



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:20 am BST

PDB ID : 2JFK
Title : Structure of the MAT domain of human FAS with malonyl-CoA
Authors : Bunkoczi, G.; Kavanagh, K.; Hozjan, V.; Rojkova, A.; Watt, S.; Wu, X.; Arrowsmith, C.H.; Edwards, A.; Sundstrom, M.; Weigelt, J.; Smith, S.; Oppermann, U.
Deposited on : 2007-02-02
Resolution : 2.40 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

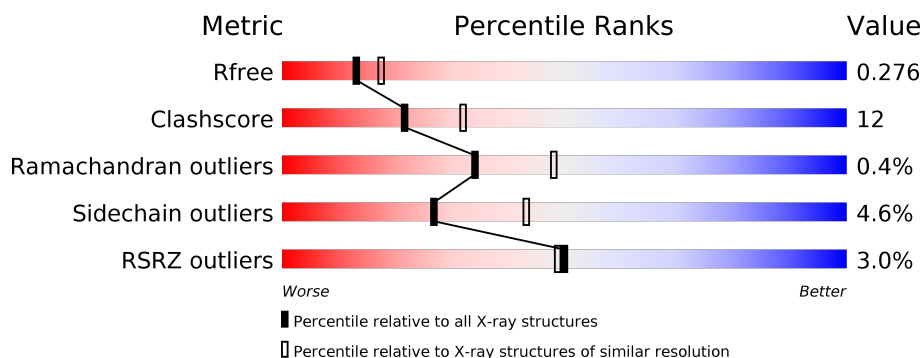
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	433	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	B	433	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>7%</div> </div> </div>
1	C	433	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	D	433	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12143 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	401	Total	C	N	O	S	0	2	0
			2984	1908	515	540	21			
1	B	404	Total	C	N	O	S	0	2	0
			3025	1931	521	552	21			
1	C	405	Total	C	N	O	S	0	2	0
			3024	1932	523	548	21			
1	D	410	Total	C	N	O	S	0	2	0
			3036	1936	526	554	20			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	MET	-	expression tag	UNP P49327
A	400	HIS	-	expression tag	UNP P49327
A	401	HIS	-	expression tag	UNP P49327
A	402	HIS	-	expression tag	UNP P49327
A	403	HIS	-	expression tag	UNP P49327
A	404	HIS	-	expression tag	UNP P49327
A	405	HIS	-	expression tag	UNP P49327
A	406	SER	-	expression tag	UNP P49327
A	407	SER	-	expression tag	UNP P49327
A	408	GLY	-	expression tag	UNP P49327
A	409	VAL	-	expression tag	UNP P49327
A	410	ASP	-	expression tag	UNP P49327
A	411	LEU	-	expression tag	UNP P49327
A	412	GLY	-	expression tag	UNP P49327
A	413	THR	-	expression tag	UNP P49327
A	414	GLU	-	expression tag	UNP P49327
A	415	ASN	-	expression tag	UNP P49327
A	416	LEU	-	expression tag	UNP P49327
A	417	TYR	-	expression tag	UNP P49327
A	418	PHE	-	expression tag	UNP P49327
A	419	GLN	-	expression tag	UNP P49327

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Chain	Residue	Modelled	Actual	Comment	Reference
A	420	SER	-	expression tag	UNP P49327
A	421	MET	-	expression tag	UNP P49327
B	399	MET	-	expression tag	UNP P49327
B	400	HIS	-	expression tag	UNP P49327
B	401	HIS	-	expression tag	UNP P49327
B	402	HIS	-	expression tag	UNP P49327
B	403	HIS	-	expression tag	UNP P49327
B	404	HIS	-	expression tag	UNP P49327
B	405	HIS	-	expression tag	UNP P49327
B	406	SER	-	expression tag	UNP P49327
B	407	SER	-	expression tag	UNP P49327
B	408	GLY	-	expression tag	UNP P49327
B	409	VAL	-	expression tag	UNP P49327
B	410	ASP	-	expression tag	UNP P49327
B	411	LEU	-	expression tag	UNP P49327
B	412	GLY	-	expression tag	UNP P49327
B	413	THR	-	expression tag	UNP P49327
B	414	GLU	-	expression tag	UNP P49327
B	415	ASN	-	expression tag	UNP P49327
B	416	LEU	-	expression tag	UNP P49327
B	417	TYR	-	expression tag	UNP P49327
B	418	PHE	-	expression tag	UNP P49327
B	419	GLN	-	expression tag	UNP P49327
B	420	SER	-	expression tag	UNP P49327
B	421	MET	-	expression tag	UNP P49327
C	399	MET	-	expression tag	UNP P49327
C	400	HIS	-	expression tag	UNP P49327
C	401	HIS	-	expression tag	UNP P49327
C	402	HIS	-	expression tag	UNP P49327
C	403	HIS	-	expression tag	UNP P49327
C	404	HIS	-	expression tag	UNP P49327
C	405	HIS	-	expression tag	UNP P49327
C	406	SER	-	expression tag	UNP P49327
C	407	SER	-	expression tag	UNP P49327
C	408	GLY	-	expression tag	UNP P49327
C	409	VAL	-	expression tag	UNP P49327
C	410	ASP	-	expression tag	UNP P49327
C	411	LEU	-	expression tag	UNP P49327
C	412	GLY	-	expression tag	UNP P49327
C	413	THR	-	expression tag	UNP P49327
C	414	GLU	-	expression tag	UNP P49327
C	415	ASN	-	expression tag	UNP P49327

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Chain	Residue	Modelled	Actual	Comment	Reference
C	416	LEU	-	expression tag	UNP P49327
C	417	TYR	-	expression tag	UNP P49327
C	418	PHE	-	expression tag	UNP P49327
C	419	GLN	-	expression tag	UNP P49327
C	420	SER	-	expression tag	UNP P49327
C	421	MET	-	expression tag	UNP P49327
D	399	MET	-	expression tag	UNP P49327
D	400	HIS	-	expression tag	UNP P49327
D	401	HIS	-	expression tag	UNP P49327
D	402	HIS	-	expression tag	UNP P49327
D	403	HIS	-	expression tag	UNP P49327
D	404	HIS	-	expression tag	UNP P49327
D	405	HIS	-	expression tag	UNP P49327
D	406	SER	-	expression tag	UNP P49327
D	407	SER	-	expression tag	UNP P49327
D	408	GLY	-	expression tag	UNP P49327
D	409	VAL	-	expression tag	UNP P49327
D	410	ASP	-	expression tag	UNP P49327
D	411	LEU	-	expression tag	UNP P49327
D	412	GLY	-	expression tag	UNP P49327
D	413	THR	-	expression tag	UNP P49327
D	414	GLU	-	expression tag	UNP P49327
D	415	ASN	-	expression tag	UNP P49327
D	416	LEU	-	expression tag	UNP P49327
D	417	TYR	-	expression tag	UNP P49327
D	418	PHE	-	expression tag	UNP P49327
D	419	GLN	-	expression tag	UNP P49327
D	420	SER	-	expression tag	UNP P49327
D	421	MET	-	expression tag	UNP P49327

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			7	4	1	1	1		
2	B	1	Total	C	N	O	S	0	0
			8	5	1	1	1		
2	C	1	Total	C	N	O	S	0	0
			9	5	2	1	1		
2	D	1	Total	C	N	O	S	0	0
			12	7	2	2	1		

