Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:24 AM BST

PDB ID	:	6ROP
Title	:	KS-MAT DI-DOMAIN OF MOUSE FAS WITH OCTANOYL COA
Authors	:	Paithankar, K.S.; Rittner, A.; Grininger, M.
Deposited on	:	2019-05-13
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

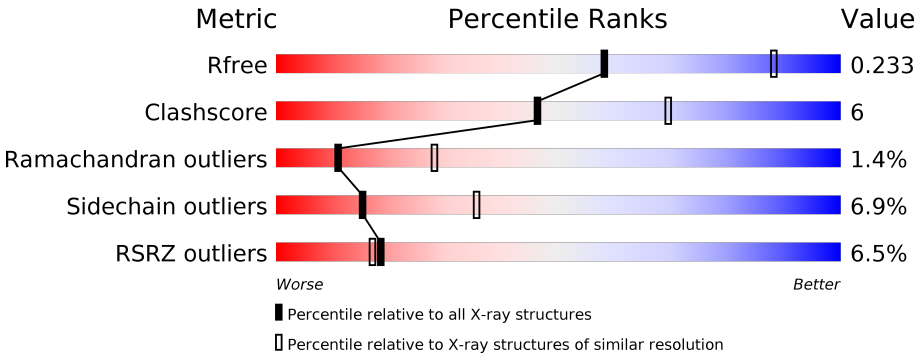
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	3% 84% 15%
1	B	852	9% 76% 20%
1	C	852	10% 77% 20%
1	D	852	4% 81% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25764 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.

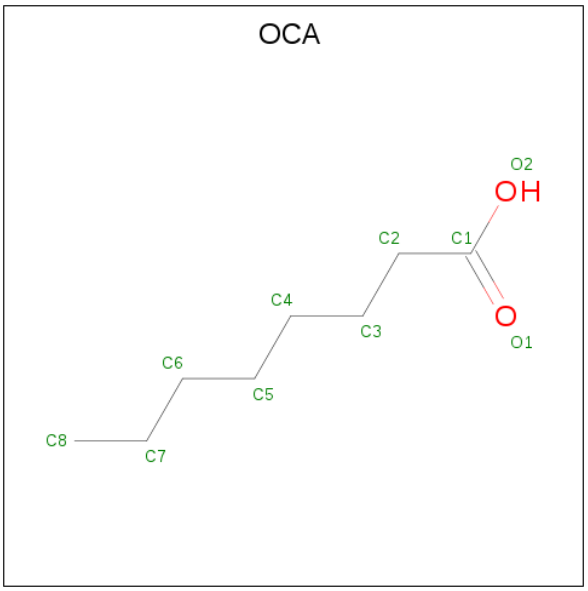
- Molecule 1 is a protein called Fatty acid synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	852	Total	C	N	O	S	0	0	0
			6477	4094	1137	1214	32			
1	B	831	Total	C	N	O	S	0	0	0
			6295	3978	1102	1184	31			
1	C	847	Total	C	N	O	S	0	0	0
			6413	4051	1125	1207	30			
1	D	852	Total	C	N	O	S	0	0	0
			6477	4094	1137	1214	32			

There are 4 discrepancies between the modelled and reference sequences:

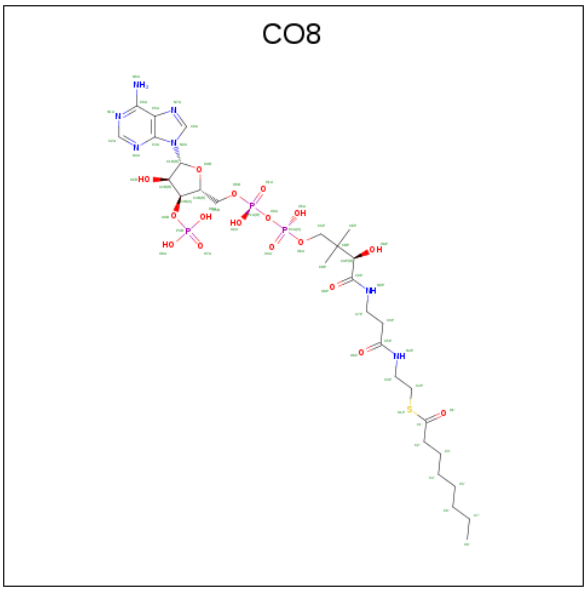
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P19096
B	1	SER	-	expression tag	UNP P19096
C	1	SER	-	expression tag	UNP P19096
D	1	SER	-	expression tag	UNP P19096

- Molecule 2 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula: $C_8H_{16}O_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 8 1	0	0
2	B	1	Total C O 9 8 1	0	0
2	C	1	Total C O 9 8 1	0	0
2	D	1	Total C O 9 8 1	0	0
2	D	1	Total C O 9 8 1	0	0

- Molecule 3 is OCTANOYL-COENZYME A (three-letter code: CO8) (formula: $C_{29}H_{50}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by author).



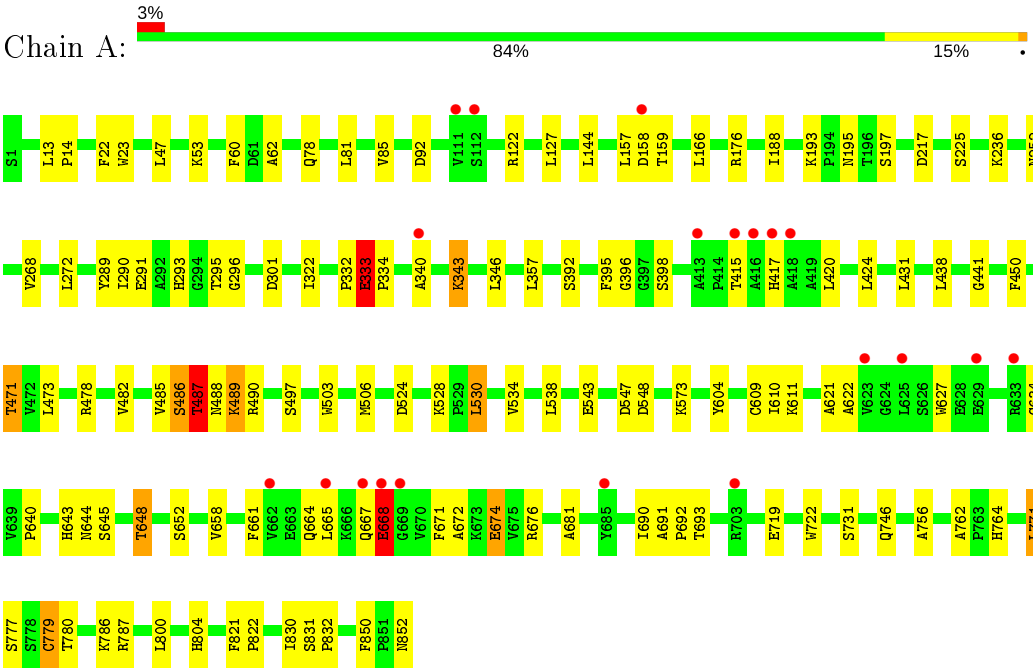
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		

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.

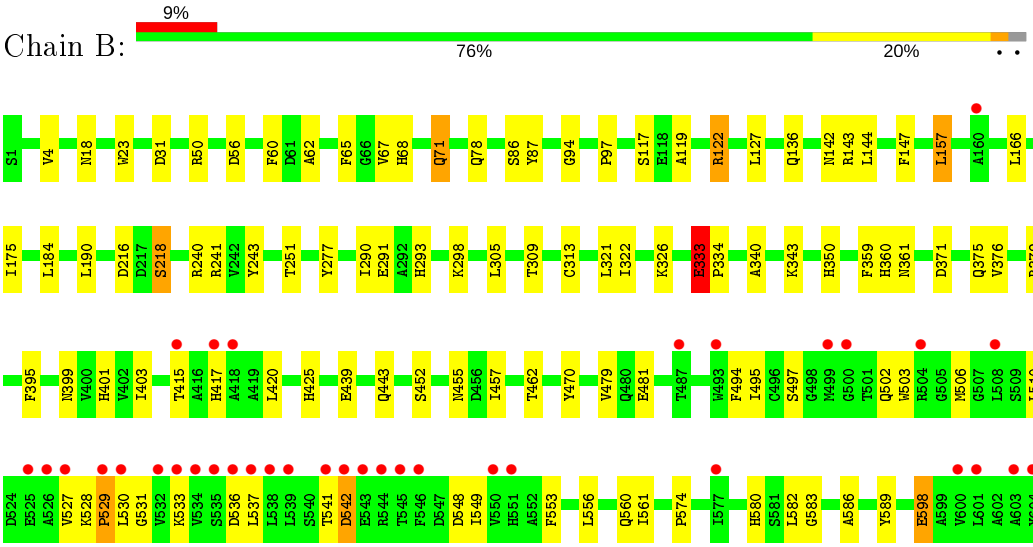
- Molecule 1: Fatty acid synthase

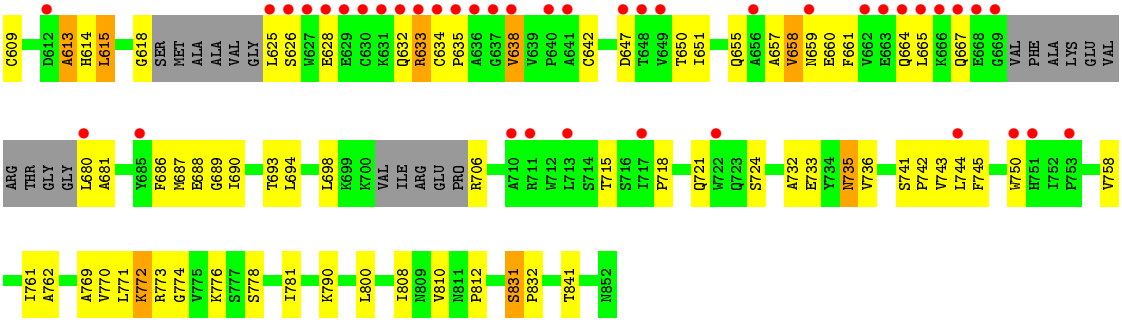
Chain A:



- Molecule 1: Fatty acid synthase

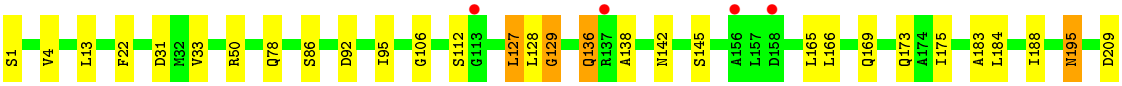
Chain B:

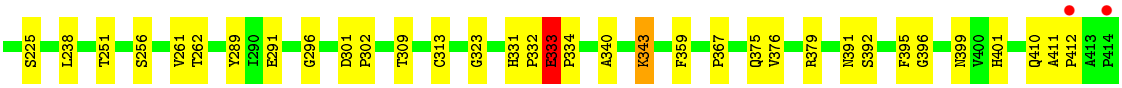


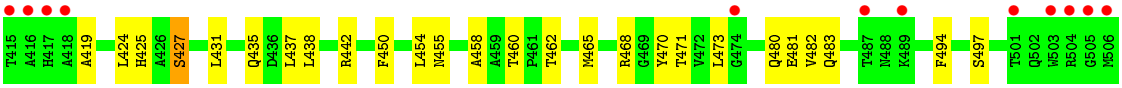


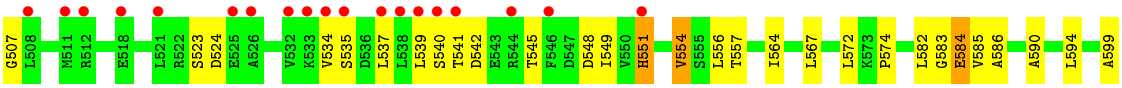
• Molecule 1: Fatty acid synthase

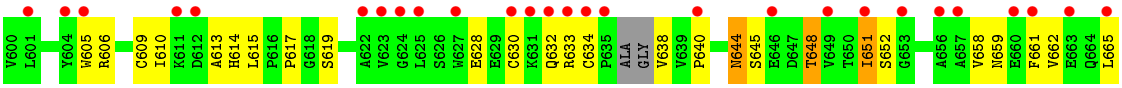
Chain C:

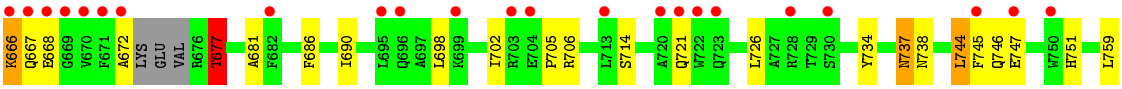


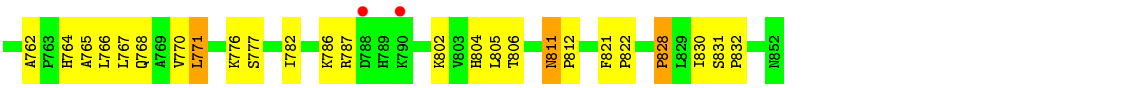


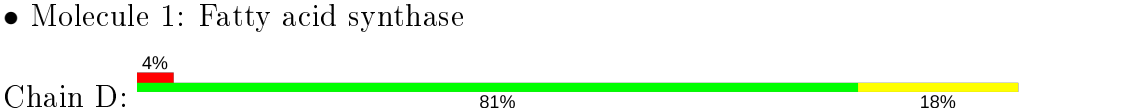


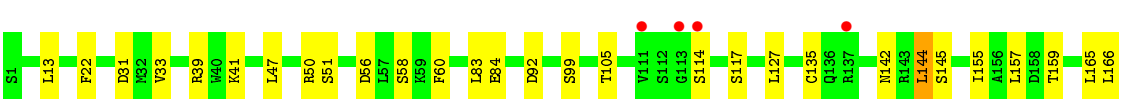


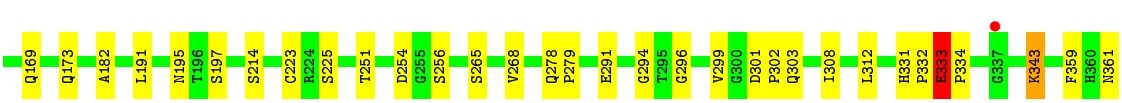






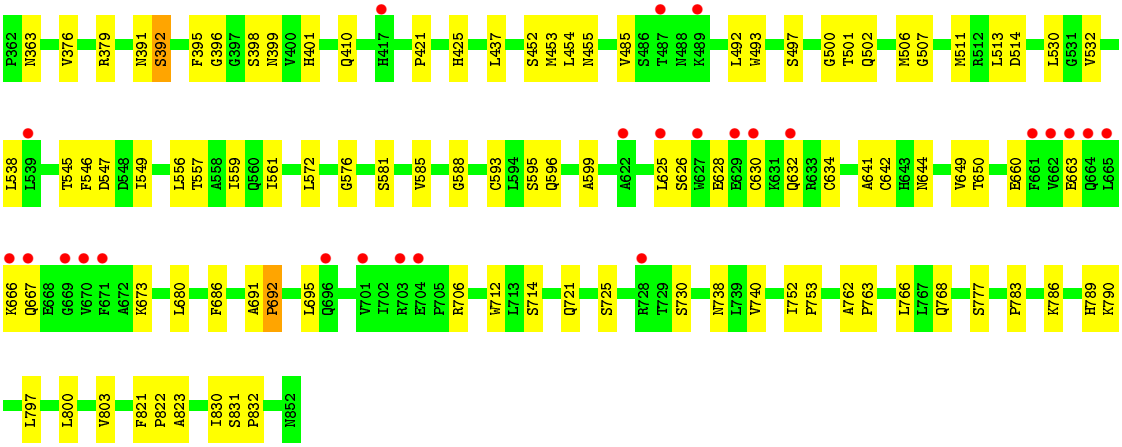






• Molecule 1: Fatty acid synthase

Chain D:


P362 N363 V376 R379 N391 S392 F395 G396 G397 S398 N399 V400 H401 Q410 H417 P421 H425 L437 S452 M453 L454 N455 V485 S486 T487 N488 K489 L492 W493 S497 G500 T501 Q502 M506 G507 M511 R512 L513 D514 L530 G531 V532
L538 L539 T545 F546 D547 D548 I549 L556 T557 A558 I559 Q560 I561 L572 G576 S581 V585 G588 C593 L594 S595 Q596 A599 A622 L625 S626 W627 E628 E629 C630 K631 Q632 R633 C634 A641 C642 H643 N644 V649 T650 E660 F661 V662 E663 Q664 L665
K666 Q667 E668 G669 V670 F671 A672 K673 L680 F686 A691 P692 L695 Q696 V701 I702 R703 E704 P705 R706 W712 L713 S714 Q721 S725 R728 T729 S730 N738 L739 V740 I752 P753 A762 P763 L766 L767 Q768 S777 P783 K786 H789 K790
L797 L800 V803 F821 P822 A823 I830 S831 P832 N862

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	147.44Å 354.11Å 218.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.70 48.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.00-2.70) 98.2 (48.02-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.184 , 0.233 0.189 , 0.233	Depositor DCC
R_{free} test set	7707 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25764	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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: OCA, CO8

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	0.68	0/6624	0.84	1/9009 (0.0%)
1	B	0.71	2/6437 (0.0%)	0.85	3/8758 (0.0%)
1	C	0.69	0/6556	0.83	1/8920 (0.0%)
1	D	0.69	0/6624	0.86	1/9009 (0.0%)
All	All	0.69	2/26241 (0.0%)	0.84	6/35696 (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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	598	GLU	CD-OE1	9.48	1.36	1.25
1	B	706	ARG	CZ-NH2	-8.53	1.22	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	706	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	A	333	GLU	CB-CA-C	6.42	123.23	110.40
1	B	333	GLU	CB-CA-C	6.17	122.75	110.40
1	B	706	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	333	GLU	CB-CA-C	5.63	121.65	110.40
1	C	333	GLU	CB-CA-C	5.32	121.04	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	598	GLU	Sidechain

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	6477	0	6460	63	0
1	B	6295	0	6228	82	0
1	C	6413	0	6372	102	0
1	D	6477	0	6459	77	0
2	A	9	0	15	0	0
2	B	9	0	15	0	0
2	C	9	0	15	1	0
2	D	18	0	30	2	0
3	D	57	0	46	4	0
All	All	25764	0	25640	323	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 6.

