Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:47 PM GMT

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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

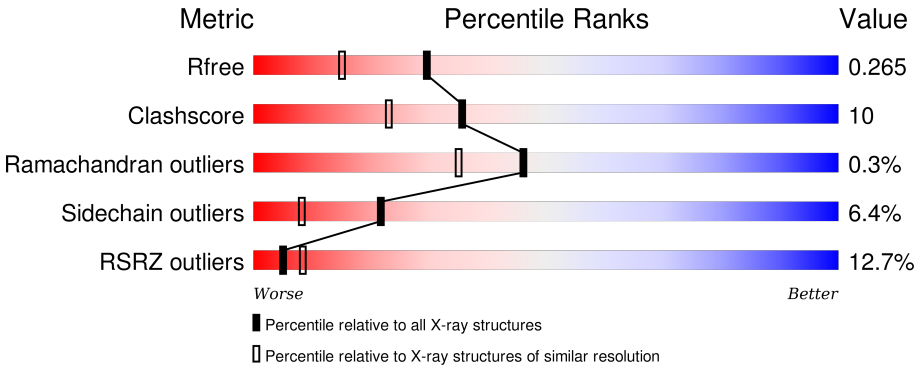
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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	84% 13%
1	B	392	81% 17%
1	C	392	19% 75% 23%
1	D	392	30% 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	A	1393	-	-	-	X
3	CAA	B	2393	-	-	-	X

2 Entry composition

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.

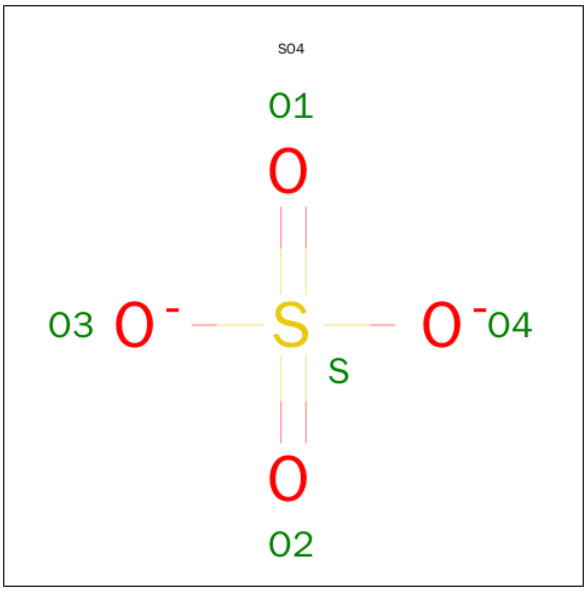
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

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:

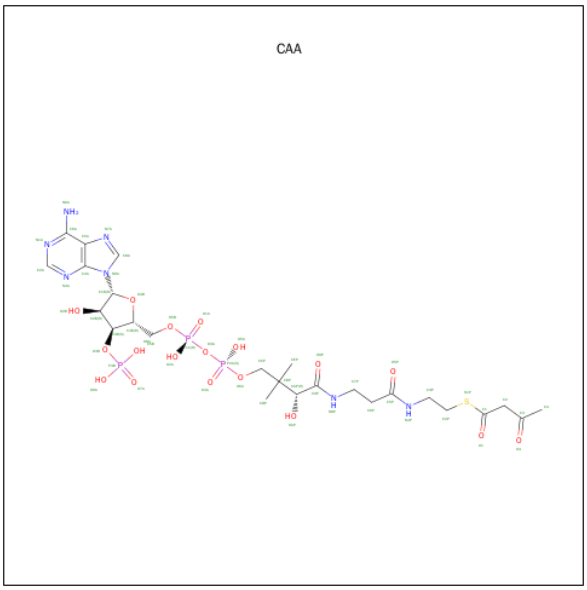
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	INSERTION	UNP P07097
A	89	ALA	CYS	ENGINEERED	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	10	ALA	-	INSERTION	UNP P07097
B	89	ALA	CYS	ENGINEERED	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	10	ALA	-	INSERTION	UNP P07097
C	89	ALA	CYS	ENGINEERED	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 O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- 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	C	N	O	P	S	0	0
			54	25	7	18	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 4 is water.

