



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 06:15 AM EDT

PDB ID : 8DO8
Title : Crystal structure ATG9 HDIR in complex with the ATG13:ATG101 HORMA dimer
Authors : Buffalo, C.Z.; Ren, X.; Yokom, A.L.; Hurley, J.H.
Deposited on : 2022-07-12
Resolution : 2.41 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

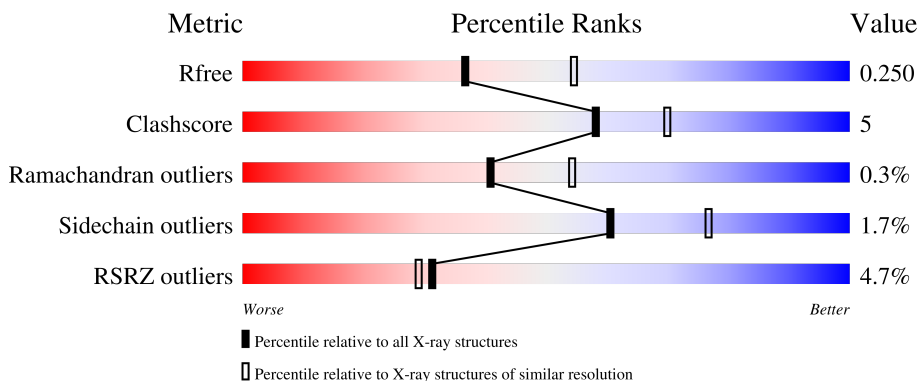
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	218	 3% 72% 11% 17%
1	C	218	 6% 75% 12% 13%
1	E	218	 .. 95%
1	F	218	 .. 96%
2	B	197	 5% 85% 12% ..

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Mol	Chain	Length	Quality of chain
2	D	197	

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	A	202	-	-	-	X
3	GOL	A	204	-	-	-	X
3	GOL	A	207	-	-	-	X
3	GOL	C	206	-	-	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6271 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 Autophagy-related protein 101.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	2	0
			1398	893	227	269	9			
1	C	190	Total	C	N	O	S	0	0	0
			1435	914	239	273	9			
1	E	10	Total	C	N	O		0	0	0
			77	49	13	15				
1	F	8	Total	C	N	O		0	0	0
			56	36	11	9				

