



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:52 PM GMT

PDB ID : 4DKM
Title : Crystal Structure of Amphioxus GFPc1a
Authors : Deheyne, 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

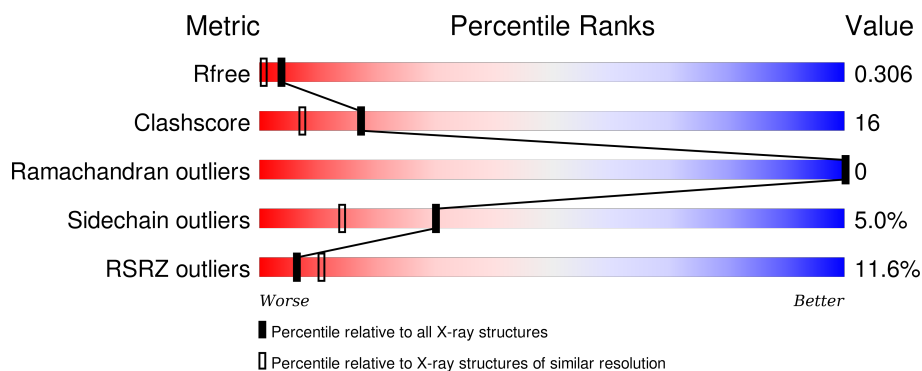
1 Overall quality at a glance

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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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. 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	<div> <div>8%</div> <div>72%</div> <div>26%</div> <div>.</div> </div>
1	B	214	<div> <div>10%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>
1	C	214	<div> <div>7%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>
1	D	214	<div> <div>10%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>
1	E	214	<div> <div>12%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	214	<div><div></div><div>9%</div><div>72%</div><div>25%</div><div></div></div>
1	G	214	<div><div></div><div>17%</div><div>73%</div><div>24%</div><div></div></div>
1	H	214	<div><div></div><div>18%</div><div>73%</div><div>25%</div><div></div></div>

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

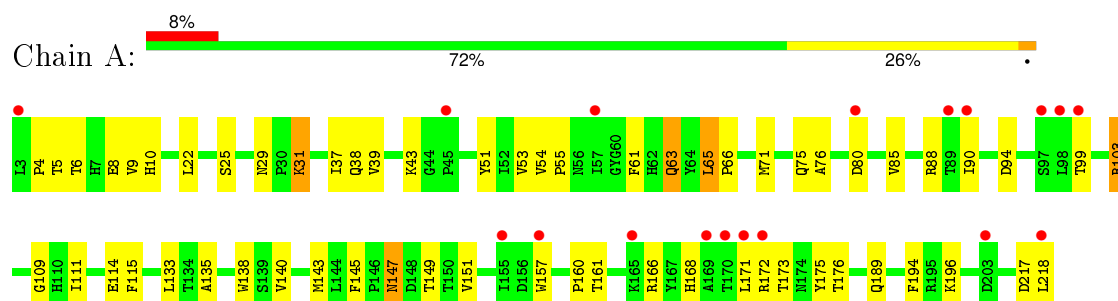
- Molecule 2 is water.

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

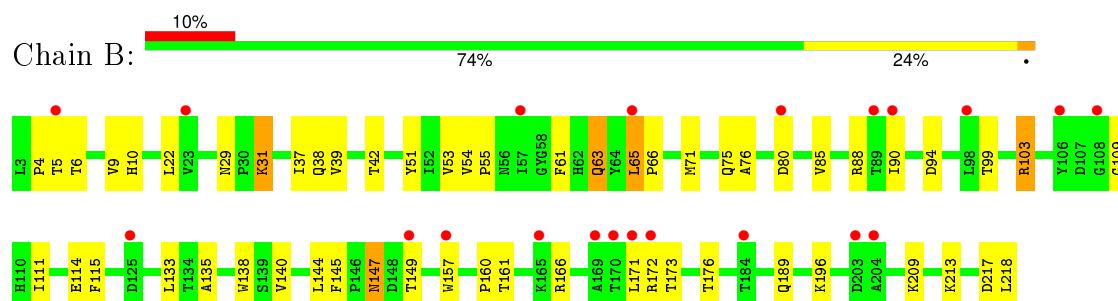
3 Residue-property plots [i](#)

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.

