



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2018 – 02:34 PM EST

PDB ID : 5MY2
Title : KS-MAT DI-DOMAIN OF MOUSE FAS
Authors : Paithankar, K.S.; Rittner, A.; Vu Huu, K.; Grininger, M.
Deposited on : 2017-01-25
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

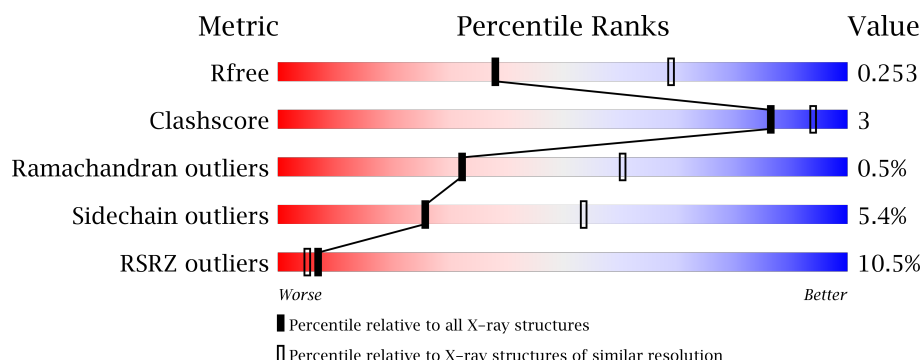
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	852	<div> <div>5%</div> <div>90%</div> <div>10%</div> <div>.</div> </div>
1	B	852	<div> <div>14%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	C	852	<div> <div>17%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	D	852	<div> <div>6%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25831 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 Fatty acid synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	852	Total	C	N	O	S	0	0	0
			6469	4089	1136	1212	32			
1	B	844	Total	C	N	O	S	0	0	0
			6410	4054	1123	1201	32			
1	C	848	Total	C	N	O	S	0	0	0
			6439	4072	1128	1207	32			
1	D	852	Total	C	N	O	S	0	0	0
			6465	4087	1136	1210	32			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P19096
B	1	SER	-	expression tag	UNP P19096
C	1	SER	-	expression tag	UNP P19096
D	1	SER	-	expression tag	UNP P19096