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	expression tag	UNP Q9BSB4
A	-18	GLY	-	expression tag	UNP Q9BSB4
A	-17	THR	-	expression tag	UNP Q9BSB4
A	-16	SER	-	expression tag	UNP Q9BSB4
A	-15	GLU	-	expression tag	UNP Q9BSB4
A	-14	ASP	-	expression tag	UNP Q9BSB4
A	-13	GLU	-	expression tag	UNP Q9BSB4
A	-12	LEU	-	expression tag	UNP Q9BSB4
A	-11	PRO	-	expression tag	UNP Q9BSB4
A	-10	PRO	-	expression tag	UNP Q9BSB4
A	-9	GLN	-	expression tag	UNP Q9BSB4
A	-8	VAL	-	expression tag	UNP Q9BSB4
A	-7	HIS	-	expression tag	UNP Q9BSB4
A	-6	LYS	-	expression tag	UNP Q9BSB4
A	-5	VAL	-	expression tag	UNP Q9BSB4
A	-4	GLY	-	expression tag	UNP Q9BSB4
A	-3	SER	-	expression tag	UNP Q9BSB4
A	-2	ASP	-	expression tag	UNP Q9BSB4
A	-1	GLU	-	expression tag	UNP Q9BSB4
A	0	ALA	-	expression tag	UNP Q9BSB4
C	-19	GLY	-	expression tag	UNP Q9BSB4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	GLY	-	expression tag	UNP Q9BSB4
C	-17	THR	-	expression tag	UNP Q9BSB4
C	-16	SER	-	expression tag	UNP Q9BSB4
C	-15	GLU	-	expression tag	UNP Q9BSB4
C	-14	ASP	-	expression tag	UNP Q9BSB4
C	-13	GLU	-	expression tag	UNP Q9BSB4
C	-12	LEU	-	expression tag	UNP Q9BSB4
C	-11	PRO	-	expression tag	UNP Q9BSB4
C	-10	PRO	-	expression tag	UNP Q9BSB4
C	-9	GLN	-	expression tag	UNP Q9BSB4
C	-8	VAL	-	expression tag	UNP Q9BSB4
C	-7	HIS	-	expression tag	UNP Q9BSB4
C	-6	LYS	-	expression tag	UNP Q9BSB4
C	-5	VAL	-	expression tag	UNP Q9BSB4
C	-4	GLY	-	expression tag	UNP Q9BSB4
C	-3	SER	-	expression tag	UNP Q9BSB4
C	-2	ASP	-	expression tag	UNP Q9BSB4
C	-1	GLU	-	expression tag	UNP Q9BSB4
C	0	ALA	-	expression tag	UNP Q9BSB4
E	825	GLY	-	expression tag	UNP Q9BSB4
E	826	GLY	-	expression tag	UNP Q9BSB4
E	827	THR	-	expression tag	UNP Q9BSB4
E	828	SER	-	expression tag	UNP Q9BSB4
E	829	GLU	-	expression tag	UNP Q9BSB4
E	830	ASP	-	expression tag	UNP Q9BSB4
E	831	GLU	-	expression tag	UNP Q9BSB4
E	832	LEU	-	expression tag	UNP Q9BSB4
E	833	PRO	-	expression tag	UNP Q9BSB4
E	834	PRO	-	expression tag	UNP Q9BSB4
E	835	GLN	-	expression tag	UNP Q9BSB4
E	836	VAL	-	expression tag	UNP Q9BSB4
E	837	HIS	-	expression tag	UNP Q9BSB4
E	838	LYS	-	expression tag	UNP Q9BSB4
E	839	VAL	-	expression tag	UNP Q9BSB4
E	840	GLY	-	expression tag	UNP Q9BSB4
E	841	SER	-	expression tag	UNP Q9BSB4
E	842	ASP	-	expression tag	UNP Q9BSB4
E	843	GLU	-	expression tag	UNP Q9BSB4
E	844	ALA	-	expression tag	UNP Q9BSB4
F	825	GLY	-	expression tag	UNP Q9BSB4
F	826	GLY	-	expression tag	UNP Q9BSB4
F	827	THR	-	expression tag	UNP Q9BSB4

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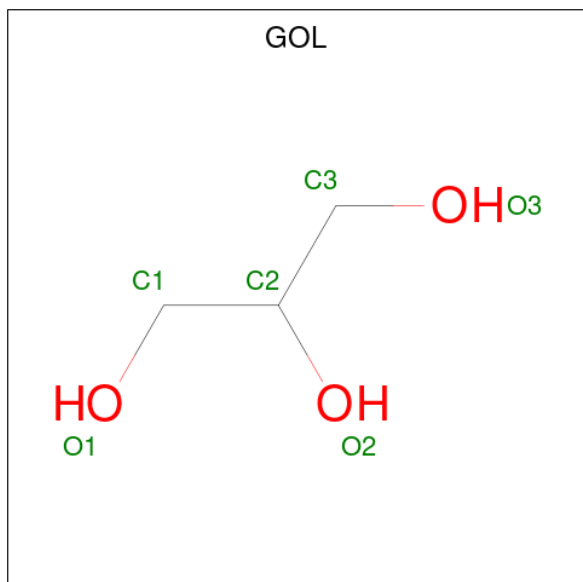
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Chain	Residue	Modelled	Actual	Comment	Reference
F	828	SER	-	expression tag	UNP Q9BSB4
F	829	GLU	-	expression tag	UNP Q9BSB4
F	830	ASP	-	expression tag	UNP Q9BSB4
F	831	GLU	-	expression tag	UNP Q9BSB4
F	832	LEU	-	expression tag	UNP Q9BSB4
F	833	PRO	-	expression tag	UNP Q9BSB4
F	834	PRO	-	expression tag	UNP Q9BSB4
F	835	GLN	-	expression tag	UNP Q9BSB4
F	836	VAL	-	expression tag	UNP Q9BSB4
F	837	HIS	-	expression tag	UNP Q9BSB4
F	838	LYS	-	expression tag	UNP Q9BSB4
F	839	VAL	-	expression tag	UNP Q9BSB4
F	840	GLY	-	expression tag	UNP Q9BSB4
F	841	SER	-	expression tag	UNP Q9BSB4
F	842	ASP	-	expression tag	UNP Q9BSB4
F	843	GLU	-	expression tag	UNP Q9BSB4
F	844	ALA	-	expression tag	UNP Q9BSB4