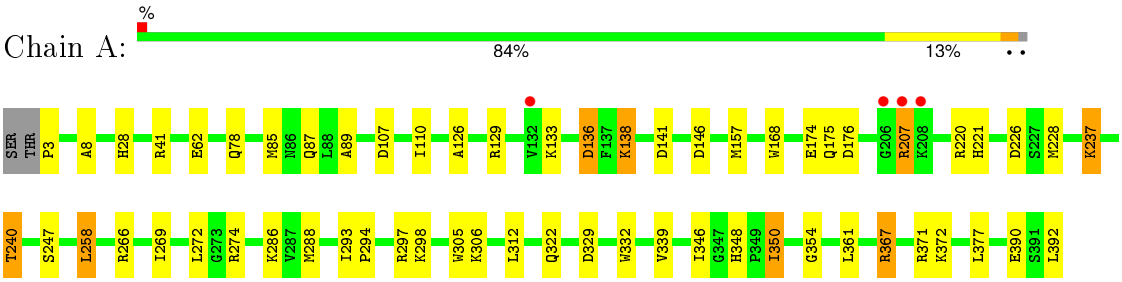
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	360	Total	O	0	0
			360	360		
4	B	372	Total	O	0	0
			372	372		
4	C	127	Total	O	0	0
			127	127		
4	D	143	Total	O	0	0
			143	143		

3 Residue-property plots (i)

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

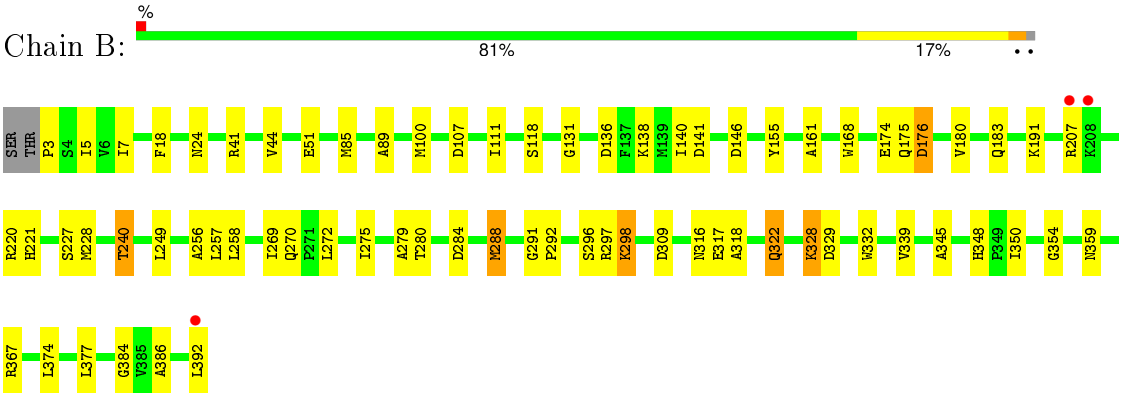
- Molecule 1: Acetyl-CoA acetyltransferase

Chain A:



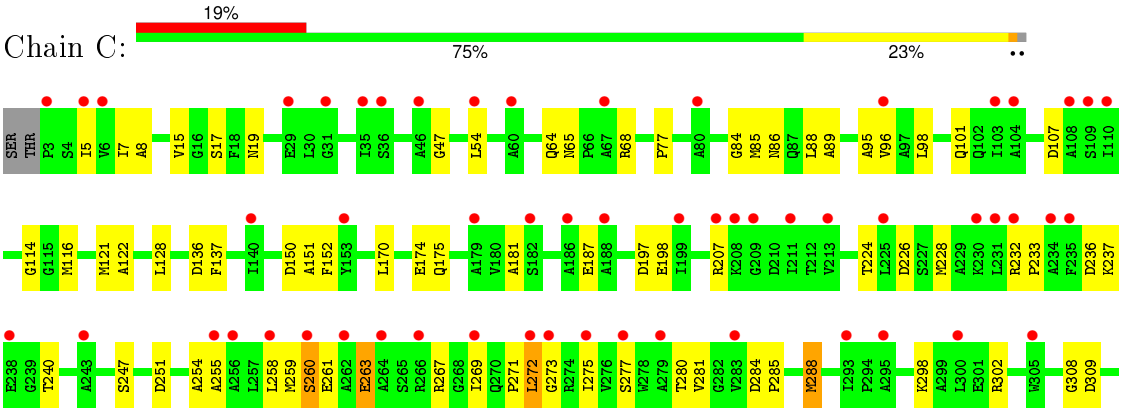
- Molecule 1: Acetyl-CoA acetyltransferase

