WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:04 AM GMT

PDB ID : 2VU1
Title : BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. COMPLEX OF WITH O-PANTHETEINE-11-PIVALATE.
Authors : Kursula, P.; Schmitz, W.; Wierenga, R.K.
Deposited on : 2008-05-19
Resolution : 1.51 Å(reported)

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 1.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.255
Clashscore		9
Ramachandran outliers		0.3%
Sidechain outliers		3.4%
RSRZ outliers		9.9%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
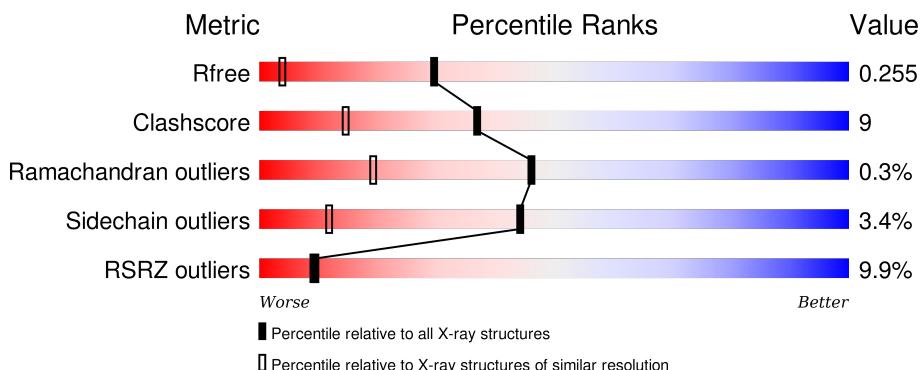
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2658 (1.54-1.50)
Clashscore	102246	2887 (1.54-1.50)
Ramachandran outliers	100387	2818 (1.54-1.50)
Sidechain outliers	100360	2816 (1.54-1.50)
RSRZ outliers	91569	2660 (1.54-1.50)

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% / 84% / 15% / •
1	B	392	2% / 87% / 13% / •
1	C	392	8% / 81% / 18%
1	D	392	28% / 72% / 26% / ••
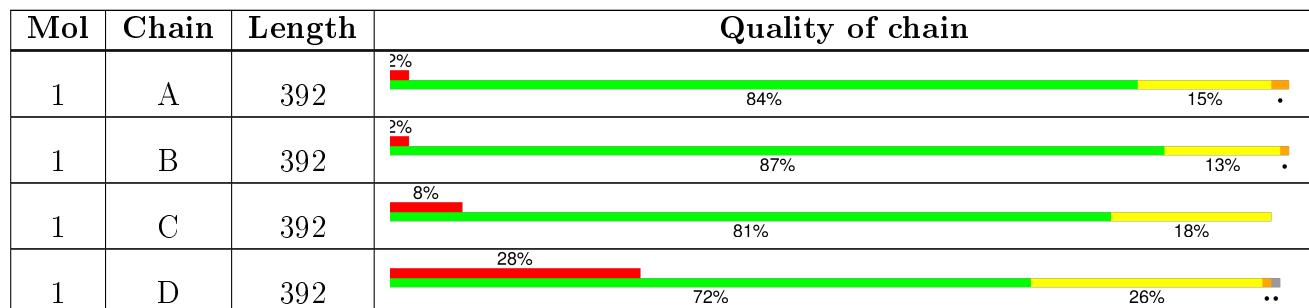
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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	OPI	A	1393	-	-	-	X
2	OPI	B	1393	-	-	-	X
4	SO4	A	1396	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12631 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 2909	C 1819	N 520	O 547	S 23	0	16	0
1	B	392	Total 2903	C 1811	N 521	O 549	S 22	0	13	0
1	C	391	Total 2828	C 1755	N 511	O 541	S 21	0	0	0
1	D	390	Total 2821	C 1751	N 510	O 539	S 21	0	0	0

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
D	11	ALA	-	INSERTION	UNP P07097
D	129	ARG	ALA	CONFLICT	UNP P07097

- Molecule 2 is PANTOTHENYL-AMINOETHANOL-11-PIVALIC ACID (three-letter code: OPI) (formula: $C_{16}H_{30}N_2O_6$).
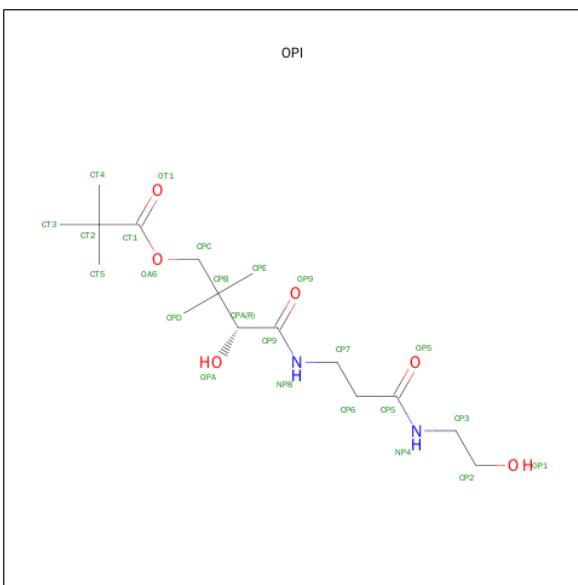
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	16	2	6		
2	B	1	Total	C	N	O	0	0
			24	16	2	6		

