



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:50 AM UTC

PDB ID : 5MY2 / pdb_00005my2
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

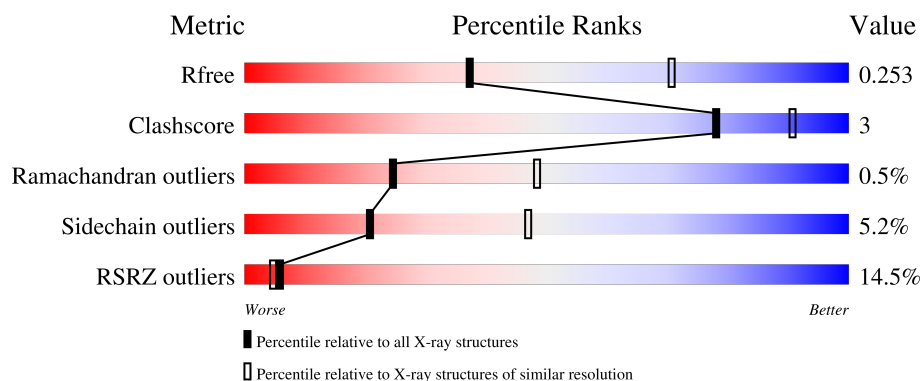
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	4% 89% 10%
1	B	852	21% 88% 10%
1	C	852	23% 89% 9%
1	D	852	9% 86% 12%

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 (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).

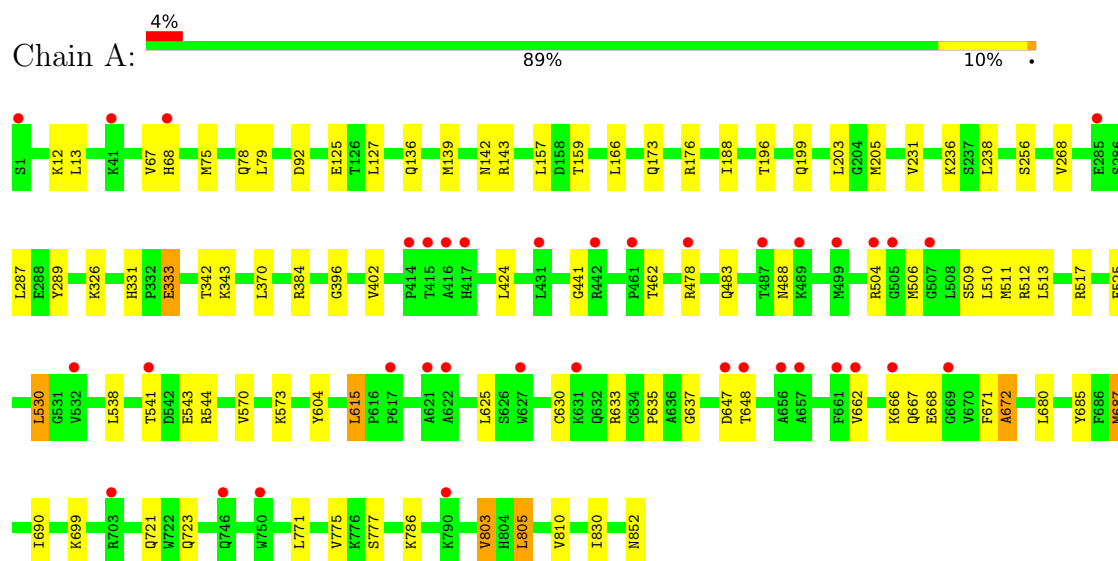


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

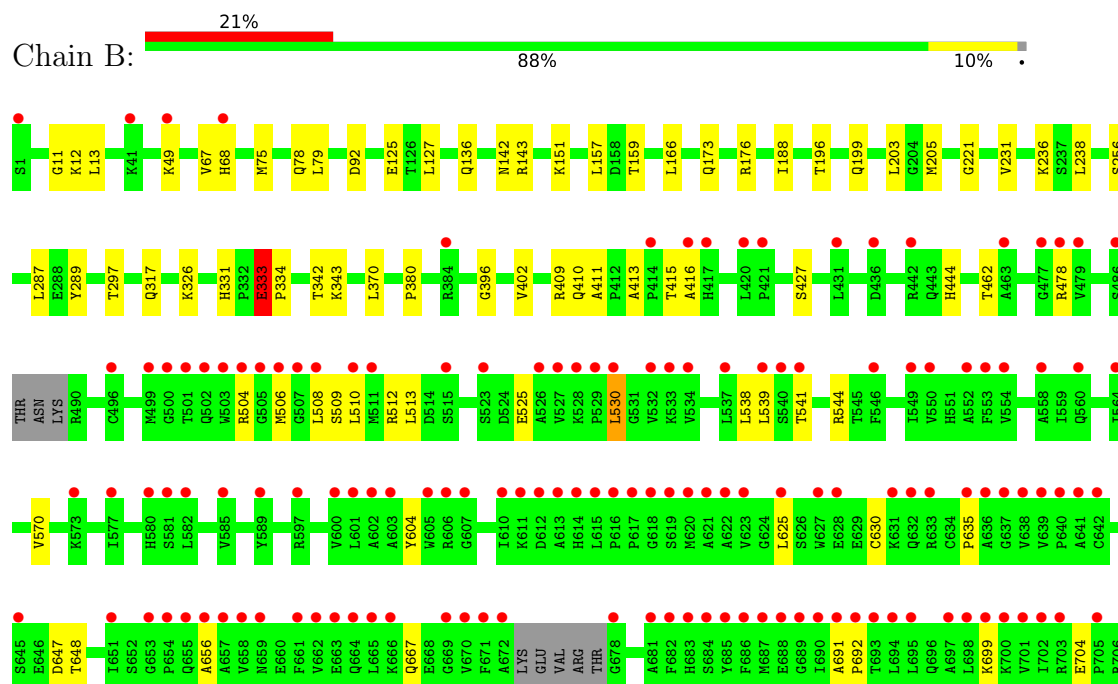
3 Residue-property plots [i](#)

