Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2017 – 03:16 PM EST

PDB ID	:	5B1H
Title	:	Crystal structure of cystathionine beta-synthase from Lactobacillus plantarum
Authors	:	Matoba, Y.; Sugiyama, M.
Deposited on	:	2015-12-04
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

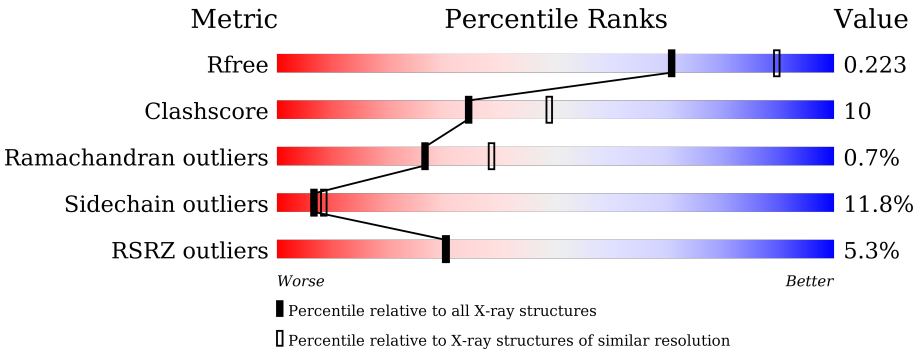
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	311	5% 74% 20%
1	B	311	5% 72% 22%
1	C	311	6% 72% 22%
1	D	311	5% 74% 20%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	406	-	-	-	X
3	GOL	A	407	-	-	-	X
3	GOL	B	403	-	-	-	X
3	GOL	B	405	-	-	-	X
3	GOL	B	406	-	-	-	X
3	GOL	C	405	-	-	-	X
3	GOL	C	406	-	-	-	X
3	GOL	D	404	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9736 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 Cystathionine beta-synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	P	S	0	2	0
			2294	1454	401	431	1	7			
1	B	303	Total	C	N	O	P	S	0	3	0
			2299	1457	403	431	1	7			
1	C	303	Total	C	N	O	P	S	0	2	0
			2294	1454	401	431	1	7			
1	D	303	Total	C	N	O	P	S	0	3	0
			2299	1457	403	431	1	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	304	LEU	-	expression tag	UNP F9UT54
A	305	GLU	-	expression tag	UNP F9UT54
A	306	HIS	-	expression tag	UNP F9UT54
A	307	HIS	-	expression tag	UNP F9UT54
A	308	HIS	-	expression tag	UNP F9UT54
A	309	HIS	-	expression tag	UNP F9UT54
A	310	HIS	-	expression tag	UNP F9UT54
A	311	HIS	-	expression tag	UNP F9UT54
B	304	LEU	-	expression tag	UNP F9UT54
B	305	GLU	-	expression tag	UNP F9UT54
B	306	HIS	-	expression tag	UNP F9UT54
B	307	HIS	-	expression tag	UNP F9UT54
B	308	HIS	-	expression tag	UNP F9UT54
B	309	HIS	-	expression tag	UNP F9UT54
B	310	HIS	-	expression tag	UNP F9UT54
B	311	HIS	-	expression tag	UNP F9UT54
C	304	LEU	-	expression tag	UNP F9UT54
C	305	GLU	-	expression tag	UNP F9UT54
C	306	HIS	-	expression tag	UNP F9UT54
C	307	HIS	-	expression tag	UNP F9UT54
C	308	HIS	-	expression tag	UNP F9UT54

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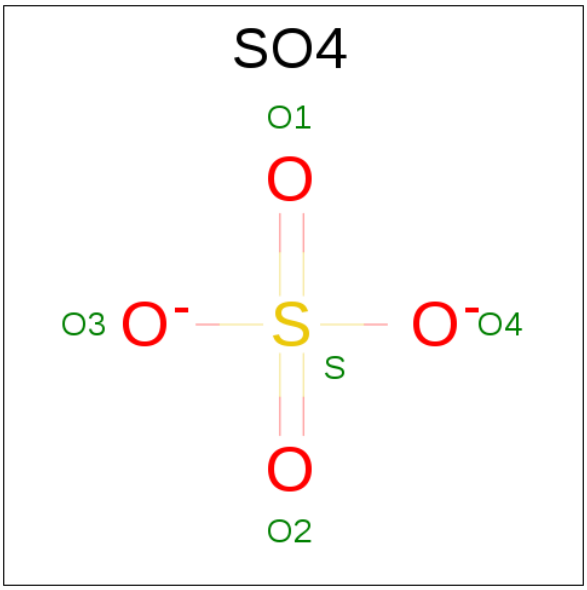
Chain	Residue	Modelled	Actual	Comment	Reference
C	309	HIS	-	expression tag	UNP F9UT54
C	310	HIS	-	expression tag	UNP F9UT54
C	311	HIS	-	expression tag	UNP F9UT54
D	304	LEU	-	expression tag	UNP F9UT54
D	305	GLU	-	expression tag	UNP F9UT54
D	306	HIS	-	expression tag	UNP F9UT54
D	307	HIS	-	expression tag	UNP F9UT54
D	308	HIS	-	expression tag	UNP F9UT54
D	309	HIS	-	expression tag	UNP F9UT54
D	310	HIS	-	expression tag	UNP F9UT54
D	311	HIS	-	expression tag	UNP F9UT54