- Molecule 2 is a protein called Autophagy-related protein 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	192	Total 1448	C 926	N 244	O 269	S 9	0	1	0
2	D	190	Total 1442	C 923	N 246	O 265	S 8	0	1	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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	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	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	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		

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

- Molecule 4 is water.

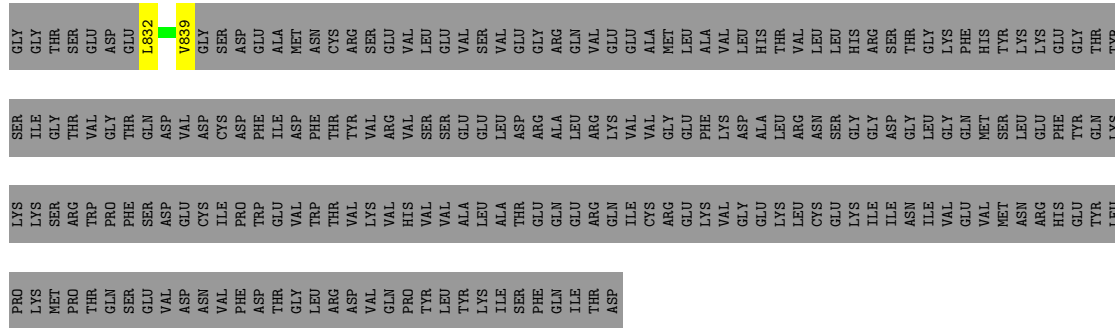
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	49	Total O 49 49	0	0
4	B	45	Total O 45 45	0	0
4	C	45	Total O 45 45	0	0

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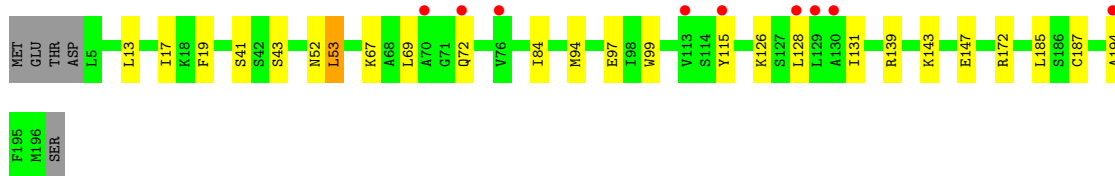
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	45	Total 45	O 45	0	0
4	E	1	Total 1	O 1	0	0
4	F	2	Total 2	O 2	0	0

Chain F: .. 96%



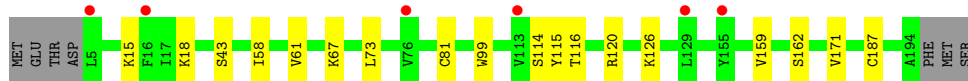
• Molecule 2: Autophagy-related protein 13

Chain B: 5% 85% 12% ..