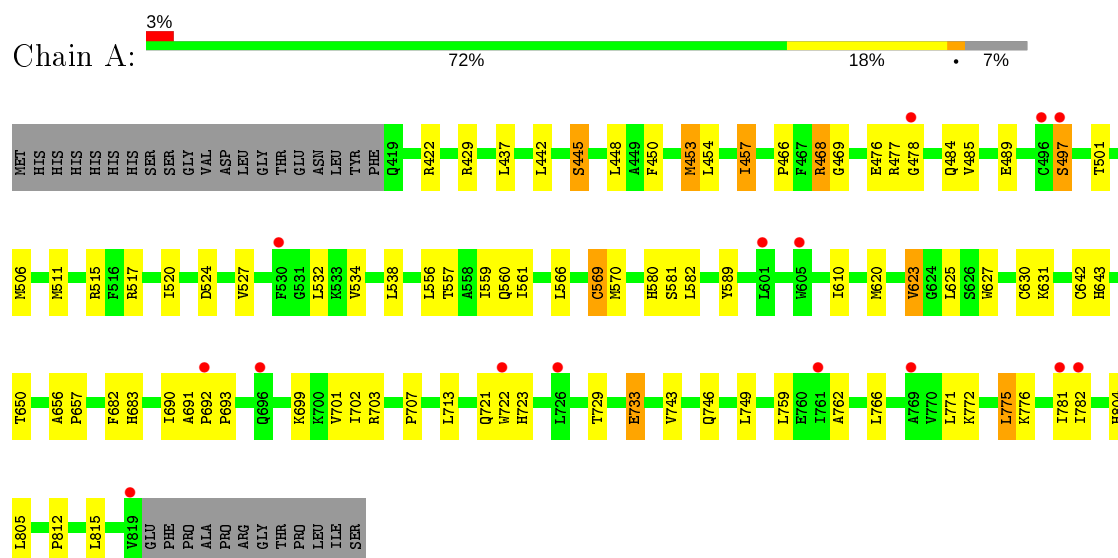
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	5	Total	O	0	0
			5	5		
3	C	20	Total	O	0	0
			20	20		
3	D	8	Total	O	0	0
			8	8		

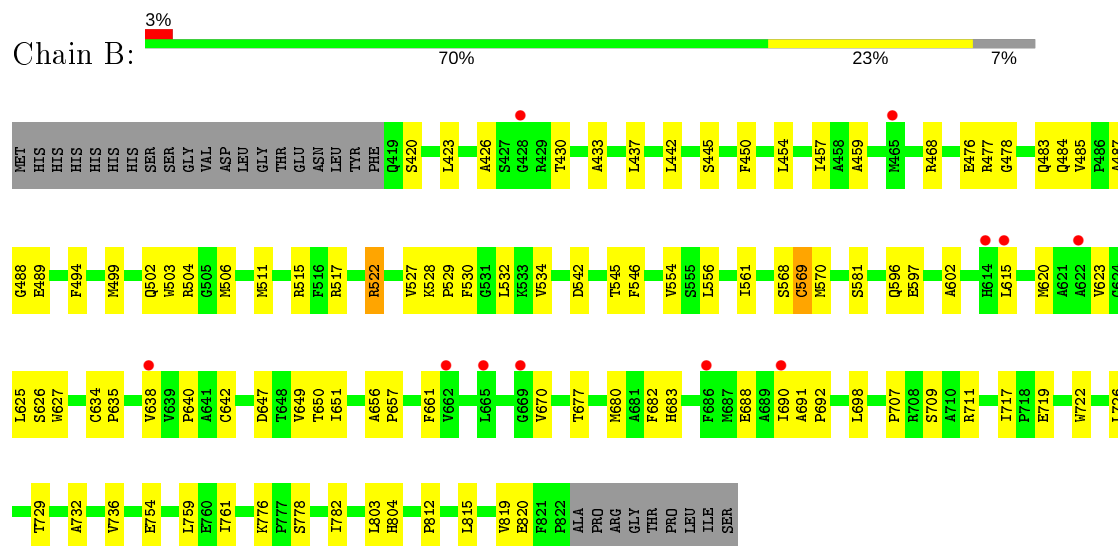
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

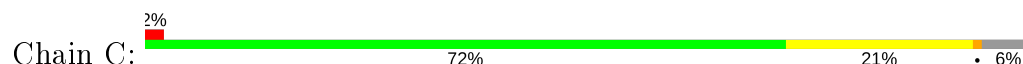
• Molecule 1: FATTY ACID SYNTHASE

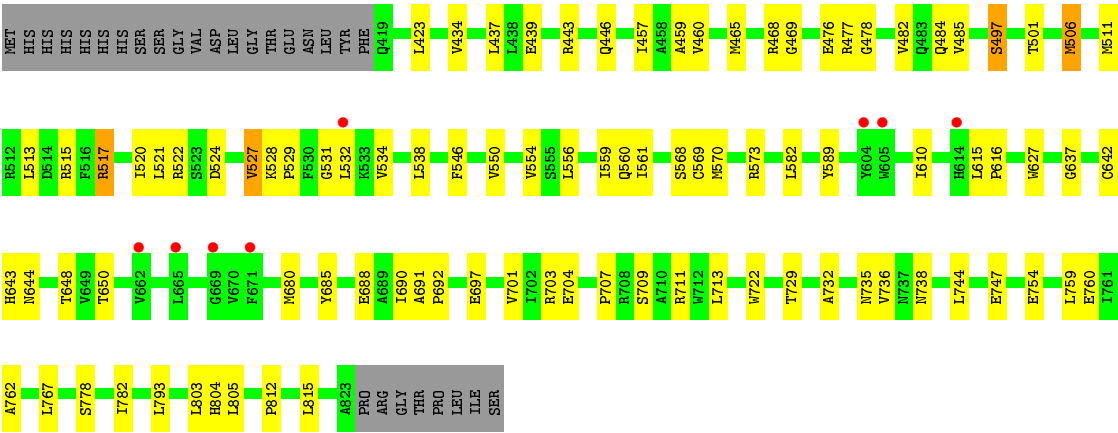


• Molecule 1: FATTY ACID SYNTHASE

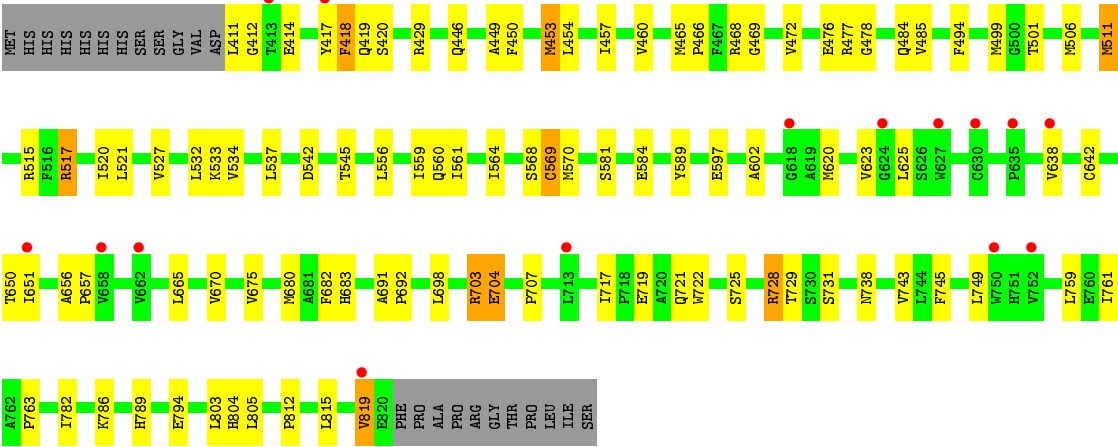


• Molecule 1: FATTY ACID SYNTHASE





● Molecule 1: FATTY ACID SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.92Å 91.41Å 261.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.96 – 2.40 40.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.96-2.40) 99.6 (40.95-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.271 0.231 , 0.276	Depositor DCC
R_{free} test set	3902 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12143	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: COA, MCS

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	0.60	2/3054 (0.1%)	0.69	3/4163 (0.1%)
1	B	0.57	0/3095	0.67	0/4218
1	C	0.64	1/3096 (0.0%)	0.74	0/4222
1	D	0.48	0/3103	0.63	0/4230
All	All	0.58	3/12348 (0.0%)	0.68	3/16833 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	733	GLU	CD-OE1	12.43	1.39	1.25
1	A	733	GLU	CD-OE2	8.94	1.35	1.25
1	C	527	VAL	CB-CG2	6.00	1.65	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	733	GLU	OE1-CD-OE2	5.59	130.01	123.30
1	A	457	ILE	CB-CA-C	-5.43	100.75	111.60
1	A	468	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	487	ALA	Peptide
1	B	488	GLY	Peptide
1	D	411	LEU	Peptide
1	D	412	GLY	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	2984	0	2884	64	0
1	B	3025	0	2942	74	0
1	C	3024	0	2926	75	0
1	D	3036	0	2939	76	0
2	A	7	0	6	0	0
2	B	8	0	8	0	0
2	C	9	0	10	0	0
2	D	12	0	11	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	20	0	0	0	0
3	D	8	0	0	0	0
All	All	12143	0	11726	283	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 12.