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

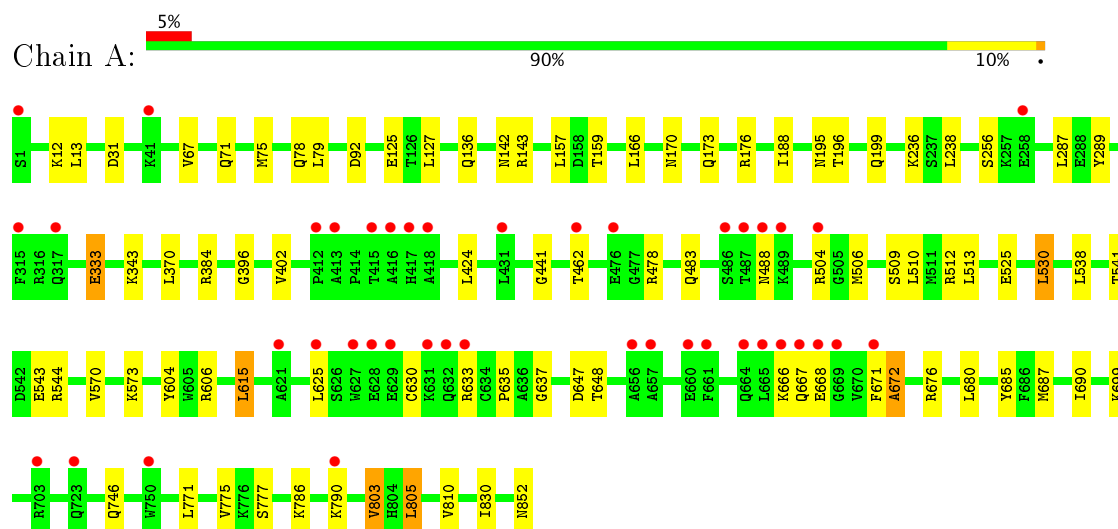


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

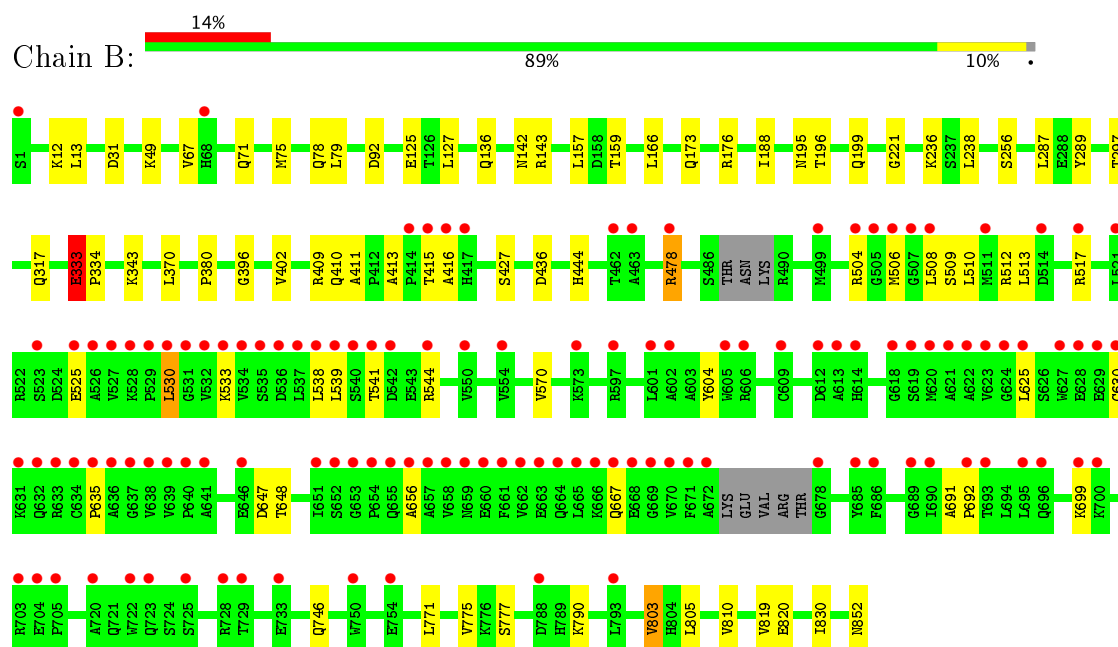
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

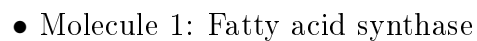
• Molecule 1: Fatty acid synthase



• Molecule 1: Fatty acid synthase



• Molecule 1: Fatty acid synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	216.56Å 345.81Å 145.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	183.54 – 2.70 43.75 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (183.54-2.70) 99.2 (43.75-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.217 , 0.251 0.221 , 0.253	Depositor DCC
R_{free} test set	7262 reflections (5.17%)	DCC
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25831	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.74% 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, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0.64	0/6616	0.82	3/9000 (0.0%)
1	B	0.63	0/6555	0.80	5/8914 (0.1%)
1	C	0.62	0/6583	0.82	11/8951 (0.1%)
1	D	0.66	1/6612 (0.0%)	0.84	14/8995 (0.2%)
All	All	0.64	1/26366 (0.0%)	0.82	33/35860 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	ASP	CB-CG	-5.16	1.41	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	798	THR	N-CA-CB	7.90	125.30	110.30
1	C	209	ASP	N-CA-CB	-7.79	96.57	110.60
1	D	209	ASP	N-CA-CB	-7.38	97.32	110.60
1	D	209	ASP	CB-CA-C	-6.99	96.42	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	ASP	CB-CA-C	-6.82	96.76	110.40
1	D	661	PHE	CB-CG-CD2	6.48	125.34	120.80
1	D	706	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	409	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	209	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	278	GLN	CA-CB-CG	6.04	126.68	113.40
1	D	132	MET	CG-SD-CE	6.02	109.84	100.20
1	D	478	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	D	790	LYS	CA-CB-CG	5.91	126.41	113.40
1	B	478	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	31	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	31	ASP	CB-CG-OD1	5.54	123.28	118.30
1	D	128	LEU	CA-CB-CG	5.52	128.00	115.30
1	D	570	VAL	CA-CB-CG2	5.45	119.07	110.90
1	B	31	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	384	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	209	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	333	GLU	CB-CA-C	5.28	120.95	110.40
1	D	333	GLU	CB-CA-C	5.26	120.92	110.40
1	A	606	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	384	ARG	CG-CD-NE	5.23	122.78	111.80
1	C	447	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	130	TYR	CA-CB-CG	-5.08	103.74	113.40
1	C	333	GLU	CB-CA-C	5.08	120.55	110.40
1	C	31	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	706	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	333	GLU	CB-CA-C	5.02	120.44	110.40
1	B	517	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	379	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	541	THR	Peptide
1	B	416	ALA	Peptide
1	B	541	THR	Peptide
1	C	541	THR	Peptide
1	D	541	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	6469	0	6446	26	1
1	B	6410	0	6385	32	1
1	C	6439	0	6417	33	0
1	D	6465	0	6442	48	0
2	D	48	0	32	3	0
All	All	25831	0	25722	130	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 3.

