



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2020 – 06:13 PM EST

PDB ID : 6MYB
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

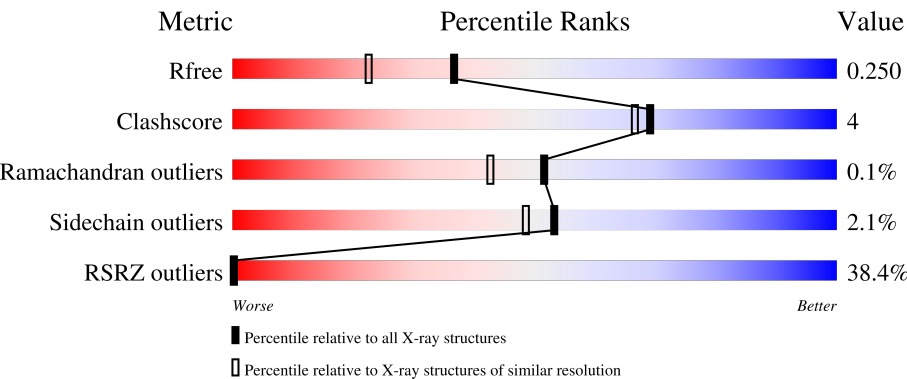
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

1 Overall quality at a glance i

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on 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	<div><div>26%</div><div><div></div><div>91%</div><div>6%</div><div>.</div></div></div>
1	B	223	<div><div>26%</div><div><div></div><div>87%</div><div>9%</div><div>..</div></div></div>
1	C	223	<div><div>28%</div><div><div></div><div>92%</div><div>.</div><div>..</div></div></div>
1	D	223	<div><div>44%</div><div><div></div><div>89%</div><div>7%</div><div>..</div></div></div>
1	E	223	<div><div>48%</div><div><div></div><div>84%</div><div>11%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	223	<div><div></div><div>50%</div><div></div><div>89%</div><div></div><div>7%</div><div></div><div>• •</div></div>
1	G	223	<div><div></div><div>35%</div><div></div><div>81%</div><div></div><div>15%</div><div></div><div>• •</div></div>
1	H	223	<div><div></div><div>39%</div><div></div><div>84%</div><div></div><div>13%</div><div></div><div>•</div></div>

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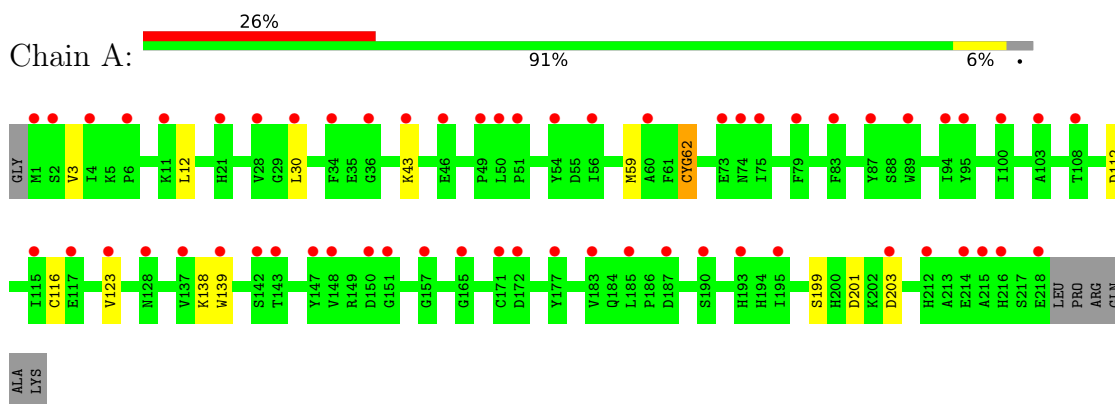
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	96	Total 96	O 96	0	0
2	H	108	Total 108	O 108	0	0

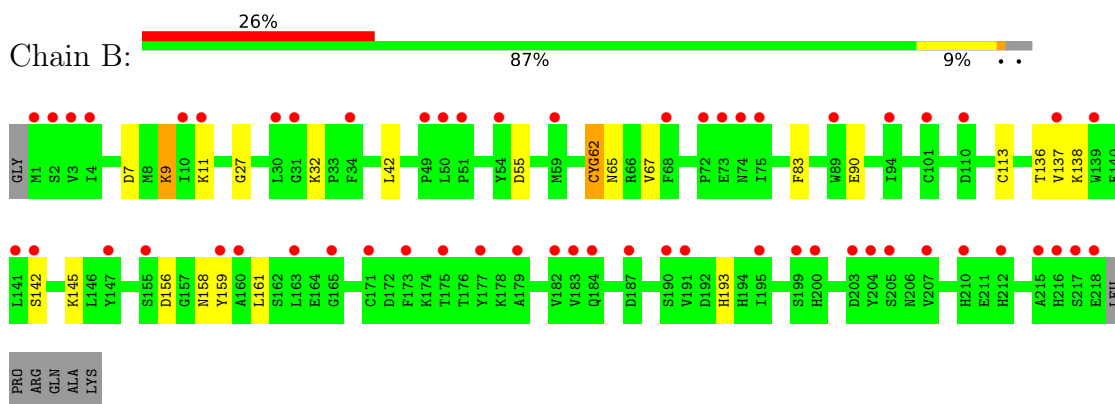
3 Residue-property plots [i](#)

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.

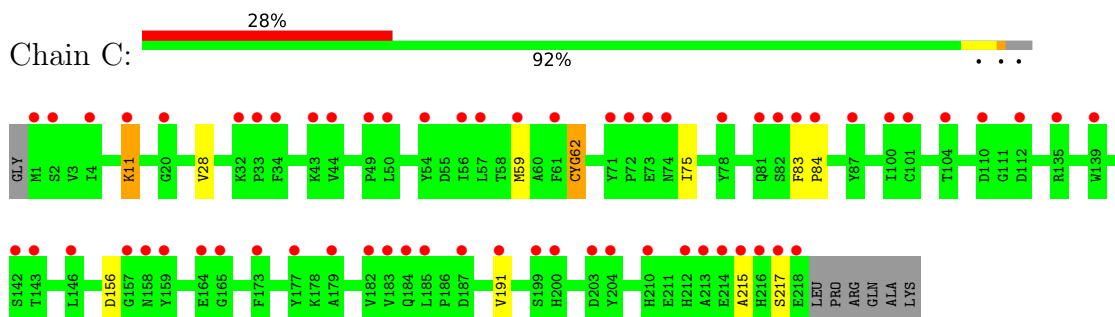
• Molecule 1: Photoswitchable protein Tetrdon