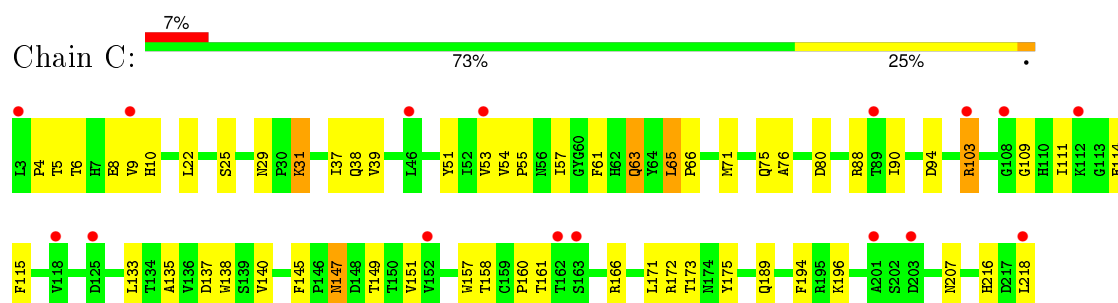
- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a



- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a

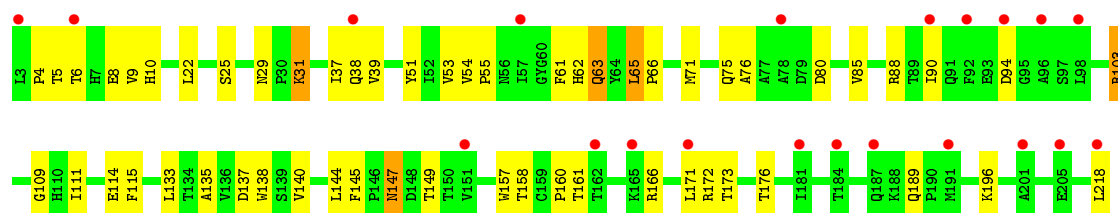


- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a

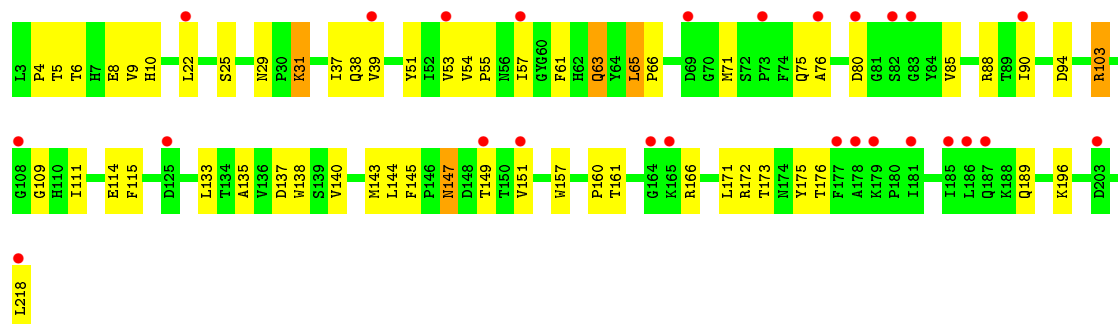


- Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a

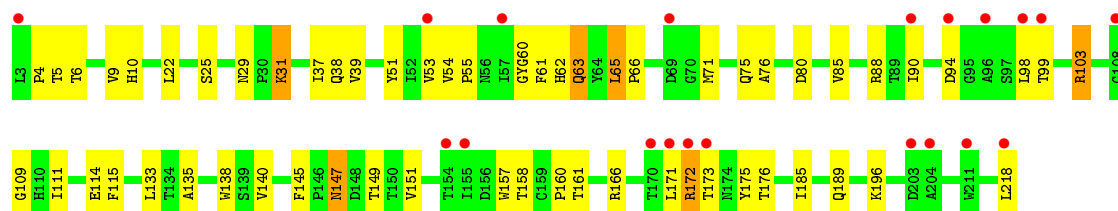




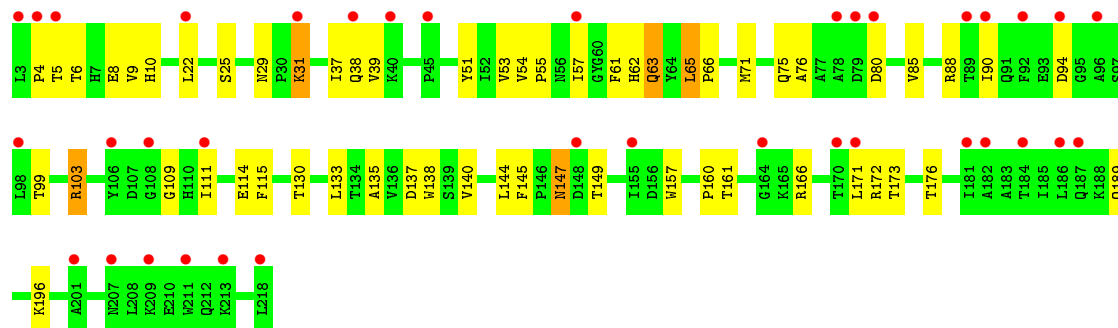
• Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a



• Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a

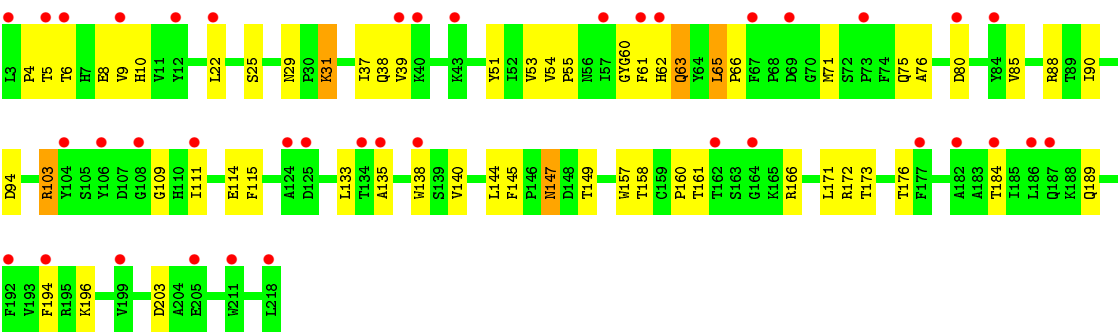


• Molecule 1: Amphioxus Green Fluorescent Protein, GFPc1a



• 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	158.76 Å 130.46 Å 106.33 Å 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 1.95 Å)	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 , 36.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.39	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 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	54	0
1	B	1672	0	1599	59	0
1	C	1672	0	1599	54	0
1	D	1672	0	1599	54	0
1	E	1672	0	1599	53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 16.

All (422) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:PRO:HG3	1:H:166:ARG:HH12	1.42	0.84
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	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

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
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%)	30	14
1	B	179/179 (100%)	170 (95%)	9 (5%)	30	14
1	C	179/179 (100%)	170 (95%)	9 (5%)	30	14
1	D	179/179 (100%)	170 (95%)	9 (5%)	30	14
1	E	179/179 (100%)	170 (95%)	9 (5%)	30	14
1	F	179/179 (100%)	170 (95%)	9 (5%)	30	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	179/179 (100%)	170 (95%)	9 (5%)	30	14
1	H	179/179 (100%)	170 (95%)	9 (5%)	30	14
All	All	1432/1432 (100%)	1360 (95%)	72 (5%)	30	14