• Molecule 2: Autophagy-related protein 13

Chain D: 3% 87% 9% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.45Å 139.86Å 147.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.41 – 2.41 39.41 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.41-2.41) 99.8 (39.41-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.42Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.204 , 0.251 0.202 , 0.250	Depositor DCC
R_{free} test set	1152 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtrriage
Anisotropy	0.291	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 71.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6271	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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

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	0.31	0/1432	0.51	0/1948
1	C	0.30	0/1464	0.50	0/1994
1	E	0.25	0/79	0.44	0/109
1	F	0.25	0/58	0.40	0/80
2	B	0.30	0/1472	0.56	0/1999
2	D	0.30	0/1465	0.55	0/1987
All	All	0.30	0/5970	0.53	0/8117

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	1398	0	1284	16	0
1	C	1435	0	1317	17	0
1	E	77	0	69	4	0
1	F	56	0	45	2	0
2	B	1448	0	1428	18	0
2	D	1442	0	1444	11	0
3	A	78	0	104	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	64	1	0
3	C	60	0	80	1	0
3	D	36	0	48	2	0
3	E	6	0	8	0	0
4	A	49	0	0	3	0
4	B	45	0	0	1	0
4	C	45	0	0	1	0
4	D	45	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
All	All	6271	0	5891	57	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 5.

All (57) 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:172:ARG:NH2	4:B:301:HOH:O	2.26	0.69
2:B:94:MET:HE1	2:B:194:ALA:HB3	1.84	0.58
1:C:31:HIS:CD2	1:C:159:MET:HG3	2.40	0.57
1:C:31:HIS:CG	1:C:159:MET:HG3	2.41	0.55
2:B:19:PHE:HZ	1:E:830:ASP:HB3	1.72	0.55
1:A:6:GLU:HG3	1:A:158:VAL:HG11	1.89	0.55
1:A:147:LYS:O	1:A:151:LYS:HG2	2.08	0.54
1:A:63:THR:HG1	3:A:205:GOL:HO3	1.54	0.54
2:B:53:LEU:HD11	2:B:126:LYS:HG3	1.90	0.54
3:C:203:GOL:H2	2:D:171:VAL:HA	1.90	0.53
1:A:61:ASP:OD2	2:B:139:ARG:NH1	2.41	0.53
1:C:62:PHE:HA	3:D:201:GOL:H32	1.91	0.53
1:A:183:ARG:O	2:B:43:SER:HB2	2.09	0.52
2:B:69:LEU:HD22	2:B:72:GLN:O	2.09	0.52
1:C:184:ASP:N	1:C:184:ASP:OD1	2.43	0.52
2:B:19:PHE:CZ	1:E:830:ASP:HB3	2.44	0.51
1:A:156:VAL:HG21	2:B:131:ILE:HG12	1.93	0.51
1:C:78:LYS:O	1:C:82:GLU:HG3	2.11	0.50
2:D:99:TRP:CE3	2:D:187:CYS:HB2	2.46	0.50
2:B:115:TYR:CZ	1:E:837:HIS:HA	2.47	0.49
2:D:116:THR:O	2:D:120:ARG:HG3	2.12	0.49
1:C:95:LEU:HB3	1:C:197:THR:HG23	1.93	0.49