All (283) 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:A:468:ARG:HD3	1:A:485:VAL:HG21	1.33	1.06
1:B:570:MET:HE3	1:B:815:LEU:HD21	1.38	1.05
1:A:570:MET:HE2	1:A:815:LEU:HG	1.52	0.91
1:D:570:MET:HE3	1:D:812:PRO:HA	1.52	0.89
1:B:615:LEU:HD11	1:B:690:ILE:HD11	1.53	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:ARG:HD3	1:C:485:VAL:HG21	1.58	0.86
1:C:570:MET:HE2	1:C:815:LEU:HG	1.55	0.86
1:B:468:ARG:HD3	1:B:485:VAL:HG21	1.59	0.83
1:C:550:VAL:O	1:C:554:VAL:HG23	1.80	0.81
1:A:506:MET:HE3	1:A:559:ILE:HD12	1.64	0.80
1:D:707:PRO:HA	1:D:729:THR:HG22	1.63	0.78
1:A:527:VAL:CG1	1:A:532:LEU:HB2	2.14	0.78
1:C:642:MCS:HBC2	1:C:650:THR:HB	1.64	0.78
1:D:453:MET:CE	1:D:457:ILE:HD11	2.13	0.78
1:C:732:ALA:O	1:C:736:VAL:HG23	1.83	0.77
1:C:615:LEU:HD11	1:C:690:ILE:HD11	1.66	0.77
1:B:570:MET:HE3	1:B:815:LEU:CD2	2.14	0.77
1:B:642:MCS:HBC2	1:B:650:THR:HB	1.67	0.77
1:C:527:VAL:CG1	1:C:532:LEU:HB2	2.15	0.76
1:D:642:MCS:HBC2	1:D:650:THR:HB	1.68	0.76
1:D:453:MET:HE1	1:D:457:ILE:HD11	1.66	0.75
1:C:570:MET:CE	1:C:815:LEU:HD11	2.17	0.75
1:D:499:MET:HE1	1:D:682:PHE:CD1	2.22	0.75
1:D:542:ASP:O	1:D:545:THR:HG22	1.87	0.74
1:A:506:MET:CE	1:A:559:ILE:HD12	2.18	0.73
1:D:468:ARG:HD3	1:D:485:VAL:HG21	1.69	0.73
1:D:453:MET:HE2	1:D:457:ILE:CD1	2.19	0.72
1:A:527:VAL:HG12	1:A:532:LEU:HB2	1.73	0.71
1:B:625:LEU:HD21	1:B:670:VAL:HG11	1.72	0.70
1:C:610:ILE:HG23	1:C:680:MET:CE	2.21	0.70
1:C:754:GLU:O	1:C:778:SER:OG	2.06	0.70
1:D:560:GLN:O	1:D:564:ILE:HD12	1.91	0.69
1:C:610:ILE:HG23	1:C:680:MET:HE2	1.75	0.68
1:C:759:LEU:HD21	1:C:803:LEU:HD21	1.75	0.68
1:B:499:MET:HE1	1:B:682:PHE:CD1	2.29	0.67
1:D:717:ILE:HG23	1:D:721:GLN:HB2	1.77	0.67
1:C:434:VAL:HG11	1:C:482:VAL:HG22	1.78	0.66
1:A:610:ILE:HA	1:A:690:ILE:HD13	1.75	0.66
1:C:570:MET:HE3	1:C:815:LEU:HD11	1.76	0.66
1:A:570:MET:HE3	1:A:815:LEU:HD11	1.78	0.66
1:A:581:SER:HB2	1:A:683:HIS:NE2	2.11	0.66
1:A:527:VAL:O	1:A:527:VAL:HG12	1.96	0.65
1:A:759:LEU:HD23	1:A:782:ILE:HB	1.78	0.65
1:B:691:ALA:HB3	1:B:692:PRO:HD3	1.78	0.65
1:A:642:MCS:HBC2	1:A:650:THR:HB	1.79	0.65
1:B:426:ALA:HB1	1:B:437:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:MET:CE	1:D:812:PRO:HA	2.25	0.65
1:A:566:LEU:HD22	1:A:815:LEU:HD22	1.79	0.64
1:B:527:VAL:O	1:B:527:VAL:HG12	1.97	0.64
1:C:527:VAL:HG11	1:C:532:LEU:HB2	1.80	0.64
1:A:497:SER:OG	1:A:762:ALA:HB2	1.98	0.64
1:D:453:MET:CE	1:D:457:ILE:CD1	2.74	0.64
1:B:570:MET:CE	1:B:815:LEU:HD11	2.28	0.63
1:A:527:VAL:HG11	1:A:532:LEU:HB2	1.81	0.63
1:C:697:GLU:O	1:C:701:VAL:HG23	1.99	0.63
1:A:570:MET:CE	1:A:815:LEU:HG	2.26	0.63
1:C:691:ALA:HB3	1:C:692:PRO:HD3	1.81	0.63
1:D:584:GLU:OE1	1:D:738:ASN:ND2	2.32	0.62
1:B:570:MET:CE	1:B:815:LEU:HD21	2.24	0.62
1:D:728:ARG:HD3	1:D:729:THR:HG23	1.80	0.62
1:B:527:VAL:HG11	1:B:532:LEU:HD12	1.82	0.62
1:A:691:ALA:HB3	1:A:692:PRO:HD3	1.82	0.61
1:C:570:MET:HE2	1:C:815:LEU:CG	2.29	0.61
1:B:499:MET:HE3	1:B:682:PHE:CE1	2.35	0.61
1:C:556:LEU:O	1:C:560:GLN:HG3	2.00	0.61
1:C:468:ARG:HD3	1:C:485:VAL:CG2	2.29	0.61
1:D:707:PRO:CA	1:D:729:THR:HG22	2.30	0.61
1:C:570:MET:CE	1:C:815:LEU:CD1	2.79	0.60
1:C:434:VAL:CG1	1:C:482:VAL:HG22	2.31	0.60
1:B:542:ASP:O	1:B:545:THR:HG22	2.02	0.60
1:D:534:VAL:HA	1:D:537:LEU:HD12	1.84	0.60
1:A:561:ILE:HG23	1:A:589:TYR:CE1	2.37	0.60
1:D:417:TYR:O	1:D:419:GLN:N	2.34	0.60
1:D:527:VAL:CG1	1:D:532:LEU:HB2	2.31	0.60
1:D:728:ARG:CD	1:D:729:THR:HG23	2.32	0.59
1:D:556:LEU:HD23	1:D:763:PRO:HG3	1.85	0.59
1:D:656:ALA:HB3	1:D:657:PRO:CD	2.32	0.59
1:C:423:LEU:HD23	1:C:812:PRO:HG3	1.85	0.59
1:D:527:VAL:HG12	1:D:527:VAL:O	2.02	0.59
1:C:556:LEU:HD12	1:C:582:LEU:HD23	1.85	0.58
1:D:717:ILE:CG2	1:D:721:GLN:HB2	2.32	0.58
1:D:642:MCS:HAG2	1:D:650:THR:HG21	1.84	0.58
1:C:561:ILE:HG23	1:C:589:TYR:CE1	2.38	0.58
1:D:759:LEU:HD23	1:D:782:ILE:HB	1.86	0.58
1:B:754:GLU:HA	1:B:776:LYS:HD2	1.85	0.58
1:C:570:MET:CE	1:C:815:LEU:CG	2.81	0.58
1:D:515[A]:ARG:HD2	1:D:569[A]:CYS:SG	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:728:ARG:NE	1:D:729:THR:HG23	2.18	0.58
1:C:570:MET:CE	1:C:815:LEU:HG	2.30	0.58
1:B:527:VAL:CG1	1:B:532:LEU:HB2	2.34	0.57
1:D:703:ARG:O	1:D:704:GLU:HG3	2.05	0.57
1:C:437:LEU:HD13	1:D:453:MET:CE	2.34	0.57
1:B:620:MET:HG3	1:B:677:THR:HG21	1.86	0.56
1:C:468:ARG:CD	1:C:485:VAL:HG21	2.32	0.56
1:D:691:ALA:HB3	1:D:692:PRO:HD3	1.87	0.56
1:C:459:ALA:O	1:D:429:ARG:NH2	2.39	0.55
1:C:527:VAL:HG12	1:C:532:LEU:HB2	1.88	0.55
1:C:627:TRP:CZ3	1:C:643:HIS:HB2	2.41	0.55
1:B:499:MET:CE	1:B:682:PHE:CE1	2.89	0.55
1:C:637:GLY:O	1:C:685:TYR:OH	2.20	0.55
1:B:450:PHE:CE2	1:B:454:LEU:HD11	2.42	0.55
1:B:561:ILE:HG21	1:B:596:GLN:HG3	1.87	0.55
1:D:569[A]:CYS:SG	1:D:815:LEU:HD23	2.47	0.55
1:C:506:MET:HE2	1:C:546:PHE:CZ	2.42	0.55
1:A:569[A]:CYS:SG	1:A:815:LEU:HD23	2.48	0.54
1:A:627:TRP:CZ3	1:A:643:HIS:HB2	2.43	0.54
1:A:570:MET:CE	1:A:815:LEU:CG	2.85	0.54
1:C:531:GLY:O	1:C:532:LEU:HD23	2.08	0.54
1:A:749:LEU:HD22	1:A:775:LEU:HD21	1.89	0.54
1:C:527:VAL:HG12	1:C:527:VAL:O	2.07	0.54
1:A:570:MET:HE2	1:A:815:LEU:CG	2.32	0.54
1:C:524:ASP:OD1	1:C:534:VAL:HB	2.07	0.54
1:B:430:THR:O	1:B:433:ALA:HB3	2.08	0.53
1:D:665:LEU:HD22	1:D:670:VAL:HG11	1.90	0.53
1:A:453:MET:HE1	1:A:454:LEU:HD23	1.91	0.53
1:B:423:LEU:HD23	1:B:812:PRO:HG3	1.90	0.53
1:B:581:SER:HB3	1:B:683:HIS:NE2	2.23	0.53
1:B:656:ALA:HB3	1:B:657:PRO:CD	2.39	0.53
1:C:497:SER:HB3	1:C:767:LEU:HD12	1.90	0.53
1:B:759:LEU:HD23	1:B:782:ILE:HB	1.91	0.53
1:B:707:PRO:HA	1:B:729:THR:HG22	1.91	0.53
1:D:469:GLY:HA2	1:D:805:LEU:HD21	1.89	0.53
1:D:527:VAL:HG11	1:D:532:LEU:HB2	1.90	0.52
1:B:627:TRP:CZ3	1:B:640:PRO:HB2	2.43	0.52
1:C:497:SER:OG	1:C:762:ALA:HB2	2.10	0.52
1:D:468:ARG:HG2	1:D:804:HIS:NE2	2.24	0.52
1:C:506:MET:O	1:C:538:LEU:HD22	2.09	0.52
1:D:499:MET:CE	1:D:682:PHE:CE1	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:ALA:O	1:B:736:VAL:HG23	2.09	0.52
1:A:429:ARG:HA	1:A:466:PRO:HD2	1.92	0.52
1:B:527:VAL:HG11	1:B:532:LEU:HB2	1.91	0.52
1:D:499:MET:HE3	1:D:682:PHE:CE1	2.45	0.52
1:A:713:LEU:HD22	1:A:722:TRP:CZ3	2.46	0.51
1:B:442:LEU:O	1:B:445:SER:OG	2.28	0.51
1:B:620:MET:CG	1:B:677:THR:HG21	2.41	0.51
1:C:437:LEU:HD13	1:D:453:MET:HE1	1.92	0.51
1:D:638:VAL:CG1	1:D:651:ILE:HD12	2.39	0.51
1:B:570:MET:HE2	1:B:815:LEU:HD11	1.93	0.51
1:C:610:ILE:HG23	1:C:680:MET:HE1	1.91	0.51
1:D:506:MET:HB3	1:D:559:ILE:HD11	1.93	0.51
1:A:656:ALA:HB3	1:A:657:PRO:CD	2.41	0.51
1:D:680:MET:HB3	1:D:682:PHE:CE1	2.45	0.51
1:B:570:MET:CE	1:B:815:LEU:CG	2.89	0.50
1:B:627:TRP:CZ3	1:B:649:VAL:HG13	2.46	0.50
1:B:627:TRP:HZ3	1:B:649:VAL:HG13	1.75	0.50
1:A:771:LEU:HB3	1:A:781:ILE:HD13	1.93	0.50
1:B:602:ALA:HA	1:B:698:LEU:HD21	1.94	0.50