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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
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 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	3.75	7 (35%)	25,27,29	4.79	10 (40%)
1	CR2	B	58	1	20,20,21	3.75	8 (40%)	25,27,29	4.56	10 (40%)
1	CR2	C	60	1	20,20,21	3.78	7 (35%)	25,27,29	4.89	10 (40%)
1	CR2	D	60	1	20,20,21	3.81	7 (35%)	25,27,29	4.75	10 (40%)
1	CR2	E	60	1	20,20,21	3.95	8 (40%)	25,27,29	4.83	10 (40%)
1	CR2	F	60	1	20,20,21	3.85	7 (35%)	25,27,29	4.75	10 (40%)
1	CR2	G	60	1	20,20,21	3.80	7 (35%)	25,27,29	4.75	10 (40%)
1	CR2	H	60	1	20,20,21	3.84	7 (35%)	25,27,29	4.72	10 (40%)

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	-	0/6/25/26	0/2/2/2
1	CR2	B	58	1	-	0/6/25/26	0/2/2/2
1	CR2	C	60	1	-	0/6/25/26	0/2/2/2
1	CR2	D	60	1	-	0/6/25/26	0/2/2/2
1	CR2	E	60	1	-	0/6/25/26	0/2/2/2
1	CR2	F	60	1	-	0/6/25/26	0/2/2/2
1	CR2	G	60	1	-	0/6/25/26	0/2/2/2
1	CR2	H	60	1	-	0/6/25/26	0/2/2/2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	60	CR2	CA2-N2	-8.45	1.20	1.38
1	C	60	CR2	CA2-N2	-8.24	1.20	1.38
1	A	60	CR2	CA2-N2	-8.17	1.20	1.38
1	G	60	CR2	CA2-N2	-8.09	1.20	1.38
1	D	60	CR2	CA2-N2	-8.02	1.20	1.38
1	E	60	CR2	CA2-N2	-7.95	1.21	1.38
1	B	58	CR2	CA2-N2	-7.91	1.21	1.38
1	H	60	CR2	CA2-N2	-7.77	1.21	1.38
1	F	60	CR2	C2-N3	-5.93	1.27	1.39
1	E	60	CR2	C2-N3	-5.70	1.27	1.39
1	D	60	CR2	C2-N3	-5.66	1.27	1.39
1	H	60	CR2	C2-N3	-5.58	1.27	1.39
1	A	60	CR2	C2-N3	-5.53	1.28	1.39
1	B	58	CR2	C2-N3	-5.53	1.28	1.39
1	C	60	CR2	C2-N3	-5.49	1.28	1.39
1	G	60	CR2	C2-N3	-5.45	1.28	1.39
1	A	60	CR2	OH-CZ	-4.81	1.25	1.37
1	F	60	CR2	OH-CZ	-4.79	1.25	1.37
1	H	60	CR2	OH-CZ	-4.70	1.25	1.37
1	B	58	CR2	OH-CZ	-4.66	1.25	1.37
1	D	60	CR2	OH-CZ	-4.56	1.26	1.37
1	C	60	CR2	OH-CZ	-4.55	1.26	1.37
1	G	60	CR2	OH-CZ	-4.50	1.26	1.37
1	E	60	CR2	OH-CZ	-4.32	1.26	1.37
1	C	60	CR2	C1-N3	-4.12	1.30	1.37
1	E	60	CR2	C1-N3	-3.80	1.31	1.37
1	G	60	CR2	C1-N3	-3.72	1.31	1.37
1	F	60	CR2	C1-N3	-3.71	1.31	1.37
1	A	60	CR2	C1-N3	-3.35	1.32	1.37
1	H	60	CR2	C1-N3	-3.26	1.32	1.37
1	D	60	CR2	C1-N3	-2.98	1.32	1.37
1	G	60	CR2	CE2-CZ	-2.94	1.32	1.38
1	H	60	CR2	CE2-CZ	-2.89	1.33	1.38
1	E	60	CR2	CE2-CZ	-2.87	1.33	1.38
1	E	60	CR2	CA3-N3	-2.87	1.42	1.47
1	A	60	CR2	CE2-CZ	-2.79	1.33	1.38
1	D	60	CR2	CE2-CZ	-2.75	1.33	1.38
1	B	58	CR2	CE2-CZ	-2.72	1.33	1.38
1	B	58	CR2	C1-N3	-2.69	1.33	1.37
1	F	60	CR2	CE2-CZ	-2.60	1.33	1.38
1	F	60	CR2	CA3-N3	-2.49	1.43	1.47
1	D	60	CR2	CA3-N3	-2.46	1.43	1.47
1	G	60	CR2	CA3-N3	-2.45	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	CR2	CE2-CZ	-2.40	1.34	1.38
1	B	58	CR2	CA3-N3	-2.31	1.43	1.47
1	A	60	CR2	CA3-N3	-2.26	1.43	1.47
1	H	60	CR2	CA3-N3	-2.25	1.43	1.47
1	C	60	CR2	CA3-N3	-2.15	1.43	1.47
1	E	60	CR2	CA2-C2	-2.12	1.46	1.48
1	B	58	CR2	CA1-C1	2.96	1.52	1.49
1	C	60	CR2	CB2-CA2	11.20	1.45	1.35
1	A	60	CR2	CB2-CA2	11.33	1.45	1.35
1	B	58	CR2	CB2-CA2	11.33	1.45	1.35
1	F	60	CR2	CB2-CA2	11.43	1.45	1.35
1	G	60	CR2	CB2-CA2	11.57	1.45	1.35
1	D	60	CR2	CB2-CA2	11.88	1.45	1.35
1	H	60	CR2	CB2-CA2	12.17	1.45	1.35
1	E	60	CR2	CB2-CA2	12.35	1.46	1.35

