Full wwPDB X-ray Structure Validation Report (i)

Jun 1, 2021 – 06:11 PM EDT

PDB ID	:	7LC0
Title	:	Structure of D-Glucosaminate-6-phosphate Ammonia-lyase
Authors	:	Phillips, R.S.
Deposited on	:	2021-01-09
Resolution	:	2.60 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 (1)) were used in the production of this report:

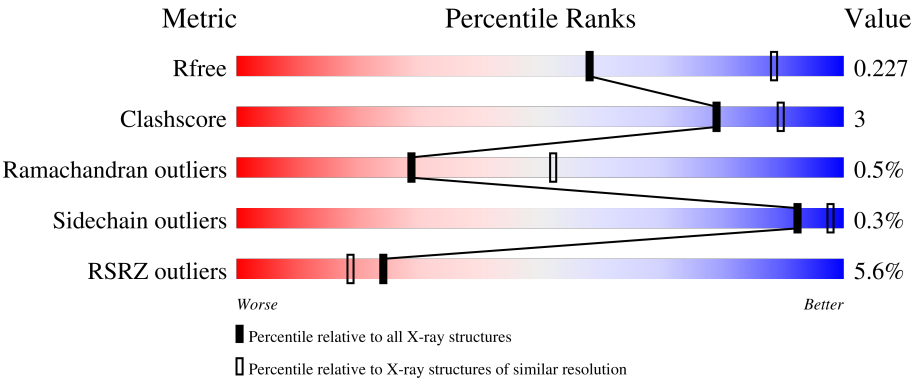
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.19
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.19

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	369	7% 90% 10%
1	B	369	% 95% 5%
1	C	369	2% 92% 8%
1	D	369	2% 92% 8%
1	E	369	2% 90% 9%

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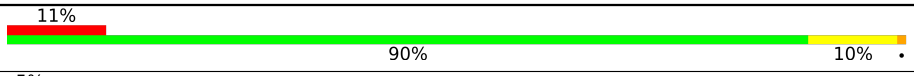
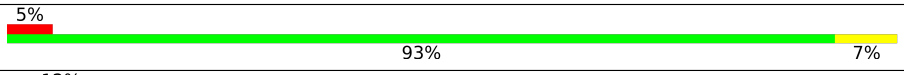
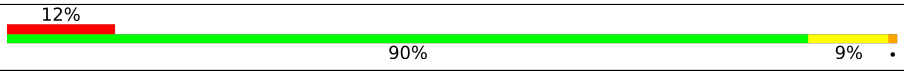
Mol	Chain	Length	Quality of chain
1	F	369	
1	G	369	
1	H	369	

2 Entry composition (i)

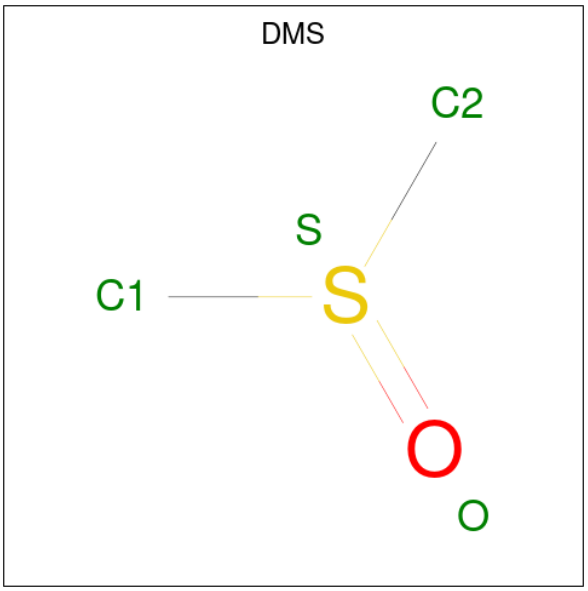
There are 7 unique types of molecules in this entry. The entry contains 22539 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative selenocysteine synthase (L-seryl-tRNA(Ser) selenium transferase).

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	P	S	Se	0	0	0
			2774	1731	497	530	1	4	11			
1	B	369	Total	C	N	O	P	S	Se	0	0	0
			2774	1731	497	530	1	4	11			
1	C	369	Total	C	N	O	P	S	Se	0	0	0
			2774	1731	497	530	1	4	11			
1	D	369	Total	C	N	O	P	S	Se	0	0	0
			2774	1731	497	530	1	4	11			
1	E	369	Total	C	N	O	P	S	Se	0	0	0
			2774	1731	497	530	1	4	11			
1	F	369	Total	C	N	O	P	S	Se	0	0	0
			2774	1731	497	530	1	4	11			
1	G	369	Total	C	N	O	P	S	Se	0	0	0
			2774	1731	497	530	1	4	11			
1	H	369	Total	C	N	O	P	S	Se	0	0	0
			2774	1731	497	530	1	4	11			

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	E	1	Total	C	O	S	0	0
			4	2	1	1		
2	E	1	Total	C	O	S	0	0
			4	2	1	1		
2	E	1	Total	C	O	S	0	0
			4	2	1	1		
2	F	1	Total	C	O	S	0	0
			4	2	1	1		
2	F	1	Total	C	O	S	0	0
			4	2	1	1		

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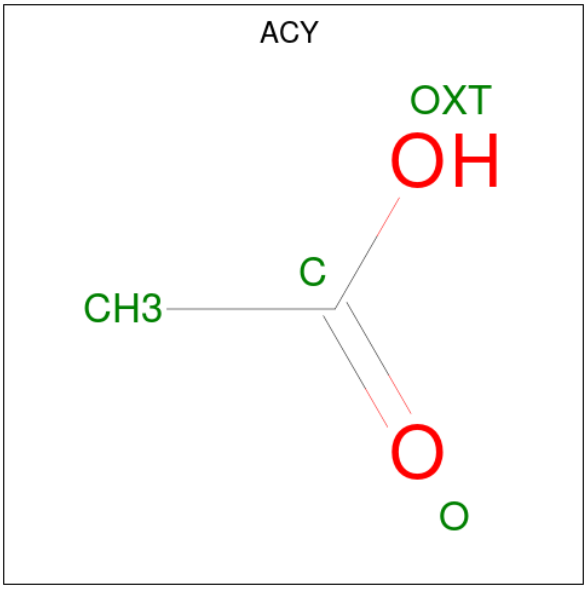
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O S 4 2 1 1	0	0
2	F	1	Total C O S 4 2 1 1	0	0
2	G	1	Total C O S 4 2 1 1	0	0
2	G	1	Total C O S 4 2 1 1	0	0
2	G	1	Total C O S 4 2 1 1	0	0

