



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 09:30 am BST

PDB ID : 5MY2
Title : KS-MAT DI-DOMAIN OF MOUSE FAS
Authors : Paithankar, K.S.; Rittner, A.; Vu Huu, K.; Gringer, 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

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.

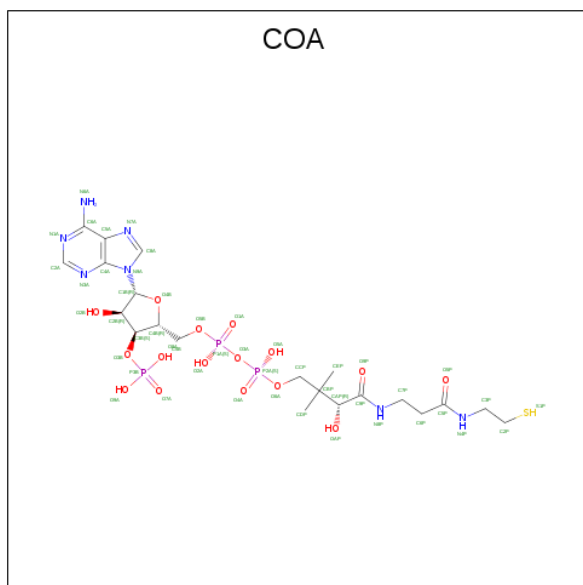
- Molecule 1 is a protein called Fatty acid synthase.

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

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: $C_{21}H_{36}N_7O_{16}P_3S$).