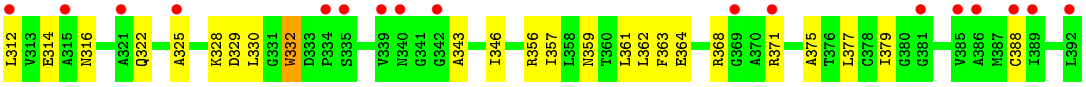
Chain B:



- Molecule 1: Acetyl-CoA acetyltransferase

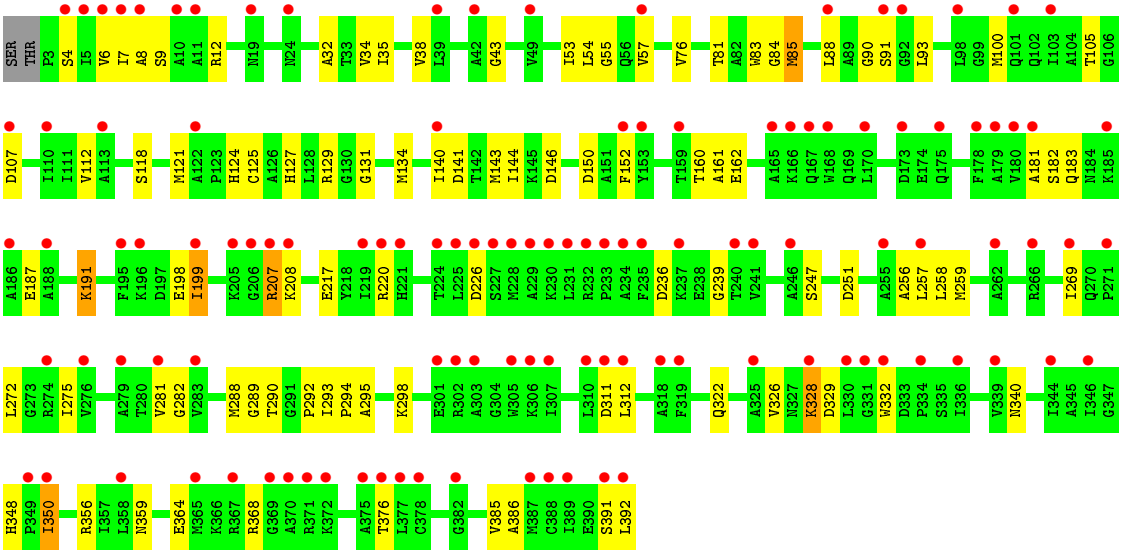
Chain C:





• Molecule 1: Acetyl-CoA acetyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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) 87.8 (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 5.1.19	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)	0.36 , 55.9	EDS
Estimated twinning fraction	0.166 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Outliers	0 of 141630 reflections	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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(^{o})	Ideal(^{o})
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:D:83:TRP:CZ2	4:D:489:HOH:O	2.33	0.80
1:C:151:ALA:HB3	4:C:519:HOH:O	1.81	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:D:385:VAL:HG22	4:D:510:HOH:O	1.94	0.68
1:A:371:ARG:HD2	4:A:454:HOH:O	1.92	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
1:D:183:GLN:HG2	4:D:461:HOH:O	1.98	0.63
4:C:504:HOH:O	1:D:140:ILE:HD13	1.99	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:D:124:HIS:HA	1:D:140:ILE:O	2.05	0.57
1:B:316:ASN:HB3	4:B:9738:HOH: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:C:316:ASN:ND2	1:C:377:LEU:HD23	2.25	0.51
1:A:174:GLU:OE2	4:A:442:HOH:O	2.19	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:D:275:ILE:HG21	4:D:535:HOH:O	2.13	0.48
1:B:7:ILE:HG23	1:B:256:ALA:HB1	1.95	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:6:VAL:O	1:D:258:LEU:CD1	2.62	0.48
1:D:217:GLU:HA	4:D:476:HOH:O	2.12	0.48
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.76	0.48
1:C:95:ALA:HA	1:C:98:LEU:HD12	1.95	0.48
1:C:280:THR:HG23	1:D:81:THR:HG21	1.96	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:C:152:PHE:CE2	4:C:519:HOH:O	2.56	0.46
1:B:270:GLN:NE2	1:B:392:LEU:OXT	2.48	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:D:12:ARG:O	1:D:199:ILE:HA	2.17	0.45
1:B:131:GLY:HA2	1:D:131:GLY:HA2	1.98	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:B:168:TRP:HH2	1:B:329:ASP:HB2	1.82	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:A:28:HIS:ND1	1:A:62:GLU:OE2	2.43	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:D:247[B]:SER:OG	1:D:348:HIS:HB2	2.17	0.45
1:C:101:GLN:HG2	1:D:105:THR:HG21	1.98	0.45
1:B:183:GLN:HA	1:B:345:ALA:HB2	1.99	0.45
1:D:386:ALA:N	4:D:510:HOH:O	2.50	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:B:138:LYS:HB2	1:B:140:ILE:HD11	1.99	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:83:TRP:HE3	1:D:84:GLY:O	2.00	0.44
1:D:281:VAL:HG23	4:D:503:HOH:O	2.17	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:B:317:GLU:OE2	4:B:9724:HOH:O	2.21	0.43
1:A:274:ARG:NH2	1:A:390:GLU:OE1	2.51	0.43
1:D:161:ALA:HA	4:D:459:HOH:O	2.18	0.43
1:A:85:MET:HA	1:B:85:MET:HA	2.00	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:HD22	1:B:258:LEU:N	2.34	0.42
1:D:57:VAL:HG21	1:D:350:ILE:CG2	2.48	0.42
1:D:162:GLU:HG3	4:D:523:HOH:O	2.18	0.42
1:D:293:ILE:HB	1:D:294:PRO:CD	2.50	0.42
1:C:86:ASN:OD1	1:C:88:LEU:HD23	2.19	0.42
1:A:346:ILE:O	1:A:346:ILE:HG22	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:275:ILE:CG2	4:B:466:HOH:O	2.68	0.42
1:B:131:GLY:HA2	1:D:131:GLY:CA	2.50	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:18:PHE:HB2	1:B:249:LEU:O	2.19	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:76:VAL:HB	4:D:396:HOH:O	2.20	0.41
1:D:100:MET:SD	1:D:100:MET:C	2.98	0.41
1:C:356:ARG:NH2	1:C:357:ILE:HG22	2.35	0.41
1:C:346:ILE:HD13	1:C:356:ARG:NH1	2.35	0.41
1:C:7:ILE:O	1:C:272:LEU:N	2.54	0.41
1:C:54:LEU:HD13	1:C:116:MET:CE	2.50	0.41
1:D:54:LEU:O	1:D:84:GLY:HA2	2.20	0.41
1:C:89:ALA:CB	4:C:400:HOH:O	2.66	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:B:176:ASP:O	1:B:180:VAL:HG23	2.21	0.41
1:B:275:ILE:HG21	4:B:466:HOH:O	2.21	0.41
1:D:55:GLY:HA2	4:D:502:HOH:O	2.21	0.41
1:D:290:THR:O	1:D:294:PRO:HD2	2.21	0.41
1:A:237:LYS:HA	1:A:237:LYS:HD2	1.87	0.41
1:A:247[B]:SER:OG	1:A:348:HIS:HB2	2.21	0.41
1:D:257:LEU:C	1:D:257:LEU:HD23	2.41	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:C:84:GLY:HA3	4:C:515:HOH:O	2.21	0.40
1:B:257:LEU:C	1:B:257:LEU:CD2	2.90	0.40
1:A:157:MET:CG	4:A:467:HOH:O	2.54	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:D:88:LEU:O	1:D:91:SER:CB	2.70	0.40
1:D:208:LYS:C	4:D:519:HOH:O	2.60	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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	34 21
1	B	389/392 (99%)	374 (96%)	14 (4%)	1 (0%)	46 35
1	C	389/392 (99%)	370 (95%)	19 (5%)	0	100 100
1	D	389/392 (99%)	366 (94%)	22 (6%)	1 (0%)	46 35
All	All	1556/1568 (99%)	1479 (95%)	73 (5%)	4 (0%)	46 35

