Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:04 AM GMT

PDB ID	:	2VU0
Title	:	BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. COMPLEX OF THE OXIDISED ENZYME WITH COENZYME A.
Authors	:	Kursula, P.; Wierenga, R.K.
Deposited on	:	2008-05-19
Resolution	:	1.87 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:

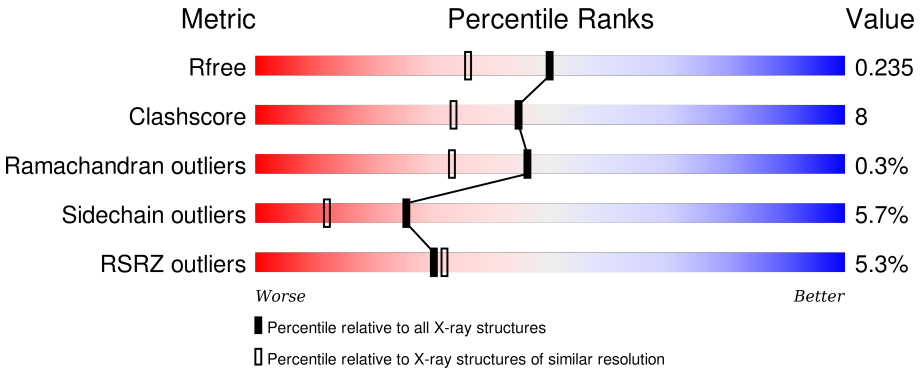
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.87 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	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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	2% 83% 14%
1	B	392	% 86% 12%
1	C	392	4% 83% 16%
1	D	392	14% 82% 16%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	COA	B	1393	-	-	-	X
4	SO4	A	1395	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12643 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.

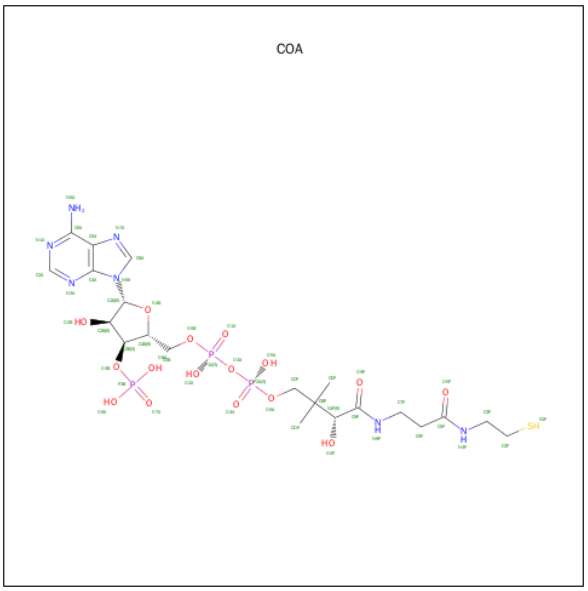
- Molecule 1 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	7	0
			2864	1781	514	548	21			
1	B	391	Total	C	N	O	S	0	10	0
			2869	1788	512	548	21			
1	C	391	Total	C	N	O	S	0	0	0
			2828	1755	511	541	21			
1	D	390	Total	C	N	O	S	0	0	0
			2821	1751	510	539	21			

There are 8 discrepancies between the modelled and reference sequences:

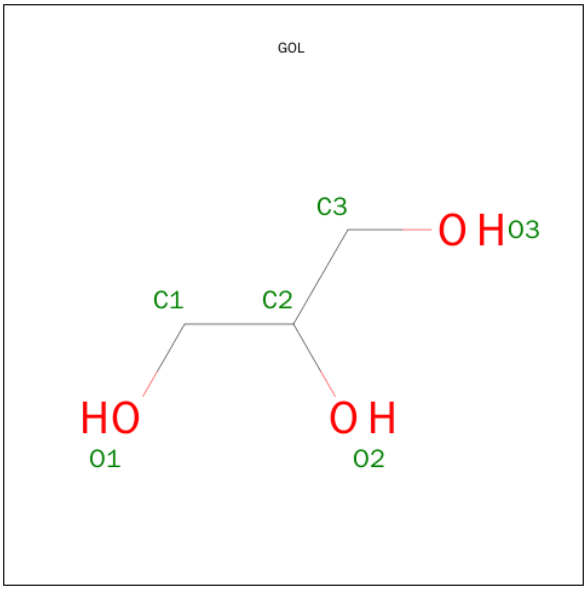
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ALA	-	INSERTION	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	11	ALA	-	INSERTION	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	11	ALA	-	INSERTION	UNP P07097
C	129	ARG	ALA	CONFLICT	UNP P07097
A	11	ALA	-	INSERTION	UNP P07097
D	129	ARG	ALA	CONFLICT	UNP P07097

