Full wwPDB X-ray Structure Validation Report ⓘ

Apr 8, 2024 – 12:32 PM EDT

PDB ID	:	8SBF
Title	:	Full-length structure of the LysR-type transcriptional regulator, ACIAD0746, from Acinetobacter baylyi
Authors	:	Momany, C.; Nune, M.; Brondani, J.C.; Afful, D.; Neidle, E.; Galloway, N.R.
Deposited on	:	2023-04-03
Resolution	:	2.29 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:

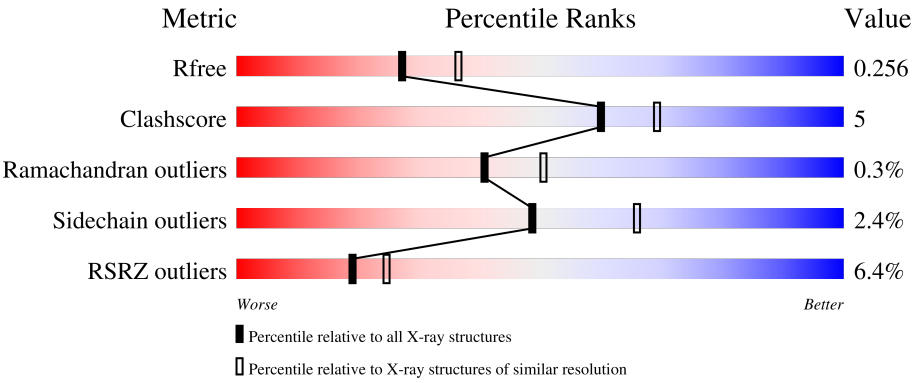
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	300	89% 9%
1	B	300	6% 87% 10%
1	C	300	3% 89% 9%
1	D	300	15% 79% 18%

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
4	GOL	B	402	-	-	-	X
4	GOL	B	403	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19224 atoms, of which 9401 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 transcriptional regulator (LysR family).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	H	N	O	S	0	3	0
			4655	1461	2349	410	421	14			
1	C	295	Total	C	H	N	O	S	0	1	0
			4646	1459	2343	409	421	14			
1	B	295	Total	C	H	N	O	S	0	1	0
			4656	1461	2350	411	420	14			
1	D	293	Total	C	H	N	O	S	0	1	0
			4626	1452	2335	408	417	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	HIS	-	expression tag	UNP Q6FE56
A	297	HIS	-	expression tag	UNP Q6FE56
A	298	HIS	-	expression tag	UNP Q6FE56
A	299	HIS	-	expression tag	UNP Q6FE56
A	300	HIS	-	expression tag	UNP Q6FE56
C	296	HIS	-	expression tag	UNP Q6FE56
C	297	HIS	-	expression tag	UNP Q6FE56
C	298	HIS	-	expression tag	UNP Q6FE56
C	299	HIS	-	expression tag	UNP Q6FE56
C	300	HIS	-	expression tag	UNP Q6FE56
B	296	HIS	-	expression tag	UNP Q6FE56
B	297	HIS	-	expression tag	UNP Q6FE56
B	298	HIS	-	expression tag	UNP Q6FE56
B	299	HIS	-	expression tag	UNP Q6FE56
B	300	HIS	-	expression tag	UNP Q6FE56
D	296	HIS	-	expression tag	UNP Q6FE56
D	297	HIS	-	expression tag	UNP Q6FE56
D	298	HIS	-	expression tag	UNP Q6FE56
D	299	HIS	-	expression tag	UNP Q6FE56
D	300	HIS	-	expression tag	UNP Q6FE56

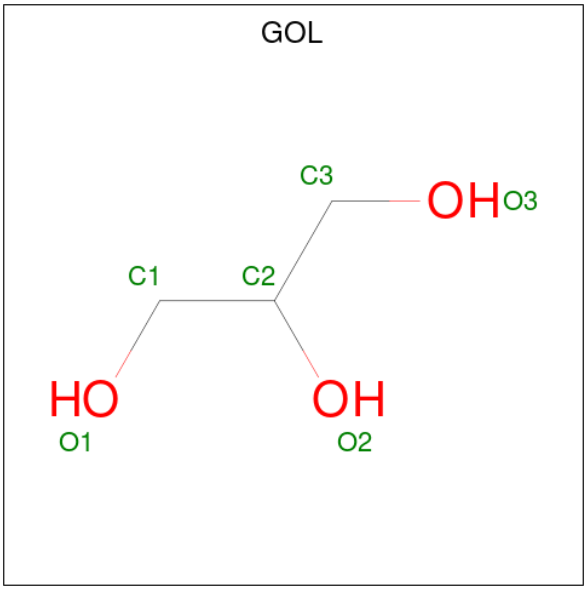
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0

- Molecule 5 is water.