1:C:101:GLU:O	1:C:190:TYR:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:LEU:HD13	2:B:185:LEU:HD21	1.96	0.48
1:A:108:SER:OG	1:C:109:ARG:NH2	2.46	0.48
1:C:4:ARG:HH12	1:C:164:TYR:HB3	1.78	0.47
1:C:38:HIS:NE2	2:D:43:SER:O	2.44	0.47
1:A:77:ARG:NH2	4:A:305:HOH:O	2.47	0.47
2:B:52:ASN:HB2	3:B:206:GOL:H11	1.96	0.47
1:C:24:VAL:HG13	1:C:155:ILE:HD11	1.96	0.47
1:C:43:GLY:O	1:F:839:VAL:N	2.40	0.46
1:A:103:TYR:HA	1:A:118:PRO:HA	1.98	0.46
2:D:81:CYS:SG	2:D:159:VAL:HG22	2.56	0.46
2:B:13:LEU:O	2:B:17:ILE:HD12	2.15	0.45
2:B:84:ILE:HB	2:B:97:GLU:HG2	1.98	0.45
1:C:84:LYS:NZ	4:C:306:HOH:O	2.50	0.44
1:A:99:SER:OG	1:A:123:THR:HG22	2.17	0.44
1:A:103:TYR:CD2	1:A:116:CYS:HB3	2.53	0.44
1:C:73:ASP:O	1:C:77:ARG:HG3	2.17	0.44
1:A:67:VAL:HG21	1:A:72:LEU:HD23	2.00	0.43
2:D:99:TRP:CZ3	2:D:187:CYS:HB2	2.53	0.43
2:D:81:CYS:HA	2:D:99:TRP:O	2.19	0.43
2:B:99:TRP:CE3	2:B:187:CYS:HB2	2.53	0.43
1:A:36:LYS:HE3	1:A:36:LYS:HB3	1.92	0.43
4:A:333:HOH:O	2:B:139:ARG:HD3	2.19	0.43
1:A:184:ASP:HB3	2:B:41:SER:HB3	2.01	0.42
2:D:126:LYS:HE3	3:D:202:GOL:H2	2.01	0.42
2:D:18:LYS:HB2	2:D:73:LEU:HD21	2.01	0.42
2:D:58:ILE:HG22	2:D:61:VAL:H	1.85	0.42
1:C:12:VAL:HB	1:C:16:GLN:HB2	2.02	0.41
1:C:99:SER:HA	1:C:122:TRP:O	2.20	0.41
1:E:832:LEU:HD23	1:E:832:LEU:HA	1.87	0.41
2:D:15:LYS:NZ	1:F:832:LEU:O	2.50	0.41
1:A:105:LYS:O	1:A:176:ASN:HB3	2.21	0.40
1:C:21:MET:HE2	1:C:21:MET:HB3	1.94	0.40
1:A:175:ASP:HB2	4:A:336:HOH:O	2.21	0.40
2:B:13:LEU:HD12	2:B:13:LEU:HA	1.89	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	177/218 (81%)	174 (98%)	3 (2%)	0	100	100
1	C	186/218 (85%)	183 (98%)	3 (2%)	0	100	100
1	E	8/218 (4%)	8 (100%)	0	0	100	100
1	F	6/218 (3%)	6 (100%)	0	0	100	100
2	B	191/197 (97%)	183 (96%)	8 (4%)	0	100	100
2	D	189/197 (96%)	184 (97%)	3 (2%)	2 (1%)	14	19
All	All	757/1266 (60%)	738 (98%)	17 (2%)	2 (0%)	41	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	115	TYR
2	D	114	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	146/196 (74%)	145 (99%)	1 (1%)	84	92
1	C	147/196 (75%)	145 (99%)	2 (1%)	67	81
1	E	9/196 (5%)	8 (89%)	1 (11%)	6	8
1	F	5/196 (3%)	5 (100%)	0	100	100
2	B	151/173 (87%)	147 (97%)	4 (3%)	46	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	151/173 (87%)	149 (99%)	2 (1%)	69	83
All	All	609/1130 (54%)	599 (98%)	10 (2%)	60	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
2	B	53	LEU
2	B	67	LYS
2	B	143	LYS
2	B	147	GLU
1	C	3	CYS
1	C	175	ASP
2	D	67	LYS
2	D	162	SER
1	E	831	GLU

