Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 03:33 PM JST

PDB ID	:	7CZ0
Title	:	Crystal structure of a thermostable green fluorescent protein (TGP) with a synthetic nanobody (Sb92)
Authors	:	Cai, H.; Yao, H.; Li, T.; Hutter, C.; Tang, Y.; Li, Y.; Seeger, M.; Li, D.
Deposited on	:	2020-09-06
Resolution	:	2.77 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:

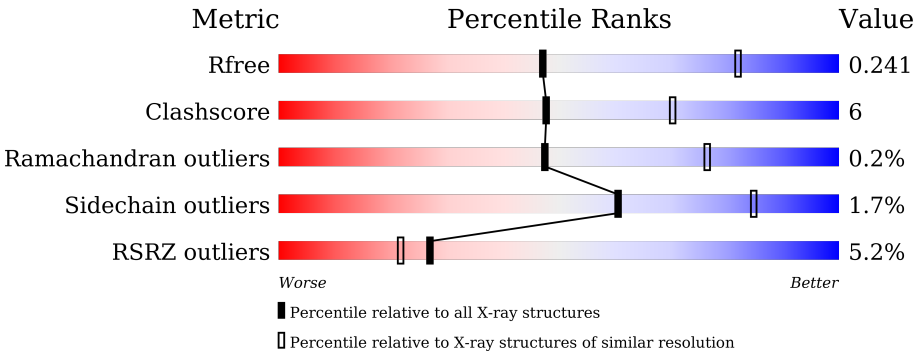
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 <=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	232	82% 10% 7%
1	B	232	81% 11% 7%
1	C	232	% 77% 16% 7%
1	D	232	82% 9% • 7%
2	E	144	5% 74% 8% 17%
2	F	144	3% 72% 11% 17%

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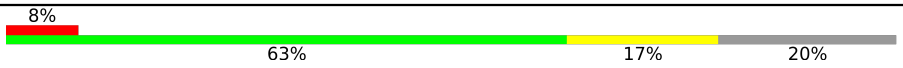
Mol	Chain	Length	Quality of chain
2	G	144	
2	H	144	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	302	-	-	-	X
3	GOL	B	306	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10620 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.

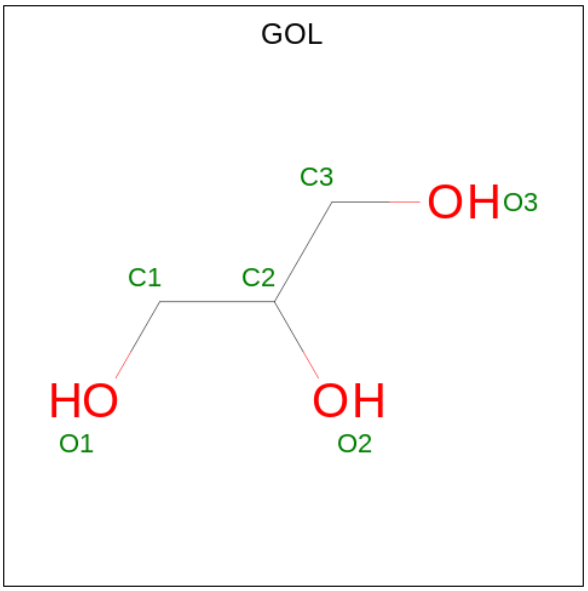
- Molecule 1 is a protein called Thermostable green fluorescent protein (TGP).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1756	1123	286	337	10			
1	B	216	Total	C	N	O	S	0	0	0
			1761	1126	287	338	10			
1	C	216	Total	C	N	O	S	0	0	0
			1761	1126	287	338	10			
1	D	215	Total	C	N	O	S	0	1	0
			1762	1128	287	337	10			

- Molecule 2 is a protein called Synthetic nanobody (Sybody) 92 recognizing the thermostable green fluorescent protein (TGP).

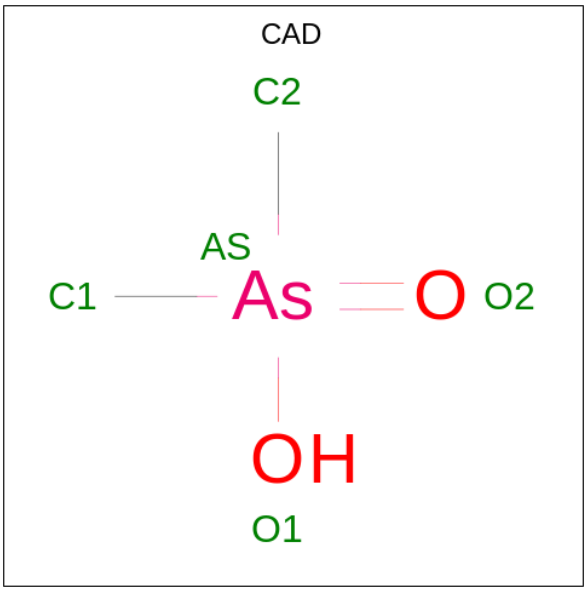
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	119	Total	C	N	O	S	0	0	0
			911	566	164	177	4			
2	F	119	Total	C	N	O	S	0	0	0
			911	566	164	177	4			
2	G	115	Total	C	N	O	S	0	1	0
			889	555	162	168	4			
2	H	109	Total	C	N	O	S	0	0	0
			785	491	138	152	4			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



