Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 04:27 PM EST

PDB ID	:	1LWJ
Title	:	CRYSTAL STRUCTURE OF T. MARITIMA 4-ALPHA-GLUCANOTRANSFERASE/ACARBOSE COMPLEX
Authors	:	Roujeinikova, A.; Raasch, C.; Sedelnikova, S.; Liebl, W.; Rice, D.W.
Deposited on	:	2002-05-31
Resolution	:	2.50 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:

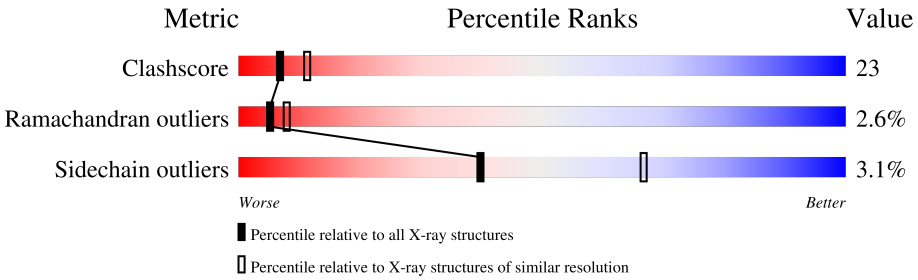
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	441	55% 42% .
1	B	441	51% 46% .

2 Entry composition

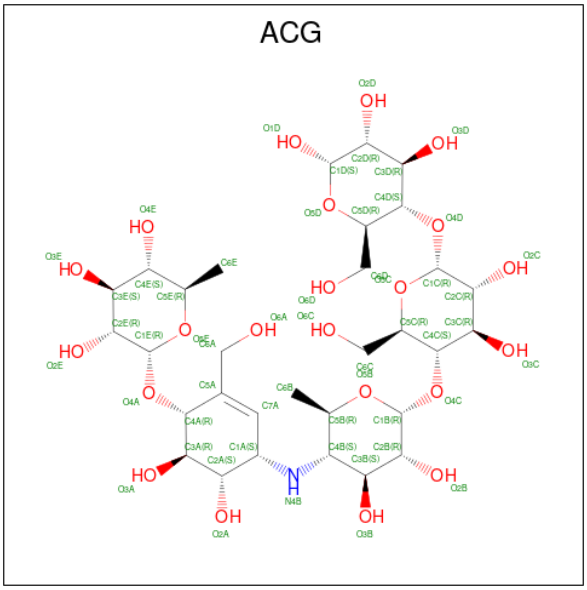
There are 4 unique types of molecules in this entry. The entry contains 7463 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-ALPHA-GLUCANOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3656	2380	604	657	15			
1	B	441	Total	C	N	O	S	0	0	0
			3656	2380	604	657	15			

- Molecule 2 is MODIFIED ACARBOSE PENTASACCHARIDE (three-letter code: ACG) (formula: $C_{31}H_{53}NO_{22}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			54	31	1	22		
2	B	1	Total	C	N	O	0	0
			54	31	1	22		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0
4	B	24	Total O 24 24	0	0

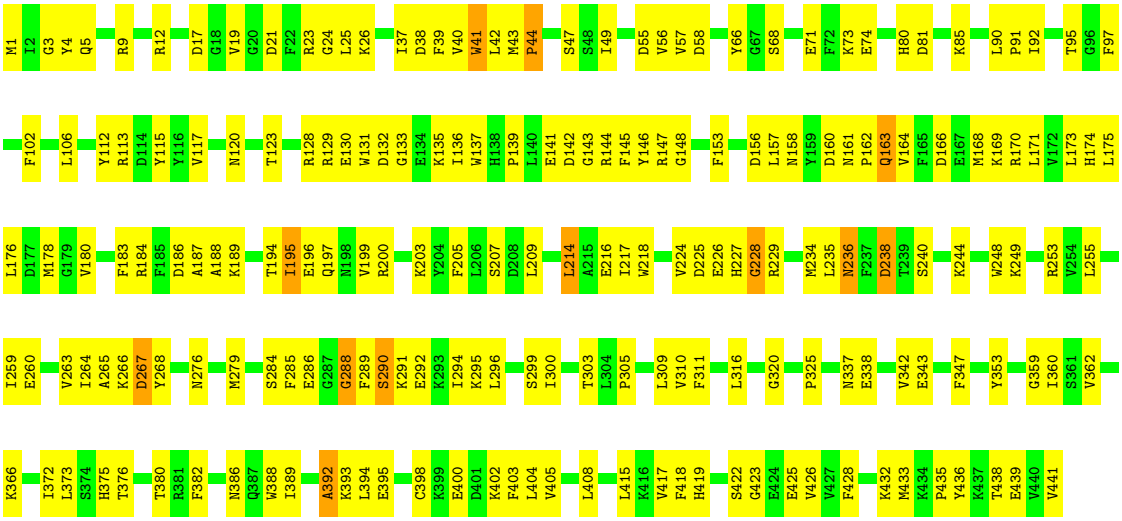
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

