



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:36 AM UTC

PDB ID : 6MYG / pdb_00006myg
Title : Mouse Gamma S Crystallin L16 Octamer
Authors : Sagar, V.; Wistow, G.J.
Deposited on : 2018-11-01
Resolution : 2.92 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

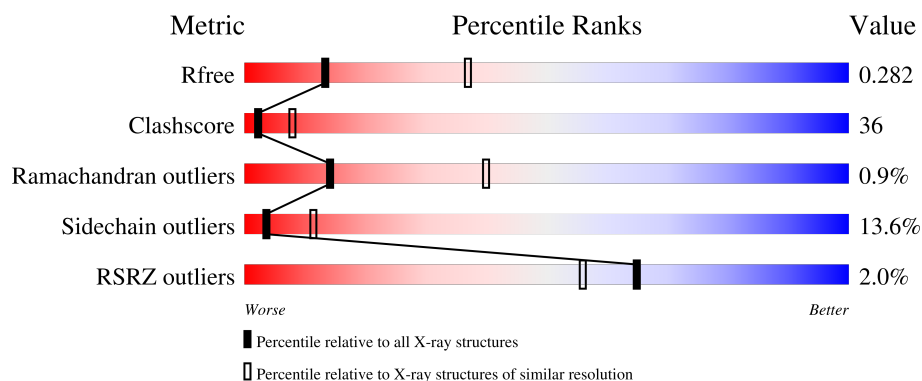
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	178	2% 53% 39% 7% ..
1	B	178	% 54% 37% 7% .
1	C	178	3% 48% 45% 6% .
1	D	178	2% 37% 51% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5544 atoms, of which 41 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 Gamma-crystallin S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	174	Total	C	N	O	S	0	2	0
			1386	883	239	253	11			
1	A	177	Total	C	N	O	S	0	2	0
			1418	898	253	256	11			
1	C	176	Total	C	N	O	S	0	3	0
			1376	874	239	251	12			
1	D	173	Total	C	H	N	O	S	0	1
			1327	814	41	222	239	11		1

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	LEU	GLN	conflict	UNP O35486
A	16	LEU	GLN	conflict	UNP O35486
C	16	LEU	GLN	conflict	UNP O35486
D	16	LEU	GLN	conflict	UNP O35486

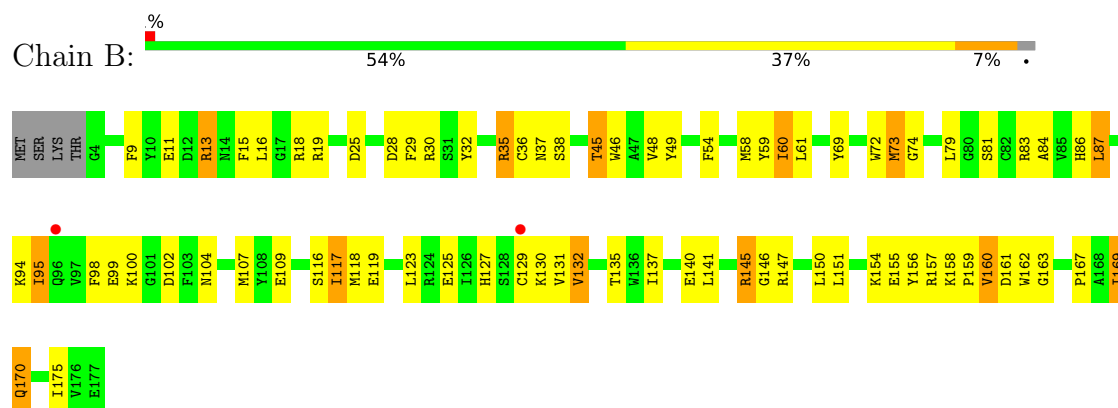
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	9	Total	O	0	0
			9	9		
2	A	9	Total	O	0	0
			9	9		
2	C	9	Total	O	0	0
			9	9		
2	D	10	Total	O	0	0
			10	10		

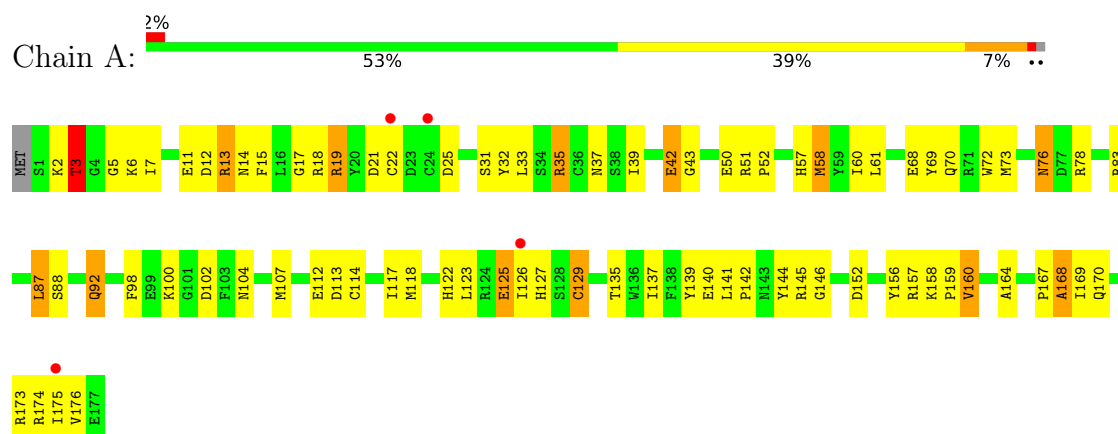
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