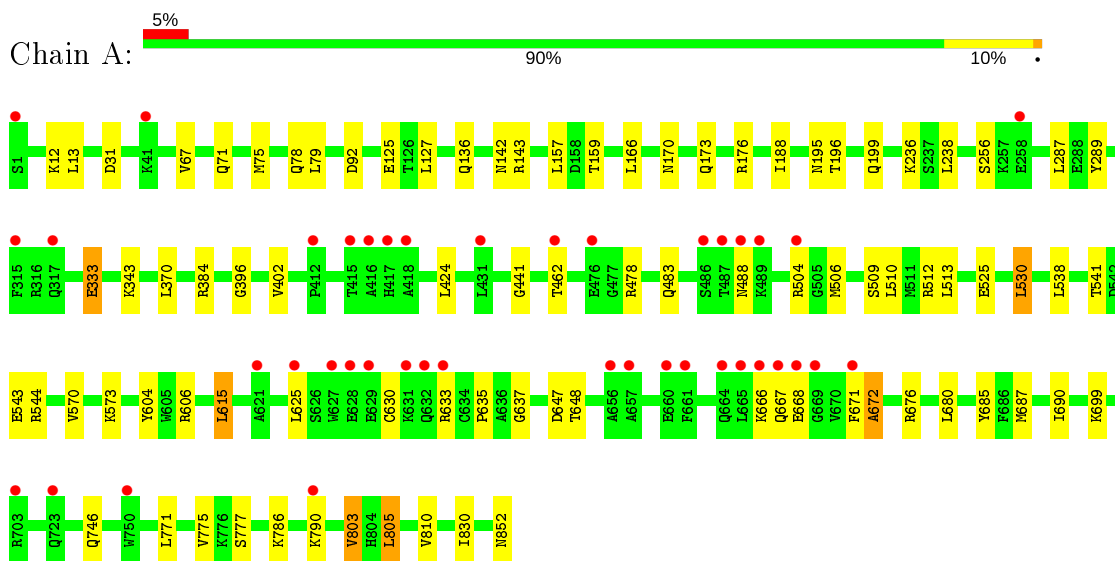


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	D	1	48	21	7	16	3	1	0	0

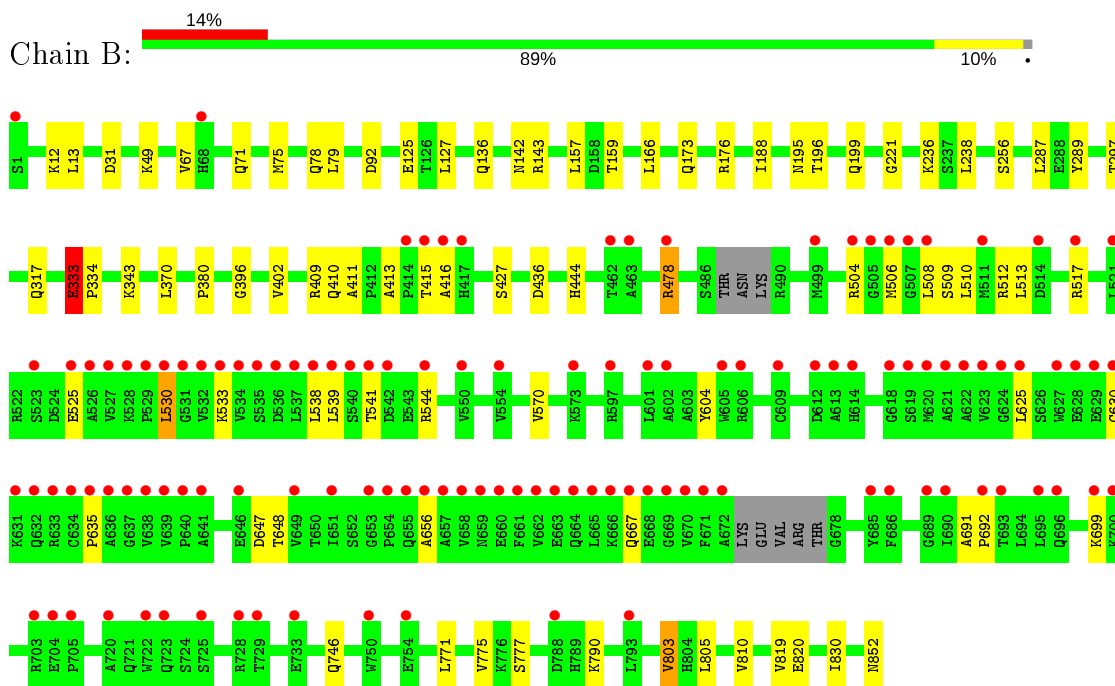
3 Residue-property plots [i](#)