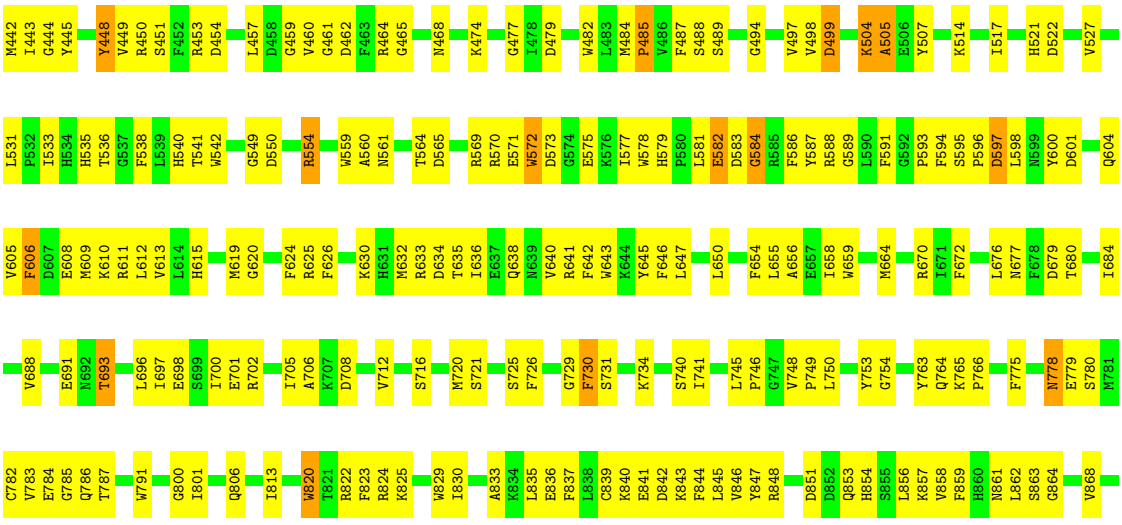
• Molecule 1: 4-ALPHA-GLUCANOTRANSFERASE

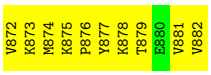
Chain A:



• Molecule 1: 4-ALPHA-GLUCANOTRANSFERASE

Chain B:




V872
K873
M874
K875
P876
Y877
K878
T879
E880
V881
V882

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	94.54Å 181.35Å 197.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.225 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7463	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACG, CA