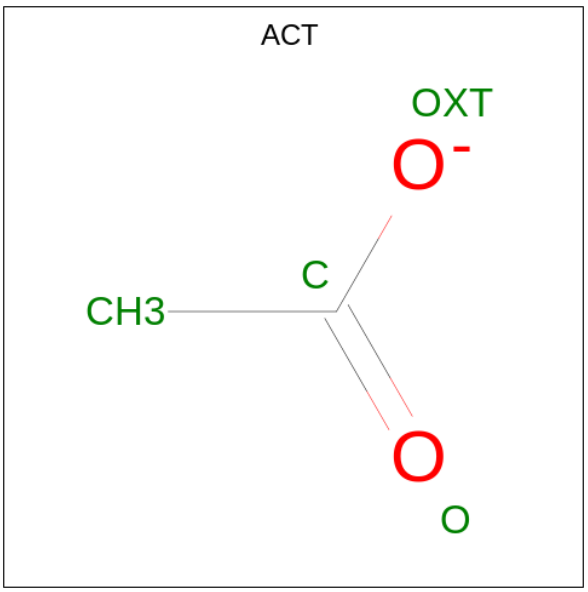
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



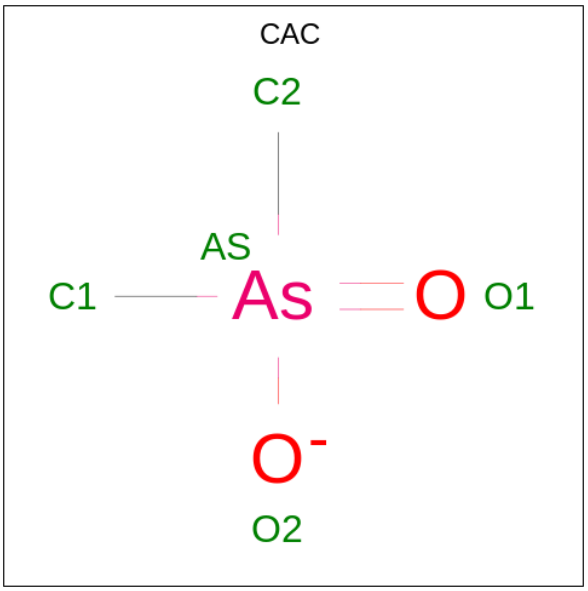
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



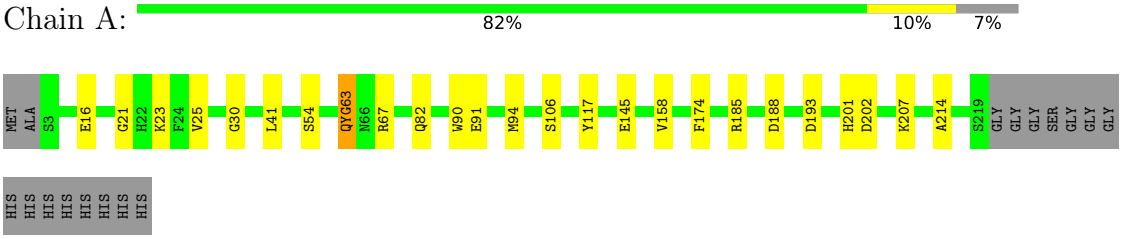
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
6	D	1	5	1	2	2	0	0

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.

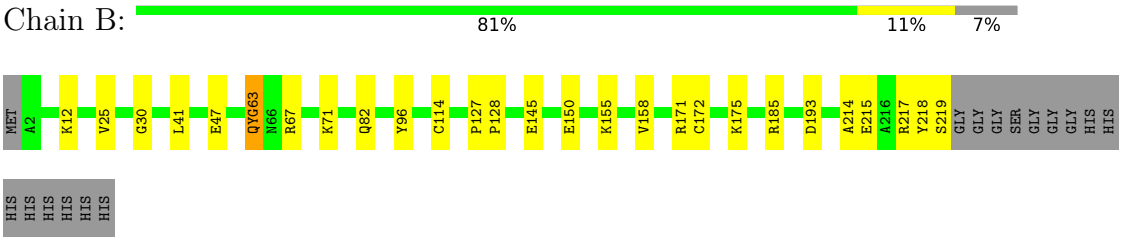
• Molecule 1: Thermostable green fluorescent protein (TGP)

Chain A:



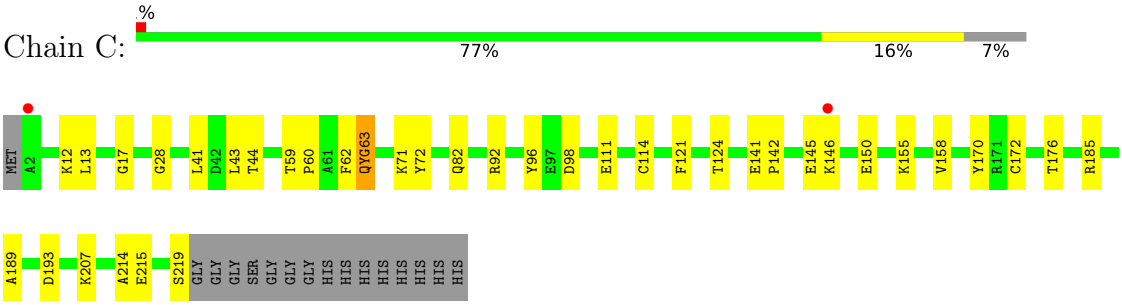
• Molecule 1: Thermostable green fluorescent protein (TGP)

Chain B:



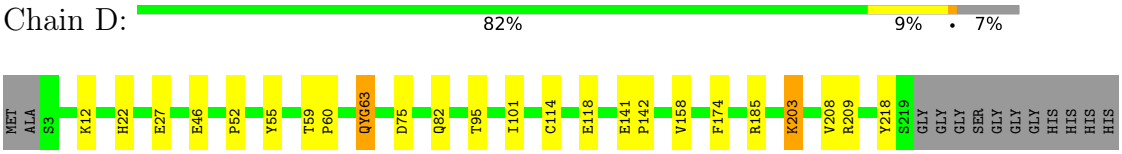
• Molecule 1: Thermostable green fluorescent protein (TGP)

Chain C:



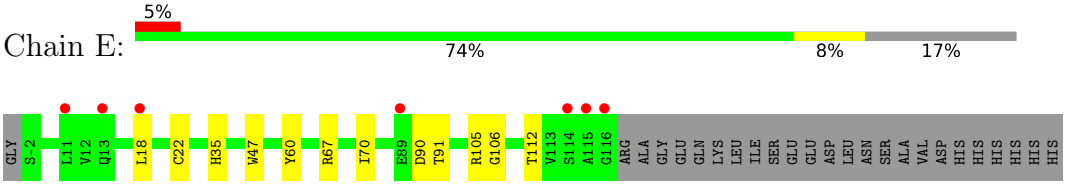
• Molecule 1: Thermostable green fluorescent protein (TGP)

Chain D:



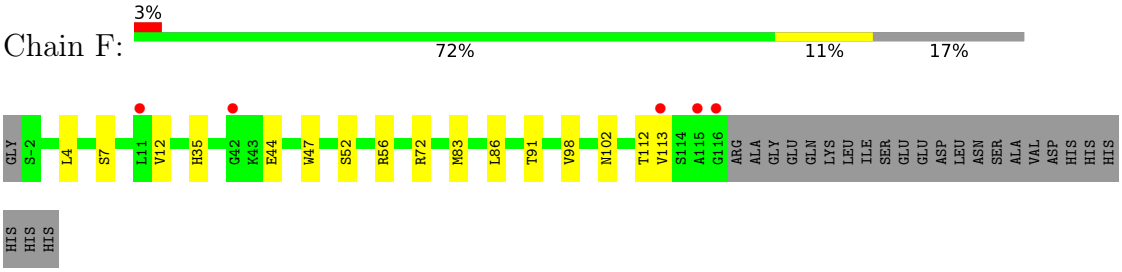
• Molecule 2: Synthetic nanobody (Sybody) 92 recognizing the thermostable green fluorescent protein (TGP)

Chain E:



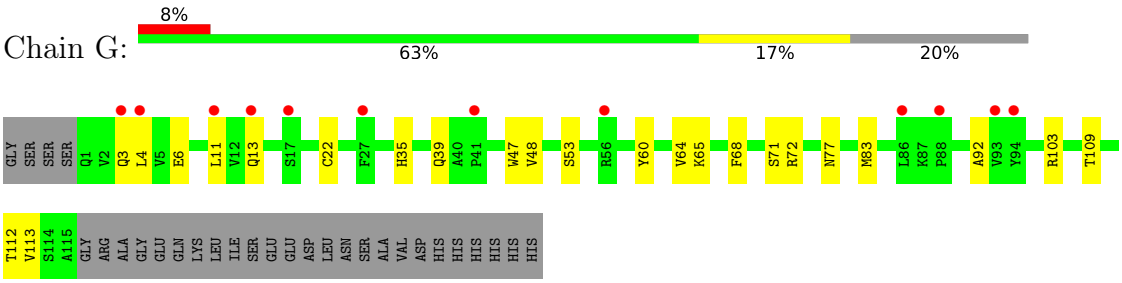
• Molecule 2: Synthetic nanobody (Sybody) 92 recognizing the thermostable green fluorescent protein (TGP)

Chain F:



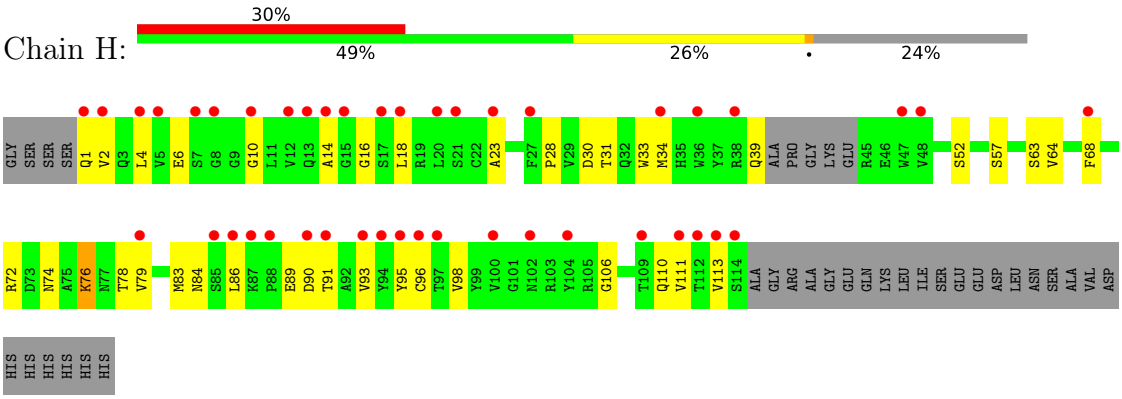
• Molecule 2: Synthetic nanobody (Sybody) 92 recognizing the thermostable green fluorescent protein (TGP)

Chain G:



• Molecule 2: Synthetic nanobody (Sybody) 92 recognizing the thermostable green fluorescent protein (TGP)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	95.25Å 130.15Å 171.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.62 – 2.77 47.62 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.62-2.77) 99.9 (47.62-2.77)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.202 , 0.241 0.204 , 0.241	Depositor DCC
R_{free} test set	2724 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10620	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1533e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, CRQ, ACT, CAD, GOL

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	0.29	0/1777	0.50	0/2398
1	B	0.30	0/1782	0.51	0/2405
1	C	0.28	0/1782	0.51	0/2405
1	D	0.28	0/1786	0.50	0/2409
2	E	0.27	0/930	0.46	0/1260
2	F	0.27	0/930	0.45	0/1260
2	G	0.27	0/911	0.51	0/1236
2	H	0.30	0/801	0.55	0/1094
All	All	0.28	0/10699	0.50	0/14467

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1756	0	1677	15	0
1	B	1761	0	1682	17	0
1	C	1761	0	1682	23	0
1	D	1762	0	1690	17	0
2	E	911	0	878	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	911	0	878	10	0
2	G	889	0	858	13	0
2	H	785	0	703	26	0
3	A	24	0	32	1	0
3	B	30	0	40	2	0
3	C	6	0	8	1	0
3	D	6	0	8	0	0
4	A	5	0	0	0	0
5	B	4	0	3	0	0
5	D	4	0	3	0	0
6	D	5	0	0	0	0
All	All	10620	0	10142	126	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 6.