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



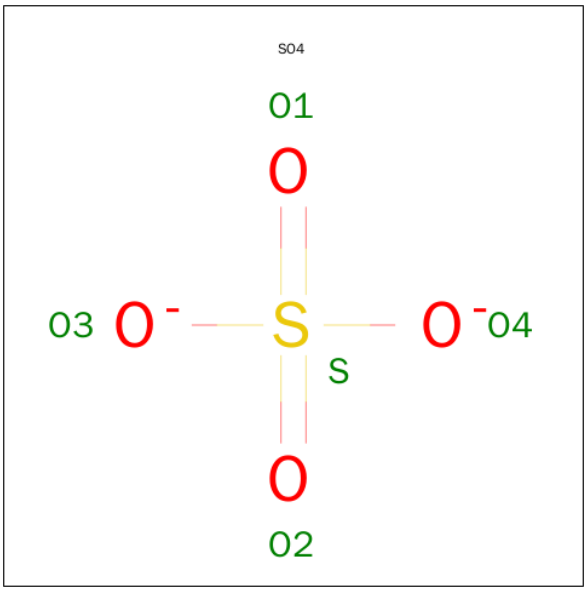
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

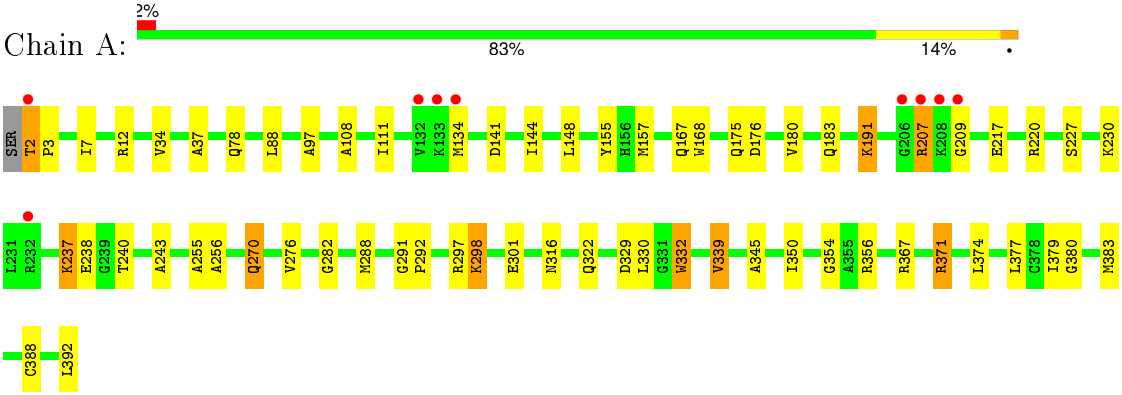
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	401	Total O 401 401	0	0
5	B	392	Total O 392 392	0	0
5	C	191	Total O 191 191	0	0
5	D	155	Total O 155 155	0	0

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.

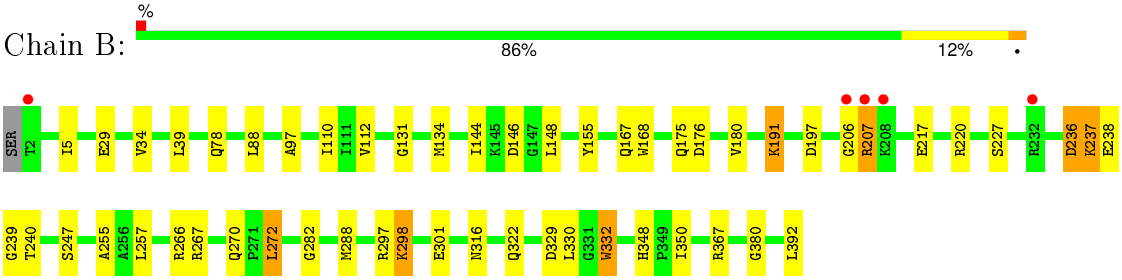
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain A:



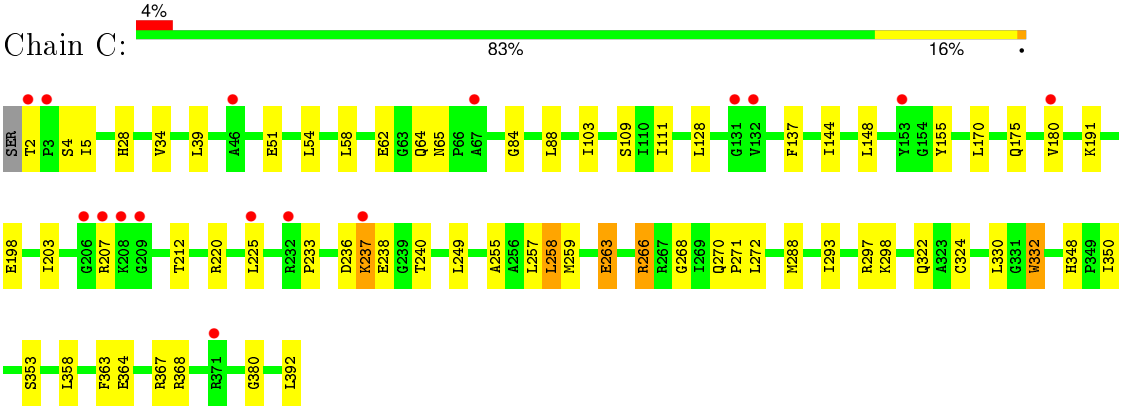
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain B:



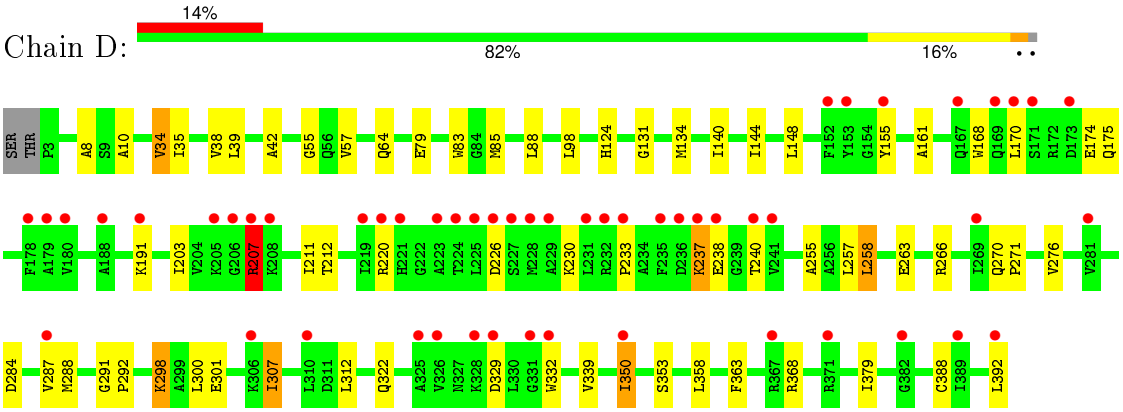
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain C:



- Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain D:


14%
82%
16%
SER THR P3 A8 S9 A10 V34 I35 V38 L39 A42 G55 Q56 V57 Q64 E79 W83 G84 M85 L88 L98 H124 G131 M134 I140 I144 L148 F152 Y153 G154 Y155 A161 Q167 W168 Q169 L170 S171 R172 D173 E174 Q175
F178 A179 V180 A188 K191 I203 V204 K205 G206 R207 K208 I211 T212 I219 R220 H221 G222 A223 T224 L225 D226 S227 M228 A229 K230 L231 R232 P233 A234 F235 D236 K237 E238 G239 T240 V241 A255 A256 L257 L258 E263 R266 I269 Q270 P271 V276 V281
D284 V287 M288 G291 P292 K298 A299 L300 E301 K306 I307 L310 D311 L312 Q322 A325 V326 N327 K328 D329 L330 G331 W332 V339 I350 S353 L358 F363 R367 R368 R371 I379 G382 C388 I389 L392

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.40Å 79.06Å 148.80Å 90.00° 92.66° 90.00°	Depositor
Resolution (Å)	20.00 – 1.87 19.72 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-1.87) 85.4 (19.72-1.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.55 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.229 0.201 , 0.235	Depositor DCC
R_{free} test set	7205 reflections (4.80%)	DCC
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 22.5	EDS
Estimated twinning fraction	0.118 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 157220 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12643	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: COA, GOL, CSO, 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	1.04	3/2919 (0.1%)	0.95	7/3941 (0.2%)
1	B	0.99	3/2933 (0.1%)	0.91	6/3960 (0.2%)
1	C	0.61	0/2862	0.71	2/3864 (0.1%)
1	D	0.60	0/2855	0.71	1/3853 (0.0%)
All	All	0.84	6/11569 (0.1%)	0.83	16/15618 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	GLU	CB-CG	-6.19	1.40	1.52
1	B	217	GLU	CB-CG	-6.08	1.40	1.52
1	A	97	ALA	CA-CB	5.88	1.64	1.52
1	B	97	ALA	CA-CB	5.51	1.64	1.52
1	A	37	ALA	CA-CB	5.41	1.63	1.52
1	B	217	GLU	CD-OE2	-5.15	1.20	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	367	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	B	367	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	371	ARG	NE-CZ-NH2	6.75	123.68	120.30
1	A	141	ASP	CB-CG-OD2	6.33	124.00	118.30
1	D	207	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	371	ARG	NE-CZ-NH1	-5.99	117.30	120.30
1	A	339	VAL	CG1-CB-CG2	5.99	120.48	110.90
1	A	367	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	146	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	266	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	236	ASP	CB-CG-OD2	-5.20	113.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	267	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	141	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	B	266	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	272	LEU	CB-CG-CD1	5.08	119.63	111.00
1	C	367	ARG	NE-CZ-NH1	5.05	122.82	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	2864	0	2885	49	0
1	B	2869	0	2908	42	0
1	C	2828	0	2833	42	0
1	D	2821	0	2827	55	0
2	A	48	0	32	4	0
2	B	48	0	32	5	0
3	A	6	0	8	0	0
4	A	10	0	0	1	0
4	B	10	0	0	0	0
5	A	401	0	0	8	1
5	B	392	0	0	6	0
5	C	191	0	0	3	0
5	D	155	0	0	8	0
All	All	12643	0	11525	181	1

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 8.