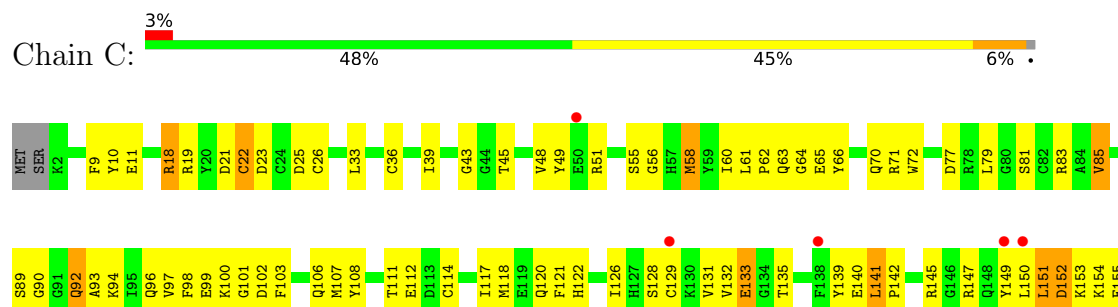
• Molecule 1: Gamma-crystallin S



• Molecule 1: Gamma-crystallin S

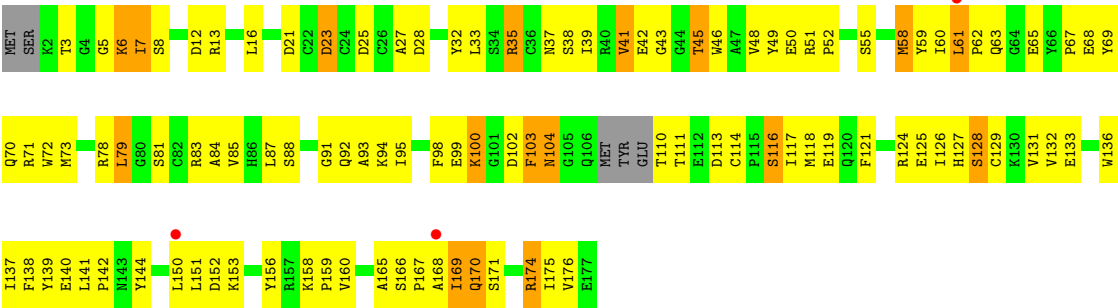


• Molecule 1: Gamma-crystallin S





● Molecule 1: Gamma-crystallin S



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	61.09Å 77.59Å 154.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.92 48.00 – 2.92	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.00-2.92) 89.4 (48.00-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.15 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.205 , 0.284 (Not available) , 0.282	Depositor DCC
R_{free} test set	851 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 82.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5544	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.50	0/1462	0.71	0/1975
1	B	0.45	0/1428	0.65	0/1933
1	C	0.42	0/1418	0.68	1/1927 (0.1%)
1	D	0.50	1/1323 (0.1%)	0.68	2/1796 (0.1%)
All	All	0.47	1/5631 (0.0%)	0.68	3/7631 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	170	GLN	CA-CB	5.19	1.63	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	PHE	N-CA-C	6.38	119.12	109.23
1	D	100	LYS	N-CA-C	5.71	118.76	110.42
1	C	155	GLU	N-CA-C	5.01	117.91	109.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1418	0	1323	86	1
1	B	1386	0	1259	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1376	0	1210	112	0
1	D	1286	41	1106	111	0
2	A	9	0	0	0	0
2	B	9	0	0	1	0
2	C	9	0	0	1	0
2	D	10	0	0	1	0
All	All	5503	41	4898	375	1

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 36.

