



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 02:21 AM UTC

PDB ID : 2RFL / pdb_00002rfl
Title : Crystal structure of the putative phosphohistidine phosphatase SixA from *Agrobacterium tumefaciens*
Authors : Kim, Y.; Binkowski, T.; Xu, X.; Edwards, A.M.; Savchenko, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-10-01
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

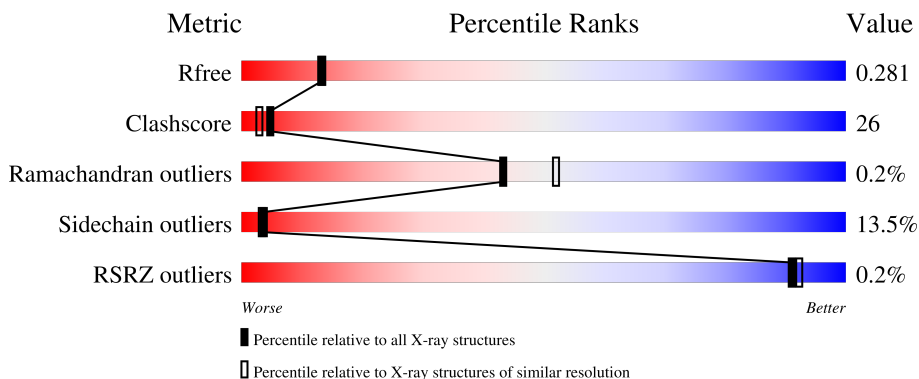
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	173	 44% 38% 5% 14%
1	B	173	 52% 30% 6% 11%
1	C	173	 41% 35% 11% 13%
1	D	173	 46% 33% 6% 15%
1	E	173	 52% 27% 10% 11%

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Mol	Chain	Length	Quality of chain
1	F	173	 41% 37% 6% 15%
1	G	173	 52% 29% 7% 11%
1	H	173	 51% 32% 7% 10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10362 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 Putative phosphohistidine phosphatase SixA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	149	1186	749	210	222	1	4	0	1	0
1	B	154	1245	784	219	237	1	4	0	4	0
1	C	151	1226	774	217	230	1	4	0	4	0
1	D	147	1195	750	209	231	1	4	0	5	0
1	E	154	1258	792	224	237	1	4	0	6	0
1	F	147	1178	741	207	225	1	4	0	3	0
1	G	154	1217	768	217	227	1	4	0	1	0
1	H	156	1257	791	223	238	1	4	0	4	0

There are 32 discrepancies between the modelled and reference sequences:

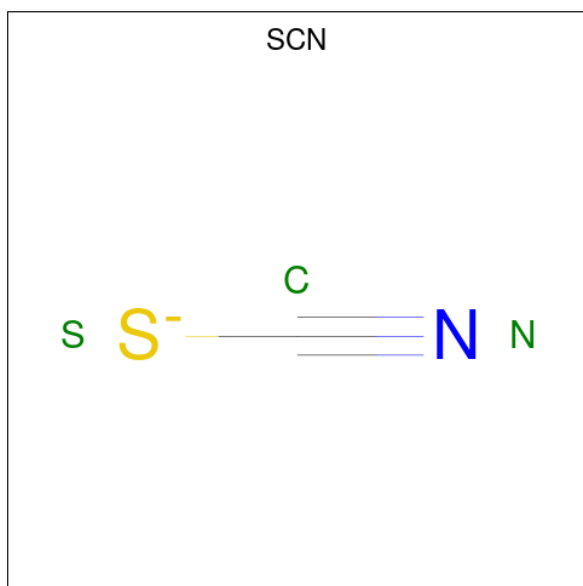
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8UFN9
A	0	HIS	-	expression tag	UNP Q8UFN9
A	170	GLY	-	expression tag	UNP Q8UFN9
A	171	SER	-	expression tag	UNP Q8UFN9
B	-1	GLY	-	expression tag	UNP Q8UFN9
B	0	HIS	-	expression tag	UNP Q8UFN9
B	170	GLY	-	expression tag	UNP Q8UFN9
B	171	SER	-	expression tag	UNP Q8UFN9
C	-1	GLY	-	expression tag	UNP Q8UFN9
C	0	HIS	-	expression tag	UNP Q8UFN9
C	170	GLY	-	expression tag	UNP Q8UFN9
C	171	SER	-	expression tag	UNP Q8UFN9
D	-1	GLY	-	expression tag	UNP Q8UFN9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP Q8UFN9
D	170	GLY	-	expression tag	UNP Q8UFN9
D	171	SER	-	expression tag	UNP Q8UFN9
E	-1	GLY	-	expression tag	UNP Q8UFN9
E	0	HIS	-	expression tag	UNP Q8UFN9
E	170	GLY	-	expression tag	UNP Q8UFN9
E	171	SER	-	expression tag	UNP Q8UFN9
F	-1	GLY	-	expression tag	UNP Q8UFN9
F	0	HIS	-	expression tag	UNP Q8UFN9
F	170	GLY	-	expression tag	UNP Q8UFN9
F	171	SER	-	expression tag	UNP Q8UFN9
G	-1	GLY	-	expression tag	UNP Q8UFN9
G	0	HIS	-	expression tag	UNP Q8UFN9
G	170	GLY	-	expression tag	UNP Q8UFN9
G	171	SER	-	expression tag	UNP Q8UFN9
H	-1	GLY	-	expression tag	UNP Q8UFN9
H	0	HIS	-	expression tag	UNP Q8UFN9
H	170	GLY	-	expression tag	UNP Q8UFN9
H	171	SER	-	expression tag	UNP Q8UFN9

- Molecule 2 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



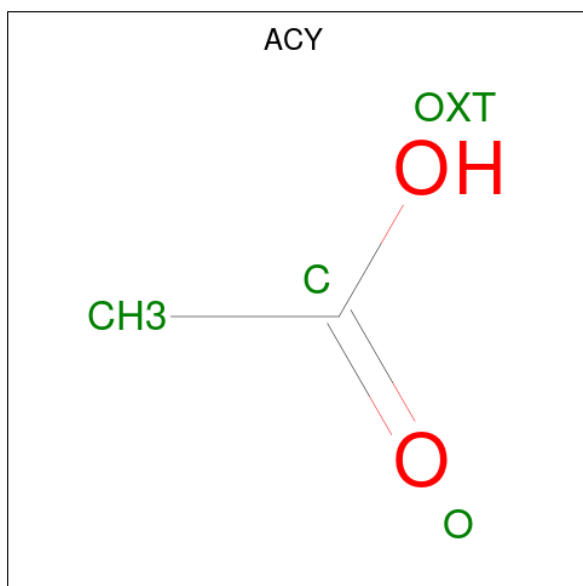
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
2	A	1	3	1	1	1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

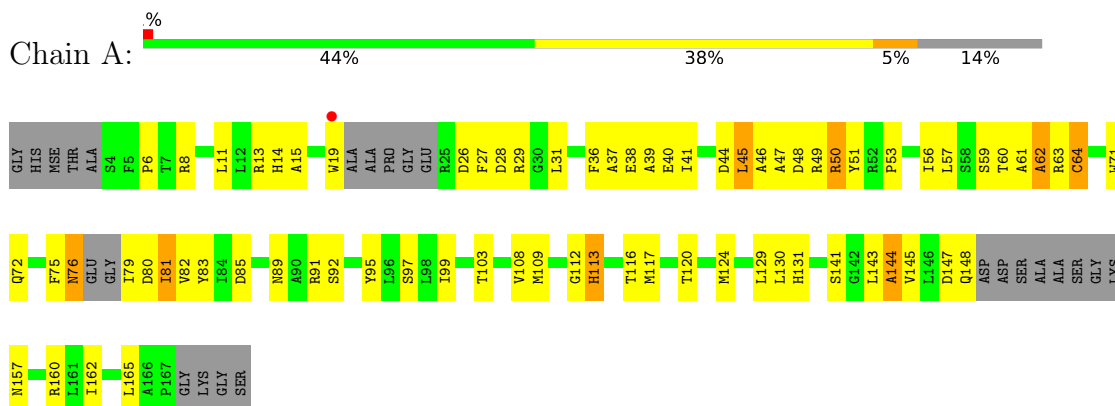
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	81	Total O 81 81	0	0
5	B	71	Total O 71 71	0	0
5	C	75	Total O 75 75	0	0
5	D	68	Total O 68 68	0	0
5	E	77	Total O 77 77	0	0
5	F	63	Total O 63 63	0	0
5	G	66	Total O 66 66	0	0
5	H	80	Total O 80 80	0	0