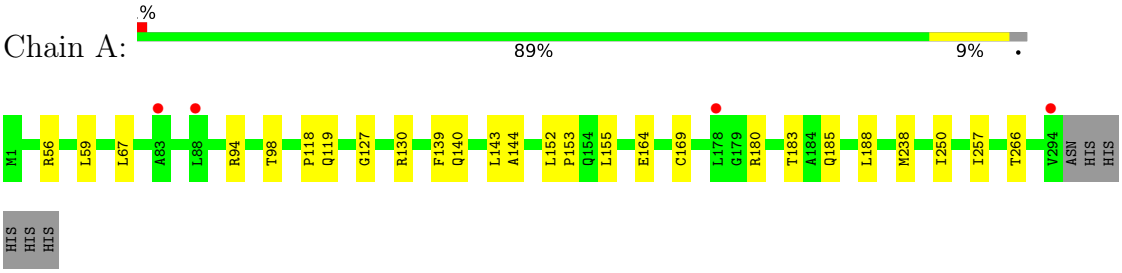
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	159	Total O 159 159	0	0
5	C	184	Total O 187 187	0	3
5	B	136	Total O 138 138	0	2
5	D	105	Total O 108 108	0	3

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.

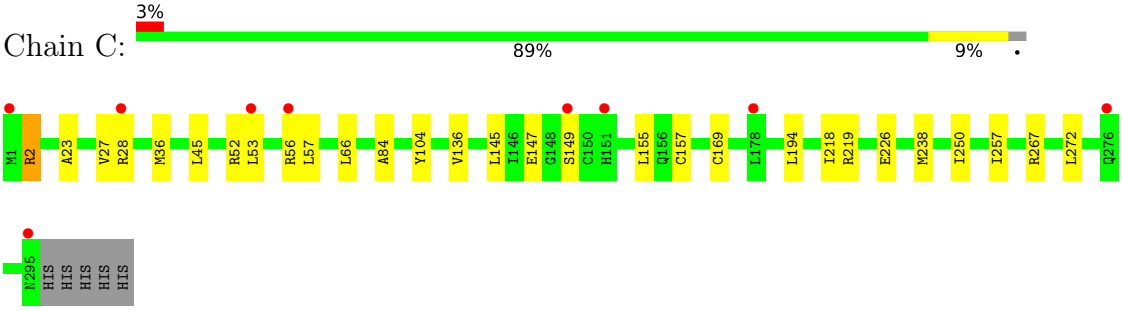
• Molecule 1: Putative transcriptional regulator (LysR family)

Chain A:



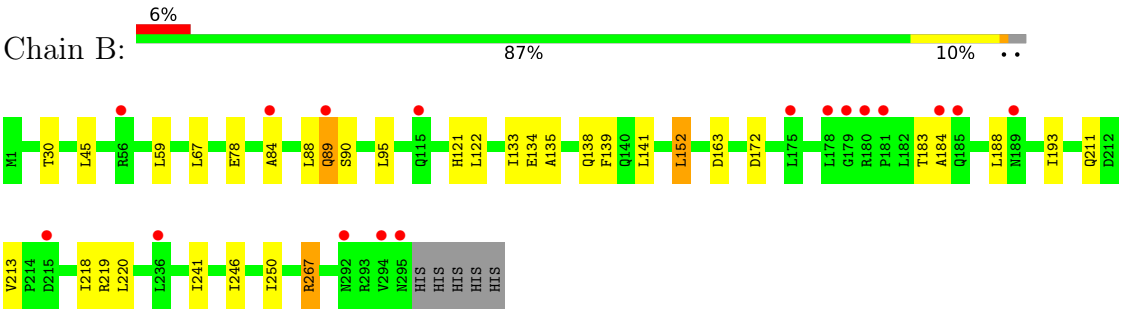
• Molecule 1: Putative transcriptional regulator (LysR family)