All (181) 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:134:MET:HE2	1:C:144:ILE:HD11	1.46	0.97
1:B:191:LYS:HB3	1:B:191:LYS:NZ	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:HB3	1:B:191:LYS:HZ2	1.34	0.87
1:D:144:ILE:CD1	1:D:148:LEU:HD12	2.10	0.82
1:A:230:LYS:HE3	5:A:2276:HOH:O	1.80	0.81
1:D:191:LYS:NZ	1:D:191:LYS:HB3	1.98	0.79
1:A:175:GLN:HE22	1:A:240:THR:CG2	1.96	0.78
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.66	0.78
1:D:207:ARG:HH11	1:D:207:ARG:HG2	1.47	0.76
1:D:57:VAL:HG21	1:D:350:ILE:CG2	2.16	0.74
1:B:298:LYS:HE2	1:B:301:GLU:OE1	1.90	0.72
1:B:237:LYS:HD2	1:B:237:LYS:N	2.05	0.71
1:B:29:GLU:OE1	5:B:2042:HOH:O	2.09	0.70
1:B:134:MET:CE	1:C:144:ILE:HD11	2.22	0.69
1:B:175:GLN:HE22	1:B:240[A]:THR:CG2	2.06	0.69
1:D:98:LEU:HB3	5:D:2062:HOH:O	1.93	0.68
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.57	0.68
1:A:207:ARG:HH11	1:A:207:ARG:HG2	1.59	0.68
1:C:144:ILE:HD13	1:C:148:LEU:HD12	1.76	0.68
1:D:257:LEU:C	1:D:257:LEU:HD23	2.14	0.67
1:D:339:VAL:HG11	1:D:368:ARG:NH2	2.09	0.67
1:C:268:GLY:HA2	5:C:2139:HOH:O	1.97	0.64
1:D:237:LYS:N	1:D:237:LYS:HD2	2.12	0.64
1:D:191:LYS:NZ	1:D:191:LYS:CB	2.61	0.64
1:C:191:LYS:HB3	1:C:191:LYS:NZ	2.11	0.64
1:C:5:ILE:HD12	1:C:103:ILE:HG21	1.80	0.63
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.33	0.63
1:D:144:ILE:HD12	1:D:148:LEU:HD12	1.79	0.63
1:B:191:LYS:NZ	1:B:191:LYS:CB	2.58	0.62
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.34	0.62
1:C:34:VAL:HB	5:C:2013:HOH:O	1.98	0.62
1:B:144:ILE:HD13	1:B:148:LEU:HD12	1.79	0.62
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.35	0.61
1:C:258:LEU:HD22	1:C:258:LEU:N	2.15	0.61
1:A:144:ILE:HD13	1:A:148:LEU:HD12	1.83	0.61
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.65	0.60
1:A:144:ILE:CD1	1:A:148:LEU:HD12	2.31	0.60
1:B:175:GLN:HE22	1:B:240[A]:THR:HG21	1.65	0.60
1:C:28:HIS:ND1	1:C:62:GLU:OE2	2.26	0.60
1:C:237:LYS:N	1:C:237:LYS:HD2	2.16	0.60
1:D:144:ILE:HD13	1:D:148:LEU:HD12	1.82	0.59
1:A:157:MET:HG3	2:A:1393:COA:S1P	2.41	0.59
1:D:300:LEU:HD13	1:D:307:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.67	0.59
1:D:276:VAL:HG22	1:D:388:CYS:O	2.05	0.57
1:B:112:VAL:HG22	1:B:257[B]:LEU:HD13	1.85	0.57
1:A:209:GLY:HA2	5:A:2249:HOH:O	2.03	0.57
1:B:197:ASP:OD1	5:B:2225:HOH:O	2.17	0.57
1:A:78:GLN:NE2	5:A:2116:HOH:O	2.35	0.57
1:D:191:LYS:HB3	1:D:191:LYS:HZ3	1.70	0.56
1:A:34[A]:VAL:HG12	1:A:255:ALA:HB3	1.86	0.56
1:A:191:LYS:HZ3	1:A:191:LYS:CB	2.18	0.56
1:A:276[A]:VAL:HG23	1:A:388:CYS:HB2	1.88	0.56
1:A:191:LYS:HG3	5:A:2221:HOH:O	2.06	0.56
1:D:191:LYS:HZ2	1:D:191:LYS:CB	2.19	0.56
1:C:257:LEU:CD2	1:C:259:MET:HE2	2.36	0.55
1:A:297[B]:ARG:NH2	1:A:329:ASP:OD1	2.39	0.55