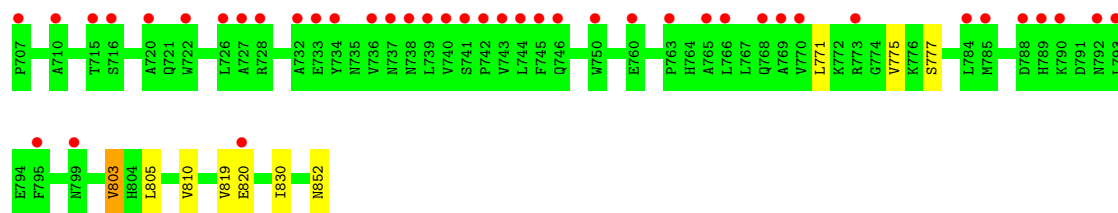
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

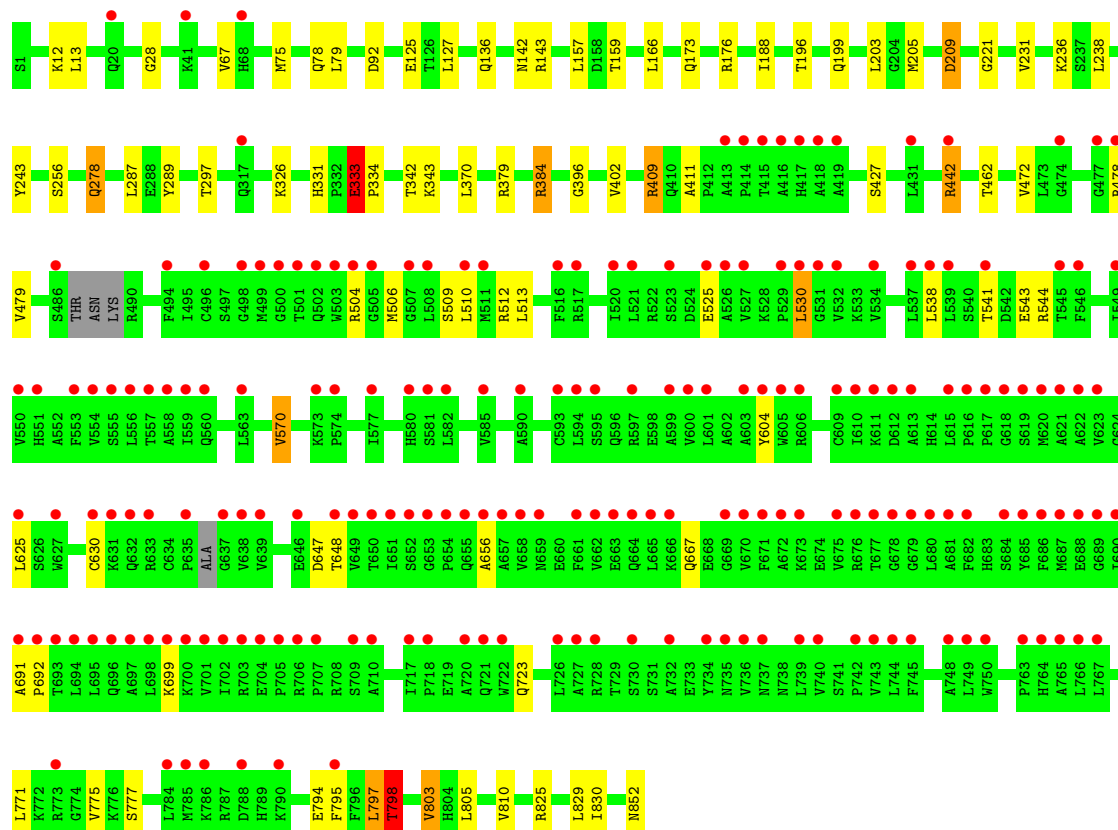
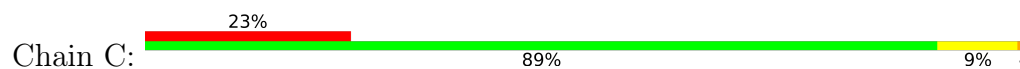


• Molecule 1: Fatty acid synthase

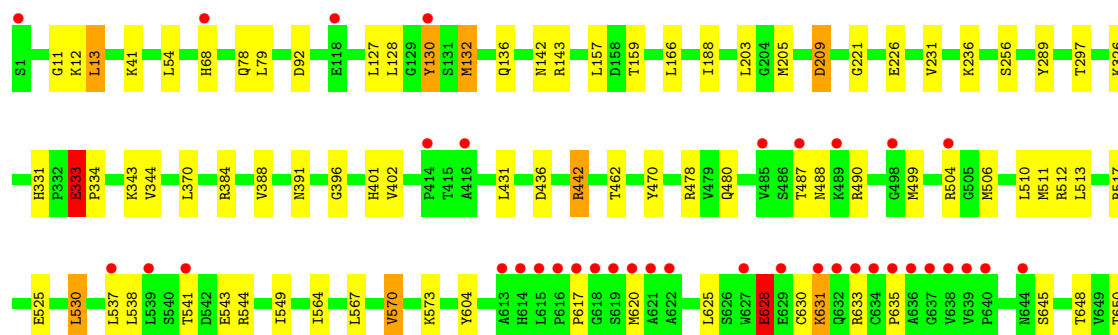
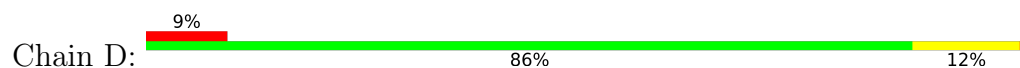


