



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:39 AM UTC

PDB ID : 5MY0 / pdb_00005my0
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 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

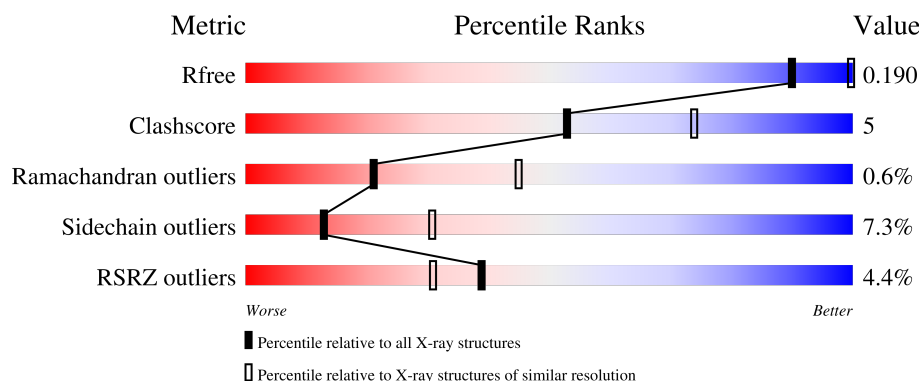
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	3% 89% 11%
1	D	852	2% 86% 12%
2	B	852	7% 87% 12%
2	C	852	7% 83% 15%

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

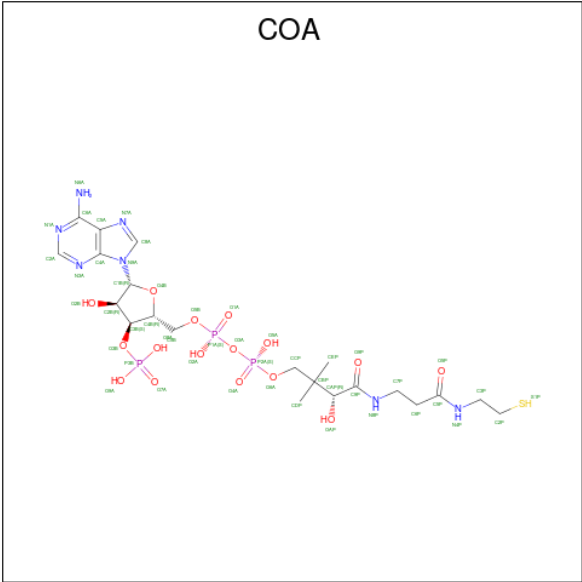
- Molecule 2 is a protein called Fatty acid synthase.

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:

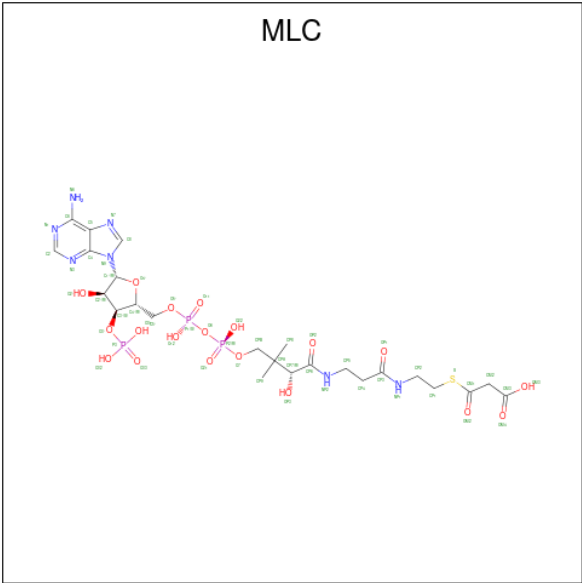
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP P19096
C	1	SER	-	expression tag	UNP P19096

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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 (CCD ID: MLC) (formula: $C_{24}H_{38}N_7O_{19}P_3S$).

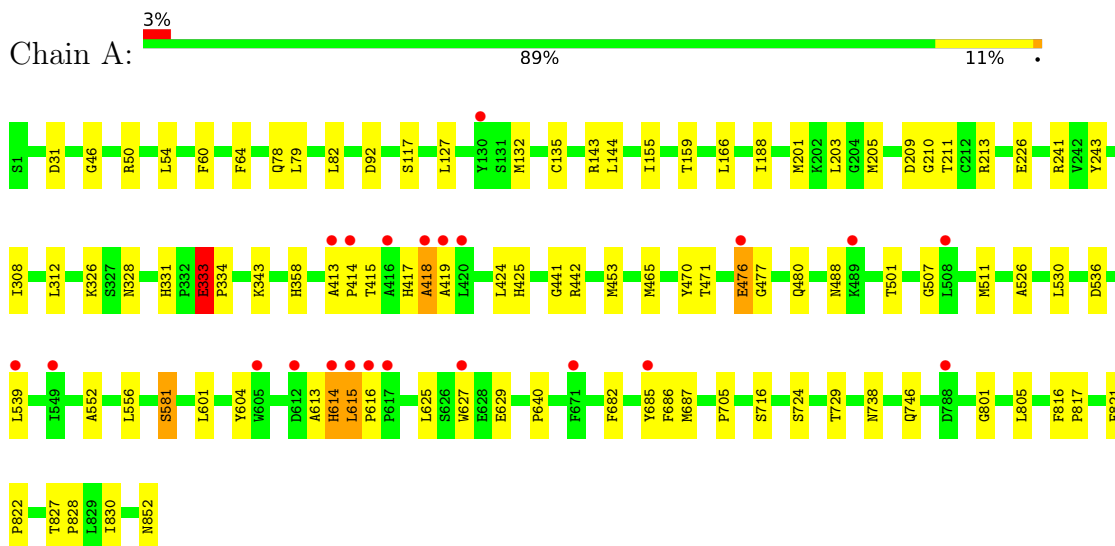


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	C	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		

