:F:98:LEU:HB3	2.02	0.41
1:C:57:ILE:HD12	1:C:57:ILE:HA	1.92	0.41
1:B:31:LYS:HA	1:B:31:LYS:HE2	2.02	0.41
1:E:166:ARG:HG2	1:E:166:ARG:NH1	2.35	0.41
1:A:51:TYR:CD2	1:A:135:ALA:HA	2.54	0.41
1:E:57:ILE:HA	1:E:57:ILE:HD12	1.93	0.41
1:G:9:VAL:HG22	1:G:61:PHE:HZ	1.80	0.41
1:H:25:SER:C	1:H:37:ILE:HG13	2.41	0.41
1:B:9:VAL:HG23	1:B:37:ILE:CD1	2.50	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:63:GLN:CG	1:B:111:ILE:HD13	2.40	0.41
1:C:25:SER:C	1:C:37:ILE:HG13	2.40	0.41
1:F:85:VAL:HG12	1:F:176:THR:HB	2.02	0.41
1:H:63:GLN:CG	1:H:111:ILE:HD13	2.38	0.41
1:H:62:HIS:N	1:H:63:GLN:HE21	2.17	0.41
1:H:147:ASN:HD22	1:H:147:ASN:C	2.23	0.41
1:B:166:ARG:NH1	1:B:166:ARG:HG2	2.35	0.41
1:A:8:GLU:HA	1:A:25:SER:HA	2.02	0.41
1:F:218:LEU:HA	1:F:218:LEU:HD23	1.92	0.41
1:E:61:PHE:CA	1:E:63:GLN:HE21	2.34	0.41
1:D:62:HIS:N	1:D:63:GLN:HE21	2.18	0.41
1:F:31:LYS:HA	1:F:31:LYS:HE2	2.03	0.41
1:H:31:LYS:HE2	1:H:31:LYS:HA	2.02	0.41
1:E:137:ASP:OD2	1:E:166:ARG:NH1	2.54	0.40
1:H:8:GLU:HA	1:H:25:SER:HA	2.02	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:G:62:HIS:N	1:G:63:GLN:HE21	2.20	0.40
1:C:147:ASN:HD22	1:C:147:ASN:C	2.25	0.40
1:E:8:GLU:HA	1:E:25:SER:HA	2.03	0.40
1:C:151:VAL:HB	1:C:175:TYR:HB2	2.02	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	Distance(Å)	Clash(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

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	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%)	34	16
1	B	179/179 (100%)	170 (95%)	9 (5%)	34	16
1	C	179/179 (100%)	170 (95%)	9 (5%)	34	16
1	D	179/179 (100%)	170 (95%)	9 (5%)	34	16
1	E	179/179 (100%)	170 (95%)	9 (5%)	34	16
1	F	179/179 (100%)	170 (95%)	9 (5%)	34	16
1	G	179/179 (100%)	170 (95%)	9 (5%)	34	16
1	H	179/179 (100%)	170 (95%)	9 (5%)	34	16
All	All	1432/1432 (100%)	1360 (95%)	72 (5%)	34	16

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	53	VAL
1	A	63	GLN
1	A	65	LEU

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Mol	Chain	Res	Type
1	A	94	ASP
1	A	103	ARG
1	A	147	ASN
1	A	157	TRP
1	A	172	ARG
1	B	31	LYS
1	B	53	VAL
1	B	63	GLN
1	B	65	LEU
1	B	94	ASP
1	B	103	ARG
1	B	147	ASN
1	B	157	TRP
1	B	172	ARG
1	C	31	LYS
1	C	53	VAL
1	C	63	GLN
1	C	65	LEU
1	C	94	ASP
1	C	103	ARG
1	C	147	ASN
1	C	157	TRP
1	C	172	ARG
1	D	31	LYS
1	D	53	VAL
1	D	63	GLN
1	D	65	LEU
1	D	94	ASP
1	D	103	ARG
1	D	147	ASN
1	D	157	TRP
1	D	172	ARG
1	E	31	LYS
1	E	53	VAL
1	E	63	GLN
1	E	65	LEU
1	E	94	ASP
1	E	103	ARG
1	E	147	ASN
1	E	157	TRP
1	E	172	ARG
1	F	31	LYS

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Mol	Chain	Res	Type