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
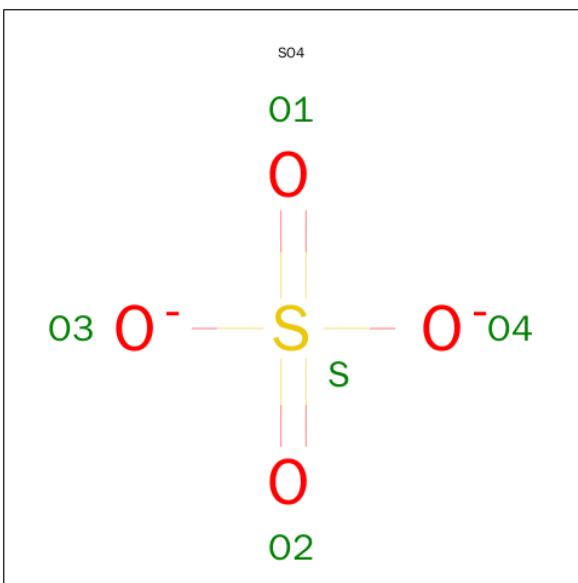
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total O S 5 4 1			0	0
4	A	1	Total O S 5 4 1			0	0
4	B	1	Total O S 5 4 1			0	0
4	B	1	Total O S 5 4 1			0	0
4	D	1	Total O S 5 4 1			0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	408	Total O 408 408		0	0
5	B	398	Total O 398 398		1	0
5	C	144	Total O 144 144		0	0
5	D	146	Total O 146 146		0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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
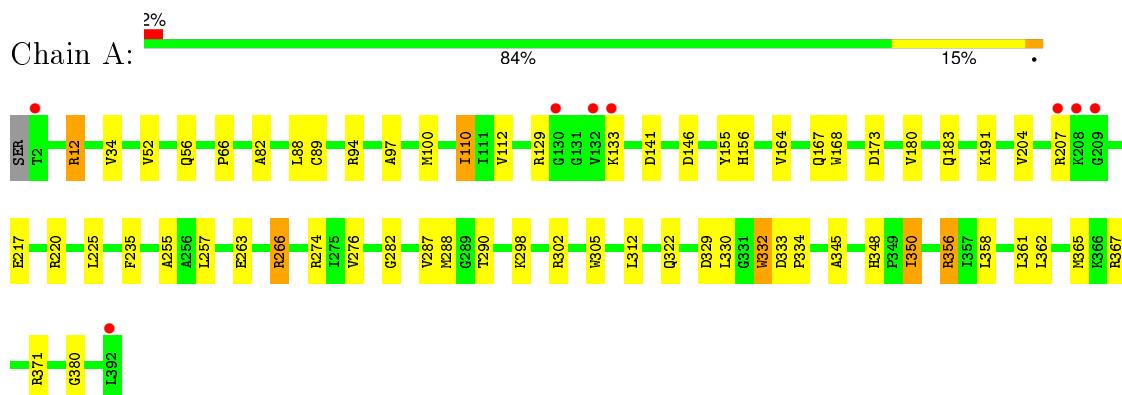
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE
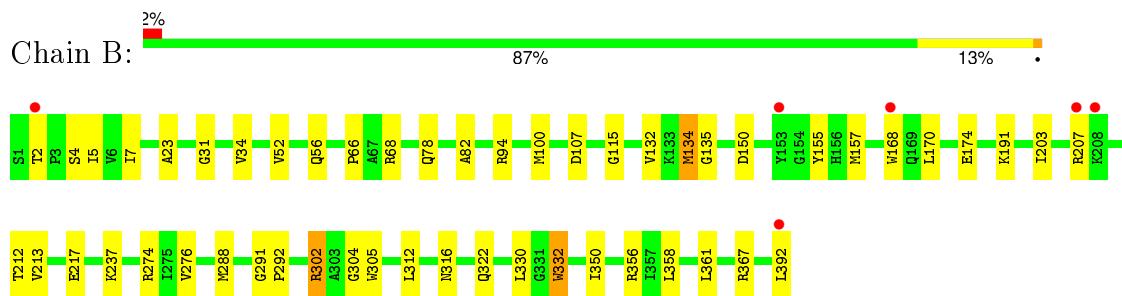
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE
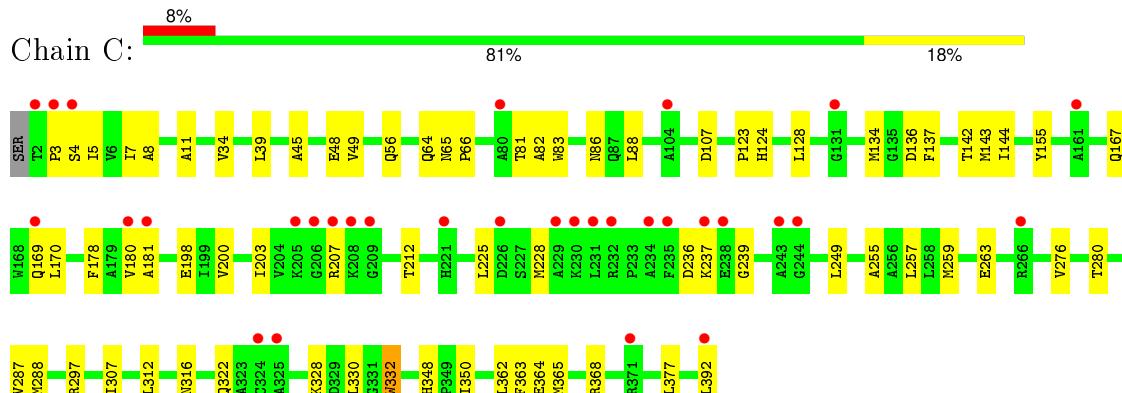
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE
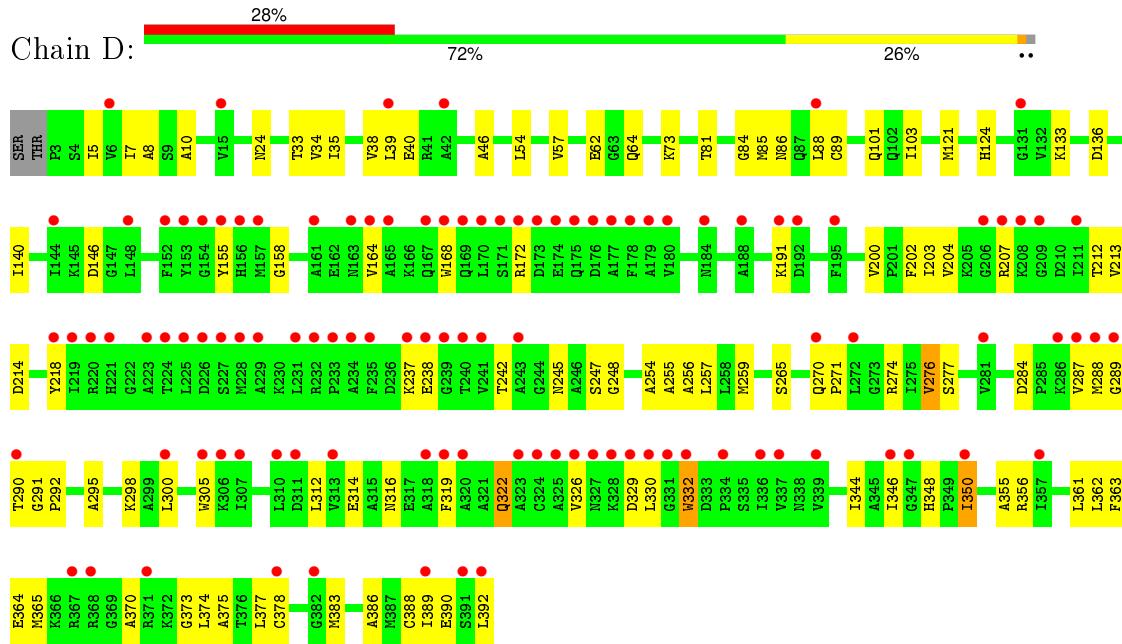
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.30Å 78.74Å 148.34Å 90.00° 92.93° 90.00°	Depositor
Resolution (Å)	20.00 – 1.51 19.98 – 1.51	Depositor EDS
% Data completeness (in resolution range)	92.5 (20.00-1.51) 79.9 (19.98-1.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.3.0028	Depositor
R, R_{free}	0.215 , 0.247 0.225 , 0.255	Depositor DCC
R_{free} test set	2810 reflections (1.01%)	DCC
Wilson B-factor (Å^2)	13.1	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.1	EDS
Estimated twinning fraction	0.136 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.37, < L^2 > = 0.20$	Xtriage
Outliers	0 of 280845 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12631	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CSO, SO4, OPI