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	0.45	0/3769	0.66	0/5096
1	B	0.47	0/3769	0.68	1/5096 (0.0%)
All	All	0.46	0/7538	0.67	1/10192 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	448	TYR	N-CA-C	-5.07	97.30	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3656	0	3506	157	1
1	B	3656	0	3503	183	0
2	A	54	0	53	4	0
2	B	54	0	53	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	17	0	0	1	0
4	B	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7463	0	7115	337	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (337) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:ILE:HD12	1:B:813:ILE:H	1.28	0.96
1:A:129:ARG:HD2	1:A:132:ASP:OD2	1.68	0.92
1:B:839:CYS:HB3	1:B:846:VAL:HB	1.49	0.92
1:A:224:VAL:HG13	1:A:234:MET:HE2	1.54	0.89
1:A:229:ARG:HG2	1:A:267:ASP:HB2	1.57	0.84
1:B:610:LYS:HE2	1:B:646:PHE:O	1.83	0.78
1:B:740:SER:HA	1:B:820:TRP:NE1	1.99	0.76
1:B:635:THR:HB	1:B:638:GLN:HG3	1.67	0.76
1:B:861:ASN:O	1:B:877:TYR:HA	1.85	0.75
1:B:836:GLU:OE1	1:B:848:ARG:NH1	2.21	0.74
1:A:372:ILE:HD12	1:A:372:ILE:N	2.03	0.73
1:B:858:VAL:HG22	1:B:881:VAL:HG12	1.69	0.73
1:A:372:ILE:HD12	1:A:372:ILE:H	1.53	0.72
1:B:830:ILE:HA	1:B:833:ALA:HB2	1.71	0.71
1:A:394:LEU:HD23	1:A:395:GLU:N	2.05	0.71
1:B:700:ILE:HD13	1:B:745:LEU:HD21	1.73	0.71
1:A:90:LEU:HG	1:A:92:ILE:HG23	1.71	0.71
1:B:656:ALA:HB2	1:B:672:PHE:CE2	2.26	0.71
1:B:538:PHE:HB2	1:B:594:PHE:HA	1.73	0.70
1:A:284:SER:HA	1:A:288:GLY:HA2	1.73	0.70
1:B:868:VAL:HG13	1:B:873:LYS:N	2.07	0.69
1:A:200:ARG:HH11	1:A:203:LYS:HE2	1.57	0.69
1:A:214:LEU:HD22	1:A:235:LEU:HG	1.75	0.68
1:B:656:ALA:HB2	1:B:672:PHE:CD2	2.28	0.68
1:A:425:GLU:OE1	1:A:432:LYS:HB3	1.92	0.68
1:A:12:ARG:HD3	1:A:24:GLY:O	1.92	0.68
1:B:593:PRO:HG2	1:B:594:PHE:CE1	2.29	0.68
1:A:400:GLU:HG3	1:A:403:PHE:CZ	2.28	0.68
1:B:868:VAL:HG22	1:B:873:LYS:CB	2.24	0.68
1:A:4:TYR:HB2	1:A:37:ILE:HD12	1.75	0.67
1:A:200:ARG:NH1	1:A:203:LYS:HE2	2.10	0.67
1:A:402:LYS:HD3	1:A:422:SER:HB3	1.74	0.67
1:B:813:ILE:H	1:B:813:ILE:CD1	2.06	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:THR:CG2	1:B:862:LEU:HD22	2.25	0.67
1:B:726:PHE:HD2	1:B:730:PHE:CE2	2.14	0.66
1:A:229:ARG:HG2	1:A:267:ASP:CB	2.25	0.66
1:B:676:LEU:HD23	1:B:712:VAL:HB	1.76	0.66
1:B:453:ARG:HD3	1:B:465:GLY:O	1.95	0.66
1:A:228:GLY:HA2	1:A:234:MET:HG3	1.78	0.65
1:A:296:LEU:O	1:A:300:ILE:HG13	1.96	0.65
1:A:176:LEU:HD23	1:A:180:VAL:O	1.96	0.65
1:B:868:VAL:HG13	1:B:872:VAL:C	2.17	0.65
1:A:136:ILE:HD12	1:A:147:ARG:HD2	1.77	0.65
1:B:861:ASN:ND2	1:B:876:PRO:HA	2.12	0.65
1:B:654:PHE:O	1:B:672:PHE:HB3	1.96	0.65
1:B:659:TRP:HB3	2:B:988:ACG:H3C	1.78	0.64
1:B:864:GLY:HA2	1:B:876:PRO:HB3	1.79	0.64
1:B:531:LEU:HG	1:B:533:ILE:HG23	1.80	0.64
1:B:571:GLU:HG2	1:B:572:TRP:HE3	1.62	0.64
1:B:444:GLY:C	1:B:750:LEU:HD12	2.18	0.64
1:A:169:LYS:HE2	1:A:205:PHE:O	1.97	0.64
1:A:418:PHE:HB3	1:A:433:MET:HG2	1.79	0.64
1:A:73:LYS:HE2	1:A:178:MET:HG3	1.80	0.63
1:A:290:SER:OG	1:A:292:GLU:HG2	1.97	0.63
1:A:195:ILE:O	1:A:199:VAL:HG23	1.98	0.63
1:B:701:GLU:HA	1:B:705:ILE:HD12	1.78	0.63
1:A:184:ARG:NH1	1:A:186:ASP:HB2	2.14	0.63
1:B:497:VAL:HG12	1:B:499:ASP:H	1.63	0.63
1:B:693:THR:HG22	1:B:862:LEU:HD22	1.80	0.62
1:A:236:ASN:HD21	1:A:238:ASP:HB3	1.64	0.62
1:A:386:ASN:HD22	1:A:388:TRP:HE1	1.45	0.62
1:B:577:ILE:HG22	1:B:588:ARG:CG	2.30	0.62
1:B:632:MET:O	1:B:633:ARG:HD2	2.00	0.62
1:A:112:TYR:O	1:A:115:TYR:HB2	2.00	0.61
1:B:464:ARG:O	1:B:468:ASN:ND2	2.32	0.61
1:A:372:ILE:H	1:A:372:ILE:CD1	2.13	0.60
1:B:450:ARG:HG3	1:B:460:VAL:HG13	1.83	0.60
1:A:255:LEU:O	1:A:259:ILE:HG13	2.00	0.60
1:B:488:SER:O	1:B:498:VAL:HG22	2.01	0.60
1:A:403:PHE:CE1	1:A:426:VAL:HG21	2.36	0.60
1:B:578:TRP:CZ2	1:B:588:ARG:HD3	2.37	0.60
1:B:670:ARG:HB2	1:B:708:ASP:OD2	2.01	0.60
1:A:144:ARG:C	1:A:145:PHE:HD1	2.04	0.60