1:B:570:MET:HE2	1:B:815:LEU:HG	1.94	0.50
1:D:561:ILE:HG23	1:D:589:TYR:CE1	2.47	0.50
1:B:468:ARG:HG2	1:B:804:HIS:NE2	2.27	0.49
1:C:538:LEU:HD21	1:C:559:ILE:HD11	1.93	0.49
1:A:699:LYS:HZ3	1:A:733:GLU:CD	2.14	0.49
1:A:476:GLU:O	1:A:478:GLY:N	2.43	0.49
1:B:499:MET:CE	1:B:682:PHE:CD1	2.96	0.49
1:C:497:SER:HB3	1:C:767:LEU:CD1	2.42	0.49
1:A:581:SER:OG	1:A:582:LEU:N	2.44	0.48
1:D:501:THR:OG1	1:D:556:LEU:HD22	2.13	0.48
1:A:580:HIS:CD2	1:A:743:VAL:HG11	2.48	0.48
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.94	0.48
1:D:453:MET:HE2	1:D:457:ILE:HD12	1.96	0.48
1:D:476:GLU:C	1:D:478:GLY:H	2.17	0.48
1:D:623:VAL:HG12	1:D:625:LEU:HG	1.95	0.48
1:C:556:LEU:HD12	1:C:582:LEU:CD2	2.43	0.47
1:A:476:GLU:C	1:A:478:GLY:H	2.17	0.47
1:B:759:LEU:HD21	1:B:803:LEU:HD21	1.96	0.47
1:A:701:VAL:HB	1:A:702:ILE:HD12	1.95	0.47
1:B:430:THR:HG23	1:B:433:ALA:H	1.80	0.47
1:D:499:MET:CE	1:D:682:PHE:CD1	2.97	0.47
1:D:527:VAL:HG12	1:D:532:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:GLU:O	1:D:478:GLY:N	2.45	0.47
1:A:557:THR:O	1:A:561:ILE:HD12	2.15	0.46
1:A:772:LYS:O	1:A:775:LEU:O	2.33	0.46
1:B:625:LEU:HD21	1:B:670:VAL:CG1	2.42	0.46
1:C:476:GLU:C	1:C:478:GLY:H	2.19	0.46
1:A:556:LEU:O	1:A:560:GLN:HG3	2.16	0.46
1:D:581:SER:HB2	1:D:683:HIS:NE2	2.30	0.46
1:B:570:MET:HE2	1:B:815:LEU:CD1	2.45	0.46
1:C:703:ARG:O	1:C:704:GLU:HG2	2.15	0.46
1:A:623:VAL:HG13	1:A:625:LEU:HG	1.96	0.46
1:B:717:ILE:HD11	1:B:726:LEU:HG	1.98	0.46
1:D:418:PHE:O	1:D:420:SER:N	2.46	0.46
1:B:534:VAL:HG22	1:B:554:VAL:HG12	1.98	0.46
1:B:502:GLN:HG3	1:B:546:PHE:HB3	1.97	0.46
1:B:529:PRO:O	1:B:530:PHE:CB	2.63	0.45
1:C:615:LEU:HD12	1:C:680:MET:CE	2.47	0.45
1:B:499:MET:HE2	1:B:499:MET:HB2	1.77	0.45
1:B:569[A]:CYS:SG	1:B:815:LEU:HD23	2.56	0.45
1:B:476:GLU:C	1:B:478:GLY:H	2.18	0.45
1:B:503:TRP:O	1:B:506:MET:HG3	2.16	0.45
1:B:570:MET:HE2	1:B:815:LEU:CG	2.46	0.45
1:A:702:ILE:O	1:A:702:ILE:HG22	2.15	0.45
1:A:699:LYS:NZ	1:A:733:GLU:OE2	2.47	0.45
1:C:501:THR:OG1	1:C:556:LEU:CD2	2.65	0.45
1:A:723:HIS:CG	1:A:723:HIS:O	2.70	0.45
1:B:623:VAL:HG12	1:B:625:LEU:HG	1.98	0.45
1:C:615:LEU:HD12	1:C:680:MET:HE3	1.98	0.44
1:A:506:MET:HE2	1:A:559:ILE:HD12	1.98	0.44
1:A:570:MET:HE3	1:A:815:LEU:CD1	2.47	0.44
1:B:635:PRO:HD3	1:B:661:PHE:CE1	2.51	0.44
1:C:468:ARG:HG2	1:C:804:HIS:NE2	2.32	0.44
1:D:494:PHE:HB3	1:D:761:ILE:HD12	1.98	0.44
1:D:511:MET:HE1	1:D:520:ILE:HG21	1.99	0.44
1:A:511:MET:HE1	1:A:520:ILE:HG21	2.00	0.44
1:B:819:VAL:HG23	1:B:820:GLU:HG3	1.99	0.44
1:C:610:ILE:CG2	1:C:680:MET:HE2	2.47	0.44
1:D:745:PHE:CE2	1:D:749:LEU:HD11	2.53	0.44
1:C:476:GLU:O	1:C:478:GLY:N	2.50	0.44
1:A:442:LEU:O	1:A:445:SER:OG	2.34	0.43
1:A:501:THR:HG22	1:A:766:LEU:HD22	2.00	0.43
1:C:517:ARG:O	1:C:521:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:760:GLU:OE1	1:C:767:LEU:HB2	2.17	0.43
1:A:450:PHE:CE2	1:A:454:LEU:HD11	2.53	0.43
1:A:707:PRO:HA	1:A:729:THR:HG22	2.00	0.43
1:B:709:SER:OG	1:B:711:ARG:HD3	2.18	0.43
1:C:759:LEU:HD23	1:C:782:ILE:HB	2.01	0.43
1:A:506:MET:O	1:A:538:LEU:HD22	2.17	0.43
1:C:513:LEU:HD21	1:C:793:LEU:HD11	2.01	0.43
1:C:570:MET:HE3	1:C:815:LEU:HD21	2.00	0.43
1:D:656:ALA:HB3	1:D:657:PRO:HD3	1.99	0.43
1:D:786:LYS:HB3	1:D:789:HIS:HB2	2.00	0.43
1:C:511:MET:HE3	1:C:520:ILE:HB	2.01	0.43
1:C:713:LEU:HD22	1:C:722:TRP:CZ3	2.54	0.43
1:C:644:ASN:HD22	1:C:648:THR:HG22	1.83	0.43
1:D:450:PHE:CE2	1:D:454:LEU:HD11	2.53	0.42
1:B:527:VAL:HG12	1:B:532:LEU:HB2	2.00	0.42
1:A:454:LEU:HA	1:A:457:ILE:HD12	2.01	0.42
1:C:642:MCS:HBC2	1:C:650:THR:CB	2.44	0.42
1:D:449:ALA:HA	1:D:819:VAL:HG11	2.01	0.42
1:A:422:ARG:NH1	1:A:448:LEU:HD22	2.33	0.42
1:D:517:ARG:O	1:D:521:LEU:HG	2.20	0.42
1:A:524:ASP:OD1	1:A:534:VAL:HB	2.19	0.42
1:D:506:MET:HE2	1:D:506:MET:HB3	1.72	0.42
1:D:642:MCS:HA	1:D:743:VAL:HB	2.01	0.42
1:A:776:LYS:N	1:A:776:LYS:HD2	2.35	0.42
1:D:472:VAL:HG11	1:D:794:GLU:HG3	2.02	0.42
1:A:429:ARG:HH21	1:B:459:ALA:CB	2.33	0.42
1:A:437:LEU:HD21	1:B:457:ILE:HD11	2.02	0.42
1:B:635:PRO:HD3	1:B:661:PHE:CD1	2.55	0.42
1:B:494:PHE:HB3	1:B:761:ILE:HD12	2.02	0.42
1:B:719:GLU:HA	1:B:722:TRP:CD1	2.55	0.42
1:B:719:GLU:HA	1:B:722:TRP:CE2	2.54	0.42
1:A:527:VAL:O	1:A:527:VAL:CG1	2.67	0.42
1:A:570:MET:CE	1:A:812:PRO:HA	2.50	0.42
1:B:570:MET:CE	1:B:815:LEU:CD2	2.93	0.42
1:C:627:TRP:CE3	1:C:643:HIS:HB2	2.54	0.42
1:A:692:PRO:HB2	1:A:693:PRO:HD3	2.01	0.41
1:B:430:THR:CG2	1:B:433:ALA:HB2	2.49	0.41
1:C:528:LYS:HB2	1:C:529:PRO:HD3	2.01	0.41
1:C:707:PRO:HA	1:C:729:THR:HG22	2.01	0.41
1:C:735:ASN:O	1:C:738:ASN:HB3	2.19	0.41
1:D:719:GLU:HA	1:D:722:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:ARG:HB3	1:B:596:GLN:OE1	2.20	0.41
1:C:506:MET:HB3	1:C:559:ILE:CD1	2.51	0.41
1:C:469:GLY:HA2	1:C:805:LEU:HD21	2.01	0.41
1:A:630:CYS:O	1:A:631:LYS:C	2.57	0.41
1:B:476:GLU:O	1:B:478:GLY:N	2.50	0.41
1:C:615:LEU:HB3	1:C:616:PRO:CD	2.51	0.41
1:C:506:MET:HB3	1:C:559:ILE:HD11	2.03	0.41
1:D:656:ALA:CB	1:D:657:PRO:CD	2.99	0.41
1:D:683:HIS:CE1	1:D:738:ASN:O	2.74	0.41
1:A:506:MET:HB3	1:A:559:ILE:CD1	2.51	0.41
1:A:656:ALA:HB3	1:A:657:PRO:HD3	2.02	0.41
1:B:528:LYS:N	1:B:529:PRO:HD2	2.35	0.41
1:B:719:GLU:HA	1:B:722:TRP:CD2	2.55	0.41
1:D:803:LEU:HD23	1:D:803:LEU:HA	1.95	0.41
1:C:744:LEU:HB3	1:C:747:GLU:CG	2.50	0.41
1:A:620:MET:SD	1:A:682:PHE:HB2	2.60	0.41
1:B:570:MET:CE	1:B:815:LEU:CD1	2.96	0.40
1:B:638:VAL:HG11	1:B:651:ILE:HD12	2.02	0.40
1:A:468:ARG:HG2	1:A:804:HIS:NE2	2.36	0.40
1:C:457:ILE:O	1:C:460:VAL:HG23	2.21	0.40
1:C:465:MET:HE2	1:D:460:VAL:HG22	2.03	0.40
1:D:602:ALA:HA	1:D:698:LEU:HD21	2.03	0.40
1:D:620:MET:O	1:D:675:VAL:HG22	2.21	0.40
1:D:719:GLU:HG3	1:D:722:TRP:CZ3	2.56	0.40
1:B:502:GLN:HB3	1:B:556:LEU:HD21	2.02	0.40
1:C:709:SER:OG	1:C:711:ARG:HD3	2.20	0.40
1:D:414:GLU:HB3	1:D:419:GLN:HG2	2.03	0.40
1:B:719:GLU:HA	1:B:722:TRP:CG	2.56	0.40
1:C:439:GLU:O	1:C:443:ARG:HG2	2.22	0.40
1:D:465:MET:HA	1:D:466:PRO:HD2	1.94	0.40
1:D:501:THR:OG1	1:D:556:LEU:CD2	2.69	0.40
1:D:623:VAL:CG1	1:D:625:LEU:HG	2.52	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	400/433 (92%)	380 (95%)	19 (5%)	1 (0%)	41	55
1	B	403/433 (93%)	387 (96%)	15 (4%)	1 (0%)	47	62
1	C	404/433 (93%)	383 (95%)	20 (5%)	1 (0%)	47	62
1	D	409/433 (94%)	386 (94%)	20 (5%)	3 (1%)	22	32
All	All	1616/1732 (93%)	1536 (95%)	74 (5%)	6 (0%)	34	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	418	PHE
1	A	477	ARG
1	D	477	ARG
1	B	477	ARG
1	C	477	ARG
1	D	819	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/358 (84%)	287 (95%)	14 (5%)	26	42
1	B	312/358 (87%)	293 (94%)	19 (6%)	18	30
1	C	308/358 (86%)	296 (96%)	12 (4%)	32	50
1	D	306/358 (86%)	291 (95%)	15 (5%)	25	40
All	All	1227/1432 (86%)	1167 (95%)	60 (5%)	27	40

