Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2018 – 11:45 AM EST

PDB ID	:	1M1O
Title	:	Crystal structure of biosynthetic thiolase, C89A mutant, complexed with acetoacetyl-CoA
Authors	:	Kursula, P.; Ojala, J.; Lambeir, A.-M.; Wierenga, R.K.
Deposited on	:	2002-06-20
Resolution	:	1.95 Å(reported)

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

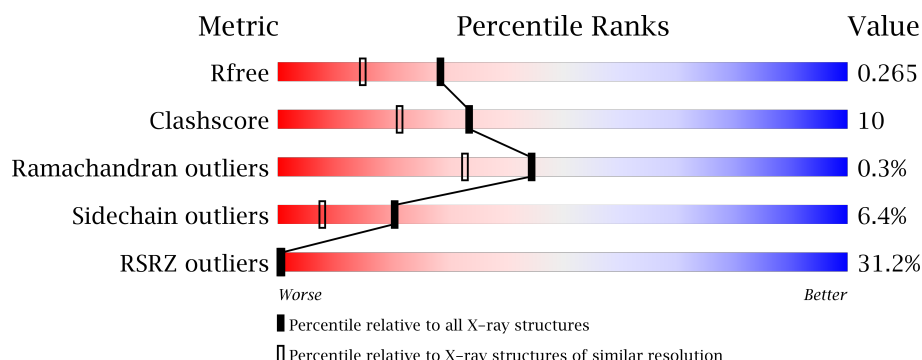|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

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 1.95 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	Percentile Ranks	Value
Rfree		0.265
Clashscore		10
Ramachandran outliers		0.3%
Sidechain outliers		6.4%
RSRZ outliers		31.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	392	23% / 84% / 13% ••
1	B	392	21% / 81% / 17% ••
1	C	392	32% / 75% / 23% ••
1	D	392	48% / 74% / 23% ••

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	CAA	B	2393	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12414 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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	1	0
			2821	1752	510	539	20			
1	B	390	Total	C	N	O	S	0	1	0
			2821	1752	510	539	20			
1	C	390	Total	C	N	O	S	0	1	0
			2821	1752	510	539	20			
1	D	390	Total	C	N	O	S	0	1	0
			2821	1752	510	539	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	INSERTION	UNP P07097
A	89	ALA	CYS	ENGINEERED	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	10	ALA	-	INSERTION	UNP P07097
B	89	ALA	CYS	ENGINEERED	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	10	ALA	-	INSERTION	UNP P07097
C	89	ALA	CYS	ENGINEERED	UNP P07097
C	129	ARG	ALA	CONFLICT	UNP P07097
D	10	ALA	-	INSERTION	UNP P07097
D	89	ALA	CYS	ENGINEERED	UNP P07097
D	129	ARG	ALA	CONFLICT	UNP P07097

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

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

- Molecule 3 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$).
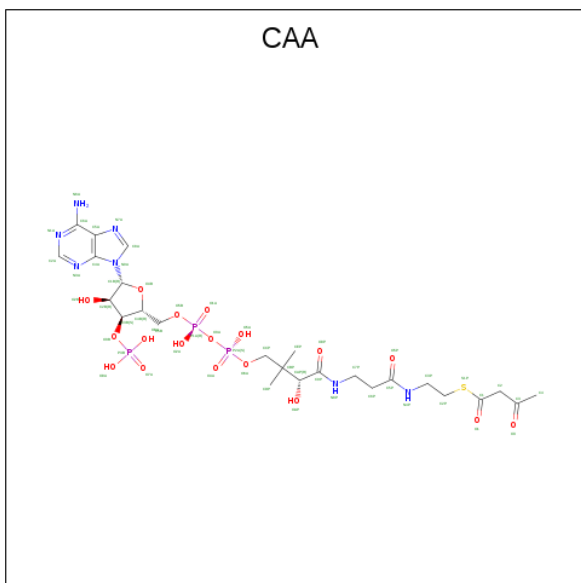
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 54	C 25	N 7	O 18	P 3	S 1	0	0
3	B	1	Total 54	C 25	N 7	O 18	P 3	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	360	Total 360	O 360	0	0
4	B	372	Total 372	O 372	0	0
4	C	127	Total 127	O 127	0	0
4	D	143	Total 143	O 143	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Acetyl-CoA acetyltransferase
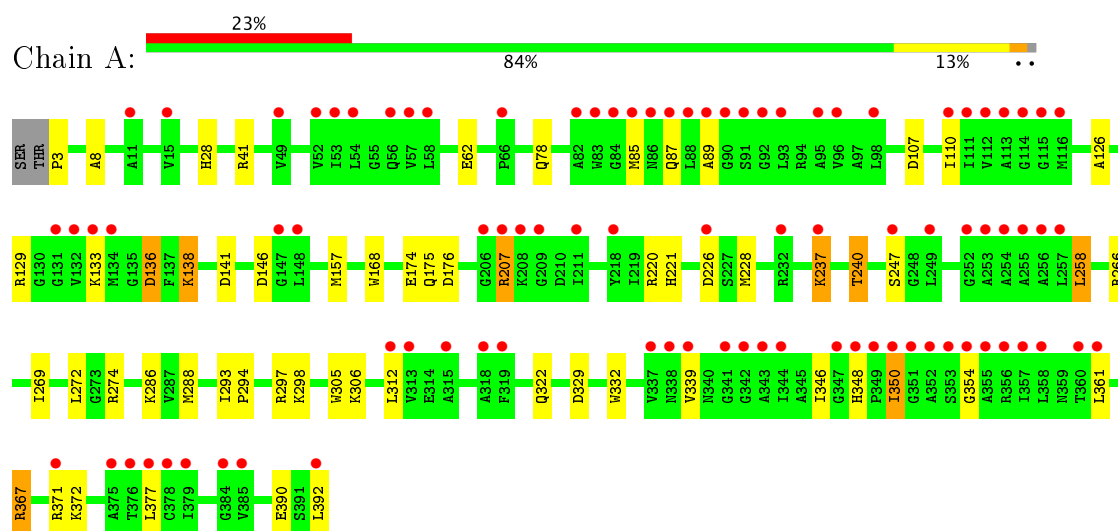
Chain A:
23%
84%
13%