All (375) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:HG	1:A:135:THR:HG21	1.21	1.09
1:B:140:GLU:HG2	1:B:141:LEU:HD22	1.32	1.05
1:A:6:LYS:HE3	1:A:21:ASP:HB3	1.44	0.99
1:B:137:ILE:HD11	1:B:175:ILE:HD11	1.44	0.98
1:C:117:ILE:HD11	1:C:170:GLN:HG2	1.46	0.98
1:C:156:TYR:CD1	1:C:161:ASP:HB2	1.99	0.97
1:B:151:LEU:HD11	1:B:162:TRP:HB3	1.47	0.96
1:D:23:ASP:OD2	2:D:201:HOH:O	1.82	0.95
1:B:130:LYS:HG2	1:B:155:GLU:HG2	1.48	0.95
1:D:159:PRO:HB3	1:D:167:PRO:HB3	1.51	0.93
1:B:150:LEU:HB2	1:A:58:MET:HE1	1.52	0.92
1:A:7:ILE:CG2	1:A:22:CYS:HB3	2.00	0.92
1:C:150:LEU:C	1:C:151:LEU:HD23	1.96	0.90
1:B:49:TYR:OH	1:B:83:ARG:NH1	2.04	0.89
1:A:118:MET:CE	1:A:122:HIS:HA	2.02	0.89
1:D:133:GLU:HA	1:D:153:LYS:HG3	1.56	0.88
1:B:13:ARG:HG3	1:B:13:ARG:HH11	1.38	0.88
1:D:159:PRO:CB	1:D:167:PRO:HB3	2.04	0.87
1:D:45:THR:HG23	1:D:62:PRO:HA	1.57	0.86
1:C:48:VAL:HG12	1:C:79:LEU:HD22	1.57	0.86
1:C:39:ILE:HG13	1:C:72:TRP:CZ3	2.12	0.85
1:C:156:TYR:HD1	1:C:161:ASP:HB2	1.42	0.83
1:A:7:ILE:HG23	1:A:22:CYS:HB3	1.61	0.81
1:A:118:MET:HE1	1:A:122:HIS:HA	1.60	0.81
1:B:145[B]:ARG:HG2	1:A:73:MET:HE1	1.63	0.80
1:A:39:ILE:HG13	1:A:72:TRP:CZ3	2.17	0.80
1:D:168:ALA:O	1:D:170:GLN:HG3	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLU:HG2	1:B:141:LEU:CD2	2.13	0.79
1:B:13:ARG:HH11	1:B:13:ARG:CG	1.94	0.79
1:B:48:VAL:HG12	1:B:79:LEU:HD22	1.64	0.79
1:C:93:ALA:O	1:C:111:THR:OG1	2.02	0.78
1:C:71:ARG:HA	1:C:71:ARG:NE	1.98	0.78
1:C:70:GLN:OE1	1:C:70:GLN:N	2.14	0.78
1:C:117:ILE:HG13	1:C:170:GLN:HA	1.66	0.76
1:A:5:GLY:HA2	1:A:43:GLY:HA3	1.67	0.75
1:C:97:VAL:HB	1:C:126:ILE:HD12	1.67	0.75
1:D:99:GLU:HA	1:D:127:HIS:H	1.50	0.75
1:C:93:ALA:HA	1:C:133:GLU:HG2	1.69	0.75
1:B:158:LYS:HD3	1:B:159:PRO:HD2	1.66	0.75
1:C:131:VAL:HG13	1:C:153:LYS:HA	1.67	0.75
1:D:95:ILE:HD12	1:D:131:VAL:HA	1.68	0.75
1:C:93:ALA:HB1	1:C:133:GLU:O	1.87	0.74
1:B:151:LEU:CD1	1:B:162:TRP:HB3	2.17	0.73
1:B:175:ILE:CG2	1:A:87:LEU:HD23	2.18	0.73
1:D:100:LYS:HA	1:D:127:HIS:HB3	1.70	0.73
1:C:71:ARG:HA	1:C:71:ARG:CZ	2.18	0.73
1:C:149:TYR:HE2	1:C:163:GLY:O	1.72	0.73
1:B:11:GLU:OE2	1:B:18:ARG:HG3	1.89	0.72
1:C:117:ILE:CG1	1:C:170:GLN:HA	2.18	0.72
1:A:25:ASP:OD1	1:A:83:ARG:HA	1.89	0.72
1:B:150:LEU:CB	1:A:58:MET:HE1	2.20	0.72
1:C:107[B]:MET:N	1:C:107[B]:MET:SD	2.63	0.72
1:A:11:GLU:HG3	1:A:33:LEU:HD23	1.72	0.71
1:D:93:ALA:O	1:D:111:THR:OG1	2.08	0.71
1:A:137:ILE:HD11	1:A:175:ILE:HD11	1.72	0.71
1:C:117:ILE:CD1	1:C:170:GLN:HG2	2.21	0.71
1:A:135:THR:HG22	1:A:152:ASP:HA	1.72	0.71
1:D:95:ILE:CD1	1:D:131:VAL:HA	2.20	0.71
1:B:15:PHE:O	1:B:16:LEU:HD23	1.91	0.71
1:D:100:LYS:HA	1:D:127:HIS:CB	2.21	0.70
1:D:138:PHE:HB3	1:D:169:ILE:HG22	1.73	0.70
1:A:11:GLU:HG3	1:A:33:LEU:CD2	2.22	0.70
1:D:49:TYR:CD2	1:D:58:MET:HB2	2.27	0.70
1:D:49:TYR:CE2	1:D:58:MET:HB2	2.27	0.70
1:D:6:LYS:HE3	1:D:21:ASP:HB3	1.73	0.69
1:A:2:LYS:O	1:A:3:THR:O	2.10	0.69
1:C:156:TYR:CE1	1:C:161:ASP:HB2	2.26	0.69
1:A:60:ILE:C	1:A:61:LEU:HD12	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ASP:O	1:D:128:SER:OG	2.06	0.69
1:C:45:THR:HG22	1:C:85:VAL:HG11	1.75	0.69
1:A:168:ALA:O	1:A:169:ILE:HD13	1.92	0.68
1:C:117:ILE:HD11	1:C:170:GLN:CG	2.22	0.68
1:D:42:GLU:HG3	1:D:43:GLY:N	2.06	0.68
1:D:169:ILE:HD12	1:D:169:ILE:N	2.07	0.68
1:C:117:ILE:HD12	1:C:118:MET:N	2.08	0.68