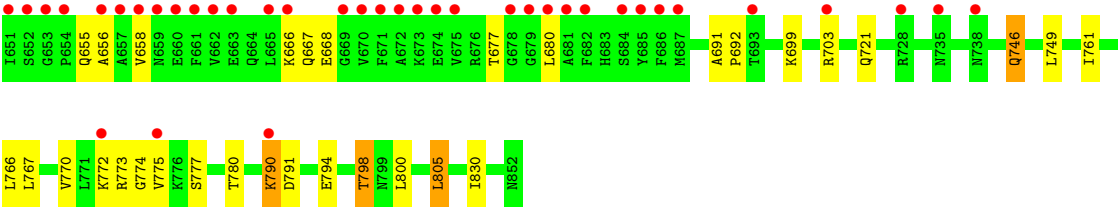


● Molecule 1: Fatty acid synthase



● 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 – 2.70 183.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (183.54-2.70) 99.2 (183.54-2.70)	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	7264 reflections (3.95%)	wwPDB-VP
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 , 38.1	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	0.88	0/6616	1.00	5/9000 (0.1%)
1	B	0.86	1/6555 (0.0%)	0.98	5/8914 (0.1%)
1	C	0.85	1/6583 (0.0%)	1.00	11/8951 (0.1%)
1	D	0.90	0/6612	1.02	12/8995 (0.1%)
All	All	0.87	2/26366 (0.0%)	1.00	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	797	LEU	C-N	-5.89	1.25	1.33
1	B	409	ARG	C-O	-5.65	1.16	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	798	THR	N-CA-CB	8.77	125.30	110.49
1	C	209	ASP	N-CA-CB	-8.23	96.57	110.49
1	D	209	ASP	N-CA-CB	-7.79	97.32	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	209	ASP	CB-CA-C	-7.03	96.42	110.42
1	C	209	ASP	CB-CA-C	-6.86	96.76	110.42
1	C	278	GLN	CA-CB-CG	6.29	126.68	114.10
1	D	790	LYS	CA-CB-CG	6.15	126.41	114.10
1	C	409	ARG	CB-CA-C	-6.10	101.24	109.71
1	D	333	GLU	CA-C-N	-6.00	113.44	119.56
1	D	333	GLU	C-N-CA	-6.00	113.44	119.56
1	A	333	GLU	CA-C-N	-5.65	113.80	119.56
1	A	333	GLU	C-N-CA	-5.65	113.80	119.56
1	D	130	TYR	CA-CB-CG	-5.64	103.74	113.90
1	A	68	HIS	CB-CA-C	5.59	117.49	109.11
1	A	333	GLU	CB-CA-C	5.47	120.95	110.17
1	B	333	GLU	CA-C-N	-5.47	113.98	119.56
1	B	333	GLU	C-N-CA	-5.47	113.98	119.56
1	D	333	GLU	CB-CA-C	5.46	120.92	110.17
1	D	11	GLY	N-CA-C	5.42	118.63	110.18
1	C	333	GLU	CA-C-N	-5.40	114.06	119.56
1	C	333	GLU	C-N-CA	-5.40	114.06	119.56
1	B	68	HIS	CB-CA-C	5.39	117.20	109.11
1	D	68	HIS	CB-CA-C	5.30	117.06	109.11
1	C	333	GLU	CB-CA-C	5.27	120.55	110.17
1	B	333	GLU	CB-CA-C	5.21	120.44	110.17
1	D	209	ASP	N-CA-C	5.21	121.89	110.80
1	C	797	LEU	CB-CA-C	-5.21	102.82	111.41
1	C	209	ASP	N-CA-C	5.20	121.88	110.80
1	D	628	GLU	CB-CA-C	5.20	119.69	110.85
1	D	570	VAL	CA-CB-CG2	5.10	119.07	110.40
1	C	442	ARG	N-CA-C	-5.08	104.83	111.02
1	B	11	GLY	N-CA-C	5.03	118.03	110.18
1	A	687	MET	CA-C-O	5.03	125.17	119.18

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	32	1
1	B	6410	0	6385	36	1
1	C	6439	0	6417	35	0
1	D	6465	0	6442	53	0
2	D	48	0	32	4	0
All	All	25831	0	25722	145	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 (145) 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:C:203:LEU:HD13	1:C:205:MET:HE3	1.71	0.72
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:A:203:LEU:HD13	1:A:205:MET:HE3	1.77	0.65
1:B:203:LEU:HD13	1:B:205:MET:HE3	1.79	0.65
1:D:203:LEU:HD13	1:D:205:MET:HE3	1.78	0.65
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:79:LEU:HD21	1:B:143:ARG:HG3	1.84	0.59
1:B:771:LEU:O	1:B:775:VAL:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:132:MET:HE3	1:D:132:MET:HA	1.89	0.54
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:B:12:LYS:C	1:B:13:LEU:HG	2.35	0.51
1:A:12:LYS:C	1:A:13:LEU:HG	2.35	0.51
1:D:127:LEU:HD12	1:D:127:LEU:C	2.36	0.51
1:D:746:GLN:HE22	1:D:774:GLY:CA	2.23	0.51
1:C:127:LEU:C	1:C:127:LEU:HD12	2.36	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:680:LEU:CD2	1:A:687:MET:HE1	2.41	0.50
1:B:67:VAL:HG11	1:B:75:MET:HE2	1.92	0.50
1:D:289:TYR:OH	1:D:343:LYS:NZ	2.45	0.49
1:A:67:VAL:HG11	1:A:75:MET:HE2	1.93	0.49
1:B:173:GLN:HE22	1:B:176:ARG:NH1	2.11	0.49
1:B:127:LEU:C	1:B:127:LEU:HD12	2.37	0.49
1:A:127:LEU:C	1:A:127:LEU:HD12	2.37	0.49
1:C:12:LYS:C	1:C:13:LEU:HG	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:THR:HG21	1:A:166:LEU:HD22	1.95	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:78:GLN:HB3	1:D:188:ILE:HD12	1.96	0.48
1:C:67:VAL:HG11	1:C:75:MET:HE2	1.96	0.47
1:C:78:GLN:HB3	1:C:188:ILE:HD12	1.95	0.47
1:D:12:LYS:C	1:D:13:LEU:HD22	2.40	0.47
1:D:132:MET:HE2	1:D:136:GLN:HB2	1.97	0.47
1:B:803:VAL:HG22	1:B:810:VAL:HG21	1.97	0.46
1:D:499:MET:HE3	1:D:677:THR:HA	1.97	0.46
1:D:650:THR:OG1	2:D:900:COA:O5P	2.33	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:HA	1:D:132:MET:CE	2.46	0.46
1:A:680:LEU:HD22	1:A:687:MET:HE1	1.97	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:470:TYR:HD1	1:D:805:LEU:HD13	1.81	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: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:HD22	1:D:13:LEU:N	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:D:506:MET:O	1:D:538:LEU:HD22	2.17	0.45
1:A:268:VAL:HG22	1:B:151:LYS:HZ3	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:GLY:HA2	1:C:297:THR:HG22	1.99	0.45
1:B:415:THR:CG2	1:B:819:VAL:HA	2.48	0.44
1:C:326:LYS:HE3	1:C:331:HIS:HD1	1.82	0.44
1:C:530:LEU:HD23	1:C:604:TYR:CD2	2.53	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
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: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:326:LYS:HE3	1:A:331:HIS:HD1	1.84	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:326:LYS:HE3	1:B:331:HIS:HD1	1.85	0.41
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: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:C:570:VAL:HG13	1:C:570:VAL:O	2.21	0.41
1:D:766:LEU:HD21	2:D:900:COA:H71	2.03	0.41
1:A:139:MET:HE1	1:B:396:GLY:HA3	2.03	0.41
1:A:511:MET:HE3	1:A:517:ARG:HG3	2.02	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
1:D:511:MET:HE3	1:D:517:ARG:HG3	2.04	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%)	24	48
1	B	838/852 (98%)	796 (95%)	39 (5%)	3 (0%)	30	54
1	C	842/852 (99%)	801 (95%)	37 (4%)	4 (0%)	24	48
1	D	850/852 (100%)	806 (95%)	38 (4%)	6 (1%)	18	41
All	All	3380/3408 (99%)	3212 (95%)	151 (4%)	17 (0%)	24	48