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

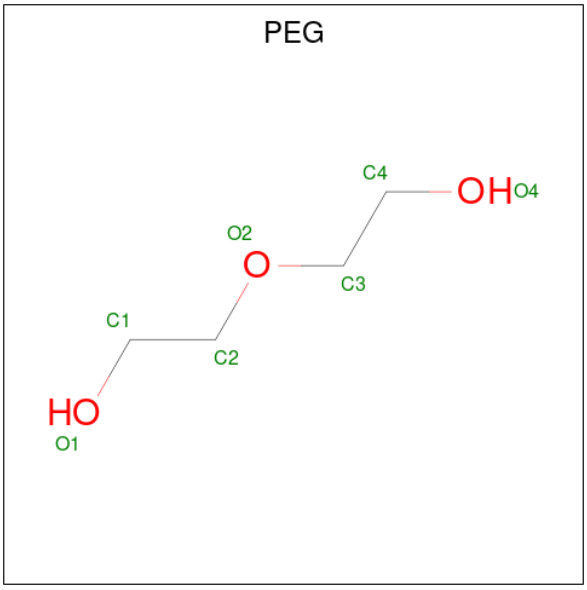
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	3	Total Mg 3 3	0	0
4	H	3	Total Mg 3 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 7 4 3	0	0

- Molecule 7 is water.

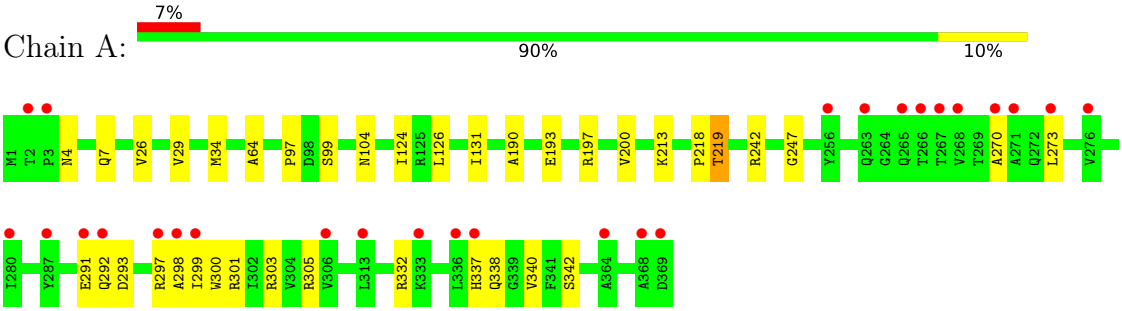
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	35	Total O 35 35	0	0
7	B	30	Total O 30 30	0	0
7	C	25	Total O 25 25	0	0
7	D	37	Total O 37 37	0	0
7	E	22	Total O 22 22	0	0
7	F	27	Total O 27 27	0	0
7	G	30	Total O 30 30	0	0
7	H	26	Total O 26 26	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

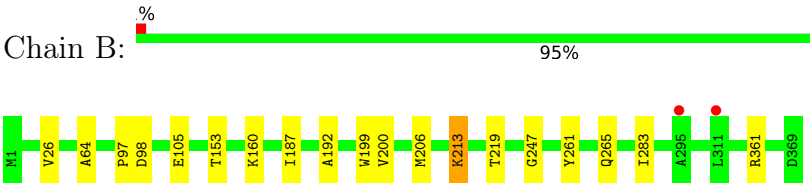
• Molecule 1: Putative selenocysteine synthase (L-seryl-tRNA(Ser) selenium transferase)

Chain A:



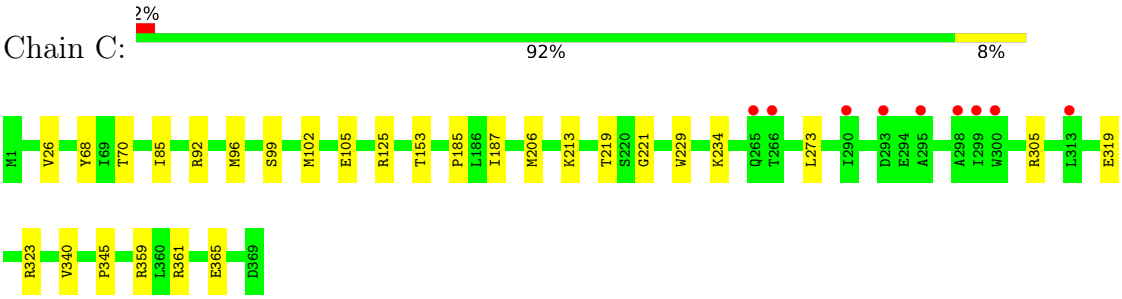
• Molecule 1: Putative selenocysteine synthase (L-seryl-tRNA(Ser) selenium transferase)

Chain B:



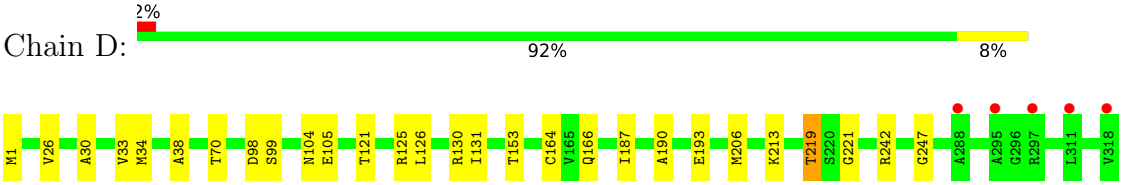
• Molecule 1: Putative selenocysteine synthase (L-seryl-tRNA(Ser) selenium transferase)

Chain C:



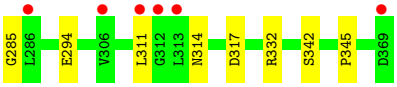
• Molecule 1: Putative selenocysteine synthase (L-seryl-tRNA(Ser) selenium transferase)

Chain D:



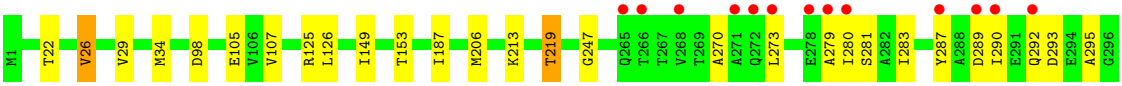
• Molecule 1: Putative selenocysteine synthase (L-seryl-tRNA(Ser) selenium transferase)

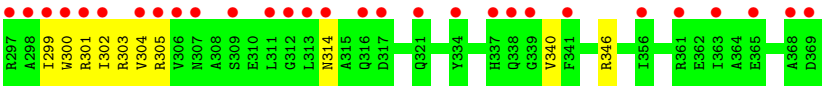
Chain E:



• Molecule 1: Putative selenocysteine synthase (L-seryl-tRNA(Ser) selenium transferase)

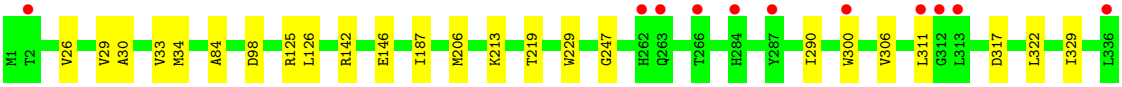
Chain F:

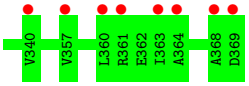




• Molecule 1: Putative selenocysteine synthase (L-seryl-tRNA(Ser) selenium transferase)

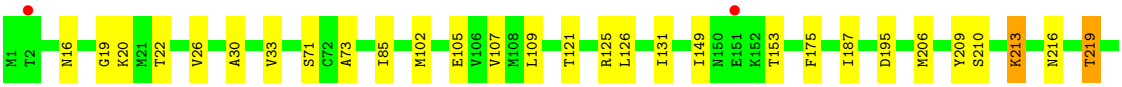
Chain G:

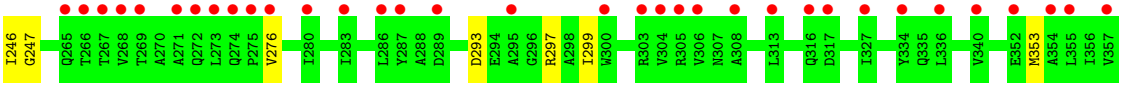


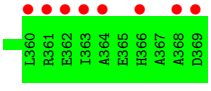


• Molecule 1: Putative selenocysteine synthase (L-seryl-tRNA(Ser) selenium transferase)

Chain H:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.09Å 205.57Å 164.03Å 90.00° 95.19° 90.00°	Depositor
Resolution (Å)	49.02 – 2.60 49.02 – 2.60	Depositor EDS
% Data completeness (in resolution range)	80.2 (49.02-2.60) 80.2 (49.02-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.193 , 0.228 0.193 , 0.227	Depositor DCC
R_{free} test set	1985 reflections (2.27%)	wwPDB-VP
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22539	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: ACY, LLP, CL, DMS, MG, PEG

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	0.23	0/2780	0.40	0/3750
1	B	0.23	0/2780	0.40	0/3750
1	C	0.23	0/2780	0.40	0/3750
1	D	0.23	0/2780	0.40	0/3750
1	E	0.23	0/2780	0.40	0/3750
1	F	0.24	0/2780	0.41	0/3750
1	G	0.23	0/2780	0.40	0/3750
1	H	0.23	0/2780	0.41	0/3750
All	All	0.23	0/22240	0.40	0/30000

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	2774	0	2778	23	0
1	B	2774	0	2778	10	0
1	C	2774	0	2778	16	0
1	D	2774	0	2778	18	0
1	E	2774	0	2778	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2774	0	2778	25	0
1	G	2774	0	2778	14	0
1	H	2774	0	2778	21	0
2	A	8	0	12	0	0
2	B	12	0	18	0	0
2	C	4	0	6	0	0
2	D	12	0	18	0	0
2	E	12	0	18	1	0
2	F	16	0	24	0	0
2	G	12	0	18	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	E	12	0	9	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
5	B	1	0	0	0	0
6	C	7	0	10	1	0
7	A	35	0	0	1	0
7	B	30	0	0	0	0
7	C	25	0	0	0	0
7	D	37	0	0	1	0
7	E	22	0	0	0	0
7	F	27	0	0	0	0
7	G	30	0	0	0	0
7	H	26	0	0	0	0
All	All	22539	0	22363	127	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 3.