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

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%)	23 9
1	B	277/278 (100%)	261 (94%)	16 (6%)	25 10
1	C	277/278 (100%)	260 (94%)	17 (6%)	23 9
1	D	277/278 (100%)	256 (92%)	21 (8%)	16 5
All	All	1108/1112 (100%)	1037 (94%)	71 (6%)	22 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	-	45,56,56	1.50	6 (13%)	58,83,83	2.39	10 (17%)
2	SO4	A	9720	-	4,4,4	0.64	0	6,6,6	0.38	0
2	SO4	A	9722	-	4,4,4	0.26	0	6,6,6	0.46	0
3	CAA	B	2393	-	45,56,56	1.63	8 (17%)	58,83,83	2.76	13 (22%)
2	SO4	B	9719	-	4,4,4	0.15	0	6,6,6	0.33	0
2	SO4	B	9721	-	4,4,4	0.53	0	6,6,6	0.55	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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2393	CAA	O3-C3	-2.52	1.13	1.21
3	B	2393	CAA	O1-C1	-2.49	1.17	1.21
3	A	1393	CAA	C5A-C4A	2.05	1.45	1.40
3	B	2393	CAA	C5A-C4A	2.41	1.45	1.40
3	A	1393	CAA	C1-S1P	2.63	1.81	1.76
3	B	2393	CAA	C1-S1P	3.03	1.82	1.76
3	A	1393	CAA	P1A-O2A	3.62	1.70	1.54
3	B	2393	CAA	P1A-O2A	3.68	1.70	1.54
3	B	2393	CAA	P2A-O5A	3.80	1.71	1.54
3	A	1393	CAA	P2A-O5A	3.97	1.71	1.54
3	A	1393	CAA	P3B-O9A	4.39	1.70	1.54
3	A	1393	CAA	P3B-O8A	4.58	1.71	1.54
3	B	2393	CAA	P3B-O8A	4.70	1.71	1.54
3	B	2393	CAA	P3B-O9A	4.89	1.72	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1393	CAA	N3A-C2A-N1A	-8.03	122.75	128.89
3	B	2393	CAA	N3A-C2A-N1A	-7.67	123.02	128.89
3	B	2393	CAA	C1B-N9A-C4A	-5.25	119.02	126.94
3	B	2393	CAA	P2A-O3A-P1A	-5.13	118.32	132.73
3	B	2393	CAA	C4B-O4B-C1B	-4.85	104.39	109.72
3	A	1393	CAA	C1B-N9A-C4A	-4.36	120.36	126.94
3	A	1393	CAA	P2A-O3A-P1A	-3.02	124.24	132.73
3	A	1393	CAA	O3-C3-C2	-2.96	108.82	120.96
3	A	1393	CAA	C2P-S1P-C1	-2.77	92.23	102.09
3	B	2393	CAA	C3P-C2P-S1P	-2.59	104.42	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2393	CAA	O3-C3-C2	-2.26	111.71	120.96
3	B	2393	CAA	C6P-C5P-N4P	-2.01	112.96	116.46
3	A	1393	CAA	C2A-N1A-C6A	2.04	122.41	118.77
3	B	2393	CAA	O1-C1-S1P	2.15	124.54	122.83
3	A	1393	CAA	O3A-P2A-O6A	2.17	108.69	102.94
3	A	1393	CAA	C4-C3-C2	2.18	126.66	118.35
3	B	2393	CAA	C2A-N1A-C6A	2.26	122.81	118.77
3	B	2393	CAA	C4-C3-C2	2.61	128.31	118.35
3	B	2393	CAA	C3-C2-C1	2.74	125.53	114.06
3	B	2393	CAA	O4B-C1B-N9A	2.92	114.21	108.10
3	A	1393	CAA	C3-C2-C1	4.59	133.29	114.06
3	A	1393	CAA	C2-C1-S1P	12.59	126.06	113.50
3	B	2393	CAA	C2-C1-S1P	15.43	128.89	113.50