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	1.11	3/2986 (0.1%)	1.06	11/4031 (0.3%)
1	B	1.07	7/2976 (0.2%)	1.01	8/4015 (0.2%)
1	C	0.63	0/2862	0.72	1/3864 (0.0%)
1	D	0.57	0/2855	0.69	1/3853 (0.0%)
All	All	0.88	10/11679 (0.1%)	0.89	21/15763 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	115	GLY	N-CA	-6.20	1.36	1.46
1	B	168	TRP	CB-CG	5.85	1.60	1.50
1	A	217	GLU	CB-CG	-5.76	1.41	1.52
1	B	23	ALA	CA-CB	-5.61	1.40	1.52
1	A	362	LEU	C-O	-5.55	1.12	1.23
1	B	217	GLU	CB-CG	-5.43	1.41	1.52
1	B	7	ILE	CA-CB	-5.31	1.42	1.54
1	B	213	VAL	CB-CG2	5.05	1.63	1.52
1	A	110	ILE	C-O	5.03	1.32	1.23
1	B	304	GLY	C-O	-5.02	1.15	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	A	146	ASP	CB-CG-OD1	8.58	126.02	118.30
1	B	367	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	A	367	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	129	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	B	367	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	358	LEU	CB-CG-CD1	6.18	121.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	367	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	12	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	136	ASP	CB-CG-OD1	5.97	123.68	118.30
1	A	141	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	356	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	266[A]	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	266[B]	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	302[A]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	302[B]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	358	LEU	CB-CG-CD1	5.40	120.17	111.00
1	B	68	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	C	136	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	94	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	356	ARG	NE-CZ-NH2	-5.02	117.79	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	2909	0	2972	44	0
1	B	2903	0	2956	39	0
1	C	2828	0	2833	53	0
1	D	2821	0	2827	87	0
2	A	24	0	30	4	0
2	B	24	0	30	3	0
3	A	1	0	0	0	0
4	A	10	0	0	2	0
4	B	10	0	0	0	0
4	D	5	0	0	0	0
5	A	408	0	0	8	2
5	B	398	0	0	9	2
5	C	144	0	0	11	0
5	D	146	0	0	22	0
All	All	12631	0	11648	218	4

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 9.