1:C:131:VAL:HG11	1:C:152:ASP:O	1.93	0.68
1:A:118:MET:HE3	1:A:122:HIS:HA	1.75	0.68
1:B:145[A]:ARG:HG2	1:A:73:MET:CE	2.24	0.68
1:C:126:ILE:HG13	1:C:169:ILE:HD11	1.76	0.68
1:C:96:GLN:CB	1:C:107[A]:MET:HE2	2.24	0.67
1:B:145[B]:ARG:NH1	2:B:201:HOH:O	2.27	0.67
1:B:151:LEU:HD11	1:B:162:TRP:CB	2.22	0.67
1:D:113:ASP:OD1	1:D:144:TYR:OH	2.09	0.67
1:D:133:GLU:CA	1:D:153:LYS:HG3	2.25	0.66
1:D:165:ALA:O	1:D:167:PRO:HD3	1.95	0.66
1:A:113:ASP:OD1	1:A:174:ARG:HG2	1.95	0.66
1:C:11:GLU:OE2	1:C:18:ARG:HD2	1.95	0.66
1:B:60:ILE:O	1:B:61:LEU:HD23	1.96	0.66
1:B:60:ILE:C	1:B:61:LEU:HD23	2.21	0.65
1:A:140:GLU:HB3	1:A:146:GLY:HA3	1.78	0.65
1:C:101:GLY:O	1:C:103:PHE:N	2.24	0.65
1:A:42:GLU:HA	1:C:19:ARG:HH22	1.60	0.65
1:B:145[B]:ARG:HG2	1:A:73:MET:CE	2.25	0.65
1:D:48:VAL:HB	1:D:79:LEU:HD13	1.77	0.65
1:C:128:SER:OG	1:C:157:ARG:O	2.11	0.65
1:A:102:ASP:OD2	1:A:158[B]:LYS:HE3	1.97	0.64
1:D:98:PHE:HB3	1:D:103:PHE:HA	1.79	0.64
1:D:49:TYR:OH	1:D:58:MET:HE2	1.97	0.64
1:C:48:VAL:CG1	1:C:79:LEU:HD22	2.27	0.64
1:C:11:GLU:CD	1:C:18:ARG:HD2	2.23	0.63
1:C:141:LEU:HG	1:C:142:PRO:N	2.13	0.63
1:B:19:ARG:NH1	1:D:65:GLU:OE1	2.31	0.63
1:B:175:ILE:HG21	1:A:87:LEU:HD23	1.80	0.63
1:A:33:LEU:HD22	1:A:35:ARG:O	1.98	0.63
1:D:5:GLY:HA2	1:D:43:GLY:HA3	1.80	0.63
1:A:6:LYS:CE	1:A:21:ASP:HB3	2.26	0.62
1:D:41:VAL:HG22	1:D:63:GLN:HA	1.81	0.61
1:C:149:TYR:HB3	1:C:162:TRP:HB2	1.81	0.61
1:A:118:MET:HE1	1:A:122:HIS:CA	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:CD2	1:C:145:ARG:HB2	2.31	0.60
1:B:11:GLU:OE2	1:D:71:ARG:NH2	2.34	0.60
1:C:23:ASP:OD2	1:C:23:ASP:N	2.34	0.60
1:D:142:PRO:HD3	1:D:170:GLN:OE1	2.02	0.60
1:B:145[A]:ARG:HD3	1:B:146:GLY:N	2.11	0.60
1:C:11:GLU:HG3	1:C:18:ARG:HB2	1.83	0.60
1:B:151:LEU:HD12	1:B:156:TYR:CE1	2.37	0.60
1:C:61:LEU:HD23	1:C:66:TYR:CD1	2.37	0.60
1:B:60:ILE:HG12	1:A:137:ILE:HD13	1.84	0.60
1:D:78:ARG:O	1:D:79:LEU:HD23	2.02	0.60
1:C:139:TYR:HA	1:C:147:ARG:O	2.02	0.59
1:D:150:LEU:HD23	1:D:150:LEU:C	2.28	0.59
1:A:140:GLU:HG2	1:A:141:LEU:HD12	1.85	0.59
1:C:156:TYR:CE1	1:C:161:ASP:CB	2.84	0.59
1:A:102:ASP:OD1	1:A:157:ARG:HD3	2.03	0.59
1:B:95:ILE:HG13	1:B:131:VAL:HG22	1.84	0.59
1:C:106:GLN:HB3	1:C:108:TYR:CE1	2.39	0.58
1:C:49:TYR:OH	1:C:58:MET:HE3	2.03	0.58
1:D:45:THR:HG23	1:D:62:PRO:CA	2.32	0.58
1:D:25:ASP:CG	1:D:83:ARG:HA	2.28	0.58
1:B:87:LEU:HG	1:A:135:THR:CG2	2.14	0.58
1:B:158:LYS:CD	1:B:159:PRO:HD2	2.31	0.58
1:A:69:TYR:HB3	1:A:72:TRP:CZ2	2.38	0.58
1:C:142:PRO:HG3	1:C:170:GLN:HB3	1.86	0.58
1:D:6:LYS:HB3	1:D:42:GLU:HG2	1.85	0.58
1:C:92:GLN:O	1:C:133:GLU:HG2	2.04	0.58
1:C:98:PHE:CD1	1:C:103:PHE:HA	2.39	0.57
1:D:137:ILE:HD11	1:D:175:ILE:HD11	1.86	0.57
1:D:98:PHE:HB2	1:D:102:ASP:O	2.04	0.57
1:B:151:LEU:HD12	1:B:156:TYR:CZ	2.39	0.57
1:C:151:LEU:HD23	1:C:151:LEU:N	2.18	0.57
1:A:92:GLN:O	1:A:92:GLN:HG2	2.04	0.57
1:D:32:TYR:O	1:D:33:LEU:HD23	2.04	0.57
1:B:175:ILE:HG22	1:A:87:LEU:HD23	1.86	0.57
1:C:131:VAL:CG1	1:C:153:LYS:HA	2.35	0.57
1:D:117:ILE:O	1:D:121:PHE:O	2.23	0.56
1:C:49:TYR:HB2	1:C:81:SER:OG	2.05	0.56
1:B:118:MET:HE2	1:B:123:LEU:O	2.05	0.56
1:C:25:ASP:OD1	1:C:83:ARG:HA	2.04	0.56
1:D:13:ARG:HG2	1:D:37:ASN:HB3	1.87	0.56
1:A:87:LEU:H	1:A:87:LEU:HD12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LEU:HD23	1:D:88:SER:N	2.21	0.56