1:B:517:ILE:HD13	1:B:527:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:GLU:HA	1:B:862:LEU:HB3	1.82	0.60
1:B:697:ILE:HD11	1:B:845:LEU:CD1	2.32	0.60
1:A:303:THR:HG21	1:A:438:THR:HG21	1.84	0.60
1:B:554:ARG:HG3	1:B:554:ARG:HH11	1.67	0.60
1:B:696:LEU:O	1:B:700:ILE:HG13	2.02	0.60
1:A:173:LEU:CD2	1:A:209:LEU:HD21	2.31	0.59
1:A:214:LEU:CD2	1:A:235:LEU:HG	2.32	0.59
1:A:337:ASN:ND2	1:A:342:VAL:HB	2.16	0.59
1:A:120:ASN:HB3	1:A:123:THR:HG23	1.85	0.59
1:B:632:MET:HG3	1:B:643:TRP:CZ2	2.37	0.59
1:B:859:PHE:HE2	1:B:882:VAL:HG23	1.67	0.59
1:B:448:TYR:CE2	1:B:450:ARG:HB3	2.37	0.59
1:A:153:PHE:CZ	1:B:780:SER:HB2	2.38	0.59
1:A:217:ILE:HD12	1:A:234:MET:CE	2.33	0.58
1:B:820:TRP:HA	1:B:820:TRP:CE3	2.38	0.58
1:B:691:GLU:OE2	1:B:877:TYR:HE1	1.86	0.58
1:A:189:LYS:HB2	1:A:217:ILE:HA	1.84	0.58
1:A:240:SER:O	1:A:244:LYS:HE2	2.04	0.58
1:B:442:MET:HA	1:B:479:ASP:OD1	2.04	0.58
1:B:636:ILE:O	1:B:640:VAL:HG23	2.04	0.58
1:A:171:LEU:O	1:A:174:HIS:HB3	2.04	0.58
1:B:655:LEU:HD11	1:B:676:LEU:HG	1.86	0.58
1:A:216:GLU:OE1	2:A:989:ACG:H1A	2.04	0.57
1:A:102:PHE:O	1:A:106:LEU:HG	2.04	0.57
1:A:309:LEU:HD13	1:A:310:VAL:N	2.18	0.57
1:A:3:GLY:C	1:A:309:LEU:HD22	2.24	0.57
1:A:21:ASP:HB2	1:A:66:TYR:O	2.04	0.57
1:A:423:GLY:HA2	1:A:435:PRO:HB3	1.87	0.57
1:B:570:ARG:NH1	1:B:573:ASP:OD1	2.38	0.57
1:B:851:ASP:OD2	1:B:854:HIS:N	2.36	0.56
1:B:754:GLY:HA2	1:B:775:PHE:HE1	1.68	0.56
1:A:128:ARG:HD3	1:A:135:LYS:HA	1.88	0.56
1:A:418:PHE:HB2	1:A:439:GLU:HB2	1.87	0.56
1:B:746:PRO:HA	1:B:830:ILE:O	2.05	0.56
1:B:835:LEU:CD1	1:B:847:TYR:HB2	2.35	0.56
1:B:859:PHE:HB3	1:B:874:MET:SD	2.46	0.56
1:B:822:ARG:O	1:B:825:LYS:HB3	2.05	0.56
1:A:139:PRO:HB3	1:A:145:PHE:CZ	2.41	0.56
1:B:851:ASP:OD1	1:B:854:HIS:HD2	1.89	0.56
1:A:263:VAL:HG11	1:A:305:PRO:HG2	1.87	0.56
1:A:49:ILE:O	1:B:459:GLY:HA3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:CD	1:A:196:GLU:H	2.09	0.55
1:B:778:ASN:HD21	1:B:782:CYS:H	1.54	0.55
1:A:117:VAL:O	1:A:146:TYR:HA	2.06	0.55
1:A:194:THR:HG23	1:A:197:GLN:OE1	2.07	0.55
1:B:630:LYS:HB2	1:B:658:ILE:HG23	1.88	0.55
1:A:184:ARG:HH11	1:A:186:ASP:HB2	1.71	0.55
1:A:200:ARG:O	1:A:203:LYS:HB3	2.07	0.55
1:A:229:ARG:HG3	1:A:229:ARG:HH11	1.72	0.55
1:A:56:VAL:HG12	1:A:58:ASP:H	1.72	0.55
1:A:260:GLU:HA	1:A:264:ILE:HD12	1.87	0.55
1:A:195:ILE:HD11	1:A:226:GLU:OE2	2.07	0.54
1:A:161:ASN:OD1	1:A:163:GLN:HB2	2.06	0.54
1:B:448:TYR:CZ	1:B:450:ARG:HB3	2.43	0.54
1:A:338:GLU:OE2	1:A:359:GLY:N	2.41	0.54
1:A:372:ILE:N	1:A:372:ILE:CD1	2.71	0.54
1:B:577:ILE:HG22	1:B:588:ARG:HG3	1.89	0.54
1:B:604:GLN:O	1:B:608:GLU:HB2	2.08	0.54
1:B:868:VAL:HG22	1:B:873:LYS:HB3	1.89	0.54
1:A:402:LYS:HB3	1:A:422:SER:HB3	1.89	0.54
1:B:454:ASP:O	1:B:785:GLY:HA2	2.08	0.53
1:B:514:LYS:HD3	1:B:619:MET:HG3	1.89	0.53
1:B:868:VAL:HG22	1:B:873:LYS:HA	1.91	0.53
1:A:5:GLN:HB3	1:A:311:PHE:HA	1.91	0.53
1:A:168:MET:O	1:A:171:LEU:HB3	2.08	0.53
1:B:589:GLY:HA2	1:B:597:ASP:OD1	2.09	0.53
1:B:655:LEU:HD13	1:B:712:VAL:HG21	1.90	0.53
1:A:158:ASN:OD1	1:A:160:ASP:HB3	2.09	0.53
1:A:405:VAL:HG13	1:A:417:VAL:O	2.09	0.53
1:B:449:VAL:O	1:B:461:GLY:HA3	2.09	0.53
1:B:559:TRP:CZ3	1:B:587:TYR:HB3	2.44	0.52
1:B:647:LEU:HD23	1:B:650:LEU:HD12	1.91	0.52
1:A:41:TRP:CD1	1:A:41:TRP:C	2.81	0.52
1:B:579:HIS:O	1:B:586:PHE:HA	2.09	0.52
1:B:843:LYS:HB3	1:B:863:SER:HB3	1.91	0.52
1:A:224:VAL:CG1	1:A:234:MET:HE2	2.33	0.52
1:A:173:LEU:HD23	1:A:209:LEU:HD21	1.92	0.52
1:B:521:HIS:HE1	1:B:620:GLY:O	1.92	0.52
1:B:698:GLU:O	1:B:702:ARG:HB2	2.09	0.52
1:A:148:GLY:HA2	1:A:156:ASP:OD1	2.10	0.52
1:B:571:GLU:HG2	1:B:572:TRP:CE3	2.44	0.51
1:B:578:TRP:CZ3	1:B:588:ARG:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:PHE:HD2	1:B:730:PHE:HE2	1.58	0.51
1:A:402:LYS:HD3	1:A:422:SER:CB	2.40	0.51
1:B:680:THR:O	1:B:684:ILE:HG13	2.11	0.51
1:A:23:ARG:O	1:A:26:LYS:HB3	2.10	0.51
1:A:291:LYS:HE3	1:A:372:ILE:CD1	2.41	0.51
1:A:376:THR:O	1:A:380:THR:HG23	2.11	0.51