All (130) 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:413:ALA:HB1	1:B:820:GLU:O	1.77	0.84
1:D:628:GLU:HA	1:D:631:LYS:HD3	1.60	0.81
1:A:615:LEU:HD21	1:A:690:ILE:HD11	1.64	0.79
1:C:794:GLU:O	1:C:797:LEU:O	2.04	0.74
1:D:391:ASN:OD1	1:D:401:HIS:HD2	1.71	0.74
1:D:794:GLU:O	1:D:798:THR:HG22	1.90	0.72
1:D:564:ILE:CD1	1:D:761:ILE:HD13	2.20	0.71
1:D:655:GLN:HA	1:D:658:VAL:HG22	1.75	0.67
1:C:396:GLY:HA3	1:D:142:ASN:HD22	1.63	0.64
1:A:79:LEU:HD21	1:A:143:ARG:HG3	1.80	0.62
1:B:410:GLN:O	1:C:825:ARG:NH2	2.32	0.62
1:B:196:THR:HA	1:B:199:GLN:HE21	1.65	0.61
1:D:746:GLN:HE22	1:D:774:GLY:HA2	1.65	0.61
1:C:157:LEU:HD13	1:C:166:LEU:HD23	1.84	0.60
1:A:771:LEU:O	1:A:775:VAL:HG12	2.02	0.59
1:C:79:LEU:HD21	1:C:143:ARG:HG3	1.83	0.59
1:B:771:LEU:O	1:B:775:VAL:HG12	2.03	0.59
1:B:79:LEU:HD21	1:B:143:ARG:HG3	1.84	0.59
1:D:79:LEU:HD21	1:D:143:ARG:HG3	1.84	0.59
1:C:196:THR:HA	1:C:199:GLN:HE21	1.67	0.58
1:C:771:LEU:O	1:C:775:VAL:HG12	2.02	0.58
1:D:633:ARG:NH2	1:D:668:GLU:OE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:LEU:HD13	1:D:166:LEU:HD23	1.86	0.57
1:A:196:THR:HA	1:A:199:GLN:HE21	1.70	0.57
1:B:157:LEU:HD13	1:B:166:LEU:HD23	1.86	0.56
1:A:157:LEU:HD13	1:A:166:LEU:HD23	1.87	0.56
1:D:326:LYS:HE3	1:D:331:HIS:HD2	1.71	0.56
1:C:159:THR:HG21	1:C:166:LEU:HD22	1.87	0.55
1:D:512:ARG:NH2	1:D:791:ASP:OD1	2.40	0.55
1:C:479:VAL:HG11	1:C:798:THR:CG2	2.37	0.55
1:C:472:VAL:HG21	1:C:798:THR:HG23	1.90	0.54
1:D:92:ASP:HA	1:D:830:ILE:HB	1.89	0.53
1:A:637:GLY:HA2	1:A:685:TYR:OH	2.08	0.53
1:A:633:ARG:NH2	1:A:668:GLU:OE2	2.42	0.53
1:D:159:THR:HG21	1:D:166:LEU:HD22	1.90	0.53
1:B:92:ASP:HA	1:B:830:ILE:HB	1.89	0.53
1:A:92:ASP:HA	1:A:830:ILE:HB	1.91	0.52
1:C:142:ASN:HD22	1:D:396:GLY:HA3	1.73	0.52
1:C:92:ASP:HA	1:C:830:ILE:HB	1.92	0.52
1:D:746:GLN:HE22	1:D:774:GLY:CA	2.23	0.51
1:C:509:SER:O	1:C:512:ARG:HD3	2.11	0.51
1:B:159:THR:HG21	1:B:166:LEU:HD22	1.92	0.51
1:D:549:ILE:HD12	1:D:680:LEU:HD13	1.92	0.51
1:B:444:HIS:CE1	1:C:384:ARG:HB3	2.47	0.50
1:B:509:SER:O	1:B:512:ARG:HD3	2.11	0.50
1:A:509:SER:O	1:A:512:ARG:HD3	2.11	0.50
1:A:67:VAL:HG11	1:A:75:MET:HE2	1.92	0.50
1:D:289:TYR:OH	1:D:343:LYS:NZ	2.45	0.49
1:B:173:GLN:HE22	1:B:176:ARG:NH1	2.11	0.49
1:A:159:THR:HG21	1:A:166:LEU:HD22	1.95	0.49
1:B:67:VAL:HG11	1:B:75:MET:HE2	1.94	0.49
1:C:289:TYR:OH	1:C:343:LYS:NZ	2.46	0.49
1:B:78:GLN:HB3	1:B:188:ILE:HD12	1.95	0.49
1:A:396:GLY:HA3	1:B:142:ASN:HD22	1.78	0.48
1:D:326:LYS:HE3	1:D:331:HIS:CD2	2.48	0.48
1:B:289:TYR:OH	1:B:343:LYS:NZ	2.46	0.48
1:A:289:TYR:OH	1:A:343:LYS:NZ	2.46	0.48
1:D:767:LEU:O	1:D:770:VAL:HG22	2.13	0.48
1:D:564:ILE:CD1	1:D:761:ILE:HG21	2.43	0.48
1:C:173:GLN:HE22	1:C:176:ARG:NH1	2.11	0.48
1:A:173:GLN:HE22	1:A:176:ARG:NH1	2.11	0.48
1:D:132:MET:HA	1:D:132:MET:HE2	1.96	0.48
1:D:78:GLN:HB3	1:D:188:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:GLN:HB3	1:C:188:ILE:HD12	1.95	0.47
1:A:12:LYS:C	1:A:13:LEU:HG	2.35	0.47