- Molecule 1: Acetyl-CoA acetyltransferase

Chain B:
21%
81%
17%

- Molecule 1: Acetyl-CoA acetyltransferase

Chain C:
32%
75%
23%
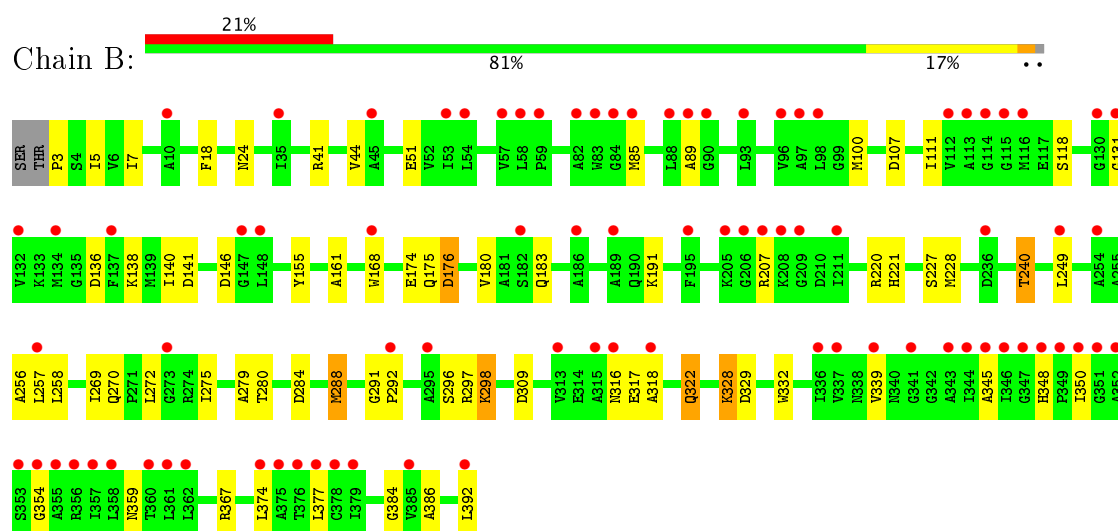
• Molecule 1: Acetyl-CoA acetyltransferase
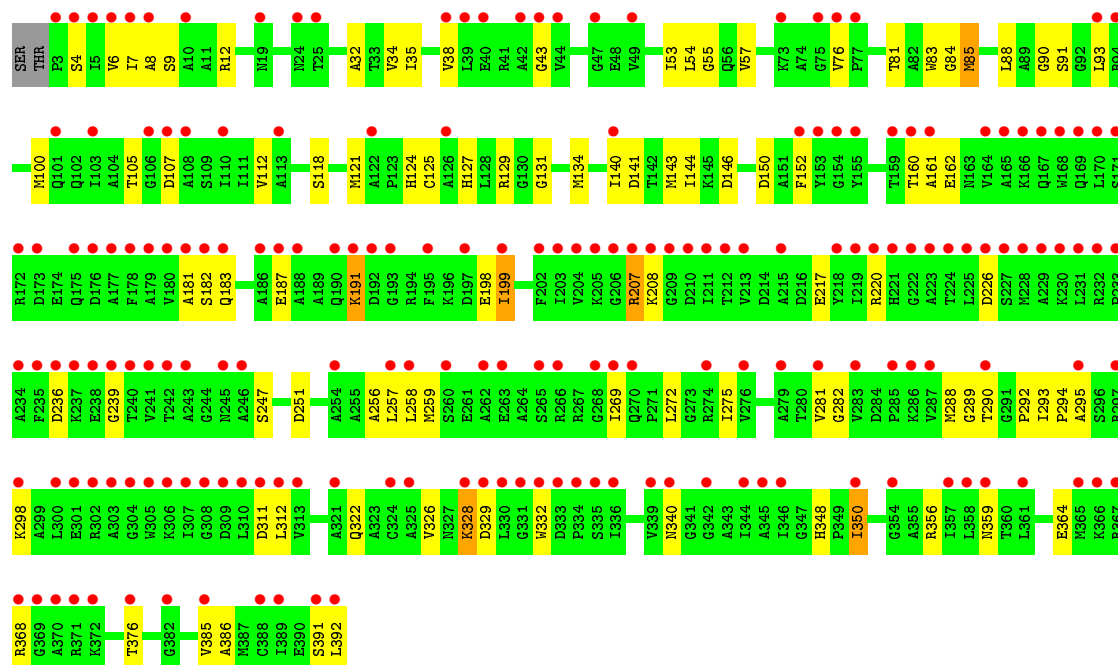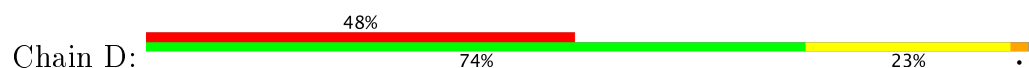
4 Data and refinement statistics (i)
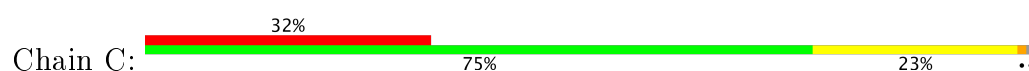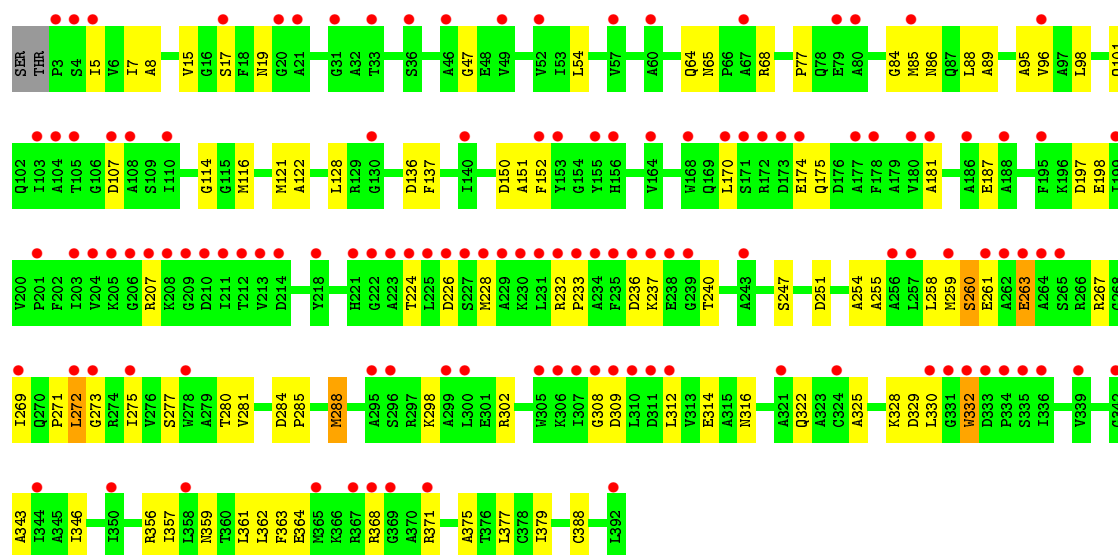
Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.22Å 79.22Å 148.29Å 90.00° 92.48° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 34.69 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.95) 99.6 (34.69-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$<I/\sigma(I)>$ [1]	2.32 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.258 0.221 , 0.265	Depositor DCC
R_{free} test set	6372 reflections (4.71%)	DCC
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 66.6	EDS
L-test for twinning [2]	$<|L|> = 0.37, <L^2> = 0.19$	Xtriage
Estimated twinning fraction	0.166 for h,-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	12414	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CAA, 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	0.96	1/2867 (0.0%)	1.02	13/3871 (0.3%)
1	B	0.94	2/2867 (0.1%)	1.00	11/3871 (0.3%)
1	C	0.64	5/2867 (0.2%)	0.78	7/3871 (0.2%)
1	D	0.61	1/2867 (0.0%)	0.77	6/3871 (0.2%)
All	All	0.81	9/11468 (0.1%)	0.90	37/15484 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	9	SER	CB-OG	10.78	1.56	1.42
1	A	126	ALA	CA-CB	-6.42	1.39	1.52
1	C	388	CYS	CB-SG	6.01	1.92	1.82
1	B	118	SER	CB-OG	5.57	1.49	1.42
1	B	386	ALA	CA-CB	-5.48	1.41	1.52
1	C	388	CYS	C-O	5.40	1.33	1.23
1	C	261	GLU	CD-OE1	5.11	1.31	1.25
1	C	260	SER	C-O	5.06	1.32	1.23
1	C	308	GLY	C-O	5.01	1.31	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	CB-CG-OD2	10.27	127.55	118.30
1	B	367	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	A	367	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	41	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	B	284	ASP	CB-CG-OD2	7.56	125.10	118.30
1	B	367	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	107	ASP	CB-CG-OD2	7.33	124.89	118.30
1	A	136	ASP	CB-CG-OD2	7.32	124.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	146	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	226	ASP	CB-CG-OD2	7.05	124.64	118.30
1	B	309	ASP	CB-CG-OD2	6.81	124.42	118.30
1	B	141	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	146	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	129	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	266	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	41	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	197	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	176	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	129	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	107	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	311	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	107	ASP	CB-CG-OD2	5.68	123.41	118.30
1	D	251	ASP	CB-CG-OD2	5.67	123.41	118.30
1	C	309	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	136	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	107	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	266	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	D	146	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	329	ASP	CB-CG-OD2	5.33	123.09	118.30
1	D	226	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	339	VAL	CG1-CB-CG2	5.20	119.23	110.90
1	C	150	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	226	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	176	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	136	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	329	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	41	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	2821	0	2828	39	0
1	B	2821	0	2828	52	0
1	C	2821	0	2828	62	0
1	D	2821	0	2828	75	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	54	0	36	6	0
3	B	54	0	36	4	0
4	A	360	0	0	20	0
4	B	372	0	0	22	0
4	C	127	0	0	23	0
4	D	143	0	0	39	0
All	All	12414	0	11384	222	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 (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:SER:HB2	4:B:408:HOH:O	1.34	1.26
1:B:100:MET:HG3	4:B:466:HOH:O	1.49	1.12
1:B:258:LEU:HG	4:B:9882:HOH:O	1.55	1.06
3:A:1393:CAA:H4'3	4:A:467:HOH:O	1.56	1.03
1:A:89:ALA:HB2	3:A:1393:CAA:H2'2	1.44	0.98
1:B:269:ILE:HD11	4:B:473:HOH:O	1.67	0.94
1:B:89:ALA:HB2	3:B:2393:CAA:H2'2	1.50	0.93
1:A:258:LEU:HG	4:A:9763:HOH:O	1.66	0.93
1:D:207:ARG:HA	4:D:524:HOH:O	1.69	0.93
1:B:175:GLN:HE22	1:B:240:THR:CG2	1.85	0.90
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.36	0.89