1:A:418:PHE:HE1	1:A:428:PHE:HD2	1.58	0.51
1:A:92:ILE:HG22	1:A:168:MET:HE1	1.94	0.50
1:A:263:VAL:CG1	1:A:305:PRO:HG2	2.41	0.50
1:A:402:LYS:CD	1:A:422:SER:HB3	2.41	0.50
1:B:542:TRP:CH2	1:B:608:GLU:HG2	2.47	0.50
1:B:462:ASP:HB2	1:B:507:TYR:O	2.12	0.50
1:A:141:GLU:C	1:A:143:GLY:H	2.15	0.50
1:B:754:GLY:HA2	1:B:775:PHE:CE1	2.46	0.50
1:A:393:LYS:O	1:A:408:LEU:HA	2.11	0.50
1:A:398:CYS:O	1:A:404:LEU:HD12	2.11	0.50
1:B:613:VAL:HG13	1:B:624:PHE:CE2	2.47	0.50
1:A:217:ILE:HD12	1:A:234:MET:HE1	1.94	0.49
1:A:128:ARG:HD2	1:A:135:LYS:N	2.27	0.49
1:B:579:HIS:CE1	1:B:593:PRO:HD3	2.48	0.49
1:B:835:LEU:HD12	1:B:836:GLU:N	2.26	0.49
1:B:868:VAL:HA	1:B:873:LYS:HA	1.94	0.49
1:A:128:ARG:HB3	1:A:133:GLY:C	2.33	0.49
1:B:786:GLN:HE21	1:B:787:THR:H	1.58	0.49
1:A:342:VAL:HG22	1:A:343:GLU:N	2.27	0.49
1:A:418:PHE:O	1:A:438:THR:HA	2.12	0.49
1:B:857:LYS:O	1:B:881:VAL:HA	2.11	0.49
1:A:25:LEU:HD21	1:A:42:LEU:HD11	1.95	0.48
1:B:498:VAL:O	1:B:499:ASP:HB2	2.13	0.48
1:B:835:LEU:HD11	1:B:847:TYR:HB2	1.95	0.48
1:B:875:LYS:HB2	1:B:878:LYS:HG3	1.95	0.48
1:A:284:SER:CA	1:A:288:GLY:HA2	2.41	0.48
1:B:716:SER:HA	1:B:720:MET:HE1	1.95	0.48
1:B:448:TYR:HD2	1:B:451:SER:HB2	1.79	0.48
1:A:173:LEU:HD21	1:A:209:LEU:HD21	1.95	0.48
1:B:830:ILE:HA	1:B:833:ALA:CB	2.43	0.48
1:B:861:ASN:HD22	1:B:876:PRO:HA	1.79	0.48
1:B:630:LYS:HB2	1:B:658:ILE:HA	1.97	0.47
1:B:626:PHE:CD2	1:B:643:TRP:CH2	3.02	0.47
1:B:765:LYS:HB3	1:B:766:PRO:HA	1.95	0.47
1:B:841:GLU:HG3	1:B:844:PHE:HE1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:THR:CB	1:B:638:GLN:HG3	2.42	0.47
1:B:443:ILE:HD12	1:B:477:GLY:O	2.14	0.47
1:B:679:ASP:OD2	1:B:702:ARG:HD2	2.15	0.47
1:B:837:PHE:HB2	1:B:840:LYS:HE3	1.97	0.47
1:B:560:ALA:HB2	1:B:578:TRP:CE3	2.50	0.47
1:A:228:GLY:HA2	1:A:234:MET:CG	2.44	0.47
1:B:697:ILE:HD11	1:B:845:LEU:HD11	1.97	0.46
1:B:868:VAL:HG13	1:B:873:LYS:CA	2.44	0.46
1:A:320:GLY:HA2	1:A:353:TYR:CD1	2.50	0.46
1:B:448:TYR:HB2	1:B:484:MET:SD	2.54	0.46
1:B:598:LEU:HD11	1:B:609:MET:HE1	1.96	0.46
1:B:778:ASN:H	1:B:778:ASN:HD22	1.63	0.46
1:A:137:TRP:CH2	1:A:147:ARG:HB2	2.51	0.46
1:A:362:VAL:O	1:A:366:LYS:HB2	2.16	0.46
1:A:9:ARG:HG3	1:A:19:VAL:HG13	1.97	0.46
1:A:17:ASP:HA	1:B:489:SER:O	2.16	0.46
1:A:160:ASP:O	1:A:162:PRO:HD3	2.14	0.46
1:B:612:LEU:O	1:B:615:HIS:HB3	2.16	0.46
1:A:295:LYS:HB3	1:A:375:HIS:NE2	2.31	0.46
1:B:829:TRP:HH2	1:B:856:LEU:HB2	1.80	0.46
1:A:97:PHE:HB2	1:A:153:PHE:HA	1.98	0.46
1:A:296:LEU:HD22	1:A:436:TYR:HA	1.98	0.46
1:B:641:ARG:O	1:B:645:TYR:CD2	2.70	0.46
1:B:841:GLU:HB2	1:B:844:PHE:CE1	2.51	0.46
1:B:535:HIS:HB3	1:B:597:ASP:HA	1.97	0.45
1:B:606:PHE:C	1:B:606:PHE:CD2	2.90	0.45
1:B:485:PRO:HB3	1:B:494:GLY:O	2.15	0.45
1:B:632:MET:HG3	1:B:642:PHE:HE2	1.81	0.45
1:B:655:LEU:HD11	1:B:676:LEU:CD2	2.46	0.45
1:A:394:LEU:HD23	1:A:394:LEU:C	2.36	0.45
1:B:600:TYR:CE1	1:B:605:VAL:HG12	2.52	0.45
1:A:175:LEU:O	1:A:178:MET:HB3	2.17	0.45
1:B:846:VAL:HA	1:B:858:VAL:O	2.17	0.45
1:A:291:LYS:HE3	1:A:372:ILE:HD11	1.98	0.45
1:A:316:LEU:HD23	1:A:373:LEU:HB2	1.99	0.45
1:A:43:MET:HB3	1:A:44:PRO:HD2	1.99	0.45
1:A:55:ASP:OD1	1:A:55:ASP:N	2.50	0.45
1:B:573:ASP:OD2	1:B:573:ASP:C	2.55	0.45
1:B:540:HIS:ND1	1:B:541:THR:N	2.65	0.45
1:B:693:THR:HG23	1:B:862:LEU:HD22	1.96	0.45
1:B:847:TYR:CE1	1:B:858:VAL:HB	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:HIS:O	1:A:228:GLY:C	2.55	0.44
2:A:989:ACG:H6D1	2:A:989:ACG:C1C	2.47	0.44
1:A:47:SER:O	1:A:57:VAL:HG22	2.17	0.44
1:A:130:GLU:HG3	1:A:131:TRP:HE3	1.82	0.44
1:B:779:GLU:OE2	1:B:800:GLY:N	2.44	0.44
1:A:266:LYS:C	1:A:268:TYR:H	2.20	0.44
1:A:303:THR:OG1	1:A:419:HIS:CE1	2.70	0.44
1:A:217:ILE:HD12	1:A:234:MET:HE3	1.98	0.44
1:A:337:ASN:HD21	1:A:342:VAL:HB	1.81	0.44
1:B:626:PHE:CD2	1:B:643:TRP:HH2	2.36	0.44
1:B:684:ILE:O	1:B:688:VAL:HG23	2.18	0.44
1:B:864:GLY:CA	1:B:876:PRO:HB3	2.47	0.44