All (323) 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:771:LEU:O	1:A:775:VAL:HG22	1.78	0.83
1:C:195:ASN:HD22	1:C:195:ASN:N	1.78	0.78
1:B:661:PHE:HA	1:B:664:GLN:HE21	1.51	0.76
1:D:391:ASN:OD1	1:D:401:HIS:HD2	1.71	0.74
1:C:136:GLN:HE22	1:C:138:ALA:HB3	1.53	0.74
1:B:31:ASP:OD2	1:B:50:ARG:NH2	2.21	0.73
1:A:438:LEU:HD22	1:A:471:THR:HG22	1.71	0.72
1:B:425:HIS:H	1:B:455:ASN:HD21	1.37	0.72
1:A:524:ASP:OD1	1:A:534:VAL:N	2.22	0.72
1:C:537:LEU:O	1:C:540:SER:HB2	1.89	0.72
1:D:425:HIS:H	1:D:455:ASN:ND2	1.88	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:MET:HE2	1:D:763:PRO:HB2	1.72	0.70
1:A:661:PHE:O	1:A:665:LEU:HB2	1.91	0.69
1:C:169:GLN:NE2	1:C:173:GLN:HE21	1.91	0.69
1:C:142:ASN:HD22	1:D:396:GLY:HA3	1.58	0.68
1:D:768:GLN:HE22	1:D:783:PRO:HD3	1.59	0.68
1:B:68:HIS:HB2	1:B:71:GLN:HE22	1.59	0.66
1:A:159:THR:HG21	1:A:166:LEU:HD22	1.77	0.66
1:B:391:ASN:OD1	1:B:401:HIS:HD2	1.78	0.66
1:C:127:LEU:C	1:C:127:LEU:HD12	2.16	0.66
1:B:608:GLN:HA	1:B:608:GLN:HE21	1.61	0.65
3:D:903:CO8:O9P	3:D:903:CO8:H132	1.94	0.65
1:C:442:ARG:NH1	1:C:480:GLN:OE1	2.28	0.65
1:C:195:ASN:HD22	1:C:195:ASN:H	1.46	0.64
1:D:39:ARG:HD2	1:D:191:LEU:O	1.97	0.64
1:C:438:LEU:HD22	1:C:471:THR:HG22	1.78	0.64
1:C:396:GLY:HA3	1:D:142:ASN:HD22	1.63	0.63
1:C:169:GLN:HE21	1:C:173:GLN:HE21	1.47	0.62
1:A:468:ARG:HD3	1:A:804:HIS:CE1	2.34	0.62
1:C:78:GLN:HG2	1:C:188:ILE:HB	1.81	0.62
1:B:169:GLN:HE21	1:B:173:GLN:HE21	1.46	0.62
1:B:4:VAL:HG22	1:B:175:ILE:HG22	1.81	0.62
1:A:503:TRP:CZ2	1:A:506:MET:HA	2.36	0.61
1:A:610:ILE:HA	1:A:690:ILE:HD11	1.82	0.61
1:C:460:THR:HG21	1:C:465:MET:HG3	1.82	0.60
1:C:468:ARG:HD3	1:C:804:HIS:CE1	2.36	0.60
1:D:493:TRP:CE3	1:D:576:GLY:HA3	2.37	0.60
1:C:659:ASN:HA	1:C:662:VAL:HG22	1.83	0.60
1:A:158:ASP:OD2	1:B:136:GLN:NE2	2.33	0.59
1:D:425:HIS:H	1:D:455:ASN:HD21	1.48	0.59
1:B:658:VAL:O	1:B:660:GLU:N	2.30	0.59
1:C:431:LEU:CD2	1:C:435:GLN:HE22	2.15	0.59
1:B:495:ILE:O	1:B:495:ILE:HG22	2.02	0.59
1:B:609:CYS:O	1:B:613:ALA:HB3	2.03	0.58
1:D:506:MET:HE2	1:D:763:PRO:CB	2.33	0.58
1:B:119:ALA:O	1:B:122:ARG:NH1	2.36	0.58
1:B:94:GLY:O	1:B:240:ARG:NH1	2.37	0.58
1:B:23:TRP:CE2	1:B:350:HIS:CD2	2.91	0.58
1:D:308:ILE:HG23	1:D:312:LEU:HD12	1.84	0.58
1:B:68:HIS:HB2	1:B:71:GLN:NE2	2.18	0.58
1:C:450:PHE:CE1	1:C:828:PRO:HB2	2.39	0.58
1:A:23:TRP:HB2	1:A:346:LEU:HD13	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:GLN:HA	1:D:506:MET:CE	2.33	0.57
1:A:291:GLU:HG2	1:A:340:ALA:HB1	1.86	0.57
1:A:667:GLN:O	1:A:668:GLU:HB2	2.03	0.57
1:C:136:GLN:HE22	1:C:138:ALA:CB	2.16	0.57
1:A:450:PHE:CE2	1:A:454:LEU:HD11	2.39	0.57
1:C:424:LEU:HA	1:C:455:ASN:HD21	1.70	0.57
1:D:157:LEU:HD13	1:D:166:LEU:HD23	1.87	0.57
1:D:686:PHE:CD1	1:D:740:VAL:HG11	2.40	0.57
1:B:127:LEU:HD12	1:B:127:LEU:C	2.26	0.56
1:A:254:ASP:HA	1:A:268:VAL:HG11	1.88	0.56
1:B:290:ILE:HG23	1:B:322:ILE:HG13	1.88	0.56
1:C:537:LEU:O	1:C:540:SER:CB	2.55	0.55
1:D:159:THR:HG21	1:D:166:LEU:HD22	1.88	0.55
1:B:744:LEU:O	1:B:744:LEU:HG	2.06	0.55
1:A:127:LEU:C	1:A:127:LEU:HD12	2.27	0.55
1:C:425:HIS:H	1:C:455:ASN:ND2	2.04	0.55
1:C:767:LEU:HA	1:C:770:VAL:HG22	1.89	0.55
1:B:497:SER:HB2	1:B:762:ALA:HB2	1.89	0.55
1:D:821:PHE:HA	1:D:822:PRO:C	2.27	0.54
1:B:698:LEU:HB3	1:B:732:ALA:HB1	1.89	0.54
1:A:627:TRP:CE3	1:A:643:HIS:HB2	2.42	0.54
1:B:169:GLN:NE2	1:B:173:GLN:HE21	2.05	0.54
1:B:241:ARG:HD2	1:B:243:TYR:CE2	2.42	0.54
1:C:261:VAL:HG13	1:C:262:THR:HG23	1.90	0.54
1:A:333:GLU:CB	1:A:334:PRO:CD	2.86	0.54
1:B:586:ALA:O	1:B:589:TYR:N	2.40	0.54
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.89	0.54
1:D:117:SER:HB3	1:D:135:CYS:HB3	1.90	0.53
1:D:768:GLN:NE2	1:D:783:PRO:HD3	2.22	0.53
1:B:360:HIS:C	1:B:361:ASN:HD22	2.10	0.53
1:C:391:ASN:OD1	1:C:401:HIS:HD2	1.91	0.53
1:C:634:CYS:HB3	1:C:661:PHE:CE2	2.43	0.53
1:C:470:TYR:CE1	1:C:481:GLU:HB2	2.44	0.53
1:B:251:THR:HA	1:B:399:ASN:O	2.08	0.53
1:B:638:VAL:HB	1:B:658:VAL:HG22	1.91	0.53
1:C:494:PHE:CD2	1:C:574:PRO:HB3	2.43	0.53
1:B:769:ALA:O	1:B:772:LYS:HE3	2.08	0.53
1:C:450:PHE:CD1	1:C:828:PRO:HB2	2.44	0.53
1:C:567:LEU:O	1:C:572:LEU:HB2	2.08	0.53
1:D:251:THR:HA	1:D:399:ASN:O	2.09	0.53
1:B:439:GLU:OE2	1:B:443:GLN:NE2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LEU:C	1:D:127:LEU:HD12	2.29	0.53
1:A:486:SER:O	1:A:487:THR:HB	2.09	0.52
1:C:582:LEU:O	1:C:585:VAL:HG12	2.10	0.52
1:B:694:LEU:HD13	1:B:736:VAL:HG12	1.90	0.52
1:B:216:ASP:OD2	1:B:218:SER:OG	2.28	0.52
1:C:13:LEU:HD13	1:C:22:PHE:CD2	2.45	0.52
1:D:507:GLY:O	1:D:511:MET:HG2	2.10	0.52
1:B:613:ALA:O	1:B:615:LEU:HD23	2.09	0.52
1:C:359:PHE:CZ	1:C:376:VAL:HG21	2.45	0.52
1:A:81:LEU:O	1:A:85:VAL:HG23	2.10	0.51
1:C:609:CYS:O	1:C:613:ALA:HB3	2.10	0.51
1:B:425:HIS:H	1:B:455:ASN:ND2	2.06	0.51
1:C:764:HIS:CD2	1:C:787:ARG:HB3	2.46	0.51
1:A:14:PRO:HA	1:A:53:LYS:O	2.11	0.51
1:C:427:SER:OG	1:C:458:ALA:O	2.28	0.51
1:A:691:ALA:HB3	1:A:692:PRO:HD3	1.92	0.51
1:C:165:LEU:HD22	1:C:392:SER:HB2	1.92	0.51
1:C:309:THR:O	1:C:313:CYS:HB2	2.11	0.51
1:B:541:THR:OG1	1:B:542:ASP:N	2.43	0.51
3:D:903:CO8:OAP	3:D:903:CO8:H71	2.11	0.51
1:A:645:SER:HA	1:A:746:GLN:HE21	1.75	0.51
1:C:634:CYS:SG	1:C:638:VAL:O	2.67	0.50
1:B:503:TRP:CH2	1:B:506:MET:HA	2.46	0.50
1:C:658:VAL:O	1:C:662:VAL:HG13	2.11	0.50
1:A:296:GLY:HA2	1:A:301:ASP:OD2	2.11	0.50
1:C:195:ASN:H	1:C:195:ASN:ND2	2.07	0.50
2:D:902:OCA:H21	3:D:903:CO8:H3'1	1.94	0.50
1:A:548:ASP:C	1:A:548:ASP:OD1	2.50	0.50
1:D:831:SER:OG	1:D:832:PRO:HD3	2.11	0.50
1:C:31:ASP:OD2	1:C:50:ARG:NH2	2.44	0.50
1:C:291:GLU:HG2	1:C:340:ALA:HB1	1.94	0.49
1:D:359:PHE:CZ	1:D:376:VAL:HG21	2.47	0.49
1:C:13:LEU:HD13	1:C:22:PHE:CG	2.48	0.49
1:D:663:GLU:O	1:D:667:GLN:HG2	2.13	0.49
1:D:588:GLY:HA2	1:D:712:TRP:CZ3	2.48	0.49
1:D:831:SER:N	1:D:832:PRO:CD	2.76	0.49
1:A:764:HIS:HD2	1:A:787:ARG:H	1.60	0.49
1:D:493:TRP:CZ3	1:D:576:GLY:HA3	2.48	0.49
1:C:640:PRO:HA	1:C:651:ILE:HG22	1.95	0.49
1:D:492:LEU:HD22	1:D:572:LEU:HD22	1.94	0.49
1:B:580:HIS:HB2	1:B:745:PHE:HE2	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:HIS:HE1	1:B:810:VAL:HB	1.77	0.49
1:C:301:ASP:HB2	1:C:302:PRO:HD3	1.94	0.49
1:D:502:GLN:HA	1:D:506:MET:HE1	1.93	0.49
1:A:438:LEU:HD22	1:A:471:THR:CG2	2.43	0.48
1:B:528:LYS:N	1:B:529:PRO:CD	2.76	0.48
1:B:721:GLN:O	1:B:724:SER:HB3	2.13	0.48
1:B:638:VAL:O	1:B:638:VAL:HG13	2.13	0.48
1:B:618:GLY:HA3	1:B:681:ALA:HB2	1.94	0.48
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.48	0.48
1:B:65:PHE:HA	1:B:147:PHE:CE1	2.47	0.48
1:D:291:GLU:OE1	1:D:343:LYS:HE2	2.14	0.48
1:A:193:LYS:HG3	1:A:850:PHE:CG	2.49	0.48
1:A:547:ASP:OD1	1:A:676:ARG:NH2	2.46	0.48
1:B:420:LEU:HD21	1:B:512:ARG:HB3	1.95	0.48
1:D:497:SER:HB2	1:D:762:ALA:HB2	1.95	0.48
1:C:425:HIS:H	1:C:455:ASN:HD21	1.61	0.48
1:C:136:GLN:NE2	1:C:138:ALA:HB3	2.25	0.48
1:C:225:SER:O	1:C:332:PRO:HA	2.14	0.48
1:C:584:GLU:OE1	1:C:738:ASN:ND2	2.46	0.47
1:D:333:GLU:CB	1:D:334:PRO:CD	2.92	0.47
1:D:425:HIS:N	1:D:455:ASN:HD21	2.11	0.47
1:D:800:LEU:O	1:D:803:VAL:HB	2.14	0.47
1:B:580:HIS:HB2	1:B:745:PHE:CE2	2.49	0.47
1:C:92:ASP:HA	1:C:830:ILE:HB	1.96	0.47
1:C:802:LYS:O	1:C:806:THR:HG23	2.14	0.47
1:A:289:TYR:OH	1:A:343:LYS:HE3	2.15	0.47
1:B:528:LYS:HG3	1:B:529:PRO:HD3	1.97	0.47
1:C:606:ARG:O	1:C:610:ILE:HD13	2.15	0.47
1:C:166:LEU:HD21	1:D:155:ILE:HG12	1.97	0.47
1:B:293:HIS:O	1:B:326:LYS:HD2	2.14	0.47
1:C:765:ALA:HB1	1:C:768:GLN:HG2	1.96	0.47
1:C:666:LYS:HD2	1:C:672:ALA:HB2	1.97	0.47
1:C:767:LEU:O	1:C:771:LEU:HB2	2.14	0.47
1:D:545:THR:HG23	1:D:546:PHE:CD2	2.50	0.47
1:C:564:ILE:HD13	1:C:590:ALA:HB2	1.97	0.47
1:C:610:ILE:N	1:C:610:ILE:HD12	2.30	0.47
1:A:756:ALA:O	1:A:779:CYS:HA	2.15	0.47
1:B:758:VAL:CG2	1:B:781:ILE:HA	2.45	0.47
1:D:92:ASP:HA	1:D:830:ILE:HB	1.96	0.47
1:B:642:CYS:HB2	1:B:650:THR:CG2	2.44	0.46
1:C:50:ARG:HD3	1:C:209:ASP:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:HIS:CD2	1:A:295:THR:HG23	2.50	0.46
1:D:56:ASP:OD1	1:D:58:SER:N	2.41	0.46
1:A:47:LEU:HD22	1:A:197:SER:HB3	1.98	0.46
1:D:157:LEU:C	1:D:157:LEU:HD12	2.36	0.46
1:C:333:GLU:CB	1:C:334:PRO:CD	2.93	0.46
1:A:497:SER:HB2	1:A:762:ALA:HB2	1.98	0.46
1:D:165:LEU:HD22	1:D:392:SER:HB2	1.97	0.46
1:C:594:LEU:HB3	1:C:599:ALA:HB2	1.98	0.45
3:D:903:CO8:H2B	3:D:903:CO8:N3A	2.31	0.45
1:D:296:GLY:HA2	1:D:301:ASP:OD2	2.16	0.45
1:A:13:LEU:HD13	1:A:22:PHE:CD2	2.51	0.45
1:B:361:ASN:HD22	1:B:361:ASN:N	2.14	0.45
1:B:715:THR:HA	1:B:744:LEU:HD23	1.99	0.45
1:D:265:SER:OG	1:D:268:VAL:HG23	2.17	0.45
1:B:18:ASN:CG	1:B:832:PRO:HB3	2.37	0.45
1:B:277:TYR:CE1	1:B:403:ILE:HD11	2.50	0.45
1:B:698:LEU:HD13	1:B:735:ASN:HD21	1.82	0.45
1:D:13:LEU:HD13	1:D:22:PHE:CD2	2.51	0.45
1:A:622:ALA:O	1:A:672:ALA:HA	2.17	0.45
1:A:490:ARG:NH2	1:A:780:THR:OG1	2.43	0.45
1:C:410:GLN:O	1:C:412:PRO:HD3	2.17	0.45
1:C:431:LEU:HD21	1:C:435:GLN:HE22	1.81	0.45
1:B:333:GLU:HB2	1:B:334:PRO:HD2	1.97	0.45
1:B:494:PHE:CE2	1:B:574:PRO:HG3	2.52	0.45
1:D:60:PHE:HA	1:D:84:GLU:OE2	2.17	0.45
1:B:687:MET:O	1:B:689:GLY:N	2.50	0.44
1:C:483:GLN:HE21	1:C:805:LEU:CD2	2.30	0.44
1:D:549:ILE:HD12	1:D:680:LEU:HD22	1.99	0.44
1:B:309:THR:O	1:B:313:CYS:HB2	2.17	0.44
1:C:633:ARG:O	1:C:661:PHE:CZ	2.70	0.44
1:D:593:CYS:O	1:D:706:ARG:HD2	2.16	0.44
1:A:489:LYS:HE3	1:A:489:LYS:HA	1.98	0.44
1:A:627:TRP:HB2	1:A:643:HIS:NE2	2.33	0.44
1:B:635:PRO:HD2	1:B:661:PHE:CE2	2.52	0.44
1:B:333:GLU:CB	1:B:334:PRO:CD	2.96	0.44
1:B:553:PHE:O	1:B:582:LEU:HD21	2.18	0.44
1:B:800:LEU:HD22	1:B:810:VAL:HG11	1.99	0.44
1:C:605:TRP:CE3	1:C:605:TRP:HA	2.53	0.44
1:D:667:GLN:HE21	1:D:667:GLN:HA	1.83	0.44
1:A:78:GLN:HB3	1:A:188:ILE:HD12	1.99	0.44
1:A:396:GLY:HA3	1:B:142:ASN:HD22	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:HIS:O	1:A:420:LEU:HD22	2.18	0.44
1:A:290:ILE:HG23	1:A:322:ILE:HG13	2.00	0.43
1:B:549:ILE:O	1:B:553:PHE:HB2	2.17	0.43
1:B:800:LEU:HD23	1:B:800:LEU:HA	1.83	0.43
1:C:86:SER:HB3	1:C:184:LEU:HD21	1.99	0.43
1:C:652:SER:OG	1:C:681:ALA:HB1	2.18	0.43
1:C:744:LEU:HD12	1:C:747:GLU:HG2	2.00	0.43
1:C:4:VAL:HG22	1:C:175:ILE:HG22	2.01	0.43
1:B:608:GLN:HA	1:B:608:GLN:NE2	2.31	0.43
1:B:157:LEU:HD13	1:B:166:LEU:HD23	1.99	0.43
1:B:560:GLN:HG2	1:B:761:ILE:HG22	2.01	0.43
1:A:252:ASN:ND2	1:A:272:LEU:HB2	2.33	0.43
1:D:301:ASP:HB2	1:D:302:PRO:HD3	2.01	0.43
1:D:628:GLU:OE1	1:D:628:GLU:HA	2.18	0.43
1:A:487:THR:HG22	1:A:488:ASN:N	2.34	0.43
1:C:548:ASP:O	1:C:551:HIS:N	2.52	0.43
1:C:630:CYS:SG	1:C:640:PRO:HG3	2.59	0.43
1:D:13:LEU:HD13	1:D:22:PHE:CE2	2.53	0.43
1:B:78:GLN:HG3	1:B:190:LEU:HD12	2.00	0.43
1:C:524:ASP:OD1	1:C:534:VAL:HG22	2.19	0.43
1:C:811:ASN:O	1:C:811:ASN:CG	2.57	0.43
1:B:523:SER:OG	1:B:561:ILE:HD11	2.19	0.43
1:B:741:SER:HB3	1:B:742:PRO:HD2	2.00	0.43
1:B:831:SER:N	1:B:832:PRO:CD	2.82	0.43
1:C:644:ASN:HB2	1:C:648:THR:O	2.19	0.43
1:C:714:SER:OG	1:C:734:TYR:OH	2.21	0.42
1:D:105:THR:HA	1:D:182:ALA:O	2.19	0.42
1:D:278:GLN:HB2	1:D:279:PRO:HD3	2.01	0.42
1:A:534:VAL:O	1:A:538:LEU:HG	2.18	0.42
1:B:425:HIS:CE1	1:B:812:PRO:HD3	2.54	0.42
1:C:610:ILE:N	1:C:610:ILE:CD1	2.82	0.42
1:C:831:SER:N	1:C:832:PRO:CD	2.81	0.42
1:C:677:THR:OG1	1:C:677:THR:O	2.35	0.42
1:D:493:TRP:CD2	1:D:576:GLY:HA3	2.54	0.42
1:A:60:PHE:O	1:A:62:ALA:N	2.53	0.42
1:C:33:VAL:CG1	1:C:50:ARG:HB3	2.49	0.42
1:C:551:HIS:O	1:C:554:VAL:HG12	2.19	0.42
1:A:831:SER:N	1:A:832:PRO:CD	2.82	0.42
1:B:86:SER:HB3	1:B:184:LEU:HD21	2.00	0.42
1:B:62:ALA:HB1	1:B:67:VAL:O	2.19	0.42
1:B:470:TYR:CE1	1:B:481:GLU:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ALA:HA	1:A:674:GLU:HA	2.01	0.42
1:A:821:PHE:HA	1:A:822:PRO:C	2.40	0.42
1:B:359:PHE:CZ	1:B:376:VAL:HG21	2.55	0.42
1:B:635:PRO:O	1:B:638:VAL:HG12	2.20	0.42
1:C:333:GLU:HB2	1:C:334:PRO:HD2	2.01	0.42
1:C:702:ILE:HG22	1:C:705:PRO:HG3	2.01	0.42
1:D:691:ALA:HB3	1:D:692:PRO:CD	2.49	0.42
1:C:128:LEU:O	1:C:129:GLY:C	2.57	0.42
1:C:821:PHE:HA	1:C:822:PRO:C	2.41	0.42
1:A:225:SER:O	1:A:332:PRO:HA	2.19	0.42
1:A:485:VAL:CG1	1:A:486:SER:H	2.33	0.42
1:C:112:SER:HB3	2:C:901:OCA:H61	2.02	0.42
1:C:251:THR:HA	1:C:399:ASN:O	2.20	0.42
1:A:92:ASP:HA	1:A:830:ILE:HB	2.01	0.41
1:C:615:LEU:HD21	1:C:686:PHE:CD2	2.55	0.41
1:D:437:LEU:HD22	1:D:454:LEU:HD22	2.02	0.41
1:B:321:LEU:HD23	1:B:375:GLN:HB3	2.02	0.41
1:B:65:PHE:O	1:B:67:VAL:HG23	2.19	0.41
1:D:559:ILE:HG21	1:D:763:PRO:HB3	2.02	0.41
1:C:296:GLY:HA2	1:C:301:ASP:OD2	2.20	0.41
1:C:659:ASN:CA	1:C:662:VAL:HG22	2.50	0.41
1:D:500:GLY:O	1:D:766:LEU:HD22	2.20	0.41
1:D:641:ALA:HB1	2:D:902:OCA:C5	2.51	0.41
1:B:87:TYR:CE1	1:B:97:PRO:HG2	2.55	0.41
1:C:127:LEU:CD1	1:C:127:LEU:C	2.87	0.41
1:D:225:SER:O	1:D:332:PRO:HA	2.20	0.41
1:D:83:LEU:HD23	1:D:144:LEU:HD12	2.03	0.41
1:A:431:LEU:HD12	1:A:482:VAL:HG11	2.02	0.41
1:A:627:TRP:CZ3	1:A:643:HIS:HB2	2.56	0.41
1:C:343:LYS:HD2	1:C:343:LYS:C	2.41	0.41
1:C:759:LEU:HD23	1:C:782:ILE:HB	2.02	0.41
1:C:497:SER:HB2	1:C:762:ALA:HB2	2.02	0.41
1:A:800:LEU:HA	1:A:800:LEU:HD23	1.81	0.41
1:C:106:GLY:O	1:C:183:ALA:HA	2.20	0.41
1:C:437:LEU:HD22	1:C:454:LEU:HD22	2.02	0.41
1:C:583:GLY:O	1:C:586:ALA:N	2.52	0.41
1:C:726:LEU:HD21	1:C:737:ASN:OD1	2.21	0.41
1:D:299:VAL:O	1:D:303:GLN:HG2	2.20	0.41
1:D:453:MET:HE1	1:D:823:ALA:CB	2.50	0.41
1:A:627:TRP:HB2	1:A:643:HIS:CE1	2.55	0.41
1:B:528:LYS:H	1:B:529:PRO:CD	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:ILE:HG21	1:D:596:GLN:HG3	2.03	0.41
1:D:501:THR:HG22	1:D:766:LEU:HB2	2.03	0.41
1:D:752:ILE:HA	1:D:753:PRO:HD3	1.89	0.41
1:D:254:ASP:HA	1:D:268:VAL:HG11	2.03	0.41
1:D:642:CYS:HB2	1:D:650:THR:HB	2.02	0.41
1:A:719:GLU:HA	1:A:722:TRP:CE2	2.56	0.41
1:D:31:ASP:OD2	1:D:50:ARG:NH2	2.48	0.41
1:D:33:VAL:CG1	1:D:50:ARG:HB3	2.51	0.41
1:C:425:HIS:CE1	1:C:812:PRO:HG3	2.56	0.40
1:D:302:PRO:HG3	1:D:363:ASN:ND2	2.36	0.40
1:D:421:PRO:HB2	1:D:797:LEU:HD12	2.02	0.40
1:A:424:LEU:CD2	1:A:441:GLY:HA3	2.51	0.40
1:A:530:LEU:HG	1:A:604:TYR:CE2	2.56	0.40
1:D:51:SER:HA	1:D:223:CYS:SG	2.60	0.40
1:A:652:SER:HB2	1:A:681:ALA:HB1	2.03	0.40
1:C:745:PHE:CZ	1:C:767:LEU:HD23	2.57	0.40
1:D:47:LEU:HD22	1:D:197:SER:HB3	2.02	0.40
1:D:549:ILE:CD1	1:D:680:LEU:HD22	2.52	0.40
1:C:585:VAL:HG13	1:C:586:ALA:N	2.36	0.40
1:D:169:GLN:HE21	1:D:173:GLN:HE21	1.69	0.40
1:D:585:VAL:HG12	1:D:599:ALA:HB1	2.02	0.40
1:D:493:TRP:CD2	1:D:752:ILE:HG12	2.56	0.40
1:A:644:ASN:HD22	1:A:648:THR:HG22	1.86	0.40
1:A:609:CYS:O	1:A:690:ILE:HD11	2.22	0.40
1:C:289:TYR:OH	1:C:323:GLY:HA3	2.22	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	850/852 (100%)	792 (93%)	52 (6%)	6 (1%)	22 46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	823/852 (97%)	729 (89%)	74 (9%)	20 (2%)	6 15
1	C	841/852 (99%)	727 (86%)	100 (12%)	14 (2%)	9 23
1	D	850/852 (100%)	806 (95%)	36 (4%)	8 (1%)	17 40
All	All	3364/3408 (99%)	3054 (91%)	262 (8%)	48 (1%)	11 28