All (218) 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:274[A]:ARG:NH1	1:B:276[A]:VAL:HG12	1.45	1.28
1:D:164:VAL:HG21	5:D:2122:HOH:O	1.47	1.11
1:A:164:VAL:HG22	1:A:287[B]:VAL:HG23	1.38	1.06
1:D:88:LEU:CD2	5:D:2059:HOH:O	2.09	1.00
1:D:146:ASP:O	5:D:2059:HOH:O	1.82	0.95
1:B:174:GLU:OE2	5:B:2203:HOH:O	1.87	0.93
1:D:88:LEU:HD22	5:D:2059:HOH:O	1.74	0.86
1:C:280:THR:HG23	1:D:81:THR:HG21	1.59	0.84
1:A:287[B]:VAL:HG22	1:A:290:THR:HG23	1.60	0.82
1:D:85:MET:HB2	5:D:2035:HOH:O	1.79	0.82
1:C:257:LEU:CD1	1:C:259:MET:HE2	2.10	0.81
1:B:274[A]:ARG:CZ	1:B:276[A]:VAL:HG12	2.10	0.80
1:A:312[A]:LEU:HD23	1:A:361:LEU:HD12	1.65	0.77
1:A:164:VAL:CG2	1:A:287[B]:VAL:HG23	2.15	0.77
1:D:88:LEU:HD21	5:D:2059:HOH:O	1.75	0.76
1:B:2:THR:HG22	5:B:2001:HOH:O	1.85	0.76
1:A:89[B]:CSO:SG	5:A:2134:HOH:O	2.43	0.76
1:A:287[B]:VAL:CG2	1:A:290:THR:HG23	2.15	0.75
1:A:173:ASP:OD2	5:A:2202:HOH:O	2.04	0.75
1:B:274[A]:ARG:NH1	1:B:276[A]:VAL:CG1	2.39	0.74
1:C:7:ILE:HD13	1:C:362:LEU:HD11	1.70	0.73
1:B:274[A]:ARG:HH12	1:B:276[A]:VAL:HG12	1.53	0.70
1:D:8:ALA:HB3	1:D:257:LEU:HD12	1.73	0.70
1:A:274:ARG:CZ	1:A:276[A]:VAL:HG12	2.22	0.69
1:B:191:LYS:HB3	1:B:191:LYS:NZ	2.07	0.69
1:D:204:VAL:HG23	5:D:2092:HOH:O	1.93	0.68
1:D:326:VAL:HG22	5:D:2123:HOH:O	1.92	0.68
1:A:287[B]:VAL:HG22	1:A:290:THR:CG2	2.23	0.68
1:D:326:VAL:CG2	5:D:2123:HOH:O	2.42	0.68
1:D:7:ILE:HG23	1:D:256:ALA:HB1	1.75	0.68
1:D:322:GLN:O	1:D:326:VAL:HG23	1.94	0.66
1:D:34:VAL:HG12	1:D:255:ALA:HB3	1.78	0.66
1:C:257:LEU:HD11	1:C:259:MET:CE	2.26	0.66
1:A:110:ILE:HG23	1:A:257[A]:LEU:HD21	1.78	0.66
1:A:110:ILE:CG2	1:A:257[A]:LEU:HD21	2.26	0.65
1:D:257:LEU:CD1	1:D:259:MET:HE2	2.27	0.64
1:A:287[B]:VAL:CG2	1:A:290:THR:CG2	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.80	0.64
1:C:257:LEU:CD1	1:C:259:MET:CE	2.75	0.63
1:C:257:LEU:HD11	1:C:259:MET:HE2	1.79	0.63
1:B:4:SER:C	1:B:5[B]:ILE:HD13	2.20	0.62
1:A:89[A]:CSO:SG	1:A:348[A]:HIS:NE2	2.72	0.62
1:B:132:VAL:HG13	1:B:132:VAL:O	2.00	0.62
1:D:8:ALA:CB	1:D:257:LEU:HD12	2.29	0.61
1:B:132:VAL:HG13	1:C:124:HIS:CE1	2.35	0.61
1:C:316:ASN:ND2	5:C:2127:HOH:O	2.17	0.60
1:A:191:LYS:HG3	5:A:2215:HOH:O	2.00	0.60
1:D:316:ASN:OD1	5:D:2134:HOH:O	2.16	0.60
1:B:135:GLY:HA2	1:C:144:ILE:HD12	1.85	0.58
1:D:34:VAL:CG1	1:D:255:ALA:HB3	2.33	0.58
1:C:34:VAL:HG12	1:C:255:ALA:HB3	1.85	0.57
1:B:191:LYS:NZ	1:B:191:LYS:CB	2.68	0.57
1:C:200:VAL:HG11	5:C:2003:HOH:O	2.05	0.57
1:D:365:MET:HG2	1:D:370:ALA:HB3	1.86	0.57
1:C:81:THR:HG22	1:D:383:MET:HG2	1.86	0.57
1:D:35:ILE:O	1:D:38:VAL:HG22	2.06	0.56
1:D:57:VAL:HG21	1:D:350:ILE:CG2	2.36	0.56
1:D:330:LEU:HD13	1:D:332:TRP:CH2	2.41	0.55
1:C:307:ILE:HD12	5:C:2122:HOH:O	2.07	0.55
1:B:312[A]:LEU:HD23	1:B:361:LEU:HD12	1.87	0.55
1:D:290:THR:HA	5:D:2123:HOH:O	2.06	0.55
1:B:56:GLN:HE22	1:B:66:PRO:HB2	1.72	0.54
1:C:312:LEU:HD23	1:C:365:MET:HG3	1.88	0.54
1:B:134:MET:HG3	1:C:144:ILE:HD11	1.89	0.54
1:B:330:LEU:HD13	1:B:332:TRP:CH2	2.43	0.54
1:C:82:ALA:HB2	5:C:2038:HOH:O	2.09	0.53
1:D:86:ASN:N	5:D:2035:HOH:O	2.38	0.53
1:C:203:ILE:CD1	1:C:212:THR:OG1	2.56	0.53
1:C:170:LEU:HD21	1:C:328:LYS:HE3	1.89	0.53
1:C:34:VAL:HG22	5:C:2003:HOH:O	2.10	0.52
1:C:200:VAL:CG1	5:C:2003:HOH:O	2.57	0.52
