Full wwPDB X-ray Structure Validation Report (i)

Jan 24, 2021 – 01:33 PM EST

PDB ID	:	3BH1
Title	:	Crystal structure of protein DIP2346 from Corynebacterium diphtheriae
Authors	:	Patskovsky, Y.; Sridhar, V.; Bonanno, J.B.; Gilmore, M.; Iizuka, M.; Groshong, C.; Gheyi, T.; Wasserman, S.R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-11-27
Resolution	:	2.51 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 (i) symbol.

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

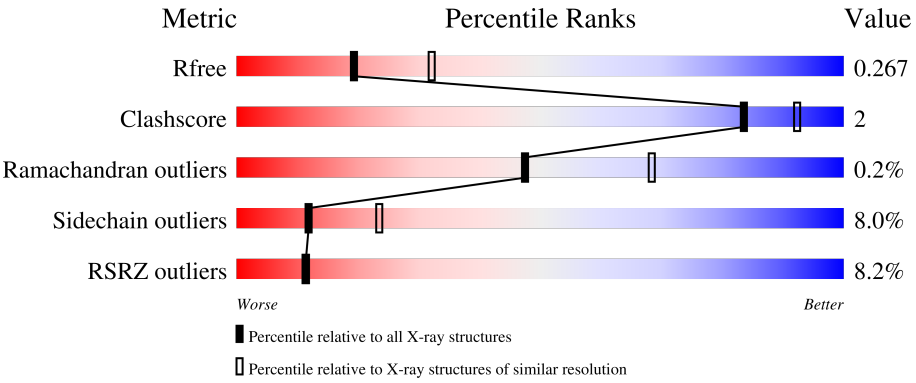
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	507	85% 10% • •
1	B	507	3% 84% 11% • •
1	C	507	14% 84% 10% • 5%
1	D	507	14% 83% 12% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15333 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 UPF0371 protein DIP2346.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	7	0
			3811	2384	677	733	17			
1	B	486	Total	C	N	O	S	0	7	0
			3819	2387	679	736	17			
1	C	483	Total	C	N	O	S	0	3	0
			3771	2359	672	722	18			
1	D	487	Total	C	N	O	S	0	2	0
			3791	2369	674	731	17			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q6NEC9
A	0	SER	-	expression tag	UNP Q6NEC9
A	1	LEU	-	expression tag	UNP Q6NEC9
A	498	GLU	-	expression tag	UNP Q6NEC9
A	499	GLY	-	expression tag	UNP Q6NEC9
A	500	HIS	-	expression tag	UNP Q6NEC9
A	501	HIS	-	expression tag	UNP Q6NEC9
A	502	HIS	-	expression tag	UNP Q6NEC9
A	503	HIS	-	expression tag	UNP Q6NEC9
A	504	HIS	-	expression tag	UNP Q6NEC9
A	505	HIS	-	expression tag	UNP Q6NEC9
B	-1	MET	-	expression tag	UNP Q6NEC9
B	0	SER	-	expression tag	UNP Q6NEC9
B	1	LEU	-	expression tag	UNP Q6NEC9
B	498	GLU	-	expression tag	UNP Q6NEC9
B	499	GLY	-	expression tag	UNP Q6NEC9
B	500	HIS	-	expression tag	UNP Q6NEC9
B	501	HIS	-	expression tag	UNP Q6NEC9
B	502	HIS	-	expression tag	UNP Q6NEC9
B	503	HIS	-	expression tag	UNP Q6NEC9
B	504	HIS	-	expression tag	UNP Q6NEC9