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

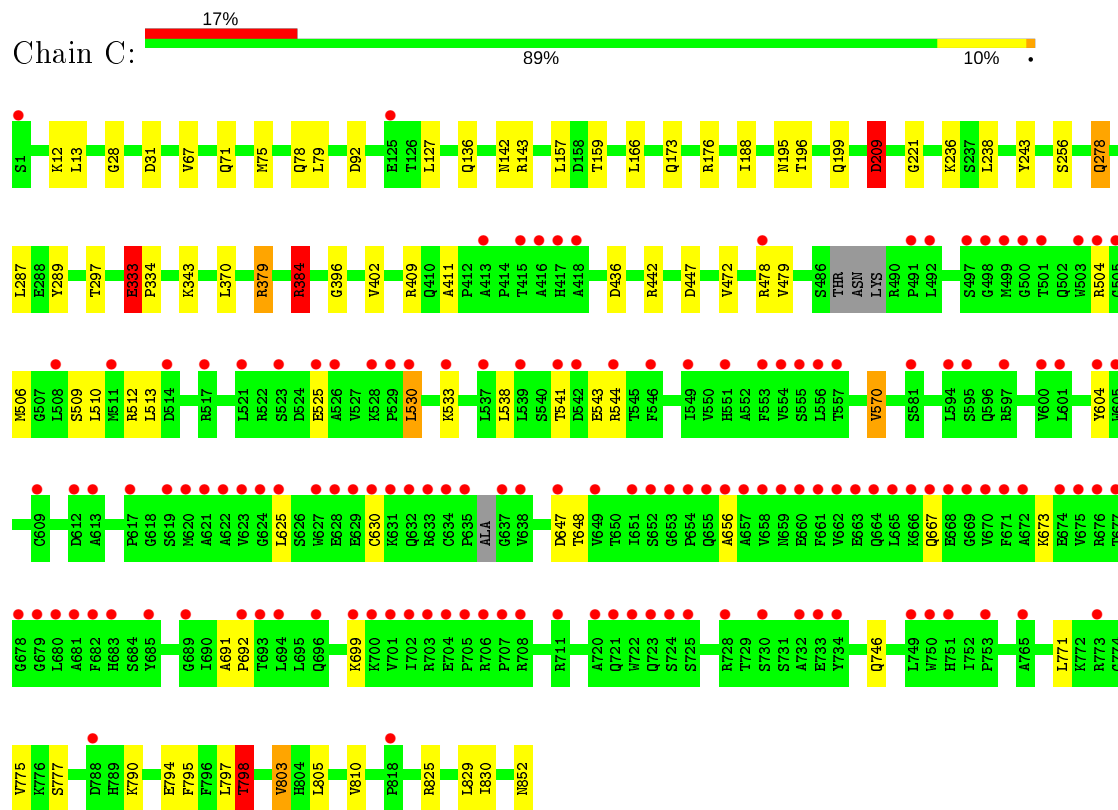
- Molecule 1: Fatty acid synthase



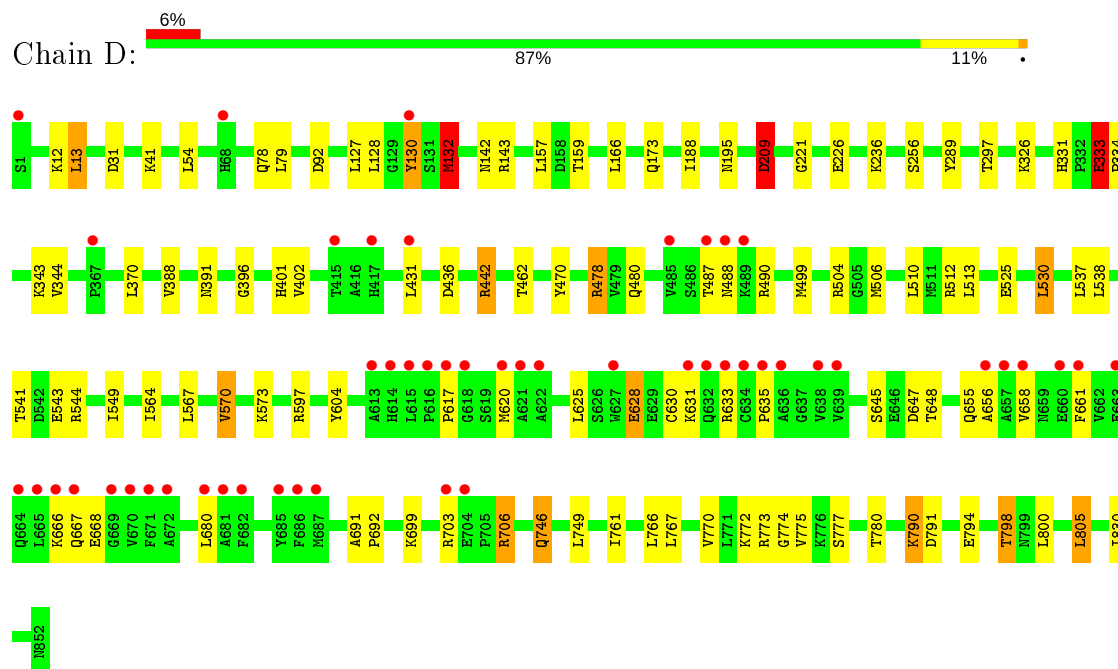
- Molecule 1: Fatty acid synthase



- 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 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)	Xtrriage
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 (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtrriage
Anisotropy	0.806	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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: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:530:LEU:HD23	1:B:604:TYR:CD2	2.51	0.45
1:B:317:GLN:HE21	1:C:442:ARG:HH12	1.64	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

Continued on next page...

Continued from previous page...

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%)	29	54
1	B	838/852 (98%)	796 (95%)	39 (5%)	3 (0%)	34	60
1	C	842/852 (99%)	801 (95%)	37 (4%)	4 (0%)	29	54
1	D	850/852 (100%)	806 (95%)	38 (4%)	6 (1%)	22	46
All	All	3380/3408 (99%)	3212 (95%)	151 (4%)	17 (0%)	29	54

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 [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	700/702 (100%)	661 (94%)	39 (6%)	21	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	694/702 (99%)	660 (95%)	34 (5%)	25	52
1	C	697/702 (99%)	658 (94%)	39 (6%)	21	45
1	D	699/702 (100%)	659 (94%)	40 (6%)	20	44
All	All	2790/2808 (99%)	2638 (95%)	152 (5%)	22	47