1:A:248:TRP:CE3	1:A:249:LYS:HG3	2.53	0.44
1:A:299:SER:O	1:A:303:THR:HG23	2.17	0.44
1:B:783:VAL:HG13	1:B:783:VAL:O	2.17	0.44
1:A:236:ASN:ND2	1:A:238:ASP:HB3	2.31	0.44
1:B:445:TYR:CZ	1:B:753:TYR:HA	2.53	0.44
1:B:868:VAL:HG22	1:B:873:LYS:CA	2.47	0.44
1:B:569:ARG:HH11	1:B:575:GLU:HA	1.83	0.44
1:B:700:ILE:HG21	1:B:835:LEU:HD21	1.99	0.44
1:A:91:PRO:HA	1:A:186:ASP:HB3	1.98	0.43
1:A:95:THR:HG23	1:A:157:LEU:HD21	2.00	0.43
1:A:285:PHE:O	1:A:286:GLU:HB2	2.17	0.43
1:B:697:ILE:HD11	1:B:845:LEU:HD13	1.99	0.43
1:A:389:ILE:HA	1:A:392:ALA:HB2	2.00	0.43
1:B:725:SER:HA	1:B:729:GLY:CA	2.48	0.43
1:A:184:ARG:NH1	1:A:186:ASP:CB	2.80	0.43
1:B:549:GLY:O	1:B:550:ASP:C	2.56	0.43
1:B:820:TRP:HA	1:B:820:TRP:HE3	1.81	0.43
1:B:487:PHE:CE2	1:B:531:LEU:HD12	2.53	0.43
1:B:720:MET:C	1:B:763:TYR:HB2	2.39	0.43
1:A:144:ARG:C	1:A:145:PHE:CD1	2.89	0.43
1:A:284:SER:HA	1:A:288:GLY:CA	2.45	0.43
1:B:691:GLU:OE2	1:B:877:TYR:CE1	2.68	0.43
1:A:102:PHE:CE2	1:A:106:LEU:HD21	2.53	0.43
1:A:200:ARG:HH11	1:A:203:LYS:CE	2.29	0.43
1:B:454:ASP:OD2	1:B:457:LEU:HA	2.18	0.43
1:B:570:ARG:HH21	1:B:591:PHE:HA	1.83	0.43
1:B:630:LYS:HG3	1:B:664:MET:CE	2.48	0.43
1:A:74:GLU:O	1:A:74:GLU:HG2	2.17	0.43
1:A:342:VAL:CG2	1:A:343:GLU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:CYS:HB3	1:A:405:VAL:HB	2.00	0.43
1:A:186:ASP:O	1:A:187:ALA:HB3	2.19	0.43
1:B:748:VAL:HA	1:B:749:PRO:HD2	1.94	0.43
1:A:158:ASN:O	1:A:164:VAL:HG21	2.19	0.42
1:B:561:ASN:HB3	1:B:564:THR:OG1	2.19	0.42
1:B:601:ASP:OD2	1:B:633:ARG:NH2	2.51	0.42
1:B:564:THR:HG21	1:B:578:TRP:CZ2	2.54	0.42
1:B:581:LEU:O	1:B:583:ASP:N	2.52	0.42
1:A:290:SER:O	1:A:294:ILE:HG13	2.19	0.42
1:B:691:GLU:OE1	1:B:863:SER:HA	2.19	0.42
1:B:778:ASN:HD22	1:B:778:ASN:N	2.17	0.42
1:B:801:ILE:HA	1:B:806:GLN:HE21	1.83	0.42
1:A:386:ASN:ND2	1:A:388:TRP:HE1	2.14	0.42
1:B:813:ILE:HD12	1:B:813:ILE:N	2.12	0.42
1:B:859:PHE:O	1:B:879:THR:HA	2.19	0.42
1:B:697:ILE:O	1:B:701:GLU:HB2	2.19	0.42
1:A:218:TRP:NE1	2:A:989:ACG:H5D	2.34	0.42
1:A:433:MET:HA	1:A:439:GLU:OE1	2.20	0.42
1:A:225:ASP:O	1:A:229:ARG:NH1	2.53	0.42
1:B:521:HIS:CE1	1:B:620:GLY:O	2.72	0.42
1:B:572:TRP:CG	1:B:573:ASP:N	2.88	0.41
1:A:168:MET:O	1:A:171:LEU:N	2.53	0.41
1:B:763:TYR:O	1:B:764:GLN:HB3	2.20	0.41
1:B:859:PHE:HE2	1:B:882:VAL:CG2	2.31	0.41
1:A:1:MET:HA	1:A:38:ASP:OD2	2.19	0.41
1:A:3:GLY:CA	1:A:39:PHE:CE1	3.03	0.41
1:B:531:LEU:HD22	1:B:624:PHE:CD1	2.54	0.41
1:B:835:LEU:HD12	1:B:836:GLU:H	1.85	0.41
1:A:40:VAL:O	1:A:40:VAL:HG23	2.20	0.41
1:B:595:SER:N	1:B:596:PRO:CD	2.83	0.41
1:A:176:LEU:C	1:A:178:MET:N	2.73	0.41
1:A:218:TRP:CZ3	2:A:989:ACG:H6C2	2.56	0.41
1:A:299:SER:HB3	1:A:438:THR:OG1	2.21	0.41
1:B:542:TRP:CZ2	1:B:608:GLU:HG2	2.55	0.41
1:A:80:HIS:O	1:A:81:ASP:C	2.59	0.41
1:A:276:ASN:OD1	1:A:279:MET:HG2	2.20	0.41
1:A:405:VAL:HA	1:A:417:VAL:O	2.21	0.41
1:A:415:LEU:HD12	1:A:441:VAL:OXT	2.20	0.41
1:B:584:GLY:O	1:B:586:PHE:HD1	2.04	0.41
1:B:474:LYS:HD2	1:B:474:LYS:HA	1.85	0.41
1:B:659:TRP:CD2	2:B:988:ACG:H5C	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:LEU:HD11	1:B:676:LEU:CG	2.52	0.40
1:A:85:LYS:NZ	4:A:996:HOH:O	2.54	0.40
1:A:195:ILE:O	1:A:195:ILE:HD12	2.21	0.40
1:A:325:PRO:HG2	1:B:791:TRP:CE2	2.55	0.40
1:B:611:ARG:HG2	1:B:611:ARG:HH11	1.85	0.40
1:B:632:MET:HG3	1:B:643:TRP:CE2	2.55	0.40
1:B:684:ILE:HG23	1:B:741:ILE:HG21	2.01	0.40
1:B:721:SER:N	1:B:763:TYR:HB2	2.37	0.40
1:A:68:SER:OG	1:A:71:GLU:HG3	2.21	0.40
1:B:536:THR:HG23	1:B:598:LEU:HD21	2.02	0.40
1:B:625:ARG:HA	1:B:655:LEU:O	2.20	0.40
1:A:113:ARG:O	1:A:113:ARG:HG2	2.22	0.40
1:A:180:VAL:HG11	1:A:183:PHE:CE1	2.56	0.40
1:B:823:PHE:CD1	1:B:824:ARG:N	2.90	0.40
1:B:504:LYS:O	1:B:505:ALA:C	2.60	0.40
1:B:581:LEU:O	1:B:582:GLU:C	2.60	0.40
1:B:835:LEU:HD11	1:B:847:TYR:CB	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASP:OD1	1:A:166:ASP:OD1[4_555]	1.84	0.36