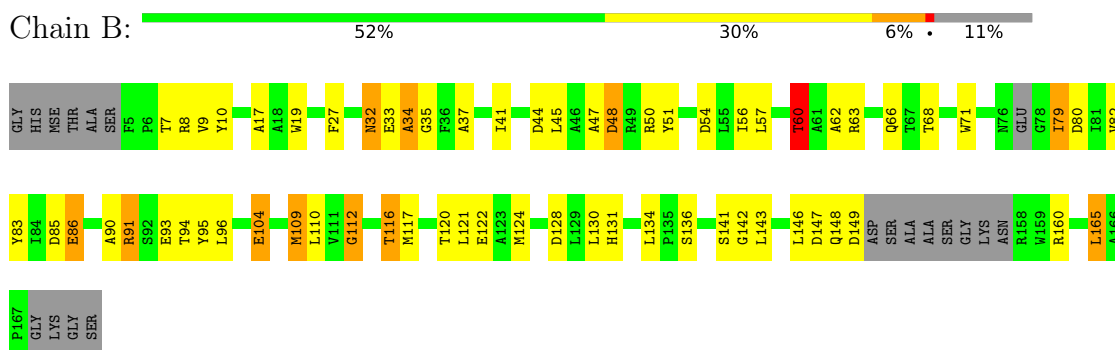
3 Residue-property plots [i](#)

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.

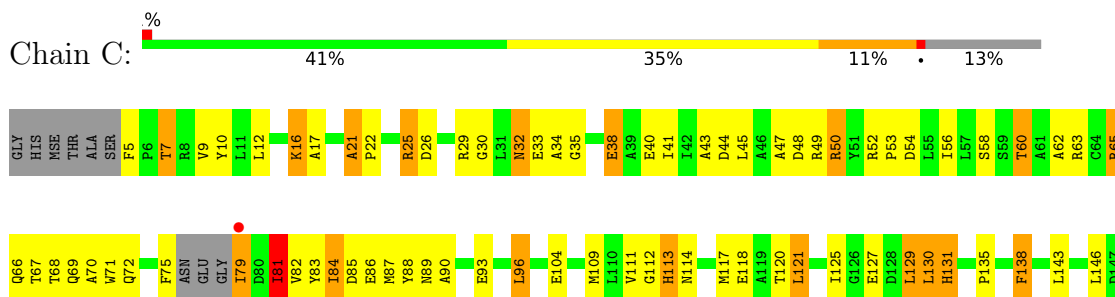
- Molecule 1: Putative phosphohistidine phosphatase SixA

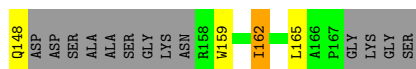


- Molecule 1: Putative phosphohistidine phosphatase SixA

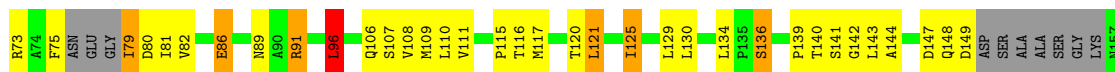
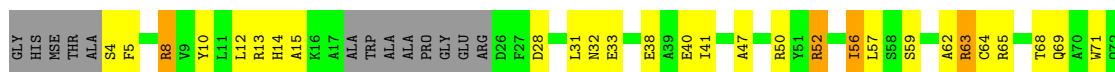


