



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:04 AM GMT

PDB ID : 2VTZ
Title : BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. COMPLEX OF THE C89A MUTANT WITH COENZYME A.
Authors : Kursula, P.; Merilainen, G.; Wierenga, R.K.
Deposited on : 2008-05-19
Resolution : 2.30 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 ⓘ symbol.

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

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

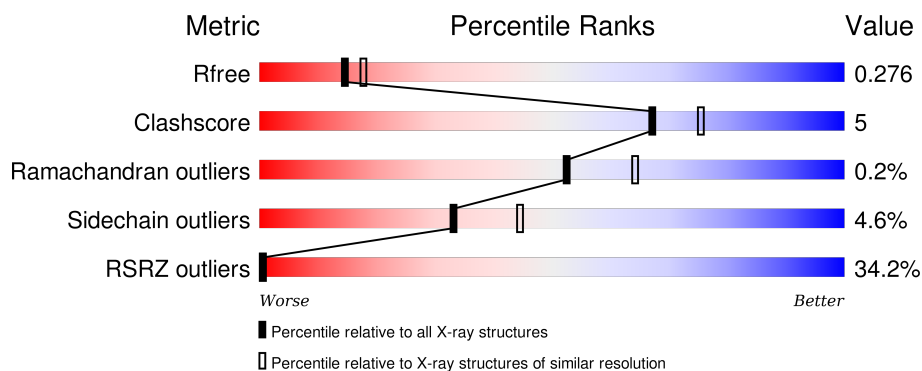
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 $\leq 5\%$. 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	<div> <div>5%</div> <div>88%</div> <div>11% ..</div> </div>
1	B	392	<div> <div>4%</div> <div>84%</div> <div>15% .</div> </div>
1	C	392	<div> <div>53%</div> <div>88%</div> <div>11% ..</div> </div>
1	D	392	<div> <div>75%</div> <div>89%</div> <div>10% .</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	COA	A	1393	-	-	-	X
2	COA	B	1393	-	-	-	X
2	COA	C	1393	-	-	-	X
2	COA	D	1393	-	-	-	X
3	SO4	A	1396	-	-	-	X
3	SO4	B	1396	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12275 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	389	Total	C	N	O	S	0	0	0
			2812	1746	509	537	20			
1	B	389	Total	C	N	O	S	0	0	0
			2812	1746	509	537	20			
1	C	389	Total	C	N	O	S	0	0	0
			2812	1746	509	537	20			
1	D	389	Total	C	N	O	S	0	0	0
			2812	1746	509	537	20			

There are 8 discrepancies between the modelled and reference sequences:

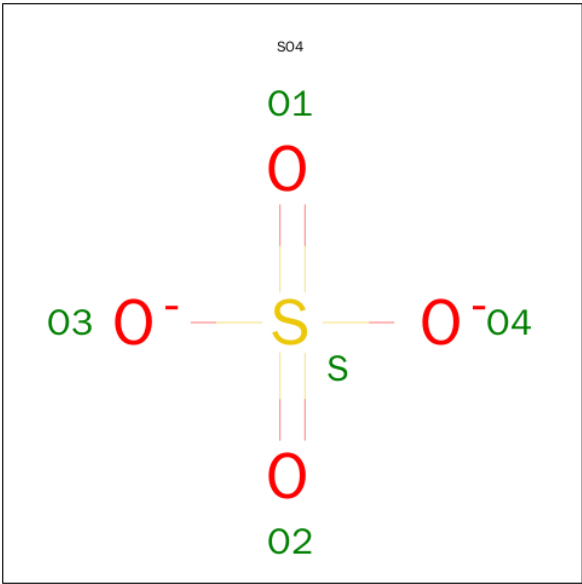
Chain	Residue	Modelled	Actual	Comment	Reference
A	89	ALA	CYS	ENGINEERED MUTATION	UNP P07097
B	89	ALA	CYS	ENGINEERED MUTATION	UNP P07097
C	89	ALA	CYS	ENGINEERED MUTATION	UNP P07097
D	89	ALA	CYS	ENGINEERED MUTATION	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	129	ARG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

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

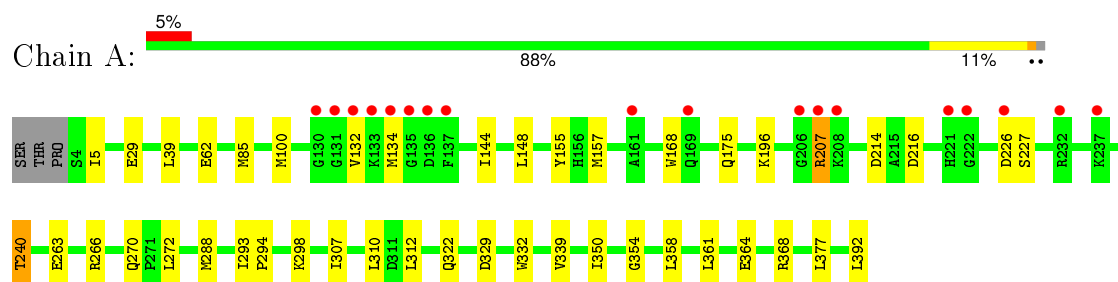
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	336	Total O 336 336	0	0
4	B	308	Total O 308 308	0	0
4	C	94	Total O 94 94	0	0
4	D	67	Total O 67 67	0	0