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	CR2	O2-C2-CA2	-18.46	120.98	130.95
1	E	60	CR2	O2-C2-CA2	-18.07	121.19	130.95
1	A	60	CR2	O2-C2-CA2	-17.69	121.40	130.95
1	G	60	CR2	O2-C2-CA2	-17.68	121.40	130.95
1	D	60	CR2	O2-C2-CA2	-17.67	121.41	130.95
1	F	60	CR2	O2-C2-CA2	-17.66	121.41	130.95
1	H	60	CR2	O2-C2-CA2	-17.43	121.53	130.95
1	B	58	CR2	O2-C2-CA2	-16.58	121.99	130.95
1	E	60	CR2	C2-CA2-N2	-3.37	106.22	108.91
1	G	60	CR2	C2-CA2-N2	-3.22	106.34	108.91
1	C	60	CR2	C2-CA2-N2	-3.21	106.35	108.91
1	E	60	CR2	CA3-N3-C1	-3.14	123.22	127.91
1	F	60	CR2	C2-CA2-N2	-3.10	106.43	108.91
1	H	60	CR2	C2-CA2-N2	-3.10	106.44	108.91
1	A	60	CR2	CA3-N3-C1	-3.06	123.34	127.91
1	F	60	CR2	CA3-N3-C1	-3.01	123.42	127.91
1	B	58	CR2	C2-CA2-N2	-2.99	106.52	108.91
1	D	60	CR2	C2-CA2-N2	-2.96	106.55	108.91
1	D	60	CR2	CA3-N3-C1	-2.95	123.50	127.91
1	H	60	CR2	CA3-N3-C1	-2.93	123.53	127.91
1	B	58	CR2	CA3-N3-C1	-2.92	123.56	127.91
1	A	60	CR2	C2-CA2-N2	-2.90	106.59	108.91
1	G	60	CR2	CA3-N3-C1	-2.87	123.62	127.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	CR2	CA3-N3-C1	-2.81	123.72	127.91
1	G	60	CR2	CE1-CZ-CE2	2.18	122.90	119.79
1	E	60	CR2	CE1-CZ-CE2	2.18	122.90	119.79
1	H	60	CR2	CE1-CZ-CE2	2.22	122.96	119.79
1	C	60	CR2	CE1-CZ-CE2	2.27	123.03	119.79
1	D	60	CR2	CE1-CZ-CE2	2.27	123.03	119.79
1	B	58	CR2	CE1-CZ-CE2	2.33	123.12	119.79
1	F	60	CR2	CE1-CZ-CE2	2.34	123.12	119.79
1	A	60	CR2	CE1-CZ-CE2	2.45	123.29	119.79
1	B	58	CR2	O2-C2-N3	3.28	131.59	124.50
1	G	60	CR2	O2-C2-N3	3.34	131.70	124.50
1	D	60	CR2	O2-C2-N3	3.39	131.81	124.50
1	H	60	CR2	O2-C2-N3	3.40	131.83	124.50
1	F	60	CR2	O2-C2-N3	3.41	131.85	124.50
1	A	60	CR2	O2-C2-N3	3.44	131.92	124.50
1	E	60	CR2	O2-C2-N3	3.48	132.01	124.50
1	C	60	CR2	O2-C2-N3	3.52	132.10	124.50
