



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:25 PM UTC

PDB ID : 6MYB / pdb_00006myb
Title : Room-temperature structure of deuterated Tetdron (isomorph 1)
Authors : Dajnowicz, S.; Kovalevsky, A.
Deposited on : 2018-11-01
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

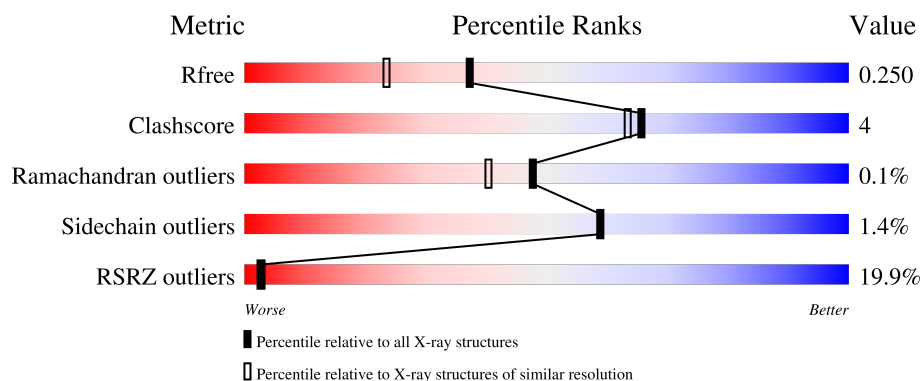
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	223	14% 91% 5% .
1	B	223	11% 87% 10% .
1	C	223	14% 91% 5% .
1	D	223	23% 89% 7% ..
1	E	223	30% 85% 10% ..

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Mol	Chain	Length	Quality of chain
1	F	223	29% 89% 7%
1	G	223	14% 82% 14%
1	H	223	18% 85% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14664 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 Photoswitchable protein Tetdron.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1735	1105	291	327	12			
1	B	216	Total	C	N	O	S	0	1	0
			1738	1107	291	328	12			
1	C	216	Total	C	N	O	S	0	0	0
			1735	1105	291	327	12			
1	D	216	Total	C	N	O	S	0	0	0
			1735	1105	291	327	12			
1	E	216	Total	C	N	O	S	0	0	0
			1735	1105	291	327	12			
1	F	216	Total	C	N	O	S	0	0	0
			1735	1105	291	327	12			
1	G	216	Total	C	N	O	S	0	1	0
			1738	1107	291	328	12			
1	H	216	Total	C	N	O	S	0	0	0
			1735	1105	291	327	12			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	109	Total	O	0	0
			109	109		
2	B	116	Total	O	0	0
			116	116		
2	C	101	Total	O	0	0
			101	101		
2	D	83	Total	O	0	0
			83	83		
2	E	84	Total	O	0	0
			84	84		
2	F	81	Total	O	0	0
			81	81		

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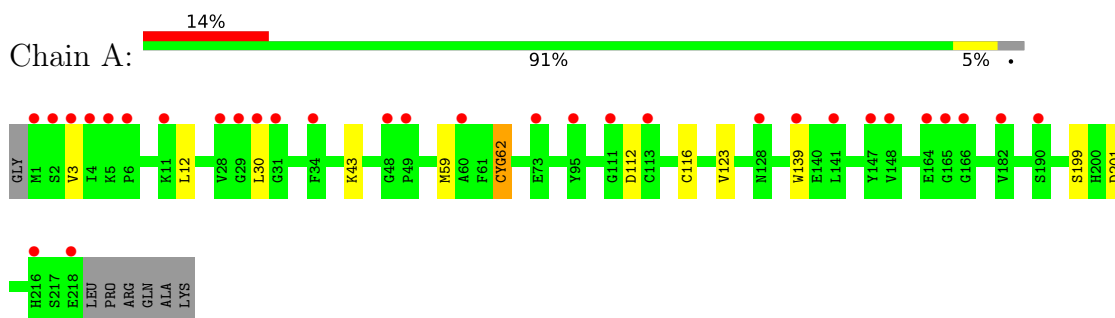
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	96	Total 96	O 96	0	0
2	H	108	Total 108	O 108	0	0

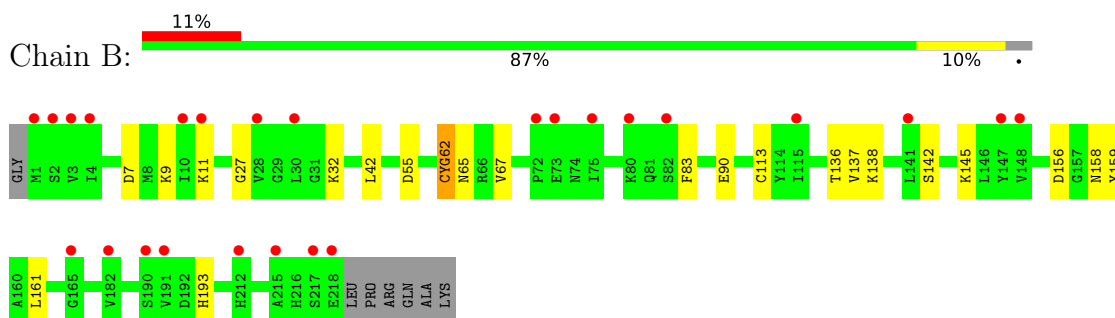
3 Residue-property plots [i](#)

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

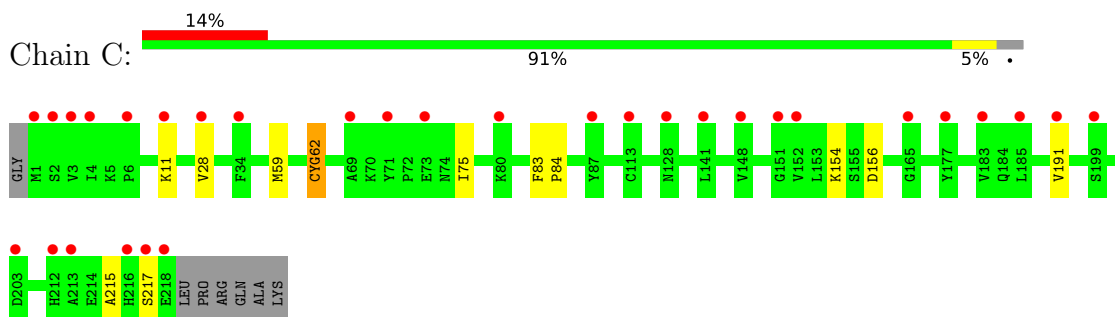
- Molecule 1: Photoswitchable protein Tetrdon



