Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:52 am BST

PDB ID	:	5MY0
Title	:	KS-MAT DI-DOMAIN OF MOUSE FAS WITH MALONYL-COA
Authors	:	Paithankar, K.S.; Rittner, A.; Huu, K.V.; Grininger, M.
Deposited on	:	2017-01-25
Resolution	:	2.94 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:

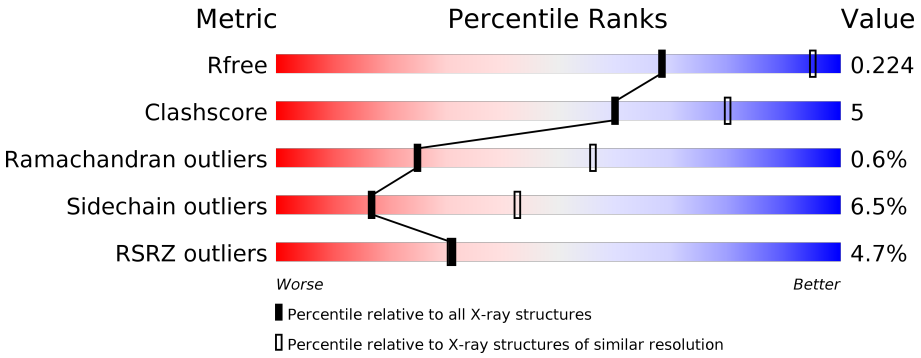
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 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 <=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	2% 85% 13%
1	D	852	2% 87% 12%
2	B	852	8% 84% 13%
2	C	852	7% 84% 15%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MLC	C	900	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25992 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
			6483	4097	1137	1217	32			
1	D	852	Total	C	N	O	S	0	0	0
			6483	4097	1137	1217	32			

There are 2 discrepancies between the modelled and reference sequences:

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

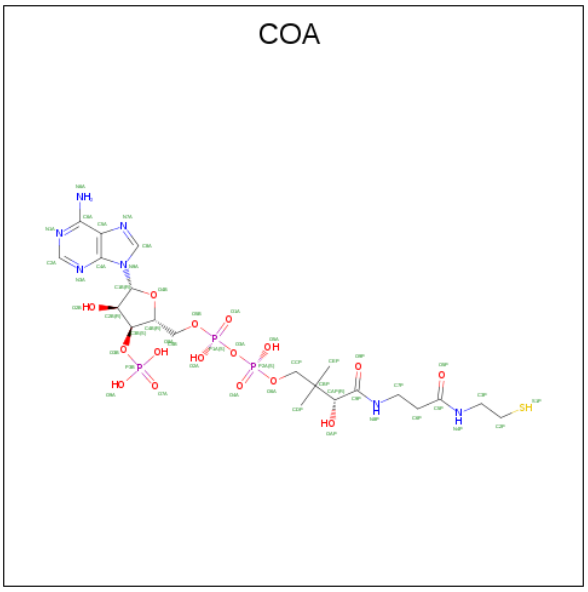
- Molecule 2 is a protein called Fatty acid synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	848	Total	C	N	O	S	0	0	0
			6441	4072	1129	1208	32			
2	C	848	Total	C	N	O	S	0	0	0
			6435	4066	1129	1208	32			

There are 2 discrepancies between the modelled and reference sequences:

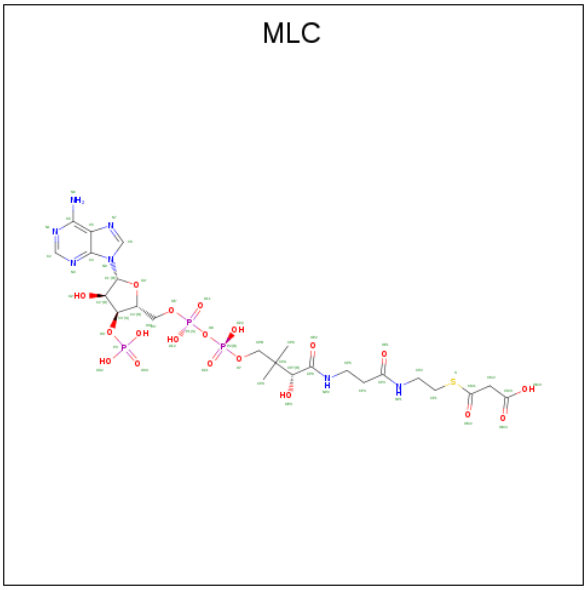
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP P19096
C	1	SER	-	expression tag	UNP P19096

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 4 is MALONYL-COENZYME A (three-letter code: MLC) (formula: $C_{24}H_{38}N_7O_{19}P_3S$).



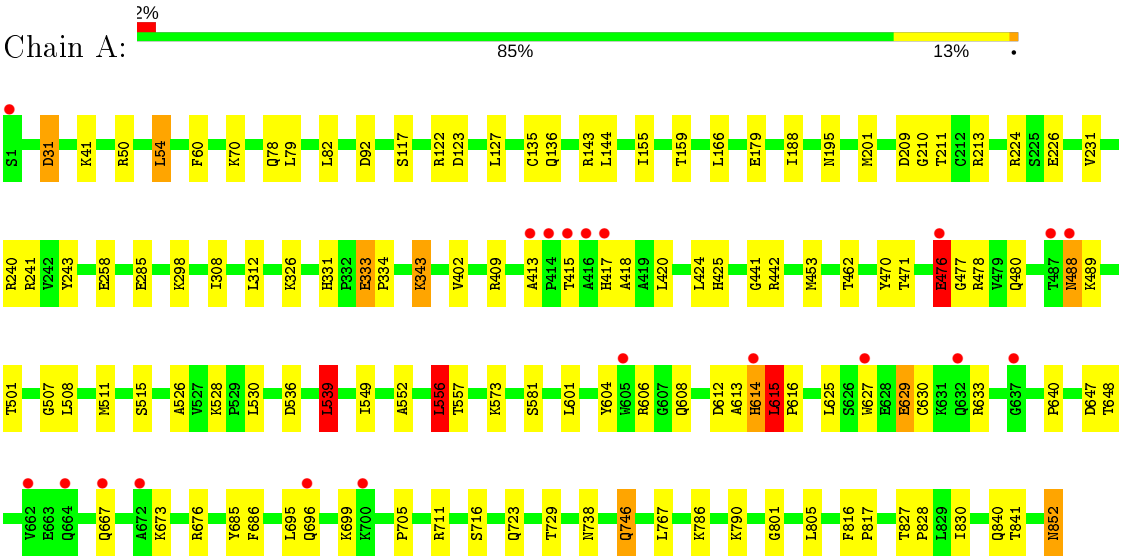
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		

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.

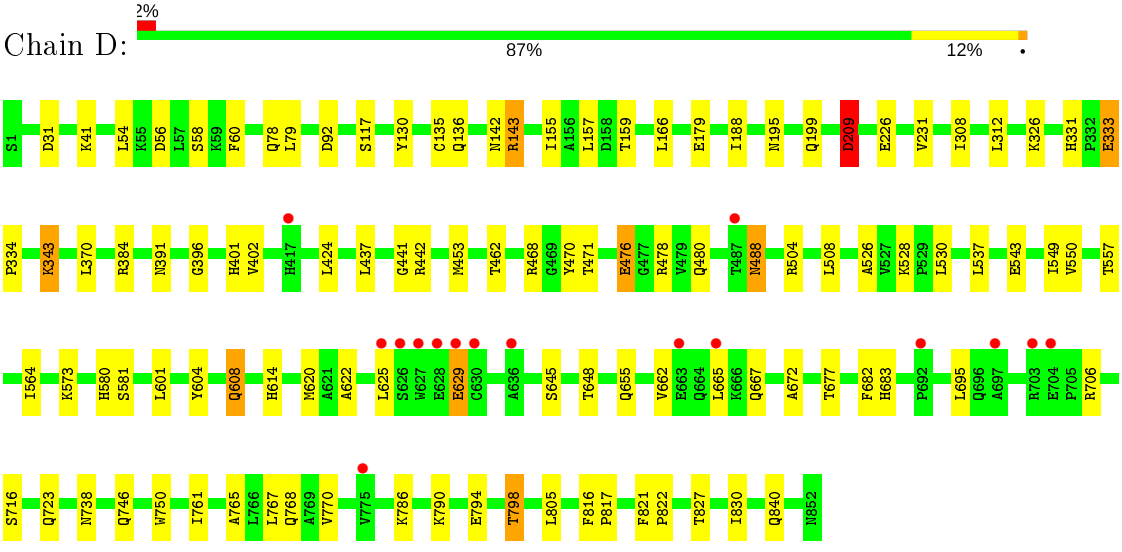
- Molecule 1: Fatty acid synthase

Chain A:



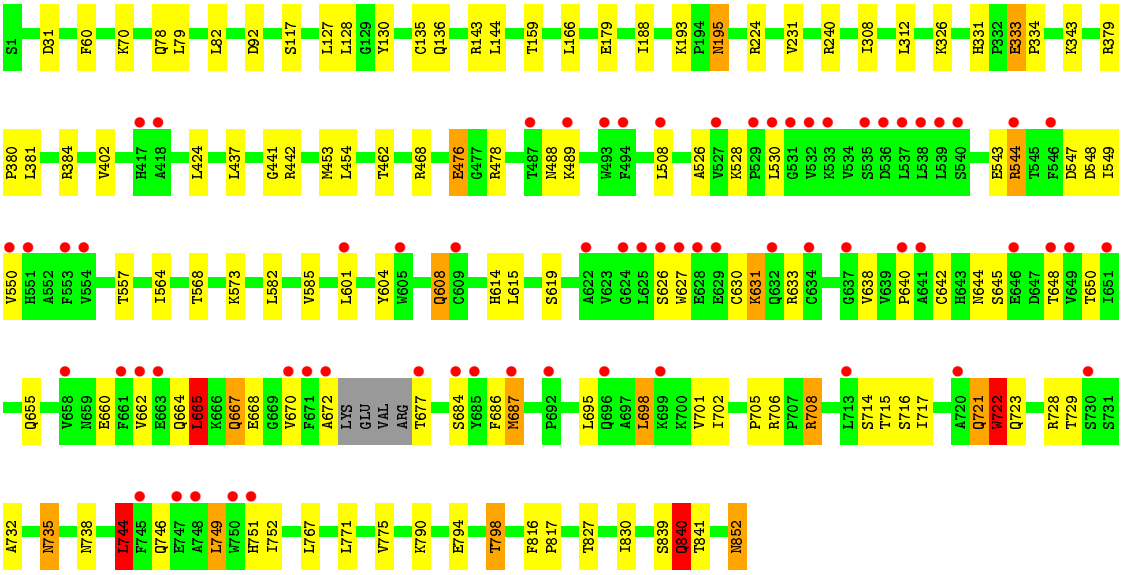
- Molecule 1: Fatty acid synthase

Chain D:

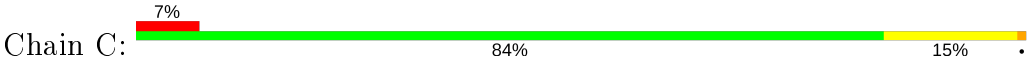


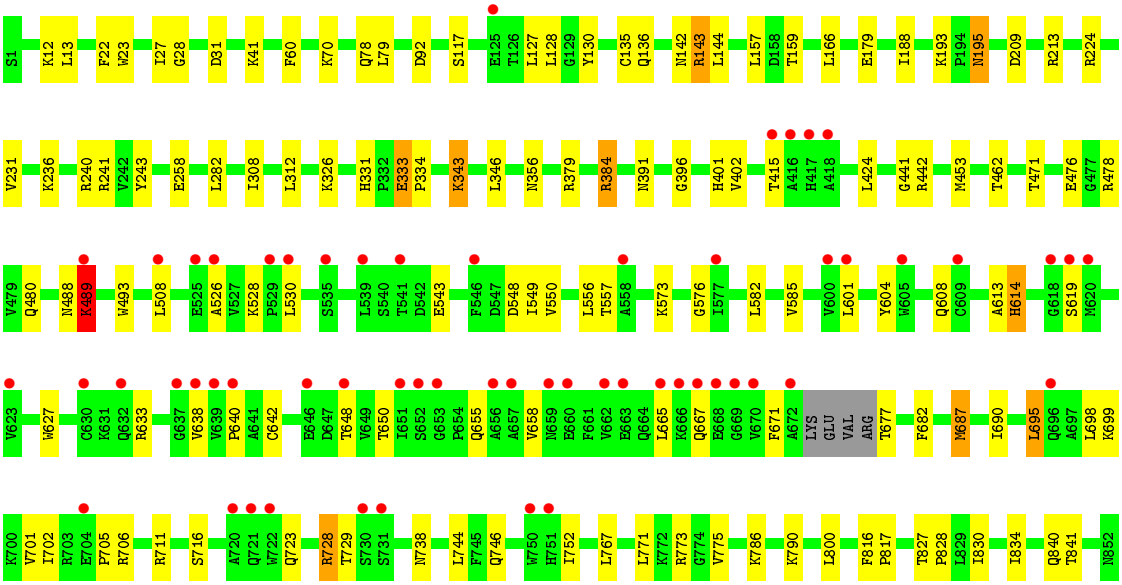
- Molecule 2: Fatty acid synthase

Chain B:



- Molecule 2: Fatty acid synthase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	147.04Å 354.39Å 217.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 2.94 49.56 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.56-2.94) 98.7 (49.56-2.94)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.188 , 0.222 0.192 , 0.224	Depositor DCC
R_{free} test set	5918 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	66.2	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25992	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, MLC, K5L

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	0.67	1/6617 (0.0%)	0.88	16/8998 (0.2%)
1	D	0.67	1/6617 (0.0%)	0.86	8/8998 (0.1%)
2	B	0.67	1/6587 (0.0%)	0.90	18/8959 (0.2%)
2	C	0.64	0/6580	0.85	8/8950 (0.1%)
All	All	0.66	3/26401 (0.0%)	0.87	50/35905 (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
2	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	840	GLN	CG-CD	7.08	1.67	1.51
1	D	209	ASP	CB-CG	-5.01	1.41	1.51
1	A	285	GLU	CG-CD	5.00	1.59	1.51

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	381	LEU	CB-CG-CD1	9.87	127.78	111.00
2	B	665	LEU	CA-CB-CG	9.26	136.61	115.30
1	D	209	ASP	N-CA-CB	-8.80	94.75	110.60
1	D	209	ASP	CB-CA-C	-8.37	93.66	110.40
2	B	840	GLN	CA-C-N	8.14	135.11	117.20
1	A	615	LEU	CA-CB-CG	8.12	133.98	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	840	GLN	C-N-CA	7.94	141.55	121.70
1	A	539	LEU	CA-CB-CG	7.79	133.21	115.30
2	C	31	ASP	CB-CG-OD1	7.36	124.92	118.30
1	D	31	ASP	CB-CG-OD1	7.04	124.64	118.30
2	B	31	ASP	CB-CG-OD1	7.01	124.61	118.30
2	B	744	LEU	CA-CB-CG	6.92	131.22	115.30
1	A	31	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	606	ARG	NE-CZ-NH1	6.81	123.71	120.30
2	B	722	TRP	CA-CB-CG	6.66	126.35	113.70
2	C	143	ARG	NE-CZ-NH2	-6.45	117.08	120.30
2	C	834	ILE	CG1-CB-CG2	-6.16	97.85	111.40
1	A	606	ARG	NE-CZ-NH2	-6.15	117.22	120.30
2	B	840	GLN	CB-CA-C	6.13	122.67	110.40
2	B	840	GLN	CA-C-O	-6.13	107.22	120.10
2	C	695	LEU	CA-CB-CG	5.99	129.08	115.30
2	B	31	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	A	488	ASN	N-CA-C	-5.88	95.12	111.00
2	B	224	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	143	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	C	31	ASP	CB-CG-OD2	-5.73	113.15	118.30
2	C	224	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	B	442	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	209	ASP	CB-CG-OD1	5.63	123.37	118.30
1	D	209	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	B	708	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	B	224	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	409	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	C	384	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	B	840	GLN	CB-CG-CD	5.41	125.67	111.60
1	A	240	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	201	MET	CG-SD-CE	-5.34	91.66	100.20
1	D	31	ASP	CB-CG-OD2	-5.29	113.54	118.30
2	B	381	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	A	539	LEU	CB-CG-CD2	5.22	119.87	111.00
1	A	224	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	556	LEU	CA-CB-CG	5.18	127.21	115.30
2	B	631	LYS	CA-CB-CG	5.14	124.72	113.40
1	A	31	ASP	CB-CG-OD2	-5.10	113.71	118.30
2	C	728	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	612	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	D	468	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	123	ASP	CB-CG-OD1	5.03	122.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	468	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	767	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	839	SER	Peptide
2	B	840	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6483	0	6456	54	0
1	D	6483	0	6456	56	0
2	B	6441	0	6419	69	0
2	C	6435	0	6412	67	0
3	A	48	0	32	0	0
3	D	48	0	32	5	0
4	C	54	0	33	1	0
All	All	25992	0	25840	240	0