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	41,50,50	0.89	1 (2%)	52,75,75	1.69	11 (21%)

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	-	-	17/44/64/64	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	2.34	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	-5.02	120.83	128.68
2	D	900	COA	C6P-C5P-N4P	4.27	123.61	116.42
2	D	900	COA	C2A-N1A-C6A	2.89	123.69	118.75
2	D	900	COA	O5P-C5P-C6P	-2.73	117.03	122.02
2	D	900	COA	C6P-C7P-N8P	2.67	117.29	111.90
2	D	900	COA	C3P-N4P-C5P	2.67	127.79	122.84
2	D	900	COA	N6A-C6A-N1A	2.63	124.03	118.57
2	D	900	COA	CEP-CBP-CCP	2.53	112.36	108.23
2	D	900	COA	CDP-CBP-CAP	-2.48	104.51	108.82
2	D	900	COA	C3B-C2B-C1B	2.35	105.10	99.89
2	D	900	COA	C1B-N9A-C4A	-2.21	122.76	126.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	900	COA	C3B-O3B-P3B-O7A
2	D	900	COA	C5B-O5B-P1A-O3A
2	D	900	COA	S1P-C2P-C3P-N4P
2	D	900	COA	C6P-C5P-N4P-C3P
2	D	900	COA	C4B-C3B-O3B-P3B
2	D	900	COA	O5P-C5P-N4P-C3P
2	D	900	COA	C5P-C6P-C7P-N8P
2	D	900	COA	C6P-C7P-N8P-C9P
2	D	900	COA	CDP-CBP-CCP-O6A
2	D	900	COA	CEP-CBP-CCP-O6A
2	D	900	COA	C3B-O3B-P3B-O9A
2	D	900	COA	P1A-O3A-P2A-O4A
2	D	900	COA	C5B-O5B-P1A-O1A
2	D	900	COA	C5B-O5B-P1A-O2A
2	D	900	COA	C2B-C3B-O3B-P3B
2	D	900	COA	C3B-C4B-C5B-O5B
2	D	900	COA	P1A-O3A-P2A-O5A

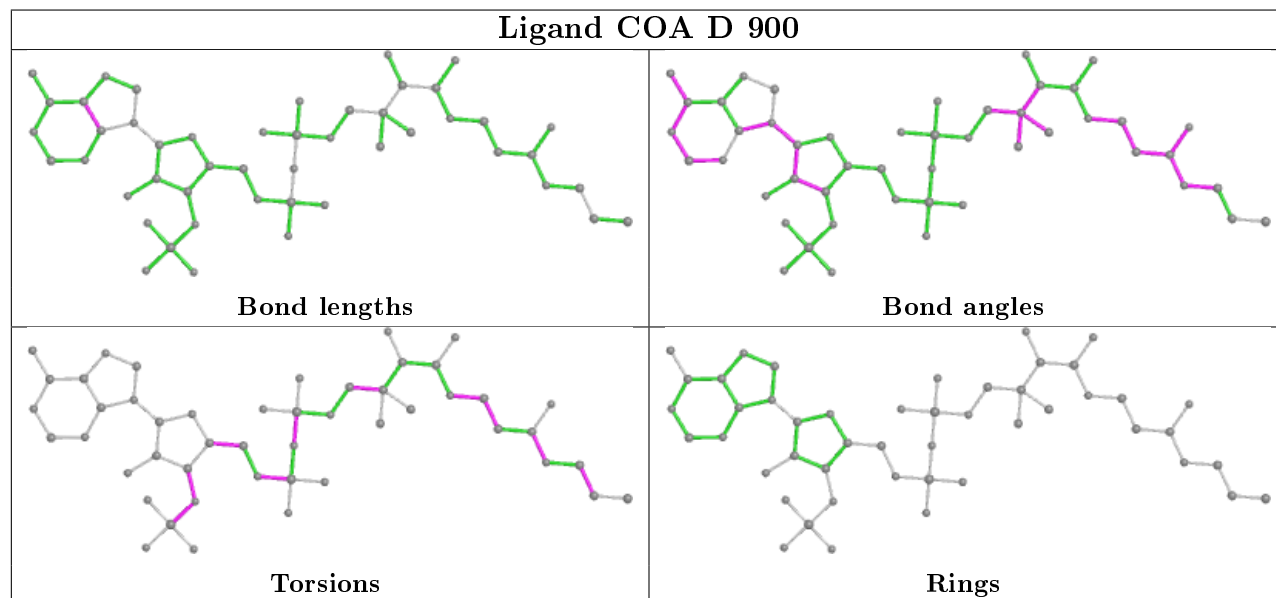
There are no ring outliers.

