



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:59 pm BST

PDB ID : 4FK5
Title : Structure of the SAGA Ubp8(S144N)/Sgf11/Sus1/Sgf73 DUB module
Authors : Samara, N.L.; Ringel, A.E.; Wolberger, C.
Deposited on : 2012-06-12
Resolution : 2.03 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 : 2.11
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) : 2.11

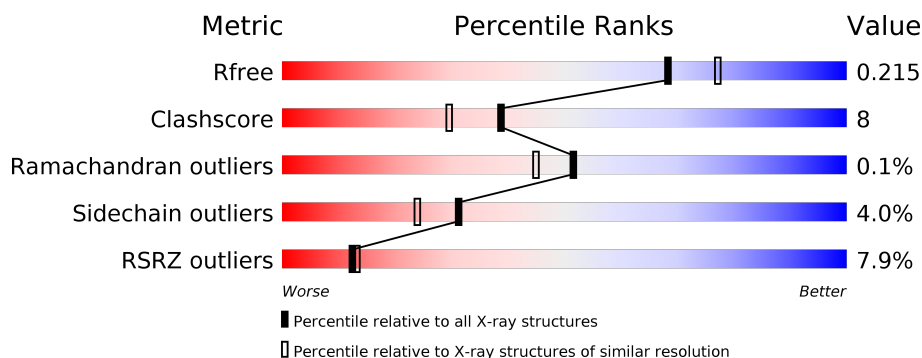
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	476	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>•</div> <div>8%</div> </div> </div>
2	B	96	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• •</div> </div> </div>
3	C	99	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>•</div> <div>7%</div> </div> </div>
4	E	96	<div> <div>15%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6139 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 Ubiquitin carboxyl-terminal hydrolase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	2	0
			3495	2217	598	644	36			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP P50102
A	-3	ALA	-	EXPRESSION TAG	UNP P50102
A	-2	ALA	-	EXPRESSION TAG	UNP P50102
A	-1	ALA	-	EXPRESSION TAG	UNP P50102
A	0	ALA	-	EXPRESSION TAG	UNP P50102
A	144	ASN	SER	ENGINEERED MUTATION	UNP P50102

- Molecule 2 is a protein called Protein SUS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total	C	N	O	S	0	3	0
			765	477	129	157	2			

- Molecule 3 is a protein called SAGA-associated factor 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	92	Total	C	N	O	S	0	0	0
			734	449	135	147	3			

- Molecule 4 is a protein called SAGA-associated factor 73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	91	Total	C	N	O	S	0	1	0
			725	457	121	143	4			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	Zn 6	0	0
5	C	1	Total 1	Zn 1	0	0
5	E	1	Total 1	Zn 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

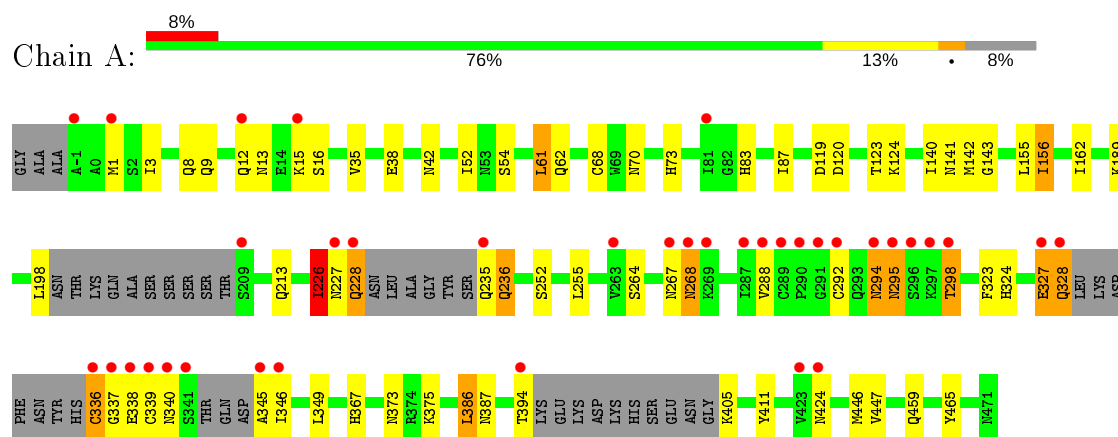
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	242	Total	O	0	0
			242	242		
8	B	43	Total	O	0	0
			43	43		
8	C	54	Total	O	0	0
			54	54		
8	E	57	Total	O	0	0
			57	57		