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

All (240) 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:D:581:K5L:OAI	1:D:581:K5L:CAK	1.79	1.31
1:A:581:K5L:CAK	1:A:581:K5L:OAI	1.82	1.27
1:A:581:K5L:CB	1:A:581:K5L:OAI	1.81	1.26
1:D:581:K5L:OAI	1:D:581:K5L:CB	1.82	1.25
1:A:209:ASP:OD2	1:A:213:ARG:NH1	1.91	1.04
2:C:209:ASP:OD2	2:C:213:ARG:NH1	1.92	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:716:SER:OG	2:B:738:ASN:HA	1.75	0.87
2:C:195:ASN:HD22	2:C:195:ASN:H	1.24	0.85
1:D:645:SER:HA	1:D:746:GLN:HE21	1.43	0.83
2:B:550:VAL:HG11	2:B:608:GLN:HG2	1.59	0.82
2:C:195:ASN:HD22	2:C:195:ASN:N	1.81	0.78
2:B:626:SER:O	2:B:630:CYS:SG	2.42	0.77
2:B:665:LEU:HD11	2:B:672:ALA:HB2	1.68	0.74
2:C:92:ASP:O	2:C:241:ARG:NH1	2.21	0.73
1:A:92:ASP:O	1:A:241:ARG:NH1	2.21	0.72
1:D:471:THR:HG22	1:D:480:GLN:HB2	1.74	0.70
1:A:471:THR:HG22	1:A:480:GLN:HB2	1.74	0.69
1:A:615:LEU:HB2	1:A:616:PRO:CD	2.21	0.69
1:A:530:LEU:HD23	1:A:604:TYR:CE1	2.28	0.69
1:D:530:LEU:HD23	1:D:604:TYR:CE1	2.27	0.69
2:C:241:ARG:NH2	2:C:828:PRO:O	2.26	0.68
1:D:564:ILE:CD1	1:D:761:ILE:HD13	2.23	0.68
2:B:530:LEU:HD23	2:B:604:TYR:CE1	2.29	0.68
2:C:530:LEU:HD23	2:C:604:TYR:CE1	2.28	0.68
2:C:471:THR:HG22	2:C:480:GLN:HB2	1.74	0.68
2:C:142:ASN:HD22	1:D:396:GLY:HA3	1.58	0.67
2:C:13:LEU:HD13	2:C:22:PHE:CD2	2.29	0.67
1:A:241:ARG:NH2	1:A:828:PRO:O	2.26	0.67
2:B:548:ASP:OD2	2:B:550:VAL:HG22	1.95	0.67
2:C:548:ASP:OD2	2:C:550:VAL:HG12	1.95	0.67
2:B:840:GLN:HA	2:B:840:GLN:HE21	1.62	0.65
2:C:582:LEU:O	2:C:585:VAL:HG12	1.99	0.63
2:B:582:LEU:O	2:B:585:VAL:HG12	1.99	0.63
1:A:501:THR:OG1	1:A:556:LEU:HD11	1.99	0.62
1:D:391:ASN:OD1	1:D:401:HIS:HD2	1.82	0.62
2:C:391:ASN:OD1	2:C:401:HIS:HD2	1.82	0.61
2:B:665:LEU:CD1	2:B:672:ALA:HB2	2.30	0.61
2:B:645:SER:OG	2:B:648:THR:HG22	2.01	0.60
1:A:615:LEU:HB2	1:A:616:PRO:HD2	1.82	0.60
2:C:619:SER:HB2	2:C:658:VAL:HG21	1.83	0.60
1:A:79:LEU:HD21	1:A:143:ARG:HG3	1.83	0.60
1:A:536:ASP:HA	1:A:539:LEU:HD22	1.85	0.59
1:D:620:MET:HE2	1:D:677:THR:HG21	1.85	0.59
2:C:442:ARG:HH12	2:C:471:THR:HG21	1.67	0.59
2:B:752:ILE:HG12	2:B:775:VAL:HG13	1.85	0.59
1:A:442:ARG:HH12	1:A:471:THR:HG21	1.68	0.58
2:C:767:LEU:O	2:C:771:LEU:HD23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:717:ILE:HG23	2:B:721:GLN:HG3	1.86	0.58
1:D:580:HIS:HE1	3:D:900:COA:H31	1.69	0.58
2:B:684:SER:H	2:B:687:MET:HE1	1.69	0.58
2:B:767:LEU:O	2:B:771:LEU:HD23	2.04	0.58
2:C:79:LEU:HD21	2:C:143:ARG:HG3	1.85	0.57
1:D:79:LEU:HD21	1:D:143:ARG:HG3	1.86	0.57
1:A:50:ARG:NH1	1:A:211:THR:OG1	2.37	0.57
2:C:619:SER:HB2	2:C:658:VAL:CG2	2.35	0.57
1:A:852:ASN:HD22	1:A:852:ASN:C	2.09	0.56
2:B:852:ASN:HD22	2:B:852:ASN:C	2.09	0.56
2:B:79:LEU:HD21	2:B:143:ARG:HG3	1.86	0.56
2:C:142:ASN:ND2	1:D:396:GLY:HA3	2.22	0.55
2:B:698:LEU:HD11	2:B:735:ASN:HB3	1.89	0.55
2:C:701:VAL:HG23	2:C:702:ILE:HG13	1.89	0.54
2:C:159:THR:HG21	2:C:166:LEU:HD22	1.88	0.54
1:D:564:ILE:HD11	1:D:761:ILE:HG21	1.90	0.53
2:C:241:ARG:HD3	2:C:243:TYR:CE2	2.44	0.53
1:A:31:ASP:OD2	1:A:50:ARG:NH2	2.41	0.53
1:A:241:ARG:HD3	1:A:243:TYR:CE2	2.44	0.53
2:B:749:LEU:O	2:B:752:ILE:HG13	2.08	0.53
1:D:159:THR:HG21	1:D:166:LEU:HD22	1.89	0.53
2:B:714:SER:HB2	2:B:722:TRP:CZ3	2.43	0.53
1:A:413:ALA:O	1:A:415:THR:HG22	2.09	0.52
1:D:564:ILE:HD11	1:D:761:ILE:HD13	1.91	0.52
2:B:326:LYS:HE3	2:B:331:HIS:CD2	2.44	0.52
2:C:326:LYS:HE3	2:C:331:HIS:CD2	2.44	0.52
1:D:471:THR:HG22	1:D:480:GLN:CB	2.39	0.52
1:D:550:VAL:HG21	1:D:608:GLN:NE2	2.25	0.52
2:B:701:VAL:HG23	2:B:702:ILE:HG13	1.92	0.52
2:C:241:ARG:HD3	2:C:243:TYR:CZ	2.45	0.52
2:B:660:GLU:OE1	2:B:660:GLU:HA	2.10	0.51
2:B:664:GLN:HA	2:B:667:GLN:HG3	1.91	0.51
1:D:326:LYS:HE3	1:D:331:HIS:CD2	2.45	0.51
2:B:715:THR:O	2:B:744:LEU:HG	2.10	0.51
1:D:746:GLN:OE1	1:D:750:TRP:NE1	2.43	0.51
1:A:241:ARG:HD3	1:A:243:TYR:CZ	2.45	0.51
2:B:752:ILE:CD1	2:B:775:VAL:HG13	2.40	0.51
2:C:453:MET:CE	2:C:827:THR:HG21	2.41	0.51
1:D:581:K5L:OAI	1:D:581:K5L:CA	2.54	0.51
1:A:159:THR:HG21	1:A:166:LEU:HD22	1.93	0.51
2:C:471:THR:HG22	2:C:480:GLN:CB	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:ASN:ND2	2:C:195:ASN:N	2.53	0.50
1:A:326:LYS:HE3	1:A:331:HIS:CD2	2.46	0.50
1:D:620:MET:CE	1:D:677:THR:HG21	2.42	0.50
1:A:471:THR:HG22	1:A:480:GLN:CB	2.39	0.50
2:B:453:MET:HE1	2:B:827:THR:HG21	1.94	0.50
2:C:195:ASN:ND2	2:C:195:ASN:H	2.01	0.50
1:D:622:ALA:HB3	3:D:900:COA:H131	1.92	0.50
2:B:453:MET:CE	2:B:827:THR:HG21	2.42	0.50
2:C:619:SER:CB	2:C:658:VAL:HG21	2.42	0.49
2:C:488:ASN:O	2:C:489:LYS:C	2.51	0.49
1:A:415:THR:HG23	1:A:417:HIS:CD2	2.47	0.49
1:D:564:ILE:CD1	1:D:761:ILE:HG21	2.43	0.48
1:A:470:TYR:HD1	1:A:805:LEU:HD13	1.78	0.48
1:D:453:MET:CE	1:D:827:THR:HG21	2.43	0.48
1:A:625:LEU:HB3	1:A:629:GLU:HG2	1.95	0.48
2:C:493:TRP:CE3	2:C:752:ILE:CD1	2.97	0.48
1:A:453:MET:CE	1:A:827:THR:HG21	2.44	0.48
2:C:128:LEU:HD13	2:C:130:TYR:CZ	2.49	0.47
2:C:308:ILE:HG23	2:C:312:LEU:HD12	1.96	0.47
2:C:671:PHE:CB	4:C:900:MLC:N7	2.77	0.47
1:D:470:TYR:HD1	1:D:805:LEU:HD13	1.78	0.47
1:D:92:ASP:HA	1:D:830:ILE:HB	1.97	0.47
1:D:625:LEU:HB3	1:D:629:GLU:HG2	1.96	0.47
1:A:581:K5L:CA	1:A:581:K5L:OAI	2.56	0.47
2:C:716:SER:HB2	2:C:738:ASN:HA	1.97	0.47
2:C:356:ASN:N	2:C:356:ASN:HD22	2.13	0.47
1:A:308:ILE:HG23	1:A:312:LEU:HD12	1.97	0.47
1:A:530:LEU:HD23	1:A:604:TYR:CD1	2.50	0.47
2:B:698:LEU:HG	2:B:732:ALA:CB	2.46	0.46
1:A:54:LEU:HD13	1:A:226:GLU:HB2	1.97	0.46
2:B:128:LEU:HD13	2:B:130:TYR:CZ	2.51	0.46
1:D:308:ILE:HG23	1:D:312:LEU:HD12	1.97	0.46
2:B:92:ASP:HA	2:B:830:ILE:HB	1.97	0.46