All (126) 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)
2:E:105:ARG:NH2	2:E:106:GLY:O	2.00	0.95
1:D:95:THR:HG22	1:D:101:ILE:CD1	2.12	0.80
3:B:301:GOL:H31	3:B:302:GOL:H32	1.70	0.74
2:G:11:LEU:HG	2:G:112:THR:HB	1.73	0.70
1:A:16:GLU:HG3	1:A:25:VAL:HG22	1.76	0.67
2:E:35:HIS:HD2	2:E:47:TRP:HE1	1.43	0.67
1:C:28:GLY:HA3	1:C:43:LEU:HD23	1.76	0.66
2:F:35:HIS:HD2	2:F:47:TRP:HE1	1.42	0.66
1:C:146:LYS:HE3	1:C:189:ALA:HB1	1.79	0.64
2:H:14:ALA:HA	2:H:113:VAL:HG13	1.80	0.64
1:D:82:GLN:HE22	1:D:185:ARG:H	1.44	0.63
2:G:6:GLU:HB3	2:G:109:THR:HG22	1.81	0.62
2:G:60:TYR:HB2	2:G:65:LYS:HG3	1.81	0.62
1:A:207:LYS:HB3	3:A:302:GOL:H32	1.81	0.61
1:C:44:THR:HG22	1:C:207:LYS:HD2	1.82	0.61
2:E:67:ARG:NH1	2:E:90:ASP:OD2	2.34	0.61
2:F:52:SER:O	2:F:72:ARG:NH1	2.34	0.60
1:B:217:ARG:HH11	1:B:217:ARG:HG2	1.68	0.59
1:B:82:GLN:HE22	1:B:185:ARG:H	1.51	0.58
2:H:95:TYR:HB2	2:H:106:GLY:O	2.03	0.58
2:G:3:GLN:NE2	2:G:4:LEU:H	2.02	0.58
1:A:82:GLN:HE22	1:A:185:ARG:H	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:THR:HG22	1:D:101:ILE:HD13	1.87	0.57
2:E:91:THR:HG23	2:E:112:THR:HA	1.85	0.56
2:H:34:MET:HG2	2:H:98:VAL:HB	1.88	0.56
1:B:96:TYR:CD2	1:B:172:CYS:HB2	2.42	0.55
2:G:48:VAL:HG23	2:G:64:VAL:HG21	1.88	0.55
2:H:4:LEU:HA	2:H:23:ALA:O	2.06	0.55
2:H:30:ASP:HB3	2:H:74:ASN:ND2	2.21	0.55
1:C:82:GLN:HE22	1:C:185:ARG:H	1.55	0.55
1:C:71:LYS:HB3	1:C:215:GLU:HG2	1.89	0.54
2:H:23:ALA:HA	2:H:78:THR:HG22	1.89	0.54
2:F:83:MET:HE2	2:F:86:LEU:HD21	1.90	0.53
1:A:91:GLU:HB3	1:C:124:THR:OG1	2.09	0.53
2:H:16:GLY:O	2:H:86:LEU:HD23	2.08	0.52
1:C:111:GLU:OE2	2:G:103:ARG:NH1	2.42	0.52
1:D:12:LYS:HD3	1:D:114:CYS:SG	2.50	0.52
2:F:91:THR:HG22	2:F:112:THR:HA	1.91	0.51
2:G:53:SER:O	2:G:72:ARG:NH2	2.42	0.51
1:D:95:THR:CG2	1:D:101:ILE:CD1	2.87	0.51
1:C:17:GLY:HA3	1:C:121:PHE:O	2.11	0.51
1:D:59:THR:OG1	1:D:60:PRO:HD3	2.11	0.51
1:B:217:ARG:HG2	1:B:217:ARG:NH1	2.27	0.50
1:C:12:LYS:HG3	1:C:114:CYS:SG	2.51	0.50
2:F:35:HIS:CD2	2:F:47:TRP:HE1	2.27	0.50
2:H:72:ARG:HG3	2:H:79:VAL:HG12	1.94	0.49
1:C:96:TYR:CD1	1:C:172:CYS:HB2	2.47	0.49
1:D:141:GLU:HG3	1:D:142:PRO:HD2	1.94	0.49
2:F:91:THR:HG22	2:F:113:VAL:H	1.78	0.48
1:B:47:GLU:HA	3:B:305:GOL:H2	1.94	0.48
1:A:21:GLY:O	1:A:23:LYS:NZ	2.45	0.48
2:H:76:LYS:O	2:H:78:THR:HG23	2.14	0.47
2:F:12:VAL:O	2:F:113:VAL:HA	2.14	0.47
1:D:95:THR:HG22	1:D:101:ILE:HD12	1.93	0.47
2:H:1:GLN:HG3	2:H:2:VAL:HG23	1.95	0.47
2:H:39:GLN:HB3	2:H:93:VAL:HG13	1.96	0.47
2:H:64:VAL:HG11	2:H:68:PHE:CD2	2.50	0.47
1:A:30:GLY:HA3	1:A:41:LEU:HD23	1.96	0.47
2:H:6:GLU:N	2:H:6:GLU:OE1	2.47	0.47
2:H:91:THR:HG21	2:H:113:VAL:H	1.80	0.47
1:C:141:GLU:HG3	1:C:142:PRO:HD2	1.98	0.46
1:A:158:VAL:HG13	1:A:174:PHE:HB2	1.96	0.46
1:B:30:GLY:HA3	1:B:41:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:VAL:HG13	1:D:174:PHE:HB2	1.98	0.46
1:D:75:ASP:OD1	1:D:75:ASP:N	2.43	0.46
2:F:91:THR:CG2	2:F:113:VAL:H	2.29	0.45
1:A:193:ASP:O	1:A:214:ALA:HA	2.15	0.45
3:C:301:GOL:O3	3:C:301:GOL:O1	2.18	0.45