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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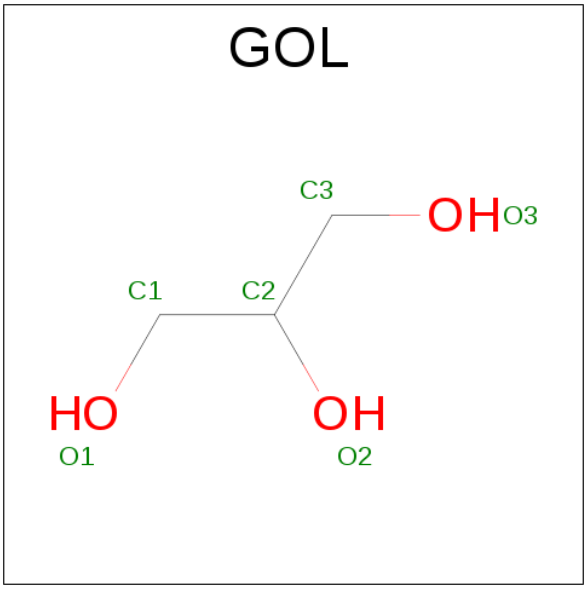
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

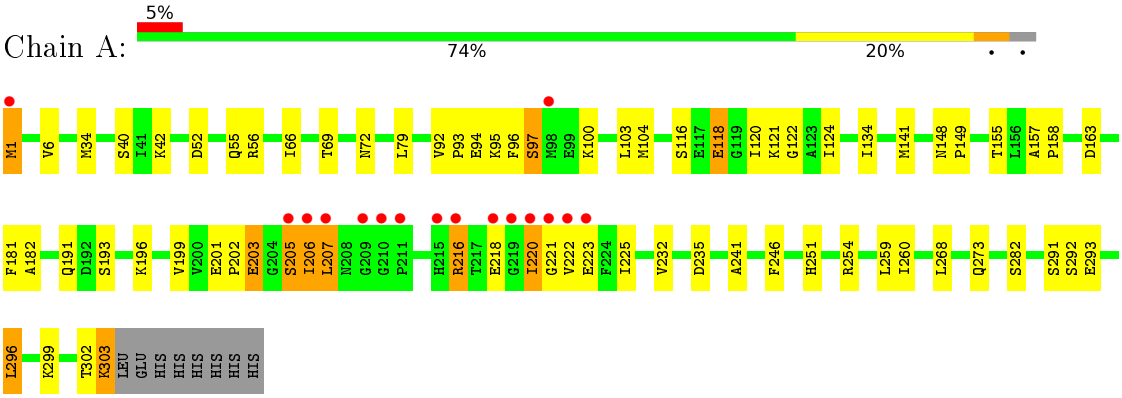
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		
4	B	107	Total	O	0	0
			107	107		
4	C	99	Total	O	0	0
			99	99		
4	D	104	Total	O	0	0
			104	104		

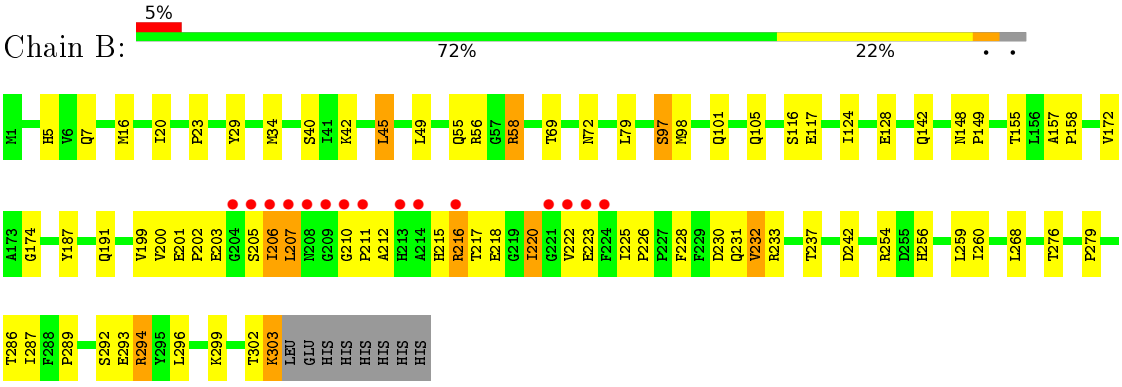
3 Residue-property plots (i)

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

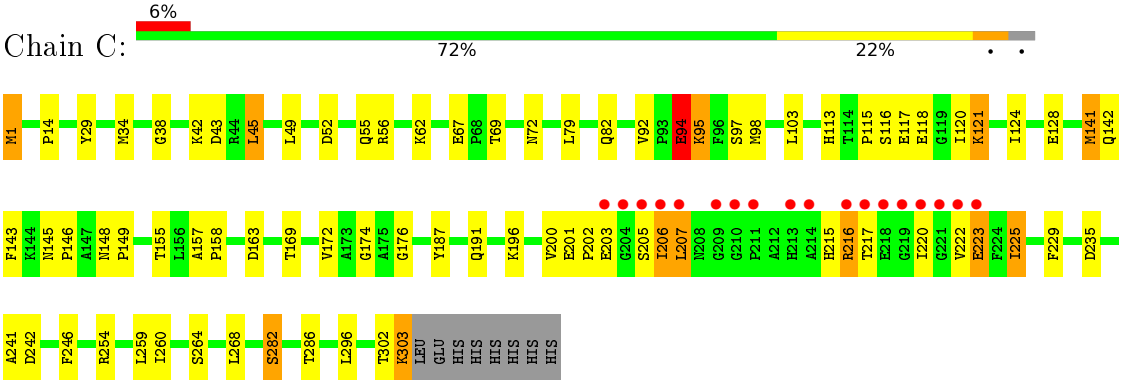
- Molecule 1: Cystathionine beta-synthase