1 monomer is involved in 3 short contacts:

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

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 [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	852/852 (100%)	0.14	41 (4%) 30 28	22, 44, 85, 131	0
1	B	844/852 (99%)	0.68	121 (14%) 2 1	22, 50, 141, 264	0
1	C	848/852 (99%)	0.73	143 (16%) 1 1	21, 49, 151, 240	0
1	D	852/852 (100%)	0.18	51 (5%) 21 20	22, 43, 96, 158	0
All	All	3396/3408 (99%)	0.43	356 (10%) 6 4	21, 46, 134, 264	0

All (356) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	621	ALA	12.6
1	B	665	LEU	12.5
1	B	637	GLY	9.3
1	A	656	ALA	8.6
1	C	665	LEU	8.4
1	D	665	LEU	8.4
1	B	661	PHE	8.1
1	B	664	GLN	8.0
1	C	659	ASN	7.8
1	B	662	VAL	7.7
1	C	546	PHE	7.6
1	B	667	GLN	7.1
1	C	661	PHE	6.8
1	C	663	GLU	6.6
1	C	672	ALA	6.5
1	B	658	VAL	6.5
1	B	670	VAL	6.4
1	C	629	GLU	6.4
1	D	656	ALA	6.3
1	C	521	LEU	6.0
1	C	667	GLN	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	656	ALA	6.0
1	C	632	GLN	5.9
1	C	654	PRO	5.8
1	C	622	ALA	5.8
1	B	539	LEU	5.8
1	C	676	ARG	5.8
1	B	659	ASN	5.7
1	B	507	GLY	5.5
1	C	656	ALA	5.5
1	A	661	PHE	5.5
1	B	602	ALA	5.4
1	B	651	ILE	5.4
1	C	693	THR	5.4
1	A	669	GLY	5.4
1	C	657	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	5.2
1	C	658	VAL	5.2
1	C	541	THR	5.1
1	C	660	GLU	5.1
1	C	633	ARG	5.1
1	B	632	GLN	5.0
1	D	636	ALA	5.0
1	A	633	ARG	5.0
1	B	638	VAL	5.0
1	C	662	VAL	5.0
1	C	788	ASP	5.0
1	C	619	SER	5.0
1	C	617	PRO	5.0
1	D	635	PRO	5.0
1	C	635	PRO	4.9
1	C	597	ARG	4.9
1	D	634	CYS	4.9
1	B	671	PHE	4.9
1	B	663	GLU	4.9
1	B	640	PRO	4.8
1	C	677	THR	4.8
1	B	696	GLN	4.8
1	B	527	VAL	4.7
1	B	621	ALA	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	624	GLY	4.7
1	B	631	LYS	4.7
1	C	630	CYS	4.7
1	C	508	LEU	4.7
1	B	619	SER	4.6
1	B	605	TRP	4.6
1	B	633	ARG	4.6
1	B	654	PRO	4.6
1	B	660	GLU	4.6
1	C	696	GLN	4.6
1	C	620	MET	4.6
1	A	415	THR	4.6
1	C	730	SER	4.6
1	C	669	GLY	4.5
1	B	601	LEU	4.5
1	D	661	PHE	4.5
1	B	537	LEU	4.5
1	B	639	VAL	4.5
1	B	630	CYS	4.5
1	B	625	LEU	4.5
1	B	705	PRO	4.4
1	B	695	LEU	4.4
1	D	658	VAL	4.4
1	B	655	GLN	4.3
1	B	508	LEU	4.3
1	B	533	LYS	4.3
1	C	655	GLN	4.2
1	D	613	ALA	4.2
1	B	634	CYS	4.2
1	C	724	SER	4.1
1	C	734	TYR	4.1
1	C	416	ALA	4.1
1	B	478	ARG	4.1
1	C	530	LEU	4.1
1	C	533	LYS	4.1
1	D	616	PRO	4.1