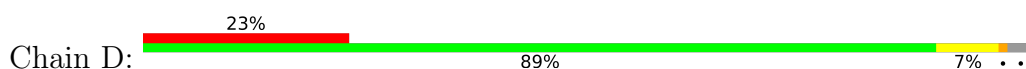
- Molecule 1: Photoswitchable protein Tetrdon

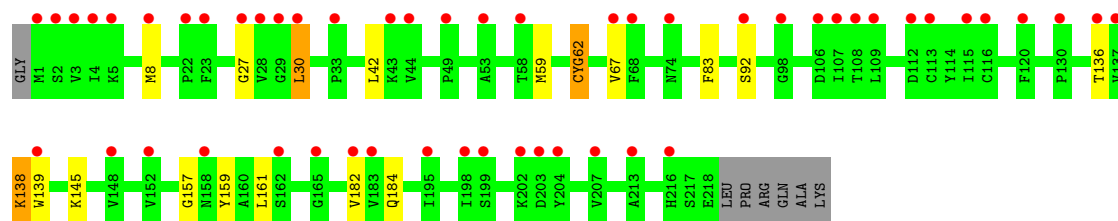


- Molecule 1: Photoswitchable protein Tetrdon

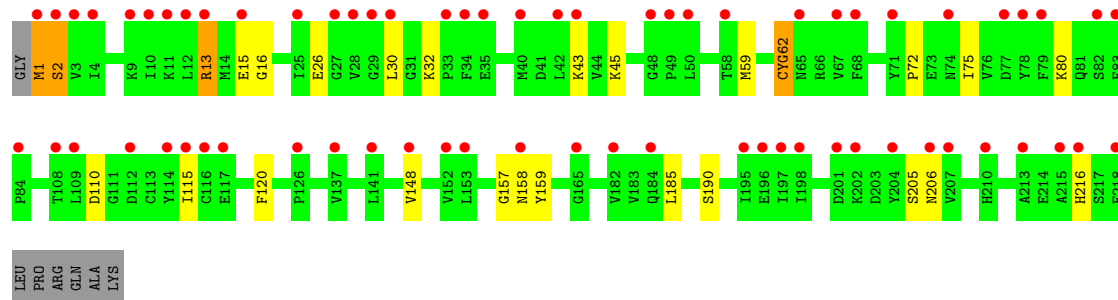
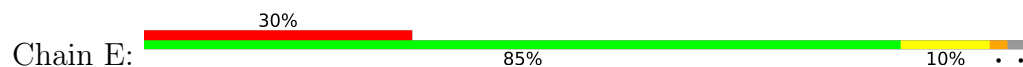


- Molecule 1: Photoswitchable protein Tetrdon

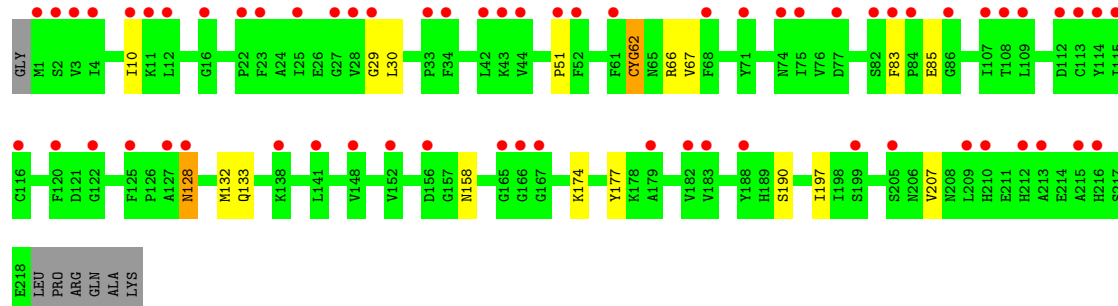
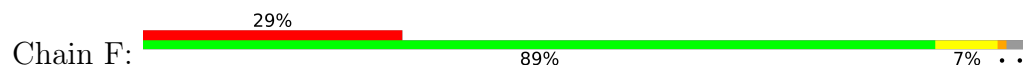




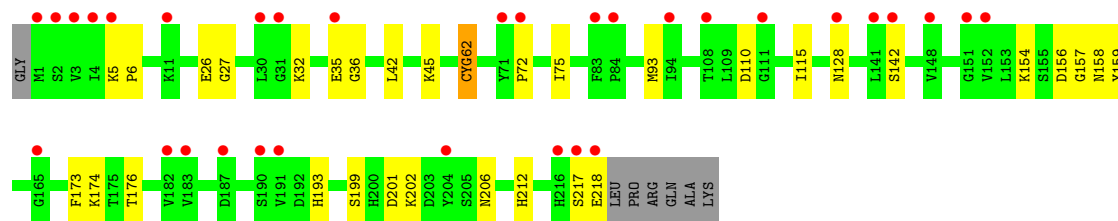
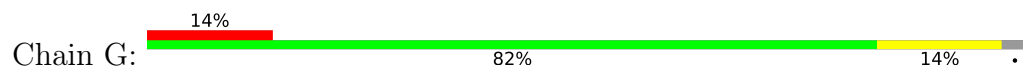
• Molecule 1: Photoswitchable protein Tetdron



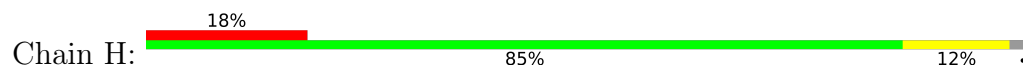
• Molecule 1: Photoswitchable protein Tetdron

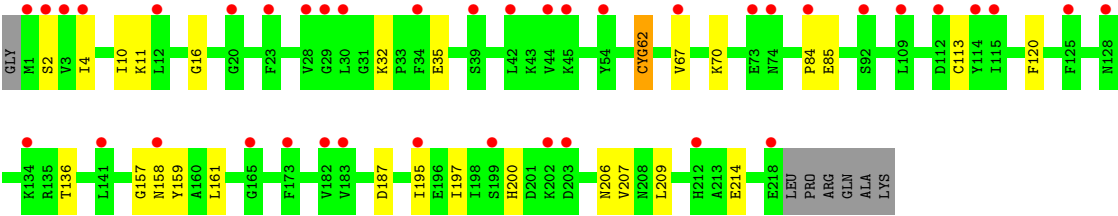


• Molecule 1: Photoswitchable protein Tetdron



• Molecule 1: Photoswitchable protein Tetdron





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.62Å 129.57Å 98.56Å 90.00° 105.36° 90.00°	Depositor
Resolution (Å)	35.63 – 1.90 35.63 – 1.90	Depositor EDS
% Data completeness (in resolution range)	85.8 (35.63-1.90) 85.7 (35.63-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.199 , 0.250 0.200 , 0.250	Depositor DCC
R_{free} test set	5905 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14664	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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](#)