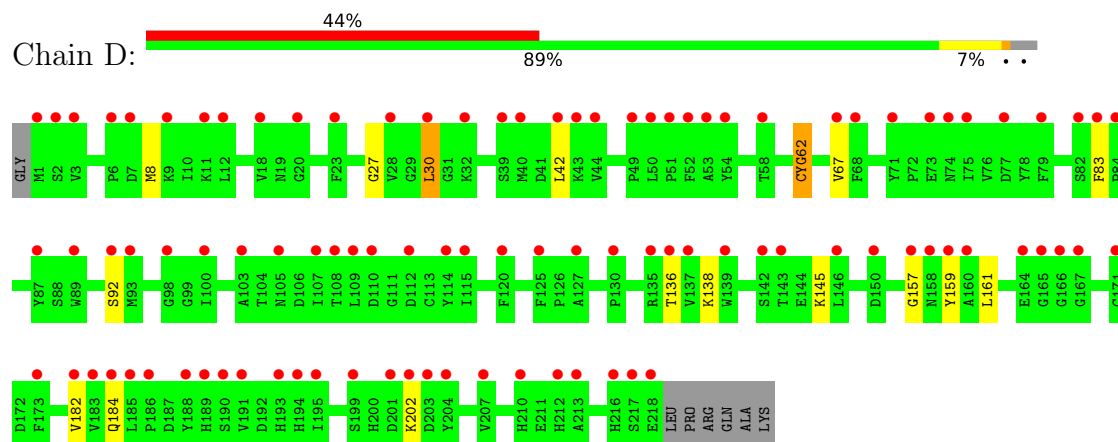
• Molecule 1: Photoswitchable protein Tetrdon



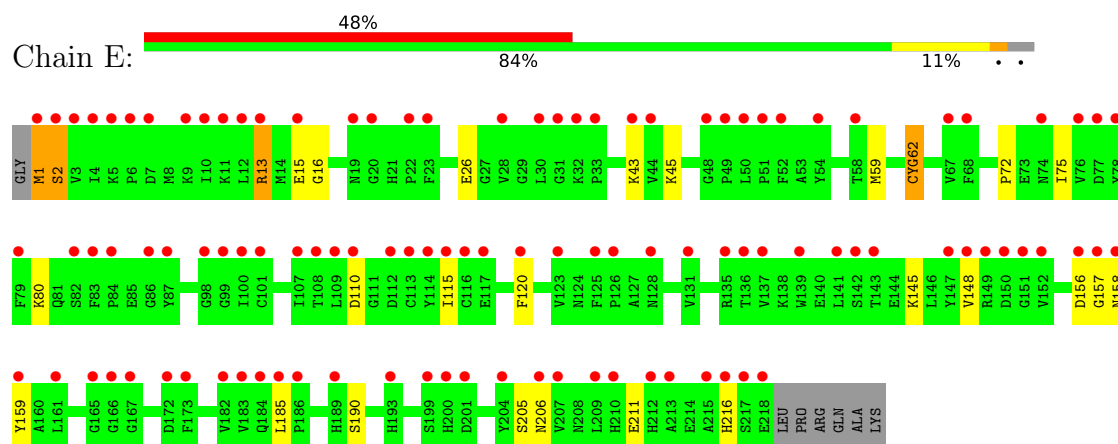
• Molecule 1: Photoswitchable protein Tetrdon



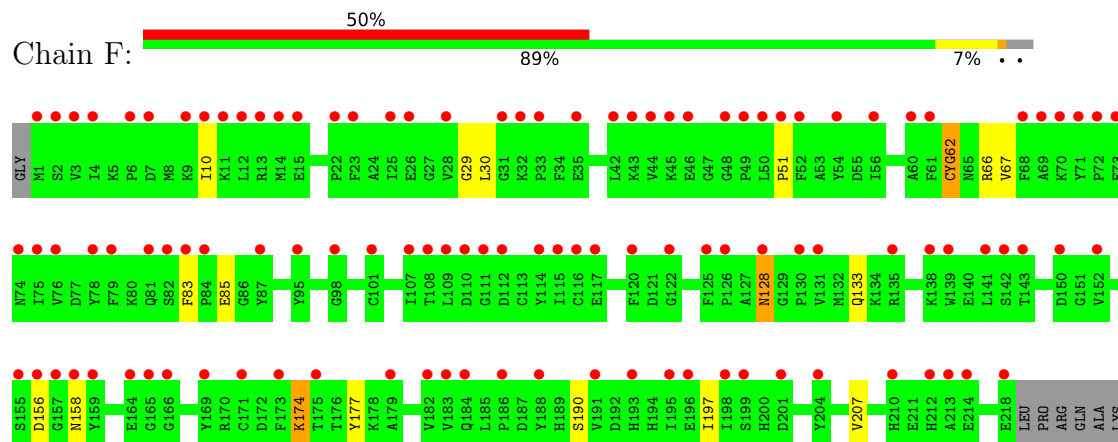
- Molecule 1: Photoswitchable protein Tetrdon



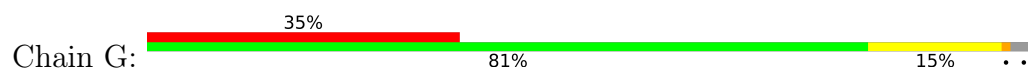
- Molecule 1: Photoswitchable protein Tetrdon

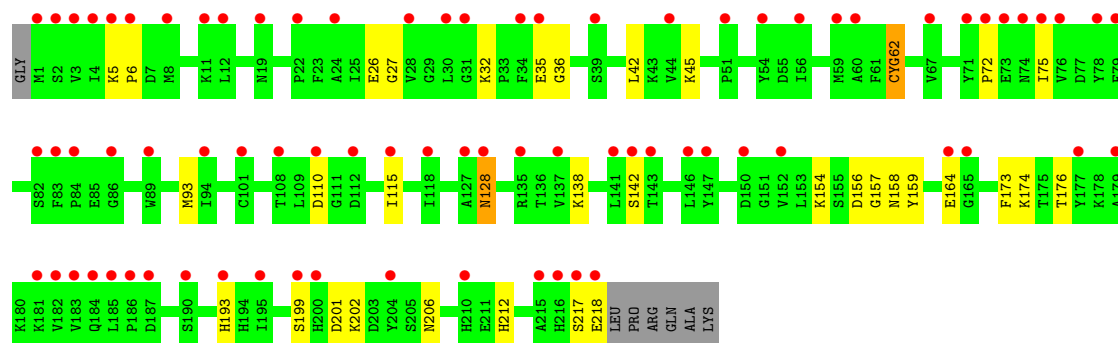


- Molecule 1: Photoswitchable protein Tetrdon

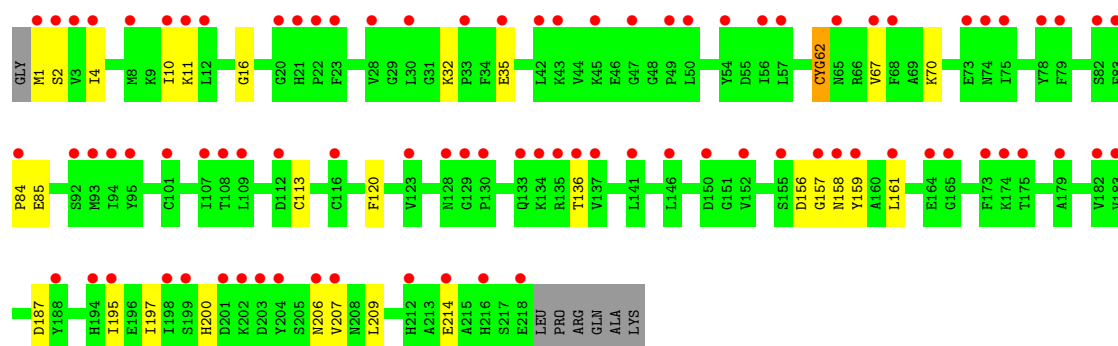
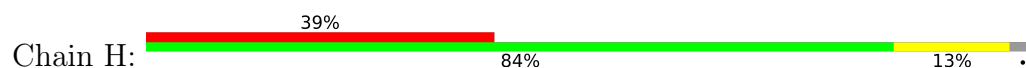