1:D:83:TRP:HZ2	5:D:2062:HOH:O	1.88	0.55
1:C:348:HIS:ND1	1:C:353:SER:OG	2.36	0.55
1:B:168:TRP:HH2	1:B:329:ASP:HB2	1.69	0.55
1:B:34[A]:VAL:HG12	1:B:255:ALA:HB3	1.89	0.54
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.71	0.54
1:D:8:ALA:HB3	1:D:257:LEU:HD22	1.91	0.53
1:C:58:LEU:O	5:C:2033:HOH:O	2.18	0.53
1:D:263:GLU:HA	1:D:266:ARG:NH1	2.24	0.53
1:B:206:GLY:C	1:B:207:ARG:HG2	2.28	0.53
1:D:257:LEU:HD23	1:D:258:LEU:N	2.23	0.53
1:B:134:MET:HE3	1:C:249:LEU:HD11	1.89	0.53
1:C:5:ILE:HD12	1:C:103:ILE:CG2	2.37	0.53
1:A:371:ARG:CZ	5:A:2387:HOH:O	2.57	0.53
1:A:2:THR:N	1:A:3:PRO:HD2	2.24	0.53
1:D:57:VAL:CG2	1:D:350:ILE:HG22	2.39	0.52
1:B:131:GLY:HA2	1:D:131:GLY:HA2	1.92	0.52
1:D:298:LYS:HE2	1:D:301:GLU:OE1	2.10	0.52
1:A:191:LYS:NZ	1:A:191:LYS:CB	2.72	0.52
1:A:237:LYS:H	1:A:237:LYS:HD2	1.75	0.51
1:D:257:LEU:C	1:D:257:LEU:CD2	2.79	0.51
1:B:227:SER:HB2	2:B:1393:COA:H2A	1.92	0.51
1:A:191:LYS:HZ3	1:A:191:LYS:HB2	1.76	0.51
1:C:34:VAL:HG12	1:C:255:ALA:HB3	1.92	0.51
1:D:191:LYS:HZ2	1:D:191:LYS:HB3	1.72	0.51
1:B:207:ARG:NH1	5:B:2234:HOH:O	2.43	0.51
1:B:297:ARG:NE	5:B:2318:HOH:O	2.44	0.51
1:B:330:LEU:HD12	1:B:332:TRP:CZ2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:LEU:HD12	1:C:332:TRP:CZ2	2.46	0.50
1:C:175:GLN:HE22	1:C:240:THR:CG2	2.25	0.50
1:A:191:LYS:NZ	1:A:191:LYS:HB2	2.27	0.49
1:B:110:ILE:CG2	1:B:257[B]:LEU:HD11	2.42	0.49
1:D:271:PRO:HD2	1:D:392:LEU:HD12	1.94	0.49
1:D:34:VAL:HG13	1:D:255:ALA:HB3	1.95	0.48
1:D:175:GLN:NE2	1:D:240:THR:OG1	2.45	0.48
1:C:5:ILE:CD1	1:C:103:ILE:CG2	2.92	0.48
1:D:79:GLU:HB2	5:D:2056:HOH:O	2.13	0.48
1:D:57:VAL:HG21	1:D:350:ILE:HG21	1.92	0.48
1:A:298:LYS:HD2	4:A:1395:SO4:O3	2.13	0.48
1:A:176:ASP:O	1:A:180:VAL:HG23	2.14	0.47
1:C:5:ILE:HD11	1:C:103:ILE:HG22	1.97	0.47
1:B:5:ILE:N	1:B:5:ILE:HD12	2.29	0.47
1:D:258:LEU:N	1:D:258:LEU:HD22	2.29	0.47
1:A:298:LYS:HE2	1:A:301:GLU:OE1	2.15	0.47
1:A:330:LEU:HD13	1:A:332:TRP:CH2	2.50	0.47
1:C:258:LEU:CD2	1:C:258:LEU:N	2.78	0.47
1:A:374:LEU:C	1:A:374:LEU:HD23	2.36	0.47
1:C:170:LEU:HD13	1:C:324:CYS:HB2	1.97	0.47
1:B:34[A]:VAL:CG1	1:B:255:ALA:HB3	2.45	0.47
1:B:131:GLY:HA2	1:D:131:GLY:CA	2.45	0.47
1:D:284:ASP:HB3	1:D:287:VAL:HG22	1.97	0.47
1:C:271:PRO:HD2	1:C:392:LEU:HD12	1.97	0.46
1:A:88:LEU:HD12	1:A:380:GLY:O	2.16	0.46
1:A:108:ALA:CB	1:A:111:ILE:HD11	2.46	0.46
1:B:112:VAL:CG2	1:B:257[B]:LEU:HD13	2.46	0.46
1:D:168:TRP:CH2	1:D:329:ASP:HB2	2.50	0.45
1:C:348:HIS:CE1	1:C:353:SER:HG	2.33	0.45
1:A:316:ASN:HB3	5:A:2353:HOH:O	2.16	0.45
1:D:203:ILE:HD13	1:D:212:THR:OG1	2.16	0.45
1:A:276[A]:VAL:CG2	1:A:388:CYS:HB2	2.46	0.45
1:D:35:ILE:O	1:D:38:VAL:HG22	2.17	0.45
1:C:293:ILE:O	1:C:297:ARG:HG3	2.17	0.45
1:A:78:GLN:O	1:B:282:GLY:HA3	2.17	0.45