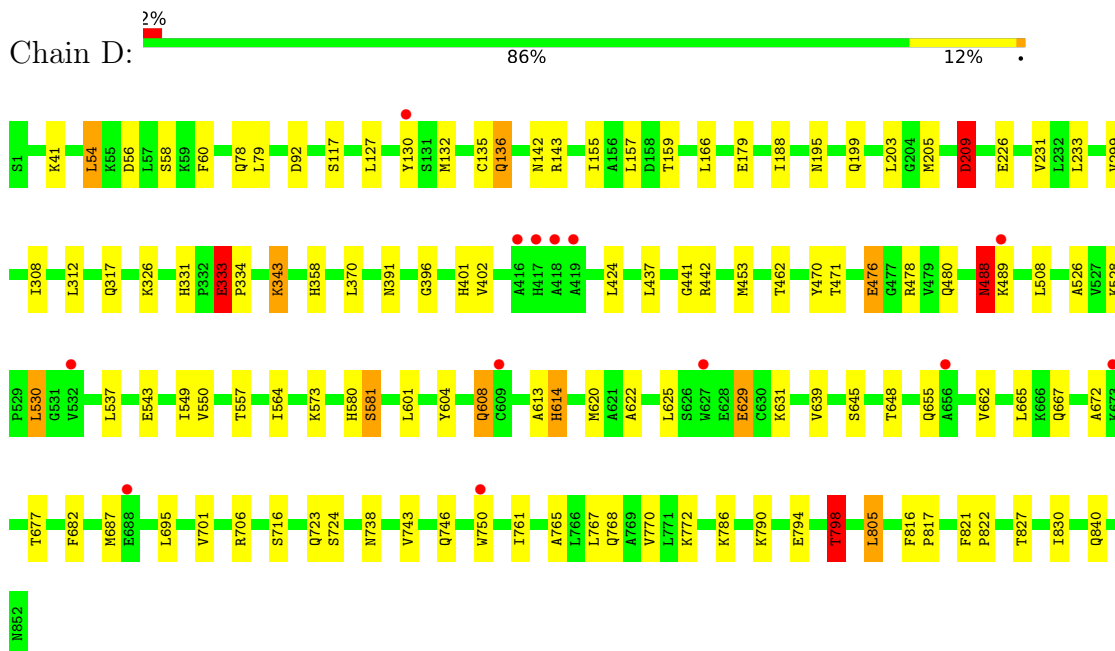
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