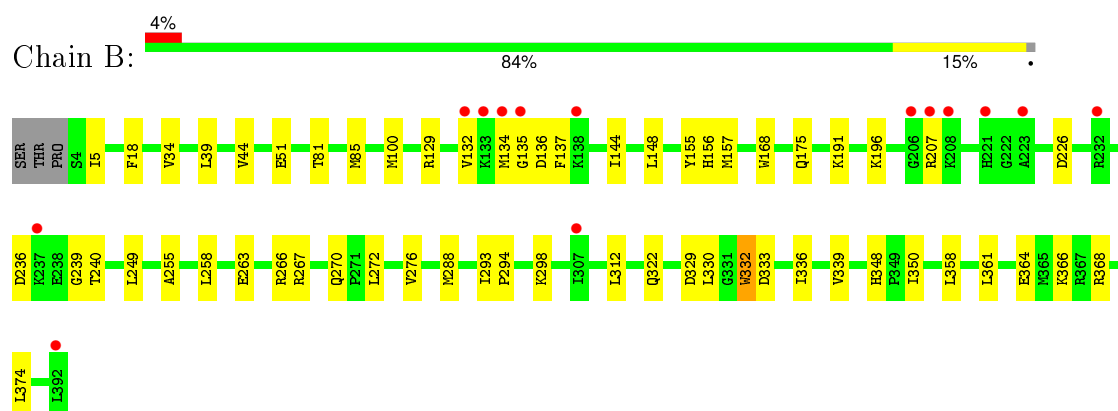
3 Residue-property plots

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.

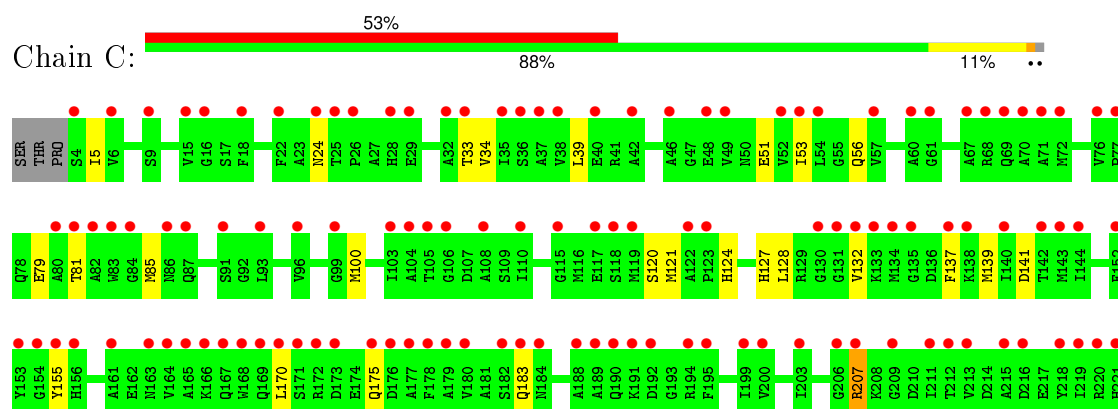
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

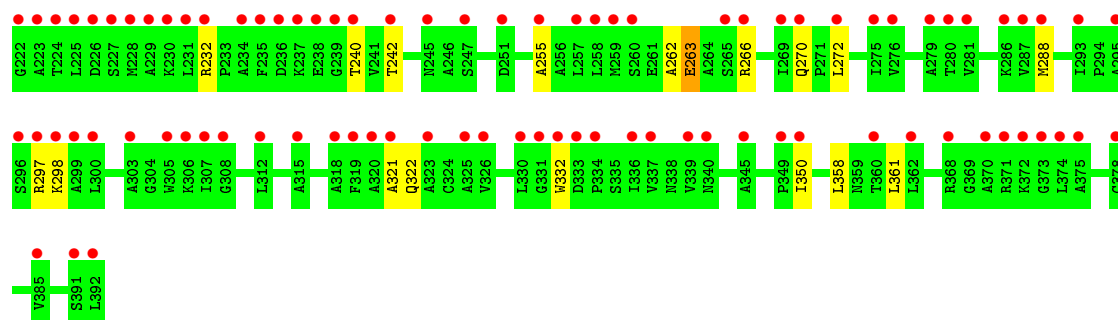


• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

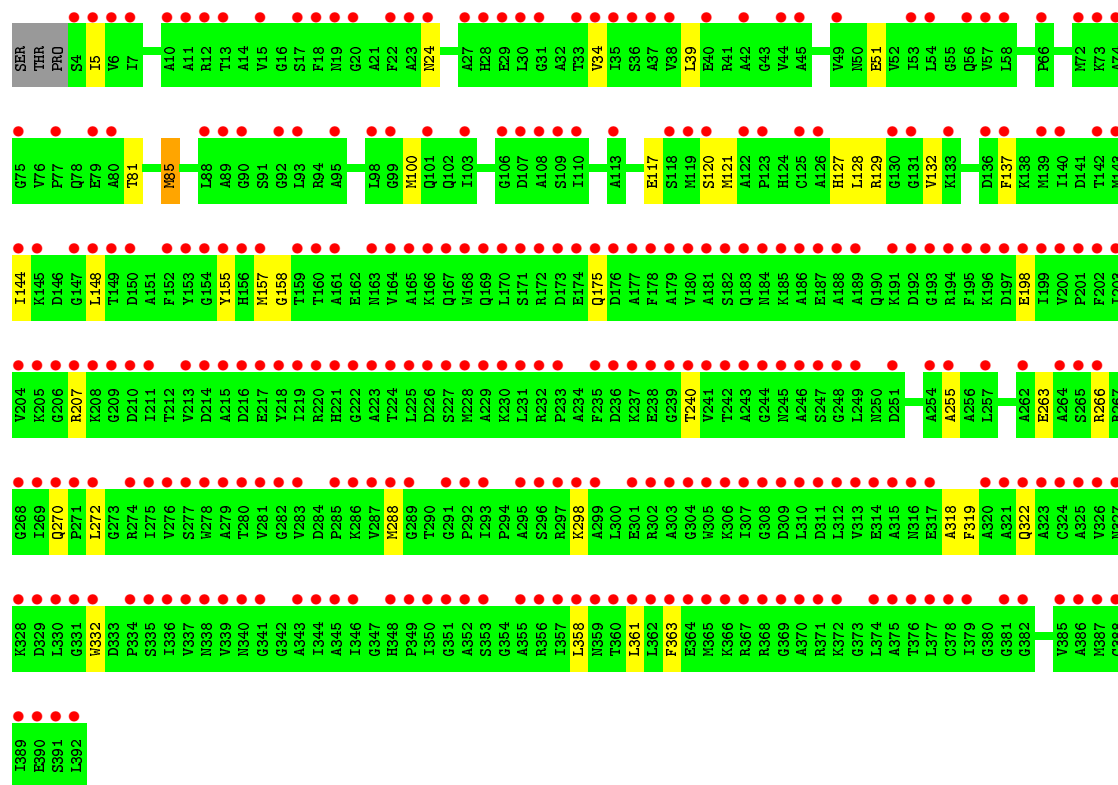
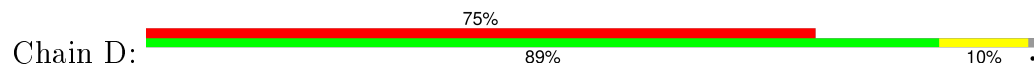