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

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	390/392 (99%)	-0.18	4 (1%) 84 89	6, 13, 27, 45	0
1	B	390/392 (99%)	-0.22	3 (0%) 87 92	6, 13, 26, 49	0
1	C	390/392 (99%)	1.20	73 (18%) 2 2	3, 14, 24, 38	0
1	D	390/392 (99%)	1.66	118 (30%) 1 0	2, 14, 24, 41	0
All	All	1560/1568 (99%)	0.62	198 (12%) 5 8	2, 14, 25, 49	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	392	LEU	9.1
1	D	382	GLY	8.2
1	D	281	VAL	7.4
1	D	229	ALA	7.1
1	C	36	SER	7.0
1	D	228	MET	6.7
1	D	279	ALA	6.2
1	D	331	GLY	6.1
1	D	170	LEU	5.9
1	C	80	ALA	5.8
1	D	246	ALA	5.7
1	D	179	ALA	5.7
1	D	235	PHE	5.5
1	D	7	ILE	5.4
1	D	232	ARG	5.2
1	D	388	CYS	5.0
1	D	307	ILE	5.0
1	C	334	PRO	5.0
1	D	186	ALA	5.0
1	C	272	LEU	4.9
1	C	295	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	231	LEU	4.8
1	D	152	PHE	4.7
1	D	219	ILE	4.6
1	A	132	VAL	4.4
1	D	208	LYS	4.4
1	D	226	ASP	4.4
1	C	321	ALA	4.4
1	D	325	ALA	4.4
1	D	376	THR	4.4
1	D	180	VAL	4.3
1	D	344	ILE	4.2
1	D	328	LYS	4.1
1	C	186	ALA	4.1
1	D	206	GLY	4.1
1	C	211	ILE	4.1
1	D	310	LEU	4.1
1	C	110	ILE	4.0
1	D	303	ALA	4.0
1	C	243	ALA	3.9
1	C	208	LYS	3.9
1	D	371	ARG	3.9
1	D	332	TRP	3.9
1	D	188	ALA	3.8
1	C	96	VAL	3.8
1	D	370	ALA	3.7
1	D	306	LYS	3.7
1	C	213	VAL	3.7
1	C	67	ALA	3.7
1	C	342	GLY	3.6
1	D	195	PHE	3.6
1	C	385	VAL	3.6
1	D	5	ILE	3.6
1	D	10	ALA	3.6
1	D	107	ASP	3.5
1	D	6	VAL	3.5
1	C	209	GLY	3.5
1	D	274	ARG	3.5
1	D	339	VAL	3.4
1	D	269	ILE	3.4
1	C	371	ARG	3.4
1	C	312	LEU	3.4
1	C	392	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	358	LEU	3.4
1	D	276	VAL	3.3
1	C	230	LYS	3.3
1	D	8	ALA	3.3
1	D	346	ILE	3.3
1	D	330	LEU	3.2
1	D	377	LEU	3.2
1	A	206	GLY	3.2
1	D	175	GLN	3.1
1	D	350	ILE	3.1
1	A	207	ARG	3.1
1	D	283	VAL	3.1
1	C	104	ALA	3.1
1	A	208	LYS	3.1
1	C	275	ILE	3.0
1	D	225	LEU	3.0
1	D	367	ARG	3.0
1	D	167	GLN	3.0
1	D	391	SER	3.0
1	D	241	VAL	3.0
1	C	234	ALA	3.0
1	C	269	ILE	3.0
1	C	46	ALA	3.0
1	C	235	PHE	3.0
1	B	207	ARG	3.0
1	C	60	ALA	2.9
1	C	108	ALA	2.9
1	C	231	LEU	2.9
1	D	336	ILE	2.9
1	D	140	ILE	2.9
1	D	207	ARG	2.9
1	D	220	ARG	2.9
1	D	221	HIS	2.9
1	D	181	ALA	2.8
1	C	339	VAL	2.8
1	C	232	ARG	2.8
