



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:19 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 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/ValidationPDFNotes.html>

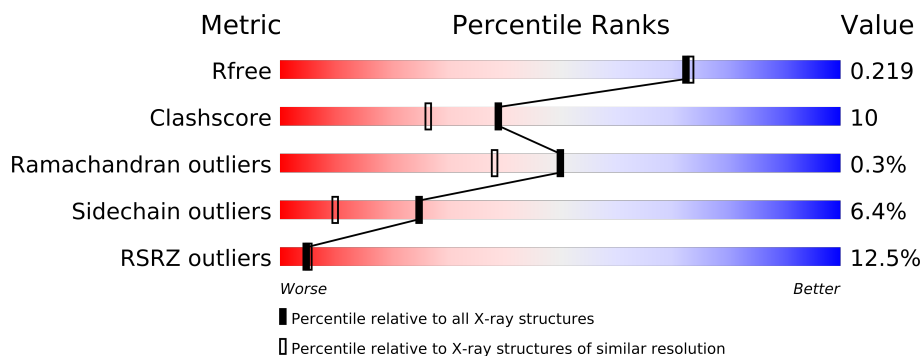
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	392	
1	B	392	
1	C	392	
1	D	392	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	9720	-	X
2	SO4	B	9721	-	X
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 hydrogen and 0 are deuterium.

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:

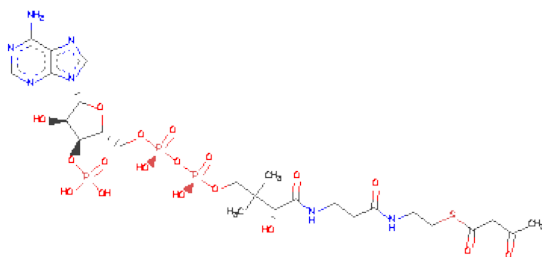
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	INSERTION	UNP P07097
A	89	ALA	CYS	ENGINEERED	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	10	ALA	-	INSERTION	UNP P07097
B	89	ALA	CYS	ENGINEERED	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	10	ALA	-	INSERTION	UNP P07097
C	89	ALA	CYS	ENGINEERED	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: O₄S).



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

- 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		

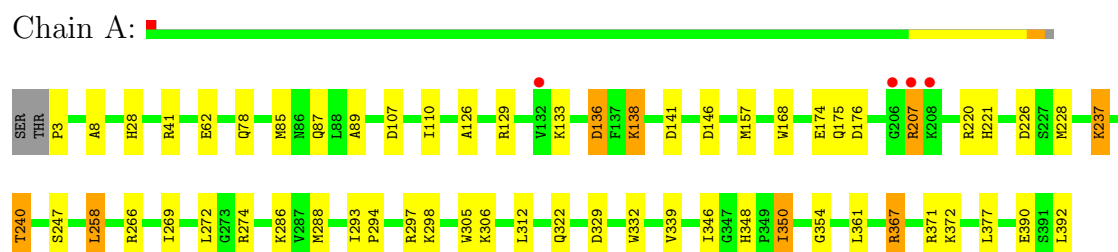
- Molecule 4 is water.

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		

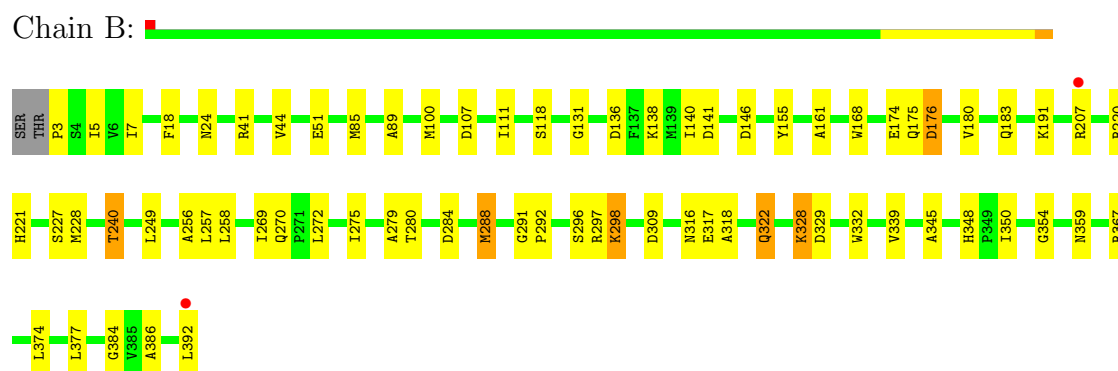
3 Residue-property plots

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.