• Molecule 1: ACETYL-COA ACETYLTRANSFERASE





• Molecule 1: ACETYL-COA ACETYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.22Å 79.57Å 148.92Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-2.30) 81.1 (19.06-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.262 0.234 , 0.276	Depositor DCC
R_{free} test set	4262 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.897	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
Estimated twinning fraction	0.186 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 85233 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12275	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: COA, 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	0.54	0/2853	0.64	0/3852
1	B	0.54	0/2853	0.66	0/3852
1	C	0.35	0/2853	0.51	0/3852
1	D	0.33	0/2853	0.50	0/3852
All	All	0.45	0/11412	0.58	0/15408

There are no bond length outliers.

There are no bond angle outliers.

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	2812	0	2819	30	0
1	B	2812	0	2819	39	0
1	C	2812	0	2819	33	0
1	D	2812	0	2819	20	0
2	A	48	0	32	0	0
2	B	48	0	32	1	0
2	C	48	0	32	0	0
2	D	48	0	32	1	0
3	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	0	0
4	A	336	0	0	15	0
4	B	308	0	0	11	0
4	C	94	0	0	15	0
4	D	67	0	0	0	0
All	All	12275	0	11404	110	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (110) 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:A:310:LEU:HD12	4:A:2275:HOH:O	1.80	0.81
1:A:310:LEU:CD1	4:A:2275:HOH:O	2.30	0.79
1:C:53:ILE:HG13	4:C:2016:HOH:O	1.85	0.76
1:A:307:ILE:HA	4:A:2275:HOH:O	1.87	0.74
1:B:44:VAL:HA	4:B:2225:HOH:O	1.93	0.67
1:A:5:ILE:HG13	1:A:100:MET:HG2	1.78	0.66
1:B:156:HIS:NE2	4:B:2136:HOH:O	2.29	0.65
1:B:226:ASP:HB3	4:B:2206:HOH:O	1.96	0.65
1:C:232:ARG:O	4:C:2066:HOH:O	2.14	0.64
1:C:33:THR:HG21	4:C:2061:HOH:O	1.98	0.64
1:A:263:GLU:HA	1:A:266:ARG:NH1	2.13	0.63
1:B:148:LEU:O	1:B:157:MET:HG2	1.99	0.62
1:D:158:GLY:HA2	1:D:319:PHE:CE2	2.35	0.61
1:A:226:ASP:HB3	4:A:2222:HOH:O	2.01	0.61
1:C:263:GLU:HA	1:C:266:ARG:NH1	2.17	0.60
1:A:196:LYS:NZ	4:A:2188:HOH:O	2.35	0.60
1:C:321:ALA:HA	4:C:2051:HOH:O	2.03	0.59
1:D:263:GLU:HA	1:D:266:ARG:NH1	2.18	0.58
2:B:1393:COA:H131	2:B:1393:COA:O9P	2.04	0.57
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.70	0.57
1:A:144:ILE:HD13	1:A:148:LEU:HD12	1.87	0.55
1:A:132:VAL:HA	4:A:2139:HOH:O	2.07	0.55
1:B:129:ARG:HA	1:D:132:VAL:O	2.07	0.55
1:B:135:GLY:N	1:C:141:ASP:OD2	2.29	0.55
1:A:29:GLU:HG2	4:A:2036:HOH:O	2.06	0.55
1:A:392:LEU:HG	4:A:2252:HOH:O	2.05	0.55
1:C:170:LEU:HB3	4:C:2051:HOH:O	2.07	0.54
1:B:196:LYS:HD2	4:B:2084:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLN:NE2	4:C:2053:HOH:O	2.39	0.53
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.23	0.52
1:C:132:VAL:HG21	1:C:137:PHE:CD1	2.45	0.52
1:C:34:VAL:HG12	1:C:255:ALA:HB3	1.92	0.52
1:A:196:LYS:HD2	4:A:2042:HOH:O	2.09	0.52
1:B:374:LEU:C	1:B:374:LEU:HD23	2.30	0.51
1:B:258:LEU:HG	4:B:2097:HOH:O	2.09	0.51
1:B:312:LEU:HD21	1:B:364:GLU:CG	2.41	0.51
1:A:214:ASP:HB2	4:A:2207:HOH:O	2.10	0.51
1:C:51:GLU:C	4:C:2016:HOH:O	2.50	0.50
1:B:366:LYS:NZ	4:B:2290:HOH:O	2.39	0.50
1:B:137:PHE:CE2	1:C:139:MET:HG3	2.46	0.50
1:A:134:MET:HA	4:A:2140:HOH:O	2.14	0.48
1:C:242:THR:HA	4:C:2066:HOH:O	2.14	0.48
1:B:339:VAL:HG11	1:B:368:ARG:NH2	2.29	0.48
1:C:262:ALA:HB3	4:C:2070:HOH:O	2.13	0.47
1:A:148:LEU:O	1:A:157:MET:HG2	2.14	0.47
1:B:137:PHE:CZ	1:C:139:MET:HG3	2.49	0.47
1:D:128:LEU:HD21	1:D:137:PHE:CE1	2.50	0.47