- Molecule 1: Cystathionine beta-synthase

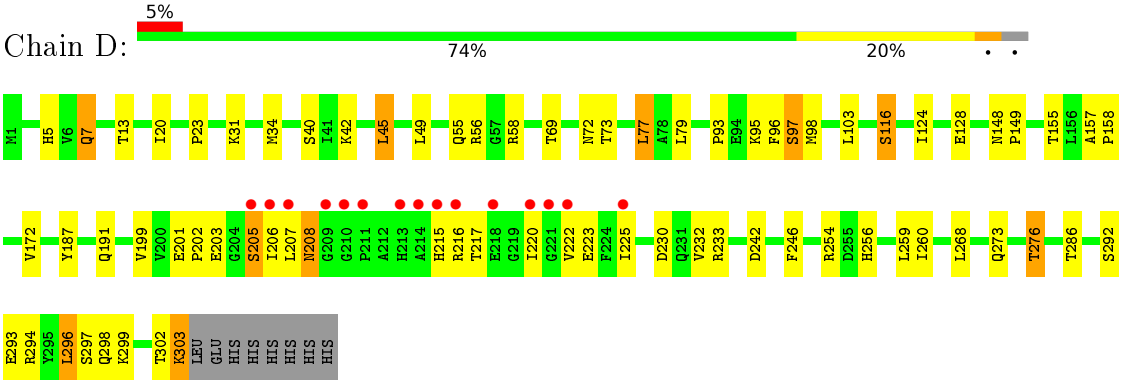


- Molecule 1: Cystathionine beta-synthase



• Molecule 1: Cystathionine beta-synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.89Å 146.34Å 82.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 2.40 46.06 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.49-2.40) 97.1 (46.06-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.189 , 0.221 0.190 , 0.223	Depositor DCC
R_{free} test set	3181 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.047 for k,h,-l 0.046 for -k,-h,-l 0.478 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9736	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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, LLP, SO4

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	0.32	0/2330	0.57	0/3171
1	B	0.33	0/2341	0.58	0/3186
1	C	0.32	0/2330	0.57	1/3171 (0.0%)
1	D	0.33	0/2341	0.59	0/3186
All	All	0.32	0/9342	0.57	1/12714 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	176	GLY	N-CA-C	-5.16	100.20	113.10

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	2294	0	2295	45	0
1	B	2299	0	2298	43	0
1	C	2294	0	2295	57	0
1	D	2299	0	2298	44	0
2	A	20	0	0	0	0
2	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	20	0	0	0	0
2	D	10	0	0	0	0
3	A	24	0	32	1	0
3	B	24	0	32	1	0
3	C	18	0	24	0	0
3	D	18	0	24	0	0
4	A	96	0	0	4	0
4	B	107	0	0	1	0
4	C	99	0	0	1	0
4	D	104	0	0	1	0
All	All	9736	0	9298	186	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 10.