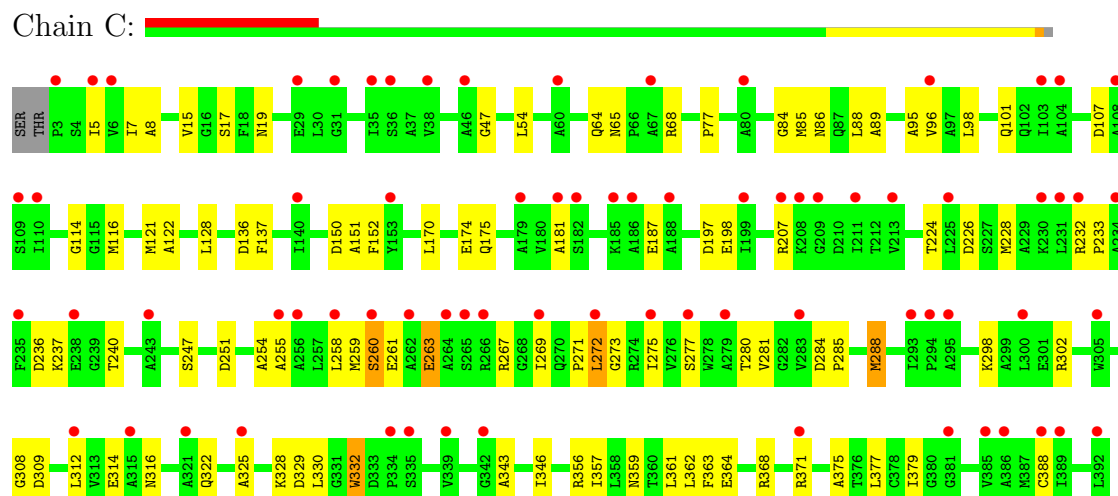
- Molecule 1: Acetyl-CoA acetyltransferase



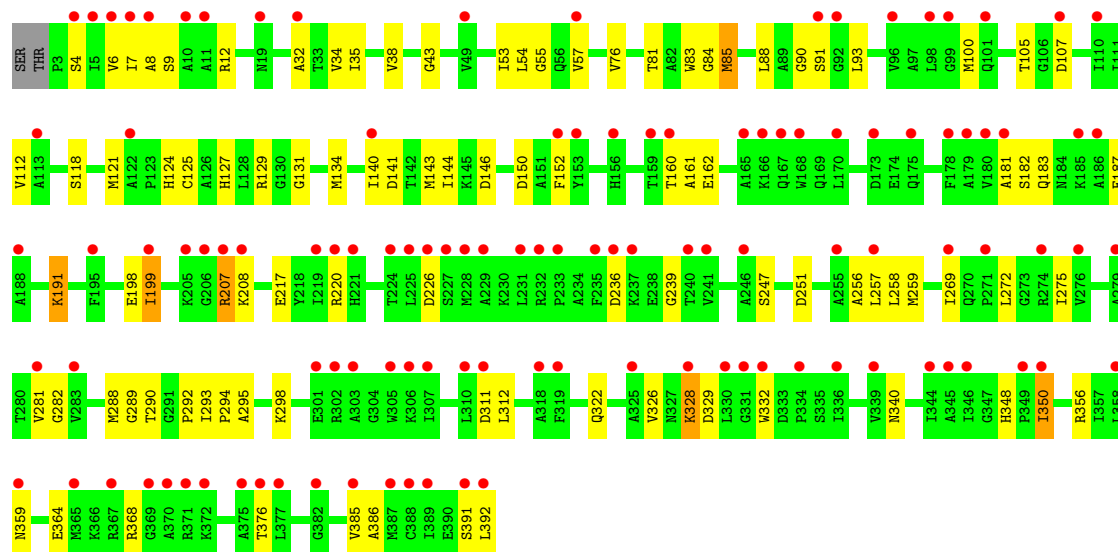
- Molecule 1: Acetyl-CoA acetyltransferase



- Molecule 1: Acetyl-CoA acetyltransferase



Chain D:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.211 , 0.258 0.201 , 0.219	Depositor DCC
R_{free} test set	6373 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 , 55.7	EDS
Estimated twinning fraction	0.166 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	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.*

¹Intensities estimated from amplitudes.