1:B:12:LYS:C	1:B:13:LEU:HG	2.35	0.47
1:C:67:VAL:HG11	1:C:75:MET:HE2	1.97	0.46
1:B:803:VAL:HG22	1:B:810:VAL:HG21	1.97	0.46
1:D:127:LEU:HD12	1:D:127:LEU:C	2.36	0.46
1:A:67:VAL:HG11	1:A:75:MET:CE	2.45	0.46
1:A:78:GLN:HB3	1:A:188:ILE:HD12	1.97	0.46
1:A:803:VAL:HG22	1:A:810:VAL:HG21	1.97	0.46
1:D:132:MET:CE	1:D:132:MET:HA	2.46	0.46
1:C:127:LEU:HD12	1:C:127:LEU:C	2.36	0.46
1:D:490:ARG:HH22	1:D:780:THR:HG23	1.81	0.46
1:D:620:MET:CE	2:D:900:COA:S1P	3.04	0.46
1:D:499:MET:HB2	2:D:900:COA:S1P	2.56	0.46
1:D:564:ILE:HD12	1:D:761:ILE:HD13	1.94	0.46
1:D:470:TYR:HD1	1:D:805:LEU:HD13	1.81	0.46
1:B:67:VAL:HG11	1:B:75:MET:CE	2.47	0.45
1:B:317:GLN:HE21	1:C:442:ARG:HH12	1.64	0.45
1:B:530:LEU:HD23	1:B:604:TYR:CD2	2.51	0.45
1:D:442:ARG:NH2	1:D:480:GLN:OE1	2.46	0.45
1:C:803:VAL:HG22	1:C:810:VAL:HG21	1.98	0.45
1:D:13:LEU:N	1:D:13:LEU:HD22	2.31	0.45
1:A:671:PHE:O	1:A:672:ALA:HB2	2.16	0.45
1:D:326:LYS:CE	1:D:331:HIS:CD2	2.99	0.45
1:C:12:LYS:C	1:C:13:LEU:HG	2.37	0.45
1:D:506:MET:O	1:D:538:LEU:HD22	2.17	0.45
1:B:221:GLY:HA2	1:B:297:THR:HG22	1.99	0.45
1:B:415:THR:HG22	1:B:819:VAL:HA	1.99	0.45
1:C:221:GLY:HA2	1:C:297:THR:HG22	1.99	0.45
1:B:127:LEU:HD12	1:B:127:LEU:C	2.37	0.44
1:B:415:THR:CG2	1:B:819:VAL:HA	2.48	0.44
1:C:530:LEU:HD23	1:C:604:TYR:CD2	2.53	0.44
1:A:127:LEU:C	1:A:127:LEU:HD12	2.37	0.44
1:A:530:LEU:HD23	1:A:604:TYR:CD2	2.53	0.44
1:C:243:TYR:OH	1:C:829:LEU:HD22	2.17	0.44
1:D:691:ALA:HB3	1:D:692:PRO:HD3	1.99	0.44
1:C:67:VAL:HG11	1:C:75:MET:CE	2.47	0.44
1:D:567:LEU:HA	1:D:570:VAL:HG22	2.00	0.44
1:B:380:PRO:HB2	1:C:28:GLY:HA2	1.99	0.43
1:C:795:PHE:O	1:C:798:THR:OG1	2.32	0.43
1:B:508:LEU:HD21	1:B:539:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:ALA:HB3	1:B:692:PRO:HD3	2.00	0.43
1:A:142:ASN:HD22	1:B:396:GLY:HA3	1.84	0.43
1:D:645:SER:HA	1:D:746:GLN:HE21	1.82	0.43
1:C:506:MET:O	1:C:538:LEU:HD22	2.19	0.43
1:B:506:MET:O	1:B:538:LEU:HD22	2.19	0.43
1:D:12:LYS:C	1:D:13:LEU:HD22	2.40	0.43
1:D:344:VAL:HG11	1:D:388:VAL:HG11	2.02	0.42
1:D:772:LYS:HG3	1:D:773:ARG:N	2.34	0.42
1:D:530:LEU:HD23	1:D:604:TYR:CD2	2.55	0.42
1:A:424:LEU:CD2	1:A:441:GLY:HA3	2.50	0.42
1:A:483:GLN:HG2	1:A:805:LEU:HD13	2.01	0.42
1:B:413:ALA:CB	1:B:820:GLU:O	2.60	0.41
1:B:411:ALA:HB3	1:C:411:ALA:HB2	2.02	0.41
1:D:54:LEU:HD13	1:D:226:GLU:HB2	2.02	0.41
1:A:506:MET:O	1:A:538:LEU:HD22	2.20	0.41
1:C:691:ALA:HB3	1:C:692:PRO:HD3	2.01	0.41
1:D:333:GLU:CB	1:D:334:PRO:CD	2.99	0.41
1:D:510:LEU:HD22	1:D:510:LEU:N	2.35	0.41
1:A:680:LEU:HB3	1:A:687:MET:HE3	2.03	0.41
1:C:333:GLU:CB	1:C:334:PRO:CD	2.99	0.41
1:D:504:ARG:HD2	1:D:543:GLU:O	2.19	0.41
1:B:333:GLU:CB	1:B:334:PRO:CD	2.99	0.41
1:D:766:LEU:HD21	2:D:900:COA:H71	2.03	0.41
1:C:570:VAL:HG13	1:C:570:VAL:O	2.21	0.41
1:D:749:LEU:HB3	1:D:775:VAL:HG22	2.03	0.41
1:D:221:GLY:HA2	1:D:297:THR:HG22	2.02	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)
1:A:615:LEU:O	1:B:317:GLN:OE1[3_657]	2.06	0.14