All (186) 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:A:1:MET:HG2	1:C:14:PRO:HA	1.43	1.00
1:A:203:GLU:HG2	1:A:241:ALA:HA	1.43	0.98
1:D:201:GLU:OE1	1:D:207:LEU:HB2	1.68	0.94
1:B:202:PRO:HD3	1:B:220:ILE:HD12	1.51	0.92
1:A:1:MET:HA	4:A:577:HOH:O	1.70	0.90
1:D:202:PRO:HD3	1:D:220:ILE:HD12	1.59	0.85
1:C:207:LEU:HD12	1:C:222:VAL:HG21	1.59	0.84
1:A:220:ILE:HG12	1:A:221:GLY:H	1.46	0.80
1:A:202:PRO:HD3	1:A:220:ILE:HD13	1.66	0.77
1:D:45:LEU:HD22	1:D:49:LEU:HG	1.67	0.76
1:C:157:ALA:HB3	1:C:158:PRO:HD3	1.68	0.76
1:C:203:GLU:O	1:C:215:HIS:HB3	1.87	0.75
1:A:207:LEU:HD12	1:A:222:VAL:HG21	1.68	0.74
1:D:157:ALA:HB3	1:D:158:PRO:HD3	1.70	0.73
1:A:157:ALA:HB3	1:A:158:PRO:HD3	1.74	0.69
1:B:45:LEU:HD22	1:B:49:LEU:HG	1.75	0.69
1:B:157:ALA:HB3	1:B:158:PRO:HD3	1.75	0.68
1:B:5[B]:HIS:CE1	1:B:7:GLN:HG2	2.29	0.67
1:C:45:LEU:HD22	1:C:49:LEU:HG	1.75	0.66
1:A:299:LYS:HB3	1:A:302:THR:HB	1.76	0.66
1:D:5[B]:HIS:ND1	1:D:7:GLN:HB2	2.11	0.65
1:D:203:GLU:O	1:D:215:HIS:HB3	1.97	0.65
1:A:220:ILE:HG12	1:A:221:GLY:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:589:HOH:O	1:C:1:MET:HG2	1.98	0.64
1:C:148:ASN:HB3	1:C:149:PRO:CD	2.28	0.64
1:D:20:ILE:HG22	1:D:256:HIS:NE2	2.13	0.63
1:A:52:ASP:O	1:A:56:ARG:HG3	1.97	0.63
1:C:115:PRO:HB2	1:C:118:GLU:HG3	1.80	0.63
1:C:121:LYS:HZ2	1:C:121:LYS:HB2	1.64	0.63
1:D:42:LLP:NZ	1:D:42:LLP:O3	2.32	0.62
1:C:42:LLP:H2'1	1:C:72:ASN:ND2	2.14	0.62
1:B:124:ILE:O	1:B:128:GLU:HG3	2.00	0.62
1:C:42:LLP:H2'1	1:C:72:ASN:HD22	1.65	0.61
1:D:302:THR:HG22	1:D:303:LYS:H	1.66	0.61
1:A:163:ASP:OD2	1:C:1:MET:HB3	2.00	0.61
1:B:203:GLU:O	1:B:215:HIS:HB3	2.01	0.60
1:B:42:LLP:O3	1:B:42:LLP:NZ	2.34	0.60
1:B:56:ARG:NH2	1:B:58:ARG:HD3	2.17	0.60
1:C:202:PRO:HD3	1:C:220:ILE:HD12	1.83	0.60
1:D:202:PRO:CD	1:D:220:ILE:HD12	2.31	0.59
1:A:148:ASN:HB3	1:A:149:PRO:CD	2.33	0.58
1:B:279:PRO:HB2	3:B:406:GOL:H12	1.85	0.58
1:B:101:GLN:O	1:B:105:GLN:HG3	2.05	0.57
1:C:203:GLU:CG	1:C:241:ALA:HA	2.34	0.57
1:D:216:ARG:HB3	1:D:246:PHE:HE1	1.70	0.57
1:C:187:TYR:O	1:C:191:GLN:HG2	2.05	0.57
1:D:217:THR:HG21	1:D:220:ILE:HD11	1.87	0.57
1:B:155:THR:O	1:B:158:PRO:HD2	2.05	0.56
1:C:203:GLU:HG2	1:C:241:ALA:HA	1.88	0.56
1:A:260:ILE:O	1:A:292:SER:HB3	2.06	0.55
1:C:42:LLP:O3	1:C:42:LLP:NZ	2.37	0.55
1:A:120:ILE:O	1:A:124:ILE:HG13	2.07	0.55
1:D:201:GLU:OE2	1:D:208:ASN:HB2	2.06	0.55
1:B:20:ILE:HG22	1:B:256:HIS:NE2	2.22	0.54
1:B:206:ILE:HD11	1:B:223:GLU:C	2.28	0.54
1:B:302:THR:HG22	1:B:303:LYS:N	2.22	0.54
1:D:216:ARG:HB3	1:D:246:PHE:CE1	2.42	0.54
1:D:42:LLP:H2'1	1:D:72:ASN:ND2	2.23	0.53
1:A:291:SER:OG	1:A:293:GLU:HG3	2.08	0.53
1:C:141:MET:CE	1:C:143:PHE:HB2	2.39	0.53
1:A:118:GLU:HB3	1:A:122:GLY:HA3	1.91	0.53
1:C:52:ASP:O	1:C:56:ARG:HG3	2.09	0.53
1:B:294:ARG:NE	4:B:501:HOH:O	2.35	0.53
1:A:66:ILE:HD11	1:A:134:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LLP:O3	1:A:42:LLP:NZ	2.40	0.52
1:C:121:LYS:HE2	1:C:223:GLU:OE1	2.09	0.52
1:B:260:ILE:O	1:B:292:SER:HB3	2.09	0.52
1:B:202:PRO:HD3	1:B:220:ILE:CD1	2.33	0.52
1:B:207:LEU:HD22	1:B:222:VAL:HG21	1.91	0.52
1:A:202:PRO:HG3	1:A:220:ILE:HG23	1.92	0.52
1:B:56:ARG:CZ	1:B:58:ARG:HD3	2.40	0.52
1:A:181:PHE:CZ	1:A:199:VAL:HG22	2.45	0.52
1:C:38:GLY:N	1:C:43:ASP:OD2	2.36	0.51
1:B:199:VAL:HG13	1:B:237:THR:HG23	1.92	0.51
1:D:13:THR:OG1	1:D:31:LYS:HE3	2.11	0.51
1:B:42:LLP:H2'1	1:B:72:ASN:ND2	2.26	0.51
1:D:302:THR:HG22	1:D:303:LYS:N	2.25	0.50
1:C:260:ILE:HB	1:C:264:SER:CB	2.41	0.50
1:A:293:GLU:HA	1:A:296:LEU:HD22	1.94	0.49
1:D:56:ARG:NH2	1:D:58:ARG:HG3	2.27	0.49
1:C:155:THR:O	1:C:158:PRO:HD2	2.11	0.49
1:D:232:VAL:HG12	1:D:233:ARG:N	2.27	0.49
1:A:42:LLP:H2'1	1:A:72:ASN:ND2	2.28	0.49
1:B:206:ILE:HD11	1:B:223:GLU:O	2.13	0.49
1:D:225:ILE:HG23	1:D:225:ILE:O	2.13	0.49
1:D:187:TYR:O	1:D:191:GLN:HG2	2.12	0.48
1:B:232:VAL:CG2	1:B:233:ARG:N	2.75	0.48
1:B:148:ASN:HB3	1:B:149:PRO:CD	2.44	0.48
1:C:206:ILE:HD12	1:C:222:VAL:O	2.14	0.48
1:D:148:ASN:HB3	1:D:149:PRO:CD	2.44	0.48
1:D:124:ILE:O	1:D:128:GLU:HG3	2.13	0.48
1:C:202:PRO:CD	1:C:220:ILE:HD12	2.44	0.48
1:D:260:ILE:O	1:D:292:SER:HB3	2.13	0.48
1:C:225:ILE:HG23	1:C:225:ILE:O	2.14	0.47
1:C:141:MET:HE3	1:C:143:PHE:HB2	1.96	0.47
1:D:155:THR:O	1:D:158:PRO:HD2	2.15	0.47
1:B:228:PHE:O	1:B:231:GLN:HG2	2.15	0.47
1:B:216:ARG:H	1:B:242:ASP:CG	2.18	0.47