1	D	166	LYS	2.8
1	D	271	PRO	2.8
1	D	349	PRO	2.8
1	D	365	MET	2.8
1	C	315	ALA	2.8
1	D	375	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	205	LYS	2.8
1	C	258	LEU	2.8
1	D	237	LYS	2.8
1	C	225	LEU	2.7
1	D	88	LEU	2.7
1	D	173	ASP	2.7
1	D	302	ARG	2.7
1	C	188	ALA	2.7
1	C	207	ARG	2.7
1	C	305	TRP	2.7
1	C	182	SER	2.6
1	D	110	ILE	2.6
1	C	386	ALA	2.6
1	B	392	LEU	2.6
1	D	227	SER	2.6
1	D	318	ALA	2.6
1	C	3	PRO	2.6
1	C	35	ILE	2.6
1	D	389	ILE	2.6
1	D	168	TRP	2.6
1	D	113	ALA	2.6
1	D	369	GLY	2.6
1	D	233	PRO	2.6
1	D	301	GLU	2.5
1	C	256	ALA	2.5
1	D	255	ALA	2.5
1	D	199	ILE	2.5
1	D	185	LYS	2.5
1	D	305	TRP	2.5
1	D	257	LEU	2.5
1	D	178	PHE	2.5
1	C	103	ILE	2.5
1	C	140	ILE	2.5
1	C	153	TYR	2.5
1	D	101	GLN	2.5
1	D	49	VAL	2.5
1	D	387	MET	2.5
1	C	238	GLU	2.4
1	C	388	CYS	2.4
1	B	208	LYS	2.4
1	D	224	THR	2.4
1	D	4	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	262	ALA	2.4
1	D	153	TYR	2.4
1	C	381	GLY	2.4
1	C	335	SER	2.4
1	C	389	ILE	2.3
1	D	19	ASN	2.3
1	C	266	ARG	2.3
1	C	5	ILE	2.3
1	C	6	VAL	2.3
1	D	57	VAL	2.3
1	C	277	SER	2.3
1	C	264	ALA	2.3
1	D	311	ASP	2.3
1	C	31	GLY	2.3
1	D	230	LYS	2.3
1	D	378	CYS	2.3
1	D	319	PHE	2.2
1	C	109	SER	2.2
1	D	24	ASN	2.2
1	D	92	GLY	2.2
1	D	266	ARG	2.2
1	C	199	ILE	2.2
1	D	196	LYS	2.2
1	C	273	GLY	2.1
1	D	11	ALA	2.1
1	D	165	ALA	2.1
1	D	234	ALA	2.1
1	C	293	ILE	2.1
1	D	103	ILE	2.1
1	D	159	THR	2.1
1	D	240	THR	2.1
1	C	54	LEU	2.1
1	D	39	LEU	2.1
1	D	122	ALA	2.1
1	C	283	VAL	2.1
1	C	260	SER	2.1
1	C	179	ALA	2.1
1	D	98	LEU	2.1
1	D	312	LEU	2.1
1	D	334	PRO	2.1
1	C	340	ASN	2.0
1	C	255	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	325	ALA	2.0
1	D	42	ALA	2.0
1	D	262	ALA	2.0
1	C	300	LEU	2.0
1	C	279	ALA	2.0
1	D	91	SER	2.0
1	C	29	GLU	2.0
1	C	369	GLY	2.0
1	D	372	LYS	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CAA	B	2393	54/54	0.85	0.22	6.02	11,52,57,60	0
3	CAA	A	1393	54/54	0.83	0.23	2.22	18,52,60,63	0
2	SO4	A	9722	5/5	0.93	0.16	1.27	58,59,61,63	0
2	SO4	B	9719	5/5	0.96	0.13	-	66,67,68,68	0
2	SO4	A	9720	5/5	0.98	0.10	-	47,48,51,53	0
2	SO4	B	9721	5/5	0.98	0.10	-	47,47,50,51	0

6.5 Other polymers (i)

There are no such residues in this entry.