1:C:43:LEU:HD13	1:C:62:PHE:CE2	2.52	0.45
1:B:175:LYS:HE3	1:B:175:LYS:HB3	1.72	0.45
1:C:59:THR:OG1	1:C:60:PRO:HD3	2.17	0.45
2:H:10:GLY:O	2:H:111:VAL:HA	2.17	0.45
2:G:39:GLN:C	2:G:92:ALA:HB1	2.37	0.45
1:C:92:ARG:HB2	1:C:176:THR:HG23	1.98	0.44
1:D:27:GLU:HG3	1:D:46:GLU:HG3	1.98	0.44
2:F:44:GLU:H	2:F:44:GLU:CD	2.21	0.44
2:H:39:GLN:HB3	2:H:93:VAL:CG1	2.47	0.44
2:H:110:GLN:OE1	2:H:111:VAL:N	2.50	0.44
1:A:82:GLN:NE2	1:A:185:ARG:H	2.14	0.44
2:H:28:PRO:O	2:H:31:THR:HG22	2.18	0.44
1:D:82:GLN:NE2	1:D:185:ARG:H	2.11	0.44
1:B:193:ASP:O	1:B:214:ALA:HA	2.17	0.44
2:H:63:SER:HB2	2:H:64:VAL:HG23	1.99	0.44
1:A:67:ARG:CZ	1:A:67:ARG:HA	2.48	0.44
2:H:91:THR:CG2	2:H:113:VAL:H	2.31	0.44
1:A:145:GLU:HA	1:A:158:VAL:HB	2.00	0.43
2:G:13:GLN:HA	2:G:113:VAL:HG23	2.00	0.43
1:C:150:GLU:HB3	1:C:155:LYS:HG3	2.01	0.43
1:C:82:GLN:HE22	1:C:185:ARG:HB2	1.83	0.43
2:H:83:MET:HB2	2:H:86:LEU:HD21	2.01	0.43
2:H:83:MET:C	2:H:84:ASN:HD22	2.22	0.43
1:B:145:GLU:HA	1:B:158:VAL:HB	2.00	0.42
1:D:55:TYR:CZ	1:D:208:VAL:HG21	2.53	0.42
1:D:118:GLU:HG3	2:H:57:SER:OG	2.19	0.42
1:C:63:CRQ:HD1	1:C:63:CRQ:N2	2.35	0.42
2:F:4:LEU:HD11	2:F:98:VAL:HG12	2.02	0.42
2:G:35:HIS:HD2	2:G:47:TRP:HE1	1.66	0.42
2:G:68:PHE:CE1	2:G:83:MET:HB3	2.54	0.42
1:A:90:TRP:CE2	1:A:106:SER:HB3	2.54	0.42
1:B:82:GLN:NE2	1:B:185:ARG:H	2.17	0.42
1:C:145:GLU:HA	1:C:158:VAL:HB	2.00	0.42
2:H:83:MET:CB	2:H:86:LEU:HD21	2.50	0.42
1:A:94:MET:HG2	1:A:174:PHE:CE1	2.54	0.41
1:C:150:GLU:HB3	1:C:155:LYS:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:60:TYR:CE2	2:E:70:ILE:HG22	2.54	0.41
2:H:89:GLU:C	2:H:91:THR:H	2.23	0.41
1:D:203:LYS:HB2	1:D:203:LYS:HE2	1.89	0.41
1:A:201:HIS:HD2	1:A:202:ASP:O	2.03	0.41
2:H:33:TRP:CD2	2:H:52:SER:HA	2.55	0.41
1:C:13:LEU:CD2	1:C:41:LEU:HD21	2.51	0.41
1:A:63:CRQ:HD1	1:A:63:CRQ:N2	2.35	0.41
1:B:12:LYS:HD2	1:B:114:CYS:SG	2.60	0.41
1:C:98:ASP:HB2	1:C:170:TYR:CE1	2.56	0.41
1:D:63:CRQ:N2	1:D:63:CRQ:HD1	2.35	0.41
1:B:63:CRQ:N2	1:B:63:CRQ:HD1	2.35	0.41
1:B:67:ARG:HA	1:B:67:ARG:CZ	2.51	0.41
1:B:150:GLU:OE1	1:B:155:LYS:NZ	2.52	0.41
2:E:35:HIS:CD2	2:E:47:TRP:HE1	2.30	0.41
2:G:71:SER:OG	2:G:72:ARG:N	2.54	0.41
1:B:25:VAL:HB	1:B:47:GLU:HB2	2.02	0.40
1:C:111:GLU:HG2	2:G:35:HIS:CD2	2.56	0.40
1:C:193:ASP:O	1:C:214:ALA:HA	2.21	0.40
1:B:71:LYS:HB3	1:B:215:GLU:HG2	2.03	0.40
2:E:18:LEU:HD23	2:E:18:LEU:HA	1.82	0.40
1:B:127:PRO:HA	1:B:128:PRO:HD3	1.99	0.40
1:D:22:HIS:CE1	1:D:52:PRO:HD3	2.57	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	210/232 (90%)	210 (100%)	0	0	100	100
1	B	211/232 (91%)	209 (99%)	2 (1%)	0	100	100
1	C	211/232 (91%)	210 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	211/232 (91%)	207 (98%)	4 (2%)	0	100 100
2	E	117/144 (81%)	114 (97%)	3 (3%)	0	100 100
2	F	117/144 (81%)	111 (95%)	6 (5%)	0	100 100
2	G	114/144 (79%)	106 (93%)	8 (7%)	0	100 100
2	H	105/144 (73%)	95 (90%)	8 (8%)	2 (2%)	8 23
All	All	1296/1504 (86%)	1262 (97%)	32 (2%)	2 (0%)	47 76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	76	LYS
2	H	90	ASP