All (127) 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:E:285:GLY:HA3	1:E:311:LEU:HB2	1.64	0.80
1:H:293:ASP:HB3	1:H:297:ARG:HB3	1.66	0.76
1:C:85:ILE:HG22	1:C:102:MSE:HE2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:293:ASP:HB2	1:H:299:ILE:HB	1.82	0.62
1:A:292:GLN:HB3	1:A:297:ARG:HA	1.84	0.60
1:A:29:VAL:HG11	1:A:34:MSE:HE3	1.83	0.60
1:C:92:ARG:HD3	1:C:102:MSE:HE3	1.84	0.59
1:D:99:SER:O	1:D:104:ASN:ND2	2.35	0.59
1:A:124:ILE:HD13	1:A:131:ILE:HD11	1.83	0.59
1:H:85:ILE:HG22	1:H:102:MSE:HE2	1.83	0.58
1:E:259:GLU:OE2	1:E:263:GLN:NE2	2.37	0.57
1:A:291:GLU:HB2	1:A:303:ARG:HB2	1.86	0.56
1:E:273:LEU:HD11	1:E:345:PRO:HG3	1.88	0.56
1:E:332:ARG:HB2	1:E:342:SER:HB2	1.87	0.56
1:C:319:GLU:OE1	1:C:323:ARG:NH1	2.35	0.56
1:F:289:ASP:OD2	1:F:303:ARG:NE	2.38	0.56
1:F:281:SER:HA	1:F:287:TYR:HA	1.88	0.55
1:F:270:ALA:HB2	1:F:300:TRP:CD1	2.41	0.55
1:B:160:LYS:HG3	1:B:199:TRP:CZ2	2.45	0.52
1:A:4:ASN:HB3	1:A:7:GLN:HG3	1.92	0.52
1:B:192:ALA:HB2	1:B:213:LLP:HD3	1.91	0.52
1:D:98:ASP:HB2	1:F:125:ARG:HD3	1.92	0.52
1:E:125:ARG:HD3	1:G:98:ASP:HB2	1.92	0.51
1:H:20:LYS:NZ	1:H:216:ASN:OD1	2.43	0.51
1:A:305:ARG:HG2	1:A:340:VAL:HG22	1.94	0.49
1:F:292:GLN:HB2	1:F:303:ARG:HD3	1.93	0.49
1:A:292:GLN:HB3	1:A:298:ALA:H	1.77	0.49
1:C:96:MSE:HE1	1:C:99:SER:HB3	1.95	0.49
1:D:105:GLU:HB2	1:D:153:THR:HA	1.94	0.49
1:E:86:THR:HG23	1:E:96:MSE:HE2	1.93	0.48
1:B:187:ILE:HG12	1:B:206:MSE:HE3	1.95	0.48
1:E:98:ASP:HB2	1:G:125:ARG:HD3	1.94	0.48
1:D:125:ARG:HD3	1:F:98:ASP:HB2	1.96	0.48
1:H:105:GLU:HB2	1:H:153:THR:HA	1.96	0.48
1:A:99:SER:O	1:A:104:ASN:ND2	2.47	0.47
1:B:98:ASP:HB2	1:C:125:ARG:HD3	1.96	0.47
1:D:130:ARG:NH1	7:D:502:HOH:O	2.46	0.47
1:H:16:ASN:ND2	1:H:19:GLY:O	2.38	0.47
1:C:305:ARG:HG2	1:C:340:VAL:HG22	1.97	0.47
1:D:1:MSE:HG3	1:D:355:LEU:HD11	1.96	0.47
1:F:22:THR:HG22	1:F:26:VAL:HG22	1.97	0.47
1:G:29:VAL:HG21	1:G:34:MSE:HE3	1.96	0.47
1:H:187:ILE:HG12	1:H:206:MSE:HE3	1.96	0.47
1:A:126:LEU:HD22	1:H:126:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:ILE:HG12	1:G:206:MSE:HE3	1.96	0.47
1:F:295:ALA:HB3	1:F:301:ARG:HH12	1.80	0.47
1:E:41:ALA:HB2	1:E:249:GLU:HB3	1.97	0.46
1:B:105:GLU:HB2	1:B:153:THR:HA	1.97	0.46
1:C:359:ARG:HH12	6:C:401:PEG:H21	1.81	0.46
1:D:38:ALA:HA	1:F:34:MSE:HG2	1.96	0.46
1:F:273:LEU:HB3	1:F:302:ILE:HD11	1.97	0.46
1:E:126:LEU:HD22	1:G:126:LEU:HD22	1.98	0.46
1:F:187:ILE:HG12	1:F:206:MSE:HE3	1.97	0.46
1:C:187:ILE:HG12	1:C:206:MSE:HE3	1.97	0.46
1:E:294:GLU:N	1:E:294:GLU:OE1	2.48	0.46
1:E:105:GLU:HB2	1:E:153:THR:HA	1.97	0.46
1:B:247:GLY:HA3	1:C:219:THR:OG1	2.17	0.45
1:D:187:ILE:HG12	1:D:206:MSE:HE3	1.98	0.45
1:F:29:VAL:HG21	1:F:34:MSE:SE	2.66	0.45
1:A:219:THR:OG1	1:H:247:GLY:HA3	2.17	0.45
1:G:142:ARG:NH1	1:G:146:GLU:OE2	2.50	0.45
1:F:289:ASP:CG	1:F:303:ARG:HE	2.20	0.45
1:E:219:THR:OG1	1:G:247:GLY:HA3	2.16	0.44
1:E:314:ASN:ND2	1:E:317:ASP:OD1	2.49	0.44
1:C:70:THR:N	1:C:221:GLY:O	2.38	0.44
1:F:299:ILE:HD13	1:F:346:ARG:HD3	1.98	0.44
1:F:305:ARG:HG2	1:F:340:VAL:HG22	1.98	0.44
1:D:164:CYS:O	1:D:166:GLN:NE2	2.51	0.44
1:D:219:THR:OG1	1:F:247:GLY:HA3	2.18	0.44
1:E:73:ALA:HB2	1:E:210:SER:HB2	1.98	0.44
1:F:280:ILE:HG21	1:F:304:VAL:HG22	2.00	0.44
1:B:64:ALA:HB2	1:B:200:VAL:HG11	2.00	0.44
1:B:261:TYR:O	1:B:265:GLN:HG3	2.17	0.44
1:D:247:GLY:HA3	1:F:219:THR:OG1	2.18	0.44
1:E:107:VAL:HG21	1:E:149:ILE:HD13	1.99	0.44
1:F:290:ILE:HD12	1:F:290:ILE:HA	1.80	0.44
1:A:247:GLY:HA3	1:H:219:THR:OG1	2.18	0.44
1:E:30:ALA:HB3	1:E:33:VAL:HG23	1.99	0.43
1:H:276:VAL:HG11	1:H:353:MSE:HE3	1.99	0.43
1:A:190:ALA:HB1	1:A:193:GLU:HB2	2.00	0.43
1:A:301:ARG:NH2	7:A:506:HOH:O	2.51	0.43
1:A:332:ARG:HD3	1:A:342:SER:HB3	1.99	0.43
1:H:213:LLP:HB3	1:H:213:LLP:HE2	1.81	0.43
1:D:242:ARG:NH2	1:F:22:THR:HG21	2.34	0.43
1:G:290:ILE:HG22	1:G:300:TRP:HE3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:ALA:HB3	1:H:33:VAL:HG23	2.00	0.43
1:A:293:ASP:H	1:A:298:ALA:HB3	1.84	0.43
1:G:84:ALA:HA	1:G:229:TRP:CZ3	2.54	0.43
1:G:306:VAL:HG13	1:G:311:LEU:HD23	2.01	0.43
1:H:73:ALA:HB2	1:H:210:SER:HB2	2.00	0.43
1:C:273:LEU:HD11	1:C:345:PRO:HG3	2.01	0.42
1:A:97:PRO:HB3	1:A:126:LEU:O	2.18	0.42
1:H:71:SER:HA	1:H:246:ILE:HB	2.01	0.42
1:D:126:LEU:HD22	1:F:126:LEU:HD22	2.02	0.42
1:C:361:ARG:O	1:C:365:GLU:HG3	2.19	0.42
1:F:107:VAL:HG21	1:F:149:ILE:HD13	2.01	0.42
1:G:30:ALA:HB3	1:G:33:VAL:HG23	2.02	0.42
1:F:279:ALA:O	1:F:283:ILE:HG12	2.19	0.42
1:A:291:GLU:HB2	1:A:303:ARG:CB	2.50	0.41
1:E:226:ARG:NH1	2:E:406:DMS:O	2.54	0.41
1:A:29:VAL:HG11	1:A:218:PRO:HD3	2.02	0.41
1:A:337:HIS:ND1	1:A:338:GLN:HG3	2.35	0.41
1:H:107:VAL:HG21	1:H:149:ILE:HD13	2.02	0.41
1:H:195:ASP:O	1:H:209:TYR:OH	2.33	0.41
1:A:64:ALA:HB2	1:A:200:VAL:HG11	2.01	0.41
1:D:70:THR:N	1:D:221:GLY:O	2.41	0.41
1:A:242:ARG:NH2	1:H:22:THR:HG21	2.36	0.41
1:E:110:ARG:NH1	1:E:135:GLY:O	2.49	0.41
1:H:121:THR:HG22	1:H:131:ILE:HG12	2.02	0.41
1:C:105:GLU:HB2	1:C:153:THR:HA	2.03	0.41
1:C:185:PRO:HB3	1:C:229:TRP:CE2	2.56	0.41
1:G:290:ILE:HG22	1:G:300:TRP:CE3	2.56	0.41
1:G:322:LEU:HB3	1:G:329:ILE:HB	2.02	0.41
1:A:97:PRO:HD2	1:H:125:ARG:HG2	2.03	0.41
1:A:270:ALA:HA	1:A:273:LEU:HD12	2.02	0.41
1:B:97:PRO:HD2	1:C:125:ARG:HG2	2.03	0.41
1:C:68:TYR:CD1	1:C:234:LYS:HG2	2.57	0.40
1:D:30:ALA:HB3	1:D:33:VAL:HG23	2.02	0.40
1:D:121:THR:HG22	1:D:131:ILE:HG12	2.03	0.40
1:E:247:GLY:HA3	1:G:219:THR:OG1	2.21	0.40
1:H:109:LEU:HG	1:H:175:PHE:HZ	1.85	0.40
1:D:34:MSE:O	1:D:38:ALA:N	2.46	0.40
1:B:283:ILE:HG12	1:B:361:ARG:HG2	2.04	0.40
1:D:190:ALA:HB1	1:D:193:GLU:HB2	2.04	0.40
1:E:187:ILE:HG12	1:E:206:MSE:HE3	2.04	0.40
1:F:105:GLU:HB2	1:F:153:THR:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:ASP:OD1	1:F:293:ASP:N	2.54	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	366/369 (99%)	355 (97%)	9 (2%)	2 (0%)	29	52
1	B	366/369 (99%)	357 (98%)	7 (2%)	2 (0%)	29	52
1	C	366/369 (99%)	354 (97%)	11 (3%)	1 (0%)	41	64
1	D	366/369 (99%)	356 (97%)	8 (2%)	2 (0%)	29	52
1	E	366/369 (99%)	356 (97%)	8 (2%)	2 (0%)	29	52
1	F	366/369 (99%)	356 (97%)	8 (2%)	2 (0%)	29	52
1	G	366/369 (99%)	355 (97%)	10 (3%)	1 (0%)	41	64
1	H	366/369 (99%)	356 (97%)	8 (2%)	2 (0%)	29	52
All	All	2928/2952 (99%)	2845 (97%)	69 (2%)	14 (0%)	29	52