- Molecule 1: Photoswitchable protein Tetrdon





• 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) 85.8 (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 0.199 , 0.250	Depositor DCC
R_{free} test set	5905 reflections (5.05%)	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)	0.32 , 55.2	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	0.39	0/1757	0.60	0/2369
1	B	0.43	0/1763	0.62	0/2377
1	C	0.40	0/1757	0.59	0/2369
1	D	0.38	0/1757	0.57	0/2369
1	E	0.39	0/1757	0.58	0/2369
1	F	0.36	0/1757	0.56	0/2369
1	G	0.42	0/1763	0.62	0/2377
1	H	0.44	0/1757	0.62	0/2369
All	All	0.40	0/14068	0.60	0/18968

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 [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	1667	11	0
1	B	1738	0	1672	15	0
1	C	1735	0	1667	6	0
1	D	1735	0	1667	10	0
1	E	1735	0	1667	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1735	0	1667	10	0
1	G	1738	0	1672	22	0
1	H	1735	0	1667	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	2	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	13346	100	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 (100) 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:B:145:LYS:NZ	2:B:301:HOH:O	2.26	0.65
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:HD1	1:B:62:GYC:O2	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:199:SER:HB2	1:G:201:ASP:HA	1.85	0.57
1:F:62:GYC:HD1	1:F:62:GYC:O2	2.08	0.54
1:B:142[B]:SER:OG	1:B:193:HIS:HB2	2.07	0.54
1:D:62:GYC:HD1	1:D:62:GYC:O2	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:A:59:MET:HE2	1:A:139:TRP:CE2	2.45	0.52
1:B:137:VAL:HG12	1:B:138:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:145:LYS:NZ	2:E:302:HOH:O	2.28	0.51
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:A:59:MET:HE2	1:A:139:TRP:CD2	2.46	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:HD1	1:G:62:GYC:O2	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:A:138:LYS:NZ	1:G:164:GLU:OE1	2.35	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:HE2	1:G:202:LYS:HB3	1.62	0.47
1:G:93:MET:HG2	1:G:173:PHE:CE1	2.51	0.46
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:G:110:ASP:HB3	1:G:115:ILE:CD1	2.47	0.45
1:A:199:SER:CB	1:G:201:ASP:HA	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
1:C:11:LYS:HG3	1:C:28:VAL:HG12	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:H:158:ASN:OD1	2.51	0.42
1:E:80:LYS:NZ	2:E:312:HOH:O	2.49	0.42
1:G:128:ASN:H	1:G:128:ASN:ND2	2.16	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: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:B:142[B]:SER:HB2	1:B:159:TYR:CD1	2.56	0.40
1:B:27:GLY:HA3	1:B:42:LEU:HD23	2.03	0.40
1:E:190:SER:HB2	1:E:216:HIS:CE1	2.56	0.40
1:E:72:PRO:HD2	1:E:75:ILE:HD12	2.02	0.40
1:A:43:LYS:NZ	2:A:306:HOH:O	2.40	0.40
1:B:9:LYS:HD2	1:B:9:LYS:N	2.36	0.40
1:F:10:ILE:N	1:F:29:GLY:O	2.50	0.40
1:A:12:LEU:HB3	1:A:116:CYS:HB2	2.02	0.40

There are no symmetry-related clashes.

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	213/223 (96%)	210 (99%)	3 (1%)	0	100	100
1	B	214/223 (96%)	212 (99%)	2 (1%)	0	100	100
1	C	213/223 (96%)	213 (100%)	0	0	100	100
1	D	213/223 (96%)	211 (99%)	2 (1%)	0	100	100
1	E	213/223 (96%)	210 (99%)	2 (1%)	1 (0%)	29	18
1	F	213/223 (96%)	210 (99%)	3 (1%)	0	100	100
1	G	214/223 (96%)	211 (99%)	3 (1%)	0	100	100
1	H	213/223 (96%)	211 (99%)	2 (1%)	0	100	100
All	All	1706/1784 (96%)	1688 (99%)	17 (1%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	SER

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	185/190 (97%)	182 (98%)	3 (2%)	62	60
1	B	186/190 (98%)	183 (98%)	3 (2%)	62	60
1	C	185/190 (97%)	182 (98%)	3 (2%)	62	60
1	D	185/190 (97%)	181 (98%)	4 (2%)	52	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	185/190 (97%)	179 (97%)	6 (3%)	39	30
1	F	185/190 (97%)	179 (97%)	6 (3%)	39	30
1	G	186/190 (98%)	183 (98%)	3 (2%)	62	60
1	H	185/190 (97%)	182 (98%)	3 (2%)	62	60
All	All	1482/1520 (98%)	1451 (98%)	31 (2%)	53	48

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	30	LEU
1	A	203	ASP
1	B	9	LYS
1	B	156	ASP
1	B	158	ASN
1	C	11	LYS
1	C	59	MET
1	C	156	ASP
1	D	30	LEU
1	D	92	SER
1	D	138	LYS
1	D	202	LYS
1	E	1	MET
1	E	13	ARG
1	E	59	MET
1	E	156	ASP
1	E	158	ASN
1	E	211	GLU
1	F	30	LEU
1	F	128	ASN
1	F	156	ASP
1	F	158	ASN
1	F	174	LYS
1	F	190	SER
1	G	128	ASN
1	G	138	LYS
1	G	158	ASN
1	H	1	MET
1	H	67	VAL
1	H	156	ASP

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

Mol	Chain	Res	Type
1	F	128	ASN
1	G	128	ASN

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	C	62	1	22,22,23	2.62	7 (31%)	26,30,32	3.67	14 (53%)
1	GYC	E	62	1	22,22,23	2.79	6 (27%)	26,30,32	3.48	10 (38%)
1	GYC	A	62	1	22,22,23	2.66	6 (27%)	26,30,32	3.27	8 (30%)
1	GYC	G	62	1	22,22,23	2.81	7 (31%)	26,30,32	3.84	10 (38%)
1	GYC	H	62	1	22,22,23	2.80	6 (27%)	26,30,32	3.49	10 (38%)
1	GYC	D	62	1	22,22,23	2.91	6 (27%)	26,30,32	3.18	9 (34%)
1	GYC	F	62	1	22,22,23	2.70	7 (31%)	26,30,32	3.26	8 (30%)
1	GYC	B	62	1	22,22,23	2.46	7 (31%)	26,30,32	3.67	11 (42%)