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	850/852 (100%)	809 (95%)	37 (4%)	4 (0%)	32	60
1	B	838/852 (98%)	796 (95%)	39 (5%)	3 (0%)	38	66
1	C	842/852 (99%)	801 (95%)	37 (4%)	4 (0%)	32	60
1	D	850/852 (100%)	806 (95%)	38 (4%)	6 (1%)	25	53
All	All	3380/3408 (99%)	3212 (95%)	151 (4%)	17 (0%)	32	60

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	GLU
1	B	333	GLU
1	C	333	GLU
1	C	798	THR
1	D	333	GLU
1	D	635	PRO
1	A	672	ALA
1	C	209	ASP
1	D	209	ASP
1	A	635	PRO
1	B	635	PRO
1	D	488	ASN
1	B	656	ALA
1	A	488	ASN
1	C	656	ALA
1	D	617	PRO
1	D	656	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	700/702 (100%)	661 (94%)	39 (6%)	25	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	694/702 (99%)	660 (95%)	34 (5%)	29	58
1	C	697/702 (99%)	658 (94%)	39 (6%)	25	51
1	D	699/702 (100%)	659 (94%)	40 (6%)	24	51
All	All	2790/2808 (99%)	2638 (95%)	152 (5%)	26	54

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	125	GLU
1	A	136	GLN
1	A	170	ASN
1	A	195	ASN
1	A	236	LYS
1	A	238	LEU
1	A	256	SER
1	A	287	LEU
1	A	370	LEU
1	A	384	ARG
1	A	402	VAL
1	A	462	THR
1	A	478	ARG
1	A	504	ARG
1	A	510	LEU
1	A	513	LEU
1	A	525	GLU
1	A	530	LEU
1	A	543	GLU
1	A	544	ARG
1	A	570	VAL
1	A	573	LYS
1	A	615	LEU
1	A	625	LEU
1	A	630	CYS
1	A	647	ASP
1	A	648	THR
1	A	666	LYS
1	A	667	GLN
1	A	676	ARG
1	A	699	LYS
1	A	746	GLN

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Mol	Chain	Res	Type
1	A	777	SER
1	A	786	LYS
1	A	790	LYS
1	A	803	VAL
1	A	805	LEU
1	A	852	ASN
1	B	49	LYS
1	B	71	GLN
1	B	125	GLU
1	B	136	GLN
1	B	195	ASN
1	B	236	LYS
1	B	238	LEU
1	B	256	SER
1	B	287	LEU
1	B	370	LEU
1	B	402	VAL
1	B	427	SER
1	B	436	ASP
1	B	478	ARG
1	B	504	ARG
1	B	510	LEU
1	B	513	LEU
1	B	525	GLU
1	B	530	LEU
1	B	533	LYS
1	B	544	ARG
1	B	570	VAL
1	B	625	LEU
1	B	630	CYS
1	B	647	ASP
1	B	648	THR
1	B	667	GLN
1	B	699	LYS
1	B	746	GLN
1	B	777	SER
1	B	790	LYS
1	B	803	VAL
1	B	805	LEU
1	B	852	ASN
1	C	71	GLN
1	C	136	GLN

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Mol	Chain	Res	Type
1	C	195	ASN
1	C	209	ASP
1	C	236	LYS
1	C	238	LEU
1	C	256	SER
1	C	278	GLN
1	C	287	LEU
1	C	370	LEU
1	C	379	ARG
1	C	384	ARG
1	C	402	VAL
1	C	409	ARG
1	C	436	ASP
1	C	478	ARG
1	C	504	ARG
1	C	510	LEU
1	C	513	LEU
1	C	525	GLU
1	C	530	LEU
1	C	533	LYS
1	C	543	GLU
1	C	544	ARG
1	C	570	VAL
1	C	625	LEU
1	C	630	CYS
1	C	647	ASP
1	C	648	THR
1	C	667	GLN
1	C	673	LYS
1	C	699	LYS
1	C	746	GLN
1	C	777	SER
1	C	790	LYS
1	C	798	THR
1	C	803	VAL
1	C	805	LEU
1	C	852	ASN
1	D	13	LEU
1	D	41	LYS
1	D	130	TYR
1	D	132	MET
1	D	173	GLN

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Mol	Chain	Res	Type
1	D	195	ASN
1	D	209	ASP
1	D	236	LYS
1	D	256	SER
1	D	370	LEU
1	D	402	VAL
1	D	431	LEU
1	D	436	ASP
1	D	442	ARG
1	D	462	THR
1	D	478	ARG
1	D	487	THR
1	D	513	LEU
1	D	525	GLU
1	D	530	LEU
1	D	537	LEU
1	D	544	ARG
1	D	573	LYS
1	D	597	ARG
1	D	625	LEU
1	D	628	GLU
1	D	630	CYS
1	D	647	ASP
1	D	648	THR
1	D	666	LYS
1	D	667	GLN
1	D	699	LYS
1	D	703	ARG
1	D	706	ARG
1	D	746	GLN
1	D	777	SER
1	D	790	LYS
1	D	798	THR
1	D	800	LEU
1	D	805	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	169	GLN
1	A	170	ASN