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	186/196 (95%)	183 (98%)	3 (2%)	62 86
1	B	186/196 (95%)	183 (98%)	3 (2%)	62 86
1	C	186/196 (95%)	184 (99%)	2 (1%)	73 90
1	D	187/196 (95%)	184 (98%)	3 (2%)	62 86
2	E	96/117 (82%)	95 (99%)	1 (1%)	76 91
2	F	96/117 (82%)	93 (97%)	3 (3%)	40 71
2	G	92/117 (79%)	90 (98%)	2 (2%)	52 80
2	H	75/117 (64%)	73 (97%)	2 (3%)	44 75
All	All	1104/1252 (88%)	1085 (98%)	19 (2%)	60 85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	SER

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Mol	Chain	Res	Type
1	A	117	TYR
1	A	188	ASP
1	B	171	ARG
1	B	218	TYR
1	B	219	SER
1	C	72	TYR
1	C	219	SER
1	D	203	LYS
1	D	209	ARG
1	D	218	TYR
2	E	22	CYS
2	F	7	SER
2	F	56	ARG
2	F	102	ASN
2	G	22	CYS
2	G	77	ASN
2	H	18	LEU
2	H	96	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	82	GLN
1	A	99	GLN
1	A	169	HIS
1	A	201	HIS
1	A	206	ASN
1	B	22	HIS
1	B	82	GLN
1	B	169	HIS
1	C	82	GLN
1	C	125	ASN
1	C	206	ASN
1	D	82	GLN
1	D	125	ASN
1	D	190	HIS
1	D	194	HIS
1	D	201	HIS
2	E	35	HIS
2	F	35	HIS
2	F	82	GLN

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Mol	Chain	Res	Type
2	F	84	ASN
2	G	3	GLN
2	G	13	GLN
2	G	35	HIS
2	H	35	HIS
2	H	84	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	CRQ	A	63	1	24,25,26	2.52	9 (37%)	27,34,36	2.58	7 (25%)
1	CRQ	C	63	1	24,25,26	2.48	8 (33%)	27,34,36	2.63	7 (25%)
1	CRQ	D	63	1	24,25,26	2.57	9 (37%)	27,34,36	2.75	7 (25%)
1	CRQ	B	63	1	24,25,26	2.48	9 (37%)	27,34,36	2.69	6 (22%)

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	CRQ	A	63	1	-	4/10/32/33	0/2/2/2
1	CRQ	C	63	1	-	3/10/32/33	0/2/2/2
1	CRQ	D	63	1	-	5/10/32/33	0/2/2/2
1	CRQ	B	63	1	-	3/10/32/33	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	CRQ	CA2-C2	6.47	1.55	1.48
1	A	63	CRQ	CA2-C2	6.42	1.54	1.48
1	C	63	CRQ	CA2-C2	6.18	1.54	1.48
1	B	63	CRQ	CA2-C2	5.85	1.54	1.48
1	D	63	CRQ	C1-N3	5.00	1.46	1.38
1	C	63	CRQ	C1-N3	4.81	1.46	1.38
1	B	63	CRQ	C1-N3	4.80	1.46	1.38
1	A	63	CRQ	C1-N3	4.74	1.46	1.38
1	D	63	CRQ	C1-N2	4.41	1.42	1.33
1	B	63	CRQ	C1-N2	4.26	1.42	1.33
1	C	63	CRQ	C1-N2	4.18	1.42	1.33
1	A	63	CRQ	C1-N2	4.03	1.42	1.33
1	D	63	CRQ	CD3-NE1	4.02	1.45	1.32
1	A	63	CRQ	CD3-NE1	3.97	1.45	1.32
1	C	63	CRQ	CD3-NE1	3.96	1.45	1.32
1	B	63	CRQ	CD3-NE1	3.93	1.45	1.32
1	A	63	CRQ	C2-N3	3.93	1.49	1.39
1	D	63	CRQ	C2-N3	3.93	1.49	1.39
1	B	63	CRQ	C2-N3	3.90	1.49	1.39
1	C	63	CRQ	C2-N3	3.86	1.48	1.39
1	A	63	CRQ	CG2-CB2	3.77	1.54	1.46
1	D	63	CRQ	CG2-CB2	3.72	1.54	1.46
1	C	63	CRQ	CG2-CB2	3.69	1.54	1.46
1	B	63	CRQ	CG2-CB2	3.49	1.53	1.46
1	B	63	CRQ	CB2-CA2	-3.05	1.32	1.35
1	A	63	CRQ	CB2-CA2	-2.85	1.32	1.35
1	D	63	CRQ	CB2-CA2	-2.61	1.32	1.35
1	C	63	CRQ	CB2-CA2	-2.48	1.33	1.35
1	B	63	CRQ	CA2-N2	2.32	1.43	1.38
1	D	63	CRQ	CA2-N2	2.29	1.43	1.38
1	C	63	CRQ	CA2-N2	2.23	1.43	1.38
1	A	63	CRQ	CA2-N2	2.19	1.43	1.38
1	B	63	CRQ	O2-C2	-2.11	1.18	1.23
1	D	63	CRQ	O2-C2	-2.10	1.18	1.23
1	A	63	CRQ	O2-C2	-2.06	1.18	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	CRQ	O2-C2-CA2	-9.05	125.88	130.96
1	D	63	CRQ	CA2-C2-N3	8.79	107.53	103.37
1	D	63	CRQ	O2-C2-CA2	-8.24	126.34	130.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	63	CRQ	CA2-C2-N3	8.07	107.19	103.37
1	B	63	CRQ	CA2-C2-N3	7.99	107.15	103.37
1	A	63	CRQ	O2-C2-CA2	-7.98	126.48	130.96
1	C	63	CRQ	O2-C2-CA2	-7.94	126.50	130.96
1	A	63	CRQ	CA2-C2-N3	7.49	106.91	103.37
1	C	63	CRQ	C2-CA2-N2	-3.85	106.24	108.93
1	D	63	CRQ	C2-CA2-N2	-3.74	106.31	108.93
1	D	63	CRQ	CG2-CB2-CA2	-3.66	125.46	129.94
1	A	63	CRQ	CG2-CB2-CA2	-3.63	125.50	129.94
1	A	63	CRQ	C2-CA2-N2	-3.43	106.53	108.93
1	B	63	CRQ	C2-CA2-N2	-3.13	106.74	108.93
1	C	63	CRQ	CG2-CB2-CA2	-3.13	126.11	129.94
1	B	63	CRQ	CG2-CB2-CA2	-2.98	126.30	129.94
1	C	63	CRQ	O3-C3-CA3	-2.93	117.54	126.39
1	C	63	CRQ	CA2-N2-C1	2.87	109.58	104.33
1	A	63	CRQ	O3-C3-CA3	-2.85	117.78	126.39
1	B	63	CRQ	O3-C3-CA3	-2.82	117.87	126.39
1	A	63	CRQ	CB2-CA2-C2	2.82	125.64	122.28
1	A	63	CRQ	CA2-N2-C1	2.69	109.25	104.33
1	D	63	CRQ	CA2-N2-C1	2.65	109.18	104.33
1	D	63	CRQ	O3-C3-CA3	-2.56	118.66	126.39
1	D	63	CRQ	CB2-CA2-C2	2.48	125.24	122.28
1	B	63	CRQ	CA2-N2-C1	2.48	108.86	104.33
1	C	63	CRQ	CB2-CA2-C2	2.43	125.17	122.28