1:B:135:GLY:O	1:C:124:HIS:NE2	2.44	0.47
1:B:100:MET:HB2	4:B:2097:HOH:O	2.14	0.47
1:C:51:GLU:HG2	4:C:2016:HOH:O	2.14	0.47
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.80	0.46
1:D:51:GLU:HA	1:D:81:THR:O	2.16	0.46
1:B:236:ASP:O	1:B:239:GLY:N	2.48	0.46
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.51	0.46
1:B:156:HIS:CD2	4:B:2136:HOH:O	2.69	0.45
1:C:128:LEU:HD21	1:C:137:PHE:CZ	2.52	0.45
1:C:120:SER:O	1:D:127:HIS:NE2	2.48	0.45
1:D:157:MET:HG3	2:D:1393:COA:S1P	2.56	0.45
1:D:318:ALA:C	1:D:319:PHE:CD1	2.89	0.45
1:B:132:VAL:HG21	1:B:137:PHE:CD1	2.51	0.45
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.52	0.45
1:D:158:GLY:HA2	1:D:319:PHE:HE2	1.77	0.45
1:B:266:ARG:HH11	1:B:266:ARG:HG3	1.82	0.45
1:A:339:VAL:HG11	1:A:368:ARG:NH2	2.32	0.44
1:B:267:ARG:NH1	4:B:2225:HOH:O	2.50	0.44
1:B:34:VAL:HG12	1:B:255:ALA:HB3	2.00	0.44
1:B:134:MET:HA	1:D:129:ARG:NH1	2.32	0.44
1:B:18:PHE:HB2	1:B:249:LEU:O	2.18	0.44
1:C:175:GLN:CG	4:C:2051:HOH:O	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:PHE:O	4:B:2012:HOH:O	2.21	0.43
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.83	0.43
1:C:85:MET:HA	1:D:85:MET:HA	1.99	0.43
1:A:354:GLY:HA2	1:A:377:LEU:HD11	2.00	0.43
1:C:51:GLU:HA	1:C:81:THR:O	2.18	0.43
1:B:136:ASP:HA	1:C:139:MET:O	2.19	0.43
1:C:79:GLU:N	1:C:79:GLU:OE1	2.51	0.43
1:B:5:ILE:HG13	1:B:100:MET:HG2	1.99	0.43
1:A:207:ARG:N	1:A:207:ARG:HD3	2.33	0.43
1:D:24:ASN:HA	1:D:121:MET:SD	2.59	0.43
1:A:293:ILE:HB	1:A:294:PRO:CD	2.49	0.43
1:D:5:ILE:HG13	1:D:100:MET:HG2	2.00	0.43
1:B:134:MET:HA	1:D:129:ARG:HH12	1.84	0.42
1:A:312:LEU:HD21	1:A:364:GLU:CG	2.50	0.42
1:D:34:VAL:HG12	1:D:255:ALA:HB3	2.01	0.42
1:C:24:ASN:HA	1:C:121:MET:SD	2.59	0.42
1:A:227:SER:OG	4:A:2221:HOH:O	2.21	0.42
1:C:127:HIS:NE2	1:D:120:SER:O	2.50	0.42
1:C:207:ARG:N	1:C:207:ARG:HD3	2.35	0.42
1:B:293:ILE:HB	1:B:294:PRO:CD	2.50	0.42
1:A:310:LEU:HG	4:A:2275:HOH:O	2.19	0.42
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.84	0.42
1:C:175:GLN:HG2	4:C:2051:HOH:O	2.20	0.42
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.85	0.42
1:C:56:GLN:N	4:C:2018:HOH:O	2.53	0.42
1:B:333:ASP:O	1:B:336:ILE:HG12	2.20	0.42
1:B:191:LYS:NZ	4:B:2160:HOH:O	2.42	0.42
1:A:62:GLU:O	1:A:62:GLU:HG2	2.20	0.41
1:B:330:LEU:HD13	1:B:332:TRP:CH2	2.55	0.41
1:D:144:ILE:HD13	1:D:148:LEU:HD12	2.01	0.41
1:C:297:ARG:HA	4:C:2079:HOH:O	2.19	0.41
1:C:5:ILE:HG13	1:C:100:MET:HG2	2.02	0.41
1:C:170:LEU:CB	4:C:2051:HOH:O	2.69	0.40
1:A:85:MET:HA	1:B:85:MET:HA	2.03	0.40
1:A:310:LEU:CG	4:A:2275:HOH:O	2.65	0.40
1:D:198:GLU:HB3	1:D:363:PHE:CD2	2.56	0.40
1:A:216:ASP:HB3	4:A:2309:HOH:O	2.20	0.40
1:B:144:ILE:HD13	1:B:148:LEU:HD12	2.02	0.40
1:A:339:VAL:HG11	1:A:368:ARG:HH21	1.86	0.40
1:B:51:GLU:HA	1:B:81:THR:O	2.22	0.40
1:B:132:VAL:O	1:D:129:ARG:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/392 (99%)	377 (97%)	9 (2%)	1 (0%)	46	57
1	B	387/392 (99%)	376 (97%)	10 (3%)	1 (0%)	46	57
1	C	387/392 (99%)	377 (97%)	9 (2%)	1 (0%)	46	57
1	D	387/392 (99%)	377 (97%)	10 (3%)	0	100	100
All	All	1548/1568 (99%)	1507 (97%)	38 (2%)	3 (0%)	52	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ILE
1	B	350	ILE
1	C	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	275/278 (99%)	263 (96%)	12 (4%)	35	46
1	B	275/278 (99%)	261 (95%)	14 (5%)	29	39
1	C	275/278 (99%)	263 (96%)	12 (4%)	35	46
1	D	275/278 (99%)	262 (95%)	13 (5%)	32	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1100/1112 (99%)	1049 (95%)	51 (5%)	33	44