2:C:530:LEU:HD23	2:C:604:TYR:CD1	2.51	0.46
2:B:705:PRO:HB3	2:B:729:THR:OG1	2.15	0.46
2:B:530:LEU:HD23	2:B:604:TYR:CD1	2.51	0.46
1:A:705:PRO:HB3	1:A:729:THR:OG1	2.15	0.46
1:D:580:HIS:HE1	3:D:900:COA:C3P	2.28	0.46
2:C:816:PHE:HB3	2:C:817:PRO:HD2	1.97	0.45
3:D:900:COA:H141	3:D:900:COA:N8P	2.31	0.45
2:B:767:LEU:HB3	2:B:771:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASP:HA	1:A:830:ILE:HB	1.98	0.45
2:B:308:ILE:HG23	2:B:312:LEU:HD12	1.98	0.45
1:D:54:LEU:HD13	1:D:226:GLU:HB2	1.98	0.45
2:B:665:LEU:HD13	2:B:670:VAL:HB	1.98	0.45
2:C:705:PRO:HB3	2:C:729:THR:OG1	2.16	0.45
2:C:127:LEU:HD13	1:D:199:GLN:HG2	1.98	0.45
2:B:662:VAL:HG13	2:B:672:ALA:HB1	1.97	0.45
2:B:840:GLN:HA	2:B:840:GLN:NE2	2.31	0.45
1:D:620:MET:HE2	1:D:677:THR:CG2	2.47	0.45
2:B:564:ILE:O	2:B:568:THR:HG23	2.16	0.45
2:B:816:PHE:HB3	2:B:817:PRO:HD2	1.98	0.45
1:D:530:LEU:HD23	1:D:604:TYR:CD1	2.52	0.45
1:D:453:MET:HE1	1:D:827:THR:HG21	1.99	0.45
1:A:50:ARG:NH1	1:A:210:GLY:O	2.49	0.44
2:B:127:LEU:HD12	2:B:127:LEU:C	2.38	0.44
2:B:752:ILE:CG1	2:B:775:VAL:HG13	2.47	0.44
2:B:642:CYS:SG	2:B:650:THR:OG1	2.73	0.44
2:B:752:ILE:O	2:B:752:ILE:HD12	2.17	0.44
1:D:343:LYS:HD2	1:D:343:LYS:C	2.38	0.44
1:D:662:VAL:HG13	1:D:672:ALA:HB1	1.98	0.44
1:A:552:ALA:O	1:A:556:LEU:HB2	2.18	0.44
2:C:767:LEU:HB3	2:C:771:LEU:CD2	2.48	0.44
2:C:92:ASP:HA	2:C:830:ILE:HB	1.99	0.44
1:D:581:K5L:OAI	3:D:900:COA:S1P	2.74	0.44
1:A:425:HIS:HE1	1:A:801:GLY:HA2	1.82	0.44
1:A:816:PHE:HB3	1:A:817:PRO:HD2	1.98	0.44
2:C:343:LYS:HD2	2:C:343:LYS:C	2.38	0.44
2:C:698:LEU:HA	2:C:701:VAL:HG22	1.99	0.44
1:A:716:SER:HB2	1:A:738:ASN:HA	1.99	0.44
2:B:698:LEU:HA	2:B:701:VAL:HG22	1.99	0.43
1:D:488:ASN:HD22	1:D:488:ASN:N	2.15	0.43
2:C:13:LEU:HD13	2:C:22:PHE:CG	2.53	0.43
1:A:343:LYS:C	1:A:343:LYS:HD2	2.39	0.43
2:C:453:MET:HE1	2:C:827:THR:HG21	1.99	0.43
2:C:682:PHE:HA	2:C:687:MET:SD	2.58	0.43
2:C:396:GLY:HA3	1:D:142:ASN:HD22	1.83	0.43
2:B:343:LYS:C	2:B:343:LYS:HD2	2.38	0.43
2:B:159:THR:HG21	2:B:166:LEU:CD2	2.49	0.43
1:D:581:K5L:CB	1:D:683:HIS:HE2	2.32	0.43
1:A:155:ILE:HG12	2:B:166:LEU:HD21	2.01	0.43
2:B:615:LEU:HD12	2:B:686:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:LEU:CD2	2:B:144:LEU:HD11	2.49	0.43
2:C:117:SER:HB2	2:C:135:CYS:HB3	2.00	0.43
1:D:117:SER:HB2	1:D:135:CYS:HB3	2.00	0.43
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.54	0.43
2:C:193:LYS:HE3	2:C:195:ASN:HB2	2.01	0.43
1:A:453:MET:HE1	1:A:827:THR:HG21	1.99	0.43
2:C:526:ALA:O	2:C:601:LEU:HD21	2.19	0.43
2:B:333:GLU:CB	2:B:334:PRO:CD	2.97	0.42
2:B:627:TRP:CZ3	2:B:640:PRO:HB2	2.54	0.42
2:B:794:GLU:O	2:B:798:THR:CG2	2.67	0.42
2:C:127:LEU:C	2:C:127:LEU:HD12	2.39	0.42
1:D:78:GLN:HB3	1:D:188:ILE:HD12	1.99	0.42
2:B:380:PRO:HB2	2:C:28:GLY:HA2	2.01	0.42
2:C:627:TRP:CZ3	2:C:640:PRO:HB2	2.54	0.42
1:A:117:SER:HB2	1:A:135:CYS:HB3	2.02	0.42
2:B:544:ARG:HB3	2:B:547:ASP:OD2	2.19	0.42
2:B:698:LEU:CD2	2:B:732:ALA:HB1	2.50	0.42
2:B:82:LEU:HD21	2:B:144:LEU:HD11	2.01	0.42
1:D:437:LEU:HA	1:D:437:LEU:HD23	1.93	0.42
1:A:82:LEU:CD2	1:A:144:LEU:HD11	2.49	0.42
1:A:746:GLN:HE21	1:A:746:GLN:HA	1.84	0.42
2:B:117:SER:HB2	2:B:135:CYS:HB3	2.01	0.42
2:B:437:LEU:HD22	2:B:454:LEU:HD22	2.01	0.42
1:A:526:ALA:O	1:A:601:LEU:HD21	2.19	0.42
2:B:78:GLN:HB3	2:B:188:ILE:HD12	2.02	0.42
2:B:526:ALA:O	2:B:601:LEU:HD21	2.19	0.42
2:B:716:SER:OG	2:B:738:ASN:CA	2.59	0.42
1:A:333:GLU:CB	1:A:334:PRO:CD	2.97	0.42
2:C:642:CYS:SG	2:C:650:THR:OG1	2.75	0.42
1:A:613:ALA:O	1:A:614:HIS:C	2.58	0.42
1:A:685:TYR:CE1	1:A:686:PHE:CD1	3.08	0.42
2:B:193:LYS:HE3	2:B:195:ASN:HB2	2.02	0.42
1:D:424:LEU:CD2	1:D:441:GLY:HA3	2.50	0.42
1:D:794:GLU:O	1:D:798:THR:CG2	2.68	0.41
1:D:716:SER:HB2	1:D:738:ASN:HA	2.02	0.41
1:D:767:LEU:O	1:D:770:VAL:HG22	2.19	0.41
1:A:507:GLY:O	1:A:511:MET:HG2	2.19	0.41
2:B:644:ASN:ND2	2:B:650:THR:HG23	2.35	0.41
2:C:12:LYS:C	2:C:13:LEU:HG	2.40	0.41
1:D:488:ASN:N	1:D:488:ASN:ND2	2.67	0.41
2:B:644:ASN:HB2	2:B:648:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:816:PHE:HB3	1:D:817:PRO:HD2	2.03	0.41
2:B:717:ILE:O	2:B:722:TRP:CZ3	2.73	0.41
2:C:424:LEU:CD2	2:C:441:GLY:HA3	2.50	0.41
1:D:526:ALA:O	1:D:601:LEU:HD21	2.20	0.41
1:A:424:LEU:CD2	1:A:441:GLY:HA3	2.51	0.41
1:A:476:GLU:HG2	1:A:477:GLY:N	2.35	0.41
2:B:708:ARG:CZ	2:B:714:SER:OG	2.69	0.41
2:C:78:GLN:HB3	2:C:188:ILE:HD12	2.03	0.41
1:D:333:GLU:CB	1:D:334:PRO:CD	2.98	0.41
2:C:333:GLU:CB	2:C:334:PRO:CD	2.99	0.41
2:C:613:ALA:O	2:C:614:HIS:C	2.59	0.41
2:C:771:LEU:O	2:C:775:VAL:HG13	2.21	0.41
1:A:127:LEU:C	1:A:127:LEU:HD12	2.42	0.41
2:B:424:LEU:CD2	2:B:441:GLY:HA3	2.51	0.40
2:B:698:LEU:HG	2:B:732:ALA:HB1	2.04	0.40
2:C:453:MET:HE3	2:C:827:THR:HG21	2.03	0.40
1:D:765:ALA:HB1	1:D:768:GLN:HG2	2.02	0.40
1:A:82:LEU:HD21	1:A:144:LEU:HD11	2.03	0.40
2:C:23:TRP:HB2	2:C:346:LEU:HD13	2.03	0.40
1:D:620:MET:HE1	1:D:682:PHE:HD2	1.86	0.40
1:A:78:GLN:HB3	1:A:188:ILE:HD12	2.02	0.40
2:C:493:TRP:CZ3	2:C:576:GLY:HA3	2.56	0.40
1:D:56:ASP:OD1	1:D:58:SER:N	2.55	0.40
2:B:664:GLN:HA	2:B:667:GLN:CG	2.52	0.40
2:C:27:ILE:HD12	2:C:27:ILE:HA	1.97	0.40
2:C:166:LEU:HD21	1:D:155:ILE:HG12	2.03	0.40
2:C:493:TRP:CD2	2:C:752:ILE:CD1	3.04	0.40
2:C:800:LEU:HA	2:C:800:LEU:HD23	1.90	0.40
1:D:821:PHE:HA	1:D:822:PRO:C	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	849/852 (100%)	813 (96%)	31 (4%)	5 (1%)	25	56
1	D	849/852 (100%)	821 (97%)	22 (3%)	6 (1%)	22	52
2	B	844/852 (99%)	811 (96%)	28 (3%)	5 (1%)	25	56
2	C	844/852 (99%)	809 (96%)	30 (4%)	5 (1%)	25	56
All	All	3386/3408 (99%)	3254 (96%)	111 (3%)	21 (1%)	25	56