1:B:89:ALA:CB	3:B:2393:CAA:H2'2	2.04	0.88
1:A:258:LEU:CD2	4:A:9763:HOH:O	2.23	0.87
1:D:35:ILE:HD12	4:D:462:HOH:O	1.77	0.83
1:C:314:GLU:HB2	4:C:501:HOH:O	1.80	0.82
1:A:258:LEU:CG	4:A:9763:HOH:O	2.22	0.81
1:C:151:ALA:HB3	4:C:519:HOH:O	1.81	0.80
1:D:83:TRP:CZ2	4:D:489:HOH:O	2.33	0.80
1:A:286:LYS:HE3	4:A:9757:HOH:O	1.81	0.80
1:D:93:LEU:HA	4:D:454:HOH:O	1.81	0.80
1:B:227:SER:OG	4:B:9734:HOH:O	2.03	0.77
1:D:32:ALA:HA	4:D:462:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:MET:HE1	4:B:413:HOH:O	1.86	0.76
1:A:157:MET:HG3	4:A:467:HOH:O	1.85	0.76
1:A:312:LEU:HD23	1:A:361:LEU:HD12	1.68	0.75
1:A:133:LYS:HA	4:A:401:HOH:O	1.85	0.75
1:B:175:GLN:NE2	1:B:240:THR:HG23	2.01	0.74
3:A:1393:CAA:N6A	4:A:9827:HOH:O	2.16	0.73
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.01	0.73
1:D:83:TRP:HZ2	4:D:489:HOH:O	1.67	0.72
1:D:88:LEU:O	1:D:91:SER:OG	2.07	0.72
1:A:89:ALA:HB2	3:A:1393:CAA:C2	2.18	0.72
1:C:281:VAL:HA	4:C:458:HOH:O	1.90	0.72
1:D:91:SER:HB3	4:D:502:HOH:O	1.88	0.71
1:C:330:LEU:HD12	1:C:332:TRP:CH2	2.26	0.71
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.55	0.70
1:C:15:VAL:HG22	4:C:480:HOH:O	1.91	0.70
1:C:5:ILE:HB	4:C:509:HOH:O	1.92	0.69
1:C:122:ALA:HA	4:C:431:HOH:O	1.93	0.69
1:A:371:ARG:HD2	4:A:454:HOH:O	1.92	0.68
1:D:385:VAL:HG22	4:D:510:HOH:O	1.94	0.68
1:B:100:MET:HE2	4:B:466:HOH:O	1.93	0.67
1:C:272:LEU:O	1:C:362:LEU:HD22	1.95	0.66
1:C:330:LEU:HD12	1:C:332:TRP:CZ2	2.31	0.66
1:A:258:LEU:HD21	4:A:9763:HOH:O	1.90	0.66
1:D:12:ARG:NE	1:D:198:GLU:OE2	2.29	0.66
1:B:257:LEU:HD23	1:B:258:LEU:N	2.12	0.65
1:A:136:ASP:OD2	4:A:409:HOH:O	2.14	0.65
1:C:275:ILE:HB	4:C:509:HOH:O	1.97	0.65
1:B:288:MET:HE1	4:B:479:HOH:O	1.96	0.64
1:D:385:VAL:HG11	4:D:532:HOH:O	1.96	0.64
1:D:112:VAL:HG12	4:D:504:HOH:O	1.97	0.64
1:A:286:LYS:CE	4:A:9757:HOH:O	2.42	0.64
1:C:275:ILE:O	4:C:418:HOH:O	2.14	0.64
1:D:90:GLY:O	4:D:532:HOH:O	2.15	0.64
1:D:312:LEU:HD13	1:D:368:ARG:HD2	1.79	0.63
4:C:504:HOH:O	1:D:140:ILE:HD13	1.99	0.63
1:D:183:GLN:HG2	4:D:461:HOH:O	1.98	0.63
1:C:375:ALA:HA	4:C:501:HOH:O	1.99	0.62
1:C:255:ALA:HB3	4:C:436:HOH:O	2.00	0.61
1:B:24:ASN:OD1	4:B:472:HOH:O	2.16	0.61
1:C:181:ALA:HB2	4:C:447:HOH:O	2.00	0.60
1:C:89:ALA:HB1	4:C:400:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ALA:HA	4:B:416:HOH:O	2.02	0.58
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.37	0.58
1:B:322:GLN:HB3	4:B:416:HOH:O	2.04	0.58
1:B:174:GLU:OE2	1:B:328:LYS:NZ	2.31	0.58
1:D:392:LEU:HD12	4:D:522:HOH:O	2.04	0.58
1:B:316:ASN:HB3	4:B:9738:HOH:O	2.05	0.57
1:D:124:HIS:HA	1:D:140:ILE:O	2.05	0.57
1:D:150:ASP:HB2	4:D:521:HOH:O	2.05	0.57
1:C:95:ALA:HB3	4:C:448:HOH:O	2.05	0.56
1:A:354:GLY:HA2	1:A:377:LEU:HD11	1.87	0.56
4:C:437:HOH:O	1:D:152:PHE:CE2	2.53	0.56
1:D:150:ASP:CG	4:D:521:HOH:O	2.45	0.56
1:C:263:GLU:O	1:C:267:ARG:HD2	2.06	0.56
1:C:8:ALA:HB1	1:C:269:ILE:HG21	1.88	0.55
1:D:326:VAL:HG23	4:D:456:HOH:O	2.06	0.55
1:C:356:ARG:HG3	4:C:480:HOH:O	2.06	0.54
1:C:330:LEU:CD1	1:C:332:TRP:CH2	2.89	0.54
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.42	0.54
1:C:312:LEU:HD23	1:C:361:LEU:HD12	1.89	0.54
1:C:7:ILE:N	1:C:273:GLY:O	2.27	0.54
1:A:175:GLN:NE2	1:A:240:THR:HG23	2.23	0.53
1:C:198:GLU:HB3	1:C:363:PHE:CD2	2.43	0.53
1:B:318:ALA:HB1	4:B:479:HOH:O	2.07	0.53
1:C:54:LEU:O	1:C:84:GLY:HA2	2.08	0.53
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.70	0.52
1:C:68:ARG:HG3	1:D:152:PHE:HZ	1.74	0.52
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.44	0.52
1:B:297:ARG:NE	4:B:9829:HOH:O	2.41	0.52
1:D:340:ASN:ND2	1:D:364:GLU:OE1	2.36	0.52
1:D:289:GLY:O	1:D:292:PRO:HD2	2.10	0.51
1:C:174:GLU:OE2	1:C:328:LYS:NZ	2.33	0.51
1:C:259:MET:HG3	1:C:260:SER:O	2.11	0.51
1:A:174:GLU:OE2	4:A:442:HOH:O	2.19	0.51
1:C:316:ASN:ND2	1:C:377:LEU:HD23	2.25	0.51
1:B:44:VAL:CG2	4:B:473:HOH:O	2.59	0.50
1:D:295:ALA:HA	4:D:503:HOH:O	2.10	0.50
1:D:6:VAL:O	1:D:258:LEU:HD13	2.12	0.50
1:C:114:GLY:HA3	1:C:254:ALA:O	2.11	0.50
1:C:64:GLN:O	1:C:65:ASN:C	2.50	0.50
1:A:87:GLN:C	4:A:444:HOH:O	2.50	0.50
1:A:89:ALA:CB	3:A:1393:CAA:H2'2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:NE	4:A:437:HOH:O	2.45	0.50
1:D:6:VAL:HG22	1:D:259:MET:O	2.11	0.50
1:A:8:ALA:HB1	1:A:269:ILE:HG21	1.94	0.49
1:C:96:VAL:HG23	4:C:448:HOH:O	2.12	0.49
1:D:236:ASP:HB3	1:D:239:GLY:HA3	1.95	0.49
1:B:296:SER:CB	4:B:408:HOH:O	2.15	0.49
1:C:114:GLY:N	4:C:448:HOH:O	2.46	0.48
1:A:89:ALA:CB	3:A:1393:CAA:C2	2.90	0.48
1:B:7:ILE:HG23	1:B:256:ALA:HB1	1.95	0.48
1:D:275:ILE:HG21	4:D:535:HOH:O	2.13	0.48
1:D:257:LEU:HD23	1:D:258:LEU:N	2.28	0.48
1:D:76:VAL:HG23	4:D:531:HOH:O	2.13	0.48
1:D:217:GLU:HA	4:D:476:HOH:O	2.12	0.48
1:D:6:VAL:O	1:D:258:LEU:CD1	2.62	0.48
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.76	0.48
1:C:280:THR:HG23	1:D:81:THR:HG21	1.96	0.48