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

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	0.32	0/1757	0.56	0/2369
1	B	0.35	0/1763	0.60	0/2377
1	C	0.36	0/1757	0.53	0/2369
1	D	0.32	1/1757 (0.1%)	0.53	0/2369
1	E	0.31	0/1757	0.52	0/2369
1	F	0.27	0/1757	0.49	0/2369
1	G	0.37	0/1763	0.57	0/2377
1	H	0.38	0/1757	0.58	0/2369
All	All	0.34	1/14068 (0.0%)	0.55	0/18968

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	LYS	C-O	-5.32	1.17	1.23

There are no bond angle outliers.

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	1735	0	1663	10	0
1	B	1738	0	1668	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1735	0	1663	6	0
1	D	1735	0	1663	12	0
1	E	1735	0	1663	15	0
1	F	1735	0	1663	11	0
1	G	1738	0	1668	21	0
1	H	1735	0	1663	17	0
2	A	109	0	0	2	0
2	B	116	0	0	1	0
2	C	101	0	0	2	0
2	D	83	0	0	1	0
2	E	84	0	0	1	0
2	F	81	0	0	1	0
2	G	96	0	0	0	0
2	H	108	0	0	2	0
All	All	14664	0	13314	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (102) 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:H:2:SER:O	1:H:4:ILE:N	2.24	0.70
1:D:184:GLN:NE2	1:F:51:PRO:HB2	2.07	0.69
1:B:7:ASP:OD1	1:B:32:LYS:NZ	2.28	0.66
1:E:13:ARG:NH1	1:E:15:GLU:OE2	2.30	0.65
1:H:10:ILE:O	1:H:11:LYS:HD2	1.97	0.64
1:H:11:LYS:HD3	1:H:113:CYS:SG	2.38	0.64
1:D:67:VAL:HG21	1:D:83:PHE:CE2	2.34	0.62
1:B:62:GYC:O2	1:B:62:GYC:HD1	2.01	0.59
1:H:32:LYS:NZ	2:H:306:HOH:O	2.34	0.59
1:E:110:ASP:HB2	1:E:115:ILE:HD11	1.84	0.59
1:F:67:VAL:HG11	1:F:83:PHE:HE2	1.68	0.58
1:F:67:VAL:HG11	1:F:83:PHE:CE2	2.39	0.57
1:D:67:VAL:HG21	1:D:83:PHE:HE2	1.67	0.57
1:A:59:MET:HE2	1:A:139:TRP:CE2	2.40	0.57
1:A:199:SER:HB2	1:G:201:ASP:HA	1.85	0.57
1:B:145:LYS:NZ	2:B:301:HOH:O	2.26	0.55
1:F:62:GYC:HD1	1:F:62:GYC:O2	2.08	0.54
1:A:43:LYS:NZ	2:A:306:HOH:O	2.40	0.54
1:B:142[B]:SER:OG	1:B:193:HIS:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:GYC:O2	1:D:62:GYC:HD1	2.06	0.54
1:H:157:GLY:HA3	1:H:159:TYR:CZ	2.42	0.53
1:E:43:LYS:HG3	1:E:206:ASN:OD1	2.08	0.53
1:B:137:VAL:HG12	1:B:138:LYS:HE2	1.91	0.52
1:B:67:VAL:HG11	1:B:83:PHE:CE2	2.45	0.52
1:E:26:GLU:HG3	1:E:45:LYS:HG3	1.91	0.52
1:F:85:GLU:N	1:F:85:GLU:OE1	2.41	0.52
1:H:195:ILE:HD11	1:H:209:LEU:HD11	1.91	0.51
1:H:16:GLY:HA3	1:H:120:PHE:O	2.11	0.51
1:C:62:GYC:O2	1:C:62:GYC:HD1	2.11	0.50
1:G:142[B]:SER:OG	1:G:193:HIS:HB2	2.11	0.50
1:G:72:PRO:HG2	1:G:75:ILE:HG13	1.94	0.50
1:G:62:GYC:O2	1:G:62:GYC:HD1	2.11	0.49
1:H:157:GLY:HA3	1:H:159:TYR:CE1	2.47	0.49
1:A:62:GYC:HD2	1:A:62:GYC:O2	2.11	0.49
1:A:112:ASP:N	2:A:307:HOH:O	2.42	0.49
1:G:156:ASP:OD1	1:G:174:LYS:NZ	2.41	0.49
1:H:62:GYC:O2	1:H:62:GYC:HD1	2.13	0.49
1:E:43:LYS:HA	1:E:205:SER:O	2.14	0.48
1:H:70:LYS:HB3	1:H:214:GLU:HG3	1.96	0.47
1:A:123:VAL:HB	1:B:90:GLU:HB3	1.96	0.47
1:B:65:ASN:OD1	1:B:67:VAL:HG22	2.14	0.47
1:G:217:SER:O	1:G:218:GLU:HG2	2.15	0.47
1:F:128:ASN:HA	1:F:133:GLN:HE21	1.80	0.47
1:G:202:LYS:HB3	1:G:202:LYS:HE2	1.62	0.47
1:D:184:GLN:NE2	1:F:132:MET:HE3	2.31	0.46
1:G:93:MET:HG2	1:G:173:PHE:CE1	2.51	0.46
1:B:142[B]:SER:HG	1:B:193:HIS:HB2	1.80	0.45
1:D:27:GLY:HA3	1:D:42:LEU:HD23	1.98	0.45
1:G:154:LYS:HD3	1:G:176:THR:HG23	1.98	0.45
1:G:32:LYS:HD3	1:G:35:GLU:OE2	2.15	0.45
1:G:157:GLY:HA3	1:G:159:TYR:CZ	2.52	0.45
1:A:199:SER:CB	1:G:201:ASP:HA	2.47	0.45
1:G:110:ASP:HB3	1:G:115:ILE:CD1	2.47	0.45
1:A:201:ASP:HA	1:G:199:SER:HB2	1.99	0.44
1:H:187:ASP:HB3	2:H:397:HOH:O	2.18	0.44
1:B:55:ASP:HB3	1:B:161:LEU:HD21	1.98	0.44
1:C:215:ALA:O	2:C:301:HOH:O	2.21	0.44
1:F:197:ILE:HG23	1:F:207:VAL:HG13	2.00	0.44
1:G:201:ASP:OD2	1:G:206:ASN:ND2	2.34	0.44
1:C:75:ILE:HD11	1:C:217:SER:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:LYS:HG3	1:C:28:VAL:HG12	1.98	0.44
1:E:30:LEU:HG	1:E:32:LYS:HZ1	1.83	0.44
1:G:142[B]:SER:HG	1:G:193:HIS:HB2	1.82	0.44
1:E:157:GLY:HA3	1:E:159:TYR:CE1	2.53	0.44
1:B:11:LYS:HG2	1:B:113:CYS:SG	2.57	0.43
1:E:62:GYC:HD1	1:E:62:GYC:O2	2.18	0.43
2:C:356:HOH:O	1:D:145:LYS:HE3	2.18	0.43
1:B:136:THR:HG21	1:B:161:LEU:HD13	2.00	0.43
1:H:200:HIS:HA	1:H:206:ASN:O	2.18	0.43
1:D:182:VAL:HG22	2:D:371:HOH:O	2.19	0.43
1:H:197:ILE:HG23	1:H:207:VAL:HG13	2.01	0.43
1:F:174:LYS:HE3	2:F:301:HOH:O	2.19	0.43
1:C:191:VAL:HG22	1:C:215:ALA:HB2	2.01	0.42
1:H:158:ASN:OD1	1:H:158:ASN:N	2.51	0.42
1:E:80:LYS:NZ	2:E:312:HOH:O	2.49	0.42
1:E:43:LYS:HG2	1:E:205:SER:O	2.20	0.42
1:D:157:GLY:HA3	1:D:159:TYR:CZ	2.55	0.42
1:F:66:ARG:NH1	1:F:177:TYR:OH	2.49	0.42
1:G:26:GLU:OE2	1:G:45:LYS:HE3	2.20	0.42
1:G:27:GLY:HA3	1:G:42:LEU:HD23	2.02	0.42
1:B:142[B]:SER:HB2	1:B:159:TYR:CE1	2.54	0.42
1:D:136:THR:HG21	1:D:161:LEU:HD13	2.01	0.42
1:G:5:LYS:HG3	1:G:6:PRO:HD2	2.01	0.41
1:H:32:LYS:HD3	1:H:35:GLU:HG3	2.02	0.41
1:C:83:PHE:HB3	1:C:84:PRO:HA	2.03	0.41
1:G:110:ASP:HB3	1:G:115:ILE:HD11	2.02	0.41
1:H:136:THR:HG21	1:H:161:LEU:HD13	2.03	0.41
1:H:84:PRO:HD2	1:H:85:GLU:OE2	2.21	0.41
1:E:1:MET:HB2	1:E:2:SER:H	1.61	0.41
1:E:148:VAL:HG21	1:E:185:LEU:HB3	2.03	0.41
1:D:8:MET:O	1:D:30:LEU:HD23	2.21	0.41
1:D:59:MET:HE3	1:D:139:TRP:CG	2.56	0.41
1:G:36:GLY:O	1:G:212:HIS:HA	2.21	0.41
1:E:16:GLY:HA3	1:E:120:PHE:O	2.20	0.40
1:A:59:MET:HE2	1:A:139:TRP:CD2	2.57	0.40
1:B:27:GLY:HA3	1:B:42:LEU:HD23	2.03	0.40
1:B:142[B]:SER:HB2	1:B:159:TYR:CD1	2.56	0.40
1:E:72:PRO:HD2	1:E:75:ILE:HD12	2.02	0.40
1:E:190:SER:HB2	1:E:216:HIS:CE1	2.56	0.40
1:B:9:LYS:N	1:B:9:LYS:HD2	2.36	0.40
1:F:10:ILE:N	1:F:29:GLY:O	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HB3	1:A:116:CYS:HB2	2.02	0.40