1	F	53	VAL
1	F	63	GLN
1	F	65	LEU
1	F	94	ASP
1	F	103	ARG
1	F	147	ASN
1	F	157	TRP
1	F	172	ARG
1	G	31	LYS
1	G	53	VAL
1	G	63	GLN
1	G	65	LEU
1	G	94	ASP
1	G	103	ARG
1	G	147	ASN
1	G	157	TRP
1	G	172	ARG
1	H	31	LYS
1	H	53	VAL
1	H	63	GLN
1	H	65	LEU
1	H	94	ASP
1	H	103	ARG
1	H	147	ASN
1	H	157	TRP
1	H	172	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	63	GLN
1	A	75	GLN
1	A	147	ASN
1	A	168	HIS
1	A	189	GLN
1	B	63	GLN
1	B	75	GLN
1	B	147	ASN
1	B	189	GLN
1	C	63	GLN
1	C	75	GLN

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Mol	Chain	Res	Type
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	147	ASN
1	D	168	HIS
1	D	189	GLN
1	E	38	GLN
1	E	63	GLN
1	E	75	GLN
1	E	147	ASN
1	E	189	GLN
1	F	63	GLN
1	F	75	GLN
1	F	147	ASN
1	F	189	GLN
1	G	38	GLN
1	G	63	GLN
1	G	75	GLN
1	G	147	ASN
1	G	189	GLN
1	H	38	GLN
1	H	63	GLN
1	H	75	GLN
1	H	147	ASN
1	H	189	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	5.82	9 (45%)	25,27,29	4.89	7 (28%)
1	CR2	B	58	1	20,20,21	5.78	9 (45%)	25,27,29	4.61	8 (32%)
1	CR2	C	60	1	20,20,21	5.85	9 (45%)	25,27,29	4.93	7 (28%)
1	CR2	D	60	1	20,20,21	5.93	9 (45%)	25,27,29	4.82	7 (28%)
1	CR2	E	60	1	20,20,21	6.08	10 (50%)	25,27,29	4.89	7 (28%)
1	CR2	F	60	1	20,20,21	5.96	9 (45%)	25,27,29	4.82	7 (28%)
1	CR2	G	60	1	20,20,21	5.98	9 (45%)	25,27,29	4.81	7 (28%)
1	CR2	H	60	1	20,20,21	5.98	9 (45%)	25,27,29	4.77	7 (28%)

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	-	0/8/25/26	0/2/2/2
1	CR2	B	58	1	-	0/8/25/26	0/2/2/2
1	CR2	C	60	1	-	0/8/25/26	0/2/2/2
1	CR2	D	60	1	-	0/8/25/26	0/2/2/2
1	CR2	E	60	1	-	0/8/25/26	0/2/2/2
1	CR2	F	60	1	-	0/8/25/26	0/2/2/2
1	CR2	G	60	1	-	0/8/25/26	0/2/2/2
1	CR2	H	60	1	-	0/8/25/26	0/2/2/2

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	60	CR2	O3-C3	17.87	1.23	1.11
1	F	60	CR2	O3-C3	17.54	1.23	1.11
1	H	60	CR2	O3-C3	17.50	1.23	1.11
1	C	60	CR2	O3-C3	17.45	1.23	1.11
1	E	60	CR2	O3-C3	17.34	1.23	1.11
1	D	60	CR2	O3-C3	17.34	1.23	1.11
1	A	60	CR2	O3-C3	17.22	1.23	1.11
1	B	58	CR2	O3-C3	17.11	1.23	1.11
1	E	60	CR2	CB2-CA2	15.91	1.46	1.35
1	H	60	CR2	CB2-CA2	15.68	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	60	CR2	CB2-CA2	15.30	1.45	1.35
1	G	60	CR2	CB2-CA2	14.91	1.45	1.35
1	F	60	CR2	CB2-CA2	14.72	1.45	1.35
1	B	58	CR2	CB2-CA2	14.60	1.45	1.35
1	A	60	CR2	CB2-CA2	14.60	1.45	1.35
1	C	60	CR2	CB2-CA2	14.43	1.45	1.35
1	F	60	CR2	CA2-N2	-8.20	1.20	1.38
1	C	60	CR2	CA2-N2	-7.99	1.20	1.38
1	A	60	CR2	CA2-N2	-7.92	1.20	1.38
1	G	60	CR2	CA2-N2	-7.84	1.20	1.38
1	D	60	CR2	CA2-N2	-7.78	1.20	1.38