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(°)	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(°)	Ideal(°)
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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (222) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	38	23
1	B	389/392 (99%)	374 (96%)	14 (4%)	1 (0%)	50	38
1	C	389/392 (99%)	370 (95%)	19 (5%)	0	100	100
1	D	389/392 (99%)	366 (94%)	22 (6%)	1 (0%)	50	38
All	All	1556/1568 (99%)	1479 (95%)	73 (5%)	4 (0%)	50	38

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%)	26	11
1	B	277/278 (100%)	261 (94%)	16 (6%)	28	12
1	C	277/278 (100%)	260 (94%)	17 (6%)	26	11
1	D	277/278 (100%)	256 (92%)	21 (8%)	19	6
All	All	1108/1112 (100%)	1037 (94%)	71 (6%)	25	10

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains 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	-	56,56,56	1.60	10 (17%)	83,83,83	2.30	16 (19%)
2	SO4	A	9720	-	4,4,4	0.65	0	6,6,6	0.38	0
2	SO4	A	9722	-	4,4,4	0.25	0	6,6,6	0.46	0
3	CAA	B	2393	-	56,56,56	1.59	10 (17%)	83,83,83	2.67	18 (21%)
2	SO4	B	9719	-	4,4,4	0.13	0	6,6,6	0.33	0
2	SO4	B	9721	-	4,4,4	0.53	0	6,6,6	0.52	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	-	-	0/55/71/71	0/1/3/3
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	-	-	0/55/71/71	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2393	CAA	P3B-O9A	4.80	1.72	1.54
3	B	2393	CAA	P3B-O8A	4.62	1.71	1.54
3	A	1393	CAA	P3B-O8A	4.50	1.71	1.54
3	A	1393	CAA	C2-C1	-4.36	1.45	1.51
3	A	1393	CAA	P3B-O9A	4.31	1.70	1.54
3	A	1393	CAA	C4A-N9A	-3.91	1.32	1.37
3	A	1393	CAA	P2A-O5A	3.78	1.71	1.55
3	B	2393	CAA	P2A-O5A	3.61	1.71	1.55
3	B	2393	CAA	C4A-N9A	-3.59	1.32	1.37
3	B	2393	CAA	P1A-O2A	3.50	1.70	1.55
3	A	1393	CAA	P1A-O2A	3.44	1.70	1.55
3	B	2393	CAA	C1-S1P	3.03	1.82	1.76
3	B	2393	CAA	C2-C1	-2.81	1.47	1.51
3	A	1393	CAA	C1-S1P	2.63	1.81	1.76
3	B	2393	CAA	O3-C3	-2.55	1.13	1.21
3	B	2393	CAA	O1-C1	-2.51	1.17	1.21
3	B	2393	CAA	C5A-C4A	2.41	1.45	1.40
3	A	1393	CAA	P1A-O3A	2.34	1.64	1.59
3	A	1393	CAA	P2A-O3A	2.18	1.63	1.59
3	A	1393	CAA	C5A-C4A	2.05	1.45	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2393	CAA	C2-C1-S1P	14.27	128.89	113.43
3	A	1393	CAA	C2-C1-S1P	11.65	126.06	113.43
3	B	2393	CAA	O1-C1-C2	-10.54	106.27	122.75
3	A	1393	CAA	O1-C1-C2	-7.82	110.53	122.75
3	A	1393	CAA	N3A-C2A-N1A	-7.13	122.75	128.71
3	B	2393	CAA	N3A-C2A-N1A	-6.80	123.02	128.71
3	B	2393	CAA	O4B-C1B-N9A	6.21	114.21	108.44
3	A	1393	CAA	N3A-C4A-N9A	5.97	136.22	125.43
3	B	2393	CAA	N3A-C4A-N9A	5.13	134.70	125.43
3	B	2393	CAA	C4B-O4B-C1B	-4.93	104.39	109.75