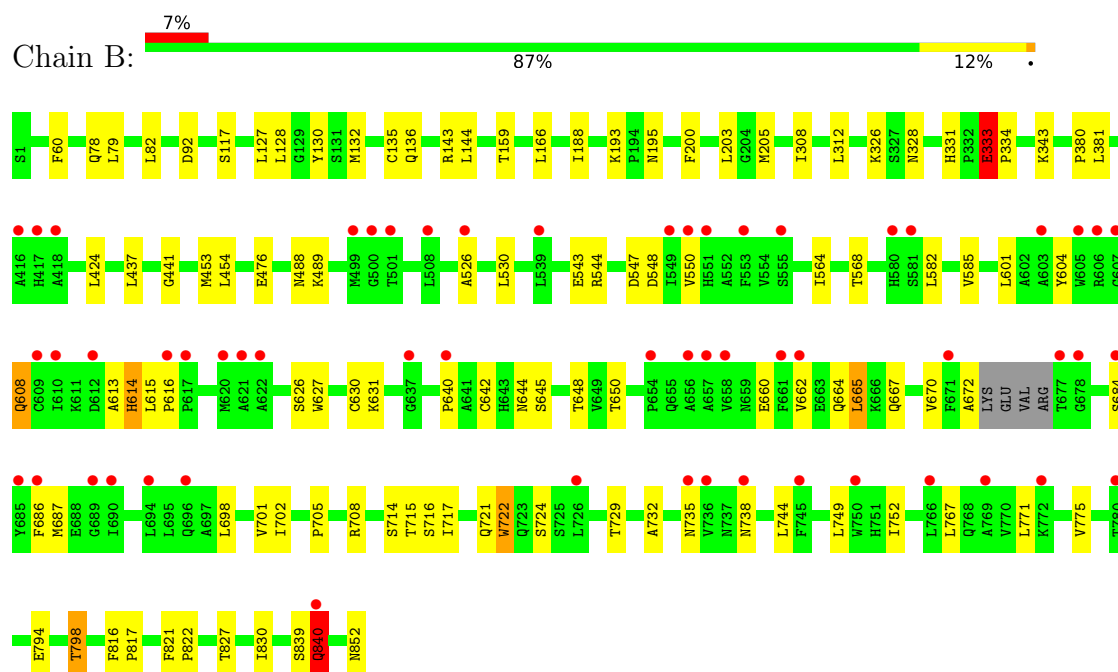
- Molecule 1: Fatty acid synthase



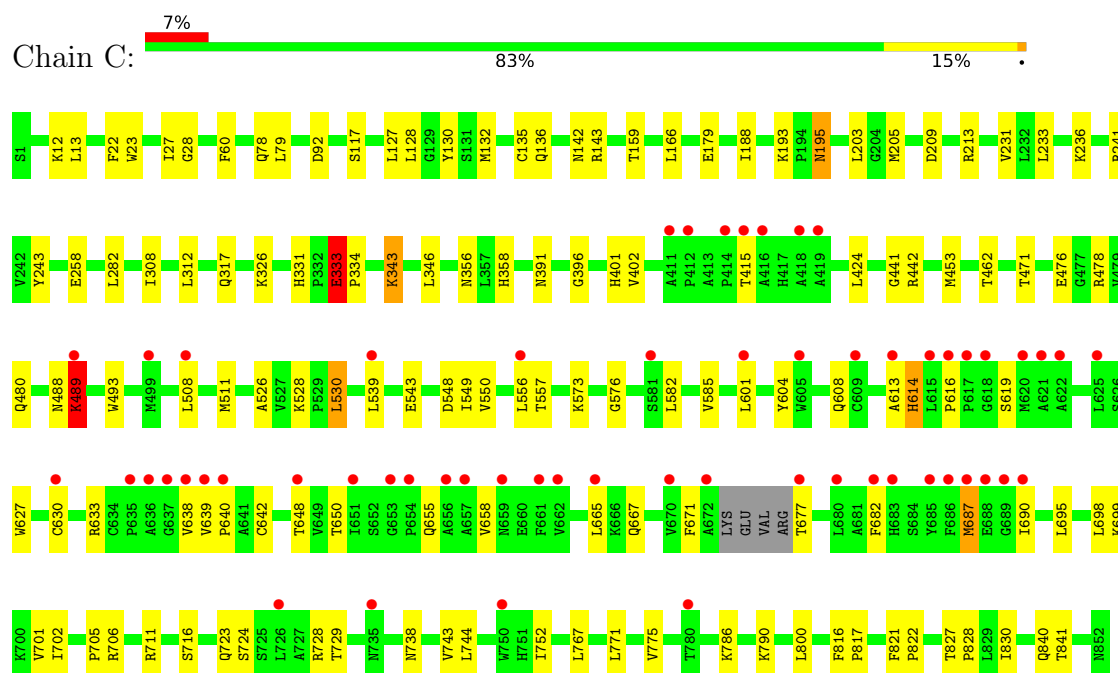
- Molecule 1: Fatty acid synthase



- Molecule 2: Fatty acid synthase



- Molecule 2: Fatty acid synthase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.188 , 0.222 (Not available) , 0.190	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)	0.32 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K5L, MLC, 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	0.91	1/6617 (0.0%)	1.04	12/8998 (0.1%)
1	D	0.90	0/6617	1.04	12/8998 (0.1%)
2	B	0.89	2/6587 (0.0%)	1.07	18/8959 (0.2%)
2	C	0.87	1/6580 (0.0%)	1.01	6/8950 (0.1%)
All	All	0.89	4/26401 (0.0%)	1.04	48/35905 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	840	GLN	CA-C	-6.98	1.43	1.52
2	B	840	GLN	CG-CD	6.12	1.67	1.52
1	A	418	ALA	CA-C	5.18	1.59	1.52
2	C	179	GLU	N-CA	5.11	1.52	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	840	GLN	CA-C-N	11.03	141.55	121.70
2	B	840	GLN	C-N-CA	11.03	141.55	121.70
1	D	209	ASP	N-CA-CB	-9.31	94.75	110.49
2	B	840	GLN	CA-C-O	-9.29	107.22	120.51
1	A	488	ASN	N-CA-C	-8.99	95.12	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	209	ASP	CB-CA-C	-8.42	93.66	110.42
2	B	840	GLN	CB-CG-CD	7.69	125.67	112.60
2	B	488	ASN	N-CA-C	-6.76	98.70	109.59
2	B	722	TRP	CA-CB-CG	6.71	126.35	113.60
1	D	488	ASN	N-CA-C	-6.46	99.20	109.59
1	A	414	PRO	CA-C-N	6.40	133.77	121.54
1	A	414	PRO	C-N-CA	6.40	133.77	121.54
1	A	328	ASN	N-CA-C	6.27	118.20	111.36
1	A	419	ALA	N-CA-C	6.26	124.14	110.80
1	A	418	ALA	N-CA-C	6.26	124.13	110.80
2	B	840	GLN	CB-CA-C	6.15	122.67	110.42
2	C	333	GLU	CA-C-N	-6.12	113.32	119.56
2	C	333	GLU	C-N-CA	-6.12	113.32	119.56
1	A	333	GLU	CA-C-N	-6.09	113.35	119.56
1	A	333	GLU	C-N-CA	-6.09	113.35	119.56
2	B	333	GLU	CA-C-N	-6.00	113.44	119.56
2	B	333	GLU	C-N-CA	-6.00	113.44	119.56
1	D	333	GLU	CA-C-N	-5.97	113.47	119.56
1	D	333	GLU	C-N-CA	-5.97	113.47	119.56
2	B	665	LEU	CA-CB-CG	5.80	136.61	116.30
2	B	381	LEU	CB-CG-CD1	5.70	127.78	110.70
1	D	798	THR	N-CA-CB	5.68	118.97	110.22
1	D	724	SER	N-CA-C	5.63	117.81	110.43
2	C	616	PRO	O-C-N	5.60	123.89	121.31
2	B	798	THR	N-CA-CB	5.51	118.71	110.22
1	D	358	HIS	N-CA-C	5.40	119.45	112.86
2	B	724	SER	N-CA-C	5.37	117.47	110.43
2	B	616	PRO	O-C-N	5.33	123.76	121.31
2	B	631	LYS	CA-CB-CG	5.31	124.72	114.10
1	A	724	SER	N-CA-C	5.31	117.38	110.43
2	C	358	HIS	N-CA-C	5.26	119.28	112.86
2	C	724	SER	N-CA-C	5.25	117.30	110.43
1	A	414	PRO	O-C-N	5.24	128.97	122.22
1	D	798	THR	CA-CB-CG2	5.21	119.36	110.50
1	D	209	ASP	N-CA-C	5.21	121.89	110.80
1	D	333	GLU	CB-CA-C	5.12	120.25	110.17
1	D	299	VAL	CB-CA-C	-5.09	105.25	111.92
2	B	608	GLN	CA-CB-CG	-5.08	103.94	114.10
1	A	615	LEU	CA-CB-CG	5.05	133.98	116.30
2	B	489	LYS	N-CA-C	-5.02	101.92	109.15
2	C	333	GLU	CB-CA-C	5.02	120.05	110.17
1	A	358	HIS	N-CA-C	5.01	118.97	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	328	ASN	N-CA-C	5.01	117.85	111.69