1:D:159:PRO:HG2	1:D:167:PRO:HG3	1.88	0.56
1:C:45:THR:HB	1:C:85:VAL:HG13	1.87	0.56
1:C:121:PHE:O	1:C:122:HIS:HB2	2.06	0.56
1:B:46:TRP:O	1:B:60:ILE:HA	2.06	0.55
1:C:45:THR:CG2	1:C:85:VAL:HG11	2.35	0.55
1:D:28:ASP:OD2	1:D:52:PRO:HB3	2.06	0.55
1:B:36:CYS:HB3	1:B:79:LEU:HD12	1.88	0.55
1:C:169:ILE:O	1:C:170:GLN:HG3	2.06	0.55
1:A:19:ARG:HD2	1:A:21:ASP:OD1	2.06	0.55
1:C:43:GLY:HA2	1:C:63[A]:GLN:HE21	1.70	0.55
1:C:150:LEU:O	1:C:151:LEU:HD23	2.05	0.55
1:C:61:LEU:HD23	1:C:66:TYR:CE1	2.42	0.54
1:C:141:LEU:HG	1:C:142:PRO:CD	2.36	0.54
1:A:50:GLU:OE2	1:A:78:ARG:NH1	2.39	0.54
1:D:159:PRO:CG	1:D:167:PRO:HB3	2.37	0.54
1:D:140:GLU:O	1:D:168:ALA:O	2.24	0.54
1:B:127:HIS:O	1:B:159:PRO:HD3	2.07	0.54
1:C:147:ARG:HG2	1:C:149:TYR:OH	2.07	0.54
1:C:19:ARG:HD2	1:C:21:ASP:OD1	2.06	0.54
1:C:45:THR:HG22	1:C:85:VAL:CG1	2.37	0.54
1:C:92:GLN:OE1	1:D:91:GLY:HA3	2.08	0.54
1:A:11:GLU:HB3	1:A:12:ASP:OD2	2.08	0.54
1:D:27:ALA:O	1:D:81:SER:HB3	2.08	0.54
1:B:156:TYR:HD2	1:B:161:ASP:HB3	1.73	0.53
1:C:22:CYS:SG	1:C:26:CYS:HB2	2.48	0.53
1:C:128:SER:O	1:C:129:CYS:HB3	2.09	0.53
1:D:142:PRO:HA	1:D:171:SER:OG	2.07	0.53
1:A:7:ILE:HG21	1:A:22:CYS:HB3	1.89	0.53
1:C:36:CYS:O	1:C:77:ASP:HB2	2.09	0.53
1:D:25:ASP:OD1	1:D:84:ALA:N	2.38	0.53
1:D:38:SER:HB2	1:D:67:PRO:HA	1.91	0.53
1:A:39:ILE:HD12	1:A:61:LEU:CD2	2.39	0.52
1:A:139:TYR:HB3	1:A:145:ARG:O	2.09	0.52
1:C:141:LEU:HD22	1:C:145:ARG:HB2	1.91	0.52
1:D:98:PHE:CB	1:D:103:PHE:HA	2.39	0.52
1:D:93:ALA:HB3	1:D:174:ARG:HH21	1.75	0.52
1:C:149:TYR:CE2	1:C:163:GLY:O	2.58	0.52
1:D:150:LEU:HD23	1:D:151:LEU:N	2.25	0.52
1:A:7:ILE:HG23	1:A:22:CYS:CB	2.36	0.52
1:C:43:GLY:HA2	1:C:63[A]:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:GLU:HA	1:D:126:ILE:HA	1.92	0.52
1:B:137:ILE:CD1	1:B:175:ILE:HD11	2.28	0.52
1:A:39:ILE:HG13	1:A:72:TRP:CH2	2.45	0.52
1:B:160:VAL:O	1:B:163:GLY:N	2.38	0.51
1:A:69:TYR:CB	1:A:72:TRP:CZ2	2.93	0.51
1:B:135:THR:HG22	1:B:175:ILE:HD12	1.92	0.51
1:D:49:TYR:HB3	1:D:55:SER:O	2.10	0.51
1:C:117:ILE:HG13	1:C:170:GLN:CA	2.38	0.51
1:D:39:ILE:HG13	1:D:72:TRP:CZ3	2.45	0.51
1:D:94:LYS:O	1:D:132:VAL:HG12	2.10	0.51
1:D:25:ASP:OD1	1:D:83:ARG:HA	2.11	0.51
1:A:157:ARG:O	1:A:158[A]:LYS:HG2	2.10	0.51
1:D:152:ASP:OD1	1:D:152:ASP:N	2.42	0.51
1:A:76:ASN:OD1	1:A:78:ARG:HG3	2.11	0.51
1:A:87:LEU:HD12	1:A:87:LEU:N	2.26	0.51
1:D:23:ASP:O	1:D:46:TRP:HH2	1.95	0.50
1:C:49:TYR:HB2	1:C:81:SER:HG	1.76	0.50
1:B:13:ARG:CG	1:B:13:ARG:NH1	2.61	0.50
1:B:154:LYS:HB3	1:B:154:LYS:HZ3	1.77	0.50
1:A:144:TYR:CD2	1:A:173:ARG:HG3	2.47	0.50
1:B:59:TYR:CE2	1:B:74:GLY:HA2	2.46	0.50
1:C:94:LYS:O	1:C:132:VAL:HG22	2.11	0.50
1:D:100:LYS:CA	1:D:127:HIS:HB3	2.40	0.50
1:D:103:PHE:CD1	1:D:103:PHE:C	2.90	0.50
1:C:147:ARG:HG2	1:C:149:TYR:CZ	2.47	0.50
1:C:150:LEU:HB3	1:D:58:MET:HE1	1.94	0.50
1:D:99:GLU:O	1:D:127:HIS:HB3	2.11	0.50
1:B:118:MET:HE2	1:B:123:LEU:C	2.37	0.49
1:B:145[A]:ARG:HG2	1:A:73:MET:HE2	1.94	0.49
1:A:37:ASN:O	1:A:68:GLU:HA	2.13	0.49
1:B:94:LYS:CB	1:B:132:VAL:HG22	2.43	0.49
1:D:70:GLN:O	1:D:73[B]:MET:HE2	2.12	0.49
1:A:18[B]:ARG:HD3	1:A:32:TYR:O	2.12	0.49
1:A:51:ARG:HB3	1:A:52:PRO:HD2	1.94	0.49
1:A:158[A]:LYS:HB3	1:A:159:PRO:HD2	1.93	0.49
1:D:139:TYR:HB2	1:D:171:SER:HB2	1.94	0.49
1:C:93:ALA:HA	1:C:133:GLU:CG	2.41	0.48