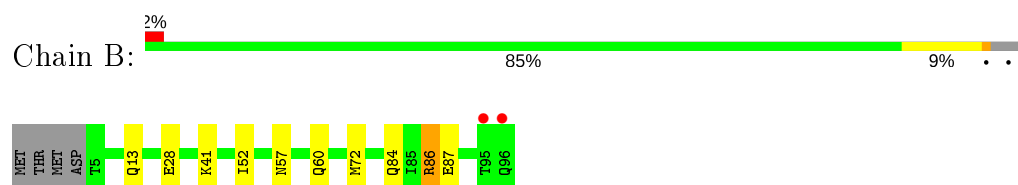
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

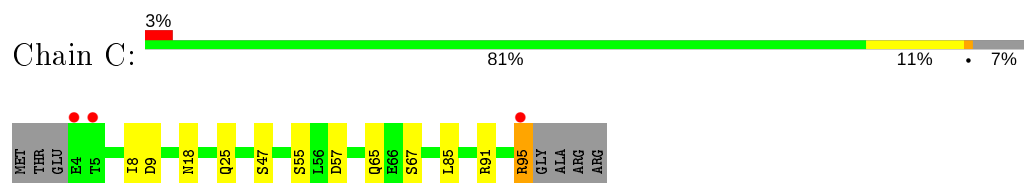
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 8



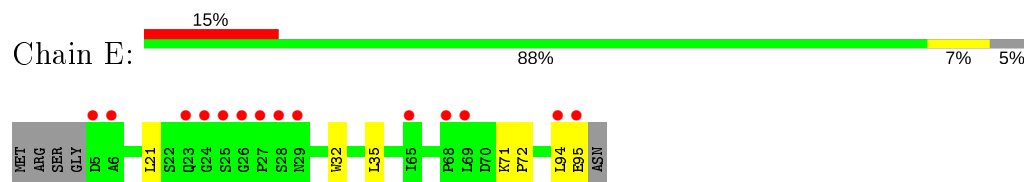
- Molecule 2: Protein SUS1



- Molecule 3: SAGA-associated factor 11



- Molecule 4: SAGA-associated factor 73



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.53Å 104.78Å 107.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.87 – 2.03 47.65 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.3 (74.87-2.03) 99.4 (47.65-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.175 , 0.212 0.181 , 0.215	Depositor DCC
R_{free} test set	3094 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6139	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, EDO

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	1.02	1/3573 (0.0%)	0.65	1/4810 (0.0%)
2	B	1.12	5/780 (0.6%)	0.64	0/1049
3	C	0.97	0/742	0.61	0/1004
4	E	0.99	1/743 (0.1%)	0.63	0/1003
All	All	1.02	7/5838 (0.1%)	0.64	1/7866 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	87	GLU	CD-OE2	9.17	1.35	1.25
2	B	86[A]	ARG	CA-C	5.72	1.67	1.52
2	B	86[B]	ARG	CA-C	5.72	1.67	1.52
4	E	32	TRP	CD2-CE2	5.59	1.48	1.41
2	B	86[A]	ARG	N-CA	-5.30	1.35	1.46
2	B	86[B]	ARG	N-CA	-5.30	1.35	1.46
1	A	73	HIS	CG-CD2	5.21	1.44	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	LEU	CB-CG-CD2	6.68	122.36	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	MET	Peptide
1	A	226	ILE	Peptide
1	A	267	ASN	Peptide

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	3495	0	3428	66	0
2	B	765	0	781	16	0
3	C	734	0	722	11	0
4	E	725	0	721	4	0
5	A	6	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	A	6	0	8	1	0
6	C	6	0	8	1	0
7	A	4	0	6	0	0
8	A	242	0	0	5	0
8	B	43	0	0	2	0
8	C	54	0	0	2	0
8	E	57	0	0	1	0
All	All	6139	0	5674	86	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 8.