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	GLU
1	A	487	THR
1	A	668	GLU
1	B	333	GLU
1	B	614	HIS
1	B	638	VAL
1	B	658	VAL
1	B	659	ASN
1	C	333	GLU
1	C	419	ALA
1	C	677	THR
1	D	333	GLU
1	D	514	ASP
1	D	789	HIS
1	A	779	CYS
1	B	548	ASP
1	B	583	GLY
1	B	657	ALA
1	B	688	GLU
1	B	690	ILE
1	C	541	THR
1	D	294	GLY
1	D	673	LYS
1	B	633	ARG
1	C	584	GLU
1	C	644	ASN
1	A	217	ASP
1	B	607	GLY
1	B	718	PRO
1	C	617	PRO
1	D	581	SER
1	B	60	PHE
1	B	647	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	774	GLY
1	C	129	GLY
1	C	411	ALA
1	C	551	HIS
1	C	614	HIS
1	D	513	LEU
1	D	644	ASN
1	B	529	PRO
1	B	613	ALA
1	C	507	GLY
1	A	635	PRO
1	C	482	VAL
1	C	549	ILE
1	B	531	GLY
1	B	527	VAL

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	702/702 (100%)	664 (95%)	38 (5%)	22	47
1	B	679/702 (97%)	620 (91%)	59 (9%)	10	23
1	C	693/702 (99%)	642 (93%)	51 (7%)	13	32
1	D	702/702 (100%)	659 (94%)	43 (6%)	18	41
All	All	2776/2808 (99%)	2585 (93%)	191 (7%)	15	35

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ARG
1	A	144	LEU
1	A	157	LEU
1	A	176	ARG
1	A	195	ASN
1	A	236	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	256	SER
1	A	343	LYS
1	A	357	LEU
1	A	392	SER
1	A	395	PHE
1	A	398	SER
1	A	415	THR
1	A	471	THR
1	A	473	LEU
1	A	478	ARG
1	A	486	SER
1	A	487	THR
1	A	489	LYS
1	A	528	LYS
1	A	530	LEU
1	A	543	GLU
1	A	573	LYS
1	A	611	LYS
1	A	634	CYS
1	A	648	THR
1	A	658	VAL
1	A	664	GLN
1	A	668	GLU
1	A	671	PHE
1	A	674	GLU
1	A	693	THR
1	A	731	SER
1	A	771	LEU
1	A	772	LYS
1	A	777	SER
1	A	786	LYS
1	A	852	ASN
1	B	56	ASP
1	B	71	GLN
1	B	117	SER
1	B	122	ARG
1	B	143	ARG
1	B	144	LEU
1	B	157	LEU
1	B	218	SER
1	B	298	LYS
1	B	305	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	343	LYS
1	B	371	ASP
1	B	379	ARG
1	B	384	ARG
1	B	395	PHE
1	B	415	THR
1	B	417	HIS
1	B	452	SER
1	B	457	ILE
1	B	462	THR
1	B	479	VAL
1	B	502	GLN
1	B	510	LEU
1	B	530	LEU
1	B	533	LYS
1	B	536	ASP
1	B	537	LEU
1	B	542	ASP
1	B	556	LEU
1	B	606	ARG
1	B	608	GLN
1	B	615	LEU
1	B	625	LEU
1	B	626	SER
1	B	628	GLU
1	B	632	GLN
1	B	633	ARG
1	B	634	CYS
1	B	651	ILE
1	B	655	GLN
1	B	665	LEU
1	B	667	GLN
1	B	680	LEU
1	B	686	PHE
1	B	693	THR
1	B	733	GLU
1	B	735	ASN
1	B	743	VAL
1	B	750	TRP
1	B	770	VAL
1	B	771	LEU
1	B	772	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	773	ARG
1	B	776	LYS
1	B	778	SER
1	B	790	LYS
1	B	808	ILE
1	B	831	SER
1	B	841	THR
1	C	1	SER
1	C	95	ILE
1	C	127	LEU
1	C	136	GLN
1	C	145	SER
1	C	195	ASN
1	C	238	LEU
1	C	256	SER
1	C	331	HIS
1	C	343	LYS
1	C	367	PRO
1	C	375	GLN
1	C	379	ARG
1	C	395	PHE
1	C	427	SER
1	C	462	THR
1	C	473	LEU
1	C	523	SER
1	C	535	SER
1	C	539	LEU
1	C	542	ASP
1	C	545	THR
1	C	554	VAL
1	C	556	LEU
1	C	557	THR
1	C	619	SER
1	C	628	GLU
1	C	632	GLN
1	C	645	SER
1	C	648	THR
1	C	651	ILE
1	C	665	LEU
1	C	666	LYS
1	C	667	GLN
1	C	668	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	677	THR
1	C	690	ILE
1	C	698	LEU
1	C	706	ARG
1	C	721	GLN
1	C	737	ASN
1	C	744	LEU
1	C	746	GLN
1	C	751	HIS
1	C	766	LEU
1	C	771	LEU
1	C	776	LYS
1	C	777	SER
1	C	786	LYS
1	C	811	ASN
1	C	828	PRO
1	D	41	LYS
1	D	99	SER
1	D	114	SER
1	D	144	LEU
1	D	145	SER
1	D	195	ASN
1	D	214	SER
1	D	256	SER
1	D	331	HIS
1	D	343	LYS
1	D	361	ASN
1	D	379	ARG
1	D	392	SER
1	D	395	PHE
1	D	398	SER
1	D	410	GLN
1	D	452	SER
1	D	485	VAL
1	D	530	LEU
1	D	532	VAL
1	D	538	LEU
1	D	547	ASP
1	D	556	LEU
1	D	557	THR
1	D	595	SER
1	D	625	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	626	SER
1	D	630	CYS
1	D	632	GLN
1	D	634	CYS
1	D	649	VAL
1	D	660	GLU
1	D	666	LYS
1	D	692	PRO
1	D	695	LEU
1	D	714	SER
1	D	721	GLN
1	D	725	SER
1	D	730	SER
1	D	738	ASN
1	D	777	SER
1	D	786	LYS
1	D	790	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	142	ASN
1	A	358	HIS
1	A	746	GLN
1	A	764	HIS
1	A	852	ASN
1	B	71	GLN
1	B	169	GLN
1	B	328	ASN
1	B	350	HIS
1	B	361	ASN
1	B	401	HIS
1	B	425	HIS
1	B	455	ASN
1	B	560	GLN
1	B	608	GLN
1	B	632	GLN
1	B	664	GLN
1	B	735	ASN
1	B	799	ASN
1	C	73	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	136	GLN
1	C	142	ASN
1	C	169	GLN
1	C	195	ASN
1	C	401	HIS
1	C	435	GLN
1	C	455	ASN
1	C	483	GLN
1	C	502	GLN
1	C	721	GLN
1	C	737	ASN
1	C	755	HIS
1	C	799	ASN
1	C	804	HIS
1	D	142	ASN
1	D	169	GLN
1	D	328	ASN
1	D	358	HIS
1	D	361	ASN
1	D	401	HIS
1	D	455	ASN
1	D	664	GLN
1	D	667	GLN
1	D	764	HIS
1	D	768	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	OCA	D	901	1	8,8,9	0.51	0	7,7,9	0.45	0
2	OCA	B	901	1	8,8,9	0.44	0	7,7,9	0.55	0
2	OCA	A	901	1	8,8,9	0.38	0	7,7,9	0.54	0
3	CO8	D	903	-	51,59,59	0.55	0	62,85,85	0.86	2 (3%)
2	OCA	D	902	1	8,8,9	0.45	0	7,7,9	0.56	0
2	OCA	C	901	1	8,8,9	0.43	0	7,7,9	0.54	0

