Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 01:34 PM JST

PDB ID	:	4U1T
Title	:	The crystal structure of holo CalE6, a methionine gamma lyase from Micromonospora echinospora
Authors	:	Song, H.G.; Guo, Z.H.
Deposited on	:	2014-07-16
Resolution	:	2.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

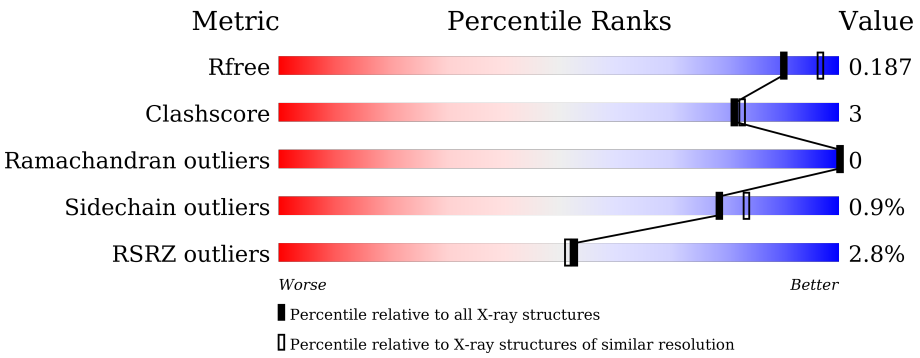
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	389	3% 87% 7% • 5%
1	B	389	3% 90% 7% •
1	C	389	2% 87% 6% 7%
1	D	389	% 86% 6% 7%
1	E	389	2% 89% 5% 6%
1	F	389	5% 92% 5% •

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Mol	Chain	Length	Quality of chain
1	G	389	2% 89% 7%
1	H	389	3% 87% 6% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24441 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 CalE6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	368	2741	1719	494	518	1	9	0	1	0
1	B	377	2816	1764	513	529	1	9	0	1	0
1	C	362	2702	1699	484	509	1	9	0	1	0
1	D	361	2696	1694	484	508	1	9	0	1	0
1	E	366	2737	1717	489	521	1	9	0	1	0
1	F	377	2826	1770	514	532	1	9	0	1	0
1	G	363	2717	1706	487	514	1	9	0	1	0
1	H	365	2729	1712	494	513	1	9	0	1	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	LEU	-	expression tag	UNP Q8KNG3
A	383	GLU	-	expression tag	UNP Q8KNG3
A	384	HIS	-	expression tag	UNP Q8KNG3
A	385	HIS	-	expression tag	UNP Q8KNG3
A	386	HIS	-	expression tag	UNP Q8KNG3
A	387	HIS	-	expression tag	UNP Q8KNG3
A	388	HIS	-	expression tag	UNP Q8KNG3
A	389	HIS	-	expression tag	UNP Q8KNG3
B	382	LEU	-	expression tag	UNP Q8KNG3
B	383	GLU	-	expression tag	UNP Q8KNG3
B	384	HIS	-	expression tag	UNP Q8KNG3
B	385	HIS	-	expression tag	UNP Q8KNG3
B	386	HIS	-	expression tag	UNP Q8KNG3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	387	HIS	-	expression tag	UNP Q8KNG3
B	388	HIS	-	expression tag	UNP Q8KNG3
B	389	HIS	-	expression tag	UNP Q8KNG3
C	382	LEU	-	expression tag	UNP Q8KNG3
C	383	GLU	-	expression tag	UNP Q8KNG3
C	384	HIS	-	expression tag	UNP Q8KNG3
C	385	HIS	-	expression tag	UNP Q8KNG3
C	386	HIS	-	expression tag	UNP Q8KNG3
C	387	HIS	-	expression tag	UNP Q8KNG3
C	388	HIS	-	expression tag	UNP Q8KNG3
C	389	HIS	-	expression tag	UNP Q8KNG3
D	382	LEU	-	expression tag	UNP Q8KNG3
D	383	GLU	-	expression tag	UNP Q8KNG3
D	384	HIS	-	expression tag	UNP Q8KNG3
D	385	HIS	-	expression tag	UNP Q8KNG3
D	386	HIS	-	expression tag	UNP Q8KNG3
D	387	HIS	-	expression tag	UNP Q8KNG3
D	388	HIS	-	expression tag	UNP Q8KNG3
D	389	HIS	-	expression tag	UNP Q8KNG3
E	382	LEU	-	expression tag	UNP Q8KNG3
E	383	GLU	-	expression tag	UNP Q8KNG3
E	384	HIS	-	expression tag	UNP Q8KNG3
E	385	HIS	-	expression tag	UNP Q8KNG3
E	386	HIS	-	expression tag	UNP Q8KNG3
E	387	HIS	-	expression tag	UNP Q8KNG3
E	388	HIS	-	expression tag	UNP Q8KNG3
E	389	HIS	-	expression tag	UNP Q8KNG3
F	382	LEU	-	expression tag	UNP Q8KNG3
F	383	GLU	-	expression tag	UNP Q8KNG3
F	384	HIS	-	expression tag	UNP Q8KNG3
F	385	HIS	-	expression tag	UNP Q8KNG3
F	386	HIS	-	expression tag	UNP Q8KNG3
F	387	HIS	-	expression tag	UNP Q8KNG3
F	388	HIS	-	expression tag	UNP Q8KNG3
F	389	HIS	-	expression tag	UNP Q8KNG3
G	382	LEU	-	expression tag	UNP Q8KNG3
G	383	GLU	-	expression tag	UNP Q8KNG3
G	384	HIS	-	expression tag	UNP Q8KNG3
G	385	HIS	-	expression tag	UNP Q8KNG3
G	386	HIS	-	expression tag	UNP Q8KNG3
G	387	HIS	-	expression tag	UNP Q8KNG3
G	388	HIS	-	expression tag	UNP Q8KNG3