1:B:287:ILE:O	1:B:289:PRO:HD3	2.15	0.47
1:A:100:LYS:O	1:A:104:MET:HG3	2.15	0.47
1:C:148:ASN:HB3	1:C:149:PRO:HD3	1.97	0.46
1:D:58:ARG:NH2	4:D:501:HOH:O	2.47	0.46
1:B:225:ILE:HD12	1:B:226:PRO:HD2	1.97	0.46
1:A:203:GLU:HB3	4:A:586:HOH:O	2.14	0.46
1:A:42:LLP:H2'1	1:A:72:ASN:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:PRO:HB2	1:D:96:PHE:CD1	2.50	0.46
1:A:93:PRO:HB2	1:A:96:PHE:CG	2.51	0.46
1:A:1:MET:N	1:C:163:ASP:OD1	2.48	0.46
1:C:95:LYS:HG2	1:C:98:MET:HE1	1.97	0.46
1:B:187:TYR:O	1:B:191:GLN:HG2	2.15	0.46
1:C:201:GLU:OE1	1:C:207:LEU:HB3	2.16	0.46
1:A:216:ARG:HB3	1:A:246:PHE:CE1	2.50	0.45
1:A:207:LEU:HB2	1:A:222:VAL:HG21	1.98	0.45
1:C:216:ARG:HB2	1:C:242:ASP:OD2	2.16	0.45
1:D:296:LEU:C	1:D:298:GLN:H	2.20	0.45
1:A:182:ALA:HA	1:A:232:VAL:HG21	1.98	0.45
1:C:121:LYS:NZ	1:C:121:LYS:HB2	2.31	0.45
1:B:215:HIS:HD2	1:B:217:THR:O	1.99	0.45
1:A:207:LEU:HD12	1:A:222:VAL:CG2	2.42	0.45
1:A:302:THR:CG2	1:A:303:LYS:N	2.80	0.45
4:A:557:HOH:O	1:C:1:MET:HG3	2.17	0.45
1:A:196:LYS:HA	1:A:235:ASP:OD2	2.17	0.44
1:B:23:PRO:HG2	1:B:276:THR:HG22	1.99	0.44
1:B:207:LEU:CD2	1:B:222:VAL:HG21	2.47	0.44
1:D:172:VAL:O	1:D:286:THR:HA	2.18	0.44
1:C:207:LEU:HD11	1:C:229:PHE:HE2	1.82	0.44
1:B:202:PRO:CD	1:B:220:ILE:HD12	2.35	0.44
1:C:45:LEU:HD22	1:C:49:LEU:CG	2.45	0.44
1:D:207:LEU:HD11	1:D:222:VAL:HG21	1.99	0.44
1:B:16:MET:O	1:B:29:TYR:HA	2.18	0.44
1:C:157:ALA:HB1	1:C:187:TYR:CD2	2.52	0.44
1:C:302:THR:HG22	1:C:303:LYS:N	2.32	0.44
1:A:181:PHE:CE2	1:A:199:VAL:HG22	2.52	0.44
1:C:117:GLU:CD	1:C:117:GLU:H	2.19	0.44
1:C:29:TYR:CD1	1:C:29:TYR:N	2.86	0.44
1:A:1:MET:HG2	1:C:14:PRO:CA	2.30	0.44
1:B:206:ILE:H	1:B:206:ILE:HG13	1.56	0.44
3:A:406:GOL:H32	4:C:505:HOH:O	2.17	0.43
1:C:207:LEU:HD11	1:C:229:PHE:CE2	2.53	0.43
1:A:251[A]:HIS:CD2	1:A:254[A]:ARG:HH12	2.37	0.43
1:D:199:VAL:HG11	1:D:207:LEU:HD13	1.99	0.43
1:A:148:ASN:HB3	1:A:149:PRO:HD3	2.00	0.43
1:B:172:VAL:O	1:B:286:THR:HA	2.18	0.43
1:D:216:ARG:HB2	1:D:242:ASP:OD2	2.18	0.43
1:D:42:LLP:H2'1	1:D:72:ASN:HD22	1.83	0.43
1:B:174:GLY:HA2	1:B:200:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ILE:HG23	1:B:225:ILE:O	2.19	0.43
1:D:201:GLU:CD	1:D:205:SER:HB3	2.39	0.43
1:B:58:ARG:HB3	1:B:58:ARG:HE	1.71	0.43
1:C:120:ILE:O	1:C:124:ILE:HG13	2.18	0.43
1:A:201:GLU:OE1	1:A:205:SER:HB3	2.19	0.42
1:B:201:GLU:OE1	1:B:207:LEU:HB3	2.19	0.42
1:B:5[B]:HIS:HE1	1:B:7:GLN:HG2	1.82	0.42
1:D:95:LYS:HG2	1:D:116:SER:HB3	2.02	0.42
1:B:206:ILE:HG23	1:B:212:ALA:HB2	2.01	0.42
1:C:196:LYS:HA	1:C:235:ASP:OD2	2.20	0.42
1:D:45:LEU:HD22	1:D:49:LEU:CG	2.43	0.42
1:D:23:PRO:HG2	1:D:276:THR:HG22	2.00	0.42
1:D:93:PRO:HB2	1:D:96:PHE:CG	2.55	0.42
1:A:225:ILE:O	1:A:225:ILE:HG23	2.20	0.42
1:C:94:GLU:HA	1:C:113:HIS:CD2	2.55	0.42
1:D:206:ILE:HG13	1:D:223:GLU:O	2.20	0.42
1:D:96:PHE:CD1	1:D:96:PHE:N	2.88	0.41
1:A:1:MET:O	1:A:1:MET:CG	2.68	0.41
1:A:155:THR:O	1:A:158:PRO:HD2	2.20	0.41
1:C:260:ILE:HB	1:C:264:SER:HB2	2.03	0.41
1:C:169:THR:HG21	1:C:282:SER:OG	2.21	0.41
1:D:73:THR:O	1:D:77:LEU:HB2	2.21	0.41
1:D:96:PHE:N	1:D:96:PHE:HD1	2.19	0.41
1:C:141:MET:HE1	1:C:143:PHE:HB2	2.01	0.41
1:A:203:GLU:HG3	1:A:203:GLU:H	1.60	0.41
1:C:206:ILE:HD13	1:C:223:GLU:O	2.21	0.41
1:C:67:GLU:OE2	1:C:142:GLN:HG2	2.21	0.40
1:C:145:ASN:HA	1:C:146:PRO:HD3	1.92	0.40
1:A:206:ILE:HG13	1:A:223:GLU:O	2.20	0.40
1:C:174:GLY:HA2	1:C:200:VAL:HB	2.02	0.40
1:C:216:ARG:HD2	1:C:246:PHE:CZ	2.56	0.40
1:C:172:VAL:O	1:C:286:THR:HA	2.20	0.40
1:B:42:LLP:H2'1	1:B:72:ASN:HD22	1.85	0.40
1:C:203:GLU:CD	1:C:241:ALA:HA	2.42	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	302/311 (97%)	290 (96%)	11 (4%)	1 (0%)	46	63
1	B	303/311 (97%)	290 (96%)	9 (3%)	4 (1%)	15	21
1	C	302/311 (97%)	293 (97%)	7 (2%)	2 (1%)	26	38
1	D	303/311 (97%)	288 (95%)	14 (5%)	1 (0%)	46	63
All	All	1210/1244 (97%)	1161 (96%)	41 (3%)	8 (1%)	26	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	97	SER
1	B	211	PRO
1	C	97	SER
1	D	97	SER
1	C	94	GLU
1	A	97	SER
1	B	220	ILE
1	B	210	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	237/243 (98%)	206 (87%)	31 (13%)	5	6
1	B	238/243 (98%)	210 (88%)	28 (12%)	6	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	237/243 (98%)	209 (88%)	28 (12%)	6 8
1	D	238/243 (98%)	213 (90%)	25 (10%)	8 12
All	All	950/972 (98%)	838 (88%)	112 (12%)	6 8