1:C:95:ALA:HA	1:C:98:LEU:HD12	1.95	0.48
1:C:19:ASN:HB2	4:C:513:HOH:O	2.13	0.47
1:B:89:ALA:HB3	3:B:2393:CAA:H2'2	1.91	0.47
1:A:78:GLN:NE2	4:A:433:HOH:O	2.24	0.47
1:C:277:SER:HB2	4:D:528:HOH:O	2.13	0.47
1:B:318:ALA:CB	4:B:479:HOH:O	2.62	0.47
1:B:374:LEU:HD23	1:B:374:LEU:C	2.36	0.47
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.97	0.47
1:D:376:THR:HG21	4:D:496:HOH:O	2.14	0.47
1:B:270:GLN:NE2	1:B:392:LEU:OXT	2.48	0.46
1:C:152:PHE:CE2	4:C:519:HOH:O	2.56	0.46
1:D:55:GLY:CA	4:D:502:HOH:O	2.64	0.46
1:C:277:SER:HB2	1:C:302:ARG:HB3	1.98	0.46
1:C:269:ILE:O	1:C:271:PRO:HD3	2.15	0.46
1:D:181:ALA:HA	4:D:529:HOH:O	2.15	0.46
1:B:354:GLY:HA2	1:B:377:LEU:HD11	1.98	0.46
1:D:281:VAL:HG12	1:D:282:GLY:N	2.31	0.46
1:B:257:LEU:C	1:B:257:LEU:HD23	2.36	0.46
1:C:85:MET:HA	1:D:85:MET:HA	1.98	0.46
1:B:131:GLY:HA2	1:D:131:GLY:HA2	1.98	0.45
1:D:12:ARG:O	1:D:199:ILE:HA	2.17	0.45
1:D:160:THR:HG21	4:D:521:HOH:O	2.16	0.45
1:D:7:ILE:HG23	1:D:256:ALA:HB1	1.98	0.45
1:D:272:LEU:C	4:D:530:HOH:O	2.54	0.45
1:A:28:HIS:ND1	1:A:62:GLU:OE2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:THR:HA	1:B:384:GLY:O	2.17	0.45
1:B:168:TRP:HH2	1:B:329:ASP:HB2	1.82	0.45
1:D:118:SER:OG	1:D:121:MET:HB2	2.17	0.45
1:B:279:ALA:CB	1:B:298:LYS:HB3	2.47	0.45
1:B:183:GLN:HA	1:B:345:ALA:HB2	1.99	0.45
1:C:101:GLN:HG2	1:D:105:THR:HG21	1.98	0.45
1:D:247[B]:SER:OG	1:D:348:HIS:HB2	2.17	0.45
1:B:138:LYS:HB2	1:B:140:ILE:HD11	1.99	0.45
1:C:272:LEU:O	1:C:362:LEU:CD2	2.62	0.45
1:D:150:ASP:CB	4:D:521:HOH:O	2.64	0.45
1:D:386:ALA:N	4:D:510:HOH:O	2.50	0.45
1:C:121:MET:HA	1:D:127:HIS:CD2	2.52	0.44
1:C:54:LEU:HD13	1:C:116:MET:SD	2.58	0.44
1:C:288:MET:HB2	1:C:379:ILE:O	2.17	0.44
1:C:5:ILE:N	1:C:5:ILE:HD13	2.33	0.44
1:B:44:VAL:HG23	4:B:473:HOH:O	2.17	0.44
1:D:281:VAL:HG23	4:D:503:HOH:O	2.17	0.44
1:D:83:TRP:HE3	1:D:84:GLY:O	2.00	0.44
1:C:88:LEU:HB3	4:C:443:HOH:O	2.18	0.44
1:A:3:PRO:N	4:A:9961:HOH:O	2.51	0.43
1:C:47:GLY:HA2	1:C:77:PRO:HG3	2.00	0.43
1:D:328:LYS:HG3	4:D:453:HOH:O	2.18	0.43
1:D:93:LEU:HB3	4:D:532:HOH:O	2.17	0.43
1:B:51:GLU:HB3	1:B:111:ILE:CD1	2.48	0.43
1:A:274:ARG:NH2	1:A:390:GLU:OE1	2.51	0.43
1:B:317:GLU:OE2	4:B:9724:HOH:O	2.21	0.43
1:A:85:MET:HA	1:B:85:MET:HA	2.00	0.43
1:D:161:ALA:HA	4:D:459:HOH:O	2.18	0.43
1:A:138:LYS:O	4:A:9793:HOH:O	2.22	0.43
1:D:141:ASP:OD1	1:D:143:MET:HB3	2.19	0.43
1:B:258:LEU:N	1:B:258:LEU:HD22	2.34	0.42
1:D:162:GLU:HG3	4:D:523:HOH:O	2.18	0.42
1:D:57:VAL:HG21	1:D:350:ILE:CG2	2.48	0.42
1:D:293:ILE:HB	1:D:294:PRO:CD	2.50	0.42
1:A:346:ILE:O	1:A:346:ILE:HG22	2.19	0.42
1:C:86:ASN:OD1	1:C:88:LEU:HD23	2.19	0.42
1:A:293:ILE:HB	1:A:294:PRO:CD	2.50	0.42
1:D:191:LYS:HA	4:D:431:HOH:O	2.19	0.42
1:D:43:GLY:HA3	4:D:507:HOH:O	2.19	0.42
1:B:18:PHE:HB2	1:B:249:LEU:O	2.19	0.42
1:B:275:ILE:CG2	4:B:466:HOH:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:GLU:O	1:C:368:ARG:HG2	2.19	0.42
1:B:131:GLY:HA2	1:D:131:GLY:CA	2.50	0.42
1:A:306:LYS:NZ	4:A:472:HOH:O	2.52	0.42
1:D:8:ALA:HB1	1:D:269:ILE:HG21	2.01	0.42
1:B:89:ALA:HB2	3:B:2393:CAA:C2	2.36	0.42
1:C:284:ASP:OD1	1:C:285:PRO:HD2	2.20	0.42
1:D:100:MET:C	1:D:100:MET:SD	2.98	0.41
1:D:76:VAL:HB	4:D:396:HOH:O	2.20	0.41
1:C:356:ARG:NH2	1:C:357:ILE:HG22	2.35	0.41
1:C:7:ILE:O	1:C:272:LEU:N	2.54	0.41
1:C:346:ILE:HD13	1:C:356:ARG:NH1	2.35	0.41
1:C:54:LEU:HD13	1:C:116:MET:CE	2.50	0.41
1:C:89:ALA:CB	4:C:400:HOH:O	2.66	0.41
1:D:54:LEU:O	1:D:84:GLY:HA2	2.20	0.41
1:B:176:ASP:O	1:B:180:VAL:HG23	2.21	0.41
1:B:44:VAL:HG22	4:B:473:HOH:O	2.20	0.41
1:D:35:ILE:HG22	4:D:531:HOH:O	2.20	0.41
1:A:237:LYS:HA	1:A:237:LYS:HD2	1.87	0.41
1:B:275:ILE:HG21	4:B:466:HOH:O	2.21	0.41
1:A:247[B]:SER:OG	1:A:348:HIS:HB2	2.21	0.41
1:D:290:THR:O	1:D:294:PRO:HD2	2.21	0.41
1:D:55:GLY:HA2	4:D:502:HOH:O	2.21	0.41
1:A:305:TRP:CE2	1:A:372:LYS:HD3	2.55	0.41
1:C:170:LEU:HD11	1:C:325:ALA:HB2	2.02	0.41
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.86	0.41
1:D:257:LEU:C	1:D:257:LEU:HD23	2.41	0.41
1:C:84:GLY:HA3	4:C:515:HOH:O	2.21	0.40
1:A:157:MET:CG	4:A:467:HOH:O	2.54	0.40
1:B:257:LEU:C	1:B:257:LEU:CD2	2.90	0.40
1:B:291:GLY:N	1:B:292:PRO:CD	2.83	0.40
1:A:350:ILE:HD13	1:A:350:ILE:HG21	1.91	0.40
1:D:34:VAL:O	1:D:38:VAL:HG13	2.20	0.40
1:C:233:PRO:HB2	1:C:236:ASP:O	2.21	0.40
1:C:247[B]:SER:OG	1:C:343:ALA:O	2.39	0.40
1:D:208:LYS:C	4:D:519:HOH:O	2.60	0.40
1:D:88:LEU:O	1:D:91:SER:CB	2.70	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	389/392 (99%)	369 (95%)	18 (5%)	2 (0%)	32	19
1	B	389/392 (99%)	374 (96%)	14 (4%)	1 (0%)	44	33
1	C	389/392 (99%)	370 (95%)	19 (5%)	0	100	100
1	D	389/392 (99%)	366 (94%)	22 (6%)	1 (0%)	44	33
All	All	1556/1568 (99%)	1479 (95%)	73 (5%)	4 (0%)	44	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ARG
1	A	350	ILE
1	D	350	ILE
1	B	350	ILE