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	C	62	1	-	4/9/29/30	0/2/2/2
1	GYC	E	62	1	-	3/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYC	A	62	1	-	3/9/29/30	0/2/2/2
1	GYC	G	62	1	-	4/9/29/30	0/2/2/2
1	GYC	H	62	1	-	3/9/29/30	0/2/2/2
1	GYC	D	62	1	-	3/9/29/30	0/2/2/2
1	GYC	F	62	1	-	3/9/29/30	0/2/2/2
1	GYC	B	62	1	-	3/9/29/30	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	62	GYC	CA2-C2	8.89	1.57	1.48
1	D	62	GYC	CA2-C2	8.82	1.57	1.48
1	H	62	GYC	CA2-C2	8.42	1.56	1.48
1	E	62	GYC	CA2-C2	7.90	1.56	1.48
1	A	62	GYC	CA2-C2	7.81	1.56	1.48
1	F	62	GYC	CA2-C2	7.48	1.56	1.48
1	C	62	GYC	CA2-C2	7.14	1.55	1.48
1	B	62	GYC	CA2-C2	6.38	1.54	1.48
1	F	62	GYC	C1-N2	6.13	1.41	1.32
1	E	62	GYC	C1-N2	6.10	1.41	1.32
1	D	62	GYC	C1-N2	5.98	1.41	1.32
1	A	62	GYC	C1-N2	5.86	1.40	1.32
1	C	62	GYC	C1-N2	5.59	1.40	1.32
1	H	62	GYC	C1-N2	5.54	1.40	1.32
1	G	62	GYC	C1-N2	5.34	1.40	1.32
1	H	62	GYC	C1-N3	5.08	1.45	1.37
1	B	62	GYC	C1-N3	5.01	1.45	1.37
1	E	62	GYC	C1-N3	4.86	1.45	1.37
1	G	62	GYC	C1-N3	4.73	1.45	1.37
1	D	62	GYC	C1-N3	4.73	1.45	1.37
1	A	62	GYC	C1-N3	4.61	1.44	1.37
1	B	62	GYC	C1-N2	4.45	1.38	1.32
1	C	62	GYC	C1-N3	4.41	1.44	1.37
1	E	62	GYC	C2-N3	4.19	1.49	1.39
1	F	62	GYC	C1-N3	4.18	1.44	1.37
1	D	62	GYC	C2-N3	4.10	1.49	1.39
1	C	62	GYC	C2-N3	4.00	1.49	1.39
1	F	62	GYC	C2-N3	3.97	1.49	1.39
1	C	62	GYC	CB2-CA2	-3.96	1.31	1.35
1	G	62	GYC	C2-N3	3.89	1.49	1.39
1	B	62	GYC	C2-N3	3.86	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	GYC	CB2-CA2	-3.76	1.32	1.35
1	H	62	GYC	C2-N3	3.71	1.48	1.39
1	A	62	GYC	C2-N3	3.58	1.48	1.39
1	F	62	GYC	CG2-CB2	3.40	1.53	1.46
1	E	62	GYC	CG2-CB2	3.25	1.53	1.46
1	H	62	GYC	CB2-CA2	-3.15	1.32	1.35
1	B	62	GYC	CB2-CA2	-3.04	1.32	1.35
1	A	62	GYC	CB2-CA2	-3.03	1.32	1.35
1	H	62	GYC	CG2-CB2	3.03	1.52	1.46
1	D	62	GYC	CG2-CB2	2.86	1.52	1.46
1	G	62	GYC	CG2-CB2	2.83	1.52	1.46
1	E	62	GYC	CB2-CA2	-2.77	1.32	1.35
1	G	62	GYC	CB2-CA2	-2.73	1.32	1.35
1	B	62	GYC	CG2-CB2	2.72	1.52	1.46
1	F	62	GYC	CB2-CA2	-2.62	1.32	1.35
1	C	62	GYC	CG2-CB2	2.40	1.51	1.46
1	B	62	GYC	O2-C2	-2.32	1.18	1.23
1	C	62	GYC	O2-C2	-2.31	1.18	1.23
1	F	62	GYC	O2-C2	-2.30	1.18	1.23
1	A	62	GYC	CG2-CB2	2.07	1.50	1.46
1	G	62	GYC	O2-C2	-2.04	1.18	1.23