1:B:11:GLU:CD	1:B:18:ARG:HG3	2.38	0.48
1:A:167:PRO:O	1:A:169:ILE:HG12	2.13	0.48
1:C:117:ILE:HD12	1:C:118:MET:H	1.76	0.48
1:D:126:ILE:O	1:D:169:ILE:HD11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ILE:HB	1:D:136:TRP:CE2	2.48	0.48
1:D:12:ASP:HB2	1:D:16:LEU:O	2.13	0.48
1:D:73[B]:MET:HE2	1:D:73[B]:MET:H	1.77	0.48
1:D:110:THR:HG22	1:D:111:THR:N	2.27	0.48
1:C:98:PHE:CG	1:C:103:PHE:HA	2.48	0.48
1:C:133:GLU:OE2	1:D:92:GLN:N	2.44	0.48
1:C:151:LEU:HD21	1:C:162:TRP:HB3	1.94	0.48
1:B:19:ARG:NH2	1:D:42:GLU:O	2.46	0.48
1:C:141:LEU:HG	1:C:142:PRO:HD2	1.96	0.48
1:D:99:GLU:CA	1:D:127:HIS:H	2.24	0.48
1:D:103:PHE:O	1:D:104:ASN:ND2	2.46	0.48
1:B:49:TYR:CE1	1:B:58:MET:HG3	2.49	0.48
1:A:127:HIS:O	1:A:158[A]:LYS:HA	2.14	0.48
1:B:130:LYS:CG	1:B:155:GLU:HG2	2.32	0.47
1:C:10:TYR:CE2	1:C:19:ARG:HG3	2.48	0.47
1:D:138:PHE:HB3	1:D:169:ILE:CG2	2.42	0.47
1:A:76:ASN:HD22	1:A:76:ASN:H	1.62	0.47
1:D:42:GLU:CG	1:D:43:GLY:N	2.78	0.47
1:B:116:SER:HB3	1:B:119:GLU:HB2	1.97	0.47
1:D:51:ARG:HB3	1:D:52:PRO:CD	2.45	0.47
1:B:9:PHE:O	1:B:19:ARG:HA	2.15	0.47
1:B:145[A]:ARG:CD	1:B:146:GLY:N	2.74	0.46
1:D:110:THR:HG22	1:D:111:THR:H	1.78	0.46
1:D:141:LEU:HB3	1:D:142:PRO:HD2	1.96	0.46
1:A:100:LYS:HB2	1:A:104:ASN:C	2.40	0.46
1:D:126:ILE:H	1:D:169:ILE:CD1	2.27	0.46
1:C:39:ILE:HG13	1:C:72:TRP:CH2	2.49	0.46
1:C:62:PRO:O	1:C:63[A]:GLN:C	2.57	0.46
1:C:131:VAL:HG13	1:C:154:LYS:H	1.80	0.46
1:D:116:SER:HB3	1:D:119:GLU:CB	2.46	0.46
1:B:87:LEU:HD13	1:B:87:LEU:HA	1.81	0.46
1:C:106:GLN:HB3	1:C:108:TYR:HE1	1.81	0.46
1:D:94:LYS:CB	1:D:132:VAL:HG11	2.46	0.46
1:D:151:LEU:HB3	1:D:156:TYR:CE1	2.51	0.46
1:C:126:ILE:CG1	1:C:169:ILE:HD11	2.44	0.46
1:A:18[B]:ARG:HG2	1:A:18[B]:ARG:HH21	1.81	0.45
1:D:99:GLU:CB	1:D:125:GLU:O	2.64	0.45
1:B:98:PHE:CE2	1:B:107:MET:HG3	2.51	0.45
1:A:137:ILE:HD11	1:A:175:ILE:CD1	2.45	0.45
1:D:60:ILE:C	1:D:61:LEU:HD23	2.41	0.45
1:B:54:PHE:CD2	1:B:81:SER:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ILE:CD1	1:D:175:ILE:HD11	2.45	0.45
1:D:71:ARG:O	1:D:71:ARG:NH1	2.43	0.45
1:B:28:ASP:OD2	1:B:30:ARG:N	2.48	0.45
1:A:117:ILE:HG12	1:A:170:GLN:HA	1.99	0.45
1:B:11:GLU:O	1:B:35:ARG:HD2	2.16	0.45
1:B:100:LYS:HB2	1:B:104:ASN:OD1	2.17	0.45
1:B:37:ASN:O	1:B:38:SER:HB3	2.16	0.45
1:C:64:GLY:C	1:C:65:GLU:OE2	2.60	0.44
1:B:150:LEU:C	1:B:151:LEU:HD22	2.42	0.44
1:A:114:CYS:SG	1:A:117:ILE:HD13	2.57	0.44
1:A:125:GLU:C	1:A:126:ILE:HG12	2.42	0.44
1:C:25:ASP:CG	1:C:83:ARG:HG3	2.42	0.44
1:D:152:ASP:OD1	1:D:156:TYR:OH	2.35	0.44
1:B:151:LEU:HD22	1:B:151:LEU:N	2.33	0.44
1:A:140:GLU:CG	1:A:141:LEU:HD12	2.46	0.44
1:B:25:ASP:CG	1:B:83:ARG:HB2	2.42	0.44
1:B:86:HIS:O	1:B:87:LEU:C	2.61	0.44
1:B:117:ILE:HD11	1:B:169:ILE:O	2.18	0.44
1:A:118:MET:HE3	1:A:118:MET:HA	2.00	0.44
1:A:129:CYS:HG	1:A:156:TYR:HD2	1.64	0.44
1:C:132:VAL:HG23	1:C:133:GLU:N	2.32	0.44
1:C:71:ARG:NE	1:C:71:ARG:CA	2.73	0.44
1:D:93:ALA:HB3	1:D:174:ARG:NH2	2.33	0.44
1:A:14:ASN:O	1:A:15:PHE:HB2	2.18	0.44
1:B:69:TYR:HA	1:B:72:TRP:CH2	2.53	0.43
1:A:11:GLU:HG2	1:A:35:ARG:HD2	1.98	0.43
1:C:141:LEU:HD21	1:C:145:ARG:HB2	2.00	0.43
1:D:127:HIS:O	1:D:158:LYS:HA	2.18	0.43
1:B:60:ILE:O	1:B:60:ILE:HG13	2.19	0.43
1:D:102:ASP:HA	1:D:128:SER:CB	2.48	0.43
1:A:39:ILE:HD12	1:A:61:LEU:HD21	2.00	0.43
1:A:160:VAL:HA	1:A:164:ALA:O	2.19	0.43