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	SER
1	A	453	MET
1	A	484	GLN
1	A	489	GLU
1	A	497	SER
1	A	515	ARG
1	A	517	ARG
1	A	569[A]	CYS
1	A	569[B]	CYS
1	A	623	VAL
1	A	703	ARG
1	A	721	GLN
1	A	746	GLN
1	A	775	LEU
1	B	420	SER
1	B	483	GLN
1	B	484	GLN
1	B	489	GLU
1	B	504	ARG
1	B	511	MET
1	B	515	ARG
1	B	517	ARG
1	B	522	ARG
1	B	568	SER
1	B	569[A]	CYS
1	B	569[B]	CYS
1	B	597	GLU
1	B	626	SER
1	B	634	CYS
1	B	647	ASP
1	B	680	MET
1	B	688	GLU
1	B	778	SER
1	C	446	GLN
1	C	484	GLN
1	C	497	SER
1	C	506	MET
1	C	515	ARG
1	C	517	ARG
1	C	522	ARG
1	C	568	SER
1	C	569[A]	CYS
1	C	569[B]	CYS

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Mol	Chain	Res	Type
1	C	573	ARG
1	C	688	GLU
1	D	446	GLN
1	D	453	MET
1	D	484	GLN
1	D	511	MET
1	D	517	ARG
1	D	533	LYS
1	D	568	SER
1	D	569[A]	CYS
1	D	569[B]	CYS
1	D	597	GLU
1	D	703	ARG
1	D	704	GLU
1	D	725	SER
1	D	728	ARG
1	D	731	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	MCS	C	642	1	6,11,12	3.77	3 (50%)	4,13,15	11.38	4 (100%)
1	MCS	A	642	1	6,11,12	1.83	1 (16%)	4,13,15	5.05	4 (100%)
1	MCS	D	642	1	6,11,12	1.80	2 (33%)	4,13,15	6.00	3 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MCS	B	642	1	6,11,12	2.04	3 (50%)	4,13,15	12.87	4 (100%)