1:D:289:GLY:O	1:D:292:PRO:HD2	2.10	0.52
1:C:64:GLN:HG2	5:D:2059:HOH:O	2.09	0.52
1:D:362:LEU:CD2	1:D:389:ILE:HG21	2.40	0.52
1:C:39:LEU:HD21	1:C:49:VAL:HG23	1.92	0.52
1:B:302[B]:ARG:NH1	5:B:2328:HOH:O	2.43	0.52
1:A:302[B]:ARG:NH1	5:A:2341:HOH:O	2.29	0.51
1:B:203:ILE:HD13	1:B:212:THR:OG1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:GLN:NE2	1:C:287:VAL:HG11	2.26	0.51
1:D:274:ARG:HB2	1:D:392:LEU:HD21	1.93	0.51
1:D:85:MET:CE	5:D:2035:HOH:O	2.59	0.51
1:C:83:TRP:HE3	5:D:2035:HOH:O	1.94	0.51
1:D:295:ALA:O	1:D:386:ALA:HB3	2.11	0.50
1:C:34:VAL:HA	5:C:2003:HOH:O	2.10	0.50
1:D:276:VAL:HG22	1:D:388:CYS:HB2	1.93	0.50
1:D:172:ARG:HB3	5:D:2074:HOH:O	2.10	0.50
1:C:11:ALA:HB1	5:C:2003:HOH:O	2.11	0.50
1:D:5:ILE:HD12	1:D:103:ILE:CG2	2.41	0.50
1:A:89[A]:CSO:SG	1:A:350:ILE:HG23	2.51	0.50
1:D:254:ALA:HB3	1:D:355:ALA:HB3	1.93	0.50
1:D:204:VAL:CG2	5:D:2092:HOH:O	2.56	0.50
1:C:39:LEU:HD21	1:C:49:VAL:CG2	2.42	0.50
1:A:302[A]:ARG:NH1	5:A:2342:HOH:O	0.65	0.50
1:D:374:LEU:HD12	1:D:388:CYS:SG	2.51	0.50
1:D:326:VAL:HG12	1:D:330:LEU:HD12	1.94	0.50
1:D:203:ILE:HD13	1:D:212:THR:OG1	2.12	0.50
1:D:213:VAL:HG23	5:D:2092:HOH:O	2.12	0.49
1:C:170:LEU:CD2	1:C:328:LYS:HE3	2.42	0.49
1:D:242:THR:HG23	1:D:245:ASN:HD21	1.78	0.49
1:A:235:PHE:HE1	2:A:1393:OPI:HT32	1.77	0.49
1:C:169:GLN:NE2	5:C:2069:HOH:O	2.46	0.49
1:B:291:GLY:N	1:B:292:PRO:CD	2.75	0.48
1:B:150:ASP:HB2	5:B:2182:HOH:O	2.12	0.48
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.49	0.48
1:C:8:ALA:HB3	1:C:257:LEU:HD12	1.95	0.48
1:D:276:VAL:HG22	1:D:388:CYS:CB	2.44	0.48
1:C:280:THR:CG2	1:D:81:THR:HG21	2.38	0.48
1:D:326:VAL:CG1	1:D:330:LEU:HD12	2.43	0.48
1:A:330:LEU:HD13	1:A:332:TRP:CH2	2.48	0.48
2:A:1393:OPI:NP8	2:A:1393:OPI:HPC1	2.29	0.48
1:D:287:VAL:HG23	1:D:287:VAL:O	2.14	0.48
1:D:362:LEU:HD23	1:D:389:ILE:HG21	1.95	0.47
1:C:330:LEU:HD12	1:C:332:TRP:CZ2	2.50	0.47
1:B:191:LYS:HZ2	1:B:191:LYS:HB3	1.78	0.47
1:C:316:ASN:HD21	1:C:348:HIS:CE1	2.33	0.47
1:C:11:ALA:CB	5:C:2003:HOH:O	2.62	0.47
1:A:180:VAL:HG21	1:A:225:LEU:HA	1.96	0.47
1:D:312:LEU:O	1:D:373:GLY:HA2	2.14	0.47
1:C:297:ARG:NH1	1:C:307:ILE:HD11	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:MET:HE1	1:C:249:LEU:HD13	1.97	0.47
1:D:39:LEU:HD13	1:D:46:ALA:HA	1.96	0.46
1:A:56:GLN:HE22	1:A:66:PRO:HB2	1.80	0.46
1:D:361:LEU:HD22	1:D:375:ALA:HB2	1.96	0.46
1:D:5:ILE:HD12	1:D:103:ILE:HG22	1.98	0.46
1:D:284:ASP:HB3	1:D:287:VAL:HG22	1.98	0.46
1:D:292:PRO:HD3	1:D:378:CYS:HB3	1.98	0.46
1:D:271:PRO:HD2	1:D:392:LEU:HD12	1.98	0.46
1:A:263:GLU:HA	1:A:266[A]:ARG:CZ	2.46	0.46
1:C:316:ASN:ND2	1:C:377:LEU:HD23	2.30	0.46
2:B:1393:OPI:CT5	2:B:1393:OPI:CPC	2.93	0.46
1:A:112:VAL:HG22	1:A:257[A]:LEU:HD23	1.96	0.46
1:D:54:LEU:O	1:D:84:GLY:HA2	2.16	0.46
1:D:168:TRP:CH2	1:D:329:ASP:HB2	2.50	0.46
1:B:157:MET:CE	5:B:2182:HOH:O	2.63	0.46
1:A:298:LYS:HE3	4:A:1396:SO4:O3	2.16	0.46
1:A:167:GLN:NE2	5:A:2193:HOH:O	2.46	0.45
1:B:174:GLU:OE1	5:B:2200:HOH:O	2.21	0.45
1:D:257:LEU:HD11	1:D:259:MET:HE2	1.96	0.45
1:B:392[B]:LEU:H	1:B:392[B]:LEU:HD23	1.81	0.45
1:C:88:LEU:HD11	1:D:64:GLN:HB3	1.98	0.45
1:D:158:GLY:HA2	1:D:319:PHE:CE2	2.51	0.45
1:A:276[A]:VAL:HG21	1:A:305:TRP:CZ2	2.51	0.45
1:D:271:PRO:HG2	1:D:392:LEU:HD12	1.98	0.45