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 ⓘ

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	62	0
1	D	6483	0	6456	58	0
2	B	6441	0	6419	77	0
2	C	6435	0	6412	70	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	259	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 (259) 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:OAI	1:A:581:K5L:CAK	1.82	1.27
1:A:581:K5L:OAI	1:A:581:K5L:CB	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
2:B:716:SER:OG	2:B:738:ASN:HA	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:ASN:H	2:C:195:ASN:HD22	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:D:453:MET:HE1	1:D:827:THR:HG21	1.74	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
1:A:453:MET:HE1	1:A:827:THR:HG21	1.75	0.67
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:453:MET:HE1	2:C:827:THR:HG21	1.79	0.64
2:B:453:MET:HE1	2:B:827:THR:HG21	1.80	0.64
2:C:582:LEU:O	2:C:585:VAL:HG12	1.99	0.63
1:A:132:MET:HE3	2:B:200:PHE:CE1	2.34	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
1:A:852:ASN:C	1:A:852:ASN:HD22	2.09	0.61
2:B:665:LEU:CD1	2:B:672:ALA:HB2	2.30	0.61
2:B:852:ASN:C	2:B:852:ASN:HD22	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:684:SER:H	2:B:687:MET:HE1	1.65	0.60
1:A:536:ASP:HA	1:A:539:LEU:HD22	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
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: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
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
2:C:488:ASN:O	2:C:489:LYS:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:132:MET:HE2	2:C:136:GLN:HG3	1.92	0.50
2:C:471:THR:HG22	2:C:480:GLN:CB	2.39	0.50
1:D:132:MET:HE2	1:D:136:GLN:HG3	1.94	0.50
1:D:620:MET:CE	1:D:677:THR:HG21	2.42	0.50
2:C:195:ASN:N	2:C:195:ASN:ND2	2.53	0.50
1:A:326:LYS:HE3	1:A:331:HIS:CD2	2.46	0.50
1:A:471:THR:HG22	1:A:480:GLN:CB	2.39	0.50
2:C:195:ASN:H	2:C:195:ASN:ND2	2.01	0.50
1:D:622:ALA:HB3	3:D:900:COA:H131	1.92	0.50
2:C:619:SER:CB	2:C:658:VAL:HG21	2.42	0.49
2:B:127:LEU:C	2:B:127:LEU:HD12	2.38	0.49
1:A:415:THR:HG23	1:A:417:HIS:CD2	2.47	0.49
1:D:343:LYS:HD2	1:D:343:LYS:C	2.38	0.49
2:B:203:LEU:HD13	2:B:205:MET:HE3	1.94	0.49
1:A:132:MET:HE3	2:B:200:PHE:CD1	2.48	0.48
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
2:C:343:LYS:C	2:C:343:LYS:HD2	2.38	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:343:LYS:C	1:A:343:LYS:HD2	2.39	0.48
2:B:343:LYS:HD2	2:B:343:LYS:C	2.38	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
2:B:132:MET:HE2	2:B:136:GLN:HG3	1.95	0.47
1:A:453:MET:CE	1:A:827:THR:HG21	2.44	0.47
2:B:453:MET:CE	2:B:827:THR:HG21	2.42	0.47
2:C:127:LEU:C	2:C:127:LEU:HD12	2.39	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:OAI	1:A:581:K5L:CA	2.56	0.47
2:C:716:SER:HB2	2:C:738:ASN:HA	1.97	0.47
2:C:203:LEU:HD13	2:C:205:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:LEU:HD23	1:A:604:TYR:CD1	2.50	0.47
1:A:613:ALA:O	1:A:614:HIS:C	2.58	0.46
2:B:698:LEU:HG	2:B:732:ALA:CB	2.46	0.46
2:C:511:MET:HE2	2:C:539:LEU:CD2	2.45	0.46
1:A:54:LEU:HD13	1:A:226:GLU:HB2	1.97	0.46
1:D:620:MET:HE2	1:D:677:THR:HG21	1.97	0.46
1:A:46:GLY:O	1:A:201:MET:HE1	2.15	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:12:LYS:C	2:C:13:LEU:HG	2.40	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
1:A:203:LEU:HD13	1:A:205:MET:HE3	1.98	0.45
2:C:816:PHE:HB3	2:C:817:PRO:HD2	1.97	0.45
2:B:642:CYS:SG	2:B:650:THR:OG1	2.73	0.45
3:D:900:COA:H141	3:D:900:COA:N8P	2.31	0.45
1:A:127:LEU:C	1:A:127:LEU:HD12	2.42	0.45
2:B:767:LEU:HB3	2:B:771:LEU:CD2	2.46	0.45
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:821:PHE:HA	1:D:822:PRO:C	2.42	0.45
2:B:564:ILE:O	2:B:568:THR:HG23	2.16	0.45
2:B:613:ALA:O	2:B:614:HIS:C	2.59	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:A:50:ARG:NH1	1:A:210:GLY:O	2.49	0.44
2:B:752:ILE:CG1	2:B:775:VAL:HG13	2.47	0.44
2:C:821:PHE:HA	2:C:822:PRO:C	2.42	0.44
2:B:752:ILE:HD12	2:B:752:ILE:O	2.17	0.44
2:C:613:ALA:O	2:C:614:HIS:C	2.59	0.44
1:D:662:VAL:HG13	1:D:672:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ALA:O	1:A:556:LEU:HB2	2.18	0.44
2:C:92:ASP:HA	2:C:830:ILE:HB	1.99	0.44
2:C:767:LEU:HB3	2:C:771:LEU:CD2	2.48	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:698:LEU:HA	2:C:701:VAL:HG22	1.99	0.44
2:B:667:GLN:HE21	2:B:667:GLN:C	2.25	0.44
2:B:821:PHE:HA	2:B:822:PRO:C	2.43	0.44
1:A:716:SER:HB2	1:A:738:ASN:HA	1.99	0.44
1:D:613:ALA:O	1:D:614:HIS:C	2.60	0.44
1:A:64:PHE:CE1	1:A:465:MET:HE2	2.52	0.44
1:D:127:LEU:HD12	1:D:127:LEU:C	2.43	0.44
2:B:698:LEU:HA	2:B:701:VAL:HG22	1.99	0.43
1:D:488:ASN:N	1:D:488:ASN:HD22	2.15	0.43
2:C:13:LEU:HD13	2:C:22:PHE:CG	2.53	0.43
2:C:396:GLY:HA3	1:D:142:ASN:HD22	1.83	0.43
2:C:682:PHE:HA	2:C:687:MET:SD	2.58	0.43
2:B:159:THR:HG21	2:B:166:LEU:CD2	2.49	0.43
1:A:155:ILE:HG12	2:B:166:LEU:HD21	2.01	0.43
2:B:82:LEU:CD2	2:B:144:LEU:HD11	2.49	0.43
2:B:615:LEU:HD12	2:B:686:PHE:CD2	2.54	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
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
1:D:78:GLN:HB3	1:D:188:ILE:HD12	1.99	0.42
1:D:682:PHE:HA	1:D:687:MET:HE3	2.01	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
1:A:821:PHE:HA	1:A:822:PRO:C	2.44	0.42
2:B:82:LEU:HD21	2:B:144:LEU:HD11	2.01	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
1:D:437:LEU:HD23	1:D:437:LEU:HA	1.93	0.42
1:A:82:LEU:CD2	1:A:144:LEU:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:488:ASN:N	1:D:488:ASN:ND2	2.67	0.41
1:A:852:ASN:C	1:A:852:ASN:ND2	2.78	0.41
2:B:644:ASN:HB2	2:B:648:THR:HG23	2.02	0.41
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:A:682:PHE:HA	1:A:687:MET:HE3	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:771:LEU:O	2:C:775:VAL:HG13	2.21	0.41
2:B:852:ASN:C	2:B:852:ASN:ND2	2.78	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	2:C:800:LEU:HA	1.90	0.40
1:D:203:LEU:HD13	1:D:205:MET:HE3	2.02	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%)	21	45
1	D	849/852 (100%)	821 (97%)	22 (3%)	6 (1%)	18	40
2	B	844/852 (99%)	811 (96%)	28 (3%)	5 (1%)	21	45
2	C	844/852 (99%)	809 (96%)	30 (4%)	5 (1%)	21	45
All	All	3386/3408 (99%)	3254 (96%)	111 (3%)	21 (1%)	21	45

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

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Mol	Chain	Res	Type
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 ⓘ

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	D	701/701 (100%)	655 (93%)	46 (7%)	15	35
2	C	548/702 (78%)	503 (92%)	45 (8%)	10	26
All	All	1249/1403 (89%)	1158 (93%)	91 (7%)	13	31

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	195	ASN
2	C	231	VAL
2	C	233	LEU
2	C	236	LYS
2	C	258	GLU
2	C	282	LEU
2	C	317	GLN
2	C	343	LYS
2	C	402	VAL
2	C	415	THR
2	C	462	THR

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Mol	Chain	Res	Type
2	C	476	GLU
2	C	478	ARG
2	C	489	LYS
2	C	508	LEU
2	C	528	LYS
2	C	530	LEU
2	C	549	ILE
2	C	556	LEU
2	C	557	THR
2	C	573	LYS
2	C	608	GLN
2	C	630	CYS
2	C	633	ARG
2	C	638	VAL
2	C	639	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	743	VAL
2	C	744	LEU
2	C	786	LYS
2	C	790	LYS
2	C	840	GLN
2	C	841	THR
1	D	41	LYS
1	D	54	LEU
1	D	130	TYR
1	D	136	GLN
1	D	157	LEU
1	D	179	GLU
1	D	195	ASN
1	D	209	ASP