Chain C:



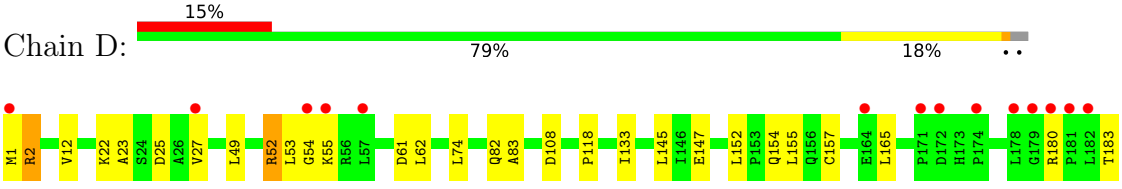
• Molecule 1: Putative transcriptional regulator (LysR family)

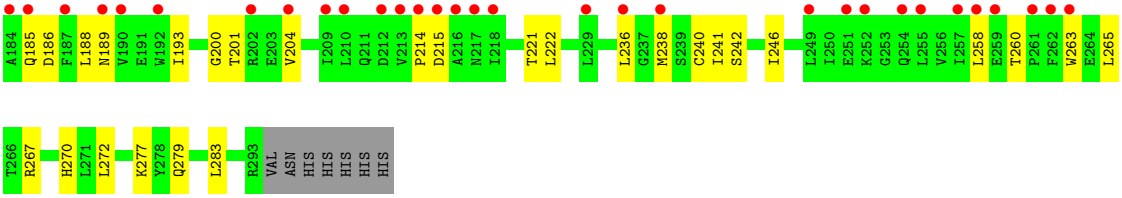
Chain B:



• Molecule 1: Putative transcriptional regulator (LysR family)

Chain D:




A184
Q185
D186
F187
L188
N189
V190
E191
W192
I193
G200
T201
R202
E203
V204
I209
L210
Q211
D212
V213
P214
D215
A216
N217
I218
T221
L222
L229
L236
G237
M238
S239
C240
I241
S242
I246
L249
I250
E251
K252
G253
Q254
L255
V256
I257
L258
E259
T260
P261
F262
W263
E264
L265

T266
R267
H270
L271
L272
K277
Y278
Q279
L283
R293
VAL
ASN
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.60Å 109.69Å 110.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.45 – 2.29 48.77 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.7 (26.45-2.29) 95.1 (48.77-2.29)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.211 , 0.258 0.211 , 0.256	Depositor DCC
R_{free} test set	2912 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k 0.015 for -l,-k,-h 0.015 for k,h,-l 0.004 for k,l,h 0.004 for l,h,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19224	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NA, GOL, MG

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	0.25	0/2356	0.49	0/3193
1	B	0.25	0/2348	0.50	0/3182
1	C	0.25	0/2345	0.49	0/3179
1	D	0.25	0/2333	0.51	0/3161
All	All	0.25	0/9382	0.50	0/12715