1:B:203:ILE:CD1	1:B:212:THR:OG1	2.66	0.44
1:A:204:VAL:O	5:A:2245:HOH:O	2.20	0.44
1:C:3:PRO:HB2	1:C:5:ILE:HD11	1.98	0.44
1:B:274[A]:ARG:HD2	5:B:2307:HOH:O	2.18	0.44
1:A:274:ARG:NH1	1:A:276[A]:VAL:HG12	2.32	0.44
1:C:364:GLU:O	1:C:368:ARG:HG3	2.18	0.44
1:D:85:MET:HE2	5:D:2035:HOH:O	2.17	0.43
1:B:52:VAL:O	1:B:82:ALA:HA	2.18	0.43
1:D:257:LEU:HD11	1:D:259:MET:CE	2.49	0.43
1:D:257:LEU:CD1	1:D:259:MET:CE	2.97	0.43
1:B:4:SER:O	1:B:5[B]:ILE:HD13	2.18	0.43
1:D:291:GLY:N	1:D:292:PRO:CD	2.81	0.43
1:A:97:ALA:O	1:A:100[A]:MET:HB3	2.19	0.43
1:C:123:PRO:O	1:C:142:THR:HG23	2.17	0.43
1:D:300:LEU:HD23	1:D:305:TRP:HB2	2.00	0.43
1:D:276:VAL:HG11	1:D:390:GLU:HB2	2.00	0.43
1:C:45:ALA:HB3	1:C:48:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:HE3	5:B:2090:HOH:O	2.18	0.43
2:A:1393:OPI:HT52	2:A:1393:OPI:HPC1	2.01	0.42
1:C:107:ASP:OD2	1:D:101:GLN:NE2	2.48	0.42
1:D:326:VAL:HG11	5:D:2124:HOH:O	2.18	0.42
1:B:316:ASN:HB3	5:B:2346:HOH:O	2.18	0.42
1:C:180:VAL:HG21	1:C:225:LEU:HA	2.01	0.42
1:B:5[B]:ILE:HB	1:B:100[B]:MET:HG3	2.01	0.42
1:C:307:ILE:CD1	5:C:2122:HOH:O	2.66	0.42
1:D:326:VAL:HG23	5:D:2123:HOH:O	2.13	0.42
1:D:191:LYS:CB	1:D:191:LYS:NZ	2.82	0.42
1:C:392:LEU:HD22	1:C:392:LEU:N	2.34	0.42
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.85	0.42
1:C:236:ASP:HB3	1:C:239:GLY:HA3	2.01	0.42
1:D:57:VAL:HG13	1:D:88:LEU:HD23	2.02	0.42
1:D:289:GLY:HA2	1:D:378:CYS:CB	2.50	0.42
1:D:312:LEU:HD21	1:D:364:GLU:HG3	2.01	0.42
1:D:346:ILE:HD13	1:D:356:ARG:NH1	2.33	0.42
1:C:198:GLU:HB3	1:C:363:PHE:CD2	2.54	0.42
1:B:191:LYS:HZ1	1:B:191:LYS:HB3	1.82	0.42
1:D:214:ASP:N	1:D:214:ASP:OD1	2.51	0.42
2:B:1393:OPI:HPC1	2:B:1393:OPI:HT52	2.01	0.42
1:D:218:TYR:CZ	1:D:248:GLY:HA3	2.55	0.42
1:D:24:ASN:HA	1:D:121:MET:SD	2.60	0.41
1:D:89:CSO:O	1:D:377:LEU:HD22	2.20	0.41
1:D:62:GLU:O	1:D:62:GLU:HG2	2.21	0.41
1:D:298:LYS:HE2	5:D:2127:HOH:O	2.20	0.41
1:A:361:LEU:O	1:A:365:MET:HG3	2.21	0.41
2:B:1393:OPI:HPD3	2:B:1393:OPI:HP8	1.85	0.41
1:A:52:VAL:O	1:A:82:ALA:HA	2.20	0.41
1:A:88:LEU:HD12	1:A:380:GLY:O	2.20	0.41
1:A:12:ARG:HD2	1:A:356:ARG:HG2	2.02	0.41
1:B:31:GLY:HA2	1:B:34[B]:VAL:HG22	2.01	0.41
1:A:302[B]:ARG:NH1	1:B:107:ASP:OD1	2.53	0.41
1:A:183:GLN:HA	1:A:345:ALA:HB2	2.03	0.41
1:C:64:GLN:O	1:C:65:ASN:C	2.59	0.41
1:D:200:VAL:HG13	1:D:200:VAL:O	2.20	0.41
1:C:86:ASN:C	1:C:86:ASN:OD1	2.58	0.41
1:B:132:VAL:CG1	1:B:132:VAL:O	2.68	0.41
1:D:124:HIS:HA	1:D:140:ILE:O	2.20	0.41
1:A:156:HIS:CD2	2:A:1393:OPI:HT43	2.56	0.41
1:D:316:ASN:HD21	1:D:348:HIS:CE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:THR:HG1	1:D:202:PHE:HD1	1.69	0.40
1:A:220:ARG:NH2	5:A:2269:HOH:O	2.54	0.40
1:A:34[A]:VAL:HG12	1:A:255:ALA:HB3	2.02	0.40
1:D:7:ILE:HD13	1:D:362:LEU:HD11	2.02	0.40
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.56	0.40
1:C:56:GLN:HE22	1:C:66:PRO:HG2	1.86	0.40
1:D:247:SER:HA	1:D:344:ILE:HA	2.03	0.40
1:B:276[A]:VAL:HG21	1:B:305:TRP:CZ2	2.56	0.40
1:C:178:PHE:O	1:C:181:ALA:HB3	2.21	0.40
1:D:10:ALA:HB3	1:D:363:PHE:HE1	1.84	0.40
1:A:266[A]:ARG:NH2	4:A:1395:SO4:O2	2.55	0.40
1:A:333:ASP:HA	1:A:334:PRO:HD2	1.97	0.40
1:A:282:GLY:HA3	1:B:78:GLN:O	2.21	0.40
1:D:314:GLU:HG3	1:D:361:LEU:HB2	2.04	0.40