All (86) 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:B:86[A]:ARG:HD3	3:C:9:ASP:OD1	1.66	0.94
1:A:236:GLN:HE21	1:A:424:ASN:HD22	1.18	0.91
1:A:236:GLN:HE21	1:A:424:ASN:ND2	1.69	0.89
1:A:13:ASN:HD22	1:A:16:SER:H	1.22	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:MET:CE	8:A:736:HOH:O	2.35	0.74
1:A:264:SER:O	1:A:268:ASN:CB	2.38	0.71
1:A:295:ASN:HD21	1:A:298:THR:HG22	1.54	0.71
2:B:86[A]:ARG:CD	3:C:9:ASP:OD1	2.40	0.70
2:B:57:ASN:HD22	2:B:60:GLN:H	1.37	0.69
1:A:70:ASN:HD21	3:C:25:GLN:HE22	1.38	0.69
1:A:140:ILE:H	1:A:213:GLN:HE22	1.40	0.69
3:C:91:ARG:HD2	8:C:214:HOH:O	1.94	0.68
1:A:264:SER:O	1:A:268:ASN:HB3	1.95	0.67
1:A:141:ASN:OD1	1:A:143:GLY:HA2	1.95	0.66
1:A:189:LYS:HD2	1:A:198:LEU:HD11	1.79	0.65
1:A:42:ASN:HB3	4:E:35:LEU:HD11	1.81	0.63
1:A:156:ILE:O	1:A:162:ILE:HD11	2.01	0.61
1:A:140:ILE:H	1:A:213:GLN:NE2	2.00	0.59
2:B:86[B]:ARG:HG3	3:C:8:ILE:CG2	2.33	0.59
1:A:446:MET:HE2	8:A:736:HOH:O	1.99	0.58
6:C:102:GOL:H32	8:E:253:HOH:O	2.03	0.58
1:A:119:ASP:O	1:A:123:THR:HG23	2.04	0.57
2:B:41:LYS:HB3	2:B:72:MET:CE	2.33	0.57
1:A:446:MET:HE3	8:A:736:HOH:O	1.99	0.57
1:A:226:ILE:HG22	1:A:227:ASN:H	1.69	0.56
1:A:336:CYS:SG	1:A:337:GLY:N	2.77	0.56
1:A:338:GLU:O	1:A:340:ASN:N	2.38	0.56
1:A:324:HIS:HD2	1:A:349:LEU:O	1.88	0.56
1:A:226:ILE:HG22	1:A:227:ASN:N	2.21	0.56
1:A:375:LYS:HZ1	1:A:459:GLN:HE22	1.55	0.54
2:B:86[B]:ARG:HG3	3:C:8:ILE:HG22	1.90	0.54
4:E:71:LYS:HB2	4:E:72:PRO:HD2	1.90	0.53
1:A:227:ASN:O	1:A:228:GLN:C	2.47	0.53
1:A:324:HIS:HE1	8:A:668:HOH:O	1.91	0.53
1:A:295:ASN:ND2	1:A:298:THR:HG22	2.24	0.52
1:A:3:ILE:HB	1:A:8:GLN:OE1	2.10	0.52
1:A:189:LYS:CD	1:A:198:LEU:HD11	2.40	0.52
1:A:288:VAL:HG12	1:A:346:ILE:HB	1.91	0.51
1:A:13:ASN:ND2	1:A:16:SER:H	2.00	0.51
1:A:235:GLN:NE2	1:A:236:GLN:OE1	2.43	0.51
1:A:52:ILE:H	2:B:13:GLN:NE2	2.10	0.49
1:A:226:ILE:N	1:A:226:ILE:CD1	2.75	0.49
1:A:367:HIS:ND1	1:A:373:ASN:ND2	2.60	0.49
1:A:264:SER:O	1:A:268:ASN:CA	2.60	0.49
1:A:375:LYS:NZ	1:A:459:GLN:HE22	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:ND2	1:A:339:CYS:SG	2.86	0.49