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

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Mol	Chain	Res	Type
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%)	662 (95%)	38 (5%)	20	45
1	B	694/702 (99%)	662 (95%)	32 (5%)	24	51
1	C	697/702 (99%)	660 (95%)	37 (5%)	20	46
1	D	699/702 (100%)	660 (94%)	39 (6%)	19	44
All	All	2790/2808 (99%)	2644 (95%)	146 (5%)	21	47

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	GLU
1	A	136	GLN
1	A	231	VAL
1	A	236	LYS
1	A	238	LEU
1	A	256	SER
1	A	287	LEU
1	A	342	THR
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

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Mol	Chain	Res	Type
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	662	VAL
1	A	666	LYS
1	A	667	GLN
1	A	699	LYS
1	A	721	GLN
1	A	723	GLN
1	A	777	SER
1	A	786	LYS
1	A	803	VAL
1	A	805	LEU
1	A	852	ASN
1	B	49	LYS
1	B	125	GLU
1	B	136	GLN
1	B	231	VAL
1	B	236	LYS
1	B	238	LEU
1	B	256	SER
1	B	287	LEU
1	B	342	THR
1	B	370	LEU
1	B	402	VAL
1	B	427	SER
1	B	462	THR
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	544	ARG
1	B	570	VAL
1	B	625	LEU
1	B	630	CYS

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Mol	Chain	Res	Type
1	B	647	ASP
1	B	648	THR
1	B	667	GLN
1	B	699	LYS
1	B	704	GLU
1	B	777	SER
1	B	803	VAL
1	B	805	LEU
1	B	852	ASN
1	C	125	GLU
1	C	136	GLN
1	C	231	VAL
1	C	236	LYS
1	C	238	LEU
1	C	256	SER
1	C	278	GLN
1	C	287	LEU
1	C	342	THR
1	C	370	LEU
1	C	379	ARG
1	C	384	ARG
1	C	402	VAL
1	C	409	ARG
1	C	427	SER
1	C	462	THR
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	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	699	LYS
1	C	723	GLN
1	C	777	SER

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Mol	Chain	Res	Type
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	128	LEU
1	D	130	TYR
1	D	132	MET
1	D	231	VAL
1	D	236	LYS
1	D	256	SER
1	D	370	LEU
1	D	384	ARG
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	625	LEU
1	D	628	GLU
1	D	630	CYS
1	D	631	LYS
1	D	648	THR
1	D	666	LYS
1	D	667	GLN
1	D	699	LYS
1	D	703	ARG
1	D	721	GLN
1	D	746	GLN
1	D	777	SER
1	D	790	LYS
1	D	798	THR
1	D	800	LEU

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Mol	Chain	Res	Type
1	D	805	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	169	GLN
1	A	170	ASN
1	A	173	GLN
1	A	199	GLN
1	A	271	GLN
1	A	399	ASN
1	A	410	GLN
1	A	422	HIS
1	A	480	GLN
1	A	664	GLN
1	A	723	GLN
1	A	746	GLN
1	A	755	HIS
1	A	799	ASN
1	A	833	HIS
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	399	ASN
1	B	480	GLN
1	B	664	GLN
1	B	723	GLN
1	B	746	GLN
1	B	755	HIS
1	B	799	ASN
1	B	833	HIS
1	B	852	ASN
1	C	142	ASN
1	C	169	GLN
1	C	170	ASN
1	C	173	GLN
1	C	199	GLN

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Mol	Chain	Res	Type
1	C	399	ASN
1	C	422	HIS
1	C	480	GLN
1	C	667	GLN
1	C	723	GLN
1	C	746	GLN
1	C	755	HIS
1	C	799	ASN
1	C	833	HIS
1	C	852	ASN
1	D	25	ASN
1	D	78	GLN
1	D	104	ASN
1	D	142	ASN
1	D	170	ASN
1	D	328	ASN
1	D	331	HIS
1	D	399	ASN
1	D	401	HIS
1	D	410	GLN
1	D	422	HIS
1	D	608	GLN
1	D	614	HIS
1	D	659	ASN
1	D	683	HIS
1	D	738	ASN
1	D	746	GLN
1	D	833	HIS

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 oligosaccharides 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	-	47,50,50	1.46	5 (10%)	69,75,75	1.97	20 (28%)