All (4) 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:2078:HOH:O	5:A:2211:HOH:O[2_655]	1.77	0.43
5:B:2101:HOH:O	5:B:2375:HOH:O[2_545]	2.03	0.17
5:A:2118:HOH:O	5:A:2392:HOH:O[2_655]	2.11	0.09
5:B:2064:HOH:O	5:B:2222:HOH:O[2_545]	2.14	0.06

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	403/392 (103%)	388 (96%)	14 (4%)	1 (0%)	52	25
1	B	401/392 (102%)	390 (97%)	10 (2%)	1 (0%)	52	25
1	C	388/392 (99%)	375 (97%)	11 (3%)	2 (0%)	34	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	387/392 (99%)	373 (96%)	13 (3%)	1 (0%)	46	19
All	All	1579/1568 (101%)	1526 (97%)	48 (3%)	5 (0%)	46	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	ILE
1	C	350	ILE
1	D	350	ILE
1	A	350	ILE
1	C	4	SER

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	292/278 (105%)	285 (98%)	7 (2%)	57	22
1	B	291/278 (105%)	284 (98%)	7 (2%)	57	22
1	C	277/278 (100%)	267 (96%)	10 (4%)	42	11
1	D	276/278 (99%)	262 (95%)	14 (5%)	29	4
All	All	1136/1112 (102%)	1098 (97%)	38 (3%)	44	12

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	LYS
1	A	155	TYR
1	A	207	ARG
1	A	288	MET
1	A	322	GLN
1	A	332	TRP
1	A	371	ARG
1	B	134	MET
1	B	155	TYR

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Mol	Chain	Res	Type
1	B	207	ARG
1	B	237	LYS
1	B	288	MET
1	B	322	GLN
1	B	332	TRP
1	C	134	MET
1	C	155	TYR
1	C	207	ARG
1	C	228	MET
1	C	237	LYS
1	C	263	GLU
1	C	276	VAL
1	C	288	MET
1	C	322	GLN
1	C	332	TRP
1	D	40	GLU
1	D	73	LYS
1	D	133	LYS
1	D	155	TYR
1	D	207	ARG
1	D	237	LYS
1	D	238	GLU
1	D	265	SER
1	D	270	GLN
1	D	276	VAL
1	D	277	SER
1	D	288	MET
1	D	322	GLN
1	D	332	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	78	GLN
1	A	156	HIS
1	A	184	ASN
1	B	56	GLN
1	C	56	GLN
1	C	78	GLN
1	C	156	HIS
1	C	169	GLN

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Mol	Chain	Res	Type
1	C	316	ASN
1	D	28	HIS
1	D	56	GLN
1	D	78	GLN
1	D	169	GLN
1	D	184	ASN
1	D	245	ASN
1	D	316	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