1:A:276[A]:VAL:HG22	1:A:388:CYS:O	2.16	0.45
1:C:263:GLU:HA	1:C:266:ARG:HH11	1.82	0.45
1:D:207:ARG:HH11	1:D:207:ARG:CG	2.24	0.45
1:A:282:GLY:HA3	1:B:78:GLN:O	2.17	0.45
1:C:257:LEU:C	1:C:258:LEU:HD22	2.37	0.44
1:A:7:ILE:HG23	1:A:256:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:GLY:HA2	1:A:377:LEU:HD11	1.99	0.44
1:B:316:ASN:HB3	5:B:2339:HOH:O	2.16	0.44
1:D:237:LYS:HD2	1:D:237:LYS:H	1.82	0.44
1:D:226:ASP:O	1:D:230:LYS:HG3	2.17	0.44
1:B:88:LEU:HD12	1:B:380:GLY:O	2.17	0.44
1:A:2:THR:N	1:A:3:PRO:CD	2.80	0.44
1:D:312:LEU:HD13	1:D:368:ARG:HD2	1.98	0.44
1:B:131:GLY:CA	1:D:131:GLY:CA	2.95	0.44
1:C:233:PRO:HB2	1:C:236:ASP:O	2.17	0.44
1:C:203:ILE:HD13	1:C:212:THR:OG1	2.18	0.43
1:D:10:ALA:HB3	1:D:363:PHE:HE1	1.82	0.43
1:D:233:PRO:HG3	5:D:2121:HOH:O	2.17	0.43
1:A:227:SER:HB2	2:A:1393:COA:H2A	2.01	0.43
1:B:39:LEU:HD23	1:B:257[B]:LEU:CD2	2.49	0.43
1:D:161:ALA:N	5:D:2084:HOH:O	2.52	0.43
1:A:237:LYS:N	1:A:237:LYS:HD2	2.34	0.43
2:B:1393:COA:CDP	5:B:2272:HOH:O	2.66	0.43
1:C:271:PRO:HG2	1:C:392:LEU:CD1	2.49	0.43
1:A:12:ARG:HD2	1:A:356:ARG:HG2	2.01	0.43
1:C:263:GLU:OE1	1:C:266:ARG:NH1	2.52	0.43
1:C:364:GLU:O	1:C:368:ARG:HG2	2.18	0.43
1:B:110:ILE:HG23	1:B:257[B]:LEU:HD11	2.01	0.42
1:B:220:ARG:NH1	2:B:1393:COA:C6A	2.82	0.42
1:C:180:VAL:HG21	1:C:225:LEU:HA	2.02	0.42
1:B:176:ASP:O	1:B:180:VAL:HG23	2.19	0.42
1:D:226:ASP:HB2	5:D:2119:HOH:O	2.18	0.42
1:B:220:ARG:NH1	2:B:1393:COA:N1A	2.68	0.42
1:B:236:ASP:O	1:B:239:GLY:N	2.52	0.42
1:D:42:ALA:CB	1:D:257:LEU:HD13	2.50	0.42
1:C:64:GLN:O	1:C:65:ASN:C	2.59	0.41
1:D:170:LEU:HD22	1:D:174:GLU:OE2	2.21	0.41
1:D:88:LEU:HB2	1:D:379:ILE:HG23	2.02	0.41
1:A:227:SER:CB	2:A:1393:COA:H2A	2.49	0.41
1:C:51:GLU:HB3	1:C:111:ILE:CD1	2.50	0.41
1:A:270:GLN:HG2	5:A:2307:HOH:O	2.20	0.41
1:D:124:HIS:HA	1:D:140:ILE:O	2.20	0.41
1:A:371:ARG:HG2	5:A:2392:HOH:O	2.18	0.41
1:C:88:LEU:HD11	1:D:64:GLN:HB3	2.02	0.41
1:C:128:LEU:HD21	1:C:137:PHE:CZ	2.56	0.41
1:A:183:GLN:HA	1:A:345:ALA:HB2	2.02	0.41
1:D:339:VAL:HG12	1:D:339:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:GLY:N	1:D:292:PRO:CD	2.84	0.41
1:B:247[B]:SER:OG	1:B:348:HIS:HB2	2.21	0.41
1:D:55:GLY:HA2	1:D:85:MET:O	2.21	0.41
1:D:83:TRP:CZ2	5:D:2062:HOH:O	2.57	0.40
1:C:54:LEU:O	1:C:84:GLY:HA2	2.20	0.40
1:C:198:GLU:HB3	1:C:363:PHE:CD2	2.56	0.40
1:A:291:GLY:N	1:A:292:PRO:CD	2.84	0.40
1:B:175:GLN:HE22	1:B:240[A]:THR:HG23	1.84	0.40
1:C:88:LEU:HD12	1:C:380:GLY:O	2.22	0.40
1:D:211:ILE:HD12	5:D:2105:HOH:O	2.21	0.40
1:A:243:ALA:CB	2:A:1393:COA:H51A	2.52	0.40
2:B:1393:COA:H131	2:B:1393:COA:O9P	2.22	0.40
1:A:379:ILE:HB	1:A:383:MET:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2110:HOH:O	5:A:2385:HOH:O[2_655]	2.13	0.07