- Molecule 1: Putative phosphohistidine phosphatase SixA





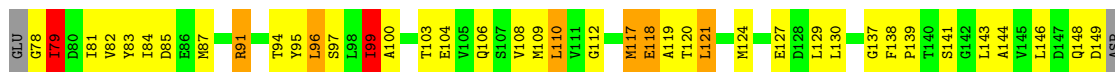
- Molecule 1: Putative phosphohistidine phosphatase SixA



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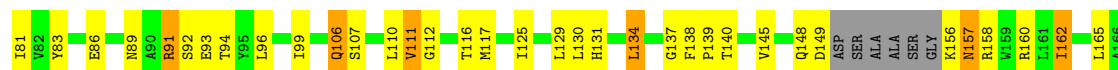




GLY
SER

- Molecule 1: Putative phosphohistidine phosphatase SixA

Chain H: 51% 32% 7% 10%



R167
GLY
LYS
GLY
SER

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.97Å 201.50Å 72.72Å 90.00° 113.98° 90.00°	Depositor
Resolution (Å)	47.25 – 2.35 47.25 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.25-2.35) 97.3 (47.25-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.283 0.230 , 0.281	Depositor DCC
R_{free} test set	6354 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtrriage
Anisotropy	0.442	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.458 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10362	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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: GOL, ACY, SCN

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	1.04	2/1204 (0.2%)	1.23	5/1626 (0.3%)
1	B	1.01	1/1266 (0.1%)	1.22	8/1712 (0.5%)
1	C	0.98	3/1246 (0.2%)	1.25	10/1684 (0.6%)
1	D	0.96	0/1211	1.22	7/1634 (0.4%)
1	E	1.14	4/1277 (0.3%)	1.32	4/1725 (0.2%)
1	F	0.96	0/1194	1.13	4/1611 (0.2%)
1	G	1.11	1/1237 (0.1%)	1.25	3/1672 (0.2%)
1	H	1.03	1/1277 (0.1%)	1.21	6/1726 (0.3%)
All	All	1.03	12/9912 (0.1%)	1.23	47/13390 (0.4%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	111	VAL	CA-CB	8.97	1.64	1.53
1	B	68	THR	CA-CB	6.29	1.63	1.53
1	G	111	VAL	CA-CB	6.08	1.60	1.53
1	A	62	ALA	CA-CB	-5.59	1.44	1.53
1	C	17	ALA	CA-CB	5.53	1.61	1.53

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	ALA	CA-C-N	8.00	128.49	119.93
1	C	21	ALA	C-N-CA	8.00	128.49	119.93
1	D	28	ASP	N-CA-C	7.53	122.50	113.16
1	F	79	ILE	N-CA-C	6.84	118.31	107.98
1	C	146	LEU	N-CA-C	6.58	119.63	108.90

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	1186	0	1158	58	0
1	B	1245	0	1198	77	0
1	C	1226	0	1193	70	1
1	D	1195	0	1153	54	0
1	E	1258	0	1223	66	0
1	F	1178	0	1143	73	1
1	G	1217	0	1190	61	0
1	H	1257	0	1224	54	0
2	A	3	0	0	0	0
3	A	6	0	8	0	0
3	G	6	0	8	0	0
4	D	4	0	3	0	0
5	A	81	0	0	7	1
5	B	71	0	0	16	0
5	C	75	0	0	23	0
5	D	68	0	0	15	0
5	E	77	0	0	9	0
5	F	63	0	0	10	1
5	G	66	0	0	14	0
5	H	80	0	0	11	0
All	All	10362	0	9501	495	2

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 26.