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

Mol	Chain	Res	Type
1	A	53	GLN
2	B	119	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

38 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	D	203	-	5,5,5	0.90	0	5,5,5	0.98	0
3	GOL	C	209	-	5,5,5	0.91	0	5,5,5	1.01	0
3	GOL	B	208	-	5,5,5	0.86	0	5,5,5	0.98	0
3	GOL	C	205	-	5,5,5	0.98	0	5,5,5	0.94	0
3	GOL	A	204	-	5,5,5	0.90	0	5,5,5	0.95	0
3	GOL	D	206	-	5,5,5	0.94	0	5,5,5	0.96	0
3	GOL	C	204	-	5,5,5	0.86	0	5,5,5	0.98	0
3	GOL	B	205	-	5,5,5	0.92	0	5,5,5	0.89	0
3	GOL	D	202	-	5,5,5	0.98	0	5,5,5	0.90	0
3	GOL	A	213	-	5,5,5	0.90	0	5,5,5	0.98	0
3	GOL	B	203	-	5,5,5	0.99	0	5,5,5	0.95	0
3	GOL	A	202	-	5,5,5	0.83	0	5,5,5	0.99	0
3	GOL	C	206	-	5,5,5	0.88	0	5,5,5	0.93	0
3	GOL	A	208	-	5,5,5	0.87	0	5,5,5	1.04	0
3	GOL	A	212	-	5,5,5	0.85	0	5,5,5	0.98	0
3	GOL	C	207	-	5,5,5	0.91	0	5,5,5	0.98	0
3	GOL	A	201	-	5,5,5	0.89	0	5,5,5	1.01	0
3	GOL	A	205	-	5,5,5	0.89	0	5,5,5	1.10	0
3	GOL	D	205	-	5,5,5	0.96	0	5,5,5	0.92	0
3	GOL	D	204	-	5,5,5	0.92	0	5,5,5	0.95	0
3	GOL	A	207	-	5,5,5	0.96	0	5,5,5	0.97	0
3	GOL	C	202	-	5,5,5	0.88	0	5,5,5	1.00	0
3	GOL	A	210	-	5,5,5	1.00	0	5,5,5	0.90	0
3	GOL	C	210	-	5,5,5	0.86	0	5,5,5	0.99	0
3	GOL	A	203	-	5,5,5	0.94	0	5,5,5	0.92	0
3	GOL	B	204	-	5,5,5	0.90	0	5,5,5	1.03	0
3	GOL	C	203	-	5,5,5	0.88	0	5,5,5	1.14	0
3	GOL	D	201	-	5,5,5	1.13	0	5,5,5	0.81	0
3	GOL	B	202	-	5,5,5	1.01	0	5,5,5	0.91	0
3	GOL	A	211	-	5,5,5	0.79	0	5,5,5	1.05	0
3	GOL	E	1101	-	5,5,5	0.83	0	5,5,5	1.04	0
3	GOL	A	206	-	5,5,5	0.87	0	5,5,5	1.02	0
3	GOL	B	206	-	5,5,5	1.10	1 (20%)	5,5,5	0.90	0
3	GOL	C	208	-	5,5,5	1.08	0	5,5,5	0.91	0
3	GOL	B	207	-	5,5,5	0.94	0	5,5,5	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	201	-	5,5,5	0.96	0	5,5,5	0.99	0
3	GOL	A	209	-	5,5,5	0.96	0	5,5,5	0.92	0
3	GOL	B	201	-	5,5,5	0.93	0	5,5,5	0.95	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	D	203	-	-	0/4/4/4	-
3	GOL	C	209	-	-	4/4/4/4	-
3	GOL	B	208	-	-	1/4/4/4	-
3	GOL	C	205	-	-	0/4/4/4	-
3	GOL	A	204	-	-	0/4/4/4	-
3	GOL	D	206	-	-	0/4/4/4	-
3	GOL	C	204	-	-	2/4/4/4	-
3	GOL	B	205	-	-	0/4/4/4	-
3	GOL	D	202	-	-	2/4/4/4	-
3	GOL	A	213	-	-	2/4/4/4	-
3	GOL	B	203	-	-	0/4/4/4	-
3	GOL	A	202	-	-	2/4/4/4	-
3	GOL	C	206	-	-	0/4/4/4	-
3	GOL	A	208	-	-	0/4/4/4	-
3	GOL	A	212	-	-	0/4/4/4	-
3	GOL	C	207	-	-	4/4/4/4	-
3	GOL	A	201	-	-	2/4/4/4	-
3	GOL	A	205	-	-	0/4/4/4	-
3	GOL	D	205	-	-	2/4/4/4	-
3	GOL	D	204	-	-	0/4/4/4	-
3	GOL	A	207	-	-	0/4/4/4	-
3	GOL	C	202	-	-	0/4/4/4	-
3	GOL	A	210	-	-	2/4/4/4	-
3	GOL	C	210	-	-	2/4/4/4	-
3	GOL	A	203	-	-	0/4/4/4	-
3	GOL	B	204	-	-	1/4/4/4	-
3	GOL	C	203	-	-	0/4/4/4	-
3	GOL	D	201	-	-	2/4/4/4	-
3	GOL	B	202	-	-	1/4/4/4	-
3	GOL	A	211	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	1101	-	-	0/4/4/4	-