1	C	750	TRP	4.1
1	C	604	TYR	4.0
1	B	614	HIS	4.0
1	C	649	VAL	4.0
1	C	418	ALA	4.0
1	B	699	LYS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	687	MET	4.0
1	D	703	ARG	4.0
1	D	631	LYS	4.0
1	C	417	HIS	4.0
1	D	614	HIS	4.0
1	B	672	ALA	4.0
1	D	487	THR	3.9
1	B	668	GLU	3.9
1	D	615	LEU	3.9
1	C	605	TRP	3.9
1	D	638	VAL	3.8
1	B	511	MET	3.8
1	B	646	GLU	3.8
1	C	689	GLY	3.8
1	B	750	TRP	3.8
1	D	489	LYS	3.8
1	C	555	SER	3.8
1	B	657	ALA	3.8
1	A	667	GLN	3.7
1	C	668	GLU	3.7
1	B	722	TRP	3.7
1	A	703	ARG	3.7
1	A	489	LYS	3.7
1	C	723	GLN	3.6
1	B	530	LEU	3.6
1	B	532	VAL	3.6
1	B	620	MET	3.6
1	B	728	ARG	3.5
1	C	733	GLU	3.5
1	C	631	LYS	3.5
1	C	612	ASP	3.5
1	C	751	HIS	3.5
1	B	704	GLU	3.4
1	A	431	LEU	3.4
1	A	631	LYS	3.4
1	C	627	TRP	3.4
1	C	600	VAL	3.4
1	A	629	GLU	3.4
1	C	664	GLN	3.4
1	B	544	ARG	3.3
1	C	681	ALA	3.3
1	B	703	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	723	GLN	3.3
1	B	1	SER	3.3
1	A	671	PHE	3.2
1	B	629	GLU	3.2
1	B	613	ALA	3.2
1	B	692	PRO	3.2
1	A	621	ALA	3.2
1	B	535	SER	3.2
1	B	541	THR	3.2
1	D	660	GLU	3.2
1	A	664	GLN	3.2
1	B	636	ALA	3.2
1	C	628	GLU	3.2
1	C	682	PHE	3.2
1	B	720	ALA	3.2
1	D	672	ALA	3.2
1	D	667	GLN	3.2
1	B	463	ALA	3.2
1	C	624	GLY	3.2
1	C	499	MET	3.1
1	B	641	ALA	3.1
1	C	702	ILE	3.1
1	D	622	ALA	3.1
1	B	462	THR	3.1
1	C	679	GLY	3.1
1	C	721	GLN	3.1
1	B	700	LYS	3.1
1	C	700	LYS	3.1
1	B	416	ALA	3.1
1	C	625	LEU	3.1
1	B	685	TYR	3.1
1	D	415	THR	3.1
1	C	725	SER	3.1
1	C	517	ARG	3.0
1	C	634	CYS	3.0
1	B	538	LEU	3.0
1	B	542	ASP	3.0
1	B	622	ALA	3.0
1	B	793	LEU	3.0
1	D	618	GLY	3.0
1	D	633	ARG	3.0
1	D	627	TRP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	657	ALA	3.0
1	B	690	ILE	3.0
1	B	597	ARG	3.0
1	D	657	ALA	3.0
1	B	628	GLU	3.0
1	C	623	VAL	3.0
1	C	703	ARG	3.0
1	C	705	PRO	3.0
1	C	653	GLY	2.9
1	B	521	LEU	2.9
1	B	525	GLU	2.9
1	C	711	ARG	2.9
1	A	665	LEU	2.9
1	B	540	SER	2.9
1	B	653	GLY	2.9
1	A	628	GLU	2.9
1	C	478	ARG	2.9
1	B	523	SER	2.9
1	D	686	PHE	2.9
1	D	621	ALA	2.9
1	C	415	THR	2.8
1	A	668	GLU	2.8
1	C	704	GLU	2.8
1	C	504	ARG	2.8
1	B	534	VAL	2.8
1	D	617	PRO	2.8
1	C	666	LYS	2.8
1	B	618	GLY	2.8
1	D	681	ALA	2.8
1	C	728	ARG	2.8
1	B	529	PRO	2.7
1	D	663	GLU	2.7
1	A	486	SER	2.7
1	B	536	ASP	2.7
1	B	517	ARG	2.7
1	D	669	GLY	2.7
1	B	729	THR	2.7
1	A	476	GLU	2.7
1	C	671	PHE	2.7
1	A	666	LYS	2.7