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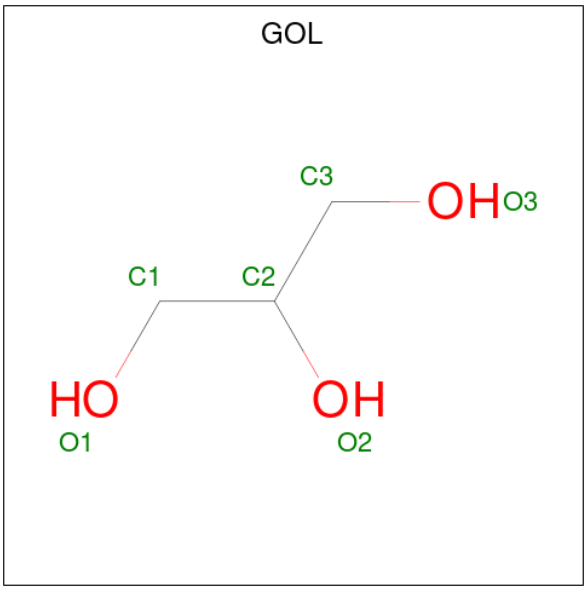
Chain	Residue	Modelled	Actual	Comment	Reference
B	505	HIS	-	expression tag	UNP Q6NEC9
C	-1	MET	-	expression tag	UNP Q6NEC9
C	0	SER	-	expression tag	UNP Q6NEC9
C	1	LEU	-	expression tag	UNP Q6NEC9
C	498	GLU	-	expression tag	UNP Q6NEC9
C	499	GLY	-	expression tag	UNP Q6NEC9
C	500	HIS	-	expression tag	UNP Q6NEC9
C	501	HIS	-	expression tag	UNP Q6NEC9
C	502	HIS	-	expression tag	UNP Q6NEC9
C	503	HIS	-	expression tag	UNP Q6NEC9
C	504	HIS	-	expression tag	UNP Q6NEC9
C	505	HIS	-	expression tag	UNP Q6NEC9
D	-1	MET	-	expression tag	UNP Q6NEC9
D	0	SER	-	expression tag	UNP Q6NEC9
D	1	LEU	-	expression tag	UNP Q6NEC9
D	498	GLU	-	expression tag	UNP Q6NEC9
D	499	GLY	-	expression tag	UNP Q6NEC9
D	500	HIS	-	expression tag	UNP Q6NEC9
D	501	HIS	-	expression tag	UNP Q6NEC9
D	502	HIS	-	expression tag	UNP Q6NEC9
D	503	HIS	-	expression tag	UNP Q6NEC9
D	504	HIS	-	expression tag	UNP Q6NEC9
D	505	HIS	-	expression tag	UNP Q6NEC9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

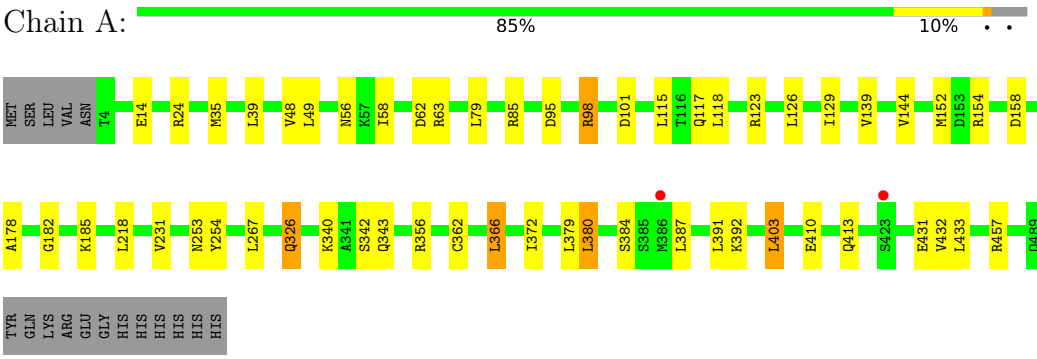
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	47	Total O 47 47	0	0
3	B	35	Total O 35 35	0	0
3	C	29	Total O 29 29	0	0
3	D	6	Total O 6 6	0	0

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.