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	OCA	D	901	1	-	3/5/6/7	-
2	OCA	B	901	1	-	3/5/6/7	-
2	OCA	A	901	1	-	3/5/6/7	-
3	CO8	D	903	-	-	25/54/74/74	0/3/3/3
2	OCA	D	902	1	-	4/5/6/7	-
2	OCA	C	901	1	-	1/5/6/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	903	CO8	C7P-C6P-C5P	2.81	117.03	112.36
3	D	903	CO8	C7P-N8P-C9P	2.22	126.54	122.59

There are no chirality outliers.

All (39) torsion outliers are listed below:

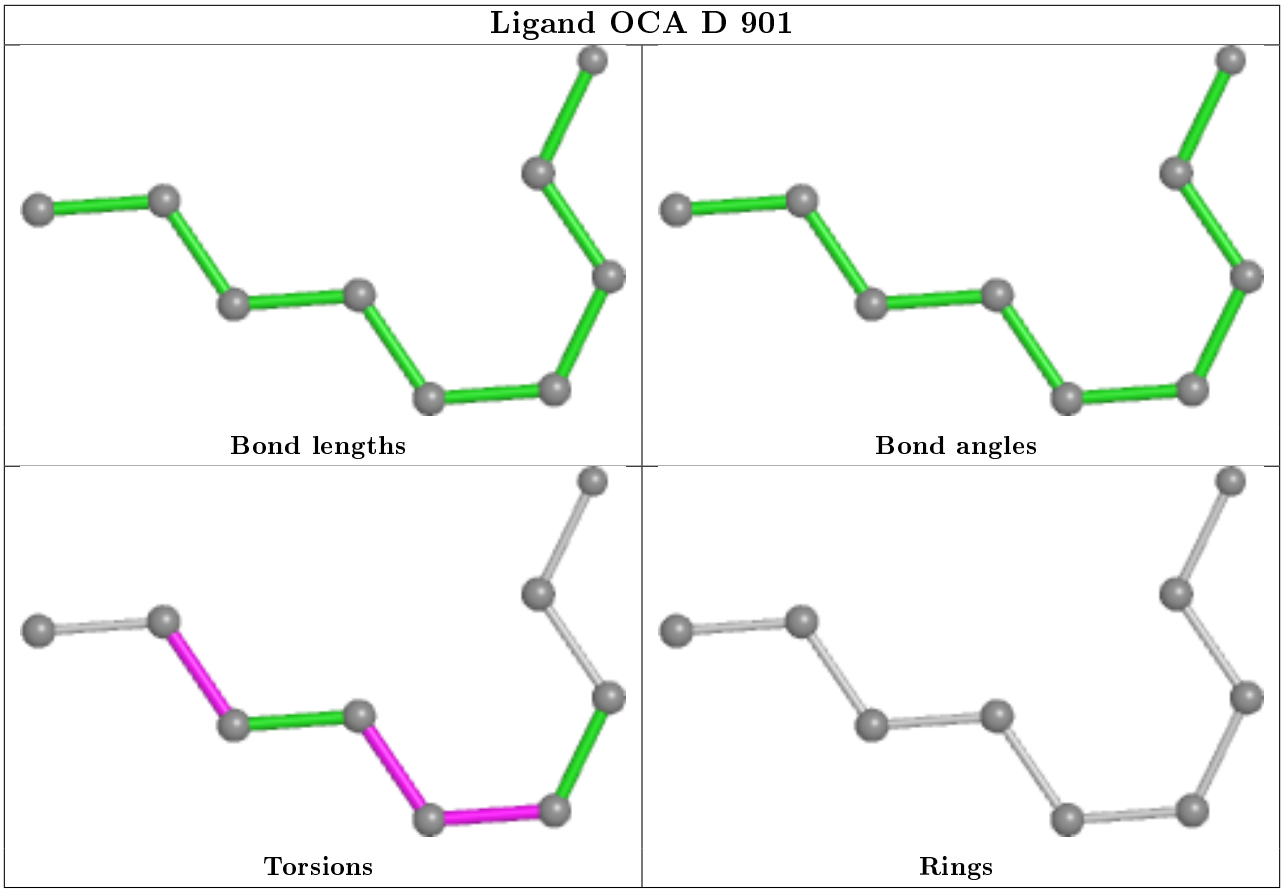
Mol	Chain	Res	Type	Atoms
3	D	903	CO8	C3B-O3B-P3B-O7A
3	D	903	CO8	C5B-O5B-P1A-O1A
3	D	903	CO8	C5B-O5B-P1A-O2A
3	D	903	CO8	CCP-O6A-P2A-O4A
3	D	903	CO8	O9P-C9P-CAP-CBP
3	D	903	CO8	N8P-C9P-CAP-CBP
3	D	903	CO8	N8P-C9P-CAP-OAP
3	D	903	CO8	CAP-C9P-N8P-C7P
3	D	903	CO8	O9P-C9P-N8P-C7P
3	D	903	CO8	S1P-C2P-C3P-N4P
3	D	903	CO8	C3P-C2P-S1P-C1'
3	D	903	CO8	C1'-C2'-C3'-C4'
3	D	903	CO8	C3B-C4B-C5B-O5B
3	D	903	CO8	O4B-C4B-C5B-O5B
2	D	901	OCA	C3-C4-C5-C6
2	A	901	OCA	C3-C4-C5-C6
2	D	901	OCA	C2-C3-C4-C5
3	D	903	CO8	C3'-C4'-C5'-C6'
3	D	903	CO8	O9P-C9P-CAP-OAP
2	A	901	OCA	C5-C6-C7-C8
2	C	901	OCA	C5-C6-C7-C8
2	A	901	OCA	C2-C3-C4-C5
2	D	902	OCA	C5-C6-C7-C8
2	D	902	OCA	C3-C4-C5-C6
3	D	903	CO8	P2A-O3A-P1A-O5B
3	D	903	CO8	S1P-C1'-C2'-C3'
3	D	903	CO8	O1'-C1'-C2'-C3'
2	D	902	OCA	C4-C5-C6-C7
3	D	903	CO8	C3B-O3B-P3B-O8A
3	D	903	CO8	C5B-O5B-P1A-O3A
2	B	901	OCA	C1-C2-C3-C4
2	D	902	OCA	C1-C2-C3-C4
3	D	903	CO8	O5P-C5P-N4P-C3P
2	D	901	OCA	C5-C6-C7-C8
3	D	903	CO8	OAP-CAP-CBP-CEP
2	B	901	OCA	C3-C4-C5-C6
2	B	901	OCA	C5-C6-C7-C8
3	D	903	CO8	OAP-CAP-CBP-CDP
3	D	903	CO8	CDP-CBP-CCP-O6A

There are no ring outliers.

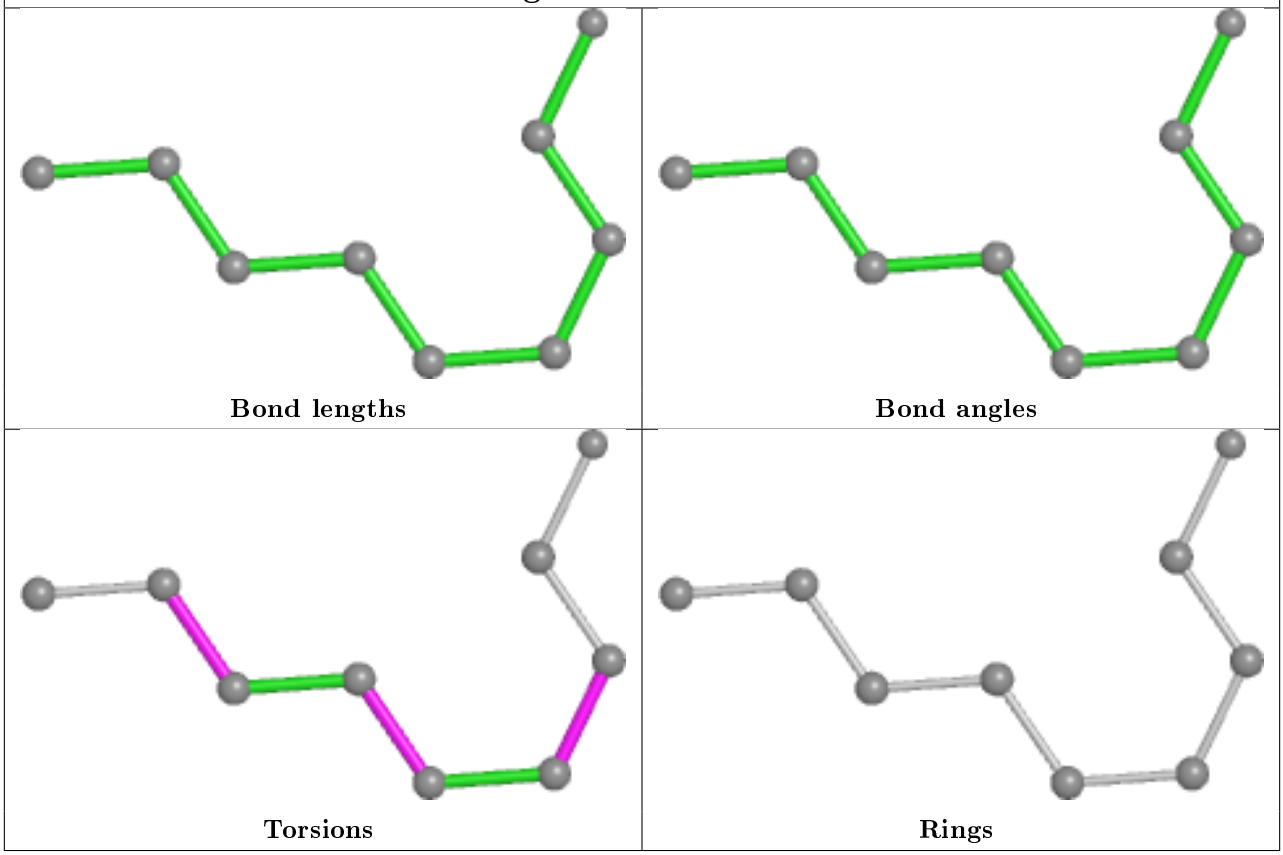
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	903	CO8	4	0
2	D	902	OCA	2	0
2	C	901	OCA	1	0