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Mol	Chain	Res	Type
1	A	173	GLN
1	A	199	GLN
1	A	271	GLN
1	A	480	GLN
1	A	667	GLN
1	A	723	GLN
1	A	799	ASN
1	A	852	ASN
1	B	142	ASN
1	B	169	GLN
1	B	170	ASN
1	B	173	GLN
1	B	199	GLN
1	B	317	GLN
1	B	480	GLN
1	B	667	GLN
1	B	723	GLN
1	B	799	ASN
1	B	852	ASN
1	C	142	ASN
1	C	169	GLN
1	C	170	ASN
1	C	173	GLN
1	C	199	GLN
1	C	480	GLN
1	C	667	GLN
1	C	723	GLN
1	C	799	ASN
1	C	852	ASN
1	D	25	ASN
1	D	142	ASN
1	D	328	ASN
1	D	331	HIS
1	D	401	HIS
1	D	608	GLN
1	D	614	HIS
1	D	659	ASN
1	D	683	HIS
1	D	746	GLN

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 ⓘ

1 ligand is 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	D	900	-	43,50,50	0.89	1 (2%)	48,75,75	2.04	11 (22%)

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	D	900	-	-	0/44/64/64	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	COA	C5A-C4A	2.94	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	COA	N3A-C2A-N1A	-9.22	120.83	128.86
2	D	900	COA	O5P-C5P-C6P	-2.65	117.03	122.01
2	D	900	COA	CDP-CBP-CAP	-2.48	104.51	108.82
2	D	900	COA	C1B-N9A-C4A	-2.24	122.76	126.64
2	D	900	COA	C3B-C2B-C1B	2.29	105.10	99.95
2	D	900	COA	C3P-N4P-C5P	2.58	127.79	122.84
2	D	900	COA	C6P-C7P-N8P	2.62	117.29	111.87
2	D	900	COA	N6A-C6A-N1A	2.66	124.03	118.77
2	D	900	COA	CEP-CBP-CCP	2.72	112.36	108.37
2	D	900	COA	C2A-N1A-C6A	2.81	123.69	118.77
2	D	900	COA	C6P-C5P-N4P	4.13	123.61	116.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	COA	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	852/852 (100%)	0.15	42 (4%) 30 29	22, 44, 85, 131	0
1	B	844/852 (99%)	0.68	122 (14%) 3 2	22, 50, 141, 264	0
1	C	848/852 (99%)	0.73	141 (16%) 2 1	21, 49, 151, 240	0
1	D	852/852 (100%)	0.18	51 (5%) 23 21	22, 43, 96, 158	0
All	All	3396/3408 (99%)	0.43	356 (10%) 7 5	21, 46, 134, 264	0