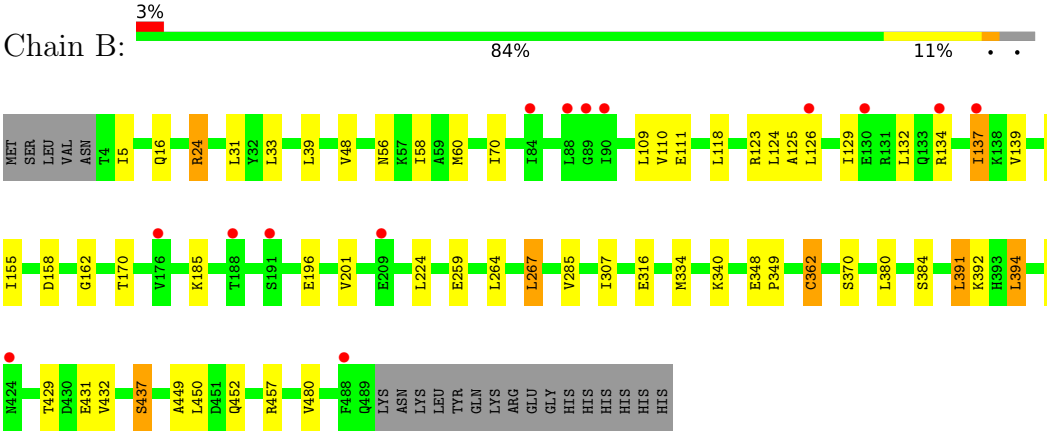
• Molecule 1: UPF0371 protein DIP2346

Chain A:



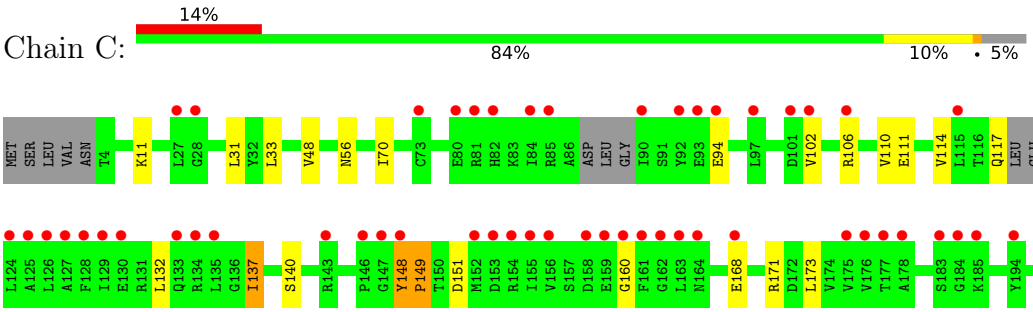
• Molecule 1: UPF0371 protein DIP2346

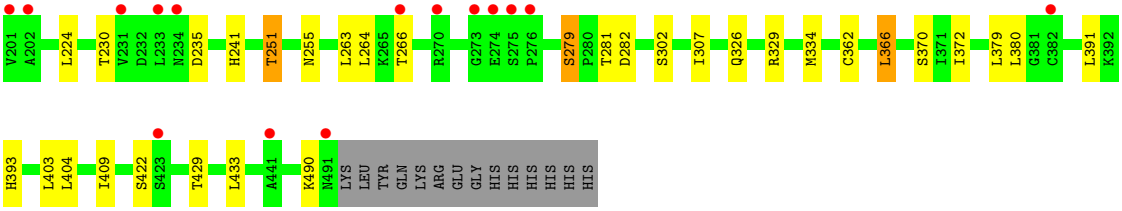
Chain B:



• Molecule 1: UPF0371 protein DIP2346

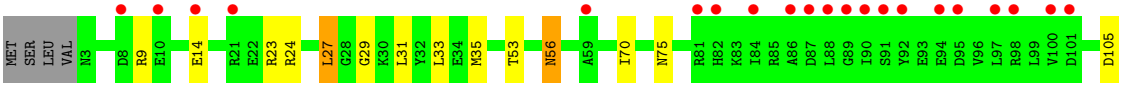
Chain C:

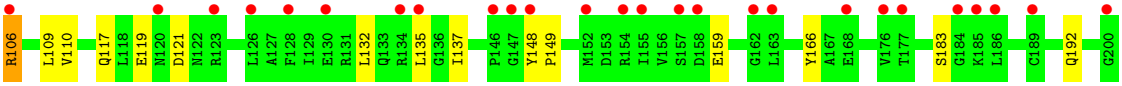


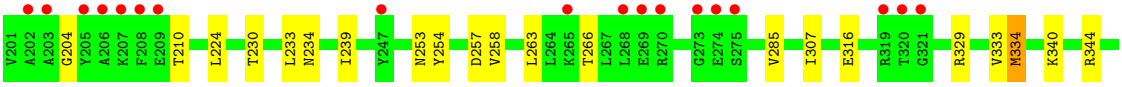


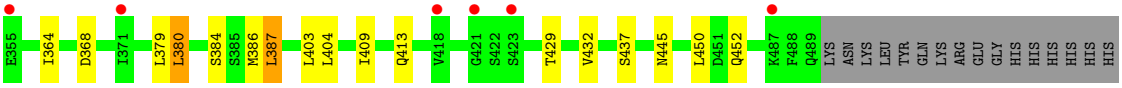
• Molecule 1: UPF0371 protein DIP2346

Chain D:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.45Å 138.94Å 98.27Å 90.00° 116.49° 90.00°	Depositor
Resolution (Å)	20.00 – 2.51 34.27 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.51) 98.7 (34.27-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.211 , 0.271 0.212 , 0.267	Depositor DCC
R_{free} test set	1544 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15333	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: 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	0.38	1/3893 (0.0%)	0.58	0/5269
1	B	0.38	1/3898 (0.0%)	0.59	0/5275
1	C	0.37	1/3839 (0.0%)	0.57	0/5191
1	D	0.37	1/3858 (0.0%)	0.54	0/5223
All	All	0.37	4/15488 (0.0%)	0.57	0/20958

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	362	CYS	CB-SG	-5.85	1.72	1.81
1	D	119	GLU	CD-OE2	5.10	1.31	1.25
1	C	362	CYS	CB-SG	-5.07	1.73	1.81
1	A	362	CYS	CB-SG	-5.04	1.73	1.81

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	3811	0	3831	18	0
1	B	3819	0	3829	20	0
1	C	3771	0	3787	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3791	0	3794	20	0
2	A	12	0	16	1	0
2	B	12	0	16	1	0
3	A	47	0	0	0	0
3	B	35	0	0	0	0
3	C	29	0	0	1	0
3	D	6	0	0	0	0
All	All	15333	0	15273	73	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 2.