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Mol	Chain	Res	Type
1	D	231	VAL
1	D	233	LEU
1	D	317	GLN
1	D	343	LYS
1	D	370	LEU
1	D	402	VAL
1	D	442	ARG
1	D	462	THR
1	D	476	GLU
1	D	478	ARG
1	D	488	ASN
1	D	489	LYS
1	D	508	LEU
1	D	528	LYS
1	D	530	LEU
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	631	LYS
1	D	639	VAL
1	D	648	THR
1	D	655	GLN
1	D	665	LEU
1	D	667	GLN
1	D	695	LEU
1	D	701	VAL
1	D	706	ARG
1	D	723	GLN
1	D	743	VAL
1	D	772	LYS
1	D	786	LYS
1	D	790	LYS
1	D	798	THR
1	D	805	LEU
1	D	840	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	189	ASN
2	C	195	ASN
2	C	271	GLN
2	C	293	HIS
2	C	331	HIS
2	C	356	ASN
2	C	401	HIS
2	C	410	GLN
2	C	417	HIS
2	C	422	HIS
2	C	488	ASN
2	C	614	HIS
2	C	738	ASN
2	C	811	ASN
1	D	25	ASN
1	D	71	GLN
1	D	104	ASN
1	D	142	ASN
1	D	170	ASN
1	D	173	GLN
1	D	271	GLN
1	D	293	HIS
1	D	331	HIS
1	D	360	HIS
1	D	399	ASN
1	D	401	HIS
1	D	422	HIS
1	D	488	ASN
1	D	580	HIS
1	D	608	GLN
1	D	614	HIS
1	D	667	GLN
1	D	746	GLN
1	D	755	HIS
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	A	581	1	10,11,12	7.47	3 (30%)	8,13,15	1.56	2 (25%)
1	K5L	D	581	1	10,11,12	7.33	3 (30%)	8,13,15	1.58	3 (37%)

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	A	581	1	-	4/9/11/13	-
1	K5L	D	581	1	-	4/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	581	K5L	OAI-CB	16.83	1.82	1.45
1	A	581	K5L	OAI-CAK	16.72	1.82	1.33
1	A	581	K5L	OAI-CB	16.08	1.81	1.45
1	D	581	K5L	OAI-CAK	15.70	1.79	1.33
1	A	581	K5L	CAG-CAJ	3.35	1.56	1.51
1	D	581	K5L	OAC-CAK	-2.08	1.16	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	581	K5L	OAB-CAJ-CAG	2.50	122.26	114.51
1	D	581	K5L	OAI-CAK-CAG	2.46	118.79	111.38
1	A	581	K5L	OAB-CAJ-OAE	-2.34	117.33	123.33
1	D	581	K5L	OAB-CAJ-CAG	2.11	121.04	114.51
1	D	581	K5L	OAI-CAK-OAC	-2.01	118.61	123.63

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	581	K5L	3	0
1	D	581	K5L	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	47,50,50	1.35	5 (10%)	69,75,75	2.03	20 (28%)
3	COA	A	900	-	47,50,50	1.51	7 (14%)	69,75,75	1.90	16 (23%)
4	MLC	C	900	-	53,56,56	1.65	9 (16%)	77,83,83	2.00	16 (20%)

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	-	-	18/48/64/64	0/3/3/3
3	COA	A	900	-	-	24/48/64/64	0/3/3/3
4	MLC	C	900	-	-	21/54/71/71	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	COA	C5A-C4A	5.49	1.48	1.39
4	C	900	MLC	C5-C4	5.12	1.48	1.39
4	C	900	MLC	P1-O6	5.01	1.64	1.59
3	D	900	COA	C5A-C4A	5.00	1.48	1.39
4	C	900	MLC	P2-O6	4.74	1.64	1.59
3	A	900	COA	P2A-O3A	3.77	1.63	1.59
3	A	900	COA	C5A-C6A	3.71	1.51	1.41
4	C	900	MLC	C5-C6	3.50	1.50	1.41
3	A	900	COA	P1A-O3A	3.31	1.63	1.59
3	D	900	COA	C5A-C6A	3.30	1.50	1.41
4	C	900	MLC	CM1-S	-3.13	1.68	1.76
4	C	900	MLC	C8-N7	2.53	1.36	1.31
3	D	900	COA	P1A-O3A	2.53	1.62	1.59
3	A	900	COA	C8A-N7A	2.40	1.36	1.31
3	A	900	COA	C4A-N3A	2.34	1.38	1.34
3	D	900	COA	OAP-CAP	2.32	1.46	1.42
4	C	900	MLC	C4-N3	2.29	1.38	1.34
4	C	900	MLC	P3-O3'	2.27	1.63	1.59
3	D	900	COA	C8A-N7A	2.19	1.35	1.31
3	A	900	COA	P3B-O3B	2.16	1.63	1.59
4	C	900	MLC	C1'-N9	2.10	1.52	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	900	MLC	CM2-CM1-S	6.48	121.86	113.63
3	A	900	COA	C5A-C4A-N3A	-6.40	117.91	126.72
4	C	900	MLC	C5-C4-N3	-5.89	118.60	126.72
3	A	900	COA	N3A-C4A-N9A	5.43	136.39	127.17
3	D	900	COA	N3A-C2A-N1A	-4.87	121.22	128.58
3	D	900	COA	C5A-C4A-N3A	-4.76	120.16	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	900	MLC	N1-C2-N3	-4.66	121.52	128.58
4	C	900	MLC	N3-C4-N9	4.66	135.10	127.17
4	C	900	MLC	C2-N3-C4	4.65	123.19	111.83
3	A	900	COA	C2A-N3A-C4A	4.62	123.12	111.83
3	D	900	COA	CEP-CBP-CAP	4.60	116.61	108.77
3	A	900	COA	N3A-C2A-N1A	-4.53	121.72	128.58
3	D	900	COA	OAP-CAP-CBP	4.23	119.98	110.18
3	D	900	COA	N3A-C4A-N9A	4.13	134.19	127.17
3	D	900	COA	C2A-N3A-C4A	4.09	121.83	111.83
3	D	900	COA	CEP-CBP-CCP	-4.05	101.54	108.22
4	C	900	MLC	OM2-CM1-S	-3.91	117.70	122.68
4	C	900	MLC	O7-CPB-CPA	3.85	116.74	110.55
4	C	900	MLC	C4-C5-N7	-3.79	106.24	110.58
3	D	900	COA	C4A-N9A-C8A	3.69	109.61	105.74
3	A	900	COA	C4A-C5A-N7A	-3.62	106.44	110.58
3	D	900	COA	C4A-C5A-N7A	-3.56	106.52	110.58
3	D	900	COA	O9P-C9P-CAP	-3.46	111.24	120.89
4	C	900	MLC	C3'-C2'-C1'	3.43	107.44	99.89
3	A	900	COA	C6P-C5P-N4P	3.35	122.45	116.34
4	C	900	MLC	C6-C5-N7	3.31	138.47	132.09
3	D	900	COA	C6A-C5A-N7A	3.21	138.27	132.09
4	C	900	MLC	C5-N7-C8	3.18	108.45	103.45
3	D	900	COA	CAP-C9P-N8P	3.17	122.50	116.48
3	A	900	COA	O5P-C5P-C6P	-3.13	116.34	122.02
3	D	900	COA	C2A-N1A-C6A	3.13	123.86	118.73
3	A	900	COA	C5A-N7A-C8A	3.04	108.23	103.45
3	D	900	COA	C2P-C3P-N4P	3.01	119.13	112.31
3	D	900	COA	C5A-N7A-C8A	3.00	108.17	103.45
3	A	900	COA	C4A-N9A-C8A	2.92	108.81	105.74
4	C	900	MLC	O4'-C1'-N9	2.74	113.36	108.09
3	D	900	COA	N9A-C8A-N7A	-2.74	110.06	113.94
4	C	900	MLC	C4-N9-C8	2.71	108.58	105.74
3	A	900	COA	C6A-C5A-N7A	2.68	137.26	132.09
3	D	900	COA	O3B-P3B-O7A	-2.49	100.47	109.33
3	D	900	COA	O3A-P1A-O1A	-2.49	103.23	110.70
4	C	900	MLC	N9-C8-N7	-2.48	110.42	113.94
3	A	900	COA	C2B-C1B-N9A	2.43	119.34	113.30
3	D	900	COA	O5P-C5P-C6P	-2.35	117.76	122.02
3	A	900	COA	CDP-CBP-CAP	2.34	112.76	108.77
3	A	900	COA	C2A-N1A-C6A	2.23	122.40	118.73
3	A	900	COA	N9A-C8A-N7A	-2.20	110.82	113.94
3	A	900	COA	C1B-N9A-C8A	-2.16	122.30	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	900	MLC	OP1-CP3-CP4	-2.08	118.25	122.02
3	A	900	COA	C2P-C3P-N4P	2.06	116.98	112.31
3	D	900	COA	O5A-P2A-O4A	2.06	122.02	112.44
4	C	900	MLC	C4-N9-C1'	-2.00	121.95	126.63