All (356) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	621	ALA	12.7
1	B	665	LEU	12.6
1	B	637	GLY	9.1
1	A	656	ALA	8.7
1	C	665	LEU	8.6
1	D	665	LEU	8.3
1	B	664	GLN	8.1
1	B	661	PHE	8.1
1	C	659	ASN	7.9
1	C	546	PHE	7.7
1	B	662	VAL	7.6
1	B	667	GLN	7.1
1	C	661	PHE	6.8
1	C	672	ALA	6.7
1	C	663	GLU	6.6
1	B	658	VAL	6.5
1	B	670	VAL	6.4
1	D	656	ALA	6.4
1	C	629	GLU	6.3
1	C	667	GLN	6.1
1	C	521	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	656	ALA	6.0
1	C	632	GLN	5.9
1	B	539	LEU	5.8
1	C	654	PRO	5.8
1	B	659	ASN	5.7
1	C	676	ARG	5.7
1	C	622	ALA	5.6
1	A	661	PHE	5.5
1	C	693	THR	5.5
1	B	507	GLY	5.5
1	C	656	ALA	5.5
1	B	651	ILE	5.4
1	C	657	ALA	5.4
1	A	669	GLY	5.4
1	B	602	ALA	5.3
1	A	417	HIS	5.3
1	B	505	GLY	5.3
1	A	750	TRP	5.3
1	B	669	GLY	5.3
1	B	632	GLN	5.2
1	D	636	ALA	5.2
1	C	658	VAL	5.1
1	C	660	GLU	5.1
1	C	633	ARG	5.1
1	C	662	VAL	5.1
1	C	541	THR	5.0
1	C	619	SER	5.0
1	B	663	GLU	5.0
1	D	635	PRO	5.0
1	C	617	PRO	5.0
1	A	633	ARG	5.0
1	B	671	PHE	4.9
1	C	597	ARG	4.9
1	C	788	ASP	4.9
1	B	640	PRO	4.9
1	B	638	VAL	4.9
1	D	634	CYS	4.8
1	B	527	VAL	4.8
1	B	624	GLY	4.7
1	B	605	TRP	4.7
1	B	660	GLU	4.7
1	B	621	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	630	CYS	4.7
1	C	635	PRO	4.6
1	B	696	GLN	4.6
1	C	677	THR	4.6
1	B	619	SER	4.6
1	B	631	LYS	4.6
1	C	669	GLY	4.6
1	B	601	LEU	4.6
1	C	508	LEU	4.6
1	B	537	LEU	4.6
1	D	661	PHE	4.5
1	B	633	ARG	4.5
1	C	696	GLN	4.5
1	C	620	MET	4.5
1	B	654	PRO	4.5
1	A	415	THR	4.5
1	B	630	CYS	4.5
1	C	730	SER	4.4
1	B	695	LEU	4.4
1	B	655	GLN	4.4
1	D	658	VAL	4.4
1	B	625	LEU	4.4
1	C	655	GLN	4.4
1	D	613	ALA	4.3
1	B	705	PRO	4.3
1	C	724	SER	4.3
1	B	508	LEU	4.3
1	C	416	ALA	4.3
1	C	418	ALA	4.2
1	C	604	TYR	4.2
1	B	639	VAL	4.2
1	B	533	LYS	4.2
1	B	478	ARG	4.2
1	B	634	CYS	4.1
1	D	616	PRO	4.1
1	C	734	TYR	4.1
1	C	533	LYS	4.1
1	B	672	ALA	4.1
1	B	699	LYS	4.1
1	D	614	HIS	4.1
1	C	750	TRP	4.1
1	D	703	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	687	MET	4.0
1	D	631	LYS	4.0
1	C	649	VAL	4.0
1	D	487	THR	4.0
1	B	668	GLU	4.0
1	C	530	LEU	3.9
1	B	614	HIS	3.9
1	C	417	HIS	3.9
1	C	605	TRP	3.9
1	B	511	MET	3.9
1	D	615	LEU	3.8
1	C	555	SER	3.8
1	C	689	GLY	3.8
1	D	638	VAL	3.8
1	D	489	LYS	3.8
1	A	667	GLN	3.8
1	B	750	TRP	3.7
1	C	723	GLN	3.7
1	C	668	GLU	3.7
1	B	722	TRP	3.7
1	A	489	LYS	3.7
1	B	646	GLU	3.7
1	A	703	ARG	3.7
1	C	612	ASP	3.6
1	B	532	VAL	3.6
1	C	733	GLU	3.6
1	B	657	ALA	3.6
1	A	431	LEU	3.5
1	C	751	HIS	3.5
1	B	728	ARG	3.5
1	B	530	LEU	3.5
1	B	620	MET	3.5
1	C	631	LYS	3.4
1	A	631	LYS	3.4
1	B	704	GLU	3.4
1	B	622	ALA	3.4
1	A	629	GLU	3.4
1	C	664	GLN	3.4
1	C	681	ALA	3.3
1	B	703	ARG	3.3
1	C	627	TRP	3.3
1	A	671	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1	SER	3.3
1	B	541	THR	3.3
1	B	720	ALA	3.3
1	D	660	GLU	3.3
1	B	723	GLN	3.3
1	D	667	GLN	3.3
1	B	535	SER	3.3
1	B	544	ARG	3.3
1	B	636	ALA	3.3
1	A	664	GLN	3.3
1	C	499	MET	3.3
1	B	629	GLU	3.2
1	C	600	VAL	3.2
1	D	622	ALA	3.2
1	C	624	GLY	3.2
1	C	700	LYS	3.2
1	A	621	ALA	3.2
1	D	672	ALA	3.2
1	C	682	PHE	3.2
1	B	463	ALA	3.2
1	B	793	LEU	3.1
1	B	613	ALA	3.1
1	C	628	GLU	3.1
1	B	462	THR	3.1
1	C	721	GLN	3.1
1	B	542	ASP	3.1
1	D	415	THR	3.1
1	D	627	TRP	3.1
1	C	702	ILE	3.1
1	B	700	LYS	3.1
1	C	625	LEU	3.1
1	B	692	PRO	3.1
1	B	416	ALA	3.0
1	B	628	GLU	3.0
1	B	641	ALA	3.0