There are no symmetry-related clashes.

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	211/223 (95%)	208 (99%)	3 (1%)	0	100	100
1	B	212/223 (95%)	211 (100%)	1 (0%)	0	100	100
1	C	211/223 (95%)	211 (100%)	0	0	100	100
1	D	211/223 (95%)	209 (99%)	2 (1%)	0	100	100
1	E	211/223 (95%)	208 (99%)	2 (1%)	1 (0%)	24	16
1	F	211/223 (95%)	208 (99%)	3 (1%)	0	100	100
1	G	212/223 (95%)	209 (99%)	3 (1%)	0	100	100
1	H	211/223 (95%)	209 (99%)	2 (1%)	0	100	100
All	All	1690/1784 (95%)	1673 (99%)	16 (1%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	SER

5.3.2 Protein sidechains [i](#)

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	185/190 (97%)	183 (99%)	2 (1%)	65	67
1	B	186/190 (98%)	184 (99%)	2 (1%)	65	67
1	C	185/190 (97%)	182 (98%)	3 (2%)	55	54
1	D	185/190 (97%)	182 (98%)	3 (2%)	55	54
1	E	185/190 (97%)	181 (98%)	4 (2%)	45	42
1	F	185/190 (97%)	181 (98%)	4 (2%)	45	42
1	G	186/190 (98%)	184 (99%)	2 (1%)	65	67
1	H	185/190 (97%)	184 (100%)	1 (0%)	81	84
All	All	1482/1520 (98%)	1461 (99%)	21 (1%)	59	59

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	30	LEU
1	B	156	ASP
1	B	158	ASN
1	C	59	MET
1	C	154	LYS
1	C	156	ASP
1	D	30	LEU
1	D	92	SER
1	D	138	LYS
1	E	1	MET
1	E	13	ARG
1	E	59	MET
1	E	158	ASN
1	F	30	LEU
1	F	128	ASN
1	F	158	ASN
1	F	190	SER
1	G	128	ASN
1	G	158	ASN
1	H	67	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	194	HIS
1	A	212	HIS
1	C	128	ASN
1	C	133	GLN
1	C	216	HIS
1	D	133	GLN
1	D	184	GLN
1	E	38	GLN
1	F	38	GLN
1	F	128	ASN
1	F	133	GLN
1	G	128	ASN
1	G	210	HIS