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	900	COA	C2B-C1B-N9A-C4A
3	A	900	COA	C2B-C1B-N9A-C8A
3	A	900	COA	CCP-O6A-P2A-O3A
3	A	900	COA	CCP-O6A-P2A-O4A
3	A	900	COA	OAP-CAP-CBP-CCP
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
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	P1A-O3A-P2A-O6A

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Mol	Chain	Res	Type	Atoms
3	A	900	COA	O4B-C4B-C5B-O5B
4	C	900	MLC	P2-O6-P1-O12
3	A	900	COA	C9P-CAP-CBP-CCP
3	A	900	COA	S1P-C2P-C3P-N4P
3	D	900	COA	S1P-C2P-C3P-N4P
4	C	900	MLC	O4'-C4'-C5'-O5'
3	A	900	COA	CCP-O6A-P2A-O5A
4	C	900	MLC	C5'-O5'-P1-O11
4	C	900	MLC	C5'-O5'-P1-O12
4	C	900	MLC	C5'-O5'-P1-O6
3	A	900	COA	C2B-C3B-O3B-P3B
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
4	C	900	MLC	CM1-CM2-CM3-OM4
3	A	900	COA	N8P-C9P-CAP-CBP
3	D	900	COA	N8P-C9P-CAP-OAP
3	A	900	COA	C3B-C4B-C5B-O5B
4	C	900	MLC	CM1-CM2-CM3-OM3
4	C	900	MLC	P2-O6-P1-O11
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	A	900	COA	C4B-C5B-O5B-P1A
3	D	900	COA	P1A-O3A-P2A-O4A
3	D	900	COA	O4B-C1B-N9A-C8A
3	D	900	COA	CBP-CCP-O6A-P2A
4	C	900	MLC	CPA-CPB-O7-P2
3	A	900	COA	CEP-CBP-CCP-O6A

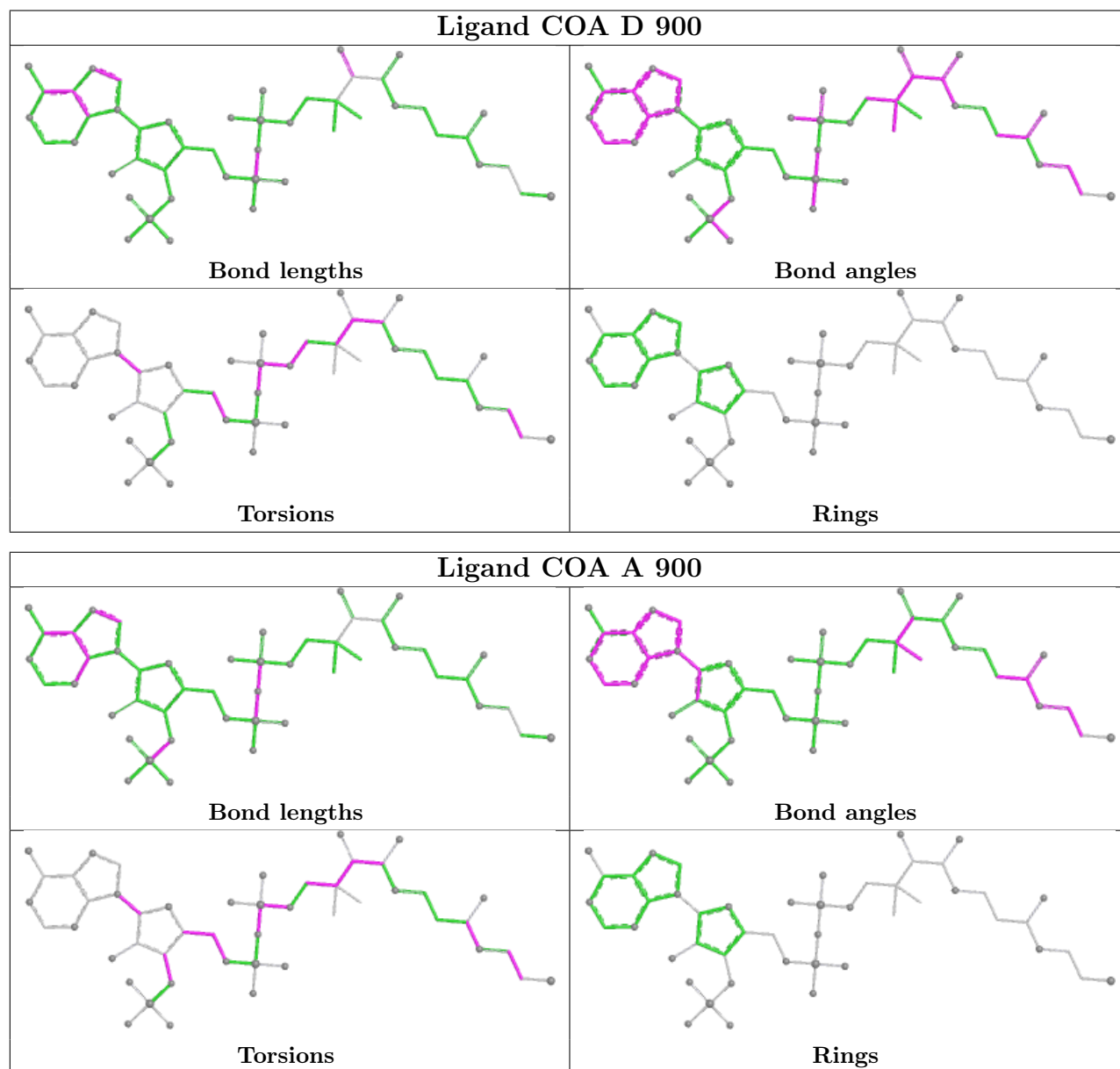
There are no ring outliers.