All (73) 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:152:MET:HE1	1:B:267:LEU:HA	1.55	0.87
1:A:253:ASN:HD22	1:A:254:TYR:H	1.34	0.73
1:B:384:SER:HB3	1:B:432:VAL:HG21	1.76	0.67
1:C:307:ILE:HG12	1:C:334:MET:HE2	1.78	0.66
1:A:182:GLY:H	2:A:506:GOL:H32	1.61	0.66
1:A:152:MET:HE1	1:A:267:LEU:HA	1.76	0.65
1:A:379:LEU:HG	1:A:380:LEU:HD13	1.79	0.65
1:A:253:ASN:ND2	1:A:254:TYR:H	1.96	0.63
1:A:384:SER:HB3	1:A:432:VAL:HG21	1.81	0.62
1:A:117:GLN:HG3	1:A:144:VAL:HG22	1.80	0.62
1:B:348:GLU:HG2	1:B:349:PRO:HD3	1.81	0.61
1:C:393:HIS:CD2	3:C:529:HOH:O	2.57	0.56
1:D:24:ARG:HB3	1:D:31:LEU:HB2	1.87	0.56
1:B:39:LEU:HB3	1:B:58:ILE:HD11	1.88	0.55
1:A:340:LYS:HG3	1:A:342:SER:H	1.72	0.55
1:A:129:ILE:HG12	1:A:139:VAL:HG11	1.90	0.53
1:B:132:LEU:HD22	1:B:137:ILE:HD11	1.89	0.53
1:B:196:GLU:HG3	1:B:201:VAL:HB	1.90	0.53
1:B:307:ILE:HG12	1:B:334:MET:HE3	1.89	0.53
1:D:27:LEU:HD12	1:D:204:GLY:HA3	1.92	0.51
1:A:35:MET:HG3	1:A:175:VAL:HG13	1.93	0.50
1:C:111:GLU:HA	1:C:137:ILE:HG22	1.93	0.50
1:B:111:GLU:HA	1:B:137:ILE:HG22	1.94	0.49
1:B:394:LEU:HD13	1:B:452:GLN:HB3	1.95	0.48
1:C:279:SER:HB2	1:C:282:ASP:H	1.77	0.48
1:B:185:LYS:H	2:B:506:GOL:H12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:THR:HG21	1:C:281:THR:HG21	1.95	0.47
1:D:132:LEU:HB3	1:D:137:ILE:HD11	1.96	0.47
1:D:253:ASN:HD22	1:D:258:VAL:HG23	1.78	0.47
1:A:326[A]:GLN:H	1:A:326[A]:GLN:HE21	1.61	0.47
1:B:125:ALA:O	1:B:129:ILE:HG12	2.14	0.47
1:D:379:LEU:HG	1:D:380:LEU:HD13	1.97	0.47
1:A:48:VAL:HG12	1:A:49:LEU:HG	1.97	0.47
1:B:158:ASP:HA	1:B:162:GLY:HA3	1.96	0.47
1:D:384:SER:HB3	1:D:432:VAL:HG21	1.97	0.47
1:B:70:ILE:HB	1:B:110:VAL:HG22	1.96	0.47
1:D:253:ASN:ND2	1:D:254:TYR:H	2.12	0.47
1:B:392:LYS:HG3	1:B:403:LEU:HD21	1.95	0.46
1:C:132:LEU:HB3	1:C:137:ILE:HG13	1.97	0.46
1:C:366:LEU:HD22	1:C:372:ILE:HD13	1.97	0.46
1:A:39:LEU:HB3	1:A:58:ILE:HD11	1.97	0.46
1:C:379:LEU:HD11	1:C:409:ILE:HG21	1.97	0.46
1:D:166:TYR:HA	1:D:192:GLN:HE22	1.81	0.45
1:A:95:ASP:OD2	1:A:98:ARG:NH1	2.49	0.45
1:C:48:VAL:HG13	1:C:302:SER:HB3	1.98	0.45
1:B:148:TYR:HA	1:B:155:ILE:HD11	1.99	0.45
1:C:149:PRO:HB2	1:C:263:LEU:HD13	1.99	0.45
1:D:70:ILE:HB	1:D:110:VAL:HG22	1.99	0.45
1:C:70:ILE:HB	1:C:110:VAL:HG22	1.98	0.45
1:A:392:LYS:HG3	1:A:403:LEU:HD21	1.98	0.45
1:C:148:TYR:HB2	1:C:149:PRO:HD3	1.99	0.45
1:C:404:LEU:HB3	1:C:409:ILE:HD11	1.99	0.44
1:D:75:ASN:HB2	1:D:183:SER:HA	1.99	0.44
1:A:366:LEU:HD22	1:A:372:ILE:HD13	1.98	0.44
1:D:387:LEU:HA	1:D:387:LEU:HD23	1.83	0.44
1:B:307:ILE:HG12	1:B:334:MET:CE	2.46	0.44
1:C:241:HIS:HB3	1:D:239:ILE:HD11	1.98	0.44
1:D:437:SER:HA	1:D:450:LEU:HD11	2.00	0.43
1:D:53:THR:O	1:D:56:ASN:HB2	2.18	0.43
1:B:437:SER:HA	1:B:450:LEU:HD11	2.00	0.43
1:C:114:VAL:HG22	1:C:140:SER:HB2	2.01	0.43
1:D:148:TYR:HA	1:D:149:PRO:HA	1.87	0.43
1:B:391:LEU:HG	1:B:449:ALA:O	2.19	0.42
1:D:253:ASN:HD21	1:D:257:ASP:HB2	1.84	0.42
1:A:152:MET:HE1	1:A:267:LEU:CA	2.47	0.42
1:D:404:LEU:HB3	1:D:409:ILE:HD11	2.02	0.42
1:B:24:ARG:HB3	1:B:31:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ALA:HB3	1:A:185[A]:LYS:HE2	2.02	0.41
1:D:307:ILE:HA	1:D:334:MET:HE3	2.04	0.40
1:C:31:LEU:HB3	1:C:173:LEU:HD12	2.02	0.40
1:B:16:GLN:HB3	1:B:60:MET:HG3	2.03	0.40
1:D:106[A]:ARG:H	1:D:106[A]:ARG:HG2	1.66	0.40
1:D:364:ILE:HB	1:D:386:MET:SD	2.61	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	491/507 (97%)	477 (97%)	14 (3%)	0	100	100
1	B	491/507 (97%)	479 (98%)	12 (2%)	0	100	100
1	C	480/507 (95%)	461 (96%)	17 (4%)	2 (0%)	34	54
1	D	487/507 (96%)	470 (96%)	16 (3%)	1 (0%)	47	68
All	All	1949/2028 (96%)	1887 (97%)	59 (3%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	29	GLY
1	C	149	PRO
1	C	160	GLY