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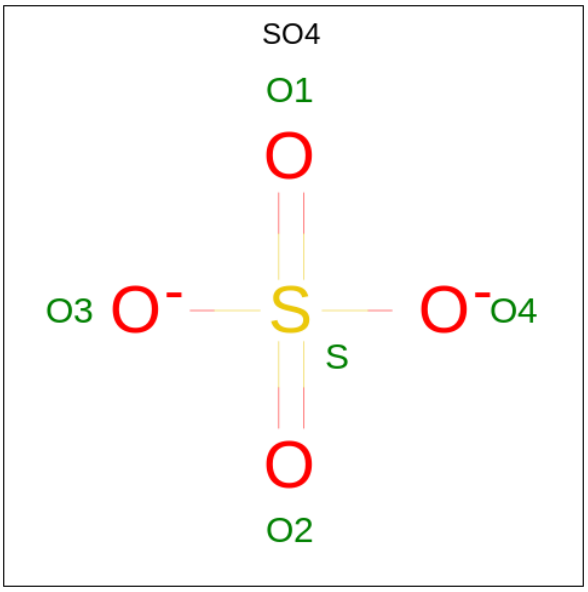
Chain	Residue	Modelled	Actual	Comment	Reference
G	389	HIS	-	expression tag	UNP Q8KNG3
H	382	LEU	-	expression tag	UNP Q8KNG3
H	383	GLU	-	expression tag	UNP Q8KNG3
H	384	HIS	-	expression tag	UNP Q8KNG3
H	385	HIS	-	expression tag	UNP Q8KNG3
H	386	HIS	-	expression tag	UNP Q8KNG3
H	387	HIS	-	expression tag	UNP Q8KNG3
H	388	HIS	-	expression tag	UNP Q8KNG3
H	389	HIS	-	expression tag	UNP Q8KNG3

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	G	1	5	4	1	0	0

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

- Molecule 3 is water.

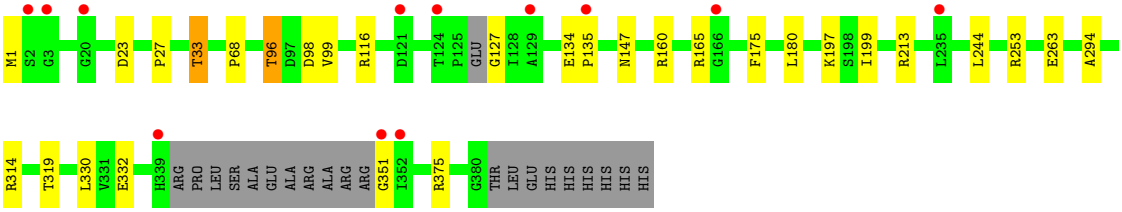
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	320	320	320	0	0
3	B	316	316	316	0	0
3	C	300	300	300	0	0
3	D	291	291	291	0	0
3	E	298	298	298	0	0
3	F	305	305	305	0	0
3	G	327	327	327	0	0
3	H	280	280	280	0	0

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.

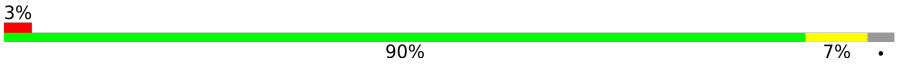
- Molecule 1: CalE6

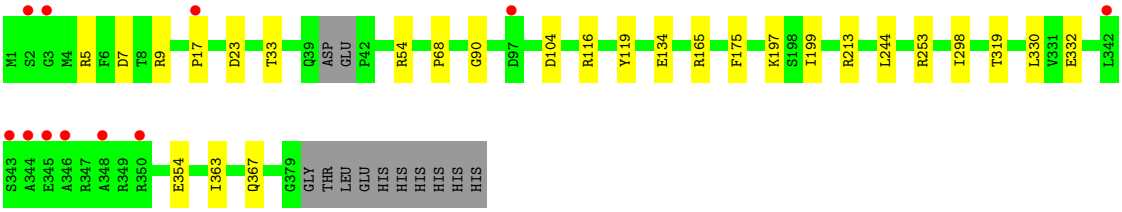
Chain A:



- Molecule 1: CalE6

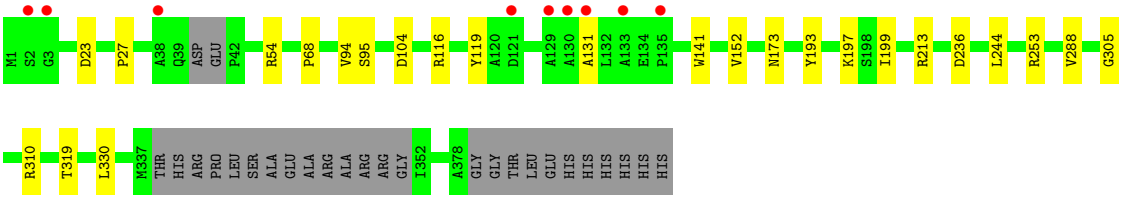
Chain B:





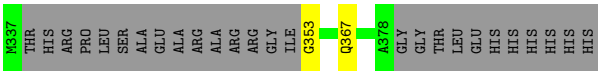
- Molecule 1: CalE6

Chain C:



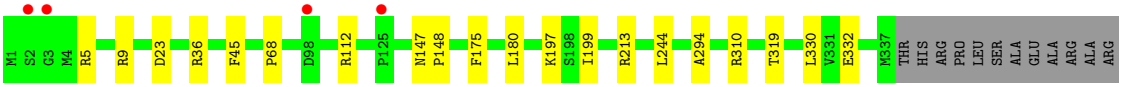
- Molecule 1: CalE6

Chain D:



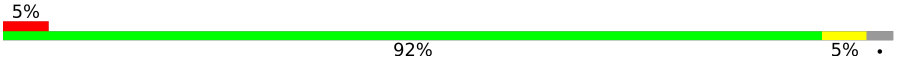
• Molecule 1: CalE6

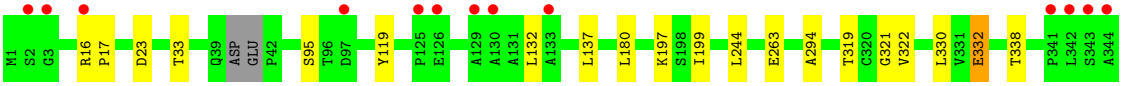
Chain E:

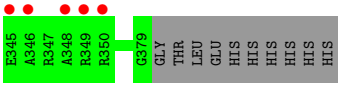


• Molecule 1: CalE6

Chain F:

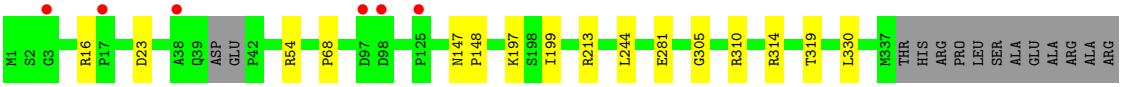


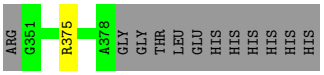




• Molecule 1: CalE6

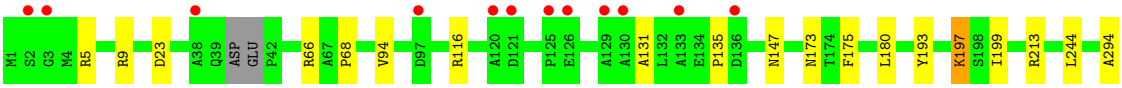
Chain G:

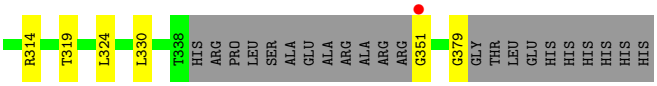




• Molecule 1: CalE6

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	146.17Å 146.22Å 348.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 2.00 47.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.66-2.00) 95.8 (47.66-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.34 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.151 , 0.184 0.156 , 0.187	Depositor DCC
R_{free} test set	12515 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 63.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.043 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	24441	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.88% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/2772	0.52	0/3782
1	B	0.40	0/2846	0.53	0/3882
1	C	0.40	0/2732	0.53	0/3727
1	D	0.36	0/2726	0.51	0/3719
1	E	0.39	0/2768	0.52	0/3777
1	F	0.39	0/2859	0.53	0/3898
1	G	0.40	0/2747	0.53	0/3746
1	H	0.37	0/2759	0.54	0/3762
All	All	0.39	0/22209	0.53	0/30293

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 (i)

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	2741	0	2705	21	0
1	B	2816	0	2786	18	0
1	C	2702	0	2676	14	0
1	D	2696	0	2667	18	0
1	E	2737	0	2702	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2826	0	2803	12	0
1	G	2717	0	2691	10	0
1	H	2729	0	2709	13	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	320	0	0	9	0
3	B	316	0	0	10	2
3	C	300	0	0	3	0
3	D	291	0	0	7	0
3	E	298	0	0	3	0
3	F	305	0	0	3	0
3	G	327	0	0	4	0
3	H	280	0	0	2	1
All	All	24441	0	21739	114	2