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	VAL
1	A	34	MET
1	A	40	SER
1	A	55	GLN
1	A	69	THR
1	A	79	LEU
1	A	92	VAL
1	A	94	GLU
1	A	95	LYS
1	A	97	SER
1	A	103	LEU
1	A	116	SER
1	A	118	GLU
1	A	121	LYS
1	A	141	MET
1	A	191	GLN
1	A	193	SER
1	A	203	GLU
1	A	205	SER
1	A	206	ILE
1	A	207	LEU
1	A	216	ARG
1	A	218	GLU
1	A	220	ILE
1	A	259	LEU
1	A	268	LEU
1	A	273	GLN
1	A	282	SER
1	A	296	LEU
1	A	303	LYS
1	B	34	MET
1	B	40	SER
1	B	45	LEU

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Mol	Chain	Res	Type
1	B	55	GLN
1	B	58	ARG
1	B	69	THR
1	B	79	LEU
1	B	97	SER
1	B	98	MET
1	B	116	SER
1	B	117	GLU
1	B	142	GLN
1	B	205	SER
1	B	206	ILE
1	B	207	LEU
1	B	216	ARG
1	B	218	GLU
1	B	230	ASP
1	B	232	VAL
1	B	254[A]	ARG
1	B	254[B]	ARG
1	B	259	LEU
1	B	268	LEU
1	B	293	GLU
1	B	294	ARG
1	B	296	LEU
1	B	299	LYS
1	B	303	LYS
1	C	1	MET
1	C	34	MET
1	C	45	LEU
1	C	55	GLN
1	C	62	LYS
1	C	69	THR
1	C	79	LEU
1	C	82	GLN
1	C	92	VAL
1	C	94	GLU
1	C	95	LYS
1	C	103	LEU
1	C	116	SER
1	C	121	LYS
1	C	128	GLU
1	C	141	MET
1	C	205	SER

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Mol	Chain	Res	Type
1	C	206	ILE
1	C	207	LEU
1	C	216	ARG
1	C	217	THR
1	C	223	GLU
1	C	225	ILE
1	C	259	LEU
1	C	268	LEU
1	C	282	SER
1	C	296	LEU
1	C	303	LYS
1	D	7	GLN
1	D	34	MET
1	D	40	SER
1	D	45	LEU
1	D	55	GLN
1	D	69	THR
1	D	77	LEU
1	D	79	LEU
1	D	97	SER
1	D	98	MET
1	D	103	LEU
1	D	116	SER
1	D	205	SER
1	D	208	ASN
1	D	230	ASP
1	D	259	LEU
1	D	268	LEU
1	D	273	GLN
1	D	276	THR
1	D	293	GLU
1	D	294	ARG
1	D	296	LEU
1	D	297	SER
1	D	299	LYS
1	D	303	LYS

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

Mol	Chain	Res	Type
1	A	101	GLN
1	A	215	HIS

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Mol	Chain	Res	Type
1	A	231	GLN
1	B	236	GLN
1	D	25	HIS
1	D	55	GLN
1	D	84	HIS
1	D	208	ASN
1	D	213	HIS
1	D	215	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	A	42	1	22,24,25	2.09	8 (36%)	28,32,34	1.25	4 (14%)
1	LLP	B	42	1	22,24,25	1.95	8 (36%)	28,32,34	1.26	4 (14%)
1	LLP	C	42	1	22,24,25	2.03	8 (36%)	28,32,34	1.23	3 (10%)
1	LLP	D	42	1	22,24,25	1.96	8 (36%)	28,32,34	1.26	3 (10%)