1:C:156:TYR:HE1	1:C:161:ASP:HB3	1.82	0.43
1:B:125:GLU:CB	1:B:167:PRO:HB2	2.49	0.43
1:D:12:ASP:OD1	1:D:35:ARG:NH1	2.52	0.43
1:B:117:ILE:HG12	1:B:170:GLN:NE2	2.34	0.42
1:A:2:LYS:C	1:A:3:THR:O	2.61	0.42
1:A:135:THR:HG22	1:A:152:ASP:CA	2.43	0.42
1:D:23:ASP:O	1:D:46:TRP:CH2	2.72	0.42
1:D:39:ILE:HG13	1:D:72:TRP:CH2	2.54	0.42
1:B:169:ILE:O	1:B:169:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:SER:O	1:C:92:GLN:HB3	2.19	0.42
1:D:60:ILE:HD13	1:D:60:ILE:HA	1.86	0.42
1:D:132:VAL:HG13	1:D:133:GLU:N	2.34	0.42
1:B:94:LYS:CB	1:B:132:VAL:CG2	2.97	0.42
1:B:127:HIS:O	1:B:158:LYS:HA	2.19	0.42
1:A:98:PHE:N	1:A:98:PHE:CD1	2.87	0.42
1:C:36:CYS:CB	1:C:79:LEU:HD12	2.50	0.42
1:A:87:LEU:O	1:A:88:SER:C	2.63	0.42
1:D:58:MET:HG2	1:D:59:TYR:N	2.30	0.42
1:B:73:MET:HB2	1:B:73:MET:HE2	1.20	0.42
1:A:117:ILE:HD13	1:A:117:ILE:N	2.35	0.42
1:D:69:TYR:CD1	1:D:70:GLN:N	2.88	0.42
1:D:138:PHE:CE2	1:D:151:LEU:HD11	2.54	0.42
1:D:159:PRO:CG	1:D:167:PRO:CB	2.98	0.42
1:B:116:SER:HB3	1:B:119:GLU:CB	2.49	0.42
1:C:131:VAL:CG1	1:C:152:ASP:O	2.66	0.42
1:B:25:ASP:OD1	1:B:83:ARG:HB2	2.20	0.42
1:B:45:THR:HA	1:B:61:LEU:O	2.20	0.41
1:C:62:PRO:O	1:C:66:TYR:OH	2.26	0.41
1:D:37:ASN:O	1:D:38:SER:HB3	2.19	0.41
1:C:51[A]:ARG:HB2	1:C:55:SER:OG	2.20	0.41
1:C:51[B]:ARG:HB2	1:C:55:SER:OG	2.20	0.41
1:C:94:LYS:C	1:C:132:VAL:HG22	2.45	0.41
1:D:114:CYS:O	1:D:171:SER:HA	2.20	0.41
1:B:100:LYS:C	1:B:127:HIS:HB2	2.45	0.41
1:A:6:LYS:HG2	1:A:7:ILE:N	2.36	0.41
1:B:46:TRP:CZ3	1:B:84:ALA:HB2	2.56	0.41
1:B:147:ARG:NH1	1:A:57:HIS:NE2	2.68	0.41
1:A:6:LYS:CG	1:A:7:ILE:N	2.82	0.41
1:C:160:VAL:HG12	1:C:161:ASP:N	2.35	0.41
1:D:95:ILE:HD12	1:D:95:ILE:HA	1.92	0.41
1:B:48:VAL:CG1	1:B:79:LEU:HD22	2.40	0.41
1:A:61:LEU:HD12	1:A:61:LEU:N	2.34	0.41
1:A:98:PHE:CD2	1:A:107:MET:HB2	2.56	0.41
1:C:142:PRO:HA	1:C:171:SER:HB3	2.02	0.41
1:B:32:TYR:CE1	1:C:176:VAL:HG13	2.56	0.41
1:C:48:VAL:HG11	1:C:79:LEU:HD13	2.02	0.41
1:C:51[A]:ARG:NH2	1:C:56:GLY:HA2	2.35	0.41
1:D:5:GLY:HA2	1:D:43:GLY:CA	2.49	0.41
1:D:50:GLU:HA	1:D:78:ARG:O	2.21	0.41
1:C:45:THR:CG2	1:C:85:VAL:CG1	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ILE:HD12	1:C:60:ILE:N	2.35	0.41
1:C:99:GLU:CB	2:C:204:HOH:O	2.69	0.41
1:C:156:TYR:CE1	1:C:161:ASP:HB3	2.54	0.41
1:D:111:THR:HG23	1:D:111:THR:O	2.21	0.40
1:D:126:ILE:H	1:D:169:ILE:HD11	1.84	0.40
1:A:142:PRO:HD3	1:A:170:GLN:HG2	2.02	0.40
1:C:114:CYS:SG	1:C:120:GLN:CB	3.09	0.40
1:C:9:PHE:CD1	1:C:39:ILE:HD13	2.55	0.40
1:D:139:TYR:CG	1:D:144:TYR:HA	2.56	0.40
1:B:94:LYS:O	1:B:132:VAL:HG22	2.22	0.40
1:B:147:ARG:NH1	1:A:57:HIS:CE1	2.89	0.40
1:C:100:LYS:O	1:C:101:GLY:C	2.65	0.40
1:C:156:TYR:HE1	1:C:161:ASP:CB	2.31	0.40
1:C:156:TYR:CB	1:C:162:TRP:HZ3	2.35	0.40
1:C:9:PHE:O	1:C:19:ARG:HA	2.22	0.40
1:D:6:LYS:CB	1:D:42:GLU:HG2	2.50	0.40
1:D:7:ILE:HG13	1:D:8:SER:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:NH2	1:A:68:GLU:OE1[2_445]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	177/178 (99%)	158 (89%)	17 (10%)	2 (1%)	11	35
1	B	174/178 (98%)	155 (89%)	19 (11%)	0	100	100
1	C	177/178 (99%)	147 (83%)	27 (15%)	3 (2%)	7	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	170/178 (96%)	142 (84%)	27 (16%)	1 (1%)	21	50
All	All	698/712 (98%)	602 (86%)	90 (13%)	6 (1%)	14	40