1	C	683	HIS	2.7
1	A	416	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	692	PRO	2.7
1	C	125	GLU	2.7
1	A	627	TRP	2.6
1	D	1	SER	2.6
1	B	68	HIS	2.6
1	B	623	VAL	2.6
1	B	725	SER	2.6
1	C	637	GLY	2.6
1	C	675	VAL	2.6
1	C	670	VAL	2.6
1	A	625	LEU	2.6
1	C	528	LYS	2.6
1	C	1	SER	2.6
1	B	627	TRP	2.6
1	B	526	ALA	2.6
1	C	732	ALA	2.6
1	C	749	LEU	2.6
1	B	609	CYS	2.5
1	C	694	LEU	2.5
1	B	666	LYS	2.5
1	D	666	LYS	2.5
1	A	632	GLN	2.5
1	C	720	ALA	2.5
1	C	525	GLU	2.5
1	B	612	ASP	2.5
1	A	790	LYS	2.5
1	C	526	ALA	2.5
1	B	528	LYS	2.5
1	C	651	ILE	2.5
1	C	706	ARG	2.5
1	B	417	HIS	2.4
1	C	549	ILE	2.4
1	D	685	TYR	2.4
1	C	539	LEU	2.4
1	B	689	GLY	2.4
1	A	1	SER	2.4
1	D	620	MET	2.4
1	D	704	GLU	2.4
1	D	130	TYR	2.4
1	B	504	ARG	2.4
1	C	674	GLU	2.4
1	D	670	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	499	MET	2.3
1	B	514	ASP	2.3
1	C	542	ASP	2.3
1	C	680	LEU	2.3
1	B	554	VAL	2.3
1	C	554	VAL	2.3
1	A	723	GLN	2.3
1	C	722	TRP	2.3
1	C	544	ARG	2.3
1	B	550	VAL	2.3
1	C	699	LYS	2.3
1	B	733	GLU	2.3
1	C	773	ARG	2.3
1	C	529	PRO	2.3
1	A	487	THR	2.3
1	B	415	THR	2.3
1	C	701	VAL	2.3
1	C	491	PRO	2.3
1	C	492	LEU	2.3
1	C	581	SER	2.3
1	C	511	MET	2.3
1	B	754	GLU	2.3
1	D	367	PRO	2.2
1	B	506	MET	2.2
1	D	682	PHE	2.2
1	C	500	GLY	2.2
1	A	317	GLN	2.2
1	D	664	GLN	2.2
1	C	652	SER	2.2
1	A	41	LYS	2.2
1	C	685	TYR	2.2
1	B	693	THR	2.2
1	B	573	LYS	2.2
1	D	485	VAL	2.2
1	C	503	TRP	2.2
1	A	488	ASN	2.2
1	A	412	PRO	2.2
1	C	556	LEU	2.2
1	C	753	PRO	2.2
1	B	788	ASP	2.2
1	C	557	THR	2.2
1	D	639	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	594	LEU	2.2
1	C	601	LEU	2.2
1	D	417	HIS	2.2
1	C	638	VAL	2.2
1	D	680	LEU	2.2
1	C	413	ALA	2.2
1	C	609	CYS	2.2
1	C	818	PRO	2.1
1	C	613	ALA	2.1
1	A	315	PHE	2.1
1	B	531	GLY	2.1
1	C	647	ASP	2.1
1	A	660	GLU	2.1
1	B	414	PRO	2.1
1	C	551	HIS	2.1
1	C	708	ARG	2.1
1	C	523	SER	2.1
1	C	505	GLY	2.1
1	C	595	SER	2.1
1	D	431	LEU	2.1
1	C	501	THR	2.1
1	D	488	ASN	2.1
1	B	686	PHE	2.1
1	C	553	PHE	2.1
1	C	537	LEU	2.1
1	C	707	PRO	2.1
1	A	462	THR	2.1
1	A	504	ARG	2.1
1	D	671	PHE	2.1
1	A	258	GLU	2.1
1	C	765	ALA	2.1
1	C	678	GLY	2.1
1	A	418	ALA	2.0
1	C	498	GLY	2.0
1	D	68	HIS	2.0
1	B	635	PRO	2.0
1	B	606	ARG	2.0
1	B	649	VAL	2.0
1	C	497	SER	2.0
1	C	514	ASP	2.0
1	D	632	GLN	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](#)