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	277/278 (100%)	260 (94%)	17 (6%)	22	8
1	B	277/278 (100%)	261 (94%)	16 (6%)	23	10
1	C	277/278 (100%)	260 (94%)	17 (6%)	22	8
1	D	277/278 (100%)	256 (92%)	21 (8%)	15	5
All	All	1108/1112 (100%)	1037 (94%)	71 (6%)	20	8

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ILE
1	A	138	LYS
1	A	207	ARG
1	A	220	ARG
1	A	221	HIS
1	A	228	MET
1	A	237	LYS
1	A	240	THR
1	A	258	LEU
1	A	272	LEU
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	332	TRP
1	A	339	VAL
1	A	367	ARG
1	A	392	LEU
1	B	3	PRO
1	B	5	ILE
1	B	155	TYR
1	B	191	LYS
1	B	207	ARG
1	B	220	ARG
1	B	221	HIS
1	B	240	THR
1	B	272	LEU
1	B	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	328	LYS
1	B	332	TRP
1	B	348	HIS
1	B	359	ASN
1	C	17	SER
1	C	187	GLU
1	C	207	ARG
1	C	224	THR
1	C	228	MET
1	C	232	ARG
1	C	237	LYS
1	C	251	ASP
1	C	258	LEU

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Mol	Chain	Res	Type
1	C	263	GLU
1	C	272	LEU
1	C	288	MET
1	C	298	LYS
1	C	322	GLN
1	C	332	TRP
1	C	359	ASN
1	C	371	ARG
1	D	4	SER
1	D	53	ILE
1	D	85	MET
1	D	125	CYS
1	D	129	ARG
1	D	134	MET
1	D	144	ILE
1	D	182	SER
1	D	187	GLU
1	D	191	LYS
1	D	199	ILE
1	D	207	ARG
1	D	220	ARG
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	328	LYS
1	D	332	TRP
1	D	356	ARG
1	D	359	ASN
1	D	391	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	175	GLN
1	A	184	ASN
1	B	78	GLN
1	B	175	GLN
1	B	184	ASN
1	B	221	HIS
1	C	78	GLN
1	C	124	HIS