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	2306	2349	2337	13	0
1	B	2306	2350	2350	29	0
1	C	2303	2343	2343	18	0
1	D	2291	2335	2335	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	18	24	24	5	0
5	A	159	0	0	0	0
5	B	138	0	0	0	0
5	C	187	0	0	0	0
5	D	108	0	0	1	0
All	All	9823	9401	9389	85	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 (85) 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:D:165:LEU:HD11	1:D:204:VAL:HG11	1.49	0.94
1:B:188:LEU:HD13	1:B:213:VAL:HG13	1.70	0.72
1:B:133:ILE:HG21	1:B:152:LEU:HD13	1.71	0.71
1:B:193:ILE:HD12	1:B:220:LEU:HD12	1.72	0.70
1:D:165:LEU:HD12	1:D:265:LEU:HB3	1.74	0.70
1:C:66:LEU:HD11	1:B:84:ALA:HB2	1.74	0.69
1:D:185:GLN:O	1:D:188:LEU:HD22	1.94	0.68
1:B:134:GLU:OE2	1:B:138:GLN:NE2	2.27	0.67
1:B:211:GLN:OE1	1:B:211:GLN:N	2.28	0.67
1:D:238:MET:HE2	1:D:258:LEU:HD11	1.77	0.66
1:A:143:LEU:HD23	1:A:144:ALA:N	2.10	0.66
1:D:23:ALA:O	1:D:27:VAL:HG22	1.97	0.65
1:C:45:LEU:HD22	1:B:84:ALA:HB3	1.78	0.65
1:D:165:LEU:HD11	1:D:204:VAL:CG1	2.28	0.62
1:D:201:THR:HG21	1:D:241:ILE:HD12	1.81	0.62
1:C:52:ARG:O	1:C:53:LEU:HD23	2.01	0.59
1:A:59:LEU:HD11	1:A:67:LEU:HD22	1.86	0.57
1:B:133:ILE:CG2	1:B:152:LEU:HD13	2.35	0.57
1:D:152:LEU:HD23	1:D:154:GLN:NE2	2.21	0.56
1:C:155:LEU:HD13	1:C:272:LEU:HD11	1.88	0.55
1:D:193:ILE:HD11	1:D:236:LEU:HD12	1.89	0.54
1:D:49:LEU:HD23	1:D:62:LEU:HD23	1.88	0.54
1:B:30:THR:HG21	4:B:402:GOL:H32	1.90	0.54
1:C:136:VAL:HG11	1:C:272:LEU:HD13	1.90	0.54
1:D:165:LEU:HD13	1:D:240:CYS:SG	2.48	0.53
1:B:246:ILE:HG22	1:B:250:ILE:HG12	1.91	0.53
1:B:246:ILE:HG22	1:B:250:ILE:CG1	2.39	0.53
1:D:157:CYS:SG	1:D:270:HIS:ND1	2.64	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:LEU:HD22	1:B:84:ALA:CB	2.40	0.51
1:B:78:GLU:HG3	4:B:403:GOL:H31	1.91	0.51
1:D:260:THR:HG21	1:D:263:TRP:HE3	1.76	0.51
1:B:59:LEU:HD11	1:B:67:LEU:HD22	1.92	0.51
1:D:52:ARG:O	1:D:53:LEU:HD22	2.10	0.51
1:B:219:ARG:NH2	1:D:118:PRO:O	2.43	0.51
1:A:118:PRO:O	1:C:219:ARG:NH2	2.41	0.50
1:D:238:MET:CE	1:D:258:LEU:HD11	2.40	0.50
1:A:153:PRO:HB3	1:B:218:ILE:HD12	1.94	0.49
1:D:241:ILE:HG22	1:D:246:ILE:HD11	1.93	0.49
1:C:28:ARG:NE	1:C:28:ARG:O	2.45	0.49
1:D:260:THR:HG21	1:D:263:TRP:CE3	2.48	0.48
1:C:104:TYR:OH	1:C:226:GLU:OE2	2.25	0.48
1:D:279:GLN:HG2	1:D:283:LEU:HD23	1.96	0.48
1:A:119:GLN:OE1	1:A:119:GLN:N	2.35	0.48
1:B:135:ALA:CB	1:B:141:LEU:HD12	2.45	0.47
1:B:135:ALA:HB3	1:B:141:LEU:HD12	1.97	0.47
1:B:193:ILE:HD11	4:B:401:GOL:H11	1.96	0.47
1:C:84:ALA:HB3	1:B:45:LEU:HD22	1.97	0.47
1:A:250:ILE:HD11	1:A:257:ILE:HG13	1.97	0.46
1:B:183:THR:HG22	1:B:184:ALA:N	2.31	0.46
1:D:165:LEU:HB3	1:D:242:SER:HA	1.97	0.46
1:A:67:LEU:HD23	1:A:139:PHE:CD2	2.51	0.46
1:A:183:THR:OG1	1:A:185:GLN:OE1	2.34	0.45
1:A:94:ARG:NH1	1:A:140:GLN:O	2.49	0.45
1:B:89:GLN:HG3	1:B:90:SER:N	2.32	0.45
1:D:12:VAL:HG21	1:D:74:LEU:HD12	1.99	0.45
1:A:169:CYS:HB3	1:A:238:MET:HG2	1.99	0.45
1:D:2:ARG:H	1:D:2:ARG:HD2	1.81	0.45
1:C:23:ALA:O	1:C:27:VAL:HG22	2.16	0.44
1:D:221:THR:O	1:D:222:LEU:HD23	2.17	0.44
1:B:121:HIS:C	1:B:122:LEU:HD23	2.38	0.44
1:D:133:ILE:HD13	1:D:272:LEU:HD21	2.00	0.44
1:D:147:GLU:HG3	1:D:200:GLY:HA3	2.00	0.44
1:D:183:THR:HG23	1:D:186:ASP:H	1.82	0.43
1:D:188:LEU:HD23	1:D:189:ASN:H	1.83	0.43
1:B:95:LEU:C	1:B:141:LEU:HD22	2.39	0.43
1:C:194:LEU:HD12	1:C:218:ILE:HD12	2.00	0.43
1:A:98:THR:HA	1:A:127:GLY:O	2.19	0.43
1:D:82:GLN:HG3	1:D:83:ALA:N	2.33	0.42
1:D:165:LEU:HD21	1:D:204:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLU:OE2	1:A:266:THR:HG22	2.19	0.42
1:D:155:LEU:HD23	1:D:272:LEU:HD11	2.02	0.42
1:B:30:THR:HG21	4:B:402:GOL:H11	2.01	0.41
1:D:277:LYS:NZ	5:D:420:HOH:O	2.53	0.41
1:C:52:ARG:HD3	1:C:57:LEU:HD21	2.02	0.41
1:C:169:CYS:HB3	1:C:238:MET:HG2	2.02	0.41
1:B:138:GLN:O	1:B:139:PHE:HB2	2.21	0.41
1:C:250:ILE:HD11	1:C:257:ILE:HG13	2.02	0.41
1:A:152:LEU:HD23	1:A:155:LEU:HG	2.02	0.41
1:B:172:ASP:OD1	1:B:172:ASP:N	2.45	0.41
1:C:147:GLU:O	1:C:267:ARG:HD2	2.20	0.40
1:B:163:ASP:OD2	1:B:267:ARG:NH1	2.54	0.40
1:C:2:ARG:N	1:C:2:ARG:HD3	2.35	0.40
1:C:145:LEU:HD12	1:C:145:LEU:N	2.36	0.40
1:B:30:THR:CB	4:B:402:GOL:H32	2.51	0.40
1:D:145:LEU:N	1:D:145:LEU:HD12	2.37	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	295/300 (98%)	285 (97%)	10 (3%)	0	100	100
1	B	294/300 (98%)	284 (97%)	9 (3%)	1 (0%)	41	50
1	C	294/300 (98%)	282 (96%)	12 (4%)	0	100	100
1	D	292/300 (97%)	280 (96%)	10 (3%)	2 (1%)	22	26
All	All	1175/1200 (98%)	1131 (96%)	41 (4%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89	GLN
1	D	54	GLY
1	D	214	PRO