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	62	GYC	CB2-CA2-C2	11.93	136.51	122.28
1	B	62	GYC	CB2-CA2-C2	11.08	135.50	122.28
1	H	62	GYC	CB2-CA2-C2	11.04	135.45	122.28
1	C	62	GYC	CB2-CA2-C2	10.59	134.91	122.28
1	A	62	GYC	CB2-CA2-C2	10.51	134.82	122.28
1	D	62	GYC	CB2-CA2-C2	10.41	134.70	122.28
1	E	62	GYC	CB2-CA2-C2	10.24	134.50	122.28
1	F	62	GYC	CB2-CA2-C2	9.71	133.87	122.28
1	H	62	GYC	CB2-CA2-N2	-8.21	117.44	128.83
1	G	62	GYC	CB2-CA2-N2	-8.13	117.55	128.83
1	B	62	GYC	CB2-CA2-N2	-7.85	117.94	128.83
1	C	62	GYC	CB2-CA2-N2	-7.78	118.03	128.83
1	D	62	GYC	CB2-CA2-N2	-7.58	118.31	128.83
1	A	62	GYC	CB2-CA2-N2	-7.58	118.32	128.83
1	E	62	GYC	CB2-CA2-N2	-6.85	119.33	128.83
1	E	62	GYC	CA2-C2-N3	6.82	106.59	103.37
1	F	62	GYC	CA2-C2-N3	6.48	106.43	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	62	GYC	CB2-CA2-N2	-6.32	120.06	128.83
1	C	62	GYC	C2-N3-C1	-6.31	104.77	107.97
1	E	62	GYC	C2-N3-C1	-6.31	104.77	107.97
1	H	62	GYC	C2-N3-C1	-6.29	104.78	107.97
1	B	62	GYC	C2-N3-C1	-5.77	105.04	107.97
1	G	62	GYC	CA2-N2-C1	5.71	109.98	105.77
1	B	62	GYC	CA2-C2-N3	5.68	106.06	103.37
1	G	62	GYC	CA2-C2-N3	5.58	106.01	103.37
1	C	62	GYC	CA2-C2-N3	5.52	105.98	103.37
1	B	62	GYC	CA2-N2-C1	5.48	109.81	105.77
1	H	62	GYC	CA2-C2-N3	5.35	105.90	103.37
1	G	62	GYC	C2-N3-C1	-5.30	105.28	107.97
1	F	62	GYC	C2-N3-C1	-5.29	105.29	107.97
1	E	62	GYC	CA2-N2-C1	4.96	109.43	105.77
1	F	62	GYC	CA2-N2-C1	4.88	109.37	105.77
1	A	62	GYC	CA2-N2-C1	4.86	109.36	105.77
1	A	62	GYC	CA2-C2-N3	4.82	105.65	103.37
1	D	62	GYC	CA2-N2-C1	4.70	109.23	105.77
1	G	62	GYC	O-C-CA3	-4.33	113.31	126.39
1	C	62	GYC	O2-C2-CA2	-4.29	128.55	130.96
1	G	62	GYC	C2-CA2-N2	-4.28	105.93	108.93
1	A	62	GYC	C2-N3-C1	-4.23	105.82	107.97
1	D	62	GYC	C2-N3-C1	-4.11	105.89	107.97
1	F	62	GYC	C2-CA2-N2	-4.09	106.07	108.93
1	G	62	GYC	CA1-CB1-SG1	-3.98	105.87	114.44
1	E	62	GYC	C2-CA2-N2	-3.94	106.17	108.93
1	C	62	GYC	CA2-N2-C1	3.89	108.64	105.77
1	D	62	GYC	CA2-C2-N3	3.87	105.20	103.37
1	H	62	GYC	CA2-N2-C1	3.75	108.54	105.77
1	C	62	GYC	CA3-N3-C2	3.60	132.06	123.80
1	B	62	GYC	C2-CA2-N2	-3.47	106.50	108.93
1	B	62	GYC	CA1-CB1-SG1	-3.43	107.04	114.44
1	C	62	GYC	CA3-N3-C1	-3.33	123.17	127.16
1	G	62	GYC	CA3-N3-C2	3.31	131.39	123.80
1	G	62	GYC	CA3-N3-C1	-3.20	123.32	127.16
1	H	62	GYC	N3-C1-N2	3.19	113.66	111.45
1	F	62	GYC	O-C-CA3	-3.16	116.85	126.39
1	D	62	GYC	O-C-CA3	-3.08	117.10	126.39
1	A	62	GYC	O-C-CA3	-3.06	117.16	126.39
1	C	62	GYC	N3-C1-N2	3.04	113.56	111.45
1	A	62	GYC	C2-CA2-N2	-3.01	106.82	108.93
1	B	62	GYC	CA3-N3-C2	2.97	130.61	123.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	GYC	O-C-CA3	-2.88	117.69	126.39
1	D	62	GYC	C2-CA2-N2	-2.78	106.98	108.93
1	B	62	GYC	O2-C2-CA2	-2.78	129.40	130.96
1	D	62	GYC	CA1-CB1-SG1	-2.75	108.51	114.44
1	C	62	GYC	C2-CA2-N2	-2.71	107.03	108.93
1	H	62	GYC	O-C-CA3	-2.67	118.32	126.39
1	B	62	GYC	O-C-CA3	-2.64	118.42	126.39
1	H	62	GYC	C2-CA2-N2	-2.60	107.11	108.93
1	C	62	GYC	CA1-CB1-SG1	-2.56	108.92	114.44
1	E	62	GYC	O2-C2-CA2	-2.55	129.53	130.96
1	E	62	GYC	CA1-CB1-SG1	-2.53	108.99	114.44
1	H	62	GYC	CA1-CB1-SG1	-2.46	109.14	114.44
1	A	62	GYC	CD2-CG2-CD1	2.44	121.25	117.64
1	B	62	GYC	CA3-N3-C1	-2.42	124.26	127.16
1	E	62	GYC	N3-C1-N2	2.28	113.03	111.45
1	H	62	GYC	CA3-N3-C2	2.26	128.98	123.80
1	C	62	GYC	CD2-CG2-CD1	2.24	120.95	117.64
1	F	62	GYC	CA3-N3-C2	2.19	128.82	123.80
1	E	62	GYC	O-C-CA3	-2.15	119.91	126.39
1	C	62	GYC	CE2-CD2-CG2	-2.01	118.63	121.25
1	D	62	GYC	CA3-N3-C2	2.00	128.39	123.80

There are no chirality outliers.

All (26) torsion outliers are listed below:

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

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

There are no ring outliers.

8 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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%)	1.74	59 (27%) 0 0	10, 19, 33, 64	0
1	B	215/223 (96%)	1.78	57 (26%) 0 0	7, 16, 30, 59	0
1	C	215/223 (96%)	1.81	63 (29%) 0 0	8, 18, 36, 65	0
1	D	215/223 (96%)	2.13	98 (45%) 0 0	12, 24, 40, 75	1 (0%)
1	E	215/223 (96%)	2.22	107 (49%) 0 0	13, 25, 44, 77	0
1	F	215/223 (96%)	2.34	111 (51%) 0 0	12, 27, 44, 87	1 (0%)
1	G	215/223 (96%)	1.97	78 (36%) 0 0	10, 20, 35, 76	0
1	H	215/223 (96%)	1.95	87 (40%) 0 0	11, 20, 33, 70	1 (0%)
All	All	1720/1784 (96%)	1.99	660 (38%) 0 0	7, 21, 39, 87	3 (0%)

All (660) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	19.3
1	B	1	MET	19.1
1	G	1	MET	17.9
1	H	1	MET	13.4
1	A	1	MET	13.2
1	F	1	MET	13.2
1	E	1	MET	12.4
1	B	2	SER	11.6
1	G	218	GLU	11.5
1	B	218	GLU	10.9
1	F	82	SER	9.4
1	A	2	SER	8.6
1	E	165	GLY	8.3
1	D	204	TYR	8.3
1	G	217	SER	8.2
1	D	1	MET	8.2