1	B	58	CR2	CA3-N3-C2	3.99	130.49	123.99
1	A	60	CR2	CA2-N2-C1	4.14	109.25	105.70
1	H	60	CR2	CA3-N3-C2	4.21	130.85	123.99
1	C	60	CR2	CA3-N3-C2	4.24	130.90	123.99
1	D	60	CR2	CA3-N3-C2	4.26	130.93	123.99
1	G	60	CR2	CA2-N2-C1	4.26	109.36	105.70
1	H	60	CR2	CA2-N2-C1	4.27	109.36	105.70
1	G	60	CR2	CA3-N3-C2	4.27	130.94	123.99
1	C	60	CR2	CA2-N2-C1	4.28	109.37	105.70
1	D	60	CR2	CA2-N2-C1	4.28	109.37	105.70
1	E	60	CR2	CA3-N3-C2	4.31	131.02	123.99
1	F	60	CR2	CA3-N3-C2	4.34	131.05	123.99
1	F	60	CR2	CA2-N2-C1	4.38	109.45	105.70
1	A	60	CR2	CA3-N3-C2	4.48	131.28	123.99
1	E	60	CR2	CA2-N2-C1	4.55	109.60	105.70
1	B	58	CR2	CA2-N2-C1	4.83	109.84	105.70
1	B	58	CR2	CA2-C2-N3	6.02	106.42	103.40
1	H	60	CR2	CA2-C2-N3	6.46	106.64	103.40
1	A	60	CR2	CA2-C2-N3	6.55	106.68	103.40
1	F	60	CR2	CA2-C2-N3	6.67	106.74	103.40
1	D	60	CR2	CA2-C2-N3	6.74	106.78	103.40
1	E	60	CR2	CA2-C2-N3	6.79	106.80	103.40
1	F	60	CR2	CG2-CB2-CA2	6.88	139.15	130.22
1	G	60	CR2	CG2-CB2-CA2	6.94	139.23	130.22
1	E	60	CR2	CG2-CB2-CA2	6.97	139.26	130.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	60	CR2	CA2-C2-N3	6.98	106.90	103.40
1	C	60	CR2	CA2-C2-N3	7.02	106.92	103.40
1	D	60	CR2	CG2-CB2-CA2	7.05	139.37	130.22
1	C	60	CR2	CG2-CB2-CA2	7.15	139.50	130.22
1	B	58	CR2	CG2-CB2-CA2	7.18	139.54	130.22
1	H	60	CR2	CG2-CB2-CA2	7.32	139.73	130.22
1	A	60	CR2	CG2-CB2-CA2	7.42	139.86	130.22
1	B	58	CR2	C3-CA3-N3	8.19	130.93	113.00
1	G	60	CR2	C3-CA3-N3	8.23	131.02	113.00
1	D	60	CR2	C3-CA3-N3	8.23	131.02	113.00
1	E	60	CR2	C3-CA3-N3	8.27	131.11	113.00
1	C	60	CR2	C3-CA3-N3	8.29	131.15	113.00
1	F	60	CR2	C3-CA3-N3	8.39	131.37	113.00
1	H	60	CR2	C3-CA3-N3	8.40	131.39	113.00
1	A	60	CR2	C3-CA3-N3	8.51	131.62	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