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	GYC	F	62	1	21,22,23	2.69	7 (33%)	26,30,32	3.05	7 (26%)
1	GYC	C	62	1	21,22,23	2.59	7 (33%)	26,30,32	3.48	12 (46%)
1	GYC	D	62	1	21,22,23	2.87	6 (28%)	26,30,32	3.06	8 (30%)
1	GYC	H	62	1	21,22,23	2.77	6 (28%)	26,30,32	3.37	9 (34%)
1	GYC	E	62	1	21,22,23	2.77	6 (28%)	26,30,32	3.29	9 (34%)
1	GYC	G	62	1	21,22,23	2.77	7 (33%)	26,30,32	3.62	9 (34%)
1	GYC	B	62	1	21,22,23	2.45	7 (33%)	26,30,32	3.50	9 (34%)
1	GYC	A	62	1	21,22,23	2.63	7 (33%)	26,30,32	3.14	8 (30%)

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	GYC	F	62	1	-	3/10/29/30	0/2/2/2
1	GYC	C	62	1	-	4/10/29/30	0/2/2/2
1	GYC	D	62	1	-	3/10/29/30	0/2/2/2
1	GYC	H	62	1	-	3/10/29/30	0/2/2/2
1	GYC	E	62	1	-	3/10/29/30	0/2/2/2
1	GYC	G	62	1	-	4/10/29/30	0/2/2/2
1	GYC	B	62	1	-	3/10/29/30	0/2/2/2
1	GYC	A	62	1	-	3/10/29/30	0/2/2/2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	62	GYC	CA2-C2	8.17	1.57	1.48
1	D	62	GYC	CA2-C2	8.11	1.57	1.48
1	H	62	GYC	CA2-C2	7.74	1.56	1.48
1	E	62	GYC	CA2-C2	7.27	1.56	1.48
1	A	62	GYC	CA2-C2	7.19	1.56	1.48
1	F	62	GYC	CA2-C2	6.88	1.56	1.48
1	C	62	GYC	CA2-C2	6.57	1.55	1.48
1	F	62	GYC	C1-N2	6.15	1.41	1.32
1	E	62	GYC	C1-N2	6.12	1.41	1.32
1	D	62	GYC	C1-N2	6.00	1.41	1.32
1	B	62	GYC	CA2-C2	5.89	1.54	1.48
1	A	62	GYC	C1-N2	5.88	1.40	1.32
1	C	62	GYC	C1-N2	5.61	1.40	1.32
1	H	62	GYC	C1-N2	5.56	1.40	1.32
1	G	62	GYC	C1-N2	5.36	1.40	1.32
1	H	62	GYC	C1-N3	5.06	1.45	1.37
1	B	62	GYC	C1-N3	4.99	1.45	1.37
1	E	62	GYC	C1-N3	4.84	1.45	1.37
1	G	62	GYC	C1-N3	4.71	1.45	1.37
1	D	62	GYC	C1-N3	4.70	1.45	1.37
1	A	62	GYC	C1-N3	4.59	1.44	1.37
1	B	62	GYC	C1-N2	4.47	1.38	1.32
1	C	62	GYC	C1-N3	4.38	1.44	1.37
1	E	62	GYC	C2-N3	4.24	1.49	1.40
1	F	62	GYC	C1-N3	4.15	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	GYC	C2-N3	4.14	1.49	1.40
1	C	62	GYC	C2-N3	4.04	1.49	1.40
1	F	62	GYC	C2-N3	4.02	1.49	1.40
1	G	62	GYC	C2-N3	3.93	1.49	1.40
1	B	62	GYC	C2-N3	3.90	1.48	1.40
1	H	62	GYC	C2-N3	3.74	1.48	1.40
1	A	62	GYC	C2-N3	3.61	1.48	1.40
1	F	62	GYC	CG2-CB2	3.55	1.53	1.46
1	C	62	GYC	CB2-CA2	-3.51	1.31	1.35
1	E	62	GYC	CG2-CB2	3.39	1.53	1.46
1	D	62	GYC	CB2-CA2	-3.34	1.32	1.35
1	H	62	GYC	CG2-CB2	3.16	1.52	1.46
1	D	62	GYC	CG2-CB2	2.99	1.52	1.46
1	G	62	GYC	CG2-CB2	2.95	1.52	1.46
1	B	62	GYC	CG2-CB2	2.84	1.52	1.46
1	H	62	GYC	CB2-CA2	-2.80	1.32	1.35
1	B	62	GYC	CB2-CA2	-2.71	1.32	1.35
1	A	62	GYC	CB2-CA2	-2.70	1.32	1.35
1	C	62	GYC	CG2-CB2	2.50	1.51	1.46
1	E	62	GYC	CB2-CA2	-2.47	1.32	1.35
1	G	62	GYC	CB2-CA2	-2.44	1.32	1.35
1	B	62	GYC	O2-C2	-2.38	1.18	1.23
1	C	62	GYC	O2-C2	-2.37	1.18	1.23
1	F	62	GYC	O2-C2	-2.35	1.18	1.23
1	F	62	GYC	CB2-CA2	-2.34	1.32	1.35
1	A	62	GYC	CG2-CB2	2.16	1.50	1.46
1	G	62	GYC	O2-C2	-2.09	1.18	1.23
1	A	62	GYC	O2-C2	-2.02	1.19	1.23