3	A	1393	CAA	C8A-N9A-C4A	4.65	110.44	106.90
3	B	2393	CAA	P2A-O3A-P1A	-4.56	118.32	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	-3.60	108.82	121.62
3	B	2393	CAA	C4-C3-C2	3.46	128.31	117.49
3	B	2393	CAA	C8A-N9A-C4A	2.98	109.17	106.90
3	A	1393	CAA	C4-C3-C2	2.94	126.66	117.49
3	A	1393	CAA	C2P-S1P-C1	-2.93	92.23	101.90
3	A	1393	CAA	CBP-CAP-C9P	-2.80	110.01	112.73
3	B	2393	CAA	O3-C3-C2	-2.78	111.71	121.62
3	B	2393	CAA	C8A-N9A-C1B	2.73	131.77	126.38
3	B	2393	CAA	C5A-C4A-N3A	-2.68	119.87	125.70
3	A	1393	CAA	O4B-C1B-N9A	-2.61	106.01	108.44
3	A	1393	CAA	C5A-C4A-N9A	-2.54	103.49	107.16
3	A	1393	CAA	P2A-O3A-P1A	-2.54	124.24	131.68
3	A	1393	CAA	C5A-C4A-N3A	-2.49	120.29	125.70
3	B	2393	CAA	C2A-N1A-C6A	2.24	122.81	118.77
3	B	2393	CAA	O9P-C9P-CAP	-2.18	116.51	120.48
3	B	2393	CAA	C2A-N3A-C4A	2.17	120.18	114.01
3	A	1393	CAA	C2A-N3A-C4A	2.16	120.15	114.01
3	B	2393	CAA	C3P-C2P-S1P	-2.15	104.42	111.04
3	B	2393	CAA	CBP-CAP-C9P	-2.04	110.75	112.73
3	A	1393	CAA	C2A-N1A-C6A	2.01	122.41	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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%)	0.01	4 (1%) 79 87	6, 13, 27, 45	0
1	B	390/392 (99%)	-0.03	2 (0%) 88 94	6, 13, 26, 49	0
1	C	390/392 (99%)	1.23	74 (18%) 2 1	3, 14, 24, 38	0
1	D	390/392 (99%)	1.65	115 (29%) 1 0	2, 14, 24, 41	0
All	All	1560/1568 (99%)	0.71	195 (12%) 5 5	2, 14, 25, 49	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	382	GLY	9.0
1	D	392	LEU	7.9
1	D	281	VAL	6.9
1	C	36	SER	6.9
1	D	229	ALA	6.8
1	D	279	ALA	6.6
1	D	228	MET	6.0
1	D	331	GLY	6.0
1	C	80	ALA	5.6
1	D	179	ALA	5.5
1	D	246	ALA	5.4
1	D	170	LEU	5.3
1	D	186	ALA	5.2
1	C	334	PRO	5.1
1	D	235	PHE	5.0
1	D	7	ILE	4.8
1	D	376	THR	4.7
1	D	232	ARG	4.6
1	C	295	ALA	4.5
1	D	307	ILE	4.5
1	D	388	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	219	ILE	4.5
1	D	206	GLY	4.4
1	C	321	ALA	4.3
1	D	188	ALA	4.3
1	D	328	LYS	4.3
1	D	325	ALA	4.2
1	D	152	PHE	4.2
1	D	180	VAL	4.2
1	C	243	ALA	4.1
1	A	132	VAL	4.1
1	C	342	GLY	4.0
1	C	186	ALA	4.0
1	D	344	ILE	4.0
1	D	303	ALA	4.0
1	D	226	ASP	4.0
1	D	231	LEU	4.0
1	D	208	LYS	3.9
1	C	209	GLY	3.9
1	D	310	LEU	3.9
1	C	272	LEU	3.8
1	C	208	LYS	3.8
1	D	107	ASP	3.8
1	C	67	ALA	3.7
1	D	332	TRP	3.7
1	D	269	ILE	3.7
1	D	371	ARG	3.7
1	C	110	ILE	3.6
1	C	211	ILE	3.6
1	D	195	PHE	3.6
1	D	358	LEU	3.5
1	D	10	ALA	3.4
1	A	206	GLY	3.4
1	D	276	VAL	3.4
1	D	350	ILE	3.4
1	C	96	VAL	3.3
1	D	274	ARG	3.3
1	D	370	ALA	3.3
1	D	5	ILE	3.3
1	C	213	VAL	3.2
1	D	6	VAL	3.2
1	D	283	VAL	3.2
1	C	275	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	367	ARG	3.2
1	D	175	GLN	3.2
1	C	60	ALA	3.2