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	248/251 (99%)	244 (98%)	4 (2%)	62	78
1	B	247/251 (98%)	243 (98%)	4 (2%)	62	78
1	C	247/251 (98%)	242 (98%)	5 (2%)	55	72
1	D	245/251 (98%)	234 (96%)	11 (4%)	27	39
All	All	987/1004 (98%)	963 (98%)	24 (2%)	49	66

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	130	ARG
1	A	180	ARG
1	A	188	LEU
1	C	2	ARG
1	C	36	MET
1	C	56	ARG
1	C	149	SER
1	C	157	CYS
1	B	88	LEU
1	B	152	LEU
1	B	241	ILE
1	B	267	ARG
1	D	1	MET
1	D	2	ARG
1	D	22	LYS
1	D	25	ASP
1	D	52	ARG
1	D	55	LYS

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Mol	Chain	Res	Type
1	D	61	ASP
1	D	108	ASP
1	D	180	ARG
1	D	215	ASP
1	D	267	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 10 ligands modelled in this entry, 7 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	$\#\|Z\| > 2$
4	GOL	B	403	-	5,5,5	0.87	0	5,5,5	1.10	0
4	GOL	B	402	-	5,5,5	0.86	0	5,5,5	1.11	1 (20%)
4	GOL	B	401	-	5,5,5	0.90	0	5,5,5	1.07	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
4	GOL	B	403	-	-	2/4/4/4	-
4	GOL	B	402	-	-	2/4/4/4	-
4	GOL	B	401	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	402	GOL	C3-C2-C1	-2.03	103.80	111.70