The worst 5 of 495 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:THR:HA	5:B:234:HOH:O	1.31	1.24
1:C:7:THR:HG22	1:C:148:GLN:OE1	1.45	1.16
1:B:90:ALA:CB	1:B:94:THR:HG21	1.76	1.15
1:B:90:ALA:HB1	1:B:94:THR:CG2	1.77	1.14
1:D:149:ASP:HB2	5:D:235:HOH:O	1.50	1.11

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ILE:O	1:F:32:ASN:ND2[2_556]	2.02	0.18
5:A:253:HOH:O	5:F:185:HOH:O[1_454]	2.19	0.01

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	142/173 (82%)	134 (94%)	8 (6%)	0	100	100
1	B	152/173 (88%)	142 (93%)	10 (7%)	0	100	100
1	C	149/173 (86%)	145 (97%)	4 (3%)	0	100	100
1	D	144/173 (83%)	136 (94%)	8 (6%)	0	100	100
1	E	154/173 (89%)	146 (95%)	7 (4%)	1 (1%)	21	24
1	F	142/173 (82%)	139 (98%)	3 (2%)	0	100	100
1	G	149/173 (86%)	140 (94%)	9 (6%)	0	100	100
1	H	154/173 (89%)	147 (96%)	6 (4%)	1 (1%)	21	24
All	All	1186/1384 (86%)	1129 (95%)	55 (5%)	2 (0%)	43	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	86	GLU
1	E	132	ALA

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	122/129 (95%)	108 (88%)	14 (12%)	5	5
1	B	126/129 (98%)	110 (87%)	16 (13%)	4	4
1	C	124/129 (96%)	104 (84%)	20 (16%)	2	2
1	D	124/129 (96%)	103 (83%)	21 (17%)	2	2
1	E	127/129 (98%)	111 (87%)	16 (13%)	4	4
1	F	121/129 (94%)	104 (86%)	17 (14%)	3	3
1	G	123/129 (95%)	102 (83%)	21 (17%)	2	1
1	H	128/129 (99%)	113 (88%)	15 (12%)	5	5
All	All	995/1032 (96%)	855 (86%)	140 (14%)	4	3

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	97	SER
1	G	121	LEU
1	H	32	ASN
1	C	131	HIS
1	C	130	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	131	HIS
1	H	131	HIS
1	H	157	ASN
1	H	148	GLN
1	E	32	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
4	ACY	D	172	-	3,3,3	0.85	0	3,3,3	1.11	0
3	GOL	G	172	-	5,5,5	0.38	0	5,5,5	0.52	0
2	SCN	A	172	-	1,2,2	1.36	0	0,1,1	-	-
3	GOL	A	173	-	5,5,5	0.42	0	5,5,5	0.57	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	G	172	-	-	2/4/4/4	-
3	GOL	A	173	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	173	GOL	O1-C1-C2-O2
3	A	173	GOL	O1-C1-C2-C3
3	A	173	GOL	C1-C2-C3-O3
3	G	172	GOL	O1-C1-C2-C3
3	G	172	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	145/173 (83%)	-1.39	1 (0%) 84 87	13, 44, 61, 74	3 (2%)
1	B	150/173 (86%)	-1.43	0 100 100	18, 43, 64, 81	7 (4%)
1	C	147/173 (84%)	-1.35	1 (0%) 84 87	17, 40, 62, 71	7 (4%)
1	D	143/173 (82%)	-1.39	0 100 100	15, 46, 75, 86	7 (4%)
1	E	150/173 (86%)	-1.48	0 100 100	15, 35, 62, 74	7 (4%)
1	F	143/173 (82%)	-1.40	0 100 100	21, 43, 69, 88	4 (2%)
1	G	150/173 (86%)	-1.42	0 100 100	20, 36, 61, 71	4 (2%)
1	H	152/173 (87%)	-1.38	0 100 100	21, 46, 67, 91	7 (4%)
All	All	1180/1384 (85%)	-1.41	2 (0%) 91 92	13, 42, 67, 91	46 (3%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	TRP	2.8
1	C	79	ILE	2.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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
3	GOL	G	172	6/6	0.98	0.07	78,81,81,83	0
4	ACY	D	172	4/4	0.98	0.05	42,42,42,42	0
2	SCN	A	172	3/3	0.99	0.05	58,58,59,59	0
3	GOL	A	173	6/6	0.99	0.03	55,55,55,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.