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	219	THR
1	E	219	THR
1	F	219	THR
1	B	219	THR
1	G	26	VAL
1	H	219	THR
1	A	219	THR
1	E	26	VAL
1	H	26	VAL

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Mol	Chain	Res	Type
1	A	26	VAL
1	B	26	VAL
1	C	26	VAL
1	F	26	VAL
1	D	26	VAL

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	277/266 (104%)	274 (99%)	3 (1%)	73 88
1	B	277/266 (104%)	277 (100%)	0	100 100
1	C	277/266 (104%)	277 (100%)	0	100 100
1	D	277/266 (104%)	277 (100%)	0	100 100
1	E	277/266 (104%)	276 (100%)	1 (0%)	91 97
1	F	277/266 (104%)	276 (100%)	1 (0%)	91 97
1	G	277/266 (104%)	276 (100%)	1 (0%)	91 97
1	H	277/266 (104%)	277 (100%)	0	100 100
All	All	2216/2128 (104%)	2210 (100%)	6 (0%)	92 98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ARG
1	A	299	ILE
1	A	300	TRP
1	E	267	THR
1	F	314	ASN
1	G	317	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	338	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 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	H	213	1	23,24,25	2.63	6 (26%)	25,32,34	1.24	3 (12%)
1	LLP	C	213	1	23,24,25	2.61	6 (26%)	25,32,34	1.36	4 (16%)
1	LLP	D	213	1	23,24,25	2.61	6 (26%)	25,32,34	1.26	3 (12%)
1	LLP	G	213	1	23,24,25	2.62	6 (26%)	25,32,34	1.25	3 (12%)
1	LLP	A	213	1	23,24,25	2.61	6 (26%)	25,32,34	1.32	4 (16%)
1	LLP	F	213	1	23,24,25	2.61	6 (26%)	25,32,34	1.27	4 (16%)
1	LLP	E	213	1	23,24,25	2.62	6 (26%)	25,32,34	1.31	4 (16%)
1	LLP	B	213	1	23,24,25	2.61	6 (26%)	25,32,34	1.30	4 (16%)