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	155	TYR
1	A	207	ARG
1	A	240	THR
1	A	270	GLN
1	A	272	LEU
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	332	TRP
1	A	358	LEU
1	A	361	LEU
1	B	39	LEU
1	B	155	TYR
1	B	207	ARG
1	B	263	GLU
1	B	270	GLN
1	B	272	LEU
1	B	276	VAL
1	B	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
1	B	348	HIS
1	B	358	LEU
1	B	361	LEU
1	C	39	LEU
1	C	155	TYR
1	C	207	ARG
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

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Mol	Chain	Res	Type
1	C	361	LEU
1	D	39	LEU
1	D	85	MET
1	D	117	GLU
1	D	155	TYR
1	D	207	ARG
1	D	270	GLN
1	D	272	LEU
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	332	TRP
1	D	358	LEU
1	D	361	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	221	HIS
1	B	78	GLN
1	B	167	GLN
1	B	175	GLN
1	B	184	ASN
1	C	175	GLN
1	C	184	ASN
1	D	175	GLN
1	D	184	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 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	1.74	3 (7%)	50,75,75	2.03	3 (6%)
3	SO4	A	1394	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	A	1395	-	4,4,4	0.21	0	6,6,6	0.20	0
3	SO4	A	1396	-	4,4,4	0.19	0	6,6,6	0.24	0
2	COA	B	1393	-	40,50,50	1.72	3 (7%)	50,75,75	1.99	6 (12%)
3	SO4	B	1394	-	4,4,4	0.23	0	6,6,6	0.26	0
3	SO4	B	1395	-	4,4,4	0.26	0	6,6,6	0.13	0
3	SO4	B	1396	-	4,4,4	0.14	0	6,6,6	0.16	0
2	COA	C	1393	-	40,50,50	1.71	3 (7%)	50,75,75	1.88	5 (10%)
2	COA	D	1393	-	40,50,50	1.72	3 (7%)	50,75,75	1.92	2 (4%)

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	SO4	A	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1396	-	-	0/0/0/0	0/0/0/0
2	COA	B	1393	-	-	0/44/64/64	0/3/3/3
3	SO4	B	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1396	-	-	0/0/0/0	0/0/0/0
2	COA	C	1393	-	-	0/44/64/64	0/3/3/3
2	COA	D	1393	-	-	0/44/64/64	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1393	COA	C2A-N1A	2.53	1.38	1.33
2	D	1393	COA	C2A-N1A	2.59	1.38	1.33
2	C	1393	COA	C2A-N1A	2.60	1.38	1.33
2	B	1393	COA	C2A-N1A	2.70	1.39	1.33
2	A	1393	COA	C2A-N3A	3.35	1.38	1.32
2	D	1393	COA	C2A-N3A	3.69	1.38	1.32
2	B	1393	COA	C2A-N3A	3.70	1.38	1.32
2	C	1393	COA	C2A-N3A	3.83	1.39	1.32
2	B	1393	COA	O9P-C9P	9.00	1.41	1.23
2	A	1393	COA	O9P-C9P	9.21	1.41	1.23
2	C	1393	COA	O9P-C9P	9.22	1.41	1.23
2	D	1393	COA	O9P-C9P	9.27	1.41	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1393	COA	N3A-C2A-N1A	-12.20	119.55	128.89
2	D	1393	COA	N3A-C2A-N1A	-11.65	119.97	128.89
2	B	1393	COA	N3A-C2A-N1A	-11.48	120.11	128.89
2	C	1393	COA	N3A-C2A-N1A	-11.30	120.24	128.89
2	D	1393	COA	P2A-O3A-P1A	-4.23	120.84	132.73
2	A	1393	COA	P2A-O3A-P1A	-3.82	121.99	132.73
2	B	1393	COA	C4B-O4B-C1B	-3.47	105.91	109.72
2	C	1393	COA	P2A-O3A-P1A	-3.42	123.12	132.73
2	B	1393	COA	P2A-O3A-P1A	-2.88	124.64	132.73
2	B	1393	COA	C2B-C1B-N9A	-2.16	110.99	114.29
2	C	1393	COA	C4A-C5A-N7A	-2.09	107.55	109.48
2	A	1393	COA	C2B-C1B-N9A	-2.05	111.17	114.29
2	C	1393	COA	C4B-O4B-C1B	2.13	112.06	109.72
2	B	1393	COA	C7P-C6P-C5P	2.16	115.87	112.31
2	C	1393	COA	C3B-C2B-C1B	2.53	106.04	99.98
2	B	1393	COA	O4B-C1B-N9A	3.00	114.37	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1393	COA	1	0
2	D	1393	COA	1	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, 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	389/392 (99%)	0.48	18 (4%) 36 45	34, 39, 47, 60	0
1	B	389/392 (99%)	0.56	14 (3%) 46 55	31, 39, 47, 60	0
1	C	389/392 (99%)	2.32	206 (52%) 0 0	35, 40, 47, 56	0
1	D	389/392 (99%)	3.60	294 (75%) 0 0	36, 39, 46, 55	0
All	All	1556/1568 (99%)	1.74	532 (34%) 0 0	31, 39, 47, 60	0

All (532) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	229	ALA	12.9
1	D	222	GLY	12.7
1	D	238	GLU	12.0
1	D	241	VAL	11.4
1	D	170	LEU	11.2
1	D	219	ILE	11.1
1	D	231	LEU	10.3
1	D	331	GLY	10.1
1	D	371	ARG	10.0
1	D	382	GLY	10.0
1	D	323	ALA	9.9
1	D	166	LYS	9.0
1	D	228	MET	8.9
1	D	153	TYR	8.9
1	D	325	ALA	8.7
1	D	207	ARG	8.7
1	D	230	LYS	8.6
1	D	367	ARG	8.5
1	D	218	TYR	8.5
1	D	188	ALA	8.5
1	D	226	ASP	8.4