3	GOL	A	206	-	-	2/4/4/4	-
3	GOL	B	206	-	-	3/4/4/4	-
3	GOL	C	208	-	-	0/4/4/4	-
3	GOL	B	207	-	-	2/4/4/4	-
3	GOL	C	201	-	-	0/4/4/4	-
3	GOL	A	209	-	-	2/4/4/4	-
3	GOL	B	201	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	206	GOL	C3-C2	2.01	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	GOL	O1-C1-C2-C3
3	A	202	GOL	O1-C1-C2-C3
3	A	206	GOL	C1-C2-C3-O3
3	A	210	GOL	O1-C1-C2-C3
3	A	211	GOL	O1-C1-C2-C3
3	A	211	GOL	C1-C2-C3-O3
3	A	213	GOL	O1-C1-C2-C3
3	B	206	GOL	C1-C2-C3-O3
3	B	207	GOL	O1-C1-C2-O2
3	B	207	GOL	O1-C1-C2-C3
3	C	204	GOL	C1-C2-C3-O3
3	C	207	GOL	C1-C2-C3-O3
3	C	210	GOL	C1-C2-C3-O3
3	D	202	GOL	C1-C2-C3-O3
3	D	202	GOL	O2-C2-C3-O3
3	A	201	GOL	O1-C1-C2-O2
3	C	210	GOL	O2-C2-C3-O3
3	A	209	GOL	C1-C2-C3-O3
3	B	204	GOL	C1-C2-C3-O3
3	C	207	GOL	O1-C1-C2-C3
3	C	209	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	C	209	GOL	C1-C2-C3-O3
3	D	201	GOL	C1-C2-C3-O3
3	A	211	GOL	O1-C1-C2-O2
3	A	211	GOL	O2-C2-C3-O3
3	A	213	GOL	O1-C1-C2-O2
3	B	206	GOL	O2-C2-C3-O3
3	C	207	GOL	O2-C2-C3-O3
3	A	202	GOL	O1-C1-C2-O2
3	A	206	GOL	O2-C2-C3-O3
3	D	201	GOL	O2-C2-C3-O3
3	C	204	GOL	O2-C2-C3-O3
3	A	210	GOL	O1-C1-C2-O2
3	D	205	GOL	O1-C1-C2-O2
3	C	207	GOL	O1-C1-C2-O2
3	D	205	GOL	O1-C1-C2-C3
3	C	209	GOL	O1-C1-C2-O2
3	C	209	GOL	O2-C2-C3-O3
3	A	209	GOL	O2-C2-C3-O3
3	B	202	GOL	O2-C2-C3-O3
3	B	206	GOL	O1-C1-C2-O2
3	B	208	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	202	GOL	1	0
3	A	205	GOL	1	0
3	C	203	GOL	1	0
3	D	201	GOL	1	0
3	B	206	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 [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	181/218 (83%)	0.36	6 (3%) 46 44	40, 64, 89, 123	0
1	C	190/218 (87%)	0.40	14 (7%) 14 13	46, 66, 99, 126	0
1	E	10/218 (4%)	0.09	1 (10%) 7 6	73, 83, 99, 117	0
1	F	8/218 (3%)	0.70	0 100 100	82, 89, 98, 109	0
2	B	192/197 (97%)	0.32	9 (4%) 31 29	41, 61, 102, 131	0
2	D	190/197 (96%)	0.25	6 (3%) 47 45	39, 63, 92, 120	0
All	All	771/1266 (60%)	0.33	36 (4%) 31 29	39, 64, 97, 131	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	93	ASP	5.0
1	C	94	GLY	4.8
2	B	115	TYR	4.3
2	B	70	ALA	4.0
1	A	194	PHE	3.4
1	C	40	LYS	3.3
2	B	194	ALA	3.3
1	A	172	SER	3.3
2	B	76	VAL	3.2
1	C	129	VAL	3.1
1	C	95	LEU	2.8
1	C	172	SER	2.7
2	D	155[A]	TYR	2.7
2	D	76	VAL	2.6
2	D	113	VAL	2.6
1	C	43	GLY	2.6
2	D	5	LEU	2.4
1	C	39	TYR	2.4
2	B	129	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	163	GLU	2.4
2	B	72	GLN	2.4
2	D	129	LEU	2.3
1	A	44	THR	2.3
2	B	113	VAL	2.3
1	C	42	GLU	2.3
1	C	126	VAL	2.3
1	E	830	ASP	2.3
1	A	30	LEU	2.3
2	B	130	ALA	2.2
1	C	195	GLN	2.2
1	C	176	ASN	2.2
1	A	41	LYS	2.1
2	B	128	LEU	2.1
2	D	16	PHE	2.1
1	C	13	GLU	2.1
1	A	39	TYR	2.0