1:A:9:GLN:HA	1:A:12:GLN:HE21	1.78	0.49
1:A:327:GLU:HG3	1:A:328:GLN:HB3	1.96	0.48
1:A:226:ILE:HD13	1:A:226:ILE:N	2.28	0.48
2:B:41:LYS:HB3	2:B:72:MET:HE1	1.96	0.48
2:B:41:LYS:HB3	2:B:72:MET:HE2	1.94	0.48
1:A:295:ASN:C	1:A:295:ASN:HD22	2.17	0.48
1:A:62:GLN:NE2	1:A:83:HIS:HA	2.27	0.48
1:A:124:LYS:HB3	4:E:94:LEU:HD22	1.96	0.48
1:A:236:GLN:NE2	1:A:424:ASN:HD22	1.99	0.48
2:B:41:LYS:HD2	8:B:124:HOH:O	2.12	0.47
1:A:328:GLN:OE1	1:A:345:ALA:O	2.32	0.47
1:A:292:CYS:SG	1:A:294:ASN:HB3	2.55	0.47
4:E:94:LEU:O	4:E:95:GLU:HG2	2.14	0.47
1:A:387:ASN:HB3	6:A:507:GOL:C1	2.46	0.46
1:A:337:GLY:HA2	1:A:338:GLU:CG	2.47	0.45
1:A:235:GLN:NE2	1:A:236:GLN:CD	2.69	0.45
1:A:288:VAL:CG1	1:A:346:ILE:HB	2.46	0.45
2:B:86[B]:ARG:HG3	3:C:8:ILE:HG21	1.98	0.44
1:A:447:VAL:O	3:C:57:ASP:HB2	2.18	0.44
2:B:86[A]:ARG:NE	3:C:9:ASP:OD1	2.50	0.44
1:A:52:ILE:H	2:B:13:GLN:HE22	1.66	0.44
1:A:13:ASN:HD21	1:A:15:LYS:HB2	1.83	0.44
1:A:236:GLN:NE2	1:A:424:ASN:ND2	2.52	0.43
2:B:28:GLU:HG2	2:B:84:GLN:HE22	1.82	0.43
1:A:337:GLY:HA2	1:A:338:GLU:HG2	2.00	0.43
1:A:35:VAL:CG2	1:A:38:GLU:HG3	2.49	0.43
1:A:235:GLN:HE21	1:A:236:GLN:CD	2.22	0.42
1:A:411:TYR:HB3	1:A:465:TYR:HB3	2.01	0.42
2:B:52:ILE:HG13	8:B:114:HOH:O	2.18	0.42
3:C:65:GLN:NE2	3:C:67:SER:OG	2.45	0.42
1:A:35:VAL:HG22	1:A:38:GLU:HG3	2.02	0.42
1:A:61:LEU:HD21	1:A:87:ILE:HD11	2.00	0.42
1:A:54:SER:O	1:A:68:CYS:HB2	2.20	0.42
2:B:84:GLN:HE21	2:B:84:GLN:HB2	1.69	0.41
1:A:9:GLN:HA	1:A:12:GLN:NE2	2.35	0.41
1:A:327:GLU:O	1:A:328:GLN:C	2.59	0.41
1:A:255[B]:LEU:HD12	8:A:807:HOH:O	2.20	0.41
1:A:235:GLN:HG3	1:A:236:GLN:HB2	2.03	0.40
1:A:162:ILE:HA	1:A:162:ILE:HD13	1.97	0.40
3:C:95:ARG:NH2	8:C:241:HOH:O	2.54	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	427/476 (90%)	417 (98%)	9 (2%)	1 (0%)	47	39
2	B	93/96 (97%)	93 (100%)	0	0	100	100
3	C	90/99 (91%)	90 (100%)	0	0	100	100
4	E	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
All	All	700/767 (91%)	686 (98%)	13 (2%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	ILE