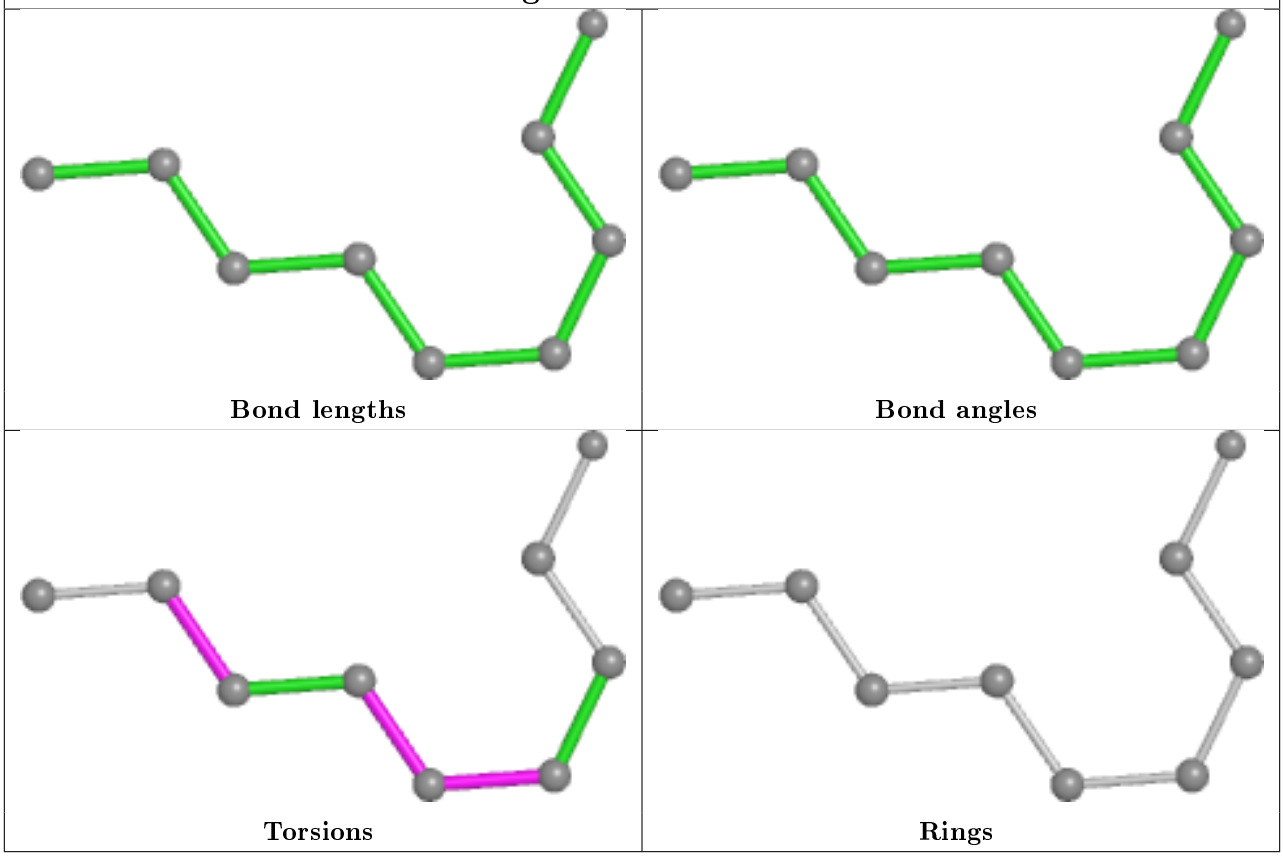
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