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	CRQ	C3-CA3-N3-C2
1	B	63	CRQ	C3-CA3-N3-C2
1	C	63	CRQ	C2-CA2-CB2-CG2
1	D	63	CRQ	C3-CA3-N3-C2
1	C	63	CRQ	N2-CA2-CB2-CG2
1	D	63	CRQ	N2-CA2-CB2-CG2
1	A	63	CRQ	CA1-CB1-CG1-CD3
1	C	63	CRQ	C3-CA3-N3-C2
1	D	63	CRQ	CA1-CB1-CG1-CD3
1	D	63	CRQ	C2-CA2-CB2-CG2
1	A	63	CRQ	N2-CA2-CB2-CG2
1	B	63	CRQ	CA1-CB1-CG1-CD3
1	B	63	CRQ	C3-CA3-N3-C1

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Mol	Chain	Res	Type	Atoms
1	A	63	CRQ	C1-CA1-CB1-CG1
1	D	63	CRQ	C1-CA1-CB1-CG1

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	CRQ	1	0
1	C	63	CRQ	1	0
1	D	63	CRQ	1	0
1	B	63	CRQ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

15 ligands 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	$\#\|Z\| > 2$
3	GOL	B	302	-	5,5,5	0.97	0	5,5,5	0.94	0
3	GOL	A	301	-	5,5,5	0.83	0	5,5,5	1.02	0
5	ACT	B	303	-	3,3,3	1.43	1 (33%)	3,3,3	1.54	0
4	CAD	A	304	-	1,4,4	3.23	1 (100%)	2,6,6	1.22	0
3	GOL	A	303	-	5,5,5	0.98	0	5,5,5	0.96	0
3	GOL	A	305	-	5,5,5	0.91	0	5,5,5	0.95	0
3	GOL	C	301	-	5,5,5	0.91	0	5,5,5	0.96	0
3	GOL	B	306	-	5,5,5	1.10	0	5,5,5	0.87	0
3	GOL	A	302	-	5,5,5	1.17	0	5,5,5	0.89	0
3	GOL	B	304	-	5,5,5	0.81	0	5,5,5	1.04	0
3	GOL	B	305	-	5,5,5	0.99	0	5,5,5	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	D	302	-	5,5,5	0.92	0	5,5,5	0.97	0
6	CAC	D	301	-	0,4,4	-	-	0,6,6	-	-
5	ACT	D	303	-	3,3,3	1.44	1 (33%)	3,3,3	1.50	0
3	GOL	B	301	-	5,5,5	1.03	0	5,5,5	0.77	0