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	418/431 (97%)	386 (92%)	32 (8%)	13 25
1	B	418/431 (97%)	385 (92%)	33 (8%)	12 24
1	C	412/431 (96%)	380 (92%)	32 (8%)	12 24
1	D	414/431 (96%)	377 (91%)	37 (9%)	9 19
All	All	1662/1724 (96%)	1528 (92%)	134 (8%)	12 23

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	24	ARG
1	A	56	ASN
1	A	62	ASP
1	A	63	ARG
1	A	79	LEU
1	A	85	ARG
1	A	98	ARG
1	A	101	ASP
1	A	115	LEU
1	A	118	LEU
1	A	123	ARG
1	A	126	LEU
1	A	154	ARG
1	A	158	ASP
1	A	170	THR
1	A	218	LEU
1	A	231	VAL
1	A	326[A]	GLN
1	A	326[B]	GLN
1	A	343	GLN
1	A	356	ARG
1	A	366	LEU
1	A	380	LEU
1	A	387	LEU
1	A	391	LEU
1	A	403	LEU
1	A	410	GLU
1	A	413	GLN
1	A	431	GLU

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Mol	Chain	Res	Type
1	A	433	LEU
1	A	457	ARG
1	B	5	ILE
1	B	24	ARG
1	B	33	LEU
1	B	48	VAL
1	B	56	ASN
1	B	109	LEU
1	B	118	LEU
1	B	123	ARG
1	B	124	LEU
1	B	126	LEU
1	B	134	ARG
1	B	137	ILE
1	B	139	VAL
1	B	170	THR
1	B	224	LEU
1	B	259	GLU
1	B	264	LEU
1	B	267	LEU
1	B	285	VAL
1	B	316	GLU
1	B	340	LYS
1	B	362	CYS
1	B	370	SER
1	B	380	LEU
1	B	391	LEU
1	B	394	LEU
1	B	399	ASP
1	B	403	LEU
1	B	429	THR
1	B	431	GLU
1	B	437	SER
1	B	457	ARG
1	B	480	VAL
1	C	11	LYS
1	C	33	LEU
1	C	56	ASN
1	C	94	GLU
1	C	102	VAL
1	C	106	ARG
1	C	117	GLN

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Mol	Chain	Res	Type
1	C	123	ARG
1	C	137	ILE
1	C	148	TYR
1	C	151	ASP
1	C	168	GLU
1	C	171	ARG
1	C	224	LEU
1	C	230	THR
1	C	235	ASP
1	C	251	THR
1	C	255	ASN
1	C	264	LEU
1	C	266	THR
1	C	279	SER
1	C	326	GLN
1	C	329	ARG
1	C	366	LEU
1	C	370	SER
1	C	380	LEU
1	C	391	LEU
1	C	403	LEU
1	C	422	SER
1	C	429	THR
1	C	433	LEU
1	C	490	LYS
1	D	9	ARG
1	D	14	GLU
1	D	23	ARG
1	D	27	LEU
1	D	33	LEU
1	D	35	MET
1	D	56	ASN
1	D	105	ASP
1	D	106[A]	ARG
1	D	106[B]	ARG
1	D	109	LEU
1	D	117	GLN
1	D	121	ASP
1	D	135	LEU
1	D	159	GLU
1	D	210	THR
1	D	224	LEU