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	402	GOL	O1-C1-C2-C3
4	B	403	GOL	O1-C1-C2-C3
4	B	401	GOL	O1-C1-C2-C3
4	B	403	GOL	O1-C1-C2-O2
4	B	402	GOL	O1-C1-C2-O2
4	B	401	GOL	O2-C2-C3-O3
4	B	401	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	GOL	1	0
4	B	402	GOL	3	0
4	B	401	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	294/300 (98%)	0.14	4 (1%) 75 80	35, 57, 87, 110	0
1	B	295/300 (98%)	0.47	17 (5%) 23 29	32, 64, 101, 122	0
1	C	295/300 (98%)	0.15	9 (3%) 49 56	30, 56, 87, 106	0
1	D	293/300 (97%)	0.82	45 (15%) 2 3	40, 88, 159, 182	0
All	All	1177/1200 (98%)	0.40	75 (6%) 19 25	30, 63, 118, 182	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	214	PRO	11.4
1	A	294	VAL	7.3
1	D	192	TRP	6.9
1	D	213	VAL	6.8
1	B	294	VAL	6.0
1	D	216	ALA	6.0
1	D	54	GLY	5.5
1	B	295	ASN	5.4
1	D	182	LEU	5.4
1	C	295	ASN	5.4
1	D	215	ASP	5.2
1	D	212	ASP	4.8
1	D	1	MET	4.6
1	D	259	GLU	4.4
1	C	151	HIS	4.3
1	D	190	VAL	4.2
1	D	255	LEU	4.2
1	C	53	LEU	4.1
1	C	1	MET	4.1
1	D	55	LYS	4.1
1	D	251	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	187	PHE	4.0
1	D	210	LEU	4.0
1	C	149	SER	3.8
1	D	252	LYS	3.8
1	C	56	ARG	3.8
1	B	292	ASN	3.7
1	A	88	LEU	3.5
1	D	238	MET	3.4
1	D	178	LEU	3.4
1	D	181	PRO	3.3
1	D	263	TRP	3.2
1	D	171	PRO	3.2
1	D	261	PRO	3.1
1	D	180	ARG	3.0
1	D	179	GLY	2.9
1	D	217	ASN	2.9
1	D	254	GLN	2.9
1	D	258	LEU	2.9
1	D	236	LEU	2.8
1	B	84	ALA	2.8
1	A	83	ALA	2.7
1	B	181	PRO	2.7
1	D	257	ILE	2.7
1	D	185	GLN	2.7
1	D	229	LEU	2.6
1	D	174	PRO	2.6
1	D	209	ILE	2.6
1	B	180	ARG	2.6
1	B	115	GLN	2.6
1	B	89	GLN	2.6
1	D	184	ALA	2.6
1	B	175	LEU	2.5
1	B	178	LEU	2.5
1	B	179	GLY	2.5
1	D	218	ILE	2.5
1	D	262	PHE	2.4
1	A	178	LEU	2.4
1	D	172	ASP	2.4
1	D	249	LEU	2.3
1	B	185	GLN	2.3
1	B	184	ALA	2.3
1	C	28	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	27	VAL	2.2
1	C	178	LEU	2.2
1	B	189	ASN	2.2
1	D	57	LEU	2.2
1	B	56	ARG	2.2
1	D	204	VAL	2.2
1	B	236	LEU	2.2
1	D	164	GLU	2.1
1	D	189	ASN	2.1
1	C	276	GLN	2.1
1	B	215	ASP	2.1
1	D	202	ARG	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, 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
4	GOL	B	402	6/6	0.55	0.55	95,133,157,169	0
4	GOL	B	403	6/6	0.60	0.54	99,135,156,163	0
2	NA	A	401	1/1	0.79	0.20	76,76,76,76	0
4	GOL	B	401	6/6	0.79	0.39	103,133,160,160	0
3	MG	B	404	1/1	0.80	0.23	85,85,85,85	0
3	MG	C	402	1/1	0.90	0.07	90,90,90,90	0
3	MG	C	401	1/1	0.93	0.09	69,69,69,69	0
3	MG	B	405	1/1	0.94	0.15	58,58,58,58	0
2	NA	B	406	1/1	0.94	0.25	74,74,74,74	0
2	NA	C	403	1/1	0.97	0.29	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.