1	E	60	CR2	CA2-N2	-7.71	1.21	1.38
1	B	58	CR2	CA2-N2	-7.67	1.21	1.38
1	H	60	CR2	CA2-N2	-7.54	1.21	1.38
1	F	60	CR2	C2-N3	-6.01	1.27	1.39
1	E	60	CR2	CA3-N3	-5.94	1.42	1.47
1	E	60	CR2	C2-N3	-5.77	1.27	1.39
1	D	60	CR2	C2-N3	-5.73	1.27	1.39
1	H	60	CR2	C2-N3	-5.65	1.27	1.39
1	A	60	CR2	C2-N3	-5.60	1.28	1.39
1	B	58	CR2	C2-N3	-5.60	1.28	1.39
1	C	60	CR2	C2-N3	-5.56	1.28	1.39
1	G	60	CR2	C2-N3	-5.52	1.28	1.39
1	F	60	CR2	CA3-N3	-5.13	1.43	1.47
1	D	60	CR2	CA3-N3	-5.06	1.43	1.47
1	G	60	CR2	CA3-N3	-5.04	1.43	1.47
1	B	58	CR2	CA3-N3	-4.74	1.43	1.47
1	A	60	CR2	CA3-N3	-4.65	1.43	1.47
1	H	60	CR2	CA3-N3	-4.61	1.43	1.47
1	A	60	CR2	OH-CZ	-4.52	1.25	1.37
1	F	60	CR2	OH-CZ	-4.50	1.25	1.37
1	H	60	CR2	OH-CZ	-4.42	1.25	1.37
1	C	60	CR2	CA3-N3	-4.39	1.43	1.47
1	B	58	CR2	OH-CZ	-4.39	1.25	1.37
1	D	60	CR2	OH-CZ	-4.29	1.26	1.37
1	C	60	CR2	OH-CZ	-4.28	1.26	1.37
1	G	60	CR2	OH-CZ	-4.24	1.26	1.37
1	C	60	CR2	C1-N3	-4.15	1.30	1.37
1	E	60	CR2	OH-CZ	-4.06	1.26	1.37
1	E	60	CR2	C1-N3	-3.82	1.31	1.37
1	G	60	CR2	C1-N3	-3.75	1.31	1.37
1	F	60	CR2	C1-N3	-3.73	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	CR2	C1-N3	-3.36	1.32	1.37
1	H	60	CR2	C1-N3	-3.28	1.32	1.37
1	D	60	CR2	C1-N3	-3.00	1.32	1.37
1	D	60	CR2	CA3-C3	2.96	1.52	1.48
1	B	58	CR2	CA3-C3	2.82	1.52	1.48
1	G	60	CR2	CE2-CZ	-2.81	1.32	1.38
1	H	60	CR2	CE2-CZ	-2.76	1.33	1.38
1	E	60	CR2	CE2-CZ	-2.74	1.33	1.38
1	G	60	CR2	CA3-C3	2.73	1.51	1.48
1	B	58	CR2	C1-N3	-2.71	1.33	1.37
1	A	60	CR2	CE2-CZ	-2.67	1.33	1.38
1	F	60	CR2	CA3-C3	2.67	1.51	1.48
1	D	60	CR2	CE2-CZ	-2.63	1.33	1.38
1	A	60	CR2	CA3-C3	2.62	1.51	1.48
1	B	58	CR2	CE2-CZ	-2.60	1.33	1.38
1	H	60	CR2	CA3-C3	2.59	1.51	1.48
1	F	60	CR2	CE2-CZ	-2.48	1.33	1.38
1	E	60	CR2	CA3-C3	2.41	1.51	1.48
1	C	60	CR2	CE2-CZ	-2.29	1.34	1.38
1	C	60	CR2	CA3-C3	2.26	1.51	1.48
1	E	60	CR2	CA2-C2	-2.07	1.46	1.48

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	CR2	O2-C2-CA2	-17.26	120.98	130.96
1	E	60	CR2	O2-C2-CA2	-16.90	121.19	130.96
1	A	60	CR2	O2-C2-CA2	-16.54	121.40	130.96
1	G	60	CR2	O2-C2-CA2	-16.53	121.40	130.96
1	D	60	CR2	O2-C2-CA2	-16.52	121.41	130.96
1	F	60	CR2	O2-C2-CA2	-16.52	121.41	130.96
1	H	60	CR2	O2-C2-CA2	-16.30	121.53	130.96
1	B	58	CR2	O2-C2-CA2	-15.51	121.99	130.96
1	A	60	CR2	CA3-N3-C2	12.56	131.28	123.46
1	F	60	CR2	CA3-N3-C2	12.20	131.05	123.46
1	E	60	CR2	CA3-N3-C2	12.14	131.02	123.46
1	G	60	CR2	CA3-N3-C2	12.02	130.94	123.46
1	D	60	CR2	CA3-N3-C2	12.01	130.93	123.46
1	C	60	CR2	CA3-N3-C2	11.96	130.90	123.46
1	H	60	CR2	CA3-N3-C2	11.87	130.85	123.46