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	MCS	C	642	1	-	2/6/11/13	-
1	MCS	A	642	1	-	2/6/11/13	-
1	MCS	D	642	1	-	2/6/11/13	-
1	MCS	B	642	1	-	2/6/11/13	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	642	MCS	CAK-SAI	7.51	1.94	1.76
1	C	642	MCS	CB-SAI	3.72	1.89	1.81
1	A	642	MCS	CAK-SAI	3.58	1.84	1.76
1	B	642	MCS	CAK-SAI	3.52	1.84	1.76
1	C	642	MCS	CB-CA	3.37	1.61	1.53
1	D	642	MCS	CB-SAI	2.81	1.87	1.81
1	D	642	MCS	CB-CA	2.47	1.59	1.53
1	B	642	MCS	CB-SAI	2.32	1.86	1.81
1	B	642	MCS	CB-CA	2.30	1.58	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	642	MCS	CAG-CAK-SAI	16.79	134.61	113.69
1	C	642	MCS	CAG-CAK-SAI	15.31	132.77	113.69
1	B	642	MCS	CB-SAI-CAK	14.86	121.62	100.84
1	C	642	MCS	CB-SAI-CAK	13.93	120.32	100.84
1	B	642	MCS	OAC-CAK-SAI	-12.35	106.58	122.61
1	C	642	MCS	OAC-CAK-SAI	-8.19	111.97	122.61
1	D	642	MCS	CB-SAI-CAK	8.02	112.05	100.84
1	A	642	MCS	CAG-CAK-SAI	7.91	123.55	113.69
1	D	642	MCS	CAG-CAK-SAI	7.19	122.65	113.69
1	D	642	MCS	OAC-CAK-SAI	-5.17	115.90	122.61
1	C	642	MCS	OAC-CAK-CAG	-4.68	115.24	123.35
1	A	642	MCS	CB-SAI-CAK	4.46	107.07	100.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	MCS	OAC-CAK-CAG	-3.15	117.89	123.35
1	A	642	MCS	OAC-CAK-SAI	-3.13	118.54	122.61
1	B	642	MCS	OAC-CAK-CAG	-2.65	118.75	123.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	642	MCS	OAC-CAK-SAI-CB
1	C	642	MCS	CAG-CAK-SAI-CB
1	A	642	MCS	OAC-CAK-SAI-CB
1	A	642	MCS	CAG-CAK-SAI-CB
1	D	642	MCS	OAC-CAK-SAI-CB
1	D	642	MCS	CAG-CAK-SAI-CB
1	B	642	MCS	OAC-CAK-SAI-CB
1	B	642	MCS	CAG-CAK-SAI-CB

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	642	MCS	2	0
1	A	642	MCS	1	0
1	D	642	MCS	3	0
1	B	642	MCS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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
2	COA	A	1820	-	5,6,50	0.65	0	5,6,75	1.27	1 (20%)
2	COA	B	1823	-	6,7,50	0.46	0	6,7,75	1.48	0
2	COA	D	1821	-	10,11,50	2.60	1 (10%)	11,12,75	0.89	0
2	COA	C	1824	-	7,8,50	0.45	0	7,8,75	1.45	1 (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
2	COA	A	1820	-	-	3/4/4/64	-
2	COA	B	1823	-	-	0/6/6/64	-
2	COA	D	1821	-	-	8/10/10/64	-
2	COA	C	1824	-	-	4/7/7/64	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1821	COA	O9P-C9P	8.12	1.41	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1824	COA	O5P-C5P-C6P	-2.76	116.97	122.02
2	A	1820	COA	C6P-C5P-N4P	2.07	119.76	116.09

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1820	COA	C6P-C5P-N4P-C3P
2	D	1821	COA	C5P-C6P-C7P-N8P
2	D	1821	COA	S1P-C2P-C3P-N4P
2	C	1824	COA	C5P-C6P-C7P-N8P
2	C	1824	COA	S1P-C2P-C3P-N4P
2	C	1824	COA	O5P-C5P-N4P-C3P
2	C	1824	COA	C6P-C5P-N4P-C3P
2	D	1821	COA	CAP-C9P-N8P-C7P
2	D	1821	COA	O9P-C9P-N8P-C7P