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	-	-	17/48/64/64	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	COA	P2A-O3A	4.60	1.64	1.59
2	D	900	COA	C5A-C4A	4.51	1.47	1.39
2	D	900	COA	P1A-O3A	4.14	1.64	1.59
2	D	900	COA	C5A-C6A	2.55	1.48	1.41
2	D	900	COA	C8A-N7A	2.24	1.36	1.31

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	COA	N3A-C2A-N1A	-5.12	120.83	128.58
2	D	900	COA	C4A-N9A-C8A	5.05	111.05	105.74
2	D	900	COA	N3A-C4A-N9A	4.82	135.37	127.17
2	D	900	COA	C5A-C4A-N3A	-4.48	120.55	126.72
2	D	900	COA	C6P-C5P-N4P	3.99	123.61	116.34
2	D	900	COA	C2A-N3A-C4A	3.93	121.42	111.83
2	D	900	COA	C2A-N1A-C6A	3.02	123.69	118.73
2	D	900	COA	N9A-C8A-N7A	-3.02	109.66	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	COA	O5P-C5P-C6P	-2.76	117.03	122.02
2	D	900	COA	C3P-N4P-C5P	2.67	127.79	122.82
2	D	900	COA	N6A-C6A-N1A	2.54	124.03	118.38
2	D	900	COA	CEP-CBP-CCP	2.51	112.36	108.22
2	D	900	COA	CDP-CBP-CAP	-2.50	104.51	108.77
2	D	900	COA	C6P-C7P-N8P	2.48	117.29	112.00
2	D	900	COA	C5A-N7A-C8A	2.43	107.26	103.45
2	D	900	COA	C6A-C5A-N7A	2.38	136.67	132.09
2	D	900	COA	C3B-C2B-C1B	2.37	105.10	99.89
2	D	900	COA	C4A-C5A-N7A	-2.29	107.97	110.58
2	D	900	COA	C5A-C6A-N6A	-2.21	117.83	123.29
2	D	900	COA	O9P-C9P-CAP	-2.02	115.24	120.89

There are no chirality outliers.

All (17) torsion outliers are listed below:

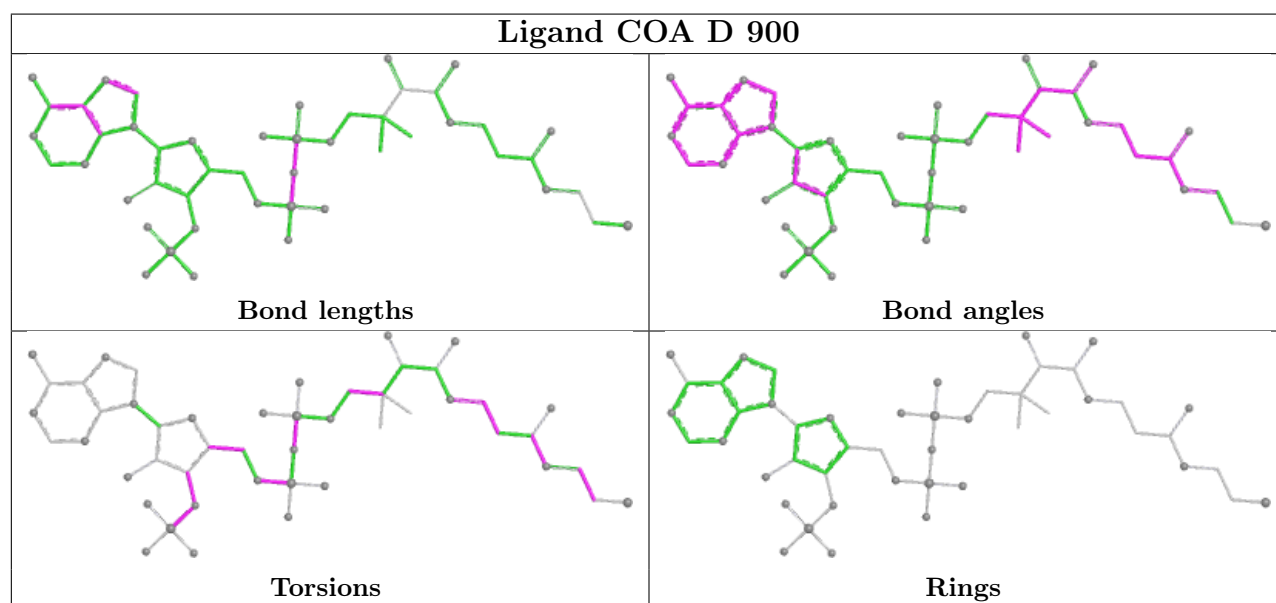
Mol	Chain	Res	Type	Atoms
2	D	900	COA	C5B-O5B-P1A-O2A
2	D	900	COA	CDP-CBP-CCP-O6A
2	D	900	COA	S1P-C2P-C3P-N4P
2	D	900	COA	C6P-C5P-N4P-C3P
2	D	900	COA	O5P-C5P-N4P-C3P
2	D	900	COA	C4B-C3B-O3B-P3B
2	D	900	COA	C5P-C6P-C7P-N8P
2	D	900	COA	C6P-C7P-N8P-C9P
2	D	900	COA	P1A-O3A-P2A-O4A
2	D	900	COA	CEP-CBP-CCP-O6A
2	D	900	COA	C5B-O5B-P1A-O1A
2	D	900	COA	C5B-O5B-P1A-O3A
2	D	900	COA	C2B-C3B-O3B-P3B
2	D	900	COA	C3B-C4B-C5B-O5B
2	D	900	COA	P1A-O3A-P2A-O5A
2	D	900	COA	C3B-O3B-P3B-O7A
2	D	900	COA	CAP-CBP-CCP-O6A

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	COA	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	0.23	37 (4%) 40 36	22, 44, 85, 131	0
1	B	844/852 (99%)	0.90	182 (21%) 2 2	22, 50, 141, 264	0
1	C	848/852 (99%)	0.92	198 (23%) 2 2	21, 49, 151, 240	0
1	D	852/852 (100%)	0.37	75 (8%) 15 13	22, 43, 96, 158	0
All	All	3396/3408 (99%)	0.61	492 (14%) 6 5	21, 46, 134, 264	0