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	H	213	1	-	5/16/17/19	0/1/1/1
1	LLP	C	213	1	-	8/16/17/19	0/1/1/1
1	LLP	D	213	1	-	6/16/17/19	0/1/1/1
1	LLP	G	213	1	-	6/16/17/19	0/1/1/1
1	LLP	A	213	1	-	7/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	F	213	1	-	6/16/17/19	0/1/1/1
1	LLP	E	213	1	-	5/16/17/19	0/1/1/1
1	LLP	B	213	1	-	8/16/17/19	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	213	LLP	C4-C4'	8.17	1.62	1.46
1	G	213	LLP	C4-C4'	8.16	1.62	1.46
1	E	213	LLP	C4-C4'	8.12	1.62	1.46
1	D	213	LLP	C4-C4'	8.11	1.62	1.46
1	F	213	LLP	C4-C4'	8.08	1.62	1.46
1	B	213	LLP	C4-C4'	8.08	1.62	1.46
1	A	213	LLP	C4-C4'	8.03	1.61	1.46
1	C	213	LLP	C4-C4'	8.02	1.61	1.46
1	G	213	LLP	C4'-NZ	4.94	1.43	1.27
1	H	213	LLP	C4'-NZ	4.94	1.43	1.27
1	D	213	LLP	C4'-NZ	4.90	1.43	1.27
1	F	213	LLP	C4'-NZ	4.89	1.43	1.27
1	E	213	LLP	C4'-NZ	4.87	1.43	1.27
1	A	213	LLP	C4'-NZ	4.87	1.43	1.27
1	B	213	LLP	C4'-NZ	4.84	1.43	1.27
1	C	213	LLP	C4'-NZ	4.84	1.43	1.27
1	C	213	LLP	C4-C5	-4.28	1.36	1.42
1	A	213	LLP	C4-C5	-4.24	1.36	1.42
1	B	213	LLP	C4-C5	-4.18	1.36	1.42
1	F	213	LLP	C4-C5	-4.16	1.36	1.42
1	E	213	LLP	C4-C5	-4.14	1.36	1.42
1	H	213	LLP	C4-C5	-4.14	1.36	1.42
1	G	213	LLP	C4-C5	-4.09	1.36	1.42
1	D	213	LLP	C4-C5	-4.06	1.36	1.42
1	B	213	LLP	C2'-C2	3.46	1.56	1.50
1	C	213	LLP	C2'-C2	3.45	1.56	1.50
1	A	213	LLP	C2'-C2	3.43	1.56	1.50
1	E	213	LLP	C2'-C2	3.43	1.56	1.50
1	H	213	LLP	C2'-C2	3.42	1.56	1.50
1	D	213	LLP	C2'-C2	3.42	1.56	1.50
1	F	213	LLP	C2'-C2	3.41	1.56	1.50
1	G	213	LLP	C2'-C2	3.37	1.56	1.50
1	E	213	LLP	C6-N1	2.99	1.40	1.34
1	B	213	LLP	C6-N1	2.97	1.40	1.34
1	F	213	LLP	C6-N1	2.96	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	213	LLP	C6-N1	2.95	1.40	1.34
1	A	213	LLP	C6-N1	2.95	1.40	1.34
1	H	213	LLP	C6-N1	2.95	1.40	1.34
1	D	213	LLP	C6-N1	2.94	1.40	1.34
1	G	213	LLP	C6-N1	2.92	1.40	1.34
1	D	213	LLP	C5'-C5	2.07	1.56	1.50
1	B	213	LLP	C5'-C5	2.06	1.56	1.50
1	E	213	LLP	C5'-C5	2.04	1.56	1.50
1	C	213	LLP	C5'-C5	2.03	1.56	1.50
1	G	213	LLP	C5'-C5	2.03	1.56	1.50
1	H	213	LLP	C5'-C5	2.02	1.56	1.50
1	F	213	LLP	C5'-C5	2.02	1.56	1.50
1	A	213	LLP	C5'-C5	2.02	1.56	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	213	LLP	C4-C4'-NZ	-3.35	108.93	124.31
1	A	213	LLP	C4-C4'-NZ	-3.28	109.27	124.31
1	B	213	LLP	C4-C4'-NZ	-3.25	109.39	124.31
1	E	213	LLP	C4-C4'-NZ	-3.22	109.53	124.31
1	D	213	LLP	C4-C4'-NZ	-3.16	109.78	124.31
1	G	213	LLP	CE-NZ-C4'	-3.15	109.21	118.90
1	F	213	LLP	C4-C4'-NZ	-3.11	110.02	124.31
1	H	213	LLP	CE-NZ-C4'	-3.08	109.43	118.90
1	A	213	LLP	CE-NZ-C4'	-3.05	109.54	118.90
1	C	213	LLP	CE-NZ-C4'	-3.04	109.56	118.90
1	E	213	LLP	CE-NZ-C4'	-3.02	109.62	118.90
1	G	213	LLP	C4-C4'-NZ	-3.00	110.52	124.31
1	F	213	LLP	CE-NZ-C4'	-2.98	109.73	118.90
1	H	213	LLP	C4-C4'-NZ	-2.98	110.62	124.31
1	B	213	LLP	CE-NZ-C4'	-2.98	109.75	118.90
1	D	213	LLP	CE-NZ-C4'	-2.90	110.00	118.90
1	C	213	LLP	C5-C6-N1	-2.49	119.67	123.82
1	A	213	LLP	C5-C6-N1	-2.44	119.76	123.82
1	F	213	LLP	C5-C6-N1	-2.39	119.83	123.82
1	G	213	LLP	C5-C6-N1	-2.38	119.86	123.82
1	B	213	LLP	C5-C6-N1	-2.36	119.88	123.82
1	H	213	LLP	C5-C6-N1	-2.36	119.88	123.82
1	E	213	LLP	C5-C6-N1	-2.36	119.89	123.82
1	D	213	LLP	C5-C6-N1	-2.33	119.93	123.82
1	C	213	LLP	C3-C4-C5	2.30	120.03	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	213	LLP	C3-C4-C5	2.22	119.96	118.26
1	B	213	LLP	C3-C4-C5	2.13	119.90	118.26
1	E	213	LLP	C3-C4-C5	2.10	119.87	118.26
1	F	213	LLP	C3-C4-C5	2.05	119.83	118.26

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	213	LLP	C4-C4'-NZ-CE
1	A	213	LLP	C-CA-CB-CG
1	B	213	LLP	C4-C4'-NZ-CE
1	B	213	LLP	N-CA-CB-CG
1	B	213	LLP	C-CA-CB-CG
1	B	213	LLP	O-C-CA-CB
1	C	213	LLP	C5'-OP4-P-OP2
1	C	213	LLP	C5'-OP4-P-OP3
1	C	213	LLP	C-CA-CB-CG
1	D	213	LLP	C4-C4'-NZ-CE
1	D	213	LLP	C-CA-CB-CG
1	E	213	LLP	C-CA-CB-CG
1	F	213	LLP	C4-C4'-NZ-CE
1	F	213	LLP	C-CA-CB-CG
1	G	213	LLP	CG-CD-CE-NZ
1	C	213	LLP	C4-C4'-NZ-CE
1	E	213	LLP	C4-C4'-NZ-CE
1	G	213	LLP	C4-C4'-NZ-CE
1	H	213	LLP	C4-C4'-NZ-CE
1	G	213	LLP	CA-CB-CG-CD
1	H	213	LLP	CA-CB-CG-CD
1	A	213	LLP	CE-CD-CG-CB
1	C	213	LLP	C3-C4-C4'-NZ
1	F	213	LLP	CE-CD-CG-CB
1	D	213	LLP	CE-CD-CG-CB
1	C	213	LLP	C5'-OP4-P-OP1
1	A	213	LLP	C3-C4-C4'-NZ
1	E	213	LLP	C3-C4-C4'-NZ
1	H	213	LLP	C3-C4-C4'-NZ
1	C	213	LLP	C5-C4-C4'-NZ
1	H	213	LLP	CG-CD-CE-NZ
1	G	213	LLP	C3-C4-C4'-NZ
1	A	213	LLP	CD-CE-NZ-C4'