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	GLU
1	A	614	HIS
2	B	333	GLU
2	C	333	GLU
1	D	209	ASP
1	D	333	GLU
2	B	614	HIS
2	C	489	LYS
2	C	614	HIS
1	D	614	HIS
1	A	418	ALA
1	A	476	GLU
2	B	476	GLU
1	D	476	GLU
2	B	543	GLU
2	C	543	GLU
1	D	60	PHE
1	A	60	PHE
2	B	60	PHE
2	C	60	PHE
1	D	543	GLU

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	701/701 (100%)	654 (93%)	47 (7%)	16	41
1	D	701/701 (100%)	664 (95%)	37 (5%)	22	52
2	B	698/702 (99%)	650 (93%)	48 (7%)	15	40
2	C	697/702 (99%)	647 (93%)	50 (7%)	14	37
All	All	2797/2806 (100%)	2615 (94%)	182 (6%)	17	43

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	54	LEU
1	A	70	LYS
1	A	122	ARG
1	A	136	GLN
1	A	179	GLU
1	A	195	ASN
1	A	231	VAL
1	A	258	GLU
1	A	298	LYS
1	A	343	LYS
1	A	402	VAL
1	A	420	LEU
1	A	462	THR
1	A	476	GLU
1	A	478	ARG
1	A	488	ASN
1	A	489	LYS
1	A	508	LEU
1	A	515	SER
1	A	528	LYS
1	A	539	LEU
1	A	549	ILE
1	A	556	LEU
1	A	557	THR
1	A	573	LYS
1	A	608	GLN
1	A	615	LEU
1	A	629	GLU
1	A	630	CYS
1	A	633	ARG
1	A	647	ASP
1	A	648	THR

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Mol	Chain	Res	Type
1	A	667	GLN
1	A	673	LYS
1	A	676	ARG
1	A	695	LEU
1	A	696	GLN
1	A	699	LYS
1	A	711	ARG
1	A	723	GLN
1	A	746	GLN
1	A	786	LYS
1	A	790	LYS
1	A	840	GLN
1	A	841	THR
1	A	852	ASN
2	B	70	LYS
2	B	136	GLN
2	B	179	GLU
2	B	195	ASN
2	B	231	VAL
2	B	240	ARG
2	B	379	ARG
2	B	384	ARG
2	B	402	VAL
2	B	462	THR
2	B	476	GLU
2	B	478	ARG
2	B	488	ASN
2	B	489	LYS
2	B	508	LEU
2	B	528	LYS
2	B	544	ARG
2	B	549	ILE
2	B	557	THR
2	B	573	LYS
2	B	608	GLN
2	B	619	SER
2	B	631	LYS
2	B	633	ARG
2	B	638	VAL
2	B	655	GLN
2	B	665	LEU
2	B	667	GLN

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Mol	Chain	Res	Type
2	B	668	GLU
2	B	677	THR
2	B	687	MET
2	B	695	LEU
2	B	698	LEU
2	B	706	ARG
2	B	721	GLN
2	B	722	TRP
2	B	723	GLN
2	B	728	ARG
2	B	735	ASN
2	B	744	LEU
2	B	746	GLN
2	B	749	LEU
2	B	751	HIS
2	B	790	LYS
2	B	798	THR
2	B	840	GLN
2	B	841	THR
2	B	852	ASN
2	C	41	LYS
2	C	70	LYS
2	C	136	GLN
2	C	144	LEU
2	C	157	LEU
2	C	179	GLU
2	C	195	ASN
2	C	231	VAL
2	C	236	LYS
2	C	240	ARG
2	C	258	GLU
2	C	282	LEU
2	C	343	LYS
2	C	379	ARG
2	C	384	ARG
2	C	402	VAL
2	C	415	THR
2	C	462	THR
2	C	476	GLU
2	C	478	ARG
2	C	489	LYS
2	C	508	LEU

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Mol	Chain	Res	Type
2	C	528	LYS
2	C	549	ILE
2	C	556	LEU
2	C	557	THR
2	C	573	LYS
2	C	608	GLN
2	C	633	ARG
2	C	638	VAL
2	C	648	THR
2	C	655	GLN
2	C	665	LEU
2	C	667	GLN
2	C	677	THR
2	C	687	MET
2	C	690	ILE
2	C	695	LEU
2	C	699	LYS
2	C	706	ARG
2	C	711	ARG
2	C	723	GLN
2	C	728	ARG
2	C	744	LEU
2	C	746	GLN
2	C	773	ARG
2	C	786	LYS
2	C	790	LYS
2	C	840	GLN
2	C	841	THR
1	D	41	LYS
1	D	130	TYR
1	D	136	GLN
1	D	157	LEU
1	D	179	GLU
1	D	195	ASN
1	D	209	ASP
1	D	231	VAL
1	D	343	LYS
1	D	370	LEU
1	D	384	ARG
1	D	402	VAL
1	D	442	ARG
1	D	462	THR

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Mol	Chain	Res	Type
1	D	476	GLU
1	D	478	ARG
1	D	488	ASN
1	D	504	ARG
1	D	508	LEU
1	D	528	LYS
1	D	537	LEU
1	D	549	ILE
1	D	557	THR
1	D	573	LYS
1	D	608	GLN
1	D	629	GLU
1	D	648	THR
1	D	655	GLN
1	D	665	LEU
1	D	667	GLN
1	D	695	LEU
1	D	706	ARG
1	D	723	GLN
1	D	786	LYS
1	D	790	LYS
1	D	798	THR
1	D	840	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	78	GLN
1	A	331	HIS
1	A	417	HIS
1	A	425	HIS
1	A	488	ASN
1	A	667	GLN
1	A	811	ASN
1	A	852	ASN
2	B	71	GLN
2	B	78	GLN
2	B	488	ASN
2	B	608	GLN
2	B	667	GLN
2	B	811	ASN

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Mol	Chain	Res	Type
2	B	840	GLN
2	B	852	ASN
2	C	71	GLN
2	C	78	GLN
2	C	142	ASN
2	C	173	GLN
2	C	189	ASN
2	C	195	ASN
2	C	356	ASN
2	C	399	ASN
2	C	401	HIS
2	C	488	ASN
2	C	667	GLN
2	C	764	HIS
2	C	811	ASN
1	D	25	ASN
1	D	71	GLN
1	D	142	ASN
1	D	173	GLN
1	D	401	HIS
1	D	488	ASN
1	D	580	HIS
1	D	608	GLN
1	D	667	GLN
1	D	746	GLN
1	D	811	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	K5L	D	581	1	7,11,12	8.63	3 (42%)	5,13,15	2.67	2 (40%)
1	K5L	A	581	1	7,11,12	8.69	2 (28%)	5,13,15	2.05	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	K5L	D	581	1	-	4/7/11/13	-
1	K5L	A	581	1	-	4/7/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	581	K5L	OAI-CAK	16.64	1.82	1.33
1	D	581	K5L	OAI-CB	16.47	1.82	1.45
1	A	581	K5L	OAI-CB	15.74	1.81	1.45
1	D	581	K5L	OAI-CAK	15.63	1.79	1.33
1	D	581	K5L	OAC-CAK	-2.10	1.16	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	581	K5L	OAI-CAK-CAG	4.55	118.79	111.07
1	A	581	K5L	OAI-CAK-CAG	3.57	117.13	111.07
1	D	581	K5L	OAI-CB-CA	-3.10	99.72	108.48
1	A	581	K5L	OAI-CB-CA	-2.41	101.68	108.48

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	581	K5L	C-CA-CB-OAI
1	D	581	K5L	N-CA-CB-OAI
1	A	581	K5L	C-CA-CB-OAI
1	A	581	K5L	N-CA-CB-OAI
1	A	581	K5L	OAC-CAK-OAI-CB
1	D	581	K5L	CAG-CAK-OAI-CB
1	D	581	K5L	OAC-CAK-OAI-CB

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Mol	Chain	Res	Type	Atoms
1	A	581	K5L	CAG-CAK-OAI-CB

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	581	K5L	5	0
1	A	581	K5L	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	COA	D	900	-	41,50,50	1.06	3 (7%)	52,75,75	1.79	11 (21%)
3	COA	A	900	-	41,50,50	1.10	6 (14%)	52,75,75	1.45	8 (15%)
4	MLC	C	900	-	44,56,56	1.11	6 (13%)	56,83,83	1.75	8 (14%)