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 (114) 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:134:GLU:O	1:A:165:ARG:NH1	2.17	0.78
1:D:90:GLY:O	3:D:501:HOH:O	2.02	0.77
1:A:263:GLU:OE2	3:A:651:HOH:O	2.00	0.77
1:B:17:PRO:O	3:B:682:HOH:O	2.04	0.76
1:B:116:ARG:NH1	3:B:732:HOH:O	2.02	0.74
1:C:95:SER:HB2	1:C:141:TRP:HB3	1.69	0.74
1:A:1:MET:N	3:A:741:HOH:O	2.21	0.73
1:B:90:GLY:O	3:B:732:HOH:O	2.07	0.72
1:C:236:ASP:OD2	3:C:595:HOH:O	2.09	0.71
1:A:351:GLY:N	3:A:803:HOH:O	2.28	0.67
1:H:351:GLY:N	3:H:692:HOH:O	2.27	0.66
1:F:263:GLU:OE2	3:F:501:HOH:O	2.14	0.66
1:D:134:GLU:O	1:D:165:ARG:NH2	2.30	0.64
1:D:1:MET:N	3:D:621:HOH:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:GLU:OE2	3:G:501:HOH:O	2.15	0.63
1:B:367:GLN:NE2	3:B:766:HOH:O	2.30	0.62
1:A:96:THR:O	1:A:99:VAL:HG13	2.00	0.62
1:A:160:ARG:NH2	3:A:744:HOH:O	2.29	0.61
1:G:305:GLY:O	1:G:310:ARG:NH1	2.34	0.61
1:D:353:GLY:N	3:D:658:HOH:O	2.34	0.60
1:E:36:ARG:HH22	1:F:322:VAL:HG22	1.67	0.59
1:D:199:ILE:HG23	1:D:244:LEU:HD13	1.84	0.58
1:A:199:ILE:HG23	1:A:244:LEU:HD13	1.86	0.58
1:H:199:ILE:HG23	1:H:244:LEU:HD13	1.86	0.57
1:B:134:GLU:O	1:B:165:ARG:NH2	2.37	0.57
1:F:16:ARG:HD2	3:F:788:HOH:O	2.04	0.57
1:A:127:GLY:N	3:A:761:HOH:O	2.36	0.56
1:E:36:ARG:HD3	1:F:321:GLY:HA2	1.87	0.56
1:G:199:ILE:HG23	1:G:244:LEU:HD13	1.88	0.55
1:D:116:ARG:HD3	3:D:501:HOH:O	2.07	0.54
1:A:351:GLY:N	3:A:809:HOH:O	2.41	0.54
1:F:319:THR:HB	1:F:330:LEU:HD23	1.90	0.53
1:G:16:ARG:HD2	3:G:654:HOH:O	2.08	0.52
1:H:68:PRO:HG2	1:H:213:ARG:HA	1.91	0.52
1:F:199:ILE:HG23	1:F:244:LEU:HD13	1.90	0.52
1:C:199:ILE:HG23	1:C:244:LEU:HD13	1.91	0.52
1:H:116:ARG:NH1	1:H:135:PRO:O	2.39	0.51
1:B:104:ASP:OD1	1:B:119:TYR:OH	2.17	0.51
1:B:199:ILE:HG23	1:B:244:LEU:HD13	1.93	0.51
1:B:68:PRO:HG2	1:B:213:ARG:HA	1.93	0.50
1:A:253:ARG:NH2	1:D:7:ASP:OD2	2.38	0.50
1:A:180:LEU:HD22	1:A:294:ALA:HB3	1.93	0.50
1:B:116:ARG:HD3	3:B:732:HOH:O	2.11	0.50
1:A:116:ARG:NH1	1:A:135:PRO:O	2.42	0.50
1:D:367:GLN:OE1	3:D:780:HOH:O	2.20	0.50
1:C:305:GLY:O	1:C:310:ARG:NH1	2.40	0.49
1:B:354:GLU:OE2	3:B:689:HOH:O	2.20	0.49
1:D:108:ASP:O	1:D:112:ARG:HG3	2.12	0.49
1:E:319:THR:HB	1:E:330:LEU:HD23	1.94	0.49
1:C:68:PRO:HG2	1:C:213:ARG:HA	1.95	0.49
1:F:180:LEU:HD22	1:F:294:ALA:HB3	1.95	0.48
1:H:197:LLP:HD3	1:H:324:LEU:HG	1.95	0.48
1:A:98:ASP:CB	3:A:734:HOH:O	2.62	0.48
1:H:5:ARG:O	1:H:9[B]:ARG:HG3	2.13	0.48
1:D:68:PRO:HG2	1:D:213:ARG:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ARG:NH2	1:F:322:VAL:HG22	2.29	0.48
1:B:54:ARG:NH1	3:B:626:HOH:O	2.41	0.47
1:E:180:LEU:HD22	1:E:294:ALA:HB3	1.96	0.47
1:D:116:ARG:NH2	1:D:134:GLU:OE2	2.45	0.47
1:B:116:ARG:NH2	1:B:134:GLU:OE1	2.47	0.47
1:E:112:ARG:NH1	3:E:772:HOH:O	2.38	0.47
1:D:180:LEU:HD22	1:D:294:ALA:HB3	1.96	0.47
1:C:54:ARG:NH1	3:C:626:HOH:O	2.38	0.47
1:G:319:THR:HB	1:G:330:LEU:HD23	1.96	0.47
1:C:310:ARG:NH2	3:C:502:HOH:O	2.48	0.46
1:A:33:THR:HG21	3:B:674:HOH:O	2.14	0.46
1:E:147:ASN:HB2	1:E:175:PHE:CZ	2.49	0.46
1:C:319:THR:HB	1:C:330:LEU:HD23	1.97	0.46
1:B:319:THR:HB	1:B:330:LEU:HD23	1.98	0.46
1:E:5:ARG:O	1:E:9[B]:ARG:HG3	2.15	0.46
1:D:319:THR:HB	1:D:330:LEU:HD23	1.96	0.46
1:A:147:ASN:HB2	1:A:175:PHE:CZ	2.50	0.46
1:G:68:PRO:HG2	1:G:213:ARG:HA	1.96	0.46
1:B:9[B]:ARG:NH2	3:B:699:HOH:O	2.46	0.45
1:E:199:ILE:HG23	1:E:244:LEU:HD13	1.97	0.45
1:H:319:THR:HB	1:H:330:LEU:HD23	1.99	0.45
1:D:197:LLP:HD3	1:D:324:LEU:HG	1.99	0.45
1:H:94:VAL:HG11	1:H:131:ALA:HB1	1.98	0.45
1:E:310:ARG:NH2	3:E:502:HOH:O	2.49	0.45
1:E:147:ASN:ND2	3:E:724:HOH:O	2.49	0.45
1:G:54:ARG:NH1	3:G:758:HOH:O	2.29	0.45
1:B:253:ARG:HD2	1:B:363:ILE:HB	1.99	0.45
1:C:94:VAL:HG11	1:C:131:ALA:HB1	1.99	0.45
1:H:180:LEU:HD22	1:H:294:ALA:HB3	1.98	0.45
1:H:66:ARG:NH1	3:H:725:HOH:O	2.50	0.44
1:E:147:ASN:HA	1:E:148:PRO:HA	1.84	0.44
1:D:9[B]:ARG:NH2	3:D:611:HOH:O	2.49	0.44
1:G:375:ARG:HG3	3:G:783:HOH:O	2.17	0.44
1:A:68:PRO:HG2	1:A:213:ARG:HA	1.99	0.44
1:C:104:ASP:OD2	1:C:119:TYR:OH	2.33	0.44
1:D:132:LEU:O	1:D:165:ARG:NE	2.46	0.43
1:D:5:ARG:O	1:D:9[B]:ARG:HG3	2.18	0.43
1:H:314:ARG:CZ	1:H:379:GLY:HA2	2.48	0.43
1:H:147:ASN:HB2	1:H:175:PHE:CZ	2.54	0.43
1:A:319:THR:HB	1:A:330:LEU:HD23	2.00	0.43
1:A:33:THR:HB	3:B:722:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ARG:HD2	3:A:516:HOH:O	2.18	0.43
1:F:95:SER:O	1:F:119:TYR:HA	2.19	0.43
1:A:27:PRO:HB2	1:C:27:PRO:HB2	2.01	0.42
1:F:17:PRO:HA	3:F:545:HOH:O	2.19	0.42
1:C:152:VAL:HG21	1:C:288:VAL:HG22	2.02	0.42
1:B:5:ARG:O	1:B:9[B]:ARG:HG3	2.19	0.42
1:E:68:PRO:HG2	1:E:213:ARG:HA	2.02	0.42
1:G:310:ARG:NE	1:G:314:ARG:NH1	2.68	0.42
1:A:375:ARG:NH1	3:A:582:HOH:O	2.52	0.42
1:H:173:ASN:HB3	1:H:193:TYR:CE1	2.54	0.42
1:D:116:ARG:NH1	3:D:501:HOH:O	2.05	0.41
1:C:173:ASN:HB3	1:C:193:TYR:CE1	2.56	0.41
1:B:7:ASP:OD2	1:C:253:ARG:NH2	2.41	0.41
1:B:175:PHE:CZ	1:B:298:ILE:HB	2.56	0.41
1:G:147:ASN:HA	1:G:148:PRO:HA	1.85	0.40
1:F:332:GLU:OE1	1:F:338:THR:HG23	2.21	0.40
1:F:132:LEU:HD22	1:F:137:LEU:HD21	2.02	0.40
1:E:36:ARG:NH2	1:E:45:PHE:HB3	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:509:HOH:O	3:H:503:HOH:O[7_454]	2.13	0.07
3:B:792:HOH:O	3:B:792:HOH:O[2_455]	2.14	0.06