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
1	LLP	A	42	1	-	0/15/17/19	0/1/1/1
1	LLP	B	42	1	-	0/15/17/19	0/1/1/1
1	LLP	C	42	1	-	0/15/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	D	42	1	-	0/15/17/19	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	LLP	O3-C3	-4.67	1.26	1.37
1	C	42	LLP	O3-C3	-4.67	1.26	1.37
1	D	42	LLP	O3-C3	-4.60	1.26	1.37
1	B	42	LLP	O3-C3	-4.51	1.26	1.37
1	D	42	LLP	OP4-C5'	-2.12	1.36	1.45
1	B	42	LLP	OP4-C5'	-2.07	1.37	1.45
1	D	42	LLP	C6-N1	2.05	1.38	1.34
1	A	42	LLP	C4-C5	2.16	1.44	1.42
1	C	42	LLP	C4-C5	2.17	1.44	1.42
1	B	42	LLP	C6-N1	2.24	1.39	1.34
1	D	42	LLP	C6-C5	2.26	1.42	1.37
1	B	42	LLP	C2-N1	2.39	1.38	1.33
1	C	42	LLP	C6-N1	2.40	1.39	1.34
1	B	42	LLP	C6-C5	2.40	1.42	1.37
1	C	42	LLP	C6-C5	2.50	1.43	1.37
1	D	42	LLP	C2-N1	2.54	1.38	1.33
1	C	42	LLP	C2-N1	2.59	1.38	1.33
1	A	42	LLP	C6-N1	2.67	1.40	1.34
1	A	42	LLP	C2-N1	2.69	1.38	1.33
1	A	42	LLP	C6-C5	2.75	1.43	1.37
1	B	42	LLP	C4-C3	2.82	1.44	1.40
1	D	42	LLP	C4-C3	3.03	1.44	1.40
1	D	42	LLP	C4'-NZ	3.07	1.36	1.27
1	A	42	LLP	C4'-NZ	3.07	1.36	1.27
1	C	42	LLP	C4'-NZ	3.18	1.36	1.27
1	B	42	LLP	C4'-NZ	3.18	1.36	1.27
1	D	42	LLP	C4-C4'	3.18	1.52	1.46
1	C	42	LLP	C4-C4'	3.19	1.52	1.46
1	A	42	LLP	C4-C4'	3.20	1.52	1.46
1	B	42	LLP	C4-C4'	3.21	1.52	1.46
1	C	42	LLP	C4-C3	3.37	1.45	1.40
1	A	42	LLP	C4-C3	3.69	1.45	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	42	LLP	CE-NZ-C4'	-2.96	110.31	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	42	LLP	C4-C4'-NZ	-2.82	109.43	125.14
1	C	42	LLP	CE-NZ-C4'	-2.80	110.78	119.14
1	B	42	LLP	C4-C4'-NZ	-2.72	110.04	125.14
1	D	42	LLP	CE-NZ-C4'	-2.65	111.24	119.14
1	B	42	LLP	CE-NZ-C4'	-2.65	111.25	119.14
1	C	42	LLP	C4-C4'-NZ	-2.58	110.78	125.14
1	A	42	LLP	C4-C4'-NZ	-2.52	111.12	125.14
1	D	42	LLP	OP3-P-OP4	-2.15	100.44	106.72
1	B	42	LLP	OP3-P-OP4	-2.14	100.48	106.72
1	A	42	LLP	O-C-CA	-2.10	120.08	125.72
1	A	42	LLP	OP3-P-OP4	-2.10	100.61	106.72
1	C	42	LLP	O-C-CA	-2.07	120.18	125.72
1	B	42	LLP	O-C-CA	-2.05	120.21	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	42	LLP	3	0
1	B	42	LLP	3	0
1	C	42	LLP	3	0
1	D	42	LLP	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