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Mol	Chain	Res	Type	RSRZ
1	D	206	GLY	8.3
1	D	328	LYS	8.3
1	C	222	GLY	8.2
1	C	224	THR	8.1
1	D	191	LYS	7.8
1	D	224	THR	7.5
1	D	179	ALA	7.4
1	D	182	SER	7.4
1	C	223	ALA	7.3
1	D	310	LEU	7.3
1	D	165	ALA	7.3
1	D	243	ALA	7.2
1	D	205	LYS	7.1
1	D	223	ALA	7.1
1	D	269	ILE	7.1
1	D	349	PRO	6.9
1	D	175	GLN	6.9
1	C	80	ALA	6.8
1	D	237	LYS	6.8
1	D	357	ILE	6.7
1	D	232	ARG	6.6
1	A	134	MET	6.5
1	D	307	ILE	6.5
1	D	186	ALA	6.3
1	D	155	TYR	6.3
1	D	301	GLU	6.2
1	D	345	ALA	6.1
1	D	303	ALA	6.1
1	D	193	GLY	6.1
1	C	280	THR	6.1
1	D	235	PHE	6.1
1	D	167	GLN	6.0
1	C	295	ALA	6.0
1	D	377	LEU	6.0
1	C	229	ALA	6.0
1	D	152	PHE	5.9
1	B	134	MET	5.9
1	C	234	ALA	5.9
1	D	271	PRO	5.9
1	D	161	ALA	5.8
1	D	247	SER	5.8
1	D	196	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	168	TRP	5.7
1	C	36	SER	5.7
1	D	326	VAL	5.7
1	D	344	ILE	5.7
1	D	178	PHE	5.7
1	D	246	ALA	5.7
1	D	245	ASN	5.6
1	C	131	GLY	5.6
1	C	269	ILE	5.6
1	D	233	PRO	5.5
1	D	160	THR	5.5
1	D	254	ALA	5.5
1	C	140	ILE	5.5
1	C	37	ALA	5.5
1	C	232	ARG	5.5
1	D	329	ASP	5.5
1	D	330	LEU	5.4
1	D	159	THR	5.4
1	D	283	VAL	5.4
1	C	156	HIS	5.4
1	D	305	TRP	5.4
1	D	336	ILE	5.4
1	D	131	GLY	5.4
1	D	248	GLY	5.4
1	C	227	SER	5.4
1	C	209	GLY	5.4
1	D	164	VAL	5.3
1	D	34	VAL	5.3
1	D	242	THR	5.3
1	C	182	SER	5.3
1	C	132	VAL	5.3
1	C	153	TYR	5.2
1	D	332	TRP	5.2
1	D	277	SER	5.2
1	A	131	GLY	5.2
1	C	237	LYS	5.2
1	D	240	THR	5.2
1	B	135	GLY	5.2
1	C	225	LEU	5.1
1	D	387	MET	5.1
1	D	37	ALA	5.1
1	C	213	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	226	ASP	5.1
1	D	306	LYS	5.0
1	D	195	PHE	5.0
1	D	108	ALA	5.0
1	C	211	ILE	5.0
1	D	346	ILE	5.0
1	D	272	LEU	5.0
1	D	368	ARG	5.0
1	D	192	ASP	5.0
1	C	391	SER	5.0
1	D	12	ARG	5.0
1	C	266	ARG	5.0
1	D	268	GLY	5.0
1	D	140	ILE	4.9
1	D	181	ALA	4.9
1	D	374	LEU	4.9
1	C	110	ILE	4.9
1	D	171	SER	4.9
1	D	225	LEU	4.9
1	D	312	LEU	4.8
1	D	239	GLY	4.8
1	D	211	ILE	4.8
1	B	208	LYS	4.8
1	C	307	ILE	4.8
1	D	220	ARG	4.8
1	D	177	ALA	4.7
1	C	235	PHE	4.7
1	C	103	ILE	4.7
1	D	327	ASN	4.7
1	C	238	GLU	4.7
1	D	315	ALA	4.6
1	D	370	ALA	4.6
1	C	230	LYS	4.6
1	D	372	LYS	4.6
1	B	206	GLY	4.6
1	D	176	ASP	4.6
1	C	315	ALA	4.5
1	D	180	VAL	4.5
1	C	33	THR	4.5
1	D	221	HIS	4.5
1	C	330	LEU	4.5
1	D	358	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	19	ASN	4.5
1	D	4	SER	4.4
1	D	365	MET	4.4
1	C	293	ILE	4.4
1	D	320	ALA	4.4
1	D	6	VAL	4.4
1	C	221	HIS	4.4
1	C	231	LEU	4.4
1	D	5	ILE	4.4
1	D	391	SER	4.3
1	D	311	ASP	4.3
1	D	154	GLY	4.3
1	C	212	THR	4.3
1	C	164	VAL	4.3
1	D	169	GLN	4.3
1	C	4	SER	4.3
1	D	204	VAL	4.3
1	C	67	ALA	4.3
1	D	119	MET	4.3
1	A	132	VAL	4.2
1	B	207	ARG	4.2
1	D	148	LEU	4.2
1	C	108	ALA	4.1
1	D	302	ARG	4.1
1	D	217	GLU	4.1
1	D	29	GLU	4.1
1	D	184	ASN	4.1
1	C	25	THR	4.1
1	C	42	ALA	4.1
1	D	362	LEU	4.0
1	D	107	ASP	4.0
1	D	24	ASN	4.0
1	D	281	VAL	4.0
1	D	20	GLY	4.0
1	C	138	LYS	4.0
1	A	207	ARG	4.0
1	D	42	ALA	4.0
1	D	321	ALA	4.0
1	D	172	ARG	4.0
1	D	189	ALA	4.0
1	C	195	PHE	4.0
1	C	76	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	285	PRO	3.9
1	C	321	ALA	3.9
1	D	173	ASP	3.9
1	D	157	MET	3.9
1	C	173	ASP	3.9
1	A	208	LYS	3.9
1	C	104	ALA	3.9
1	D	339	VAL	3.9
1	C	259	MET	3.8
1	C	306	LYS	3.8