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%)	0.91	18 (8%) 13 21	23, 40, 54, 65	0
1	B	213/214 (99%)	0.88	21 (9%) 9 15	26, 41, 54, 65	0
1	C	213/214 (99%)	0.85	16 (7%) 17 26	27, 42, 55, 65	0
1	D	213/214 (99%)	0.92	21 (9%) 9 15	30, 43, 56, 64	0
1	E	213/214 (99%)	1.01	26 (12%) 5 9	29, 43, 55, 64	0
1	F	213/214 (99%)	0.85	20 (9%) 11 17	27, 40, 55, 64	0
1	G	213/214 (99%)	1.14	37 (17%) 2 3	30, 43, 56, 65	0
1	H	213/214 (99%)	1.25	39 (18%) 2 2	33, 44, 56, 64	0
All	All	1704/1712 (99%)	0.98	198 (11%) 6 10	23, 42, 55, 65	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	218	LEU	7.0
1	H	211	TRP	5.3
1	C	203	ASP	5.0
1	H	184	THR	4.8
1	E	218	LEU	4.4
1	D	187	GLN	4.4
1	E	179	LYS	4.2
1	H	9	VAL	4.1
1	H	108	GLY	4.0
1	G	187	GLN	3.9
1	H	199	VAL	3.9
1	E	83	GLY	3.9
1	A	218	LEU	3.8
1	H	22	LEU	3.7
1	H	187	GLN	3.6
1	G	211	TRP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	5	THR	3.6
1	A	90	ILE	3.6
1	H	194	PHE	3.6
1	G	111	ILE	3.6
1	E	203	ASP	3.5
1	A	170	THR	3.5
1	D	181	ILE	3.4
1	E	181	ILE	3.4
1	C	3	LEU	3.4
1	F	69	ASP	3.4
1	G	3	LEU	3.3
1	C	201	ALA	3.3
1	E	39	VAL	3.3
1	G	45	PRO	3.2
1	D	218	LEU	3.2
1	E	57	ILE	3.1
1	F	211	TRP	3.1
1	A	98	LEU	3.1
1	E	186	LEU	3.1
1	B	108	GLY	3.1
1	H	111	ILE	3.1
1	B	90	ILE	3.0
1	H	80	ASP	3.0
1	F	171	LEU	3.0
1	B	203	ASP	3.0
1	D	191	MET	3.0
1	G	171	LEU	3.0
1	E	187	GLN	2.9
1	D	3	LEU	2.9
1	H	3	LEU	2.9
1	G	209	LYS	2.9
1	G	164	GLY	2.9
1	B	23	VAL	2.9
1	A	203	ASP	2.9
1	H	186	LEU	2.9
1	G	78	ALA	2.8
1	A	89	THR	2.8
1	H	84	TYR	2.8
1	A	171	LEU	2.8
1	C	218	LEU	2.8
1	B	171	LEU	2.7
1	G	57	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	181	ILE	2.7
1	F	170	THR	2.7
1	B	125	ASP	2.7
1	C	162	THR	2.7
1	G	218	LEU	2.7
1	F	204	ALA	2.7
1	G	80	ASP	2.7
1	H	69	ASP	2.7
1	D	90	ILE	2.6
1	D	78	ALA	2.6
1	G	106	TYR	2.6
1	E	90	ILE	2.6
1	D	184	THR	2.6
1	G	170	THR	2.6
1	A	45	PRO	2.6
1	G	90	ILE	2.6
1	H	106	TYR	2.6
1	D	162	THR	2.6
1	B	65	LEU	2.6
1	G	98	LEU	2.6
1	D	57	ILE	2.6
1	F	99	THR	2.6
1	D	151	VAL	2.5
1	F	90	ILE	2.5
1	H	12	TYR	2.5
1	E	178	ALA	2.5
1	H	125	ASP	2.5
1	E	53	VAL	2.5
1	H	39	VAL	2.5
1	F	154	THR	2.5
1	H	134	THR	2.5
1	F	203	ASP	2.5
1	C	46	LEU	2.5
1	D	98	LEU	2.5
1	G	182	ALA	2.5
1	B	80	ASP	2.5
1	C	89	THR	2.5
1	G	155	ILE	2.4
1	B	204	ALA	2.4
1	B	5	THR	2.4