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Mol	Chain	Res	Type
1	C	184	ASN
1	C	316	ASN
1	C	322	GLN
1	D	78	GLN
1	D	175	GLN
1	D	184	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5   Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6   Ligand geometry ⓘ

6 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	#$|Z| > 2$
3	CAA	A	1393	-	49,56,56	1.33	6 (12%)	57,83,83	2.51	10 (17%)
2	SO4	A	9720	-	4,4,4	0.24	0	6,6,6	0.57	0
2	SO4	A	9722	-	4,4,4	0.15	0	6,6,6	0.58	0
3	CAA	B	2393	-	49,56,56	1.48	9 (18%)	57,83,83	2.93	11 (19%)
2	SO4	B	9719	-	4,4,4	0.16	0	6,6,6	0.30	0
2	SO4	B	9721	-	4,4,4	0.20	0	6,6,6	0.47	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
3	CAA	A	1393	-	-	0/50/71/71	0/3/3/3
2	SO4	A	9720	-	-	0/0/0/0	0/0/0/0
2	SO4	A	9722	-	-	0/0/0/0	0/0/0/0
3	CAA	B	2393	-	-	0/50/71/71	0/3/3/3
2	SO4	B	9719	-	-	0/0/0/0	0/0/0/0
2	SO4	B	9721	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2393	CAA	O3-C3	-2.61	1.13	1.21
3	B	2393	CAA	O1-C1	-2.55	1.17	1.21
3	A	1393	CAA	C5A-C4A	2.05	1.45	1.40
3	B	2393	CAA	P3B-O3B	2.19	1.63	1.59
3	B	2393	CAA	C5A-C4A	2.41	1.45	1.40
3	A	1393	CAA	C1-S1P	2.65	1.81	1.76
3	A	1393	CAA	P1A-O2A	3.03	1.70	1.55
3	B	2393	CAA	C1-S1P	3.05	1.82	1.76
3	B	2393	CAA	P1A-O2A	3.08	1.70	1.55
3	B	2393	CAA	P2A-O5A	3.18	1.71	1.55
3	A	1393	CAA	P2A-O5A	3.32	1.71	1.55
3	A	1393	CAA	P3B-O9A	3.81	1.70	1.54
3	A	1393	CAA	P3B-O8A	3.98	1.71	1.54
3	B	2393	CAA	P3B-O8A	4.09	1.71	1.54
3	B	2393	CAA	P3B-O9A	4.25	1.72	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2393	CAA	O1-C1-C2	-11.16	106.27	123.08
3	A	1393	CAA	O1-C1-C2	-8.33	110.53	123.08
3	A	1393	CAA	N3A-C2A-N1A	-7.02	122.75	128.86
3	B	2393	CAA	N3A-C2A-N1A	-6.70	123.02	128.86
3	B	2393	CAA	C4B-O4B-C1B	-5.05	104.39	109.77
3	B	2393	CAA	C1B-N9A-C4A	-4.41	119.02	126.64
3	A	1393	CAA	C1B-N9A-C4A	-3.63	120.36	126.64
3	A	1393	CAA	O3-C3-C2	-3.39	108.82	121.15
3	A	1393	CAA	C2P-S1P-C1	-2.93	92.23	101.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2393	CAA	O3-C3-C2	-2.60	111.71	121.15
3	B	2393	CAA	C3P-C2P-S1P	-2.35	104.42	111.23
3	B	2393	CAA	C6P-C5P-N4P	-2.05	112.96	116.49
3	A	1393	CAA	C2A-N1A-C6A	2.08	122.41	118.77
3	A	1393	CAA	N6A-C6A-N1A	2.15	123.02	118.77
3	B	2393	CAA	C2A-N1A-C6A	2.31	122.81	118.77
3	A	1393	CAA	C4-C3-C2	2.46	126.66	117.96
3	B	2393	CAA	C3-C2-C1	2.85	125.53	113.94
3	B	2393	CAA	C4-C3-C2	2.92	128.31	117.96
3	A	1393	CAA	C3-C2-C1	4.75	133.29	113.94
3	A	1393	CAA	C2-C1-S1P	11.92	126.06	113.42
3	B	2393	CAA	C2-C1-S1P	14.59	128.89	113.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1393	CAA	6	0
3	B	2393	CAA	4	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 (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	390/392 (99%)	1.30	90 (23%)	1	1	6, 13, 27, 45	0
1	B	390/392 (99%)	1.23	84 (21%)	1	1	6, 13, 26, 49	0
1	C	390/392 (99%)	1.76	125 (32%)	0	0	3, 14, 24, 38	0
1	D	390/392 (99%)	2.25	187 (47%)	0	0	2, 14, 24, 41	0
All	All	1560/1568 (99%)	1.64	486 (31%)	0	0	2, 14, 25, 49	0