1	C	155	TYR	3.8
1	D	297	ARG	3.8
1	A	237	LYS	3.8
1	D	388	CYS	3.8
1	C	207	ARG	3.8
1	D	295	ALA	3.8
1	D	361	LEU	3.8
1	D	187	GLU	3.7
1	D	40	GLU	3.7
1	D	375	ALA	3.7
1	C	133	LYS	3.7
1	D	183	GLN	3.7
1	D	359	ASN	3.7
1	D	279	ALA	3.7
1	D	265	SER	3.7
1	D	23	ALA	3.7
1	D	313	VAL	3.7
1	C	318	ALA	3.7
1	C	312	LEU	3.6
1	A	206	GLY	3.6
1	D	389	ILE	3.6
1	A	136	ASP	3.6
1	C	130	GLY	3.6
1	D	156	HIS	3.6
1	D	199	ILE	3.6
1	C	340	ASN	3.6
1	D	392	LEU	3.6
1	D	338	ASN	3.6
1	A	133	LYS	3.5
1	C	122	ALA	3.5
1	D	308	GLY	3.5
1	C	236	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	88	LEU	3.5
1	D	291	GLY	3.5
1	C	52	VAL	3.5
1	C	296	SER	3.5
1	D	350	ILE	3.5
1	D	49	VAL	3.5
1	D	30	LEU	3.5
1	C	152	PHE	3.5
1	D	18	PHE	3.5
1	C	303	ALA	3.5
1	D	110	ILE	3.5
1	C	169	GLN	3.4
1	D	360	THR	3.4
1	D	355	ALA	3.4
1	B	133	LYS	3.4
1	D	369	GLY	3.4
1	C	392	LEU	3.4
1	D	106	GLY	3.4
1	D	93	LEU	3.4
1	D	366	LYS	3.4
1	A	135	GLY	3.4
1	D	227	SER	3.4
1	C	49	VAL	3.4
1	D	236	ASP	3.4
1	D	7	ILE	3.4
1	D	125	CYS	3.3
1	D	92	GLY	3.3
1	D	264	ALA	3.3
1	C	26	PRO	3.3
1	D	15	VAL	3.3
1	D	314	GLU	3.3
1	C	219	ILE	3.3
1	D	203	ILE	3.3
1	D	385	VAL	3.3
1	C	323	ALA	3.3
1	D	216	ASP	3.3
1	C	93	LEU	3.3
1	D	213	VAL	3.3
1	D	215	ALA	3.3
1	D	274	ARG	3.2
1	C	105	THR	3.2
1	C	167	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	79	GLU	3.2
1	D	120	SER	3.2
1	D	197	ASP	3.2
1	D	210	ASP	3.2
1	D	364	GLU	3.2
1	D	103	ILE	3.2
1	D	54	LEU	3.2
1	D	255	ALA	3.2
1	D	343	ALA	3.2
1	D	378	CYS	3.2
1	D	335	SER	3.2
1	D	133	LYS	3.2
1	D	352	ALA	3.2
1	C	40	GLU	3.2
1	D	163	ASN	3.2
1	D	390	GLU	3.2
1	D	363	PHE	3.1
1	D	282	GLY	3.1
1	D	289	GLY	3.1
1	D	10	ALA	3.1
1	C	288	MET	3.1
1	D	376	THR	3.1
1	C	220	ARG	3.1
1	C	372	LYS	3.1
1	D	143	MET	3.1
1	D	109	SER	3.1
1	A	226	ASP	3.1
1	C	333	ASP	3.1
1	C	287	VAL	3.1
1	C	375	ALA	3.1
1	D	142	THR	3.1
1	B	132	VAL	3.1
1	C	334	PRO	3.1
1	C	297	ARG	3.1
1	C	180	VAL	3.0
1	D	201	PRO	3.0
1	D	145	LYS	3.0
1	D	113	ALA	3.0
1	D	334	PRO	3.0
1	D	337	VAL	3.0
1	B	223	ALA	3.0
1	A	130	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	245	ASN	3.0
1	C	84	GLY	3.0
1	C	265	SER	3.0
1	B	221	HIS	3.0
1	D	74	ALA	3.0
1	C	137	PHE	3.0
1	C	203	ILE	3.0
1	D	244	GLY	2.9
1	C	298	LYS	2.9
1	C	165	ALA	2.9
1	C	166	LYS	2.9
1	D	80	ALA	2.9
1	D	137	PHE	2.9
1	D	249	LEU	2.9
1	C	188	ALA	2.9
1	C	61	GLY	2.9
1	C	374	LEU	2.9
1	D	185	LYS	2.9
1	D	126	ALA	2.9
1	C	200	VAL	2.9
1	D	288	MET	2.9
1	C	15	VAL	2.9
1	C	336	ILE	2.9
1	C	192	ASP	2.9
1	D	198	GLU	2.8
1	C	215	ALA	2.8
1	D	123	PRO	2.8
1	C	83	TRP	2.8
1	C	305	TRP	2.8
1	D	324	CYS	2.8
1	C	373	GLY	2.8
1	D	270	GLN	2.8
1	D	44	VAL	2.8
1	D	276	VAL	2.8
1	D	194	ARG	2.8
1	C	260	SER	2.8
1	D	17	SER	2.8
1	C	172	ARG	2.8
1	C	371	ARG	2.8
1	D	57	VAL	2.8
1	C	9	SER	2.8
1	C	16	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	90	GLY	2.8
1	C	123	PRO	2.7
1	C	171	SER	2.7
1	D	150	ASP	2.7
1	C	54	LEU	2.7
1	C	60	ALA	2.7
1	D	98	LEU	2.7
1	D	257	LEU	2.7
1	C	46	ALA	2.7
1	C	71	ALA	2.7
1	D	149	THR	2.7
1	B	237	LYS	2.7
1	C	199	ILE	2.7
1	C	275	ILE	2.7
1	D	27	ALA	2.7
1	D	118	SER	2.7
1	C	184	ASN	2.7
1	D	33	THR	2.7
1	D	348	HIS	2.7
1	C	99	GLY	2.7
1	C	175	GLN	2.7
1	C	168	TRP	2.7
1	C	87	GLN	2.7
1	C	96	VAL	2.7
1	C	370	ALA	2.6