26 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	SO4	A	401	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	402	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	A	403	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	A	404	-	4,4,4	0.20	0	6,6,6	0.05	0
3	GOL	A	405	-	5,5,5	0.28	0	5,5,5	0.18	0
3	GOL	A	406	-	5,5,5	0.31	0	5,5,5	0.24	0
3	GOL	A	407	-	5,5,5	0.20	0	5,5,5	0.23	0
3	GOL	A	408	-	5,5,5	0.24	0	5,5,5	0.21	0
2	SO4	B	401	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.11	0
3	GOL	B	403	-	5,5,5	0.28	0	5,5,5	0.20	0
3	GOL	B	404	-	5,5,5	0.30	0	5,5,5	0.24	0
3	GOL	B	405	-	5,5,5	0.29	0	5,5,5	0.20	0
3	GOL	B	406	-	5,5,5	0.29	0	5,5,5	0.23	0
2	SO4	C	401	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	402	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	C	403	-	4,4,4	0.25	0	6,6,6	0.17	0
2	SO4	C	404	-	4,4,4	0.22	0	6,6,6	0.09	0
3	GOL	C	405	-	5,5,5	0.37	0	5,5,5	0.22	0
3	GOL	C	406	-	5,5,5	0.24	0	5,5,5	0.25	0
3	GOL	C	407	-	5,5,5	0.33	0	5,5,5	0.24	0
2	SO4	D	401	-	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	D	402	-	4,4,4	0.18	0	6,6,6	0.09	0
3	GOL	D	403	-	5,5,5	0.33	0	5,5,5	0.24	0
3	GOL	D	404	-	5,5,5	0.21	0	5,5,5	0.19	0
3	GOL	D	405	-	5,5,5	0.32	0	5,5,5	0.25	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	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	A	404	-	-	0/0/0/0	0/0/0/0
3	GOL	A	405	-	-	0/4/4/4	0/0/0/0
3	GOL	A	406	-	-	0/4/4/4	0/0/0/0
3	GOL	A	407	-	-	0/4/4/4	0/0/0/0
3	GOL	A	408	-	-	0/4/4/4	0/0/0/0
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	B	406	-	-	0/4/4/4	0/0/0/0
2	SO4	C	401	-	-	0/0/0/0	0/0/0/0
2	SO4	C	402	-	-	0/0/0/0	0/0/0/0
2	SO4	C	403	-	-	0/0/0/0	0/0/0/0
2	SO4	C	404	-	-	0/0/0/0	0/0/0/0
3	GOL	C	405	-	-	0/4/4/4	0/0/0/0
3	GOL	C	406	-	-	0/4/4/4	0/0/0/0
3	GOL	C	407	-	-	0/4/4/4	0/0/0/0
2	SO4	D	401	-	-	0/0/0/0	0/0/0/0
2	SO4	D	402	-	-	0/0/0/0	0/0/0/0
3	GOL	D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	D	404	-	-	0/4/4/4	0/0/0/0
3	GOL	D	405	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406	GOL	1	0
3	B	406	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	302/311 (97%)	-0.13	16 (5%)	30	30	32, 45, 102, 117	0
1	B	302/311 (97%)	-0.07	15 (4%)	32	33	33, 44, 106, 126	0
1	C	302/311 (97%)	-0.13	18 (5%)	25	25	33, 46, 101, 120	0
1	D	302/311 (97%)	-0.11	15 (4%)	32	33	33, 44, 107, 125	0
All	All	1208/1244 (97%)	-0.11	64 (5%)	30	30	32, 45, 105, 126	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	ALA	8.6
1	B	211	PRO	7.4
1	B	222	VAL	7.2
1	A	206	ILE	6.7
1	B	210	GLY	6.7
1	D	207	LEU	6.5
1	C	206	ILE	6.3
1	D	211	PRO	6.2
1	B	209	GLY	6.1
1	D	214	ALA	6.1
1	D	206	ILE	5.9
1	D	222	VAL	5.9
1	D	210	GLY	5.8
1	A	222	VAL	5.6
1	D	209	GLY	5.4
1	C	222	VAL	5.4
1	C	216	ARG	5.0
1	B	206	ILE	4.9
1	B	207	LEU	4.8
1	B	224	PHE	4.5
1	D	221	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	208	ASN	4.2
1	D	213	HIS	4.1
1	B	221	GLY	3.9
1	C	207	LEU	3.9
1	B	213	HIS	3.9
1	A	207	LEU	3.9
1	B	205	SER	3.8
1	C	211	PRO	3.6
1	D	205	SER	3.5
1	A	205	SER	3.5
1	C	221	GLY	3.4
1	A	209	GLY	3.4
1	A	220	ILE	3.2
1	A	98	MET	3.2
1	C	209	GLY	3.2
1	C	214	ALA	3.2
1	A	221	GLY	3.2
1	C	203	GLU	3.1
1	A	219	GLY	3.0
1	A	218	GLU	2.9
1	C	218	GLU	2.8
1	C	205	SER	2.8
1	D	225	ILE	2.7
1	B	223	GLU	2.7
1	A	210	GLY	2.6
1	A	216	ARG	2.6
1	D	216	ARG	2.6
1	A	223	GLU	2.5
1	B	204	GLY	2.5
1	C	210	GLY	2.4
1	C	223	GLU	2.4
1	C	219	GLY	2.4
1	B	216	ARG	2.4
1	D	218	GLU	2.4
1	A	211	PRO	2.3
1	A	215	HIS	2.3
1	D	220	ILE	2.2
1	C	220	ILE	2.2
1	C	204	GLY	2.2
1	D	215	HIS	2.2
1	C	217	THR	2.1
1	C	213	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	LLP	B	42	24/25	0.98	0.12	-	36,40,44,45	0
1	LLP	D	42	24/25	0.98	0.12	-	35,39,42,44	0
1	LLP	A	42	24/25	0.98	0.12	-	38,46,48,48	0
1	LLP	C	42	24/25	0.97	0.14	-	37,45,47,48	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	C	405	6/6	0.91	0.26	12.53	73,74,75,76	0
3	GOL	B	406	6/6	0.94	0.20	10.67	68,70,70,71	0
3	GOL	B	405	6/6	0.88	0.29	8.23	80,81,82,82	0
3	GOL	B	403	6/6	0.87	0.24	7.67	76,83,83,84	0
3	GOL	A	406	6/6	0.86	0.30	6.90	59,63,63,65	0
3	GOL	C	406	6/6	0.90	0.25	6.19	72,74,74,74	0
3	GOL	D	404	6/6	0.80	0.36	5.64	89,91,92,92	0
3	GOL	A	407	6/6	0.94	0.19	3.40	71,72,73,74	0
3	GOL	D	403	6/6	0.86	0.14	1.79	66,74,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	D	401	5/5	0.86	0.20	1.38	125,126,126,127	0
2	SO4	B	402	5/5	0.88	0.17	1.25	111,113,113,114	0
2	SO4	C	402	5/5	0.79	0.21	1.21	124,125,125,126	0
3	GOL	A	405	6/6	0.71	0.20	0.85	95,95,96,96	0
3	GOL	C	407	6/6	0.90	0.14	0.29	72,75,76,77	0
2	SO4	A	404	5/5	0.90	0.15	0.04	116,117,117,118	0
2	SO4	B	401	5/5	0.98	0.10	-	78,80,81,82	0
2	SO4	C	401	5/5	0.93	0.10	-	91,91,92,92	0
2	SO4	C	403	5/5	0.95	0.25	-	76,79,81,81	0
2	SO4	A	402	5/5	0.87	0.28	-	97,99,100,101	0
2	SO4	C	404	5/5	0.92	0.29	-	98,100,101,102	0
3	GOL	D	405	6/6	0.93	0.19	-	74,76,77,77	0
2	SO4	D	402	5/5	0.98	0.08	-	79,80,81,82	0
3	GOL	A	408	6/6	0.89	0.18	-	71,76,76,77	0
3	GOL	B	404	6/6	0.93	0.11	-	82,85,86,86	0
2	SO4	A	403	5/5	0.90	0.28	-	80,82,85,85	0
2	SO4	A	401	5/5	0.94	0.14	-	93,93,94,94	0

6.5 Other polymers

There are no such residues in this entry.