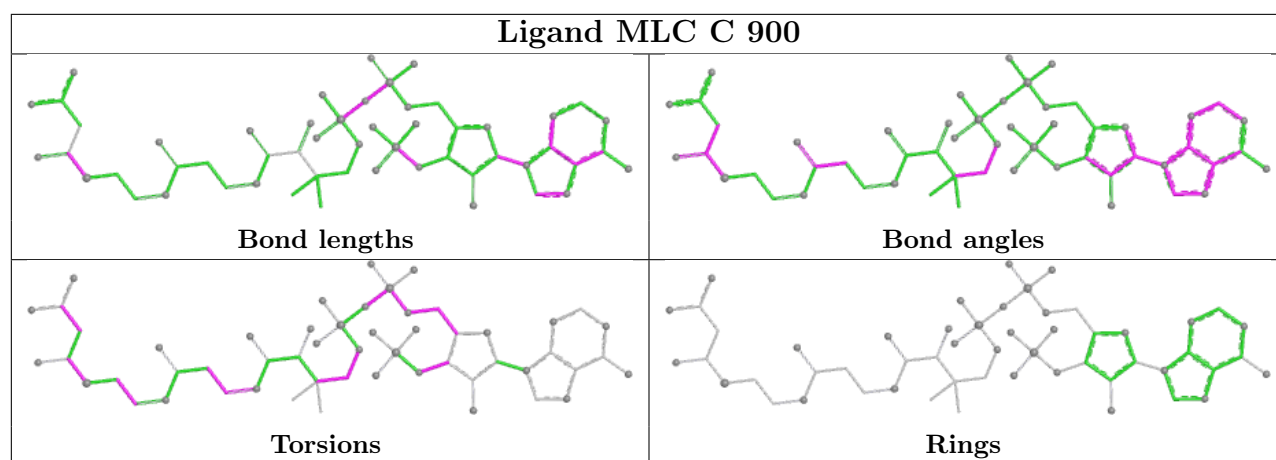
2 monomers are involved in 6 short contacts:

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 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	851/852 (99%)	-0.14	22 (2%) 57 48	29, 57, 112, 186	0
1	D	851/852 (99%)	-0.09	13 (1%) 72 65	34, 55, 106, 164	0
2	B	848/852 (99%)	0.19	57 (6%) 24 21	33, 59, 170, 240	0
2	C	848/852 (99%)	0.17	58 (6%) 23 20	34, 62, 161, 247	0
All	All	3398/3408 (99%)	0.03	150 (4%) 39 31	29, 58, 150, 247	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	677	THR	5.1
2	C	622	ALA	4.5
2	B	677	THR	4.5
2	B	622	ALA	4.4
2	B	685	TYR	4.4
2	C	416	ALA	4.4
1	A	508	LEU	4.2
2	C	657	ALA	4.2
1	D	418	ALA	4.2
2	C	662	VAL	4.1
1	D	416	ALA	4.1
2	C	689	GLY	4.0
2	B	418	ALA	4.0
2	B	662	VAL	4.0
2	C	685	TYR	3.9
2	B	607	GLY	3.9
2	B	609	CYS	3.8
1	A	614	HIS	3.8
2	C	637	GLY	3.8
1	A	130	TYR	3.7
2	C	418	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	617	PRO	3.6
1	A	418	ALA	3.6
2	B	605	TRP	3.6
2	B	610	ILE	3.6
2	C	489	LYS	3.5
1	D	627	TRP	3.5
2	C	617	PRO	3.5
2	C	653	GLY	3.5
2	B	654	PRO	3.4
1	D	417	HIS	3.4
1	A	616	PRO	3.4
2	B	606	ARG	3.3
2	B	656	ALA	3.3
2	C	656	ALA	3.3
2	C	620	MET	3.3
2	B	581	SER	3.2
2	B	726	LEU	3.2
2	C	414	PRO	3.2
2	B	416	ALA	3.2
2	B	661	PHE	3.1
2	C	499	MET	3.1
2	C	539	LEU	3.1
2	C	615	LEU	3.1
2	C	639	VAL	3.0
2	B	772	LYS	3.0
2	B	686	PHE	3.0
1	A	416	ALA	3.0
2	C	508	LEU	3.0
2	C	613	ALA	3.0
1	A	615	LEU	2.9
2	C	680	LEU	2.9
2	C	616	PRO	2.9
1	D	673	LYS	2.9
2	B	750	TRP	2.9
2	B	657	ALA	2.9
2	C	412	PRO	2.9
1	D	419	ALA	2.9
2	C	686	PHE	2.9
2	B	678	GLY	2.9
2	B	640	PRO	2.9
1	A	617	PRO	2.8
2	C	581	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	620	MET	2.8
2	C	609	CYS	2.8
2	C	672	ALA	2.8
2	C	726	LEU	2.8
1	A	414	PRO	2.8
1	D	532	VAL	2.7
2	B	694	LEU	2.7
2	C	665	LEU	2.7
2	B	735	ASN	2.6
2	B	550	VAL	2.6
2	B	658	VAL	2.6
2	B	769	ALA	2.6
2	C	654	PRO	2.6
2	B	690	ILE	2.6
2	B	553	PHE	2.6
2	C	640	PRO	2.6
2	C	688	GLU	2.6
2	B	736	VAL	2.6
2	C	415	THR	2.6
2	B	637	GLY	2.5
2	C	636	ALA	2.5
2	B	417	HIS	2.5
2	B	612	ASP	2.5
1	A	419	ALA	2.5
2	B	738	ASN	2.5
2	B	555	SER	2.5
2	C	690	ILE	2.5
2	B	603	ALA	2.4
2	B	696	GLN	2.4
2	B	539	LEU	2.4
1	A	671	PHE	2.4
1	D	656	ALA	2.4
1	D	130	TYR	2.4
2	C	601	LEU	2.4
2	B	551	HIS	2.4
2	C	638	VAL	2.3
2	C	630	CYS	2.3
2	B	621	ALA	2.3
2	C	411	ALA	2.3
2	C	750	TRP	2.3
1	A	685	TYR	2.3
2	B	616	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	635	PRO	2.3
1	A	476	GLU	2.3
2	B	840	GLN	2.3
2	C	556	LEU	2.3
2	C	625	LEU	2.3
2	B	684	SER	2.3
2	C	661	PHE	2.3
2	B	526	ALA	2.3
2	C	419	ALA	2.3
1	A	549	ILE	2.3
2	C	648	THR	2.3
2	C	618	GLY	2.3
2	C	683	HIS	2.2
1	D	609	CYS	2.2
2	C	687	MET	2.2
2	B	500	GLY	2.2
2	C	682	PHE	2.2
1	A	413	ALA	2.2
2	C	735	ASN	2.2
2	B	549	ILE	2.2
2	B	745	PHE	2.2
1	A	420	LEU	2.2
2	C	651	ILE	2.2
2	B	499	MET	2.2
2	C	780	THR	2.2
2	C	621	ALA	2.2
2	B	580	HIS	2.1
2	B	508	LEU	2.1
2	C	659	ASN	2.1
1	A	788	ASP	2.1
2	B	501	THR	2.1
2	B	780	THR	2.1
1	A	605	TRP	2.1
2	B	689	GLY	2.1
2	B	766	LEU	2.1
2	B	671	PHE	2.1
1	A	612	ASP	2.1
1	A	627	TRP	2.1
1	A	539	LEU	2.0
1	D	750	TRP	2.0
2	C	670	VAL	2.0
1	A	489	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	489	LYS	2.0
1	D	688	GLU	2.0
2	C	605	TRP	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, 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
1	K5L	D	581	12/13	0.91	0.13	59,68,77,83	0
1	K5L	A	581	12/13	0.92	0.15	58,79,99,101	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