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Mol	Chain	Res	Type	RSRZ
1	C	2	SER	8.0
1	E	2	SER	8.0
1	D	183	VAL	7.7
1	F	75	ILE	7.2
1	C	84	PRO	7.2
1	E	218	GLU	7.0
1	E	68	PHE	7.0
1	G	84	PRO	6.9
1	F	68	PHE	6.8
1	C	217	SER	6.6
1	D	49	PRO	6.6
1	E	115	ILE	6.6
1	F	110	ASP	6.4
1	D	74	ASN	6.4
1	E	33	PRO	6.4
1	B	212	HIS	6.3
1	D	3	VAL	6.1
1	F	183	VAL	6.0
1	F	2	SER	6.0
1	D	130	PRO	6.0
1	F	141	LEU	5.9
1	D	43	LYS	5.7
1	E	82	SER	5.6
1	F	165	GLY	5.5
1	H	183	VAL	5.5
1	F	204	TYR	5.4
1	E	204	TYR	5.4
1	G	2	SER	5.4
1	A	218	GLU	5.3
1	E	74	ASN	5.3
1	A	165	GLY	5.3
1	G	165	GLY	5.3
1	C	215	ALA	5.3
1	G	73	GLU	5.2
1	F	3	VAL	5.2
1	F	83	PHE	5.2
1	F	218	GLU	5.1
1	F	112	ASP	5.1
1	E	44	VAL	5.1
1	F	74	ASN	5.0
1	F	150	ASP	4.9
1	F	199	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	68	PHE	4.9
1	A	115	ILE	4.9
1	E	79	PHE	4.9
1	D	165	GLY	4.9
1	C	34	PHE	4.8
1	H	54	TYR	4.8
1	H	45	LYS	4.8
1	E	98	GLY	4.7
1	F	84	PRO	4.7
1	B	75	ILE	4.7
1	E	3	VAL	4.7
1	F	69	ALA	4.7
1	E	184	GLN	4.7
1	E	183	VAL	4.7
1	D	51	PRO	4.7
1	C	74	ASN	4.6
1	A	150	ASP	4.6
1	C	213	ALA	4.6
1	E	11	LYS	4.6
1	E	114	TYR	4.6
1	D	184	GLN	4.5
1	H	150	ASP	4.5
1	A	74	ASN	4.5
1	B	165	GLY	4.4
1	F	152	VAL	4.4
1	E	49	PRO	4.4
1	G	183	VAL	4.4
1	C	179	ALA	4.3
1	G	184	GLN	4.3
1	D	216	HIS	4.3
1	F	212	HIS	4.3
1	B	217	SER	4.3
1	C	184	GLN	4.3
1	H	130	PRO	4.3
1	F	54	TYR	4.3
1	F	107	ILE	4.3
1	C	50	LEU	4.3
1	D	2	SER	4.3
1	D	218	GLU	4.3
1	H	11	LYS	4.2
1	E	150	ASP	4.2
1	H	43	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	H	84	PRO	4.2
1	F	182	VAL	4.2
1	F	43	LYS	4.2
1	E	78	TYR	4.2
1	G	30	LEU	4.2
1	G	141	LEU	4.2
1	C	212	HIS	4.1
1	A	30	LEU	4.1
1	H	4	ILE	4.1
1	E	6	PRO	4.1
1	G	51	PRO	4.1
1	E	110	ASP	4.1
1	F	210	HIS	4.0
1	D	202	LYS	4.0
1	G	216	HIS	4.0
1	F	135	ARG	4.0
1	G	186	PRO	4.0
1	F	71	TYR	4.0
1	D	108	THR	4.0
1	A	128	ASN	4.0
1	C	158	ASN	4.0
1	D	114	TYR	4.0
1	C	216	HIS	4.0
1	G	83	PHE	3.9
1	H	123	VAL	3.9
1	D	158	ASN	3.9
1	A	157	GLY	3.9
1	G	74	ASN	3.9
1	E	15	GLU	3.9
1	F	114	TYR	3.9
1	D	23	PHE	3.9
1	B	73	GLU	3.9
1	E	113	CYS	3.8
1	C	72	PRO	3.8
1	G	185	LEU	3.8
1	E	77	ASP	3.8
1	H	33	PRO	3.8
1	C	165	GLY	3.7
1	F	139	TRP	3.7
1	F	7	ASP	3.7
1	H	93	MET	3.7
1	C	33	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	42	LEU	3.7
1	D	159	TYR	3.7
1	E	43	LYS	3.7
1	H	50	LEU	3.6
1	D	54	TYR	3.6
1	E	161	LEU	3.6
1	B	173	PHE	3.6
1	C	182	VAL	3.6
1	F	158	ASN	3.6
1	H	49	PRO	3.6
1	G	31	GLY	3.6
1	H	94	ILE	3.6
1	A	50	LEU	3.6
1	G	79	PHE	3.6
1	B	31	GLY	3.6
1	B	200	HIS	3.6
1	B	30	LEU	3.6
1	E	52	PHE	3.5
1	B	10	ILE	3.5
1	C	71	TYR	3.5
1	B	3	VAL	3.5
1	A	187	ASP	3.5
1	F	51	PRO	3.5
1	D	207	VAL	3.4
1	G	128	ASN	3.4
1	F	201	ASP	3.4
1	H	30	LEU	3.4
1	A	139	TRP	3.4
1	H	21	HIS	3.4
1	D	82	SER	3.4
1	E	84	PRO	3.4
1	F	33	PRO	3.4
1	F	116	CYS	3.4
1	F	11	LYS	3.4
1	D	30	LEU	3.4
1	G	152	VAL	3.4
1	F	10	ILE	3.4
1	G	75	ILE	3.4
1	D	201	ASP	3.4
1	E	54	TYR	3.4
1	H	74	ASN	3.3
1	A	51	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	6	PRO	3.3
1	B	210	HIS	3.3
1	H	165	GLY	3.3
1	D	11	LYS	3.3
1	D	32	LYS	3.3
1	H	218	GLU	3.3
1	H	42	LEU	3.3
1	C	218	GLU	3.3
1	F	76	VAL	3.3
1	D	199	SER	3.3
1	H	136	THR	3.3
1	F	49	PRO	3.3
1	A	43	LYS	3.2
1	C	73	GLU	3.2
1	F	4	ILE	3.2
1	E	28	VAL	3.2
1	F	159	TYR	3.2
1	C	200	HIS	3.2
1	G	82	SER	3.2
1	H	82	SER	3.2
1	D	143	THR	3.2
1	A	123	VAL	3.2
1	B	191	VAL	3.2
1	E	152	VAL	3.2
1	B	205	SER	3.2
1	E	117	GLU	3.2
1	A	148	VAL	3.2
1	C	204	TYR	3.2
1	D	217	SER	3.2
1	E	5	LYS	3.2
1	E	51	PRO	3.2
1	B	34	PHE	3.2
1	D	110	ASP	3.2
1	D	135	ARG	3.2
1	H	135	ARG	3.2
1	D	84	PRO	3.2
1	D	157	GLY	3.2
1	C	43	LYS	3.2
1	E	30	LEU	3.1
1	F	169	TYR	3.1
1	H	2	SER	3.1
1	B	101	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	83	PHE	3.1
1	A	21	HIS	3.1
1	B	141	LEU	3.1
1	G	187	ASP	3.1
1	F	108	THR	3.1
1	A	212	HIS	3.1
1	F	173	PHE	3.1
1	F	166	GLY	3.1
1	H	206	ASN	3.1
1	D	71	TYR	3.1
1	D	50	LEU	3.1