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
3	GOL	B	302	-	-	3/4/4/4	-
3	GOL	A	301	-	-	2/4/4/4	-
3	GOL	A	303	-	-	1/4/4/4	-
3	GOL	A	305	-	-	2/4/4/4	-
3	GOL	C	301	-	-	3/4/4/4	-
3	GOL	B	306	-	-	2/4/4/4	-
3	GOL	A	302	-	-	4/4/4/4	-
3	GOL	B	304	-	-	2/4/4/4	-
3	GOL	B	305	-	-	0/4/4/4	-
3	GOL	D	302	-	-	0/4/4/4	-
3	GOL	B	301	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	304	CAD	O1-AS	3.23	1.78	1.70
5	B	303	ACT	CH3-C	2.13	1.58	1.49
5	D	303	ACT	CH3-C	2.10	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	GOL	O1-C1-C2-C3
3	A	302	GOL	O1-C1-C2-C3
3	A	302	GOL	C1-C2-C3-O3
3	B	301	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	301	GOL	O2-C2-C3-O3
3	B	302	GOL	O1-C1-C2-C3
3	B	304	GOL	C1-C2-C3-O3
3	B	306	GOL	C1-C2-C3-O3
3	C	301	GOL	C1-C2-C3-O3
3	A	305	GOL	O1-C1-C2-C3
3	C	301	GOL	O1-C1-C2-C3
3	A	301	GOL	O1-C1-C2-O2
3	B	304	GOL	O2-C2-C3-O3
3	C	301	GOL	O2-C2-C3-O3
3	A	302	GOL	O1-C1-C2-O2
3	A	302	GOL	O2-C2-C3-O3
3	A	305	GOL	O1-C1-C2-O2
3	B	302	GOL	O1-C1-C2-O2
3	B	306	GOL	O2-C2-C3-O3
3	B	302	GOL	O2-C2-C3-O3
3	A	303	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	GOL	1	0
3	C	301	GOL	1	0
3	A	302	GOL	1	0
3	B	305	GOL	1	0
3	B	301	GOL	1	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	214/232 (92%)	-0.19	0 100 100	26, 40, 59, 71	0
1	B	215/232 (92%)	-0.17	0 100 100	25, 39, 58, 84	0
1	C	215/232 (92%)	-0.08	2 (0%) 84 82	29, 44, 67, 92	0
1	D	214/232 (92%)	-0.11	0 100 100	34, 48, 70, 82	0
2	E	119/144 (82%)	0.16	7 (5%) 22 17	37, 52, 87, 111	0
2	F	119/144 (82%)	0.13	5 (4%) 36 30	38, 56, 91, 109	0
2	G	115/144 (79%)	0.83	12 (10%) 6 4	53, 84, 101, 111	0
2	H	109/144 (75%)	1.59	43 (39%) 0 0	68, 104, 122, 127	0
All	All	1320/1504 (87%)	0.14	69 (5%) 27 22	25, 47, 103, 127	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	5	VAL	5.1
2	H	15	GLY	4.8
1	C	2	ALA	4.6
2	H	94	TYR	4.5
2	E	116	GLY	4.4
2	H	114	SER	4.4
2	H	12	VAL	4.3
2	H	8	GLY	4.2
2	H	111	VAL	4.0
2	H	88	PRO	4.0
2	F	116	GLY	3.9
2	H	14	ALA	3.9
2	H	13	GLN	3.8
2	H	10	GLY	3.8
2	H	113	VAL	3.7
2	H	17	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	115	ALA	3.6
2	G	13	GLN	3.6
2	G	11	LEU	3.5
2	H	4	LEU	3.4
2	G	17	SER	3.4
2	G	56[A]	ARG	3.3
2	H	18	LEU	3.3
2	H	79	VAL	3.2
2	H	38	ARG	3.2
2	G	94	TYR	3.2
2	E	11	LEU	3.1
2	G	4	LEU	3.0
2	H	90	ASP	3.0
2	H	2	VAL	3.0
2	H	23	ALA	2.9
2	F	11	LEU	2.9
2	G	86	LEU	2.9
2	F	115	ALA	2.9
2	G	41	PRO	2.8
2	H	96	CYS	2.8
2	H	7	SER	2.7
2	H	93	VAL	2.7
2	H	48	VAL	2.7
2	E	114	SER	2.6
2	H	86	LEU	2.6
2	H	85	SER	2.6
2	H	97	THR	2.6
2	H	27	PHE	2.6
2	H	68	PHE	2.6
2	H	112	THR	2.5
2	F	42	GLY	2.5
2	H	102	ASN	2.5
2	F	113	VAL	2.5
2	H	36	TRP	2.4
2	G	88	PRO	2.4
2	H	109	THR	2.3
2	H	91	THR	2.3
2	G	27	PHE	2.2
2	H	1	GLN	2.2
2	H	104	TYR	2.2
2	H	100	VAL	2.2
2	H	95	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	34	MET	2.1
2	E	89	GLU	2.1
1	C	146	LYS	2.1
2	G	3	GLN	2.1
2	H	20	LEU	2.1
2	H	87	LYS	2.0
2	E	13	GLN	2.0
2	G	93	VAL	2.0
2	H	47	TRP	2.0
2	E	18	LEU	2.0
2	H	21	SER	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, 95^{th} 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	CRQ	A	63	24/25	0.97	0.16	21,31,41,54	0
1	CRQ	B	63	24/25	0.98	0.18	25,33,38,43	0
1	CRQ	C	63	24/25	0.98	0.16	28,35,44,49	0
1	CRQ	D	63	24/25	0.98	0.14	28,38,44,51	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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, 95^{th} 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
5	ACT	D	303	4/4	0.64	0.30	74,80,85,93	0
3	GOL	B	306	6/6	0.70	0.43	49,55,65,79	0
3	GOL	B	302	6/6	0.73	0.47	55,75,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	305	6/6	0.75	0.37	67,69,79,88	0
5	ACT	B	303	4/4	0.79	0.31	56,68,73,76	0
3	GOL	A	302	6/6	0.84	0.41	38,60,68,72	0
3	GOL	A	305	6/6	0.87	0.32	51,56,60,64	0
3	GOL	B	301	6/6	0.88	0.23	47,77,80,81	0
6	CAC	D	301	5/5	0.89	0.27	48,63,87,157	0
3	GOL	D	302	6/6	0.90	0.28	59,76,83,86	0
4	CAD	A	304	5/5	0.91	0.42	61,83,118,351	0
3	GOL	C	301	6/6	0.91	0.32	63,67,68,74	0
3	GOL	A	301	6/6	0.92	0.33	52,59,64,74	0
3	GOL	B	304	6/6	0.93	0.25	54,56,70,77	0
3	GOL	A	303	6/6	0.96	0.16	42,50,52,56	0

6.5 Other polymers (i)

There are no such residues in this entry.