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	C	102	ASP
1	D	124	ARG
1	A	168	ALA
1	C	112	GLU
1	C	90	GLY

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	144/155 (93%)	127 (88%)	17 (12%)	5	16
1	B	137/155 (88%)	117 (85%)	20 (15%)	3	10
1	C	131/155 (84%)	118 (90%)	13 (10%)	7	23
1	D	116/155 (75%)	94 (81%)	22 (19%)	1	5
All	All	528/620 (85%)	456 (86%)	72 (14%)	3	11

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

Mol	Chain	Res	Type
1	B	13	ARG
1	B	29	PHE
1	B	35	ARG
1	B	45	THR
1	B	60	ILE
1	B	73	MET
1	B	87	LEU
1	B	95	ILE

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Mol	Chain	Res	Type
1	B	99	GLU
1	B	102	ASP
1	B	109	GLU
1	B	117	ILE
1	B	129	CYS
1	B	132	VAL
1	B	145[A]	ARG
1	B	145[B]	ARG
1	B	157	ARG
1	B	160	VAL
1	B	169	ILE
1	B	170	GLN
1	A	3	THR
1	A	13	ARG
1	A	19	ARG
1	A	31	SER
1	A	35	ARG
1	A	42	GLU
1	A	58	MET
1	A	70	GLN
1	A	76	ASN
1	A	87	LEU
1	A	92	GLN
1	A	112	GLU
1	A	123	LEU
1	A	125	GLU
1	A	129	CYS
1	A	160	VAL
1	A	176	VAL
1	C	18	ARG
1	C	22	CYS
1	C	33	LEU
1	C	58	MET
1	C	85	VAL
1	C	92	GLN
1	C	133	GLU
1	C	135	THR
1	C	140	GLU
1	C	141	LEU
1	C	151	LEU
1	C	152	ASP
1	C	160	VAL

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Mol	Chain	Res	Type
1	D	3	THR
1	D	6	LYS
1	D	7	ILE
1	D	23	ASP
1	D	35	ARG
1	D	41	VAL
1	D	45	THR
1	D	58	MET
1	D	61	LEU
1	D	68	GLU
1	D	79	LEU
1	D	85	VAL
1	D	104	ASN
1	D	116	SER
1	D	118	MET
1	D	128	SER
1	D	129	CYS
1	D	160	VAL
1	D	166	SER
1	D	169	ILE
1	D	174	ARG
1	D	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	127	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	177/178 (99%)	-0.03	4 (2%) 61 51	44, 92, 128, 179	2 (1%)
1	B	174/178 (97%)	-0.01	2 (1%) 78 71	51, 90, 113, 166	2 (1%)
1	C	176/178 (98%)	0.23	5 (2%) 55 45	39, 107, 158, 295	3 (1%)
1	D	173/178 (97%)	0.17	3 (1%) 69 60	30, 122, 185, 224	1 (0%)
All	All	700/712 (98%)	0.09	14 (2%) 65 56	30, 97, 167, 295	8 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	PHE	5.1
1	D	168	ALA	4.3
1	D	150	LEU	3.6
1	D	61	LEU	3.4
1	C	50	GLU	2.7
1	A	175	ILE	2.5
1	C	150	LEU	2.5
1	C	149	TYR	2.5
1	B	129	CYS	2.4
1	A	126	ILE	2.1
1	A	22	CYS	2.1
1	A	24	CYS	2.1
1	C	129	CYS	2.1
1	B	96	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.