All (486) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	LEU	7.3
1	C	209	GLY	7.1
1	D	241	VAL	7.0
1	D	310	LEU	6.6
1	D	208	LYS	6.5
1	D	186	ALA	6.4
1	D	232	ARG	6.4
1	C	231	LEU	6.3
1	D	229	ALA	6.1
1	D	181	ALA	5.9
1	C	211	ILE	5.9
1	D	180	VAL	5.7
1	C	153	TYR	5.7
1	D	203	ILE	5.5
1	D	221	HIS	5.5
1	D	207	ARG	5.5
1	D	235	PHE	5.5
1	D	303	ALA	5.4
1	D	211	ILE	5.3
1	D	107	ASP	5.3
1	D	391	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	308	GLY	5.3
1	C	208	LYS	5.3
1	A	209	GLY	5.3
1	C	234	ALA	5.2
1	D	392	LEU	5.2
1	D	228	MET	5.1
1	C	371	ARG	5.1
1	D	152	PHE	5.1
1	D	331	GLY	5.1
1	A	357	ILE	5.0
1	D	215	ALA	5.0
1	D	325	ALA	5.0
1	D	239	GLY	5.0
1	D	236	ASP	5.0
1	D	153	TYR	5.0
1	D	206	GLY	4.9
1	D	281	VAL	4.8
1	D	178	PHE	4.8
1	D	227	SER	4.8
1	D	279	ALA	4.8
1	D	209	GLY	4.8
1	A	207	ARG	4.8
1	C	334	PRO	4.7
1	D	344	ILE	4.7
1	C	181	ALA	4.7
1	B	207	ARG	4.7
1	D	307	ILE	4.7
1	D	240	THR	4.6
1	C	232	ARG	4.6
1	D	388	CYS	4.6
1	C	5	ILE	4.6
1	B	57	VAL	4.5
1	D	237	LYS	4.5
1	D	332	TRP	4.4
1	D	269	ILE	4.4
1	D	140	ILE	4.4
1	C	262	ALA	4.4
1	C	207	ARG	4.4
1	C	239	GLY	4.3
1	D	5	ILE	4.3
1	C	204	VAL	4.2
1	A	352	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	80	ALA	4.2
1	D	224	THR	4.2
1	C	312	LEU	4.2
1	D	170	LEU	4.2
1	C	235	PHE	4.2
1	A	208	LYS	4.2
1	D	306	LYS	4.1
1	C	206	GLY	4.1
1	D	195	PHE	4.1
1	A	350	ILE	4.1
1	D	262	ALA	4.1
1	D	305	TRP	4.0
1	C	140	ILE	4.0
1	D	192	ASP	4.0
1	D	371	ARG	4.0
1	B	350	ILE	4.0
1	D	6	VAL	3.9
1	C	221	HIS	3.9
1	D	233	PRO	3.9
1	D	382	GLY	3.9
1	D	226	ASP	3.9
1	D	367	ARG	3.9
1	B	357	ILE	3.9
1	D	179	ALA	3.8
1	A	57	VAL	3.8
1	A	206	GLY	3.8
1	A	378	CYS	3.8
1	D	154	GLY	3.8
1	D	103	ILE	3.8
1	C	36	SER	3.8
1	A	211	ILE	3.8
1	C	188	ALA	3.8
1	D	238	GLU	3.8
1	D	304	GLY	3.8
1	A	133	LYS	3.8
1	B	358	LEU	3.8
1	C	272	LEU	3.8
1	D	205	LYS	3.8
1	A	134	MET	3.7
1	B	361	LEU	3.7
1	D	339	VAL	3.7
1	C	205	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	212	THR	3.7
1	D	358	LEU	3.7
1	B	209	GLY	3.7
1	A	355	ALA	3.7
1	C	67	ALA	3.7
1	C	229	ALA	3.7
1	D	165	ALA	3.7
1	D	246	ALA	3.7
1	C	392	LEU	3.7
1	C	222	GLY	3.7
1	D	19	ASN	3.6
1	B	377	LEU	3.6
1	A	377	LEU	3.6
1	D	7	ILE	3.6
1	D	335	SER	3.6
1	B	93	LEU	3.6
1	C	230	LYS	3.6
1	D	230	LYS	3.6
1	A	89	ALA	3.5
1	D	340	ASN	3.5
1	A	354	GLY	3.5
1	A	379	ILE	3.5
1	D	350	ILE	3.5
1	B	113	ALA	3.5
1	C	264	ALA	3.5
1	C	333	ASP	3.5
1	D	168	TRP	3.5
1	D	243	ALA	3.5
1	D	276	VAL	3.5
1	D	309	ASP	3.5
1	D	171	SER	3.5
1	D	368	ARG	3.4
1	C	213	VAL	3.4
1	B	206	GLY	3.4
1	C	299	ALA	3.4
1	C	170	LEU	3.4
1	C	180	VAL	3.4
1	D	25	THR	3.4
1	D	166	LYS	3.4
1	C	3	PRO	3.4
1	D	370	ALA	3.4
1	C	210	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	132	VAL	3.4
1	A	237	LYS	3.4
1	D	75	GLY	3.4
1	D	295	ALA	3.4
1	A	98	LEU	3.4
1	C	309	ASP	3.4
1	C	103	ILE	3.3
1	D	336	ILE	3.3
1	A	93	LEU	3.3
1	A	337	VAL	3.3
1	D	329	ASP	3.3
1	C	20	GLY	3.3
1	C	223	ALA	3.3
1	A	358	LEU	3.3
1	D	169	GLN	3.3
1	D	225	LEU	3.3
1	A	113	ALA	3.3
1	B	54	LEU	3.3
1	D	188	ALA	3.3
1	A	88	LEU	3.2
1	B	96	VAL	3.2
1	D	385	VAL	3.2
1	B	355	ALA	3.2
1	D	234	ALA	3.2
1	A	83	TRP	3.2
1	C	243	ALA	3.2
1	A	385	VAL	3.2
1	D	301	GLU	3.2
1	C	237	LYS	3.2
1	B	254	ALA	3.2
1	D	345	ALA	3.2
1	C	226	ASP	3.2
1	C	307	ILE	3.2
1	D	210	ASP	3.2
1	D	311	ASP	3.2
1	B	208	LYS	3.2
1	C	295	ALA	3.2
1	A	148	LEU	3.1
1	D	333	ASP	3.1
1	B	112	VAL	3.1
1	D	266	ARG	3.1
1	D	223	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	361	LEU	3.1
1	D	161	ALA	3.1
1	D	177	ALA	3.1
1	C	305	TRP	3.1
1	A	342	GLY	3.1
1	D	204	VAL	3.1
1	B	344	ILE	3.1
1	D	220	ARG	3.1
1	A	313	VAL	3.1
1	D	330	LEU	3.1
1	C	156	HIS	3.1
1	D	3	PRO	3.0
1	D	376	THR	3.0
1	D	213	VAL	3.0
1	B	352	ALA	3.0
1	D	321	ALA	3.0
1	C	173	ASP	3.0
1	D	324	CYS	3.0
1	D	44	VAL	3.0
1	D	47	GLY	3.0
1	A	375	ALA	3.0
1	D	334	PRO	3.0
1	C	155	TYR	3.0
1	A	384	GLY	3.0
1	A	249	LEU	3.0
1	C	275	ILE	3.0
1	C	332	TRP	3.0
1	C	33	THR	3.0
1	D	212	THR	3.0
1	B	114	GLY	3.0
1	B	385	VAL	3.0
1	A	54	LEU	3.0
1	D	193	GLY	3.0
1	D	265	SER	3.0
1	A	343	ALA	3.0
1	A	348	HIS	3.0
1	C	233	PRO	3.0
1	D	328	LYS	3.0
1	A	252	GLY	2.9
1	B	53	ILE	2.9
1	C	130	GLY	2.9
1	D	366	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	132	VAL	2.9
1	D	187	GLU	2.9
1	C	108	ALA	2.9
1	C	186	ALA	2.9
1	D	175	GLN	2.9
1	C	60	ALA	2.9
1	D	283	VAL	2.9
1	D	300	LEU	2.9
1	C	228	MET	2.9
1	B	318	ALA	2.9
1	C	49	VAL	2.9
1	D	49	VAL	2.9
1	C	225	LEU	2.9
1	C	104	ALA	2.9
1	C	238	GLU	2.8
1	B	348	HIS	2.8
1	D	260	SER	2.8
1	B	339	VAL	2.8
1	B	115	GLY	2.8
1	A	114	GLY	2.8
1	C	339	VAL	2.8
1	A	353	SER	2.8