1	B	58	CR2	CA3-N3-C2	11.29	130.49	123.46
1	A	60	CR2	CG2-CB2-CA2	8.49	139.86	130.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	60	CR2	CG2-CB2-CA2	8.38	139.73	130.10
1	B	58	CR2	CG2-CB2-CA2	8.22	139.54	130.10
1	C	60	CR2	CG2-CB2-CA2	8.18	139.50	130.10
1	D	60	CR2	CG2-CB2-CA2	8.06	139.37	130.10
1	E	60	CR2	CG2-CB2-CA2	7.97	139.26	130.10
1	G	60	CR2	CG2-CB2-CA2	7.94	139.23	130.10
1	F	60	CR2	CG2-CB2-CA2	7.87	139.15	130.10
1	C	60	CR2	CA2-C2-N3	6.11	106.92	103.44
1	G	60	CR2	CA2-C2-N3	6.07	106.90	103.44
1	E	60	CR2	CA2-C2-N3	5.91	106.80	103.44
1	D	60	CR2	CA2-C2-N3	5.87	106.78	103.44
1	F	60	CR2	CA2-C2-N3	5.80	106.74	103.44
1	A	60	CR2	CA2-C2-N3	5.70	106.68	103.44
1	H	60	CR2	CA2-C2-N3	5.62	106.64	103.44
1	B	58	CR2	CA2-C2-N3	5.23	106.42	103.44
1	B	58	CR2	CA2-N2-C1	5.00	109.84	105.81
1	E	60	CR2	CA2-N2-C1	4.71	109.60	105.81
1	F	60	CR2	CA2-N2-C1	4.52	109.45	105.81
1	D	60	CR2	CA2-N2-C1	4.42	109.37	105.81
1	C	60	CR2	CA2-N2-C1	4.42	109.37	105.81
1	H	60	CR2	CA2-N2-C1	4.40	109.36	105.81
1	G	60	CR2	CA2-N2-C1	4.40	109.36	105.81
1	A	60	CR2	CA2-N2-C1	4.27	109.25	105.81
1	E	60	CR2	C2-CA2-N2	-3.57	106.22	108.91
1	C	60	CR2	O2-C2-N3	3.43	132.10	124.71
1	G	60	CR2	C2-CA2-N2	-3.41	106.34	108.91
1	C	60	CR2	C2-CA2-N2	-3.40	106.35	108.91
1	E	60	CR2	O2-C2-N3	3.39	132.01	124.71
1	A	60	CR2	O2-C2-N3	3.34	131.92	124.71
1	F	60	CR2	O2-C2-N3	3.31	131.85	124.71
1	H	60	CR2	O2-C2-N3	3.30	131.83	124.71
1	D	60	CR2	O2-C2-N3	3.29	131.81	124.71
1	F	60	CR2	C2-CA2-N2	-3.29	106.43	108.91
1	H	60	CR2	C2-CA2-N2	-3.29	106.44	108.91
1	G	60	CR2	O2-C2-N3	3.24	131.70	124.71
1	B	58	CR2	O2-C2-N3	3.19	131.59	124.71
1	B	58	CR2	C2-CA2-N2	-3.17	106.52	108.91
1	D	60	CR2	C2-CA2-N2	-3.14	106.55	108.91
1	A	60	CR2	C2-CA2-N2	-3.08	106.59	108.91
1	B	58	CR2	C1-CA1-N1	-2.01	108.23	112.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	214/214 (100%)	0.77	10 (4%)	30 36	23, 40, 54, 65	0
1	B	214/214 (100%)	0.79	14 (6%)	18 24	26, 41, 54, 65	0
1	C	214/214 (100%)	0.74	5 (2%)	57 65	27, 42, 55, 65	0
1	D	214/214 (100%)	0.81	16 (7%)	14 18	30, 43, 56, 64	0
1	E	214/214 (100%)	0.89	17 (7%)	13 16	29, 43, 55, 64	0
1	F	214/214 (100%)	0.75	13 (6%)	21 26	27, 40, 55, 64	0
1	G	214/214 (100%)	1.00	24 (11%)	6 6	30, 43, 56, 65	0
1	H	214/214 (100%)	1.09	29 (13%)	4 4	33, 44, 56, 64	0
All	All	1712/1712 (100%)	0.85	128 (7%)	14 18	23, 42, 55, 65	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	218	LEU	5.3
1	E	218	LEU	4.8
1	H	211	TRP	4.8
1	H	184	THR	4.3
1	C	203	ASP	4.3
1	E	179	LYS	4.2
1	D	187	GLN	4.2
1	G	187	GLN	4.1