1	D	377	LEU	3.1
1	D	339	VAL	3.1
1	D	306	LYS	3.1
1	D	241	VAL	3.1
1	C	188	ALA	3.0
1	D	375	ALA	3.0
1	C	385	VAL	3.0
1	D	391	SER	3.0
1	C	104	ALA	3.0
1	D	330	LEU	3.0
1	D	346	ILE	2.9
1	D	349	PRO	2.9
1	D	167	GLN	2.9
1	C	108	ALA	2.9
1	C	230	LYS	2.9
1	D	221	HIS	2.9
1	D	166	LYS	2.9
1	D	101	GLN	2.8
1	C	46	ALA	2.8
1	C	386	ALA	2.8
1	C	269	ILE	2.8
1	C	371	ARG	2.8
1	D	181	ALA	2.8
1	D	336	ILE	2.8
1	C	225	LEU	2.8
1	C	392	LEU	2.8
1	A	207	ARG	2.8
1	D	8	ALA	2.8
1	D	140	ILE	2.8
1	D	173	ASP	2.8
1	C	103	ILE	2.8
1	D	207	ARG	2.7
1	C	315	ALA	2.7
1	C	234	ALA	2.7
1	D	271	PRO	2.7
1	D	92	GLY	2.7
1	B	207	ARG	2.7
1	C	312	LEU	2.7
1	C	305	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	168	TRP	2.7
1	D	305	TRP	2.7
1	C	179	ALA	2.7
1	C	264	ALA	2.7
1	C	35	ILE	2.7
1	C	235	PHE	2.7
1	C	232	ARG	2.6
1	D	11	ALA	2.6
1	D	220	ARG	2.6
1	C	335	SER	2.6
1	A	208	LYS	2.6
1	C	325	ALA	2.6
1	D	165	ALA	2.6
1	C	182	SER	2.6
1	C	339	VAL	2.5
1	C	199	ILE	2.5
1	C	381	GLY	2.5
1	C	258	LEU	2.5
1	D	233	PRO	2.5
1	D	301	GLU	2.5
1	D	372	LYS	2.5
1	D	19	ASN	2.5
1	D	318	ALA	2.5
1	C	31	GLY	2.5
1	D	227	SER	2.5
1	C	231	LEU	2.5
1	C	293	ILE	2.5
1	D	110	ILE	2.5
1	D	302	ARG	2.5
1	D	387	MET	2.4
1	D	311	ASP	2.4
1	D	4	SER	2.4
1	C	140	ILE	2.4
1	D	113	ALA	2.4
1	D	389	ILE	2.4
1	D	205	LYS	2.4
1	D	237	LYS	2.4
1	D	369	GLY	2.4
1	D	159	THR	2.4
1	D	224	THR	2.4
1	D	255	ALA	2.4
1	C	256	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	3	PRO	2.4
1	C	5	ILE	2.4
1	C	207	ARG	2.3
1	C	300	LEU	2.3
1	D	345	ALA	2.3
1	D	185	LYS	2.3
1	D	240	THR	2.3
1	D	257	LEU	2.3
1	C	266	ARG	2.3
1	C	389	ILE	2.3
1	C	38	VAL	2.3
1	C	277	SER	2.3
1	D	57	VAL	2.3
1	D	96	VAL	2.3
1	D	199	ILE	2.3
1	C	153	TYR	2.2
1	C	181	ALA	2.2
1	C	262	ALA	2.2
1	D	122	ALA	2.2
1	D	178	PHE	2.2
1	D	98	LEU	2.2
1	D	91	SER	2.2
1	D	99	GLY	2.2
1	D	334	PRO	2.2
1	D	319	PHE	2.2
1	C	283	VAL	2.2
1	D	385	VAL	2.2
1	D	160	THR	2.2
1	D	365	MET	2.2
1	D	236	ASP	2.2
1	C	388	CYS	2.2
1	B	392	LEU	2.1
1	C	109	SER	2.1
1	D	156	HIS	2.1
1	C	294	PRO	2.1
1	C	29	GLU	2.1
1	C	238	GLU	2.1
1	C	6	VAL	2.1
1	D	225	LEU	2.1
1	C	255	ALA	2.1
1	D	32	ALA	2.1
1	C	265	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	185	LYS	2.0
1	C	260	SER	2.0
1	D	49	VAL	2.0
1	C	279	ALA	2.0
1	D	153	TYR	2.0
1	D	359	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	9720	5/5	0.12	13.06	47,48,51,53	0
3	CAA	B	2393	54/54	0.23	6.22	11,52,57,60	0
2	SO4	B	9721	5/5	0.13	2.65	47,47,50,51	0
3	CAA	A	1393	54/54	0.24	2.11	18,52,60,63	0
2	SO4	A	9722	5/5	0.15	1.18	58,59,61,63	0
2	SO4	B	9719	5/5	0.12	-0.22	66,67,68,68	0

6.5 Other polymers ⓘ

There are no such residues in this entry.