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	439/441 (100%)	376 (86%)	51 (12%)	12 (3%)	5	7
1	B	439/441 (100%)	387 (88%)	41 (9%)	11 (2%)	5	8
All	All	878/882 (100%)	763 (87%)	92 (10%)	23 (3%)	5	8

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PRO
1	A	207	SER
1	A	228	GLY
1	A	253	ARG
1	A	265	ALA
1	A	288	GLY
1	A	290	SER
1	B	572	TRP
1	B	582	GLU
1	B	584	GLY
1	B	693	THR
1	A	238	ASP
1	A	347	PHE
1	B	499	ASP
1	B	565	ASP
1	B	706	ALA
1	B	731	SER
1	A	142	ASP
1	A	392	ALA
1	B	485	PRO
1	A	188	ALA
1	B	505	ALA
1	B	504	LYS

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	389/393 (99%)	379 (97%)	10 (3%)	46	72
1	B	389/393 (99%)	375 (96%)	14 (4%)	35	61
All	All	778/786 (99%)	754 (97%)	24 (3%)	40	67

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	TRP
1	A	163	GLN
1	A	170	ARG
1	A	195	ILE
1	A	214	LEU
1	A	236	ASN
1	A	267	ASP
1	A	289	PHE
1	A	360	ILE
1	A	382	PHE
1	B	482	TRP
1	B	522	ASP
1	B	554	ARG
1	B	597	ASP
1	B	606	PHE
1	B	634	ASP
1	B	677	ASN
1	B	730	PHE
1	B	734	LYS
1	B	778	ASN
1	B	784	GLU
1	B	820	TRP
1	B	842	ASP
1	B	853	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	174	HIS
1	A	236	ASN
1	A	386	ASN
1	A	412	GLN
1	B	446	GLN
1	B	544	GLN
1	B	552	HIS
1	B	615	HIS
1	B	677	ASN
1	B	778	ASN
1	B	827	ASN
1	B	853	GLN
1	B	854	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	ACG	A	989	-	57,58,58	1.82	8 (14%)	73,87,87	1.70	10 (13%)
2	ACG	B	988	-	57,58,58	1.48	7 (12%)	73,87,87	1.65	9 (12%)

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	ACG	A	989	-	-	7/22/122/122	0/5/5/5
2	ACG	B	988	-	-	7/22/122/122	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	989	ACG	O4C-C4C	7.16	1.62	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	989	ACG	C4B-N4B	-5.54	1.38	1.47
2	A	989	ACG	C7A-C5A	5.10	1.39	1.32
2	B	988	ACG	O4A-C1E	5.10	1.56	1.41
2	B	988	ACG	C7A-C5A	5.00	1.39	1.32
2	A	989	ACG	C4A-C5A	3.59	1.54	1.51
2	A	989	ACG	C1A-N4B	2.68	1.52	1.47
2	B	988	ACG	O5D-C1D	2.62	1.49	1.42
2	A	989	ACG	O4A-C1E	2.60	1.49	1.41
2	B	988	ACG	C4A-C5A	2.46	1.53	1.51
2	A	989	ACG	O5B-C5B	2.24	1.49	1.44
2	B	988	ACG	O3A-C3A	-2.14	1.37	1.43
2	B	988	ACG	C1D-C2D	2.12	1.57	1.52
2	A	989	ACG	C1D-C2D	2.07	1.57	1.52
2	B	988	ACG	C1A-C7A	2.03	1.53	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	988	ACG	C7A-C1A-N4B	9.19	124.46	110.68
2	A	989	ACG	O4C-C4C-C3C	-7.28	87.92	107.28
2	A	989	ACG	O4C-C1B-C2B	5.08	121.26	108.10
2	B	988	ACG	O4C-C4C-C3C	-4.99	94.02	107.28
2	A	989	ACG	O4C-C1B-O5B	-4.75	97.41	110.67
2	A	989	ACG	O4D-C1C-O5C	4.74	123.91	110.67
2	A	989	ACG	O6A-C6A-C5A	-3.14	104.98	112.50
2	A	989	ACG	O4C-C4C-C5C	3.02	117.72	109.45
2	A	989	ACG	C3C-C4C-C5C	-2.96	104.14	110.93
2	B	988	ACG	O4C-C4C-C5C	2.91	117.42	109.45
2	B	988	ACG	O4C-C1B-C2B	2.87	115.54	108.10
2	B	988	ACG	C3C-C4C-C5C	-2.87	104.34	110.93
2	B	988	ACG	O4C-C1B-O5B	-2.81	102.83	110.67
2	A	989	ACG	O4D-C1C-C2C	-2.79	100.86	108.10
2	B	988	ACG	C1C-O4D-C4D	2.66	124.53	117.96
2	B	988	ACG	C2A-C3A-C4A	2.64	113.76	109.25
2	A	989	ACG	O2A-C2A-C3A	2.40	115.90	110.35
2	A	989	ACG	C2A-C3A-C4A	2.20	113.00	109.25
2	B	988	ACG	O2A-C2A-C3A	2.11	115.22	110.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	989	ACG	C7A-C1A-N4B-C4B
2	A	989	ACG	C4A-C5A-C6A-O6A
2	A	989	ACG	C7A-C5A-C6A-O6A
2	B	988	ACG	C7A-C1A-N4B-C4B
2	B	988	ACG	C7A-C5A-C6A-O6A
2	A	989	ACG	O5C-C5C-C6C-O6C
2	B	988	ACG	O5C-C5C-C6C-O6C
2	B	988	ACG	O5D-C5D-C6D-O6D
2	A	989	ACG	C4C-C5C-C6C-O6C
2	B	988	ACG	C4D-C5D-C6D-O6D
2	B	988	ACG	C4C-C5C-C6C-O6C
2	A	989	ACG	O5D-C5D-C6D-O6D
2	A	989	ACG	C4D-C5D-C6D-O6D
2	B	988	ACG	C4A-C5A-C6A-O6A