1	H	108	GLY	3.9
1	A	218	LEU	3.8
1	E	83	GLY	3.6
1	E	181	ILE	3.5
1	H	9	VAL	3.5
1	H	194	PHE	3.4
1	H	5	THR	3.3
1	G	57	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	181	ILE	3.2
1	G	211	TRP	3.2
1	H	199	VAL	3.2
1	H	187	GLN	3.2
1	E	57	ILE	3.1
1	H	22	LEU	3.1
1	H	124	ALA	3.1
1	D	218	LEU	3.0
1	F	204	ALA	3.0
1	B	203	ASP	3.0
1	E	203	ASP	3.0
1	C	3	LEU	2.9
1	A	90	ILE	2.9
1	G	3	LEU	2.9
1	G	164	GLY	2.9
1	A	170	THR	2.9
1	B	108	GLY	2.9
1	E	39	VAL	2.9
1	F	203	ASP	2.9
1	G	218	LEU	2.9
1	D	3	LEU	2.8
1	G	45	PRO	2.8
1	F	69	ASP	2.8
1	H	106	TYR	2.8
1	C	162	THR	2.8
1	E	186	LEU	2.8
1	G	106	TYR	2.7
1	A	203	ASP	2.7
1	A	98	LEU	2.7
1	F	211	TRP	2.7
1	C	201	ALA	2.7
1	H	57	ILE	2.7
1	D	57	ILE	2.7
1	B	171	LEU	2.6
1	D	151	VAL	2.6
1	G	111	ILE	2.6
1	B	106	TYR	2.6
1	A	171	LEU	2.6
1	H	186	LEU	2.6
1	G	44	GLY	2.5
1	B	90	ILE	2.5
1	H	3	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	209	LYS	2.5
1	B	125	ASP	2.5
1	E	90	ILE	2.5
1	F	90	ILE	2.5
1	F	171	LEU	2.5
1	D	162	THR	2.5
1	E	149	THR	2.5
1	G	181	ILE	2.4
1	B	23	VAL	2.4
1	B	172	ARG	2.4
1	G	90	ILE	2.4
1	H	84	TYR	2.4
1	E	187	GLN	2.4
1	F	99	THR	2.4
1	A	45	PRO	2.4
1	G	213	LYS	2.4
1	D	90	ILE	2.4
1	G	170	THR	2.4
1	H	69	ASP	2.3
1	H	80	ASP	2.3
1	G	96	ALA	2.3
1	G	171	LEU	2.3
1	D	191	MET	2.3
1	E	125	ASP	2.3
1	H	125	ASP	2.3
1	B	57	ILE	2.3
1	G	184	THR	2.3
1	G	98	LEU	2.3
1	B	165	LYS	2.3
1	E	178	ALA	2.3
1	B	80	ASP	2.3
1	D	98	LEU	2.3
1	B	5	THR	2.3
1	D	96	ALA	2.3
1	H	104	TYR	2.2
1	F	57	ILE	2.2
1	E	80	ASP	2.2
1	H	73	PRO	2.2
1	B	65	LEU	2.2
1	F	170	THR	2.2
1	E	82	SER	2.2
1	F	96	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	89	THR	2.2
1	D	6	THR	2.2
1	H	12	TYR	2.2
1	F	154	THR	2.2
1	H	39	VAL	2.2
1	H	177	PHE	2.2
1	G	148	ASP	2.2
1	G	182	ALA	2.1
1	A	89	THR	2.1
1	A	99	THR	2.1
1	F	108	GLY	2.1
1	H	138	TRP	2.1
1	G	40	LYS	2.1
1	D	184	THR	2.1
1	F	103	ARG	2.1
1	H	111	ILE	2.1
1	E	69	ASP	2.1
1	D	165	LYS	2.1
1	D	171	LEU	2.1
1	H	164	GLY	2.1
1	A	165	LYS	2.0
1	D	94	ASP	2.0
1	C	89	THR	2.0
1	E	158	THR	2.0
1	H	162	THR	2.0
1	G	94	ASP	2.0
1	G	108	GLY	2.0
1	H	182	ALA	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CR2	E	60	19/20	0.14	0.00	42,44,46,47	0
1	CR2	F	60	19/20	0.14	-0.39	39,41,43,44	0
1	CR2	H	60	19/20	0.15	-0.43	43,45,46,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	CR2	D	60	19/20	0.12	-0.50	41,43,45,45	0
1	CR2	G	60	19/20	0.14	-0.54	43,45,47,47	0
1	CR2	A	60	19/20	0.13	-0.65	35,41,42,43	0
1	CR2	C	60	19/20	0.12	-0.80	40,42,43,44	0
1	CR2	B	58	19/20	0.13	-0.99	36,39,41,42	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.