1	C	634	CYS	3.0
1	C	679	GLY	3.0
1	B	538	LEU	3.0
1	B	685	TYR	3.0
1	C	517	ARG	3.0
1	A	657	ALA	3.0
1	C	725	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	618	GLY	3.0
1	C	703	ARG	3.0
1	D	633	ARG	3.0
1	C	623	VAL	3.0
1	B	597	ARG	3.0
1	C	705	PRO	2.9
1	C	415	THR	2.9
1	C	666	LYS	2.9
1	A	665	LEU	2.9
1	D	657	ALA	2.9
1	B	523	SER	2.9
1	A	628	GLU	2.9
1	B	525	GLU	2.9
1	D	621	ALA	2.9
1	A	668	GLU	2.8
1	B	690	ILE	2.8
1	C	478	ARG	2.8
1	C	711	ARG	2.8
1	B	534	VAL	2.8
1	D	686	PHE	2.8
1	C	704	GLU	2.8
1	C	653	GLY	2.8
1	B	540	SER	2.8
1	B	653	GLY	2.8
1	C	504	ARG	2.8
1	C	728	ARG	2.8
1	B	521	LEU	2.8
1	C	675	VAL	2.8
1	B	618	GLY	2.8
1	D	663	GLU	2.8
1	A	666	LYS	2.8
1	B	517	ARG	2.8
1	D	669	GLY	2.8
1	B	529	PRO	2.7
1	C	720	ALA	2.7
1	D	681	ALA	2.7
1	A	486	SER	2.7
1	B	729	THR	2.7
1	A	416	ALA	2.7
1	C	670	VAL	2.7
1	C	671	PHE	2.7
1	B	536	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	68	HIS	2.7
1	A	627	TRP	2.7
1	C	683	HIS	2.7
1	B	526	ALA	2.7
1	B	627	TRP	2.7
1	C	692	PRO	2.6
1	D	1	SER	2.6
1	D	617	PRO	2.6
1	A	476	GLU	2.6
1	A	625	LEU	2.6
1	C	637	GLY	2.6
1	C	125	GLU	2.6
1	B	623	VAL	2.6
1	A	632	GLN	2.6
1	B	725	SER	2.6
1	C	1	SER	2.6
1	C	651	ILE	2.6
1	C	749	LEU	2.6
1	C	732	ALA	2.6
1	A	790	LYS	2.6
1	C	694	LEU	2.5
1	B	666	LYS	2.5
1	C	549	ILE	2.5
1	B	612	ASP	2.5
1	B	417	HIS	2.5
1	B	609	CYS	2.5
1	A	1	SER	2.5
1	C	528	LYS	2.5
1	C	539	LEU	2.5
1	D	685	TYR	2.5
1	D	620	MET	2.5
1	B	528	LYS	2.4
1	D	666	LYS	2.4
1	B	554	VAL	2.4
1	C	525	GLU	2.4
1	D	704	GLU	2.4
1	C	680	LEU	2.4
1	C	706	ARG	2.4
1	C	542	ASP	2.4
1	C	701	VAL	2.4
1	B	499	MET	2.4
1	B	504	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	130	TYR	2.4
1	C	526	ALA	2.4
1	A	317	GLN	2.3
1	A	487	THR	2.3
1	B	550	VAL	2.3
1	B	733	GLU	2.3
1	C	491	PRO	2.3
1	C	544	ARG	2.3
1	A	723	GLN	2.3
1	D	670	VAL	2.3
1	C	722	TRP	2.3
1	A	412	PRO	2.3
1	C	511	MET	2.3
1	C	554	VAL	2.3
1	C	594	LEU	2.3
1	B	415	THR	2.3
1	B	754	GLU	2.3
1	C	674	GLU	2.3
1	C	773	ARG	2.2
1	C	609	CYS	2.2
1	C	500	GLY	2.2
1	C	551	HIS	2.2
1	C	601	LEU	2.2
1	D	417	HIS	2.2
1	B	506	MET	2.2
1	C	613	ALA	2.2
1	C	699	LYS	2.2
1	C	685	TYR	2.2
1	B	514	ASP	2.2
1	D	682	PHE	2.2
1	D	664	GLN	2.2
1	A	488	ASN	2.2
1	C	492	LEU	2.2
1	C	529	PRO	2.2
1	B	788	ASP	2.2
1	A	41	LYS	2.2
1	C	581	SER	2.2
1	C	652	SER	2.2
1	D	680	LEU	2.2
1	C	503	TRP	2.2
1	A	315	PHE	2.2
1	B	573	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	367	PRO	2.2
1	C	647	ASP	2.2
1	C	556	LEU	2.2
1	D	485	VAL	2.2
1	A	660	GLU	2.2
1	C	557	THR	2.2
1	D	671	PHE	2.2
1	B	652	SER	2.1
1	D	488	ASN	2.1
1	B	414	PRO	2.1
1	C	753	PRO	2.1
1	B	689	GLY	2.1
1	A	418	ALA	2.1
1	B	693	THR	2.1
1	A	258	GLU	2.1
1	C	595	SER	2.1
1	C	505	GLY	2.1
1	C	638	VAL	2.1
1	C	413	ALA	2.1
1	D	431	LEU	2.1
1	D	639	VAL	2.1
1	B	686	PHE	2.1
1	C	537	LEU	2.1
1	C	818	PRO	2.1
1	C	765	ALA	2.1
1	A	462	THR	2.1
1	B	531	GLY	2.1
1	C	553	PHE	2.1
1	A	413	ALA	2.0
1	A	504	ARG	2.0
1	C	708	ARG	2.0
1	B	678	GLY	2.0
1	C	498	GLY	2.0
1	C	678	GLY	2.0
1	D	68	HIS	2.0
1	B	635	PRO	2.0
1	C	516	PHE	2.0
1	D	370	LEU	2.0
1	C	558	ALA	2.0
1	C	523	SER	2.0
1	B	606	ARG	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(\AA^2)	Q<0.9
2	COA	D	900	48/48	0.80	0.33	1.42	94,116,135,138	0

6.5 Other polymers [i](#)

There are no such residues in this entry.