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	395/392 (101%)	382 (97%)	12 (3%)	1 (0%)	46	33
1	B	398/392 (102%)	388 (98%)	9 (2%)	1 (0%)	46	33
1	C	388/392 (99%)	373 (96%)	13 (3%)	2 (0%)	34	20
1	D	387/392 (99%)	377 (97%)	9 (2%)	1 (0%)	46	33
All	All	1568/1568 (100%)	1520 (97%)	43 (3%)	5 (0%)	46	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	350	ILE
1	C	350	ILE
1	C	4	SER
1	A	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	284/278 (102%)	268 (94%)	16 (6%)	26 12
1	B	287/278 (103%)	274 (96%)	13 (4%)	34 19
1	C	277/278 (100%)	260 (94%)	17 (6%)	23 10
1	D	276/278 (99%)	259 (94%)	17 (6%)	23 9
All	All	1124/1112 (101%)	1061 (94%)	63 (6%)	25 12

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	134	MET
1	A	155	TYR
1	A	167	GLN
1	A	191	LYS
1	A	207	ARG
1	A	220	ARG
1	A	237	LYS
1	A	238	GLU
1	A	270	GLN
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	332	TRP
1	A	339	VAL
1	A	392	LEU
1	B	155	TYR

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Mol	Chain	Res	Type
1	B	167	GLN
1	B	191	LYS
1	B	207	ARG
1	B	237	LYS
1	B	238	GLU
1	B	270	GLN
1	B	272	LEU
1	B	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
1	B	392	LEU
1	C	2	THR
1	C	39	LEU
1	C	109	SER
1	C	155	TYR
1	C	207	ARG
1	C	220	ARG
1	C	237	LYS
1	C	238	GLU
1	C	258	LEU
1	C	263	GLU
1	C	270	GLN
1	C	272	LEU
1	C	288	MET
1	C	298	LYS
1	C	322	GLN
1	C	332	TRP
1	C	358	LEU
1	D	34	VAL
1	D	39	LEU
1	D	134	MET
1	D	155	TYR
1	D	207	ARG
1	D	220	ARG
1	D	237	LYS
1	D	238	GLU
1	D	258	LEU
1	D	270	GLN
1	D	288	MET
1	D	298	LYS
1	D	307	ILE