All (492) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	750	TRP	8.1
1	C	621	ALA	8.1
1	D	616	PRO	7.9
1	C	665	LEU	7.6
1	A	656	ALA	7.5
1	B	665	LEU	7.4
1	B	662	VAL	7.4
1	D	615	LEU	7.3
1	C	672	ALA	7.3
1	B	671	PHE	7.3
1	B	685	TYR	6.5
1	D	686	PHE	6.4
1	C	635	PRO	6.3
1	D	613	ALA	6.3
1	B	661	PHE	6.2
1	B	602	ALA	6.2
1	C	417	HIS	6.2
1	B	601	LEU	6.2
1	C	750	TRP	6.1
1	A	661	PHE	6.1
1	C	622	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	662	VAL	6.1
1	C	661	PHE	6.0
1	C	657	ALA	5.9
1	B	622	ALA	5.8
1	C	637	GLY	5.8
1	B	672	ALA	5.7
1	C	656	ALA	5.6
1	C	669	GLY	5.6
1	C	671	PHE	5.6
1	C	546	PHE	5.5
1	C	673	LYS	5.5
1	C	654	PRO	5.5
1	B	478	ARG	5.4
1	C	630	CYS	5.4
1	D	656	ALA	5.3
1	D	672	ALA	5.3
1	C	530	LEU	5.3
1	D	635	PRO	5.2
1	D	617	PRO	5.2
1	D	638	VAL	5.1
1	D	661	PHE	5.1
1	A	416	ALA	5.0
1	C	501	THR	5.0
1	B	658	VAL	5.0
1	D	657	ALA	4.9
1	B	507	GLY	4.9
1	B	619	SER	4.9
1	C	685	TYR	4.9
1	C	689	GLY	4.9
1	B	621	ALA	4.9
1	B	605	TRP	4.9
1	B	654	PRO	4.9
1	C	416	ALA	4.8
1	D	130	TYR	4.8
1	D	541	THR	4.8
1	B	750	TRP	4.8
1	C	682	PHE	4.7
1	B	539	LEU	4.7
1	B	657	ALA	4.7
1	B	656	ALA	4.7
1	B	613	ALA	4.6
1	C	766	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	555	SER	4.6
1	C	675	VAL	4.6
1	C	617	PRO	4.5
1	B	639	VAL	4.5
1	B	678	GLY	4.5
1	C	499	MET	4.5
1	B	615	LEU	4.5
1	D	654	PRO	4.5
1	C	478	ARG	4.4
1	B	689	GLY	4.4
1	B	620	MET	4.3
1	A	499	MET	4.3
1	C	620	MET	4.3
1	D	614	HIS	4.3
1	B	640	PRO	4.3
1	B	499	MET	4.3
1	D	665	LEU	4.3
1	B	637	GLY	4.2
1	C	679	GLY	4.2
1	D	680	LEU	4.2
1	A	657	ALA	4.2
1	C	585	VAL	4.2
1	C	649	VAL	4.2
1	B	691	ALA	4.2
1	B	550	VAL	4.2
1	B	614	HIS	4.1
1	D	618	GLY	4.1
1	B	736	VAL	4.1
1	D	684	SER	4.1
1	A	417	HIS	4.0
1	C	508	LEU	4.0
1	C	739	LEU	4.0
1	B	795	PHE	4.0
1	C	700	LYS	4.0
1	B	600	VAL	4.0
1	B	742	PRO	3.9
1	C	539	LEU	3.9
1	B	636	ALA	3.9
1	C	765	ALA	3.9
1	B	549	ILE	3.9
1	B	766	LEU	3.9
1	A	541	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	541	THR	3.8
1	B	416	ALA	3.8
1	C	736	VAL	3.8
1	B	606	ARG	3.8
1	C	605	TRP	3.8
1	C	734	TYR	3.8
1	C	691	ALA	3.8
1	C	613	ALA	3.8
1	D	681	ALA	3.8
1	D	658	VAL	3.8
1	C	414	PRO	3.8
1	C	549	ILE	3.8
1	B	541	THR	3.7
1	D	666	LYS	3.7
1	B	554	VAL	3.7
1	B	442	ARG	3.7
1	C	686	PHE	3.7
1	C	600	VAL	3.7
1	C	623	VAL	3.7
1	B	508	LEU	3.7
1	C	538	LEU	3.7
1	C	677	THR	3.7
1	B	617	PRO	3.7
1	C	601	LEU	3.7
1	A	622	ALA	3.7
1	C	619	SER	3.7
1	B	740	VAL	3.6
1	C	610	ILE	3.6
1	D	685	TYR	3.6
1	C	744	LEU	3.6
1	C	646	GLU	3.6
1	D	620	MET	3.6
1	C	658	VAL	3.6
1	C	521	LEU	3.6
1	D	631	LYS	3.6
1	A	478	ARG	3.5
1	B	799	ASN	3.5
1	D	738	ASN	3.5
1	B	743	VAL	3.5
1	C	556	LEU	3.5
1	C	582	LEU	3.5
1	C	590	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	698	LEU	3.5
1	C	532	VAL	3.5
1	C	551	HIS	3.5
1	D	687	MET	3.5
1	B	611	LYS	3.5
1	B	664	GLN	3.5
1	B	607	GLY	3.4
1	C	500	GLY	3.4
1	C	678	GLY	3.4
1	C	692	PRO	3.4
1	C	710	ALA	3.4
1	B	582	LEU	3.4
1	B	739	LEU	3.4
1	C	695	LEU	3.4
1	B	553	PHE	3.4
1	B	477	GLY	3.4
1	B	529	PRO	3.4
1	B	510	LEU	3.4
1	C	627	TRP	3.4
1	C	594	LEU	3.4
1	B	686	PHE	3.4
1	D	627	TRP	3.4
1	B	700	LYS	3.4
1	C	609	CYS	3.4
1	C	680	LEU	3.4
1	C	735	ASN	3.4
1	C	702	ILE	3.3
1	C	730	SER	3.3
1	D	619	SER	3.3
1	B	692	PRO	3.3
1	C	526	ALA	3.3
1	C	554	VAL	3.3
1	C	701	VAL	3.3
1	C	740	VAL	3.3
1	C	745	PHE	3.3
1	B	49	LYS	3.3
1	C	693	THR	3.3
1	D	637	GLY	3.3
1	A	790	LYS	3.3
1	C	639	VAL	3.3
1	D	682	PHE	3.3
1	B	486	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	530	LEU	3.3
1	B	537	LEU	3.3
1	B	616	PRO	3.3
1	B	769	ALA	3.3
1	C	597	ARG	3.2
1	C	418	ALA	3.2
1	A	489	LYS	3.2
1	B	760	GLU	3.2
1	C	666	LYS	3.2
1	B	701	VAL	3.2
1	D	675	VAL	3.2
1	B	765	ALA	3.2
1	C	558	ALA	3.2
1	B	534	VAL	3.2
1	B	597	ARG	3.2
1	C	606	ARG	3.2
1	B	720	ALA	3.2
1	B	690	ILE	3.2
1	B	638	VAL	3.2
1	B	682	PHE	3.2
1	C	670	VAL	3.2
1	C	728	ARG	3.1
1	B	511	MET	3.1
1	B	790	LYS	3.1
1	C	553	PHE	3.1
1	C	638	VAL	3.1
1	C	743	VAL	3.1
1	C	788	ASP	3.1
1	C	20	GLN	3.1
1	C	599	ALA	3.1
1	A	504	ARG	3.1
1	B	651	ILE	3.1
1	B	523	SER	3.1
1	C	633	ARG	3.1
1	C	529	PRO	3.1
1	C	505	GLY	3.1
1	C	507	GLY	3.1
1	B	610	ILE	3.1
1	B	770	VAL	3.1
1	C	604	TYR	3.0
1	D	489	LYS	3.0
1	B	641	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	506	MET	3.0
1	D	504	ARG	3.0
1	B	526	ALA	3.0
1	D	639	VAL	3.0
1	B	726	LEU	3.0
1	D	636	ALA	3.0
1	B	623	VAL	3.0
1	C	516	PHE	3.0
1	B	734	TYR	3.0
1	C	442	ARG	3.0
1	C	648	THR	3.0
1	A	662	VAL	3.0
1	C	625	LEU	2.9
1	D	790	LYS	2.9