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Mol	Chain	Res	Type
1	D	230	THR
1	D	233	LEU
1	D	234	ASN
1	D	263	LEU
1	D	266	THR
1	D	285	VAL
1	D	316	GLU
1	D	329	ARG
1	D	333	VAL
1	D	334	MET
1	D	340	LYS
1	D	344	ARG
1	D	368	ASP
1	D	380	LEU
1	D	387	LEU
1	D	403	LEU
1	D	413	GLN
1	D	429	THR
1	D	445	ASN
1	D	452	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	413	GLN
1	A	445	ASN
1	B	352	GLN
1	C	142	HIS
1	C	253	ASN
1	C	352	GLN
1	C	445	ASN
1	D	253	ASN
1	D	413	GLN

5.3.3 RNA

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)

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	$\#\|Z\| > 2$
2	GOL	B	506	-	5,5,5	0.35	0	5,5,5	0.50	0
2	GOL	A	507	-	5,5,5	0.38	0	5,5,5	0.18	0
2	GOL	B	507	-	5,5,5	0.37	0	5,5,5	0.31	0
2	GOL	A	506	-	5,5,5	0.34	0	5,5,5	0.41	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
2	GOL	B	506	-	-	4/4/4/4	-
2	GOL	A	507	-	-	3/4/4/4	-
2	GOL	B	507	-	-	3/4/4/4	-
2	GOL	A	506	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	507	GOL	O1-C1-C2-C3
2	B	506	GOL	C1-C2-C3-O3
2	A	506	GOL	C1-C2-C3-O3
2	B	506	GOL	O2-C2-C3-O3
2	A	507	GOL	O1-C1-C2-O2
2	A	506	GOL	O2-C2-C3-O3
2	B	506	GOL	O1-C1-C2-O2
2	B	507	GOL	O2-C2-C3-O3
2	B	506	GOL	O1-C1-C2-C3
2	B	507	GOL	O1-C1-C2-C3
2	B	507	GOL	O1-C1-C2-O2
2	A	507	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	506	GOL	1	0
2	A	506	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	486/507 (95%)	0.09	2 (0%) 92 93	45, 58, 77, 109	0
1	B	486/507 (95%)	0.23	14 (2%) 51 55	40, 58, 85, 104	0
1	C	483/507 (95%)	0.71	72 (14%) 2 2	38, 60, 98, 121	0
1	D	487/507 (96%)	0.71	71 (14%) 2 2	36, 61, 88, 107	0
All	All	1942/2028 (95%)	0.44	159 (8%) 11 11	36, 59, 88, 121	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	124	LEU	6.4
1	C	130	GLU	6.0
1	C	128	PHE	6.0
1	D	84	ILE	6.0
1	C	97	LEU	5.9
1	C	161	PHE	5.9
1	C	234	ASN	5.7
1	C	106	ARG	5.5
1	D	185	LYS	5.4
1	C	127	ALA	5.4
1	C	198	LYS	5.0
1	C	148	TYR	5.0
1	C	156	VAL	4.8
1	D	146	PRO	4.8
1	C	147	GLY	4.8
1	C	275	SER	4.7
1	C	273	GLY	4.7
1	C	231	VAL	4.6
1	C	146	PRO	4.6
1	D	274	GLU	4.5
1	C	90	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	123	ARG	4.5
1	C	201	VAL	4.4
1	C	134	ARG	4.4
1	C	154	ARG	4.4
1	C	233	LEU	4.4
1	C	121	ASP	4.3
1	D	273	GLY	4.3
1	C	153	ASP	4.3
1	D	90	ILE	4.2
1	D	81	ARG	4.2
1	C	155	ILE	4.1
1	C	84	ILE	4.1
1	D	147	GLY	4.0
1	D	88	LEU	4.0
1	C	158	ASP	4.0
1	D	123	ARG	4.0
1	C	82	HIS	3.9