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Mol	Chain	Res	Type
1	D	322	GLN
1	D	332	TRP
1	D	353	SER
1	D	358	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	C	78	GLN
1	C	175	GLN
1	C	184	ASN
1	D	78	GLN
1	D	175	GLN
1	D	184	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSO	A	89	1	3,6,7	0.55	0	1,6,8	2.82	1 (100%)
1	CSO	B	89	1	3,6,7	0.95	0	1,6,8	1.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CSO	C	89	1	3,6,7	0.62	0	1,6,8	1.80	0
1	CSO	D	89	1	3,6,7	0.37	0	1,6,8	2.31	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	A	89	1	-	0/1/5/7	0/0/0/0
1	CSO	B	89	1	-	0/1/5/7	0/0/0/0
1	CSO	C	89	1	-	0/1/5/7	0/0/0/0
1	CSO	D	89	1	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	89	CSO	O-C-CA	-2.82	118.14	125.49
1	D	89	CSO	O-C-CA	-2.31	119.47	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	COA	A	1393	-	40,50,50	1.83	3 (7%)	50,75,75	1.92	8 (16%)
3	GOL	A	1394	-	5,5,5	0.70	0	5,5,5	0.57	0
4	SO4	A	1395	-	4,4,4	0.13	0	6,6,6	0.58	0
4	SO4	A	1396	-	4,4,4	0.54	0	6,6,6	0.18	0
2	COA	B	1393	-	40,50,50	1.81	3 (7%)	50,75,75	2.47	8 (16%)
4	SO4	B	1394	-	4,4,4	0.55	0	6,6,6	0.41	0
4	SO4	B	1395	-	4,4,4	0.18	0	6,6,6	0.14	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
2	COA	A	1393	-	-	0/44/64/64	0/3/3/3
3	GOL	A	1394	-	-	0/4/4/4	0/0/0/0
4	SO4	A	1395	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1396	-	-	0/0/0/0	0/0/0/0
2	COA	B	1393	-	-	0/44/64/64	0/3/3/3
4	SO4	B	1394	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1395	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1393	COA	C2A-N1A	2.55	1.38	1.33
2	A	1393	COA	C2A-N1A	2.91	1.39	1.33
2	B	1393	COA	C2A-N3A	3.07	1.37	1.32
2	A	1393	COA	C2A-N3A	3.31	1.38	1.32
2	A	1393	COA	O9P-C9P	9.80	1.42	1.23
2	B	1393	COA	O9P-C9P	10.06	1.43	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1393	COA	N3A-C2A-N1A	-13.28	118.72	128.89
2	A	1393	COA	N3A-C2A-N1A	-10.92	120.53	128.89
2	B	1393	COA	C1B-N9A-C4A	-5.53	118.60	126.94
2	B	1393	COA	C4B-O4B-C1B	-4.27	105.03	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1393	COA	P2A-O3A-P1A	-3.80	122.06	132.73
2	B	1393	COA	C6P-C7P-N8P	-3.72	103.72	111.88
2	A	1393	COA	C1B-N9A-C4A	-3.19	122.12	126.94
2	B	1393	COA	P2A-O3A-P1A	-2.91	124.55	132.73
2	A	1393	COA	C4A-C5A-N7A	-2.45	107.22	109.48
2	B	1393	COA	CAP-C9P-N8P	-2.28	111.42	116.47
2	A	1393	COA	C2P-C3P-N4P	-2.10	108.23	112.37
2	A	1393	COA	C6P-C5P-N4P	-2.00	112.98	116.46
2	A	1393	COA	O3A-P2A-O6A	2.05	108.38	102.94
2	A	1393	COA	C7P-C6P-C5P	2.09	115.75	112.31
2	B	1393	COA	O9P-C9P-N8P	2.30	127.70	123.08
2	B	1393	COA	O4B-C1B-N9A	2.68	113.70	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1393	COA	4	0
4	A	1395	SO4	1	0
2	B	1393	COA	5	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	9 (2%) 64 66	2, 6, 17, 37	0
1	B	390/392 (99%)	0.09	5 (1%) 79 81	2, 6, 16, 36	0
1	C	390/392 (99%)	0.56	16 (4%) 41 43	2, 8, 17, 33	0
1	D	389/392 (99%)	1.00	53 (13%) 4 4	2, 8, 17, 34	0
All	All	1559/1568 (99%)	0.46	83 (5%) 30 32	2, 7, 17, 37	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	229	ALA	8.5
1	D	206	GLY	6.5
1	D	232	ARG	6.5
1	C	208	LYS	6.0
1	D	224	THR	5.6
1	D	231	LEU	5.2
1	A	208	LYS	4.9
1	D	173	ASP	4.7
1	C	206	GLY	4.4
1	A	209	GLY	4.3
1	D	207	ARG	4.0
1	C	2	THR	4.0
1	D	328	LYS	4.0
1	B	207	ARG	4.0
1	D	170	LEU	4.0
1	D	228	MET	3.9
1	D	325	ALA	3.8
1	D	331	GLY	3.8
1	A	206	GLY	3.8
1	C	207	ARG	3.8
1	A	132	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	208	LYS	3.6
1	D	306	LYS	3.6
1	C	232	ARG	3.6
1	B	208	LYS	3.5
1	A	133	LYS	3.5
1	D	238	GLU	3.5
1	A	134	MET	3.5
1	C	371	ARG	3.4
1	D	332	TRP	3.4
1	A	207	ARG	3.3
1	D	382	GLY	3.3
1	D	221	HIS	3.3
1	A	2	THR	3.2
1	D	392	LEU	3.2
1	D	180	VAL	3.1
1	D	371	ARG	3.1
1	D	227	SER	3.0
1	D	219	ILE	3.0
1	D	191	LYS	2.9
1	D	241	VAL	2.9
1	D	329	ASP	2.8
1	C	131	GLY	2.8
1	D	389	ILE	2.8
1	D	240	THR	2.8
1	D	169	GLN	2.8
1	D	153	TYR	2.8
1	D	152	PHE	2.7
1	D	223	ALA	2.7
1	C	225	LEU	2.7
1	D	225	LEU	2.7
1	D	226	ASP	2.7
1	D	167	GLN	2.6
1	D	220	ARG	2.6
1	D	310	LEU	2.6
1	C	46	ALA	2.5
1	C	67	ALA	2.5
1	D	179	ALA	2.5
1	D	287	VAL	2.5
1	D	237	LYS	2.5
1	C	153	TYR	2.5
1	D	281	VAL	2.5
1	B	2	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	232	ARG	2.4
1	D	205	LYS	2.4
1	B	232	ARG	2.2
1	C	209	GLY	2.2
1	D	326	VAL	2.2
1	D	235	PHE	2.2
1	D	236	ASP	2.2
1	C	180	VAL	2.1
1	D	350	ILE	2.1
1	D	233	PRO	2.1
1	C	237	LYS	2.1
1	D	367	ARG	2.1
1	C	132	VAL	2.1
1	C	3	PRO	2.1
1	D	178	PHE	2.1
1	D	269	ILE	2.0
1	D	155	TYR	2.0
1	D	171	SER	2.0
1	D	188	ALA	2.0
1	B	206	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
1	CSO	C	89	7/8	0.91	0.08	-	10,11,18,19	0
1	CSO	D	89	7/8	0.86	0.11	-	5,9,12,14	0
1	CSO	A	89	7/8	0.97	0.09	-	7,8,10,18	0
1	CSO	B	89	7/8	0.96	0.10	-	4,6,7,21	0

6.3 Carbohydrates (i)

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, 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
2	COA	B	1393	48/48	0.61	0.25	6.61	28,53,69,71	0
4	SO4	A	1395	5/5	0.90	0.29	4.39	42,44,45,45	0
4	SO4	B	1394	5/5	0.97	0.13	1.79	19,22,25,27	0
2	COA	A	1393	48/48	0.59	0.26	1.54	27,50,60,62	0
4	SO4	B	1395	5/5	0.89	0.19	-	42,43,44,45	0
4	SO4	A	1396	5/5	0.96	0.14	-	27,28,30,30	0
3	GOL	A	1394	6/6	0.85	0.23	-	10,17,20,20	0

6.5 Other polymers

There are no such residues in this entry.