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	362/389 (93%)	354 (98%)	8 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	373/389 (96%)	368 (99%)	5 (1%)	0	100	100
1	C	356/389 (92%)	352 (99%)	4 (1%)	0	100	100
1	D	355/389 (91%)	347 (98%)	8 (2%)	0	100	100
1	E	362/389 (93%)	355 (98%)	7 (2%)	0	100	100
1	F	373/389 (96%)	366 (98%)	7 (2%)	0	100	100
1	G	357/389 (92%)	352 (99%)	5 (1%)	0	100	100
1	H	359/389 (92%)	352 (98%)	7 (2%)	0	100	100
All	All	2897/3112 (93%)	2846 (98%)	51 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	279/304 (92%)	275 (99%)	4 (1%)	67	72
1	B	285/304 (94%)	282 (99%)	3 (1%)	73	78
1	C	275/304 (90%)	273 (99%)	2 (1%)	84	88
1	D	275/304 (90%)	272 (99%)	3 (1%)	73	78
1	E	280/304 (92%)	278 (99%)	2 (1%)	84	88
1	F	288/304 (95%)	285 (99%)	3 (1%)	76	81
1	G	278/304 (91%)	277 (100%)	1 (0%)	91	93
1	H	279/304 (92%)	278 (100%)	1 (0%)	91	93
All	All	2239/2432 (92%)	2220 (99%)	19 (1%)	78	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	33	THR