1	B	560	GLN	2.9
1	B	642	CYS	2.9
1	A	648	THR	2.9
1	C	511	MET	2.9
1	B	431	LEU	2.9
1	B	421	PRO	2.9
1	B	564	ILE	2.9
1	C	531	GLY	2.9
1	C	705	PRO	2.9
1	C	742	PRO	2.9
1	B	687	MET	2.9
1	C	486	SER	2.9
1	C	684	SER	2.9
1	B	505	GLY	2.9
1	A	431	LEU	2.9
1	B	710	ALA	2.9
1	B	503	TRP	2.8
1	C	651	ILE	2.8
1	C	415	THR	2.8
1	C	615	LEU	2.8
1	C	550	VAL	2.8
1	C	503	TRP	2.8
1	B	528	LYS	2.8
1	B	666	LYS	2.8
1	B	785	MET	2.8
1	C	676	ARG	2.8
1	C	560	GLN	2.8
1	C	721	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	533	LYS	2.8
1	C	611	LYS	2.8
1	B	792	ASN	2.8
1	B	744	LEU	2.8
1	C	419	ALA	2.8
1	C	632	GLN	2.8
1	B	702	ILE	2.8
1	B	625	LEU	2.8
1	C	474	GLY	2.8
1	C	413	ALA	2.8
1	C	697	ALA	2.8
1	D	416	ALA	2.8
1	D	621	ALA	2.8
1	B	763	PRO	2.7
1	C	664	GLN	2.7
1	B	659	ASN	2.7
1	B	683	HIS	2.7
1	B	715	THR	2.7
1	A	666	LYS	2.7
1	C	573	LYS	2.7
1	C	559	ILE	2.7
1	C	663	GLU	2.7
1	B	546	PHE	2.7
1	B	788	ASP	2.7
1	C	496	CYS	2.7
1	B	68	HIS	2.7
1	D	498	GLY	2.7
1	C	659	ASN	2.7
1	C	773	ARG	2.7
1	C	650	THR	2.7
1	C	727	ALA	2.7
1	C	785	MET	2.7
1	B	417	HIS	2.7
1	D	673	LYS	2.7
1	C	593	CYS	2.6
1	C	694	LEU	2.6
1	C	653	GLY	2.6
1	B	627	TRP	2.6
1	B	670	VAL	2.6
1	D	414	PRO	2.6
1	B	688	GLU	2.6
1	B	463	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	732	ALA	2.6
1	D	652	SER	2.6
1	C	690	ILE	2.6
1	B	384	ARG	2.6
1	D	633	ARG	2.6
1	C	707	PRO	2.6
1	B	684	SER	2.6
1	C	557	THR	2.6
1	C	687	MET	2.6
1	B	580	HIS	2.6
1	B	631	LYS	2.6
1	C	618	GLY	2.6
1	B	707	PRO	2.6
1	C	527	VAL	2.6
1	A	415	THR	2.5
1	B	515	SER	2.5
1	B	41	LYS	2.5
1	B	479	VAL	2.5
1	B	655	GLN	2.5
1	C	581	SER	2.5
1	C	537	LEU	2.5
1	C	68	HIS	2.5
1	B	502	GLN	2.5
1	B	768	GLN	2.5
1	B	618	GLY	2.5
1	D	678	GLY	2.5
1	C	763	PRO	2.5
1	C	534	VAL	2.5
1	B	501	THR	2.5
1	B	628	GLU	2.5
1	A	669	GLY	2.5
1	B	653	GLY	2.5
1	C	616	PRO	2.5
1	D	640	PRO	2.5
1	B	585	VAL	2.5
1	C	603	ALA	2.5
1	C	699	LYS	2.4
1	B	504	ARG	2.4
1	B	694	LEU	2.4
1	B	540	SER	2.4
1	C	688	GLU	2.4
1	D	663	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	532	VAL	2.4
1	B	632	GLN	2.4
1	C	655	GLN	2.4
1	C	732	ALA	2.4
1	B	633	ARG	2.4
1	C	595	SER	2.4
1	A	647	ASP	2.4
1	D	679	GLY	2.4
1	A	631	LYS	2.4
1	C	631	LYS	2.4
1	C	502	GLN	2.4
1	C	431	LEU	2.4
1	C	563	LEU	2.4
1	C	717	ILE	2.4
1	C	726	LEU	2.4
1	D	651	ILE	2.4
1	B	663	GLU	2.4
1	D	660	GLU	2.4
1	B	699	LYS	2.4
1	D	653	GLY	2.4
1	B	697	ALA	2.4
1	C	698	LEU	2.4
1	D	487	THR	2.4
1	D	68	HIS	2.4
1	B	1	SER	2.4
1	C	709	SER	2.4
1	B	414	PRO	2.4
1	A	621	ALA	2.4
1	B	603	ALA	2.4
1	D	622	ALA	2.4
1	B	420	LEU	2.3
1	B	784	LEU	2.3
1	C	523	SER	2.3
1	A	414	PRO	2.3
1	D	662	VAL	2.3
1	B	552	ALA	2.3
1	C	749	LEU	2.3
1	D	539	LEU	2.3
1	C	577	ILE	2.3
1	B	693	THR	2.3
1	B	789	HIS	2.3
1	A	41	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	733	GLU	2.3
1	B	820	GLU	2.3
1	D	118	GLU	2.3
1	D	1	SER	2.3
1	A	703	ARG	2.3
1	B	635	PRO	2.3
1	B	705	PRO	2.3
1	C	477	GLY	2.3
1	B	695	LEU	2.3
1	C	784	LEU	2.3
1	C	580	HIS	2.3
1	C	764	HIS	2.3
1	C	737	ASN	2.3
1	D	735	ASN	2.3
1	B	703	ARG	2.3
1	B	746	GLN	2.3
1	D	537	LEU	2.3
1	D	775	VAL	2.3
1	B	558	ALA	2.2
1	C	681	ALA	2.2
1	C	748	ALA	2.2
1	C	790	LYS	2.2
1	B	728	ARG	2.2
1	B	581	SER	2.2
1	B	669	GLY	2.2
1	A	532	VAL	2.2
1	B	793	LEU	2.2
1	C	510	LEU	2.2
1	C	41	LYS	2.2
1	C	494	PHE	2.2
1	C	520	ILE	2.2
1	D	634	CYS	2.2
1	C	525	GLU	2.2
1	C	545	THR	2.2
1	D	674	GLU	2.2
1	B	738	ASN	2.2
1	A	746	GLN	2.2
1	B	612	ASP	2.2
1	C	767	LEU	2.2
1	B	573	LYS	2.2
1	D	670	VAL	2.2
1	D	671	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	487	THR	2.2
1	C	703	ARG	2.2
1	C	718	PRO	2.2
1	A	507	GLY	2.2
1	A	1	SER	2.2
1	A	285	GLU	2.2
1	D	629	GLU	2.2
1	C	574	PRO	2.2
1	C	317	GLN	2.2
1	B	436	ASP	2.2
1	A	442	ARG	2.1
1	C	517	ARG	2.1
1	D	693	THR	2.1
1	B	589	TYR	2.1
1	C	786	LYS	2.1
1	A	505	GLY	2.1
1	C	652	SER	2.1
1	B	745	PHE	2.1
1	B	722	TRP	2.1
1	C	706	ARG	2.1
1	D	703	ARG	2.1
1	B	500	GLY	2.1
1	B	577	ILE	2.1
1	B	681	ALA	2.1
1	C	704	GLU	2.1
1	A	627	TRP	2.1
1	B	773	ARG	2.1
1	C	504	ARG	2.1
1	D	772	LYS	2.1
1	D	632	GLN	2.1
1	B	737	ASN	2.1
1	D	659	ASN	2.1
1	D	485	VAL	2.1
1	C	795	PHE	2.1
1	C	720	ALA	2.1
1	D	728	ARG	2.1
1	A	461	PRO	2.1
1	C	498	GLY	2.1
1	B	645	SER	2.0
1	B	741	SER	2.0
1	D	669	GLY	2.0
1	B	496	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	527	VAL	2.0
1	B	727	ALA	2.0
1	C	612	ASP	2.0
1	B	716	SER	2.0
1	C	722	TRP	2.0
1	A	617	PRO	2.0
1	C	696	GLN	2.0
1	A	68	HIS	2.0
1	D	644	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