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
3	COA	D	900	-	-	17/44/64/64	0/3/3/3
3	COA	A	900	-	-	22/44/64/64	0/3/3/3
4	MLC	C	900	-	-	20/48/71/71	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	COA	C5A-C4A	3.01	1.48	1.40
4	C	900	MLC	CM1-S	-2.97	1.68	1.76
3	D	900	COA	O4B-C1B	2.80	1.45	1.41
4	C	900	MLC	C5-C4	2.75	1.48	1.40
3	D	900	COA	C5A-C4A	2.67	1.48	1.40
3	A	900	COA	O4B-C1B	2.66	1.44	1.41
3	A	900	COA	C2A-N3A	2.57	1.36	1.32
4	C	900	MLC	C2-N3	2.32	1.35	1.32
3	A	900	COA	C4A-N3A	2.28	1.38	1.35
3	D	900	COA	OAP-CAP	2.24	1.46	1.42
4	C	900	MLC	P3-O3'	2.22	1.63	1.59
4	C	900	MLC	C4-N3	2.20	1.38	1.35
3	A	900	COA	C6A-C5A	2.16	1.51	1.43
3	A	900	COA	P3B-O3B	2.12	1.63	1.59
4	C	900	MLC	C6-C5	2.00	1.50	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	900	MLC	CM2-CM1-S	6.55	121.86	113.69
3	D	900	COA	N3A-C2A-N1A	-4.77	121.22	128.68
4	C	900	MLC	N3-C2-N1	-4.58	121.52	128.68
3	D	900	COA	CEP-CBP-CAP	4.49	116.61	108.82
3	A	900	COA	N3A-C2A-N1A	-4.45	121.72	128.68
3	D	900	COA	OAP-CAP-CBP	4.13	119.98	110.25
3	D	900	COA	CEP-CBP-CCP	-4.10	101.54	108.23
4	C	900	MLC	O7-CPB-CPA	3.85	116.74	110.55
4	C	900	MLC	OM2-CM1-S	-3.78	117.70	122.61
3	A	900	COA	C6P-C5P-N4P	3.58	122.45	116.42
4	C	900	MLC	C3'-C2'-C1'	3.41	107.44	99.89
3	D	900	COA	O9P-C9P-CAP	-3.22	111.24	121.06
3	A	900	COA	O5P-C5P-C6P	-3.10	116.34	122.02
4	C	900	MLC	C4-C5-N7	-3.03	106.24	109.40
3	D	900	COA	C2A-N1A-C6A	2.99	123.86	118.75
3	D	900	COA	C2P-C3P-N4P	2.99	119.13	112.31
3	D	900	COA	CAP-C9P-N8P	2.97	122.50	116.58
3	A	900	COA	C4A-C5A-N7A	-2.84	106.44	109.40
3	D	900	COA	C4A-C5A-N7A	-2.77	106.52	109.40
4	C	900	MLC	C1'-N9-C4	-2.67	121.95	126.64
3	A	900	COA	O4B-C1B-C2B	-2.47	103.31	106.93
3	D	900	COA	O5P-C5P-C6P	-2.33	117.76	122.02
3	D	900	COA	O3B-P3B-O7A	-2.31	100.47	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	900	COA	CDP-CBP-CAP	2.27	112.76	108.82
3	A	900	COA	C2A-N1A-C6A	2.13	122.40	118.75
4	C	900	MLC	OP1-CP3-CP4	-2.06	118.25	122.02
3	A	900	COA	C2P-C3P-N4P	2.05	116.98	112.31

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	900	COA	CCP-O6A-P2A-O3A
3	D	900	COA	CCP-O6A-P2A-O5A
3	D	900	COA	OAP-CAP-CBP-CCP
3	D	900	COA	C9P-CAP-CBP-CCP
3	D	900	COA	OAP-CAP-CBP-CDP
3	D	900	COA	C9P-CAP-CBP-CDP
3	D	900	COA	OAP-CAP-CBP-CEP
3	D	900	COA	C9P-CAP-CBP-CEP
3	D	900	COA	O9P-C9P-CAP-CBP
3	D	900	COA	N8P-C9P-CAP-CBP
3	D	900	COA	O9P-C9P-CAP-OAP
3	A	900	COA	CCP-O6A-P2A-O4A
3	A	900	COA	OAP-CAP-CBP-CCP
3	A	900	COA	S1P-C2P-C3P-N4P
4	C	900	MLC	C5'-O5'-P1-O6
4	C	900	MLC	CP7-CPA-CPB-O7
4	C	900	MLC	CP9-CPA-CPB-O7
4	C	900	MLC	CP8-CPA-CPB-O7
4	C	900	MLC	CP3-CP4-CP5-NP2
4	C	900	MLC	S-CP1-CP2-NP1
4	C	900	MLC	CM2-CM1-S-CP1
4	C	900	MLC	OM2-CM1-S-CP1
3	A	900	COA	C6P-C5P-N4P-C3P
3	A	900	COA	O5P-C5P-N4P-C3P
4	C	900	MLC	CP4-CP5-NP2-CP6
4	C	900	MLC	C4'-C5'-O5'-P1
4	C	900	MLC	C4'-C3'-O3'-P3
3	A	900	COA	C4B-C3B-O3B-P3B
4	C	900	MLC	C2'-C3'-O3'-P3
3	A	900	COA	OAP-CAP-CBP-CEP
3	D	900	COA	C4B-C5B-O5B-P1A
3	D	900	COA	S1P-C2P-C3P-N4P
3	D	900	COA	P1A-O3A-P2A-O6A

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Mol	Chain	Res	Type	Atoms
3	A	900	COA	CCP-O6A-P2A-O3A
3	A	900	COA	O4B-C4B-C5B-O5B
4	C	900	MLC	P2-O6-P1-O12
3	A	900	COA	CCP-O6A-P2A-O5A
4	C	900	MLC	C5'-O5'-P1-O11
4	C	900	MLC	C5'-O5'-P1-O12
3	A	900	COA	C9P-CAP-CBP-CCP
4	C	900	MLC	O4'-C4'-C5'-O5'
3	A	900	COA	C2B-C3B-O3B-P3B
3	A	900	COA	C3B-C4B-C5B-O5B
3	A	900	COA	OAP-CAP-CBP-CDP
3	A	900	COA	P1A-O3A-P2A-O4A
3	A	900	COA	P1A-O3A-P2A-O5A
3	A	900	COA	O9P-C9P-CAP-CBP
3	A	900	COA	N8P-C9P-CAP-CBP
4	C	900	MLC	CP2-CP1-S-CM1
4	C	900	MLC	P2-O6-P1-O11
3	D	900	COA	N8P-C9P-CAP-OAP
3	A	900	COA	C4B-C5B-O5B-P1A
4	C	900	MLC	C3'-C4'-C5'-O5'
3	A	900	COA	C9P-CAP-CBP-CDP
3	A	900	COA	C9P-CAP-CBP-CEP
3	D	900	COA	P1A-O3A-P2A-O4A
3	D	900	COA	CBP-CCP-O6A-P2A
4	C	900	MLC	CPA-CPB-O7-P2
3	A	900	COA	CEP-CBP-CCP-O6A

There are no ring outliers.

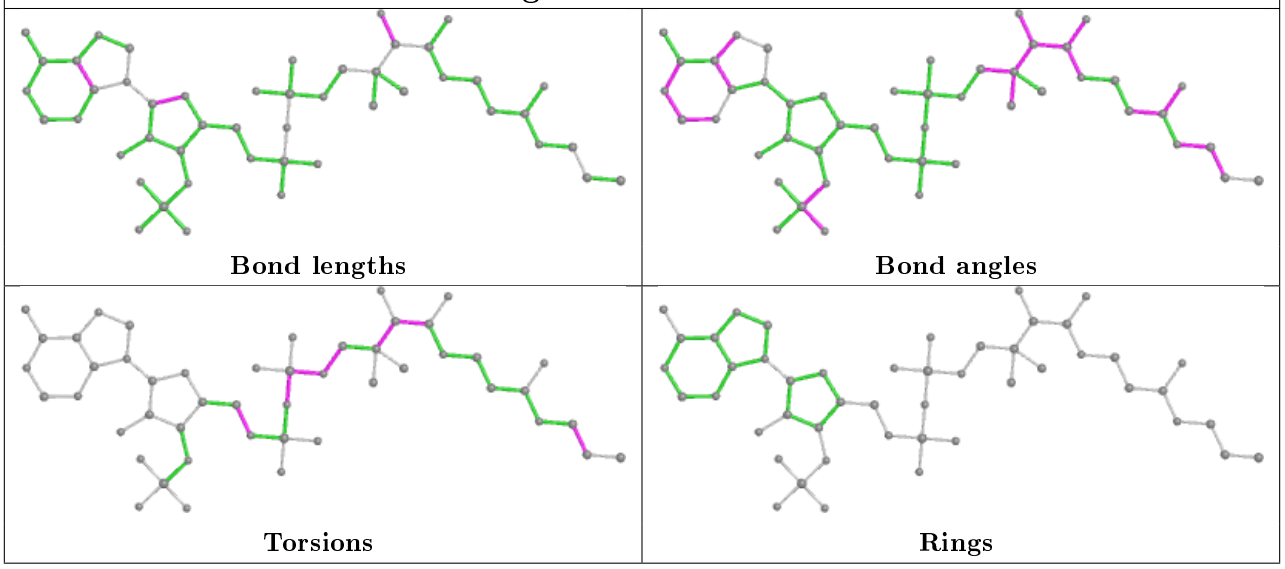
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	900	COA	5	0
4	C	900	MLC	1	0