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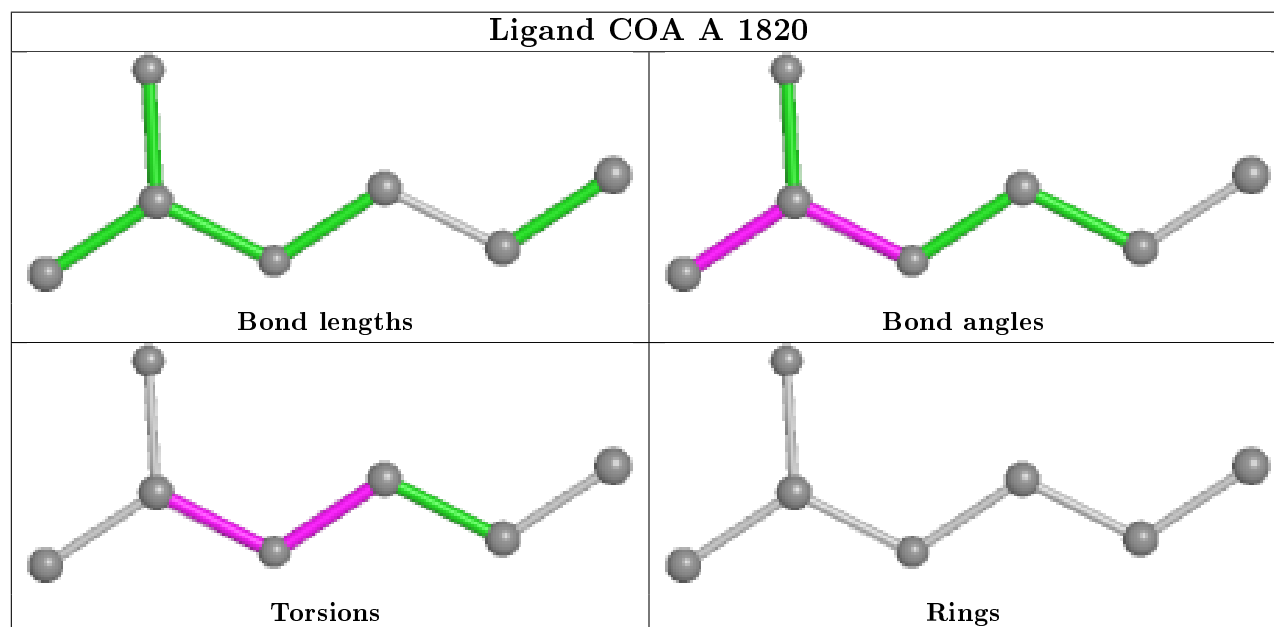
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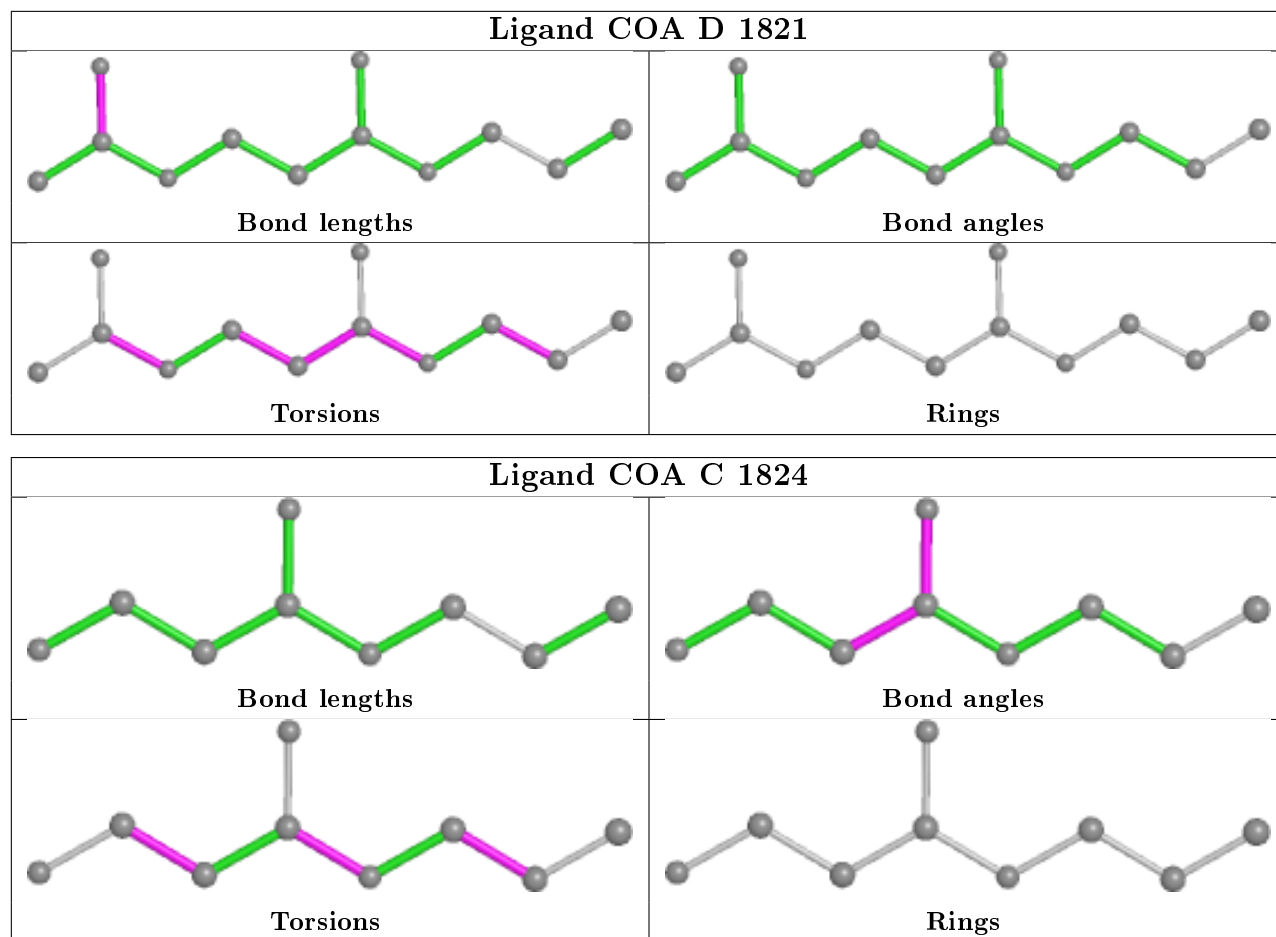
Mol	Chain	Res	Type	Atoms
2	A	1820	COA	O5P-C5P-N4P-C3P
2	D	1821	COA	N4P-C5P-C6P-C7P
2	D	1821	COA	O5P-C5P-N4P-C3P
2	D	1821	COA	C6P-C5P-N4P-C3P
2	D	1821	COA	O5P-C5P-C6P-C7P
2	A	1820	COA	C2P-C3P-N4P-C5P

There are no ring outliers.

No monomer is involved in short contacts.

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	400/433 (92%)	0.10	15 (3%) 40 39	14, 30, 43, 54	0
1	B	403/433 (93%)	-0.12	11 (2%) 54 52	21, 32, 43, 52	0
1	C	404/433 (93%)	-0.08	8 (1%) 65 63	11, 31, 42, 58	0
1	D	409/433 (94%)	0.02	15 (3%) 41 41	21, 31, 43, 63	0
All	All	1616/1732 (93%)	-0.02	49 (3%) 50 49	11, 31, 43, 63	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	530	PHE	4.2
1	A	478	GLY	3.9
1	C	605	TRP	3.8
1	D	651	ILE	3.6
1	A	692	PRO	3.6
1	B	615	LEU	3.5
1	D	630	CYS	3.5
1	D	638	VAL	3.4
1	B	665	LEU	3.4
1	A	496	CYS	3.4
1	A	497	SER	3.3
1	B	669	GLY	3.1
1	D	713	LEU	3.1
1	C	604	TYR	3.0
1	B	622	ALA	3.0
1	D	819	VAL	3.0
1	B	686	PHE	2.9
1	C	532	LEU	2.9
1	C	662	VAL	2.8
1	D	618	GLY	2.8
1	C	669	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	638	VAL	2.6
1	D	624	GLY	2.6
1	D	658	VAL	2.6
1	D	627	TRP	2.5
1	C	665	LEU	2.5
1	C	614[A]	HIS	2.5
1	C	671	PHE	2.5
1	B	662	VAL	2.4
1	A	696	GLN	2.4
1	D	752	VAL	2.4
1	A	605	TRP	2.4
1	D	413	THR	2.4
1	A	781	ILE	2.4
1	A	769	ALA	2.4
1	D	417	TYR	2.3
1	A	722	TRP	2.3
1	D	750	TRP	2.2
1	B	465	MET	2.2
1	B	690	ILE	2.2
1	B	428	GLY	2.1
1	D	635	PRO	2.1
1	A	726	LEU	2.1
1	A	782	ILE	2.1
1	A	819	VAL	2.1
1	A	761	ILE	2.1
1	B	614[A]	HIS	2.0
1	D	662	VAL	2.0
1	A	601	LEU	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	MCS	D	642	12/13	0.93	0.15	13,31,34,37	0
1	MCS	A	642	12/13	0.94	0.19	24,32,45,50	0
1	MCS	B	642	12/13	0.94	0.12	22,32,35,37	0
1	MCS	C	642	12/13	0.97	0.18	14,31,37,41	0