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	62	GYC	CB2-CA2-C2	11.68	136.51	122.36
1	B	62	GYC	CB2-CA2-C2	10.84	135.50	122.36
1	H	62	GYC	CB2-CA2-C2	10.80	135.45	122.36
1	C	62	GYC	CB2-CA2-C2	10.36	134.91	122.36
1	A	62	GYC	CB2-CA2-C2	10.28	134.82	122.36
1	D	62	GYC	CB2-CA2-C2	10.19	134.70	122.36
1	E	62	GYC	CB2-CA2-C2	10.02	134.50	122.36
1	F	62	GYC	CB2-CA2-C2	9.50	133.87	122.36
1	H	62	GYC	CB2-CA2-N2	-8.34	117.44	128.76
1	G	62	GYC	CB2-CA2-N2	-8.26	117.55	128.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	GYC	CB2-CA2-N2	-7.97	117.94	128.76
1	C	62	GYC	CB2-CA2-N2	-7.90	118.03	128.76
1	D	62	GYC	CB2-CA2-N2	-7.70	118.31	128.76
1	A	62	GYC	CB2-CA2-N2	-7.69	118.32	128.76
1	C	62	GYC	C2-N3-C1	-7.12	104.77	108.07
1	E	62	GYC	C2-N3-C1	-7.12	104.77	108.07
1	H	62	GYC	C2-N3-C1	-7.09	104.78	108.07
1	E	62	GYC	CB2-CA2-N2	-6.95	119.33	128.76
1	B	62	GYC	C2-N3-C1	-6.53	105.04	108.07
1	F	62	GYC	CB2-CA2-N2	-6.41	120.06	128.76
1	G	62	GYC	C2-N3-C1	-6.02	105.28	108.07
1	F	62	GYC	C2-N3-C1	-6.00	105.29	108.07
1	G	62	GYC	CA2-N2-C1	5.35	109.98	105.80
1	B	62	GYC	CA2-N2-C1	5.13	109.81	105.80
1	A	62	GYC	C2-N3-C1	-4.85	105.82	108.07
1	D	62	GYC	C2-N3-C1	-4.71	105.89	108.07
1	E	62	GYC	CA2-N2-C1	4.64	109.43	105.80
1	F	62	GYC	CA2-N2-C1	4.56	109.37	105.80
1	A	62	GYC	CA2-N2-C1	4.55	109.36	105.80
1	D	62	GYC	CA2-N2-C1	4.39	109.23	105.80
1	G	62	GYC	C2-CA2-N2	-4.21	105.93	108.95
1	F	62	GYC	C2-CA2-N2	-4.02	106.07	108.95
1	G	62	GYC	CA1-CB1-SG1	-3.99	105.87	114.40
1	E	62	GYC	C2-CA2-N2	-3.88	106.17	108.95
1	C	62	GYC	O2-C2-CA2	-3.87	128.55	131.02
1	C	62	GYC	CA3-N3-C2	3.82	132.06	123.67
1	E	62	GYC	CA2-C2-N3	3.68	106.59	103.50
1	C	62	GYC	CA2-N2-C1	3.64	108.64	105.80
1	G	62	GYC	CA3-N3-C2	3.51	131.39	123.67
1	H	62	GYC	CA2-N2-C1	3.50	108.54	105.80
1	F	62	GYC	CA2-C2-N3	3.49	106.43	103.50
1	B	62	GYC	CA1-CB1-SG1	-3.44	107.04	114.40
1	B	62	GYC	C2-CA2-N2	-3.42	106.50	108.95
1	B	62	GYC	CA3-N3-C2	3.16	130.61	123.67
1	B	62	GYC	CA2-C2-N3	3.04	106.06	103.50
1	G	62	GYC	CA2-C2-N3	2.99	106.01	103.50
1	A	62	GYC	C2-CA2-N2	-2.97	106.82	108.95
1	C	62	GYC	CA2-C2-N3	2.95	105.98	103.50
1	H	62	GYC	CA2-C2-N3	2.86	105.90	103.50
1	H	62	GYC	N3-C1-N2	2.77	113.66	111.48
1	D	62	GYC	CA1-CB1-SG1	-2.75	108.51	114.40
1	D	62	GYC	C2-CA2-N2	-2.74	106.98	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	62	GYC	O3-C3-CA3	-2.70	113.31	125.47
1	C	62	GYC	C2-CA2-N2	-2.68	107.03	108.95
1	C	62	GYC	N3-C1-N2	2.63	113.56	111.48
1	H	62	GYC	C2-CA2-N2	-2.56	107.11	108.95
1	C	62	GYC	CA1-CB1-SG1	-2.56	108.92	114.40
1	A	62	GYC	CA2-C2-N3	2.56	105.65	103.50
1	B	62	GYC	O2-C2-CA2	-2.54	129.40	131.02
1	E	62	GYC	CA1-CB1-SG1	-2.53	108.99	114.40
1	H	62	GYC	CA1-CB1-SG1	-2.46	109.14	114.40
1	A	62	GYC	CD2-CG2-CD1	2.43	121.25	117.65
1	H	62	GYC	CA3-N3-C2	2.42	128.98	123.67
1	E	62	GYC	O2-C2-CA2	-2.34	129.53	131.02
1	F	62	GYC	CA3-N3-C2	2.34	128.82	123.67
1	C	62	GYC	CD2-CG2-CD1	2.23	120.95	117.65
1	D	62	GYC	CA3-N3-C2	2.15	128.39	123.67
1	A	62	GYC	CA3-N3-C2	2.11	128.31	123.67
1	E	62	GYC	CA3-N3-C2	2.11	128.30	123.67
1	D	62	GYC	CA2-C2-N3	2.02	105.20	103.50
1	C	62	GYC	CE2-CD2-CG2	-2.01	118.63	121.22

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	62	GYC	C3-CA3-N3-C2
1	A	62	GYC	N2-CA2-CB2-CG2
1	A	62	GYC	C2-CA2-CB2-CG2
1	B	62	GYC	C3-CA3-N3-C2
1	B	62	GYC	C2-CA2-CB2-CG2
1	C	62	GYC	C3-CA3-N3-C2
1	C	62	GYC	C2-CA2-CB2-CG2
1	D	62	GYC	C3-CA3-N3-C2
1	D	62	GYC	N2-CA2-CB2-CG2
1	D	62	GYC	C2-CA2-CB2-CG2
1	E	62	GYC	C3-CA3-N3-C2
1	E	62	GYC	N2-CA2-CB2-CG2
1	E	62	GYC	C2-CA2-CB2-CG2
1	F	62	GYC	C3-CA3-N3-C2
1	F	62	GYC	C2-CA2-CB2-CG2
1	G	62	GYC	C3-CA3-N3-C2
1	G	62	GYC	C2-CA2-CB2-CG2
1	H	62	GYC	C3-CA3-N3-C2

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Mol	Chain	Res	Type	Atoms
1	H	62	GYC	C2-CA2-CB2-CG2
1	H	62	GYC	N2-CA2-CB2-CG2
1	B	62	GYC	N2-CA2-CB2-CG2
1	C	62	GYC	N2-CA2-CB2-CG2
1	F	62	GYC	N2-CA2-CB2-CG2
1	C	62	GYC	C3-CA3-N3-C1
1	G	62	GYC	C3-CA3-N3-C1
1	G	62	GYC	N2-CA2-CB2-CG2