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Mol	Chain	Res	Type	Atoms
1	D	213	LLP	CG-CD-CE-NZ
1	B	213	LLP	C3-C4-C4'-NZ
1	H	213	LLP	C5-C4-C4'-NZ
1	B	213	LLP	CD-CE-NZ-C4'
1	F	213	LLP	CD-CE-NZ-C4'
1	B	213	LLP	C5'-OP4-P-OP1
1	C	213	LLP	CG-CD-CE-NZ
1	D	213	LLP	C3-C4-C4'-NZ
1	F	213	LLP	C3-C4-C4'-NZ
1	E	213	LLP	CG-CD-CE-NZ
1	B	213	LLP	C5'-OP4-P-OP3
1	D	213	LLP	CD-CE-NZ-C4'
1	G	213	LLP	CE-CD-CG-CB
1	A	213	LLP	C5-C4-C4'-NZ
1	E	213	LLP	C5-C4-C4'-NZ
1	G	213	LLP	C5-C4-C4'-NZ
1	F	213	LLP	CG-CD-CE-NZ
1	A	213	LLP	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	213	LLP	1	0
1	B	213	LLP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 12 are monoatomic - leaving 25 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	$\#\|Z\|>2$
2	DMS	F	403	-	3,3,3	0.65	0	3,3,3	0.51	0
2	DMS	G	402	-	3,3,3	0.66	0	3,3,3	0.50	0
2	DMS	G	403	-	3,3,3	0.66	0	3,3,3	0.51	0
2	DMS	B	403	-	3,3,3	0.66	0	3,3,3	0.51	0
2	DMS	F	404	-	3,3,3	0.66	0	3,3,3	0.51	0
3	ACY	B	401	-	1,3,3	3.93	1 (100%)	0,3,3	0.00	-
3	ACY	E	402	-	1,3,3	4.09	1 (100%)	0,3,3	0.00	-
2	DMS	E	406	-	3,3,3	0.66	0	3,3,3	0.49	0
3	ACY	E	403	-	1,3,3	4.06	1 (100%)	0,3,3	0.00	-
6	PEG	C	401	-	6,6,6	0.49	0	5,5,5	0.28	0
3	ACY	A	402	-	1,3,3	3.50	1 (100%)	0,3,3	0.00	-
2	DMS	D	403	-	3,3,3	0.66	0	3,3,3	0.51	0
2	DMS	F	401	-	3,3,3	0.66	0	3,3,3	0.51	0
2	DMS	A	401	-	3,3,3	0.66	0	3,3,3	0.49	0
2	DMS	C	402	-	3,3,3	0.66	0	3,3,3	0.52	0
2	DMS	G	401	-	3,3,3	0.66	0	3,3,3	0.51	0
2	DMS	F	402	-	3,3,3	0.66	0	3,3,3	0.52	0
2	DMS	E	404	-	3,3,3	0.66	0	3,3,3	0.51	0
2	DMS	D	401	-	3,3,3	0.66	0	3,3,3	0.51	0
3	ACY	E	401	-	1,3,3	3.95	1 (100%)	0,3,3	0.00	-
2	DMS	D	402	-	3,3,3	0.66	0	3,3,3	0.50	0
2	DMS	B	404	-	3,3,3	0.66	0	3,3,3	0.52	0
2	DMS	B	402	-	3,3,3	0.66	0	3,3,3	0.52	0
2	DMS	A	403	-	3,3,3	0.66	0	3,3,3	0.50	0
2	DMS	E	405	-	3,3,3	0.66	0	3,3,3	0.51	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
6	PEG	C	401	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	ACY	CH3-C	4.09	1.54	1.48
3	E	403	ACY	CH3-C	4.06	1.53	1.48
3	E	401	ACY	CH3-C	3.95	1.53	1.48
3	B	401	ACY	CH3-C	3.93	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	ACY	CH3-C	3.50	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	401	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	406	DMS	1	0
6	C	401	PEG	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	357/369 (96%)	0.12	27 (7%) 13 10	41, 61, 133, 174	0
1	B	357/369 (96%)	-0.04	2 (0%) 89 88	39, 55, 89, 151	0
1	C	357/369 (96%)	-0.11	9 (2%) 57 51	34, 50, 118, 169	0
1	D	357/369 (96%)	-0.07	7 (1%) 65 60	39, 54, 98, 157	0
1	E	357/369 (96%)	0.00	9 (2%) 57 51	41, 63, 111, 166	0
1	F	357/369 (96%)	0.40	42 (11%) 4 3	39, 54, 160, 246	0
1	G	357/369 (96%)	0.07	19 (5%) 26 20	32, 57, 127, 169	0
1	H	357/369 (96%)	0.35	44 (12%) 4 2	37, 60, 142, 228	0
All	All	2856/2952 (96%)	0.09	159 (5%) 24 19	32, 57, 132, 246	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	311	LEU	12.5
1	H	271	ALA	12.5
1	F	338	GLN	8.7
1	H	313	LEU	6.3
1	A	267	THR	6.3
1	C	266	THR	6.2
1	F	368	ALA	6.1
1	F	316	GLN	6.1
1	F	271	ALA	5.7
1	A	297	ARG	5.7
1	F	268	VAL	5.7
1	F	292	GLN	5.3
1	H	369	ASP	5.3
1	F	299	ILE	5.2
1	H	280	ILE	5.1
1	H	276	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	263	GLN	5.1
1	H	286	LEU	5.1
1	D	295	ALA	5.0
1	F	337	HIS	4.9
1	F	341	PHE	4.8
1	H	334	TYR	4.8
1	F	369	ASP	4.6
1	F	313	LEU	4.5
1	F	298	ALA	4.2
1	G	313	LEU	4.2
1	E	311	LEU	4.1
1	A	271	ALA	4.1
1	F	279	ALA	4.0
1	H	295	ALA	3.9
1	A	292	GLN	3.9
1	G	266	THR	3.9
1	G	364	ALA	3.9
1	H	272	GLN	3.9
1	G	368	ALA	3.8
1	E	265	GLN	3.8
1	H	303	ARG	3.8
1	F	287	TYR	3.8
1	A	266	THR	3.7
1	H	268	VAL	3.7
1	F	312	GLY	3.6
1	G	361	ARG	3.6
1	A	270	ALA	3.6
1	F	314	ASN	3.6
1	G	300	TRP	3.6
1	F	304	VAL	3.5
1	C	295	ALA	3.5
1	H	361	ARG	3.5
1	E	306	VAL	3.5
1	A	273	LEU	3.5
1	G	284	HIS	3.4
1	H	352	GLU	3.4
1	H	363	ILE	3.4
1	F	363	ILE	3.3
1	C	313	LEU	3.3
1	F	309	SER	3.3
1	F	272	GLN	3.3
1	F	297	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	299	ILE	3.3
1	F	302	ILE	3.3
1	D	369	ASP	3.3
1	A	276	VAL	3.2
1	F	301	ARG	3.2
1	F	265	GLN	3.2
1	H	300	TRP	3.1
1	F	307	ASN	3.1
1	F	266	THR	3.1
1	A	2	THR	3.1
1	E	369	ASP	3.0
1	A	337	HIS	2.9
1	H	316	GLN	2.9
1	F	317	ASP	2.9
1	A	263	GLN	2.9
1	G	263	GLN	2.9
1	H	368	ALA	2.9
1	C	265	GLN	2.8
1	H	304	VAL	2.8
1	A	298	ALA	2.8
1	A	364	ALA	2.8
1	H	275	PRO	2.8
1	H	308	ALA	2.8
1	A	336	LEU	2.7
1	H	274	GLN	2.7
1	H	354	ALA	2.7
1	H	364	ALA	2.7
1	G	363	ILE	2.7
1	B	311	LEU	2.7
1	C	298	ALA	2.7
1	F	273	LEU	2.7
1	F	280	ILE	2.7
1	G	287	TYR	2.7
1	G	369	ASP	2.7
1	G	312	GLY	2.6
1	G	262	HIS	2.6
1	H	283	ILE	2.6
1	D	318	VAL	2.6
1	H	317	ASP	2.6
1	H	267	THR	2.6
1	F	289	ASP	2.6
1	H	306	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	355	LEU	2.5
1	H	289	ASP	2.5
1	F	278	GLU	2.5
1	A	268	VAL	2.5
1	D	311	LEU	2.5
1	A	280	ILE	2.5
1	C	299	ILE	2.5
1	E	313	LEU	2.5
1	A	333	LYS	2.5
1	F	306	VAL	2.5
1	F	321	GLN	2.5
1	G	311	LEU	2.4
1	F	300	TRP	2.4
1	H	2	THR	2.4
1	H	360	LEU	2.4
1	A	265	GLN	2.4
1	H	287	TYR	2.4
1	F	290	ILE	2.4
1	F	334	TYR	2.4
1	H	151	GLU	2.4
1	G	2	THR	2.3
1	A	369	ASP	2.3
1	G	357	VAL	2.3
1	H	269	THR	2.3
1	H	366	HIS	2.3
1	B	295	ALA	2.3
1	D	288	ALA	2.3
1	A	3	PRO	2.2
1	H	273	LEU	2.2
1	D	297	ARG	2.2
1	E	312	GLY	2.2
1	H	340	VAL	2.2
1	H	336	LEU	2.2
1	A	287	TYR	2.2
1	A	291	GLU	2.2
1	F	339	GLY	2.2
1	C	293	ASP	2.2
1	H	265	GLN	2.2
1	E	286	LEU	2.2
1	H	357	VAL	2.2
1	A	368	ALA	2.2
1	A	256	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	313	LEU	2.1
1	G	340	VAL	2.1
1	H	327	ILE	2.1
1	F	365	GLU	2.1
1	G	336	LEU	2.1
1	F	361	ARG	2.1
1	H	305	ARG	2.1
1	F	356	ILE	2.1
1	G	360	LEU	2.1
1	A	306	VAL	2.1
1	C	300	TRP	2.1
1	H	266	THR	2.1
1	H	362	GLU	2.1
1	F	305	ARG	2.0
1	C	290	ILE	2.0
1	D	368	ALA	2.0
1	E	2	THR	2.0