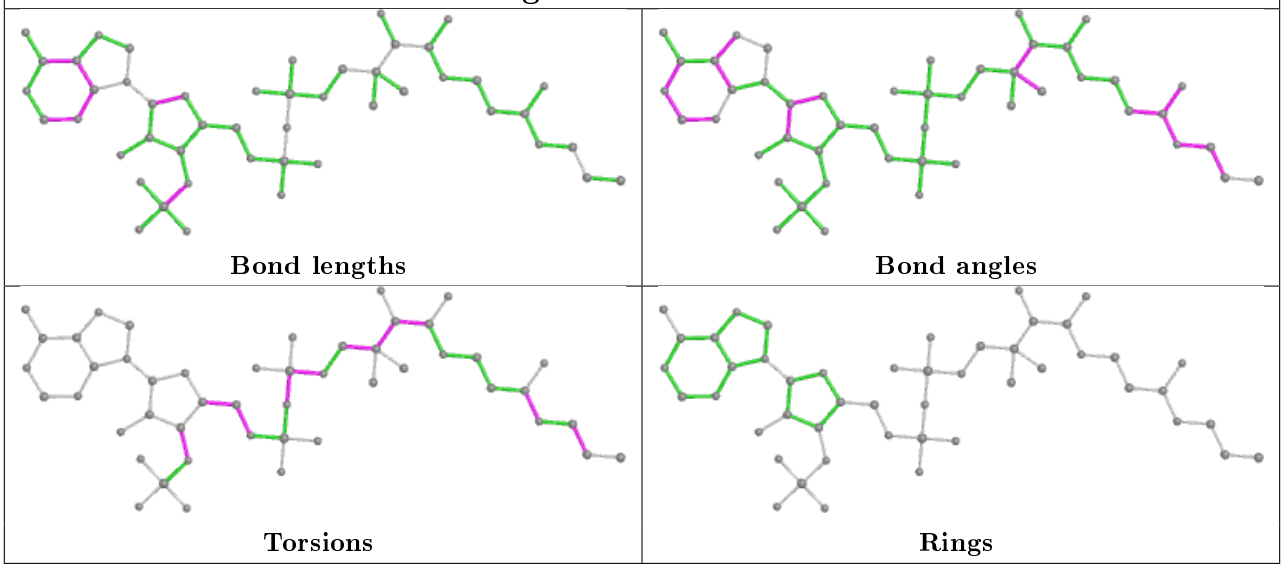
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

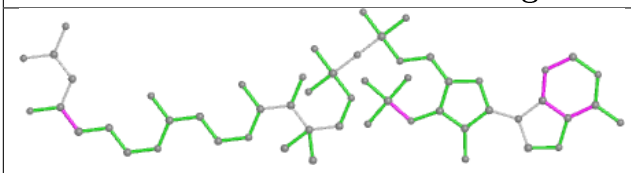
Ligand COA D 900



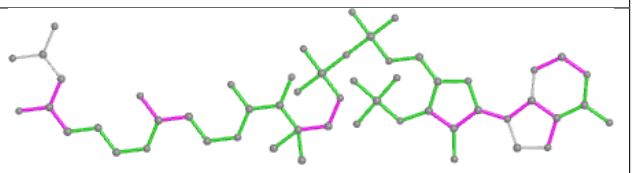
Ligand COA A 900



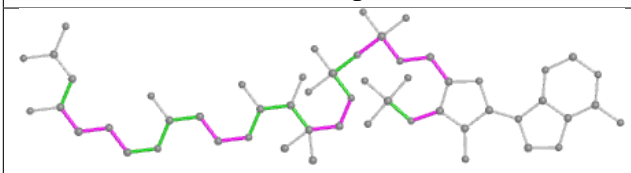
Ligand MLC C 900



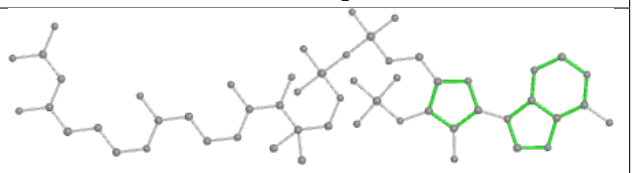
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	851/852 (99%)	0.00	20 (2%)	59	59	29, 57, 112, 186	0
1	D	851/852 (99%)	-0.02	16 (1%)	66	67	34, 55, 106, 164	0
2	B	848/852 (99%)	0.16	66 (7%)	13	11	33, 59, 170, 240	0
2	C	848/852 (99%)	0.16	58 (6%)	17	15	34, 62, 161, 247	0
All	All	3398/3408 (99%)	0.08	160 (4%)	31	31	29, 58, 150, 247	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	653	GLY	10.3
1	A	416	ALA	7.5
1	A	415	THR	7.4
2	C	417	HIS	5.7
2	C	418	ALA	5.3
2	B	671	PHE	5.2
2	C	637	GLY	5.1
2	B	661	PHE	4.9
2	C	669	GLY	4.6
2	C	526	ALA	4.6
2	B	747	GLU	4.4
2	B	627	TRP	4.4
2	C	640	PRO	4.3
2	B	662	VAL	4.3
2	B	546	PHE	4.3
2	C	539	LEU	4.2
2	C	508	LEU	4.2
2	B	696	GLN	4.2
1	A	417	HIS	4.1
2	B	624	GLY	4.1
2	B	609	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	640	PRO	4.0
1	D	636	ALA	4.0
2	B	745	PHE	3.9
2	B	531	GLY	3.9
2	B	537	LEU	3.8
2	C	750	TRP	3.8
2	B	628	GLU	3.8
2	B	625	LEU	3.7
2	C	672	ALA	3.6
2	C	667	GLN	3.6
2	C	623	VAL	3.5
2	C	670	VAL	3.5
2	B	641	ALA	3.5
1	A	696	GLN	3.5
2	C	659	ASN	3.5
2	B	626	SER	3.5
1	D	417	HIS	3.4
2	C	632	GLN	3.4
1	D	630	CYS	3.4
2	B	632	GLN	3.3
2	B	417	HIS	3.3
2	B	684	SER	3.2
2	B	544	ARG	3.2
1	A	667	GLN	3.2
2	C	605	TRP	3.2
1	D	487	THR	3.2
2	B	539	LEU	3.1
2	C	721	GLN	3.1
2	B	730	SER	3.1
2	B	720	ALA	3.1
1	D	704	GLU	3.0
2	B	651	ILE	3.0
2	B	750	TRP	3.0
2	B	646	GLU	3.0
2	C	668	GLU	3.0
2	B	487	THR	3.0
2	C	541	THR	3.0
2	C	730	SER	3.0
2	C	704	GLU	2.9
2	B	550	VAL	2.9
2	B	601	LEU	2.9
2	B	540	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	663	GLU	2.9
2	C	577	ILE	2.9
2	B	538	LEU	2.8
2	B	751	HIS	2.8
2	C	638	VAL	2.8
2	C	601	LEU	2.8
1	A	414	PRO	2.8
2	B	536	ASP	2.8
1	D	697	ALA	2.8
2	B	605	TRP	2.8
1	D	665	LEU	2.8
2	B	692	PRO	2.7
2	B	629	GLU	2.7
2	C	651	ILE	2.7
1	A	672	ALA	2.7
2	B	418	ALA	2.7
2	B	532	VAL	2.7
1	D	626	SER	2.7
1	D	628	GLU	2.7
1	D	775	VAL	2.7
1	D	703	ARG	2.6
1	A	627	TRP	2.6
2	B	622	ALA	2.6
2	B	533	LYS	2.6
2	C	525	GLU	2.6
2	B	529	PRO	2.6
2	C	662	VAL	2.6
2	C	639	VAL	2.6
2	C	609	CYS	2.5
2	B	658	VAL	2.5
2	C	666	LYS	2.5
1	A	605	TRP	2.5
2	B	489	LYS	2.5
1	D	627	TRP	2.5
2	C	722	TRP	2.5
2	C	558	ALA	2.5
2	C	535	SER	2.5
1	D	625	LEU	2.5
2	B	553	PHE	2.5
2	B	685	TYR	2.5
2	B	554	VAL	2.5
2	B	551	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	656	ALA	2.4
2	C	751	HIS	2.4
2	B	670	VAL	2.4
2	B	648	THR	2.4
1	D	629	GLU	2.4
1	A	662	VAL	2.4
2	C	660	GLU	2.4
2	B	713	LEU	2.4
2	C	125	GLU	2.4
2	C	665	LEU	2.4
2	B	672	ALA	2.3
2	B	530	LEU	2.3
2	C	618	GLY	2.3
2	C	546	PHE	2.3
2	C	529	PRO	2.3
2	B	535	SER	2.3
2	C	652	SER	2.3
1	A	700	LYS	2.3
2	B	699	LYS	2.3
2	C	619	SER	2.3
1	A	413	ALA	2.3
1	A	632	GLN	2.2
2	C	646	GLU	2.2
2	C	731	SER	2.2
2	C	630	CYS	2.2
2	B	494	PHE	2.2
2	C	530	LEU	2.2
1	D	663	GLU	2.2
2	C	620	MET	2.2
2	B	493	TRP	2.2
1	A	637	GLY	2.2
1	A	1	SER	2.2
2	C	657	ALA	2.2
2	C	720	ALA	2.2
2	B	634	CYS	2.2
2	C	696	GLN	2.2
2	B	687	MET	2.2
1	A	488	ASN	2.1
1	A	614	HIS	2.1
2	B	508	LEU	2.1
1	A	476	GLU	2.1
2	B	649	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	677	THR	2.1
2	B	637	GLY	2.1
2	C	648	THR	2.1
2	C	416	ALA	2.1
2	C	489	LYS	2.1
1	D	692	PRO	2.1
2	B	527	VAL	2.1
2	B	748	ALA	2.1
1	A	487	THR	2.0
2	C	415	THR	2.0
1	A	664	GLN	2.0
2	C	663	GLU	2.0
2	C	600	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
1	K5L	A	581	12/13	0.91	0.23	58,79,99,101	0
1	K5L	D	581	12/13	0.96	0.24	59,68,77,83	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