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 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, 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	B	206	6/6	0.43	0.36	62,68,70,81	0
3	GOL	D	204	6/6	0.51	0.34	89,94,98,100	0
3	GOL	A	207	6/6	0.55	0.45	85,94,95,98	0
3	GOL	B	207	6/6	0.60	0.32	85,87,89,99	0
3	GOL	B	203	6/6	0.60	0.30	94,105,108,111	0
3	GOL	A	206	6/6	0.61	0.32	75,80,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	212	6/6	0.64	0.24	84,87,91,97	0
3	GOL	D	205	6/6	0.65	0.38	84,89,91,98	0
3	GOL	A	202	6/6	0.69	0.52	82,88,94,95	0
3	GOL	C	205	6/6	0.70	0.39	84,101,103,106	0
3	GOL	D	202	6/6	0.70	0.25	65,69,76,79	0
3	GOL	B	205	6/6	0.71	0.34	75,79,85,90	0
3	GOL	C	206	6/6	0.72	0.40	73,86,94,95	0
3	GOL	C	204	6/6	0.73	0.32	79,89,92,92	0
3	GOL	A	209	6/6	0.74	0.25	73,81,83,83	0
3	GOL	A	204	6/6	0.75	0.45	86,88,92,93	0
3	GOL	B	202	6/6	0.75	0.19	77,81,86,90	0
3	GOL	C	207	6/6	0.77	0.28	64,75,82,91	0
3	GOL	A	208	6/6	0.77	0.28	85,87,92,94	0
3	GOL	C	201	6/6	0.81	0.29	71,76,84,84	0
3	GOL	D	206	6/6	0.81	0.22	103,108,112,117	0
3	GOL	B	204	6/6	0.82	0.19	63,72,82,85	0
3	GOL	C	210	6/6	0.82	0.23	69,76,80,81	0
3	GOL	D	203	6/6	0.83	0.21	74,78,80,81	0
3	GOL	A	203	6/6	0.85	0.26	70,79,81,81	0
3	GOL	A	201	6/6	0.86	0.29	77,84,88,94	0
3	GOL	C	208	6/6	0.86	0.15	70,80,83,85	0
3	GOL	C	202	6/6	0.87	0.36	77,85,91,103	0
3	GOL	C	209	6/6	0.87	0.17	70,73,75,78	0
3	GOL	C	203	6/6	0.87	0.11	72,77,80,85	0
3	GOL	A	205	6/6	0.87	0.14	57,65,70,72	0
3	GOL	B	208	6/6	0.88	0.26	72,75,85,87	0
3	GOL	A	213	6/6	0.89	0.12	70,74,77,82	0
3	GOL	E	1101	6/6	0.90	0.19	78,86,89,92	0
3	GOL	B	201	6/6	0.91	0.24	71,73,78,79	0
3	GOL	A	210	6/6	0.91	0.13	76,80,91,92	0
3	GOL	A	211	6/6	0.92	0.17	65,69,74,82	0
3	GOL	D	201	6/6	0.92	0.16	49,61,61,72	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.