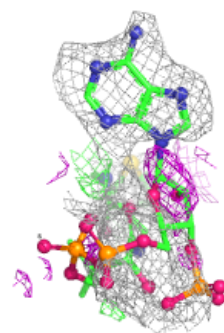
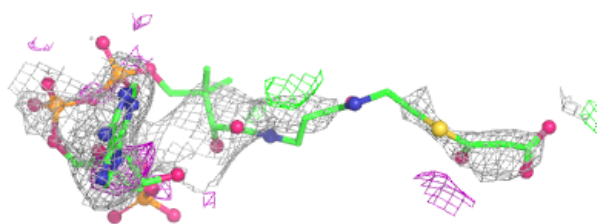
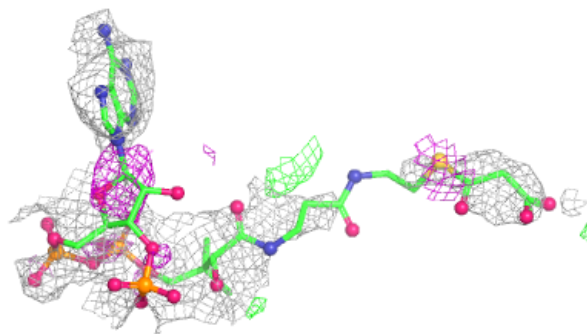
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MLC	C	900	54/54	0.66	0.16	119,164,252,262	0
3	COA	A	900	48/48	0.82	0.15	85,143,171,179	0
3	COA	D	900	48/48	0.84	0.14	66,113,130,136	0

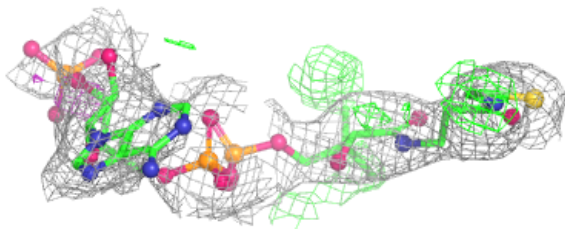
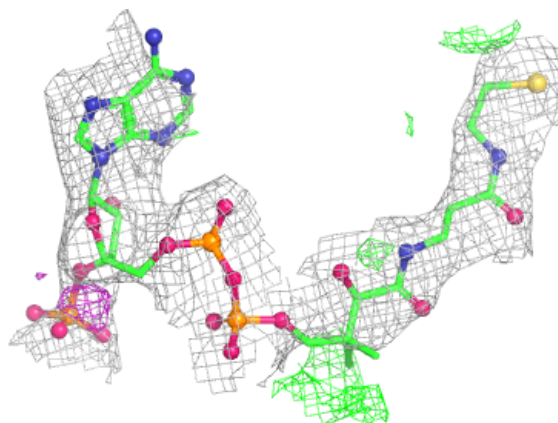
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

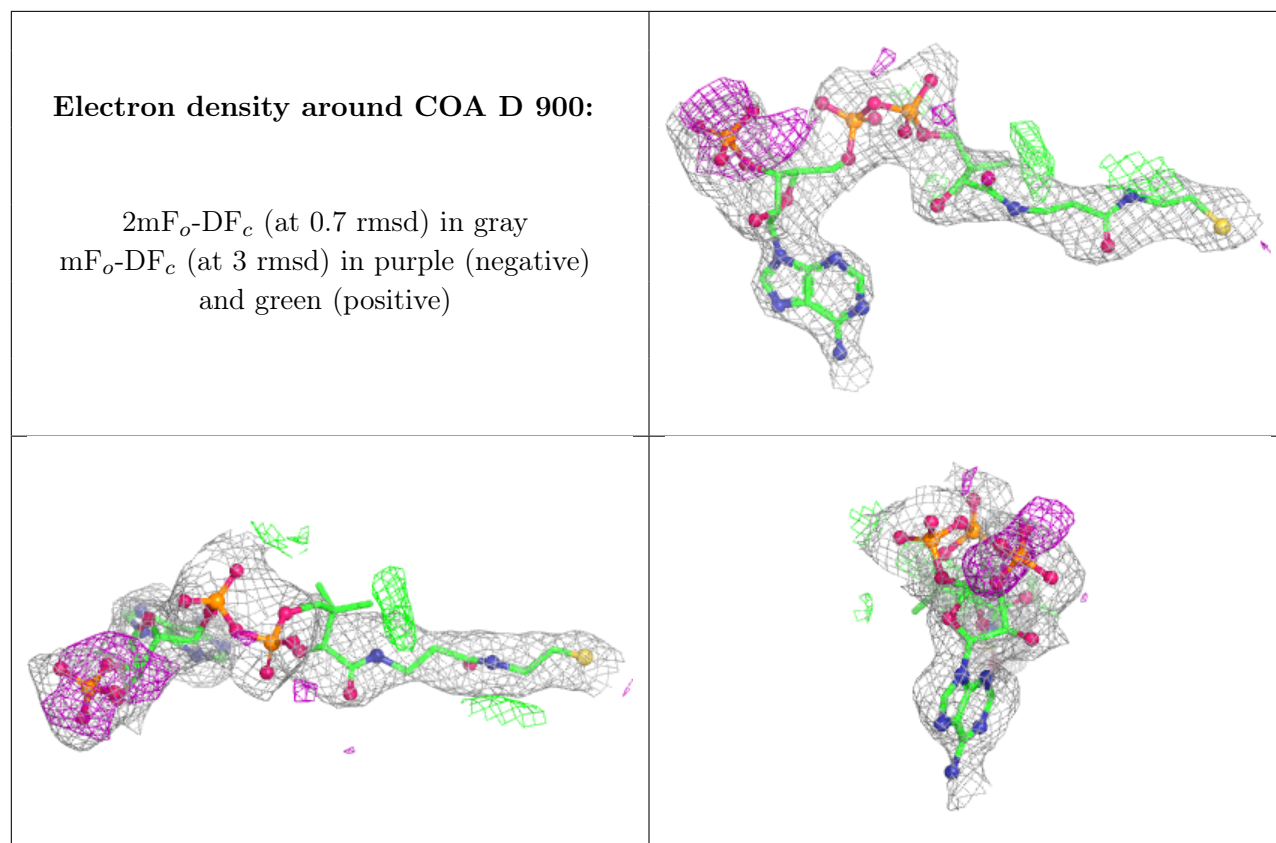
Electron density around MLC C 900:

$2mF_o-DF_c$ (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)





6.5 Other polymers ⓘ

There are no such residues in this entry.