1	F	98	LEU	2.4
1	B	172	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	106	TYR	2.4
1	B	89	THR	2.4
1	G	148	ASP	2.4
1	H	164	GLY	2.4
1	B	149	THR	2.4
1	B	57	ILE	2.3
1	A	157	TRP	2.3
1	B	98	LEU	2.3
1	H	62	HIS	2.3
1	H	182	ALA	2.3
1	A	99	THR	2.3
1	D	171	LEU	2.3
1	G	5	THR	2.3
1	E	108	GLY	2.3
1	E	164	GLY	2.3
1	H	57	ILE	2.3
1	D	6	THR	2.3
1	E	76	ALA	2.3
1	B	165	LYS	2.3
1	G	213	LYS	2.3
1	H	177	PHE	2.3
1	B	170	THR	2.3
1	H	6	THR	2.3
1	F	218	LEU	2.3
1	G	186	LEU	2.3
1	H	43	LYS	2.3
1	C	103	ARG	2.3
1	H	73	PRO	2.3
1	G	94	ASP	2.3
1	G	207	ASN	2.2
1	G	22	LEU	2.2
1	G	79	ASP	2.2
1	G	184	THR	2.2
1	A	57	ILE	2.2
1	F	96	ALA	2.2
1	G	96	ALA	2.2
1	E	125	ASP	2.2
1	B	184	THR	2.2
1	G	31	LYS	2.2
1	H	124	ALA	2.2
1	G	38	GLN	2.2
1	H	104	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	162	THR	2.2
1	H	61	PHE	2.2
1	H	192	PHE	2.2
1	G	40	LYS	2.2
1	D	94	ASP	2.2
1	C	53	VAL	2.2
1	C	152	VAL	2.2
1	G	108	GLY	2.2
1	C	125	ASP	2.2
1	A	172	ARG	2.2
1	E	177	PHE	2.1
1	A	155	ILE	2.1
1	C	112	LYS	2.1
1	E	82	SER	2.1
1	F	53	VAL	2.1
1	G	201	ALA	2.1
1	H	205	GLU	2.1
1	C	163	SER	2.1
1	E	69	ASP	2.1
1	E	22	LEU	2.1
1	C	9	VAL	2.1
1	D	205	GLU	2.1
1	G	92	PHE	2.1
1	F	3	LEU	2.1
1	A	165	LYS	2.1
1	F	173	THR	2.1
1	G	89	THR	2.1
1	C	108	GLY	2.1
1	G	4	PRO	2.1
1	B	157	TRP	2.1
1	A	169	ALA	2.1
1	B	169	ALA	2.1
1	H	135	ALA	2.1
1	D	165	LYS	2.1
1	E	165	LYS	2.1
1	E	73	PRO	2.1
1	A	80	ASP	2.1
1	D	38	GLN	2.1
1	F	94	ASP	2.1
1	F	57	ILE	2.0
1	F	155	ILE	2.0
1	F	172	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	67	PHE	2.0
1	D	96	ALA	2.0
1	C	118	VAL	2.0
1	E	149	THR	2.0
1	E	151	VAL	2.0
1	F	108	GLY	2.0
1	H	40	LYS	2.0
1	A	97	SER	2.0
1	D	201	ALA	2.0
1	D	92	PHE	2.0
1	E	185	ILE	2.0
1	A	3	LEU	2.0
1	E	80	ASP	2.0
1	H	138	TRP	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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CR2	B	58	19/20	0.93	0.12	-	36,39,41,42	0
1	CR2	A	60	19/20	0.90	0.13	-	35,41,42,43	0
1	CR2	C	60	19/20	0.89	0.12	-	40,42,43,44	0
1	CR2	E	60	19/20	0.86	0.14	-	42,44,46,47	0
1	CR2	G	60	19/20	0.86	0.14	-	43,45,47,47	0
1	CR2	H	60	19/20	0.81	0.15	-	43,45,46,47	0
1	CR2	D	60	19/20	0.88	0.11	-	41,43,45,45	0
1	CR2	F	60	19/20	0.92	0.13	-	39,41,43,44	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.