1	B	134	ARG	3.9
1	C	177	THR	3.9
1	D	320	THR	3.9
1	D	155	ILE	3.8
1	C	491	ASN	3.8
1	C	270	ARG	3.7
1	C	274	GLU	3.7
1	D	92	TYR	3.7
1	D	157	SER	3.7
1	C	125	ALA	3.6
1	D	176	VAL	3.6
1	D	189	CYS	3.5
1	C	28	GLY	3.5
1	D	269	GLU	3.5
1	C	423	SER	3.5
1	D	135	LEU	3.4
1	D	268	LEU	3.3
1	C	135	LEU	3.3
1	D	101	ASP	3.3
1	C	202	ALA	3.3
1	C	93	GLU	3.3
1	D	423	SER	3.3
1	B	84	ILE	3.2
1	C	200	GLY	3.2
1	D	355	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	162	GLY	3.2
1	C	178	ALA	3.2
1	B	130	GLU	3.2
1	D	87	ASP	3.2
1	D	128	PHE	3.1
1	B	488	PHE	3.1
1	C	160	GLY	3.1
1	D	86	ALA	3.1
1	C	133	GLN	3.0
1	D	91	SER	3.0
1	D	126	LEU	3.0
1	C	159	GLU	3.0
1	C	168	GLU	3.0
1	C	81	ARG	3.0
1	D	158	ASP	3.0
1	B	424	ASN	2.9
1	C	126	LEU	2.9
1	D	148	TYR	2.9
1	C	129	ILE	2.9
1	C	73	CYS	2.9
1	D	106[A]	ARG	2.9
1	C	152	MET	2.8
1	D	97	LEU	2.8
1	D	319	ARG	2.8
1	A	423[A]	SER	2.8
1	C	27	LEU	2.8
1	C	185	LYS	2.7
1	D	184	GLY	2.7
1	D	168	GLU	2.7
1	D	120	ASN	2.7
1	D	371	ILE	2.7
1	D	82	HIS	2.6
1	D	130	GLU	2.6
1	D	21	ARG	2.6
1	D	186	LEU	2.6
1	D	203	ALA	2.6
1	B	176	VAL	2.5
1	C	115	LEU	2.5
1	D	10	GLU	2.5
1	D	265	LYS	2.5
1	B	88	LEU	2.4
1	B	137	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	162	GLY	2.4
1	B	90	ILE	2.4
1	D	208	PHE	2.4
1	D	134	ARG	2.4
1	C	176	VAL	2.4
1	C	194	TYR	2.4
1	D	89	GLY	2.3
1	D	207	LYS	2.3
1	C	276	PRO	2.3
1	D	59	ALA	2.3
1	D	270	ARG	2.3
1	D	321	GLY	2.3
1	D	98	ARG	2.3
1	C	85	ARG	2.3
1	D	275	SER	2.3
1	C	163	LEU	2.3
1	C	94	GLU	2.3
1	D	14	GLU	2.3
1	C	102	VAL	2.2
1	D	418	VAL	2.2
1	C	197	HIS	2.2
1	D	247	TYR	2.2
1	C	441	ALA	2.2
1	D	95	ASP	2.2
1	C	382	CYS	2.2
1	D	206	ALA	2.2
1	B	209[A]	GLU	2.2
1	D	209	GLU	2.2
1	D	177	THR	2.2
1	B	89	GLY	2.2
1	D	163	LEU	2.2
1	C	80	GLU	2.2
1	A	386	MET	2.1
1	B	188	THR	2.1
1	C	184	GLY	2.1
1	D	421	GLY	2.1
1	C	183	SER	2.1
1	C	175	VAL	2.1
1	B	126	LEU	2.1
1	D	200	GLY	2.1
1	C	266	THR	2.1
1	D	154	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	8	ASP	2.1
1	D	487	LYS	2.1
1	D	152	MET	2.1
1	D	202	ALA	2.1
1	B	191	SER	2.1
1	C	164	ASN	2.1
1	C	101	ASP	2.0
1	C	92	TYR	2.0
1	D	205	TYR	2.0
1	D	94	GLU	2.0
1	D	100	VAL	2.0
1	C	143	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
2	GOL	B	506	6/6	0.91	0.17	26,64,88,90	0
2	GOL	B	507	6/6	0.93	0.17	50,60,83,94	0
2	GOL	A	507	6/6	0.95	0.16	47,61,68,79	0
2	GOL	A	506	6/6	0.96	0.22	29,63,87,88	0

6.5 Other polymers (i)

There are no such residues in this entry.