1	F	120	PHE	3.1
1	E	4	ILE	3.1
1	G	101	CYS	3.1
1	G	118	ILE	3.1
1	E	201	ASP	3.1
1	C	78	TYR	3.1
1	F	15	GLU	3.1
1	E	217	SER	3.0
1	H	195	ILE	3.0
1	F	128	ASN	3.0
1	D	77	ASP	3.0
1	H	204	TYR	3.0
1	B	72	PRO	3.0
1	B	190	SER	3.0
1	B	183	VAL	3.0
1	H	35	GLU	3.0
1	C	187	ASP	3.0
1	D	139	TRP	3.0
1	G	24	ALA	3.0
1	G	72	PRO	3.0
1	B	4	ILE	3.0
1	B	139	TRP	3.0
1	B	177	TYR	3.0
1	G	11	LYS	3.0
1	A	190	SER	3.0
1	G	60	ALA	3.0
1	G	215	ALA	3.0
1	H	134	LYS	3.0
1	D	67	VAL	3.0
1	C	4	ILE	2.9
1	D	83	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	206	ASN	2.9
1	A	73	GLU	2.9
1	A	151	GLY	2.9
1	G	108	THR	2.9
1	D	112	ASP	2.9
1	H	79	PHE	2.9
1	F	35	GLU	2.9
1	F	155	SER	2.9
1	H	92	SER	2.9
1	E	189	HIS	2.9
1	F	14	MET	2.9
1	G	204	TYR	2.9
1	C	183	VAL	2.9
1	E	109	LEU	2.9
1	F	12	LEU	2.9
1	H	146	LEU	2.9
1	D	98	GLY	2.9
1	E	48	GLY	2.9
1	H	20	GLY	2.9
1	D	7	ASP	2.9
1	A	117	GLU	2.9
1	G	4	ILE	2.9
1	G	59	MET	2.9
1	H	95	TYR	2.9
1	A	143	THR	2.9
1	H	194	HIS	2.9
1	F	157	GLY	2.9
1	H	129	GLY	2.9
1	D	193	HIS	2.8
1	E	212	HIS	2.8
1	B	187	ASP	2.8
1	E	13	ARG	2.8
1	F	46	GLU	2.8
1	H	116	CYS	2.8
1	F	193	HIS	2.8
1	C	203	ASP	2.8
1	F	32	LYS	2.8
1	F	188	TYR	2.8
1	F	164	GLU	2.8
1	E	12	LEU	2.8
1	F	171	CYS	2.8
1	B	49	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	186	PRO	2.8
1	D	28	VAL	2.8
1	E	131	VAL	2.8
1	D	142	SER	2.8
1	E	7	ASP	2.8
1	G	150	ASP	2.8
1	H	201	ASP	2.8
1	A	95	TYR	2.8
1	F	117	GLU	2.8
1	G	137	VAL	2.8
1	A	60	ALA	2.8
1	H	109	LEU	2.8
1	E	156	ASP	2.8
1	D	171	CYS	2.8
1	A	147	TYR	2.8
1	A	215	ALA	2.7
1	F	214	GLU	2.8
1	G	179	ALA	2.7
1	H	108	THR	2.7
1	D	150	ASP	2.7
1	G	56	ILE	2.7
1	G	115	ILE	2.7
1	H	75	ILE	2.7
1	B	59	MET	2.7
1	H	68	PHE	2.7
1	D	20	GLY	2.7
1	H	101	CYS	2.7
1	E	185	LEU	2.7
1	F	198	ILE	2.7
1	E	23	PHE	2.7
1	H	83	PHE	2.7
1	E	32	LYS	2.7
1	B	74	ASN	2.7
1	H	199	SER	2.7
1	H	141	LEU	2.7
1	E	20	GLY	2.7
1	E	86	GLY	2.7
1	F	184	GLN	2.7
1	B	11	LYS	2.7
1	E	136	THR	2.7
1	F	9	LYS	2.7
1	A	34	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	44	VAL	2.7
1	E	123	VAL	2.7
1	E	137	VAL	2.7
1	A	203	ASP	2.7
1	D	164	GLU	2.7
1	F	42	LEU	2.7
1	E	149	ARG	2.7
1	E	199	SER	2.7
1	C	214	GLU	2.7
1	H	203	ASP	2.7
1	A	28	VAL	2.7
1	B	147	TYR	2.7
1	B	159	TYR	2.7
1	D	109	LEU	2.7
1	F	73	GLU	2.7
1	G	143	THR	2.7
1	D	100	ILE	2.6
1	D	173	PHE	2.6
1	B	207	VAL	2.6
1	E	207	VAL	2.6
1	F	44	VAL	2.6
1	H	28	VAL	2.6
1	H	128	ASN	2.6
1	B	184	GLN	2.6
1	D	190	SER	2.6
1	D	107	ILE	2.6
1	H	47	GLY	2.6
1	D	40	MET	2.6
1	F	79	PHE	2.6
1	G	5	LYS	2.6
1	A	108	THR	2.6
1	C	143	THR	2.6
1	C	185	LEU	2.6
1	D	146	LEU	2.6
1	E	209	LEU	2.6
1	B	204	TYR	2.6
1	F	109	LEU	2.6
1	G	146	LEU	2.6
1	F	156	ASP	2.6
1	C	59	MET	2.6
1	G	39	SER	2.6
1	D	44	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	136	THR	2.6
1	H	3	VAL	2.6
1	A	193	HIS	2.6
1	D	212	HIS	2.6
1	B	199	SER	2.6
1	D	195	ILE	2.6
1	D	125	PHE	2.5
1	E	213	ALA	2.5
1	G	190	SER	2.5
1	A	89	TRP	2.5
1	E	151	GLY	2.5
1	F	48	GLY	2.5
1	H	107	ILE	2.5
1	F	13	ARG	2.5
1	C	87	TYR	2.5
1	D	160	ALA	2.5
1	E	58	THR	2.5
1	H	207	VAL	2.5
1	D	213	ALA	2.5
1	F	101	CYS	2.5
1	C	11	LYS	2.5
1	C	54	TYR	2.5
1	E	9	LYS	2.5
1	G	12	LEU	2.5
1	C	104	THR	2.5
1	D	92	SER	2.5
1	H	10	ILE	2.5
1	D	182	VAL	2.5
1	C	177	TYR	2.5
1	E	50	LEU	2.5
1	F	26	GLU	2.5
1	B	195	ILE	2.5
1	F	115	ILE	2.5
1	G	89	TRP	2.5
1	C	20	GLY	2.5
1	G	28	VAL	2.5
1	H	216	HIS	2.5
1	D	203	ASP	2.5
1	E	112	ASP	2.5
1	D	185	LEU	2.5
1	E	120	PHE	2.5
1	A	6	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	94	ILE	2.4
1	G	200	HIS	2.4
1	G	210	HIS	2.4
1	H	179	ALA	2.4
1	C	191	VAL	2.4
1	D	188	TYR	2.4
1	F	87	TYR	2.4
1	H	202	LYS	2.4
1	C	210	HIS	2.4
1	E	108	THR	2.4
1	B	110	ASP	2.4
1	D	189	HIS	2.4
1	E	200	HIS	2.4
1	G	19	ASN	2.4
1	D	137	VAL	2.4
1	D	191	VAL	2.4
1	G	110	ASP	2.4
1	C	157	GLY	2.4
1	F	72	PRO	2.4
1	H	22	PRO	2.4
1	A	79	PHE	2.4
1	A	83	PHE	2.4
1	F	142	SER	2.4
1	B	94	ILE	2.4
1	B	137	VAL	2.4
1	E	158	ASN	2.4