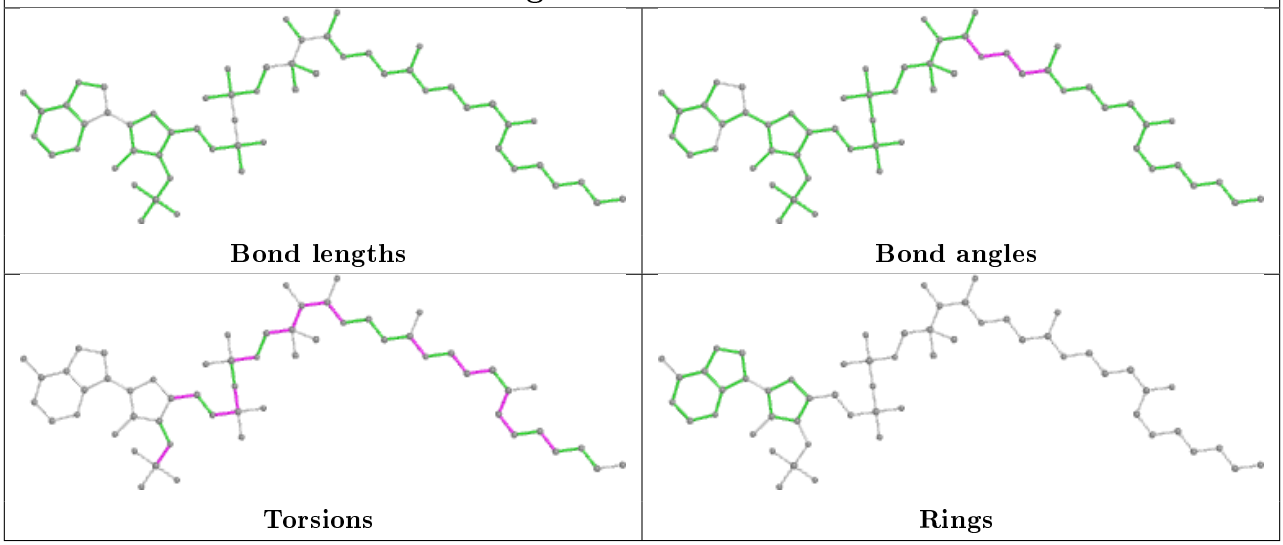
Ligand OCA B 901



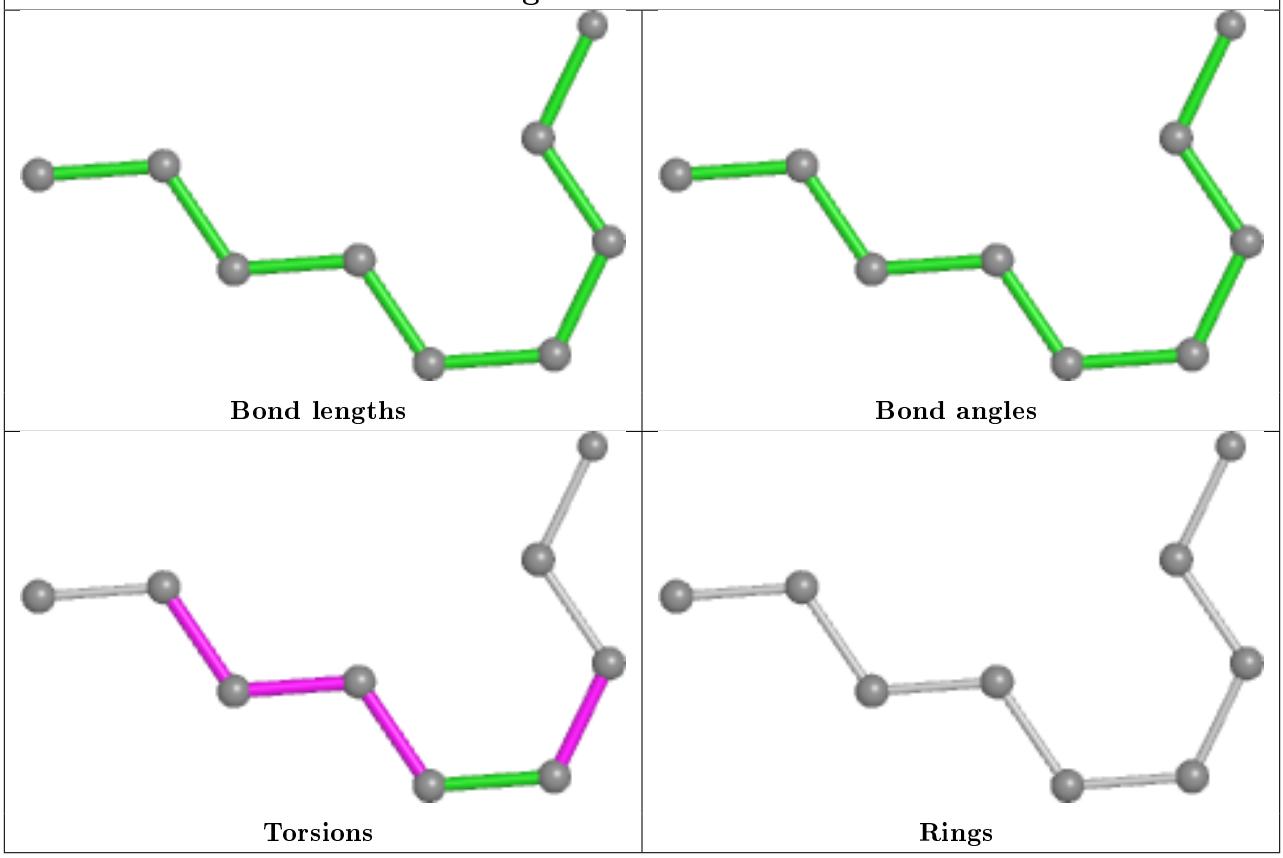
Ligand OCA A 901

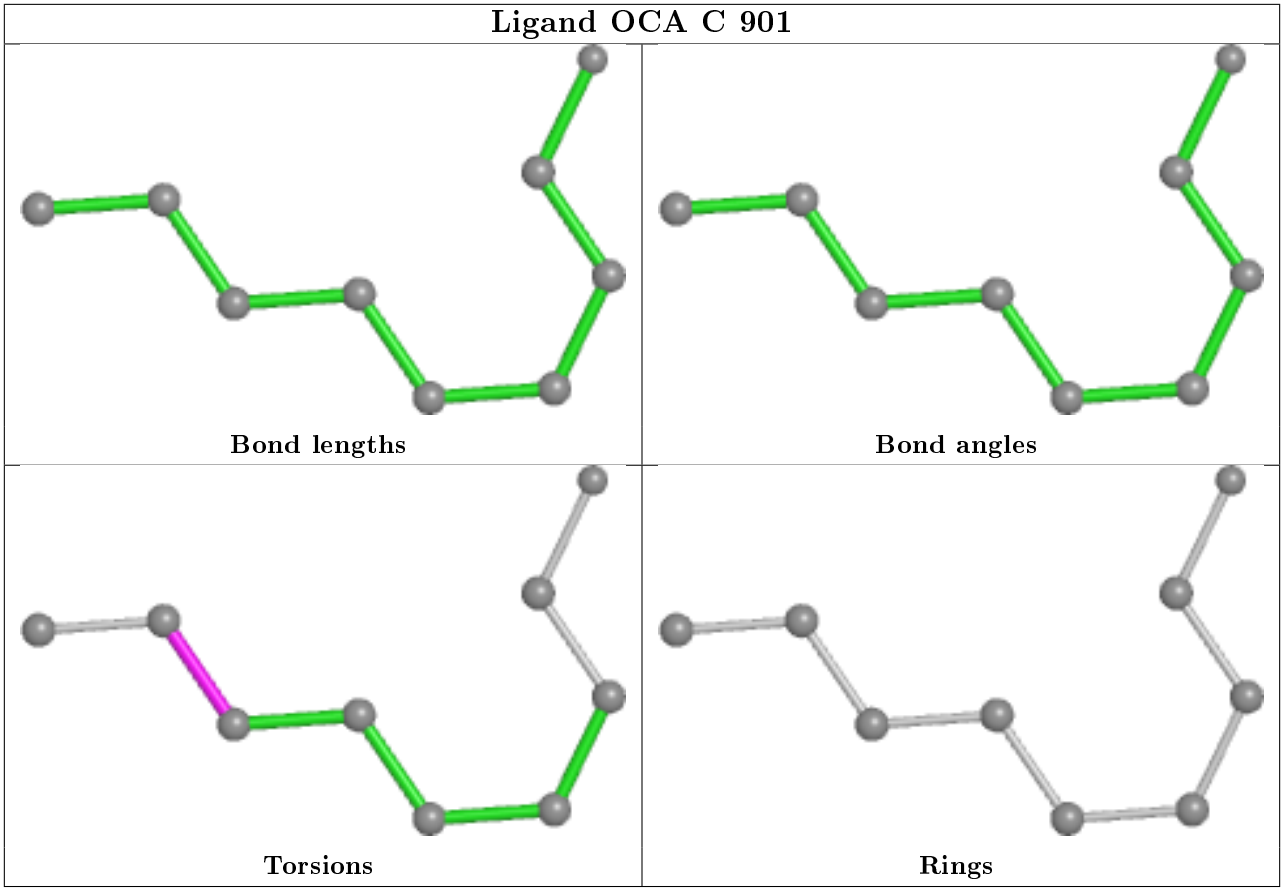


Ligand CO8 D 903



Ligand OCA D 902





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	852/852 (100%)	0.04	22 (2%) 56 57	43, 69, 118, 198	0
1	B	831/852 (97%)	0.30	78 (9%) 8 6	42, 73, 174, 212	0
1	C	847/852 (99%)	0.39	89 (10%) 6 4	45, 76, 173, 224	0
1	D	852/852 (100%)	0.02	30 (3%) 44 44	45, 68, 121, 185	0
All	All	3382/3408 (99%)	0.19	219 (6%) 18 17	42, 71, 161, 224	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	669	GLY	9.6
1	C	623	VAL	9.6
1	C	417	HIS	9.3
1	A	417	HIS	7.9
1	B	539	LEU	7.8
1	C	640	PRO	7.6
1	C	506	MET	7.5
1	C	624	GLY	7.2
1	C	539	LEU	7.0
1	D	665	LEU	6.6
1	B	542	ASP	6.4
1	B	663	GLU	6.1
1	C	418	ALA	6.1
1	B	601	LEU	6.0
1	B	625	LEU	5.9
1	B	710	ALA	5.8
1	C	656	ALA	5.7
1	C	508	LEU	5.6
1	D	417	HIS	5.5
1	B	630	CYS	5.5
1	B	640	PRO	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	546	PHE	5.4
1	B	532	VAL	5.4
1	C	661	PHE	5.3
1	B	667	GLN	5.3
1	B	546	PHE	5.3
1	B	538	LEU	5.2
1	B	744	LEU	5.1
1	C	504	ARG	5.0
1	C	622	ALA	4.9
1	B	418	ALA	4.9
1	D	671	PHE	4.7
1	C	415	THR	4.7
1	C	660	GLU	4.7
1	B	750	TRP	4.5
1	C	625	LEU	4.5
1	C	521	LEU	4.4
1	C	670	VAL	4.4
1	B	641	ALA	4.4
1	B	537	LEU	4.2
1	B	499	MET	4.2
1	B	647	ASP	4.2
1	C	416	ALA	4.1
1	B	417	HIS	4.1
1	A	416	ALA	4.1
1	C	665	LEU	4.1
1	A	418	ALA	4.1
1	B	662	VAL	4.1
1	C	728	ARG	4.0
1	B	534	VAL	4.0
1	C	672	ALA	4.0
1	B	500	GLY	4.0
1	B	541	THR	4.0
1	B	626	SER	3.9
1	B	605	TRP	3.9
1	C	541	THR	3.9
1	C	750	TRP	3.9
1	B	636	ALA	3.8
1	B	648	THR	3.8
1	C	696	GLN	3.8
1	C	649	VAL	3.8
1	B	635	PRO	3.8
1	B	668	GLU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	536	ASP	3.8
1	B	627	TRP	3.8
1	C	722	TRP	3.7
1	C	538	LEU	3.7
1	B	711	ARG	3.7
1	A	637	GLY	3.6
1	B	533	LYS	3.6
1	A	633	ARG	3.6
1	D	663	GLU	3.6
1	A	667	GLN	3.5
1	B	659	ASN	3.5
1	D	625	LEU	3.5
1	D	622	ALA	3.4
1	B	530	LEU	3.4
1	C	533	LYS	3.4
1	D	630	CYS	3.4
1	D	667	GLN	3.4
1	C	657	ALA	3.4
1	D	539	LEU	3.3
1	B	656	ALA	3.3
1	C	544	ARG	3.2
1	B	604	TYR	3.2
1	C	511	MET	3.2
1	B	666	LYS	3.2
1	B	628	GLU	3.2
1	B	638	VAL	3.2
1	A	665	LEU	3.2
1	C	730	SER	3.2
1	C	627	TRP	3.2
1	C	534	VAL	3.1
1	C	668	GLU	3.1
1	B	629	GLU	3.1
1	D	489	LYS	3.1
1	B	600	VAL	3.0
1	C	723	GLN	3.0
1	D	487	THR	3.0
1	C	632	GLN	3.0
1	B	508	LEU	3.0
1	B	722	TRP	3.0
1	B	551	HIS	2.9
1	C	601	LEU	2.9
1	C	721	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	551	HIS	2.9
1	C	666	LYS	2.9
1	B	544	ARG	2.9
1	C	713	LEU	2.9
1	B	526	ALA	2.9
1	B	685	TYR	2.9
1	C	612	ASP	2.8
1	D	629	GLU	2.8
1	B	713	LEU	2.8
1	C	501	THR	2.8
1	B	751	HIS	2.8
1	D	632	GLN	2.8
1	B	633	ARG	2.8
1	C	412	PRO	2.7
1	C	512	ARG	2.7
1	A	703	ARG	2.7
1	C	720	ALA	2.7
1	C	633	ARG	2.7
1	B	680	LEU	2.7
1	C	703	ARG	2.7
1	C	790	LYS	2.7
1	D	704	GLU	2.7
1	A	112	SER	2.7
1	D	661	PHE	2.7
1	B	603	ALA	2.6
1	D	664	GLN	2.6
1	B	527	VAL	2.6
1	B	545	THR	2.6
1	B	525	GLU	2.6
1	B	631	LYS	2.6
1	D	703	ARG	2.6
1	D	662	VAL	2.6
1	C	489	LYS	2.6
1	C	630	CYS	2.6
1	B	415	THR	2.6
1	B	649	VAL	2.6
1	D	696	GLN	2.5
1	B	637	GLY	2.5
1	C	631	LYS	2.5
1	C	503	TRP	2.5
1	A	669	GLY	2.5
1	C	653	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	670	VAL	2.5
1	B	665	LEU	2.5
1	D	111	VAL	2.5
1	C	526	ALA	2.5
1	C	604	TYR	2.5
1	C	525	GLU	2.5
1	C	474	GLY	2.5
1	C	113	GLY	2.5
1	B	535	SER	2.5
1	B	529	PRO	2.4
1	C	646	GLU	2.4
1	C	535	SER	2.4
1	B	487	THR	2.4
1	B	493	TRP	2.4
1	D	337	GLY	2.4
1	B	717	ILE	2.4
1	D	114	SER	2.4
1	A	662	VAL	2.4
1	C	605	TRP	2.4
1	C	611	LYS	2.4
1	D	627	TRP	2.4
1	A	629	GLU	2.4
1	C	663	GLU	2.4
1	C	635	PRO	2.4
1	B	669	GLY	2.3
1	D	728	ARG	2.3
1	A	111	VAL	2.3
1	C	699	LYS	2.3
1	A	668	GLU	2.3
1	C	487	THR	2.3
1	B	664	GLN	2.3
1	C	704	GLU	2.3
1	C	747	GLU	2.3
1	B	543	GLU	2.2
1	B	634	CYS	2.2
1	A	623	VAL	2.2
1	C	651	ILE	2.2
1	C	414	PRO	2.2
1	B	612	ASP	2.2
1	C	518	GLU	2.2
1	A	340	ALA	2.2
1	C	540	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	667	GLN	2.2
1	C	532	VAL	2.1
1	C	695	LEU	2.1
1	D	669	GLY	2.1
1	D	666	LYS	2.1
1	B	577	ILE	2.1
1	B	753	PRO	2.1
1	B	160	ALA	2.1
1	A	415	THR	2.1
1	B	550	VAL	2.1
1	A	638	VAL	2.1
1	D	137	ARG	2.1
1	C	137	ARG	2.1
1	C	634	CYS	2.1
1	B	632	GLN	2.1
1	C	158	ASP	2.1
1	C	505	GLY	2.1
1	C	745	PHE	2.1
1	D	113	GLY	2.1
1	C	682	PHE	2.0
1	A	413	ALA	2.0
1	A	158	ASP	2.0
1	C	788	ASP	2.0
1	A	625	LEU	2.0
1	C	537	LEU	2.0
1	B	504	ARG	2.0
1	A	685	TYR	2.0
1	C	156	ALA	2.0
1	C	671	PHE	2.0
1	D	701	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

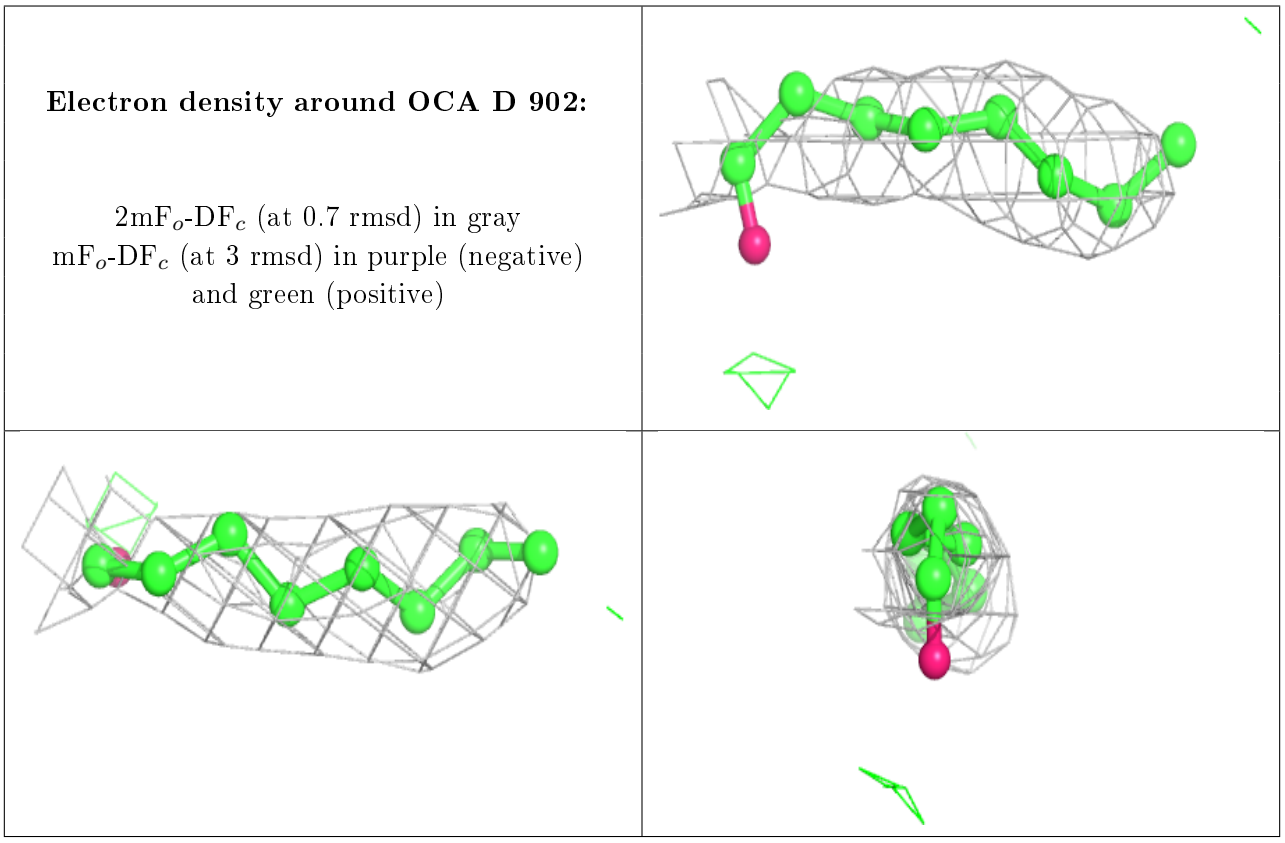
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	OCA	D	902	9/10	0.92	0.41	85,91,124,156	0
3	CO8	D	903	57/57	0.93	0.26	90,126,150,184	0
2	OCA	D	901	9/10	0.97	0.22	61,63,69,74	0
2	OCA	B	901	9/10	0.97	0.23	67,77,89,95	0
2	OCA	A	901	9/10	0.98	0.26	59,62,72,78	0
2	OCA	C	901	9/10	0.98	0.24	54,55,67,72	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.

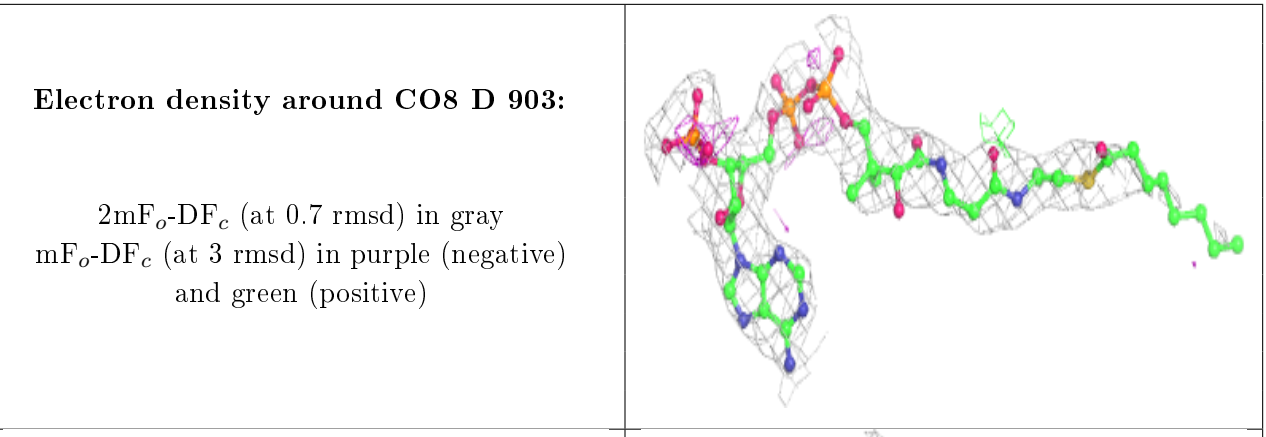
Electron density around OCA D 902:

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



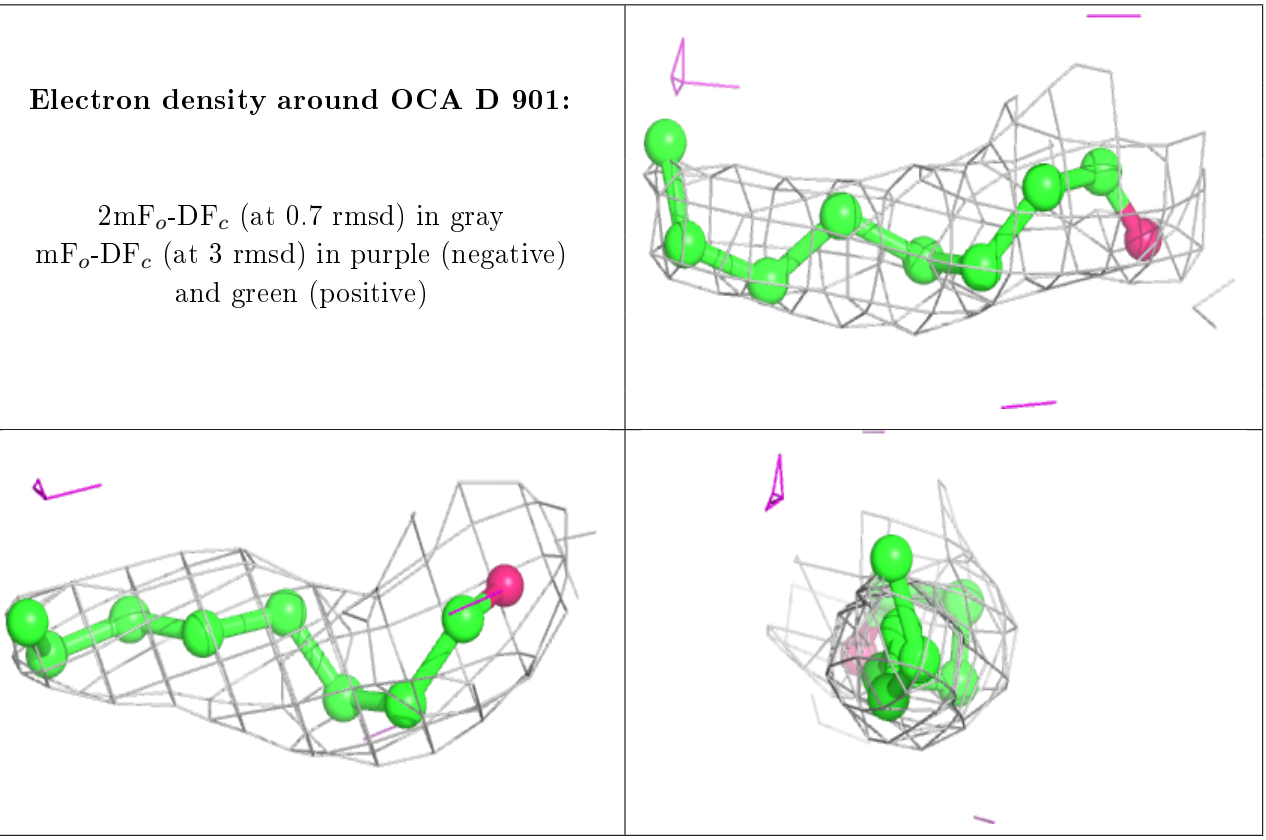
Electron density around CO8 D 903:

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



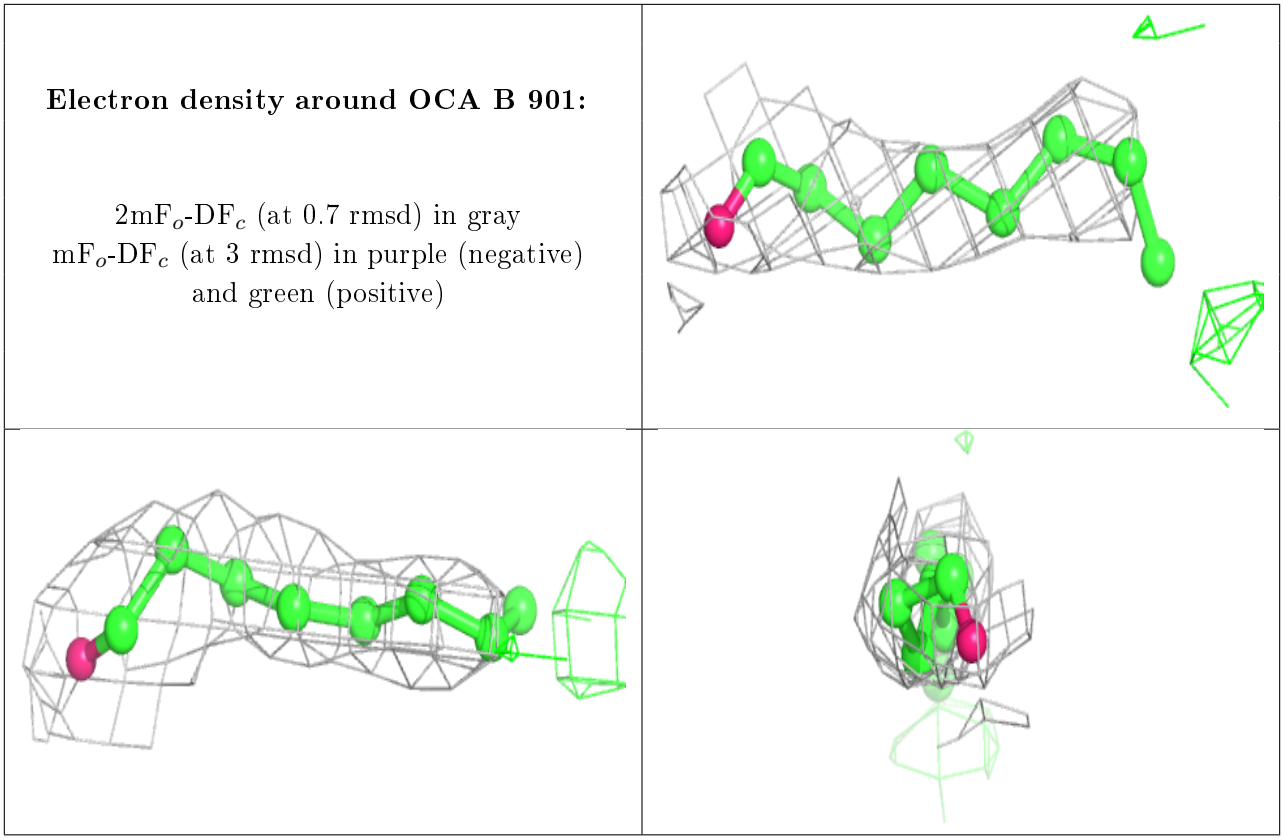
Electron density around OCA D 901:

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



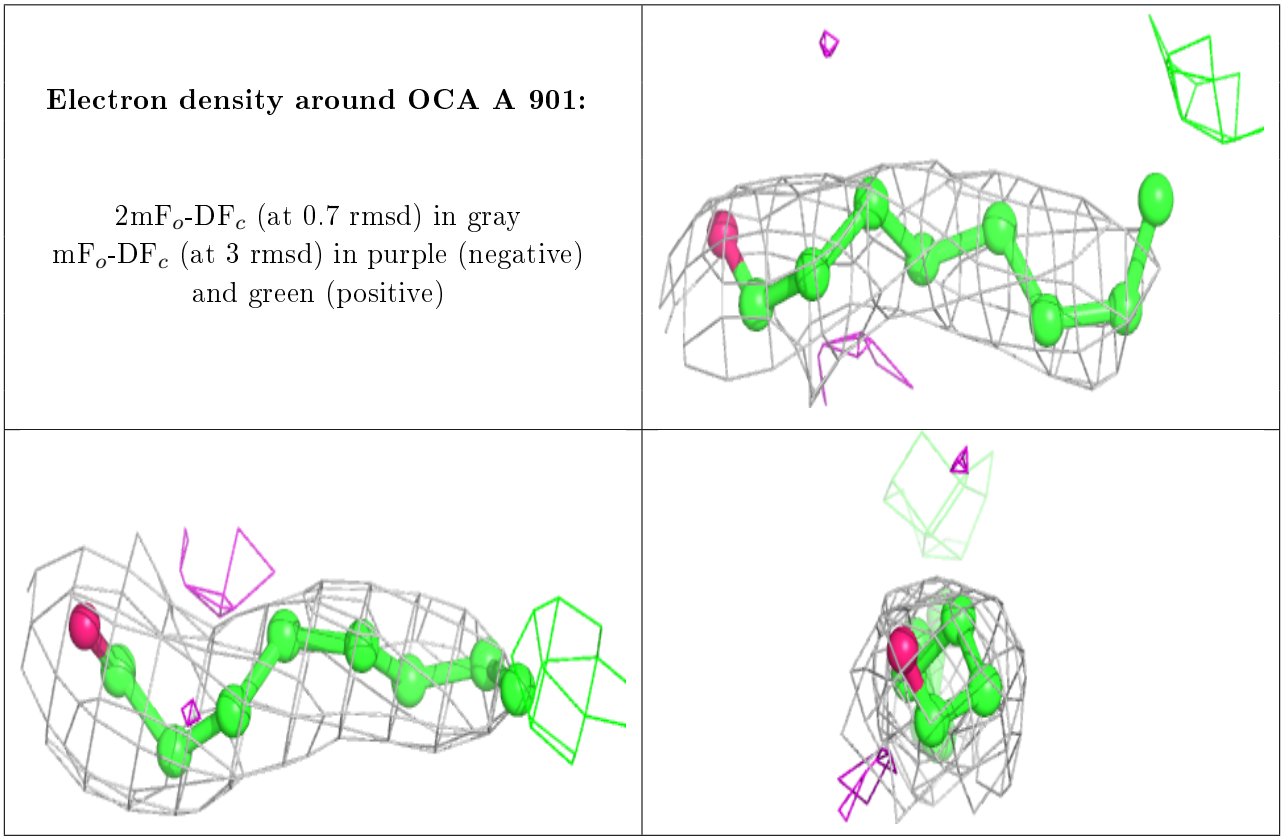
Electron density around OCA B 901:

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



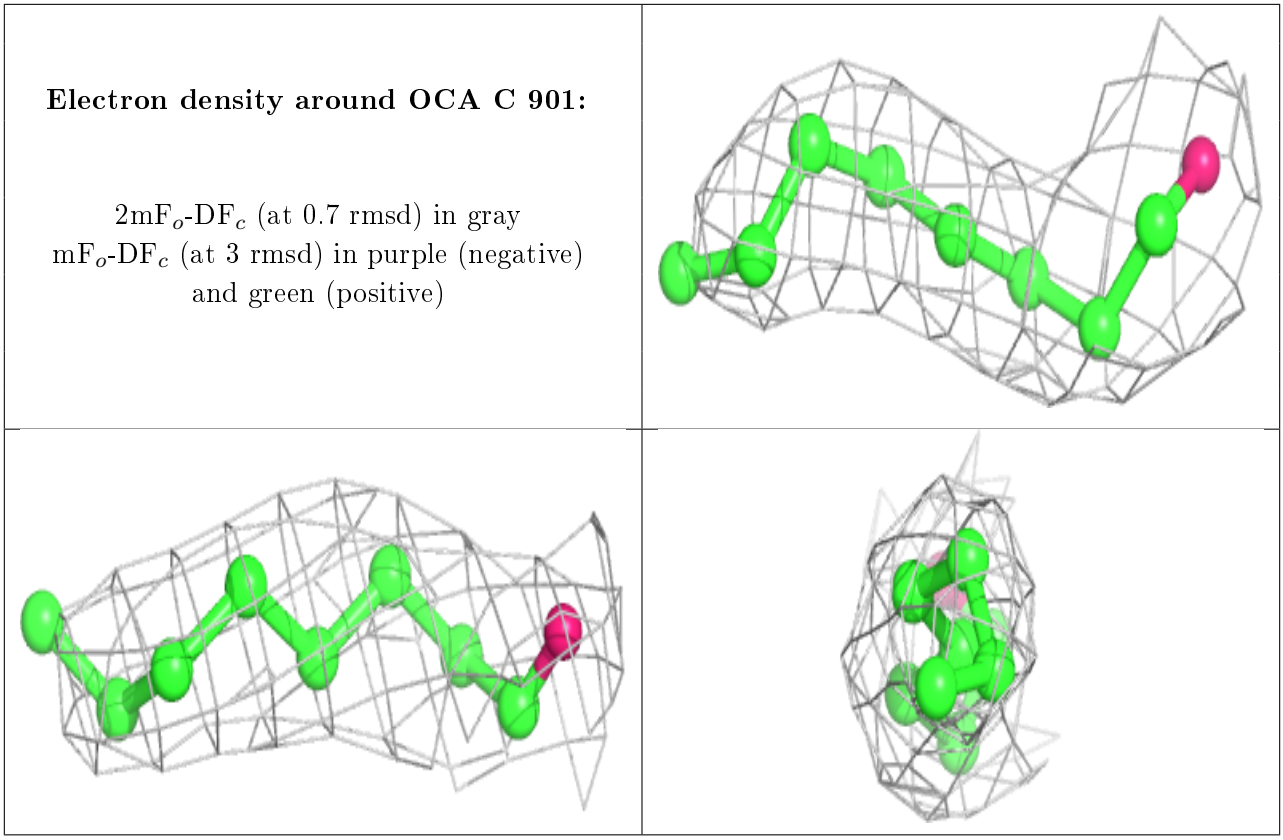
Electron density around OCA A 901:

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



Electron density around OCA C 901:

$2mF_o$-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.