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	62	GYC	1	0
1	C	62	GYC	1	0
1	D	62	GYC	1	0
1	H	62	GYC	1	0
1	E	62	GYC	1	0
1	G	62	GYC	1	0
1	B	62	GYC	1	0
1	A	62	GYC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/223 (96%)	1.11	31 (14%) 6 6	10, 19, 33, 64	0
1	B	215/223 (96%)	0.99	25 (11%) 9 10	7, 16, 30, 59	1 (0%)
1	C	215/223 (96%)	1.10	31 (14%) 6 6	8, 18, 36, 65	0
1	D	215/223 (96%)	1.48	52 (24%) 2 1	12, 24, 40, 75	1 (0%)
1	E	215/223 (96%)	1.59	67 (31%) 1 1	13, 25, 44, 77	0
1	F	215/223 (96%)	1.60	64 (29%) 1 1	12, 27, 44, 87	1 (0%)
1	G	215/223 (96%)	1.22	32 (14%) 5 6	10, 20, 35, 76	1 (0%)
1	H	215/223 (96%)	1.34	40 (18%) 3 3	11, 20, 33, 70	1 (0%)
All	All	1720/1784 (96%)	1.30	342 (19%) 3 3	7, 21, 38, 87	5 (0%)

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	183	VAL	7.0
1	C	1	MET	5.9
1	D	49	PRO	5.0
1	A	2	SER	4.8
1	A	218	GLU	4.8
1	E	115	ILE	4.8
1	E	1	MET	4.7
1	H	1	MET	4.7
1	F	28	VAL	4.7
1	E	2	SER	4.3
1	E	3	VAL	4.2
1	B	2	SER	4.2
1	G	182	VAL	4.2
1	E	114	TYR	4.1
1	C	165	GLY	4.1
1	D	207	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	75	ILE	4.1
1	A	1	MET	4.0
1	F	83	PHE	4.0
1	F	84	PRO	4.0
1	D	3	VAL	4.0
1	F	10	ILE	4.0
1	F	1	MET	4.0
1	G	1	MET	4.0
1	F	108	THR	3.9
1	C	203	ASP	3.8
1	B	1	MET	3.8
1	G	217	SER	3.8
1	D	23	PHE	3.7
1	F	27	GLY	3.7
1	F	3	VAL	3.7
1	E	74	ASN	3.7
1	F	141	LEU	3.6
1	E	197	ILE	3.6
1	D	183	VAL	3.6
1	E	30	LEU	3.5
1	D	29	GLY	3.5
1	E	11	LYS	3.5
1	D	74	ASN	3.5
1	G	165	GLY	3.5
1	H	134	LYS	3.5
1	G	84	PRO	3.4
1	E	28	VAL	3.4
1	F	183	VAL	3.4
1	H	182	VAL	3.4
1	D	53	ALA	3.4
1	G	141	LEU	3.4
1	E	165	GLY	3.3
1	H	44	VAL	3.3
1	E	218	GLU	3.3
1	E	29	GLY	3.3
1	B	75	ILE	3.2
1	D	216	HIS	3.2
1	F	212	HIS	3.2
1	F	12	LEU	3.2
1	C	11	LYS	3.2
1	E	108	THR	3.2
1	B	10	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	166	GLY	3.2
1	G	31	GLY	3.2
1	A	6	PRO	3.1
1	E	148	VAL	3.1
1	E	207	VAL	3.1
1	B	218	GLU	3.1
1	D	199	SER	3.1
1	G	4	ILE	3.1
1	A	128	ASN	3.1
1	B	72	PRO	3.1
1	B	212	HIS	3.1
1	F	29	GLY	3.1
1	H	128	ASN	3.1
1	H	199	SER	3.1
1	D	98	GLY	3.1
1	H	30	LEU	3.0
1	F	128	ASN	3.0
1	B	217	SER	3.0
1	C	3	VAL	3.0
1	D	67	VAL	3.0
1	F	2	SER	3.0
1	H	165	GLY	3.0
1	E	213	ALA	3.0
1	D	158	ASN	3.0
1	D	202	LYS	2.9
1	G	35	GLU	2.9
1	H	218	GLU	2.9
1	F	116	CYS	2.9
1	E	198	ILE	2.9
1	C	199	SER	2.9
1	D	162	SER	2.9
1	G	3	VAL	2.9
1	H	54	TYR	2.9
1	F	210	HIS	2.9
1	D	198	ILE	2.9
1	B	73	GLU	2.9
1	D	204	TYR	2.9
1	E	34	PHE	2.9
1	F	120	PHE	2.9
1	F	179	ALA	2.9
1	B	30	LEU	2.9
1	C	141	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	4	ILE	2.9
1	D	109	LEU	2.9
1	E	12	LEU	2.9
1	D	27	GLY	2.8
1	A	147	TYR	2.8
1	E	182	VAL	2.8
1	H	3	VAL	2.8
1	H	67	VAL	2.8
1	D	1	MET	2.8
1	F	188	TYR	2.8
1	C	216	HIS	2.8
1	F	51	PRO	2.8
1	D	213	ALA	2.7
1	E	158	ASN	2.7
1	D	68	PHE	2.7
1	F	34	PHE	2.7
1	D	108	THR	2.7
1	D	30	LEU	2.7
1	D	112	ASP	2.7
1	H	203	ASP	2.7
1	E	33	PRO	2.7
1	F	199	SER	2.7
1	C	218	GLU	2.7
1	C	213	ALA	2.7
1	H	73	GLU	2.7
1	D	137	VAL	2.7
1	C	69	ALA	2.6
1	H	39	SER	2.6
1	E	49	PRO	2.6
1	F	109	LEU	2.6
1	D	182	VAL	2.6
1	H	42	LEU	2.6
1	E	112	ASP	2.6
1	B	3	VAL	2.6
1	B	182	VAL	2.6
1	C	191	VAL	2.6
1	B	80	LYS	2.6
1	C	2	SER	2.6
1	E	206	ASN	2.6
1	F	74	ASN	2.6
1	E	126	PRO	2.6
1	A	30	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	4	ILE	2.6
1	A	29	GLY	2.6
1	F	213	ALA	2.6
1	G	152	VAL	2.6
1	E	68	PHE	2.5
1	C	185	LEU	2.5
1	H	141	LEU	2.5
1	D	148	VAL	2.5
1	E	84	PRO	2.5
1	F	33	PRO	2.5
1	G	151	GLY	2.5
1	H	4	ILE	2.5
1	A	182	VAL	2.5
1	H	28	VAL	2.5
1	H	84	PRO	2.5
1	A	11	LYS	2.5
1	D	5	LYS	2.5
1	E	43	LYS	2.5
1	A	141	LEU	2.5
1	D	165	GLY	2.5