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Mol	Chain	Res	Type
1	A	96	THR
1	A	332	GLU
1	B	23	ASP
1	B	33	THR
1	B	332	GLU
1	C	23	ASP
1	C	116	ARG
1	D	23	ASP
1	D	33	THR
1	D	332	GLU
1	E	23	ASP
1	E	332	GLU
1	F	23	ASP
1	F	33	THR
1	F	332	GLU
1	G	23	ASP
1	H	23	ASP

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	C	197	1	23,24,25	2.64	6 (26%)	25,32,34	1.23	2 (8%)
1	LLP	H	197	1	23,24,25	2.63	6 (26%)	25,32,34	1.30	3 (12%)
1	LLP	G	197	1	23,24,25	2.71	6 (26%)	25,32,34	1.19	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LLP	E	197	1	23,24,25	2.60	6 (26%)	25,32,34	1.29	3 (12%)
1	LLP	B	197	1	23,24,25	2.62	6 (26%)	25,32,34	1.19	3 (12%)
1	LLP	A	197	1	23,24,25	2.59	6 (26%)	25,32,34	1.32	4 (16%)
1	LLP	F	197	1	23,24,25	2.64	6 (26%)	25,32,34	1.36	4 (16%)
1	LLP	D	197	1	23,24,25	2.65	6 (26%)	25,32,34	1.20	3 (12%)