6.3 Carbohydrates [i](#)

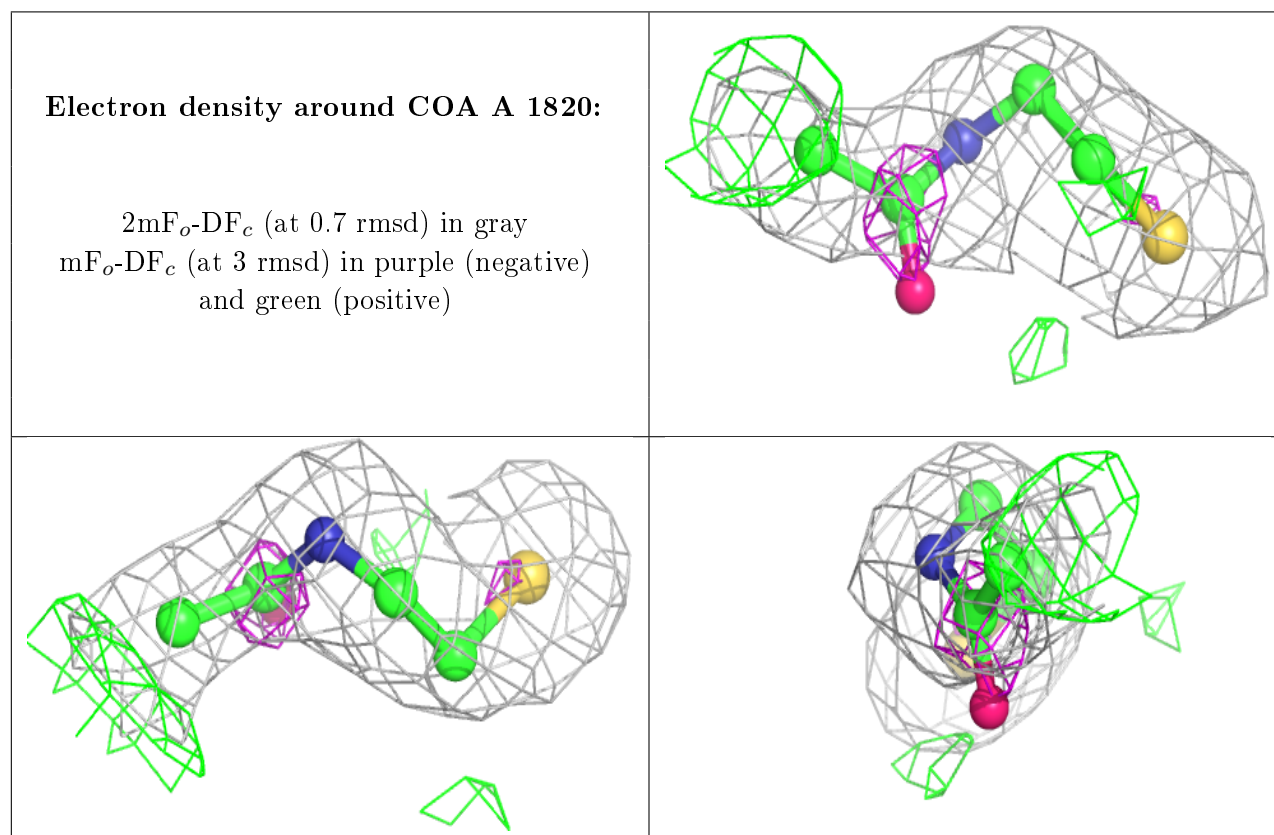
There are no carbohydrates in this entry.

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, 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.

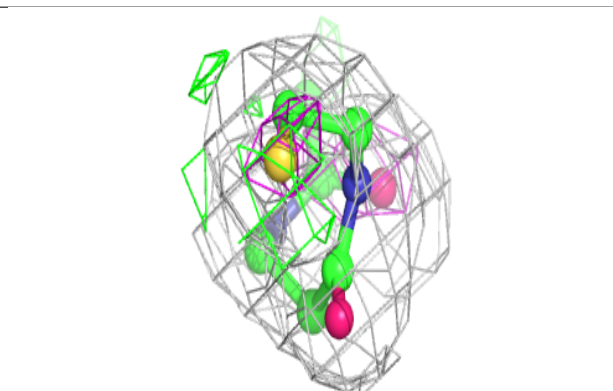
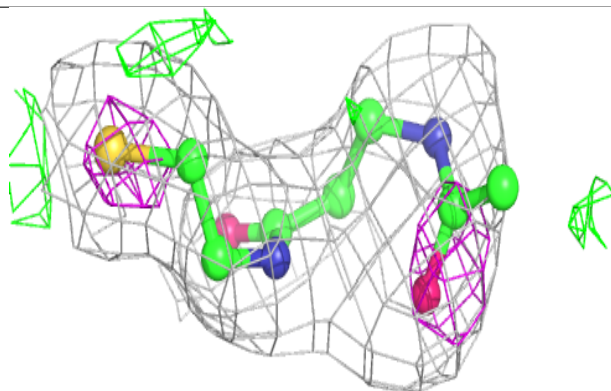
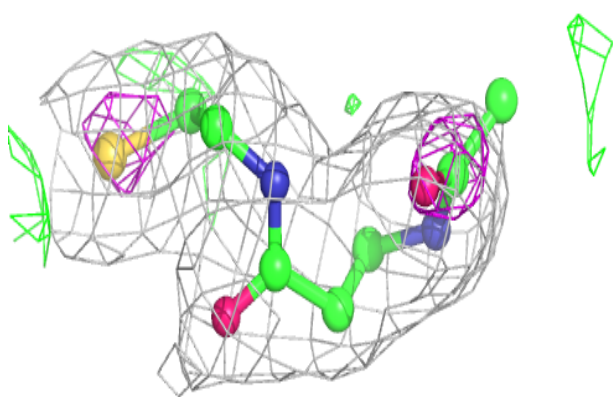
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	COA	A	1820	7/48	0.88	0.17	45,53,78,87	0
2	COA	D	1821	12/48	0.94	0.10	24,43,56,57	0
2	COA	C	1824	9/48	0.95	0.09	28,36,47,50	0
2	COA	B	1823	8/48	0.96	0.09	24,28,38,43	0

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

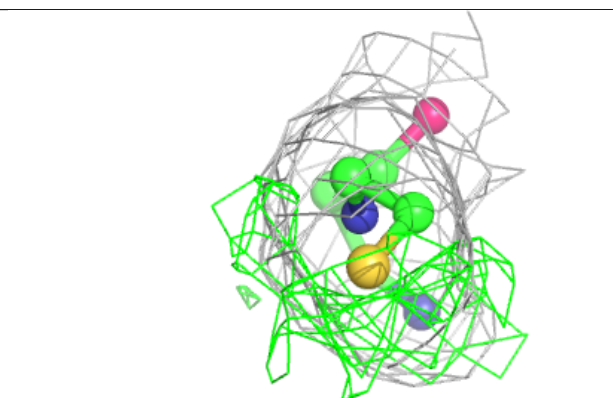
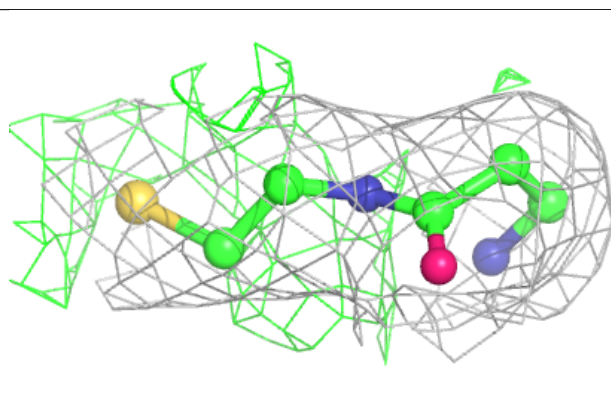
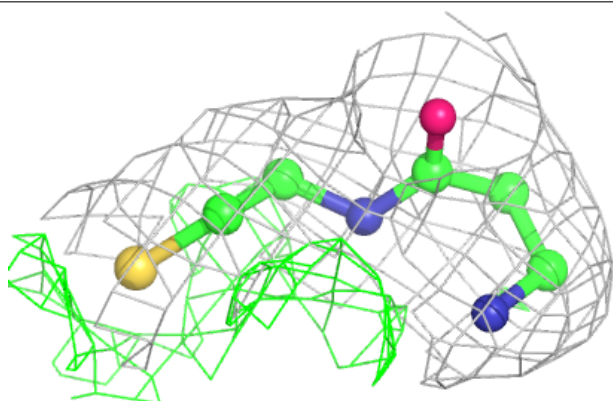


Electron density around COA D 1821:

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

**Electron density around COA C 1824:**

$2mF_o-DF_c$ (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.