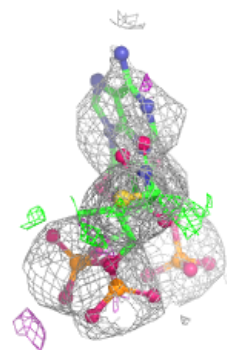
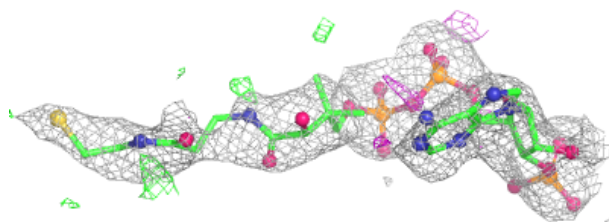
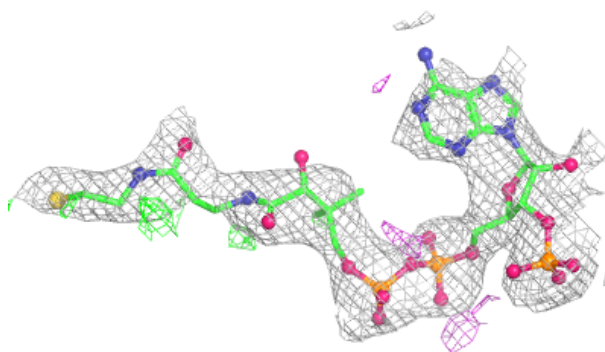
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	D	900	48/48	0.82	0.17	94,116,135,138	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around COA D 900:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.