1	D	2	SER	2.5
1	H	92	SER	2.5
1	G	148	VAL	2.5
1	G	5	LYS	2.5
1	E	27	GLY	2.4
1	E	83	PHE	2.4
1	F	52	PHE	2.4
1	E	184	GLN	2.4
1	D	136	THR	2.4
1	F	215	ALA	2.4
1	C	212	HIS	2.4
1	H	212	HIS	2.4
1	E	40	MET	2.4
1	F	114	TYR	2.4
1	A	34	PHE	2.4
1	B	4	ILE	2.4
1	E	4	ILE	2.4
1	E	13	ARG	2.4
1	B	28	VAL	2.4
1	F	165	GLY	2.4
1	E	153	LEU	2.4
1	F	11	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	209	LEU	2.4
1	H	109	LEU	2.4
1	E	204	TYR	2.4
1	E	79	PHE	2.4
1	F	77	ASP	2.4
1	D	58	THR	2.4
1	E	58	THR	2.4
1	G	108	THR	2.4
1	G	72	PRO	2.4
1	E	152	VAL	2.4
1	H	29	GLY	2.4
1	B	82	SER	2.4
1	F	156	ASP	2.3
1	C	34	PHE	2.3
1	F	23	PHE	2.3
1	A	73	GLU	2.3
1	G	94	ILE	2.3
1	A	111	GLY	2.3
1	F	86	GLY	2.3
1	G	11	LYS	2.3
1	F	152	VAL	2.3
1	E	50	LEU	2.3
1	E	109	LEU	2.3
1	F	42	LEU	2.3
1	B	147	TYR	2.3
1	C	71	TYR	2.3
1	C	87	TYR	2.3
1	F	25	ILE	2.3
1	A	148	VAL	2.3
1	D	106	ASP	2.3
1	E	201	ASP	2.3
1	C	73	GLU	2.3
1	E	196	GLU	2.3
1	E	210	HIS	2.3
1	F	216	HIS	2.3
1	B	11	LYS	2.3
1	H	173	PHE	2.3
1	C	4	ILE	2.3
1	D	115	ILE	2.3
1	E	25	ILE	2.3
1	E	48	GLY	2.3
1	H	20	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	190	SER	2.3
1	B	148	VAL	2.3
1	B	191	VAL	2.3
1	C	113	CYS	2.3
1	G	30	LEU	2.3
1	E	15	GLU	2.2
1	E	71	TYR	2.2
1	F	68	PHE	2.2
1	F	122	GLY	2.2
1	C	217	SER	2.2
1	F	205	SER	2.2
1	A	4	ILE	2.2
1	H	195	ILE	2.2
1	A	28	VAL	2.2
1	C	152	VAL	2.2
1	D	44	VAL	2.2
1	F	148	VAL	2.2
1	A	31	GLY	2.2
1	C	6	PRO	2.2
1	F	112	ASP	2.2
1	G	142[A]	SER	2.2
1	F	125	PHE	2.2
1	G	71	TYR	2.2
1	B	115	ILE	2.2
1	E	195	ILE	2.2
1	C	80	LYS	2.2
1	C	148	VAL	2.2
1	A	48	GLY	2.2
1	A	190	SER	2.2
1	B	165	GLY	2.2
1	G	2	SER	2.2
1	H	2	SER	2.2
1	H	112	ASP	2.2
1	D	22	PRO	2.2
1	D	130	PRO	2.2
1	D	107	ILE	2.2
1	D	195	ILE	2.2
1	A	5	LYS	2.2
1	C	128	ASN	2.2
1	H	74	ASN	2.2
1	A	3	VAL	2.2
1	E	137	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	183	VAL	2.2
1	E	77	ASP	2.2
1	E	82	SER	2.2
1	F	113	CYS	2.2
1	F	16	GLY	2.2
1	E	215	ALA	2.2
1	D	43	LYS	2.2
1	D	8	MET	2.1
1	A	164	GLU	2.1
1	F	61	PHE	2.1
1	H	125	PHE	2.1
1	C	177	TYR	2.1
1	G	187	ASP	2.1
1	C	183	VAL	2.1
1	D	152	VAL	2.1
1	G	190	SER	2.1
1	A	166	GLY	2.1
1	C	151	GLY	2.1
1	B	141	LEU	2.1
1	D	33	PRO	2.1
1	E	42	LEU	2.1
1	F	43	LYS	2.1
1	E	35	GLU	2.1
1	E	117	GLU	2.1
1	F	107	ILE	2.1
1	D	203	ASP	2.1
1	A	165	GLY	2.1
1	E	67	VAL	2.1
1	G	191	VAL	2.1
1	E	202	LYS	2.1
1	D	113	CYS	2.1
1	H	12	LEU	2.1
1	B	215	ALA	2.1
1	G	83	PHE	2.1
1	H	34	PHE	2.1
1	E	78	TYR	2.1
1	F	71	TYR	2.1
1	F	115	ILE	2.1
1	G	204	TYR	2.1
1	G	218	GLU	2.1
1	H	45	LYS	2.1
1	A	139	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	28	VAL	2.1
1	D	28	VAL	2.1
1	D	139	TRP	2.1
1	G	216	HIS	2.1
1	F	44	VAL	2.1
1	F	182	VAL	2.1
1	G	128	ASN	2.1
1	A	113	CYS	2.1
1	F	127	ALA	2.1
1	D	120	PHE	2.0
1	E	9	LYS	2.0
1	F	138	LYS	2.0
1	H	115	ILE	2.0
1	A	216	HIS	2.0
1	E	216	HIS	2.0
1	H	158	ASN	2.0
1	A	49	PRO	2.0
1	D	116	CYS	2.0
1	E	116	CYS	2.0
1	E	141	LEU	2.0
1	A	60	ALA	2.0
1	H	202	LYS	2.0
1	D	92	SER	2.0
1	F	82	SER	2.0
1	E	10	ILE	2.0
1	H	23	PHE	2.0
1	A	95	TYR	2.0
1	E	65	ASN	2.0
1	F	167	GLY	2.0
1	G	111	GLY	2.0
1	H	114	TYR	2.0
1	F	22	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	GYC	D	62	21/22	0.86	0.14	15,19,22,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	GYC	B	62	21/22	0.90	0.11	6,12,17,20	0
1	GYC	E	62	21/22	0.90	0.12	17,20,22,25	0
1	GYC	F	62	21/22	0.90	0.11	17,22,26,29	0
1	GYC	G	62	21/22	0.90	0.11	10,15,18,19	0
1	GYC	A	62	21/22	0.91	0.11	11,14,19,20	0
1	GYC	C	62	21/22	0.91	0.10	10,14,20,22	0
1	GYC	H	62	21/22	0.92	0.10	10,15,19,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.