5 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[A]	-	4,5,7	1.48	1 (25%)	3,5,8	1.89	2 (66%)
1	CSO	A	89[B]	-	3,6,7	1.14	0	1,6,8	1.98	0
1	CSO	B	89	1	3,6,7	0.50	0	1,6,8	2.61	1 (100%)
1	CSO	C	89	1	3,6,7	0.32	0	1,6,8	2.65	1 (100%)
1	CSO	D	89	1	3,6,7	0.46	0	1,6,8	2.24	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[A]	-	-	0/1/4/7	0/0/0/0
1	CSO	A	89[B]	-	-	0/1/5/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89[A]	CSO	CB-CA	2.71	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	89	CSO	O-C-CA	-2.65	118.59	125.49
1	B	89	CSO	O-C-CA	-2.61	118.68	125.49
1	A	89[A]	CSO	O-C-CA	-2.38	119.29	125.49
1	D	89	CSO	O-C-CA	-2.24	119.66	125.49
1	A	89[A]	CSO	CA-CB-SG	-2.11	109.65	114.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	89[A]	CSO	2	0
1	A	89[B]	CSO	1	0
1	D	89	CSO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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	OPI	A	1393	-	20,23,23	1.07	1 (5%)	28,32,32	1.90	7 (25%)
4	SO4	A	1395	-	4,4,4	0.45	0	6,6,6	0.78	0
4	SO4	A	1396	-	4,4,4	0.10	0	6,6,6	0.42	0
2	OPI	B	1393	-	20,23,23	1.14	1 (5%)	28,32,32	1.55	4 (14%)
4	SO4	B	1394	-	4,4,4	0.22	0	6,6,6	0.20	0
4	SO4	B	1395	-	4,4,4	0.31	0	6,6,6	0.73	0
4	SO4	D	1393	-	4,4,4	0.22	0	6,6,6	0.18	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	OPI	A	1393	-	-	0/32/32/32	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	OPI	B	1393	-	-	0/32/32/32	0/0/0/0
4	SO4	B	1394	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1395	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1393	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1393	OPI	OA6-CT1	4.32	1.43	1.33
2	B	1393	OPI	OA6-CT1	4.72	1.44	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1393	OPI	CPC-OA6-CT1	-4.01	111.24	116.97
2	A	1393	OPI	OA6-CT1-OT1	-3.67	116.37	124.44
2	B	1393	OPI	OA6-CT1-OT1	-3.22	117.36	124.44
2	A	1393	OPI	CP6-CP7-NP8	-3.04	105.20	111.88
2	B	1393	OPI	CPC-OA6-CT1	-2.75	113.03	116.97
2	A	1393	OPI	CP2-CP3-NP4	-2.49	106.34	111.91
2	B	1393	OPI	CT5-CT2-CT1	2.09	115.03	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1393	OPI	CPD-CPB-CPC	2.28	111.46	108.50
2	A	1393	OPI	OA6-CPC-CPB	3.01	115.61	108.84
2	A	1393	OPI	OA6-CT1-CT2	5.43	124.03	112.79
2	B	1393	OPI	OA6-CT1-CT2	5.64	124.48	112.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1393	OPI	4	0
4	A	1395	SO4	1	0
4	A	1396	SO4	1	0
2	B	1393	OPI	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	390/392 (99%)	0.08	8 (2%)	67	70	4, 9, 20, 42	0
1	B	391/392 (99%)	-0.01	6 (1%)	76	79	3, 9, 20, 44	0
1	C	390/392 (99%)	0.78	32 (8%)	14	14	4, 11, 19, 40	0
1	D	389/392 (99%)	1.48	108 (27%)	1	1	3, 10, 19, 40	0
All	All	1560/1568 (99%)	0.58	154 (9%)	9	9	3, 10, 20, 44	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	229	ALA	8.3
1	D	232	ARG	7.7
1	D	170	LEU	7.5
1	D	331	GLY	6.3
1	D	319	PHE	6.2
1	D	228	MET	6.1
1	D	219	ILE	6.0
1	D	227	SER	5.7
1	A	132	VAL	5.4
1	D	207	ARG	5.3
1	D	152	PHE	5.3
1	D	178	PHE	5.2
1	D	164	VAL	5.1
1	C	2	THR	5.1
1	D	325	ALA	4.9
1	D	153	TYR	4.8
1	D	328	LYS	4.7
1	D	289	GLY	4.5
1	A	207	ARG	4.5
1	D	224	THR	4.4
1	D	168	TRP	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	208	LYS	4.3
1	D	226	ASP	4.3
1	B	207	ARG	4.2
1	A	2	THR	4.2
1	D	326	VAL	4.2
1	D	310	LEU	4.2
1	C	324	CYS	4.1
1	D	223	ALA	4.0
1	D	339	VAL	4.0
1	D	176	ASP	3.9
1	D	209	GLY	3.9
1	D	240	THR	3.9
1	D	155	TYR	3.8
1	D	329	ASP	3.8
1	C	208	LYS	3.8
1	D	239	GLY	3.8
1	B	392[A]	LEU	3.8
1	C	207	ARG	3.8
1	D	179	ALA	3.8
1	D	225	LEU	3.7
1	C	180	VAL	3.7
1	D	332	TRP	3.7
1	D	235	PHE	3.6
1	D	177	ALA	3.6
1	D	156	HIS	3.5
1	D	367	ARG	3.5
1	D	231	LEU	3.5
1	D	392	LEU	3.5
1	A	130	GLY	3.5
1	D	174	GLU	3.3
1	D	157	MET	3.3
1	D	300	LEU	3.3
1	D	220	ARG	3.3
1	D	238	GLU	3.3
1	C	206	GLY	3.3
1	D	272	LEU	3.3
1	D	330	LEU	3.3
1	D	171	SER	3.3
1	C	237	LYS	3.3
1	D	161	ALA	3.3
1	D	382	GLY	3.2
1	D	218	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	181	ALA	3.2
1	D	165	ALA	3.1
1	D	206	GLY	3.1
1	A	133	LYS	3.1
1	D	371	ARG	3.1
1	D	391	SER	3.0
1	D	324	CYS	3.0
1	C	226	ASP	3.0
1	D	188	ALA	3.0
1	A	208	LYS	2.9
1	D	191	LYS	2.9
1	C	221	HIS	2.9
1	D	241	VAL	2.9
1	D	180	VAL	2.9
1	D	169	GLN	2.8
1	D	313	VAL	2.8
1	C	4	SER	2.8
1	D	233	PRO	2.8
1	D	154	GLY	2.8
1	D	350	ILE	2.7
1	D	237	LYS	2.7
1	D	15	VAL	2.7
1	D	334	PRO	2.7
1	D	195	PHE	2.7
1	C	209	GLY	2.7
1	C	238	GLU	2.6
1	D	167	GLN	2.6
1	D	175	GLN	2.6
1	D	305	TRP	2.6
1	D	173	ASP	2.6
1	D	311	ASP	2.6
1	D	184	ASN	2.6
1	D	287	VAL	2.6
1	C	232	ARG	2.6
1	D	163	ASN	2.5
1	D	307	ILE	2.5
1	C	371	ARG	2.5
1	C	243	ALA	2.5
1	D	42	ALA	2.5
1	D	318	ALA	2.5
1	C	3	PRO	2.5
1	C	104	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	192	ASP	2.5
1	C	161	ALA	2.5
1	D	320	ALA	2.5
1	D	323	ALA	2.5
1	C	235	PHE	2.5
1	D	88	LEU	2.5
1	D	346	ILE	2.5
1	D	6	VAL	2.4
1	D	281	VAL	2.4
1	C	266	ARG	2.4
1	D	336	ILE	2.4
1	D	389	ILE	2.4
1	A	392	LEU	2.4
1	B	2	THR	2.4
1	C	131	GLY	2.4
1	D	378	CYS	2.4
1	D	337	VAL	2.4
1	B	208	LYS	2.4
1	C	230	LYS	2.4
1	D	243	ALA	2.3
1	D	286	LYS	2.3
1	C	234	ALA	2.3
1	D	368	ARG	2.3
1	D	347	GLY	2.3
1	D	327	ASN	2.2
1	D	39	LEU	2.2
1	D	211	ILE	2.2
1	C	80	ALA	2.2
1	A	209	GLY	2.2
1	D	270	GLN	2.2
1	D	172	ARG	2.2
1	B	153	TYR	2.2
1	C	169	GLN	2.2
1	C	231	LEU	2.1
1	D	234	ALA	2.1
1	C	244	GLY	2.1
1	D	306	LYS	2.1
1	D	288	MET	2.1
1	D	148	LEU	2.1
1	C	229	ALA	2.0
1	C	325	ALA	2.0
1	D	144	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	357	ILE	2.0
1	D	221	HIS	2.0
1	B	168	TRP	2.0
1	C	205	LYS	2.0
1	C	392	LEU	2.0
1	D	131	GLY	2.0
1	D	290	THR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
1	CSO	A	89[A]	6/8	0.96	0.09	-	7,9,9,15	3
1	CSO	D	89	7/8	0.87	0.11	-	8,9,11,14	0
1	CSO	B	89	7/8	0.97	0.06	-	7,8,12,20	0
1	CSO	A	89[B]	7/8	0.96	0.09	-	2,7,9,10	4
1	CSO	C	89	7/8	0.94	0.09	-	10,11,14,15	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	OPI	B	1393	24/24	0.48	0.33	11.98	55,63,65,67	0
2	OPI	A	1393	24/24	0.67	0.20	6.49	36,46,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
4	SO4	A	1396	5/5	0.91	0.22	3.28	45,47,47,49	0
3	NA	A	1394	1/1	0.69	0.17	-	57,57,57,57	0
4	SO4	A	1395	5/5	0.97	0.11	-	33,33,36,36	0
4	SO4	B	1395	5/5	0.98	0.10	-	25,25,28,30	0
4	SO4	D	1393	5/5	0.92	0.20	-	63,64,65,65	0
4	SO4	B	1394	5/5	0.92	0.18	-	57,57,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.