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	399/429 (93%)	379 (95%)	20 (5%)	24	16
2	B	90/91 (99%)	90 (100%)	0	100	100
3	C	84/89 (94%)	79 (94%)	5 (6%)	19	11
4	E	83/86 (96%)	82 (99%)	1 (1%)	71	70
All	All	656/695 (94%)	630 (96%)	26 (4%)	31	24

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	61	LEU
1	A	120	ASP
1	A	155	LEU
1	A	156	ILE
1	A	226	ILE
1	A	228	GLN
1	A	236	GLN
1	A	252	SER
1	A	268	ASN
1	A	294	ASN
1	A	295	ASN
1	A	298	THR
1	A	323	PHE
1	A	327	GLU
1	A	328	GLN
1	A	336	CYS
1	A	386	LEU
1	A	394	THR
1	A	405	LYS
3	C	18	ASN
3	C	47	SER
3	C	55	SER
3	C	85	LEU
3	C	95	ARG
4	E	21	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	12	GLN
1	A	13	ASN
1	A	33	HIS
1	A	62	GLN
1	A	70	ASN
1	A	90	ASN
1	A	110	ASN
1	A	144	ASN
1	A	172	ASN
1	A	213	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	235	GLN
1	A	294	ASN
1	A	295	ASN
1	A	324	HIS
1	A	348	GLN
1	A	361	GLN
1	A	373	ASN
1	A	424	ASN
1	A	459	GLN
1	A	469	GLN
2	B	7	GLN
2	B	11	GLN
2	B	13	GLN
2	B	14	GLN
2	B	27	ASN
2	B	57	ASN
2	B	84	GLN
2	B	96	GLN
3	C	18	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
6	GOL	A	507	-	5,5,5	0.61	0	5,5,5	0.38	0
6	GOL	C	102	-	5,5,5	1.99	1 (20%)	5,5,5	0.78	0
7	EDO	A	508	-	3,3,3	0.70	0	2,2,2	0.15	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
6	GOL	A	507	-	-	2/4/4/4	-
6	GOL	C	102	-	-	4/4/4/4	-
7	EDO	A	508	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	102	GOL	O2-C2	4.01	1.55	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	507	GOL	O1-C1-C2-O2
6	A	507	GOL	O1-C1-C2-C3
6	C	102	GOL	O1-C1-C2-O2
6	C	102	GOL	O1-C1-C2-C3
6	C	102	GOL	C1-C2-C3-O3
6	C	102	GOL	O2-C2-C3-O3
7	A	508	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	507	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	102	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, 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	437/476 (91%)	0.38	37 (8%) 10 11	16, 31, 70, 102	5 (1%)
2	B	92/96 (95%)	0.10	2 (2%) 62 66	20, 33, 50, 75	0
3	C	92/99 (92%)	0.14	3 (3%) 46 50	23, 34, 57, 101	1 (1%)
4	E	91/96 (94%)	0.64	14 (15%) 2 1	21, 34, 71, 97	0
All	All	712/767 (92%)	0.34	56 (7%) 12 13	16, 32, 69, 102	6 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	GLY	7.7
4	E	24	GLY	6.6
1	A	289	CYS	6.5
1	A	295	ASN	5.8
1	A	292	CYS	5.8
1	A	336	CYS	5.5
1	A	269	LYS	5.3
1	A	-1	ALA	5.3
4	E	23	GLN	5.2
1	A	290	PRO	4.9
1	A	339	CYS	4.9
1	A	228	GLN	4.7
1	A	341	SER	4.7
1	A	346	ILE	4.6
1	A	288	VAL	4.3
1	A	291	GLY	4.2
1	A	328	GLN	4.1
3	C	4	GLU	4.1
1	A	268	ASN	3.9
4	E	25	SER	3.9
2	B	96	GLN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	E	26	GLY	3.7
4	E	6	ALA	3.5
4	E	95	GLU	3.5
4	E	27	PRO	3.5
1	A	235	GLN	3.5
2	B	95	THR	3.4
1	A	287	ILE	3.4
1	A	345	ALA	3.4
1	A	338	GLU	3.3
1	A	227	ASN	3.2
1	A	424	ASN	3.0
3	C	5	THR	2.7
1	A	297	LYS	2.7
1	A	294	ASN	2.7
1	A	394	THR	2.7
4	E	69	LEU	2.7
1	A	340	ASN	2.6
3	C	95	ARG	2.6
1	A	209	SER	2.6
1	A	296	SER	2.6
1	A	12	GLN	2.5
4	E	94	LEU	2.4
1	A	263	VAL	2.4
1	A	423	VAL	2.4
4	E	28	SER	2.4
4	E	29	ASN	2.4
1	A	327	GLU	2.4
4	E	65	ILE	2.4
1	A	267	ASN	2.4
1	A	1	MET	2.3
1	A	81	ILE	2.1
1	A	15	LYS	2.1
4	E	68	PRO	2.1
1	A	298	THR	2.0
4	E	5	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 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(\AA^2)	Q<0.9
6	GOL	C	102	6/6	0.74	0.28	40,47,50,55	0
6	GOL	A	507	6/6	0.76	0.21	48,67,69,72	0
7	EDO	A	508	4/4	0.93	0.10	42,52,54,58	0
5	ZN	A	506	1/1	0.97	0.09	59,59,59,59	0
5	ZN	E	101	1/1	0.97	0.08	40,40,40,40	0
5	ZN	A	504	1/1	0.99	0.06	33,33,33,33	0
5	ZN	A	502	1/1	0.99	0.08	30,30,30,30	0
5	ZN	A	503	1/1	0.99	0.07	34,34,34,34	0
5	ZN	A	501	1/1	0.99	0.08	38,38,38,38	0
5	ZN	C	101	1/1	0.99	0.07	35,35,35,35	0
5	ZN	A	505	1/1	1.00	0.10	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.