1	C	57	VAL	2.6
1	D	287	VAL	2.6
1	D	386	ALA	2.6
1	D	22	PHE	2.6
1	D	251	ASP	2.6
1	C	38	VAL	2.6
1	D	38	VAL	2.6
1	D	286	LYS	2.6
1	C	270	GLN	2.6
1	A	232	ARG	2.6
1	C	194	ARG	2.6
1	C	218	TYR	2.6
1	C	319	PHE	2.6
1	C	216	ASP	2.6
1	C	154	GLY	2.6
1	D	122	ALA	2.6
1	C	170	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	28	HIS	2.5
1	C	106	GLY	2.5
1	D	296	SER	2.5
1	C	385	VAL	2.5
1	C	183	GLN	2.5
1	C	91	SER	2.5
1	C	239	GLY	2.5
1	D	75	GLY	2.5
1	D	379	ILE	2.5
1	B	392	LEU	2.5
1	D	31	GLY	2.5
1	D	136	ASP	2.5
1	C	368	ARG	2.5
1	C	179	ALA	2.5
1	C	325	ALA	2.5
1	C	251	ASP	2.5
1	C	70	ALA	2.4
1	C	177	ALA	2.4
1	C	189	ALA	2.4
1	C	240	THR	2.4
1	D	280	THR	2.4
1	D	322	GLN	2.4
1	D	278	TRP	2.4
1	D	275	ILE	2.4
1	C	242	THR	2.4
1	C	345	ALA	2.4
1	D	45	ALA	2.4
1	C	228	MET	2.4
1	D	58	LEU	2.4
1	C	190	GLN	2.4
1	D	53	ILE	2.4
1	D	298	LYS	2.4
1	D	381	GLY	2.4
1	D	353	SER	2.4
1	C	18	PHE	2.4
1	C	320	ALA	2.4
1	B	232	ARG	2.4
1	D	316	ASN	2.4
1	C	276	VAL	2.4
1	C	281	VAL	2.4
1	C	360	THR	2.4
1	D	13	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	362	LEU	2.3
1	B	307	ILE	2.3
1	C	32	ALA	2.3
1	C	77	PRO	2.3
1	D	292	PRO	2.3
1	C	115	GLY	2.3
1	D	99	GLY	2.3
1	D	130	GLY	2.3
1	D	351	GLY	2.3
1	C	255	ALA	2.3
1	D	299	ALA	2.3
1	C	29	GLU	2.3
1	C	247	SER	2.3
1	C	72	MET	2.3
1	D	209	GLY	2.3
1	D	341	GLY	2.3
1	C	22	PHE	2.3
1	C	118	SER	2.3
1	D	208	LYS	2.3
1	C	279	ALA	2.3
1	C	339	VAL	2.3
1	D	144	ILE	2.3
1	D	89	ALA	2.3
1	C	257	LEU	2.3
1	C	300	LEU	2.3
1	D	139	MET	2.3
1	C	142	THR	2.2
1	C	337	VAL	2.2
1	D	36	SER	2.2
1	A	222	GLY	2.2
1	D	304	GLY	2.2
1	A	169	GLN	2.2
1	C	163	ASN	2.2
1	C	331	GLY	2.2
1	D	174	GLU	2.2
1	C	134	MET	2.2
1	C	86	ASN	2.2
1	C	161	ALA	2.2
1	D	317	GLU	2.2
1	D	77	PRO	2.2
1	A	221	HIS	2.2
1	C	6	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	309	ASP	2.1
1	C	326	VAL	2.1
1	A	137	PHE	2.1
1	C	119	MET	2.1
1	C	258	LEU	2.1
1	B	138	LYS	2.1
1	D	73	LYS	2.1
1	C	378	CYS	2.1
1	D	266	ARG	2.1
1	C	144	ILE	2.1
1	C	308	GLY	2.1
1	C	350	ILE	2.1
1	D	72	MET	2.1
1	C	35	ILE	2.1
1	C	191	LYS	2.1
1	D	202	PHE	2.1
1	D	101	GLN	2.1
1	D	95	ALA	2.1
1	C	28	HIS	2.1
1	D	200	VAL	2.1
1	C	332	TRP	2.1
1	C	82	ALA	2.1
1	D	340	ASN	2.1
1	D	356	ARG	2.1
1	C	176	ASP	2.1
1	D	293	ILE	2.1
1	C	24	ASN	2.1
1	D	11	ALA	2.1
1	D	262	ALA	2.1
1	D	56	GLN	2.1
1	C	349	PRO	2.1
1	C	53	ILE	2.1
1	C	178	PHE	2.0
1	C	272	LEU	2.0
1	C	117	GLU	2.0
1	D	35	ILE	2.0
1	C	206	GLY	2.0
1	D	147	GLY	2.0
1	D	214	ASP	2.0
1	A	161	ALA	2.0
1	C	135	GLY	2.0
1	C	69	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	286	LYS	2.0
1	C	81	THR	2.0
1	C	48	GLU	2.0
1	C	143	MET	2.0
1	C	299	ALA	2.0
1	C	68	ARG	2.0
1	D	66	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	B	1396	5/5	0.76	0.46	9.73	86,86,87,87	0
3	SO4	A	1396	5/5	0.77	0.46	6.93	81,82,82,83	0
2	COA	B	1393	48/48	0.76	0.31	3.36	46,72,77,78	0
2	COA	D	1393	48/48	0.22	0.66	2.31	72,72,75,76	0
2	COA	A	1393	48/48	0.79	0.27	2.11	50,68,76,77	0
2	COA	C	1393	48/48	0.56	0.40	1.15	67,69,70,71	0
3	SO4	A	1395	5/5	0.81	0.39	-	67,67,68,69	0
3	SO4	B	1395	5/5	0.98	0.23	-	44,44,45,46	0
3	SO4	B	1394	5/5	0.91	0.24	-	59,59,60,60	0
3	SO4	A	1394	5/5	0.96	0.18	-	44,44,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.