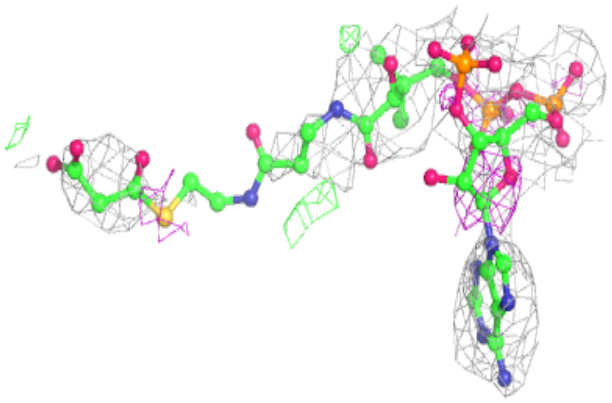
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

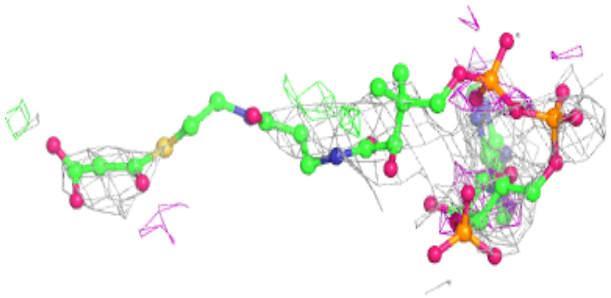
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MLC	C	900	54/54	0.64	0.40	119,164,252,262	0
3	COA	A	900	48/48	0.81	0.25	85,143,171,179	0
3	COA	D	900	48/48	0.88	0.27	66,113,130,136	0

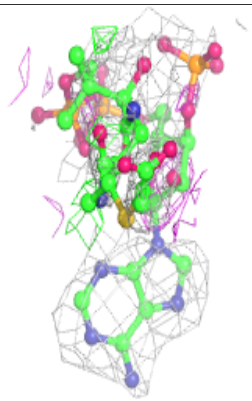
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MLC C 900:

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

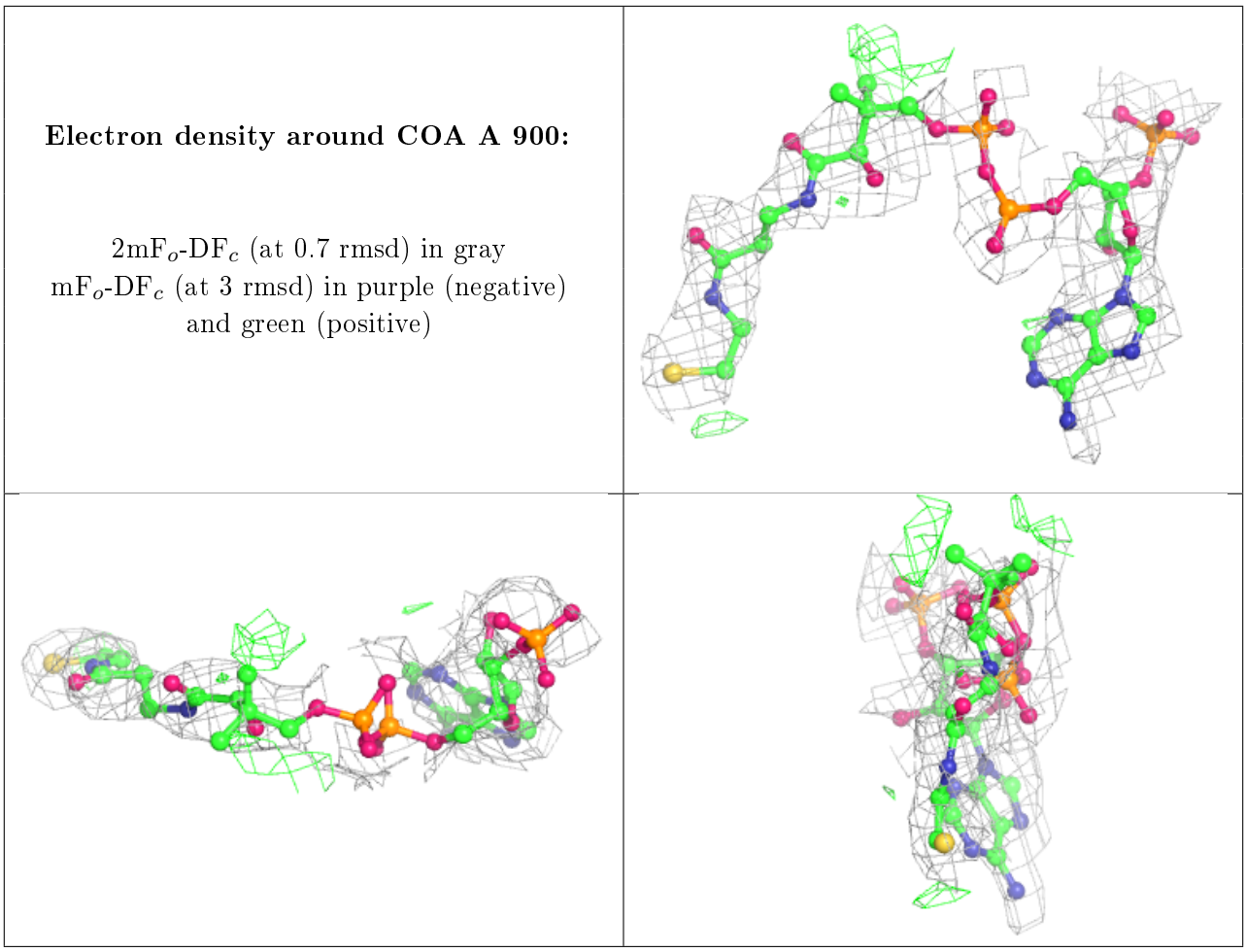






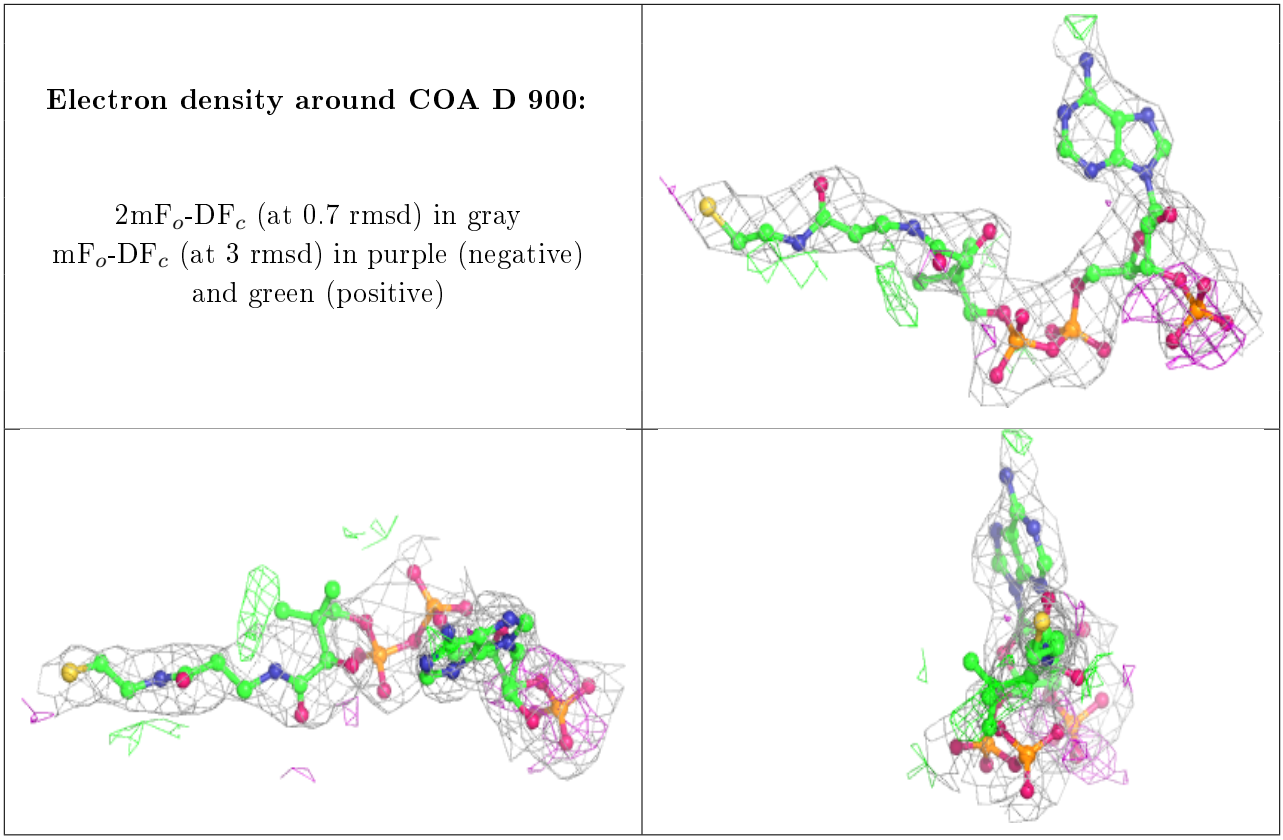
Electron density around COA A 900:

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



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

There are no such residues in this entry.