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	C	197	1	-	4/16/17/19	0/1/1/1
1	LLP	H	197	1	-	5/16/17/19	0/1/1/1
1	LLP	G	197	1	-	4/16/17/19	0/1/1/1
1	LLP	E	197	1	-	4/16/17/19	0/1/1/1
1	LLP	B	197	1	-	4/16/17/19	0/1/1/1
1	LLP	A	197	1	-	4/16/17/19	0/1/1/1
1	LLP	F	197	1	-	4/16/17/19	0/1/1/1
1	LLP	D	197	1	-	4/16/17/19	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	197	LLP	C4-C4'	8.83	1.63	1.46
1	C	197	LLP	C4-C4'	8.75	1.63	1.46
1	D	197	LLP	C4-C4'	8.59	1.63	1.46
1	F	197	LLP	C4-C4'	8.57	1.62	1.46
1	E	197	LLP	C4-C4'	8.54	1.62	1.46
1	B	197	LLP	C4-C4'	8.45	1.62	1.46
1	H	197	LLP	C4-C4'	8.45	1.62	1.46
1	A	197	LLP	C4-C4'	8.45	1.62	1.46
1	G	197	LLP	C4'-NZ	5.53	1.45	1.27
1	F	197	LLP	C4'-NZ	5.52	1.45	1.27
1	C	197	LLP	C4'-NZ	5.43	1.45	1.27
1	D	197	LLP	C4'-NZ	5.42	1.45	1.27
1	A	197	LLP	C4'-NZ	5.38	1.45	1.27
1	H	197	LLP	C4'-NZ	5.33	1.45	1.27
1	E	197	LLP	C4'-NZ	5.32	1.45	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	197	LLP	C4'-NZ	5.22	1.44	1.27
1	F	197	LLP	C2'-C2	3.97	1.57	1.50
1	G	197	LLP	C2'-C2	3.96	1.57	1.50
1	B	197	LLP	C2'-C2	3.90	1.57	1.50
1	H	197	LLP	C2'-C2	3.79	1.56	1.50
1	C	197	LLP	C2'-C2	3.76	1.56	1.50
1	A	197	LLP	C2'-C2	3.69	1.56	1.50
1	D	197	LLP	C2'-C2	3.64	1.56	1.50
1	E	197	LLP	C2'-C2	3.50	1.56	1.50
1	E	197	LLP	C6-N1	3.26	1.41	1.34
1	H	197	LLP	C6-N1	3.25	1.41	1.34
1	D	197	LLP	C6-N1	3.13	1.41	1.34
1	G	197	LLP	C6-N1	3.11	1.41	1.34
1	B	197	LLP	C6-N1	3.05	1.40	1.34
1	F	197	LLP	C6-N1	3.01	1.40	1.34
1	C	197	LLP	C6-N1	2.95	1.40	1.34
1	B	197	LLP	C4-C5	-2.93	1.38	1.42
1	G	197	LLP	C4-C5	-2.93	1.38	1.42
1	A	197	LLP	C6-N1	2.90	1.40	1.34
1	H	197	LLP	C4-C5	-2.81	1.38	1.42
1	D	197	LLP	C4-C5	-2.80	1.38	1.42
1	A	197	LLP	C4-C5	-2.79	1.38	1.42
1	C	197	LLP	C4-C5	-2.77	1.38	1.42
1	E	197	LLP	C4-C5	-2.73	1.38	1.42
1	G	197	LLP	C5'-C5	2.52	1.57	1.50
1	D	197	LLP	C5'-C5	2.52	1.57	1.50
1	F	197	LLP	C4-C5	-2.51	1.38	1.42
1	B	197	LLP	C5'-C5	2.39	1.57	1.50
1	E	197	LLP	C5'-C5	2.37	1.57	1.50
1	H	197	LLP	C5'-C5	2.34	1.57	1.50
1	C	197	LLP	C5'-C5	2.34	1.57	1.50
1	F	197	LLP	C5'-C5	2.30	1.57	1.50
1	A	197	LLP	C5'-C5	2.11	1.56	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	197	LLP	C4-C4'-NZ	-3.31	109.10	124.31
1	H	197	LLP	C4-C4'-NZ	-3.21	109.57	124.31
1	G	197	LLP	C4-C4'-NZ	-3.03	110.39	124.31
1	B	197	LLP	C4-C4'-NZ	-2.94	110.81	124.31
1	A	197	LLP	C4-C4'-NZ	-2.90	111.00	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	197	LLP	C4-C4'-NZ	-2.89	111.04	124.31
1	E	197	LLP	C4-C4'-NZ	-2.86	111.17	124.31
1	D	197	LLP	C4-C4'-NZ	-2.78	111.56	124.31
1	A	197	LLP	OP4-P-OP1	2.65	113.91	106.47
1	E	197	LLP	CE-NZ-C4'	-2.63	110.82	118.90
1	A	197	LLP	CE-NZ-C4'	-2.42	111.48	118.90
1	B	197	LLP	CE-NZ-C4'	-2.33	111.74	118.90
1	A	197	LLP	C5-C6-N1	-2.19	120.17	123.82
1	F	197	LLP	C5-C6-N1	-2.18	120.18	123.82
1	H	197	LLP	C5-C6-N1	-2.11	120.30	123.82
1	D	197	LLP	CE-NZ-C4'	-2.09	112.50	118.90
1	B	197	LLP	C5-C6-N1	-2.06	120.38	123.82
1	F	197	LLP	OP4-P-OP1	2.05	112.22	106.47
1	D	197	LLP	C5-C6-N1	-2.04	120.42	123.82
1	C	197	LLP	C4-C3-C2	2.03	121.45	120.19
1	H	197	LLP	C2'-C2-N1	2.03	121.63	117.67
1	F	197	LLP	CE-NZ-C4'	-2.01	112.74	118.90
1	E	197	LLP	OP4-P-OP1	2.01	112.11	106.47

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	197	LLP	O-C-CA-CB
1	B	197	LLP	O-C-CA-CB
1	C	197	LLP	O-C-CA-CB
1	D	197	LLP	O-C-CA-CB
1	E	197	LLP	C4-C4'-NZ-CE
1	E	197	LLP	O-C-CA-CB
1	F	197	LLP	O-C-CA-CB
1	G	197	LLP	O-C-CA-CB
1	H	197	LLP	O-C-CA-CB
1	A	197	LLP	C4-C4'-NZ-CE
1	B	197	LLP	C4-C4'-NZ-CE
1	C	197	LLP	C4-C4'-NZ-CE
1	D	197	LLP	C4-C4'-NZ-CE
1	F	197	LLP	C4-C4'-NZ-CE
1	G	197	LLP	C4-C4'-NZ-CE
1	H	197	LLP	C4-C4'-NZ-CE
1	A	197	LLP	CD-CE-NZ-C4'
1	G	197	LLP	CD-CE-NZ-C4'
1	H	197	LLP	CD-CE-NZ-C4'