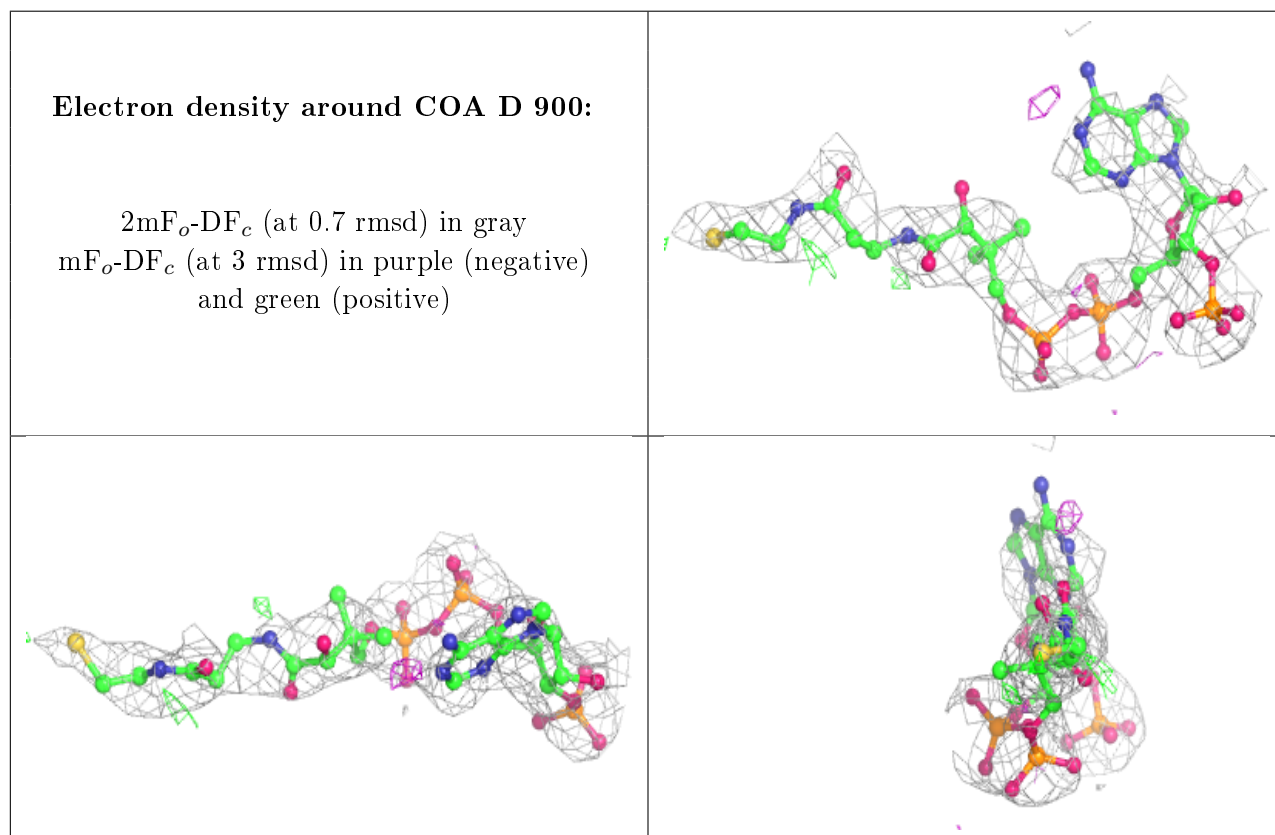
There are no carbohydrates in this entry.

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. 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	0.80	0.34	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.



6.5 Other polymers

There are no such residues in this entry.