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. 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
1	LLP	D	213	24/25	0.95	0.17	44,51,61,68	0
1	LLP	G	213	24/25	0.96	0.16	37,53,63,64	0
1	LLP	C	213	24/25	0.97	0.15	42,49,59,68	0
1	LLP	A	213	24/25	0.97	0.14	39,55,67,78	0
1	LLP	E	213	24/25	0.97	0.17	40,51,59,63	0
1	LLP	F	213	24/25	0.97	0.16	44,55,67,72	0
1	LLP	B	213	24/25	0.97	0.17	43,52,67,75	0
1	LLP	H	213	24/25	0.97	0.15	46,53,63,72	0

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
3	ACY	E	401	4/4	0.76	0.18	62,88,93,94	0
3	ACY	E	402	4/4	0.76	0.21	67,76,92,95	0
3	ACY	B	401	4/4	0.85	0.14	44,63,67,73	0
4	MG	B	405	1/1	0.87	0.08	61,61,61,61	0
2	DMS	F	403	4/4	0.88	0.14	50,59,69,94	0
3	ACY	E	403	4/4	0.88	0.29	51,52,60,76	0
4	MG	A	404	1/1	0.88	0.26	57,57,57,57	0
3	ACY	A	402	4/4	0.88	0.27	70,74,77,80	0
2	DMS	G	403	4/4	0.89	0.14	49,58,68,103	0
2	DMS	F	402	4/4	0.89	0.26	51,72,73,93	0
5	CL	B	406	1/1	0.89	0.14	66,66,66,66	0
2	DMS	E	405	4/4	0.90	0.16	47,58,74,91	0
2	DMS	C	402	4/4	0.90	0.20	44,63,72,105	0
4	MG	H	402	1/1	0.91	0.14	57,57,57,57	0
4	MG	H	403	1/1	0.91	0.29	72,72,72,72	0
4	MG	E	407	1/1	0.91	0.12	55,55,55,55	0
2	DMS	G	401	4/4	0.92	0.26	48,56,78,84	0
4	MG	C	403	1/1	0.92	0.07	53,53,53,53	0
2	DMS	B	404	4/4	0.92	0.17	57,64,72,96	0
2	DMS	E	404	4/4	0.93	0.15	68,85,89,108	0
2	DMS	B	402	4/4	0.93	0.23	57,70,79,91	0
6	PEG	C	401	7/7	0.93	0.20	68,75,78,78	0
2	DMS	F	401	4/4	0.94	0.11	64,77,82,94	0
2	DMS	G	402	4/4	0.94	0.10	56,61,77,89	0
4	MG	G	404	1/1	0.94	0.15	46,46,46,46	0
4	MG	H	401	1/1	0.94	0.20	56,56,56,56	0
2	DMS	E	406	4/4	0.95	0.18	62,73,78,87	0
2	DMS	D	401	4/4	0.95	0.12	58,74,74,90	0
2	DMS	F	404	4/4	0.95	0.36	52,61,76,87	0
4	MG	G	406	1/1	0.96	0.15	49,49,49,49	0
2	DMS	D	403	4/4	0.96	0.14	64,66,72,88	0
2	DMS	B	403	4/4	0.96	0.12	68,73,83,93	0
4	MG	F	405	1/1	0.96	0.19	52,52,52,52	0
2	DMS	A	401	4/4	0.96	0.24	70,76,85,92	0
4	MG	G	405	1/1	0.96	0.09	55,55,55,55	0
2	DMS	D	402	4/4	0.97	0.16	65,81,84,99	0
2	DMS	A	403	4/4	0.98	0.25	59,69,80,87	0

6.5 Other polymers (i)

There are no such residues in this entry.