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Mol	Chain	Res	Type	Atoms
1	C	197	LLP	CD-CE-NZ-C4'
1	E	197	LLP	CD-CE-NZ-C4'
1	D	197	LLP	C5'-OP4-P-OP1
1	F	197	LLP	CA-CB-CG-CD
1	H	197	LLP	CA-CB-CG-CD
1	B	197	LLP	CD-CE-NZ-C4'
1	D	197	LLP	CD-CE-NZ-C4'
1	G	197	LLP	C3-C4-C4'-NZ
1	F	197	LLP	CD-CE-NZ-C4'
1	A	197	LLP	N-CA-CB-CG
1	B	197	LLP	N-CA-CB-CG
1	C	197	LLP	N-CA-CB-CG
1	E	197	LLP	N-CA-CB-CG
1	H	197	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	197	LLP	1	0
1	D	197	LLP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	C	401	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	G	401	-	4,4,4	0.09	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	E	401	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	F	401	-	4,4,4	0.18	0	6,6,6	0.19	0
2	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	B	401	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	H	401	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	D	401	-	4,4,4	0.10	0	6,6,6	0.10	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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	367/389 (94%)	-0.26	12 (3%)	46	45	8, 19, 50, 89	0
1	B	376/389 (96%)	-0.25	11 (2%)	51	50	9, 20, 50, 91	0
1	C	361/389 (92%)	-0.34	9 (2%)	57	56	7, 18, 51, 93	0
1	D	360/389 (92%)	-0.32	5 (1%)	75	74	9, 22, 49, 62	0
1	E	365/389 (93%)	-0.19	9 (2%)	57	56	7, 19, 47, 77	0
1	F	376/389 (96%)	-0.13	18 (4%)	30	29	6, 19, 55, 86	0
1	G	362/389 (93%)	-0.40	6 (1%)	70	68	7, 18, 43, 73	0
1	H	364/389 (93%)	-0.25	13 (3%)	42	42	8, 20, 55, 85	0
All	All	2931/3112 (94%)	-0.27	83 (2%)	53	51	6, 19, 51, 93	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	3	GLY	4.7
1	C	38	ALA	4.6
1	B	2	SER	4.5
1	F	3	GLY	4.5
1	B	3	GLY	4.4
1	F	345	GLU	4.1
1	F	342	LEU	4.1
1	F	2	SER	4.0
1	B	17	PRO	3.9
1	B	348	ALA	3.9
1	E	98	ASP	3.9
1	F	126	GLU	3.8
1	H	3	GLY	3.8
1	F	97	ASP	3.7
1	D	38	ALA	3.6
1	H	125	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	352	ILE	3.4
1	A	2	SER	3.4
1	F	349	ARG	3.4
1	H	133	ALA	3.4
1	C	130	ALA	3.4
1	E	3	GLY	3.3
1	E	379	GLY	3.3
1	A	3	GLY	3.3
1	A	339	HIS	3.3
1	H	97	ASP	3.3
1	B	342	LEU	3.3
1	F	341	PRO	3.3
1	F	344	ALA	3.2
1	F	346	ALA	3.2
1	D	3	GLY	3.1
1	C	3	GLY	3.1
1	E	352	ILE	3.1
1	C	131	ALA	3.0
1	F	343	SER	3.0
1	G	38	ALA	3.0
1	H	351	GLY	3.0
1	E	2	SER	2.9
1	G	98	ASP	2.8
1	D	2	SER	2.8
1	H	2	SER	2.8
1	G	17	PRO	2.8
1	B	350	ARG	2.8
1	B	344	ALA	2.7
1	B	346	ALA	2.7
1	E	354	GLU	2.7
1	A	121	ASP	2.7
1	A	351	GLY	2.7
1	B	97	ASP	2.6
1	A	166	GLY	2.6
1	D	124	THR	2.5
1	E	353	GLY	2.5
1	H	136	ASP	2.5
1	F	129	ALA	2.5
1	H	126	GLU	2.5
1	C	133	ALA	2.4
1	H	38	ALA	2.4
1	H	129	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	98	ASP	2.4
1	G	97	ASP	2.4
1	C	129	ALA	2.3
1	B	345	GLU	2.3
1	A	129	ALA	2.2
1	E	125	PRO	2.2
1	F	348	ALA	2.2
1	A	235	LEU	2.2
1	F	16	ARG	2.2
1	F	125	PRO	2.2
1	A	20	GLY	2.2
1	F	133	ALA	2.2
1	C	135	PRO	2.2
1	F	130	ALA	2.1
1	H	130	ALA	2.1
1	B	343	SER	2.1
1	G	125	PRO	2.1
1	C	2	SER	2.1
1	A	135	PRO	2.1
1	C	121	ASP	2.1
1	F	350	ARG	2.1
1	A	124	THR	2.0
1	E	351	GLY	2.0
1	H	121	ASP	2.0
1	H	120	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	C	197	24/25	0.96	0.11	8,22,29,31	0
1	LLP	D	197	24/25	0.96	0.11	8,20,26,29	0
1	LLP	A	197	24/25	0.97	0.12	11,22,31,31	0
1	LLP	B	197	24/25	0.97	0.11	10,18,24,29	0
1	LLP	E	197	24/25	0.97	0.12	10,19,28,32	0
1	LLP	G	197	24/25	0.97	0.11	8,18,29,32	0
1	LLP	H	197	24/25	0.97	0.11	6,21,29,29	0
1	LLP	F	197	24/25	0.98	0.09	9,17,22,30	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	401	5/5	0.94	0.15	48,52,55,64	0
2	SO4	G	401	5/5	0.95	0.15	40,47,48,56	0
2	SO4	H	401	5/5	0.95	0.12	35,42,49,57	0
2	SO4	E	401	5/5	0.97	0.10	47,48,50,55	0
2	SO4	C	401	5/5	0.97	0.11	33,35,42,58	0
2	SO4	A	401	5/5	0.97	0.14	38,39,45,54	0
2	SO4	F	401	5/5	0.98	0.09	23,29,32,32	0
2	SO4	B	401	5/5	0.99	0.06	26,28,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.