1	C	324	CYS	2.8
1	C	195	PHE	2.8
1	D	274	ARG	2.8
1	C	265	SER	2.8
1	B	58	LEU	2.8
1	D	43	GLY	2.8
1	D	342	GLY	2.8
1	B	83	TRP	2.8
1	C	263	GLU	2.8
1	D	40	GLU	2.8
1	A	96	VAL	2.8
1	D	42	ALA	2.7
1	D	24	ASN	2.7
1	C	152	PHE	2.7
1	C	369	GLY	2.7
1	D	242	THR	2.7
1	C	342	GLY	2.7
1	D	222	GLY	2.7
1	D	191	LYS	2.7
1	C	174	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	110	ILE	2.7
1	D	167	GLN	2.7
1	B	89	ALA	2.7
1	D	113	ALA	2.7
1	D	245	ASN	2.7
1	A	49	VAL	2.7
1	B	148	LEU	2.7
1	C	79	GLU	2.7
1	B	211	ILE	2.7
1	B	337	VAL	2.7
1	A	92	GLY	2.7
1	D	285	PRO	2.7
1	C	269	ILE	2.6
1	B	347	GLY	2.6
1	D	218	TYR	2.6
1	C	335	SER	2.6
1	B	378	CYS	2.6
1	A	253	ALA	2.6
1	D	155	TYR	2.6
1	C	358	LEU	2.6
1	D	312	LEU	2.6
1	A	131	GLY	2.6
1	C	21	ALA	2.6
1	A	111	ILE	2.6
1	C	199	ILE	2.6
1	A	147	GLY	2.6
1	A	392	LEU	2.6
1	C	257	LEU	2.6
1	C	300	LEU	2.6
1	C	261	GLU	2.6
1	C	203	ILE	2.6
1	C	224	THR	2.6
1	A	15	VAL	2.6
1	B	84	GLY	2.6
1	A	95	ALA	2.5
1	A	318	ALA	2.5
1	B	362	LEU	2.5
1	C	321	ALA	2.5
1	C	4	SER	2.5
1	B	85	MET	2.5
1	B	134	MET	2.5
1	C	365	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	53	ILE	2.5
1	D	302	ARG	2.5
1	D	313	VAL	2.5
1	B	182	SER	2.5
1	B	351	GLY	2.5
1	C	278	TRP	2.5
1	A	52	VAL	2.5
1	A	351	GLY	2.5
1	D	308	GLY	2.5
1	D	369	GLY	2.5
1	D	159	THR	2.5
1	D	190	GLN	2.5
1	C	96	VAL	2.5
1	C	368	ARG	2.5
1	D	297	ARG	2.5
1	B	88	LEU	2.5
1	A	349	PRO	2.5
1	B	315	ALA	2.5
1	A	90	GLY	2.5
1	C	164	VAL	2.5
1	B	205	LYS	2.5
1	B	376	THR	2.5
1	A	115	GLY	2.4
1	B	130	GLY	2.4
1	A	247[A]	SER	2.4
1	D	258	LEU	2.4
1	D	372	LYS	2.4
1	D	176	ASP	2.4
1	C	177	ALA	2.4
1	A	360	THR	2.4
1	C	52	VAL	2.4
1	C	227	SER	2.4
1	C	296	SER	2.4
1	B	354	GLY	2.4
1	D	93	LEU	2.4
1	C	107	ASP	2.4
1	C	214	ASP	2.4
1	C	336	ILE	2.4
1	C	350	ILE	2.4
1	C	367	ARG	2.4
1	D	172	ARG	2.4
1	A	116	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	126	ALA	2.4
1	C	331	GLY	2.4
1	D	106	GLY	2.4
1	D	199	ILE	2.4
1	C	236	ASP	2.3
1	B	392	LEU	2.3
1	C	172	ARG	2.3
1	D	257	LEU	2.3
1	B	137	PHE	2.3
1	B	360	THR	2.3
1	C	105	THR	2.3
1	C	311	ASP	2.3
1	A	312	LEU	2.3
1	A	361	LEU	2.3
1	B	116	MET	2.3
1	D	359	ASN	2.3
1	B	168	TRP	2.3
1	D	4	SER	2.3
1	B	379	ILE	2.3
1	D	76	VAL	2.3
1	D	287	VAL	2.3
1	B	82	ALA	2.3
1	D	108	ALA	2.3
1	D	268	GLY	2.3
1	D	202	PHE	2.3
1	A	339	VAL	2.3
1	B	313	VAL	2.3
1	A	226	ASP	2.3
1	B	236	ASP	2.3
1	A	255	ALA	2.3
1	B	59	PRO	2.3
1	A	91	SER	2.3
1	D	183	GLN	2.3
1	A	371	ARG	2.3
1	B	90	GLY	2.3
1	B	375	ALA	2.3
1	D	254	ALA	2.3
1	D	73	LYS	2.3
1	B	341	GLY	2.2
1	D	365	MET	2.2
1	A	66	PRO	2.2
1	D	160	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	263	GLU	2.2
1	D	290	THR	2.2
1	B	257	LEU	2.2
1	A	347	GLY	2.2
1	C	178	PHE	2.2
1	B	10	ALA	2.2
1	A	344	ILE	2.2
1	B	336	ILE	2.2
1	B	374	LEU	2.2
1	C	330	LEU	2.2
1	D	298	LYS	2.2
1	D	77	PRO	2.2
1	B	195	PHE	2.2
1	D	182	SER	2.2
1	A	341	GLY	2.2
1	B	147	GLY	2.2
1	D	38	VAL	2.2
1	D	354	GLY	2.2
1	D	173	ASP	2.2
1	A	376	THR	2.2
1	D	286	LYS	2.2
1	D	8	ALA	2.2
1	A	232	ARG	2.2
1	A	87	GLN	2.2
1	B	292	PRO	2.2
1	B	349	PRO	2.2
1	B	345	ALA	2.2
1	C	85	MET	2.1
1	C	259	MET	2.1
1	A	356	ARG	2.1
1	B	98	LEU	2.1
1	B	356	ARG	2.1
1	A	11	ALA	2.1
1	A	85	MET	2.1
1	A	110	ILE	2.1
1	B	316	ASN	2.1
1	A	257	LEU	2.1
1	D	39	LEU	2.1
1	A	256	ALA	2.1
1	C	57	VAL	2.1
1	D	270	GLN	2.1
1	B	346	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	389	ILE	2.1
1	B	97	ALA	2.1
1	B	189	ALA	2.1
1	C	310	LEU	2.1
1	A	338	ASN	2.1
1	D	197	ASP	2.1
1	D	101	GLN	2.1
1	C	31	GLY	2.1
1	D	164	VAL	2.1
1	C	306	LYS	2.1
1	A	82	ALA	2.1
1	C	46	ALA	2.1
1	C	344	ILE	2.1
1	A	86	ASN	2.1
1	A	319	PHE	2.1
1	C	17	SER	2.1
1	A	315	ALA	2.1
1	B	186	ALA	2.1
1	D	10	ALA	2.1
1	A	58	LEU	2.1
1	A	84	GLY	2.1
1	A	56	GLN	2.0
1	C	171	SER	2.0
1	A	112	VAL	2.0
1	A	254	ALA	2.0
1	B	295	ALA	2.0
1	B	343	ALA	2.0
1	D	122	ALA	2.0
1	C	201	PRO	2.0
1	B	249	LEU	2.0
1	A	218	TYR	2.0
1	C	218	TYR	2.0
1	D	94	ARG	2.0
1	B	45	ALA	2.0
1	B	131	GLY	2.0
1	B	273	GLY	2.0
1	C	256	ALA	2.0
1	C	273	GLY	2.0
1	C	168	TRP	2.0
1	B	35	ILE	2.0
1	C	110	ILE	2.0
1	D	219	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	346	ILE	2.0
1	D	357	ILE	2.0
1	B	353	SER	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	CAA	B	2393	54/54	0.67	0.29	<mark>2.11</mark>	11,52,57,60	0
2	SO4	A	9722	5/5	0.92	0.19	1.67	58,59,61,63	0
3	CAA	A	1393	54/54	0.67	0.29	1.18	18,52,60,63	0
2	SO4	B	9719	5/5	0.90	0.20	-	66,67,68,68	0
2	SO4	A	9720	5/5	0.95	0.14	-	47,48,51,53	0
2	SO4	B	9721	5/5	0.95	0.19	-	47,47,50,51	0

6.5 Other polymers (i)

There are no such residues in this entry.