1	G	182	VAL	2.4
1	B	89	TRP	2.4
1	C	61	PHE	2.4
1	F	23	PHE	2.4
1	G	34	PHE	2.4
1	B	160	ALA	2.4
1	A	171	CYS	2.4
1	A	4	ILE	2.4
1	D	115	ILE	2.4
1	G	3	VAL	2.4
1	G	142[A]	SER	2.3
1	B	163	LEU	2.3
1	A	54	TYR	2.3
1	A	177	TYR	2.3
1	F	125	PHE	2.3
1	H	159	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	173	PHE	2.3
1	B	216	HIS	2.3
1	D	210	HIS	2.3
1	H	158	ASN	2.3
1	E	139	TRP	2.3
1	G	112	ASP	2.3
1	A	100	ILE	2.3
1	G	22	PRO	2.3
1	B	182	VAL	2.3
1	E	148	VAL	2.3
1	G	76	VAL	2.3
1	H	56	ILE	2.3
1	D	127	ALA	2.3
1	F	213	ALA	2.3
1	H	175	THR	2.3
1	F	186	PRO	2.3
1	H	73	GLU	2.3
1	D	87	TYR	2.3
1	A	214	GLU	2.3
1	E	167	GLY	2.3
1	F	131	VAL	2.3
1	F	56	ILE	2.3
1	A	103	ALA	2.3
1	D	53	ALA	2.3
1	C	49	PRO	2.3
1	F	78	TYR	2.3
1	D	120	PHE	2.3
1	A	216	HIS	2.3
1	B	215	ALA	2.3
1	E	215	ALA	2.3
1	F	22	PRO	2.3
1	C	82	SER	2.3
1	C	112	ASP	2.3
1	G	71	TYR	2.2
1	G	78	TYR	2.2
1	H	78	TYR	2.2
1	C	83	PHE	2.2
1	E	173	PHE	2.2
1	C	81	GLN	2.2
1	H	164	GLU	2.2
1	E	182	VAL	2.2
1	F	138	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	67	VAL	2.2
1	C	56	ILE	2.2
1	C	142	SER	2.2
1	F	195	ILE	2.2
1	G	199	SER	2.2
1	E	172	ASP	2.2
1	E	141	LEU	2.2
1	G	193	HIS	2.2
1	A	36	GLY	2.2
1	F	111	GLY	2.2
1	G	86	GLY	2.2
1	G	54	TYR	2.2
1	F	52	PHE	2.2
1	E	128	ASN	2.2
1	D	89	TRP	2.2
1	A	87	TYR	2.2
1	B	54	TYR	2.2
1	E	147	TYR	2.2
1	G	177	TYR	2.2
1	B	203	ASP	2.2
1	C	173	PHE	2.2
1	C	199	SER	2.2
1	E	193	HIS	2.2
1	F	81	GLN	2.2
1	E	67	VAL	2.2
1	A	75	ILE	2.2
1	C	57	LEU	2.2
1	E	22	PRO	2.2
1	G	6	PRO	2.2
1	D	9	LYS	2.2
1	E	143	THR	2.2
1	E	76	VAL	2.2
1	A	195	ILE	2.2
1	A	49	PRO	2.2
1	H	133	GLN	2.2
1	E	210	HIS	2.2
1	F	175	THR	2.2
1	D	166	GLY	2.2
1	E	99	GLY	2.2
1	E	157	GLY	2.2
1	F	95	TYR	2.2
1	F	122	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	157	GLY	2.2
1	A	46	GLU	2.2
1	A	183	VAL	2.2
1	H	152	VAL	2.2
1	F	126	PRO	2.1
1	H	198	ILE	2.1
1	B	175	THR	2.1
1	C	135	ARG	2.1
1	F	50	LEU	2.1
1	H	214	GLU	2.1
1	A	11	LYS	2.1
1	F	45	LYS	2.1
1	F	179	ALA	2.1
1	G	127	ALA	2.1
1	H	174	LYS	2.1
1	G	147	TYR	2.1
1	B	142[A]	SER	2.1
1	H	155	SER	2.1
1	B	51	PRO	2.1
1	D	6	PRO	2.1
1	G	44	VAL	2.1
1	D	58	THR	2.1
1	D	105	ASN	2.1
1	E	19	ASN	2.1
1	E	107	ILE	2.1
1	F	25	ILE	2.1
1	G	181	LYS	2.1
1	H	112	ASP	2.1
1	B	179	ALA	2.1
1	D	103	ALA	2.1
1	C	159	TYR	2.1
1	D	39	SER	2.1
1	C	32	LYS	2.1
1	C	110	ASP	2.1
1	F	31	GLY	2.1
1	F	98	GLY	2.1
1	C	101	CYS	2.1
1	F	143	THR	2.1
1	F	60	ALA	2.1
1	H	57	LEU	2.1
1	G	135	ARG	2.1
1	F	70	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	216	HIS	2.1
1	A	172	ASP	2.1
1	D	186	PRO	2.1
1	E	31	GLY	2.1
1	E	166	GLY	2.1
1	D	73	GLU	2.1
1	F	61	PHE	2.1
1	F	196	GLU	2.1
1	B	155	SER	2.1
1	E	100	ILE	2.1
1	H	161	LEU	2.1
1	H	212	HIS	2.1
1	E	87	TYR	2.1
1	H	23	PHE	2.1
1	H	67	VAL	2.1
1	H	137	VAL	2.1
1	H	182	VAL	2.1
1	G	164	GLU	2.1
1	A	56	ILE	2.1
1	A	94	ILE	2.1
1	C	100	ILE	2.1
1	G	195	ILE	2.1
1	B	50	LEU	2.1
1	B	171	CYS	2.1
1	D	167	GLY	2.1
1	E	116	CYS	2.1
1	H	12	LEU	2.1
1	G	8	MET	2.0
1	E	159	TYR	2.0
1	G	35	GLU	2.0
1	H	65	ASN	2.0
1	A	137	VAL	2.0
1	D	18	VAL	2.0
1	E	125	PHE	2.0
1	F	191	VAL	2.0
1	E	126	PRO	2.0
1	F	130	PRO	2.0
1	E	135	ARG	2.0
1	E	101	CYS	2.0
1	D	93	MET	2.0
1	H	8	MET	2.0
1	D	194	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	188	TYR	2.0
1	F	28	VAL	2.0
1	B	68	PHE	2.0
1	D	52	PHE	2.0
1	D	79	PHE	2.0
1	C	139	TRP	2.0
1	A	185	LEU	2.0
1	C	146	LEU	2.0
1	D	12	LEU	2.0
1	D	75	ILE	2.0
1	E	10	ILE	2.0
1	A	142	SER	2.0
1	E	142	SER	2.0
1	C	164	GLU	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	0.79	0.24	15,19,22,25	0
1	GYC	E	62	21/22	0.80	0.26	17,20,22,25	0
1	GYC	F	62	21/22	0.81	0.23	17,22,26,29	0
1	GYC	G	62	21/22	0.86	0.21	10,15,18,19	0
1	GYC	C	62	21/22	0.86	0.20	10,14,20,22	0
1	GYC	A	62	21/22	0.86	0.22	11,14,19,20	0
1	GYC	H	62	21/22	0.88	0.20	10,15,19,20	0
1	GYC	B	62	21/22	0.89	0.20	6,12,17,20	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.