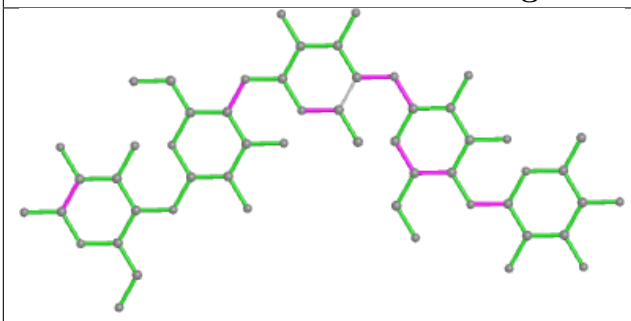
There are no ring outliers.

2 monomers are involved in 6 short contacts:

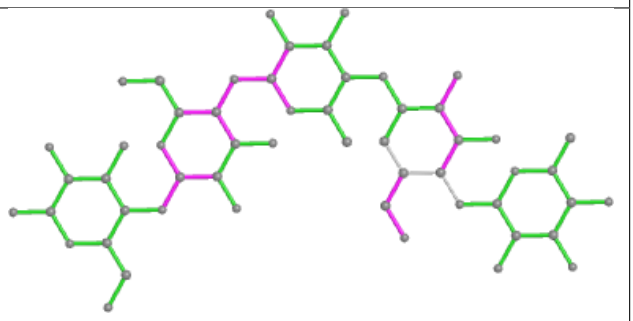
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	989	ACG	4	0
2	B	988	ACG	2	0

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.

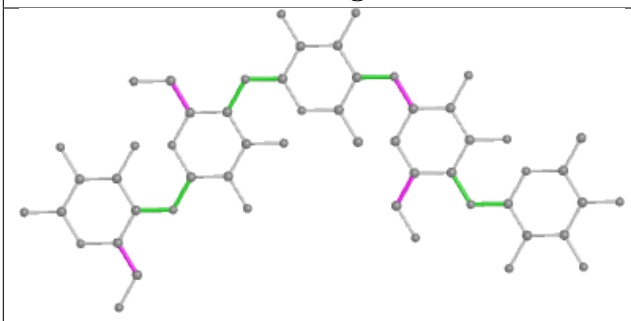
Ligand ACG A 989



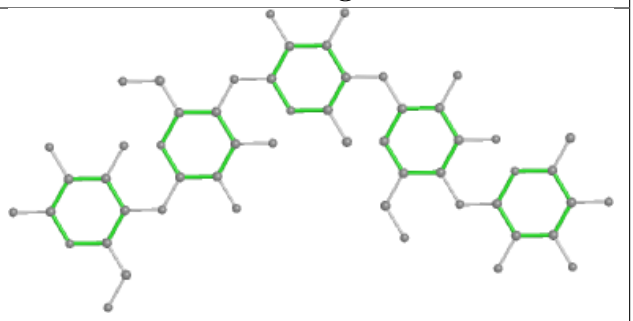
Bond lengths



Bond angles

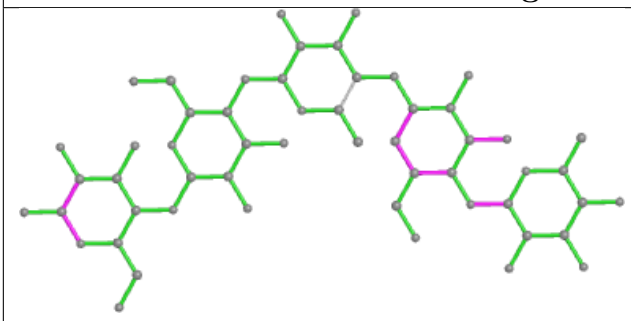


Torsions

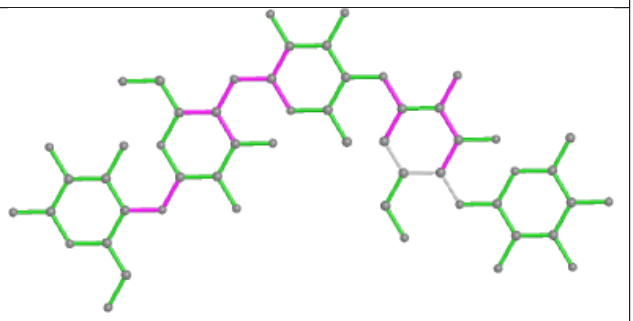


Rings

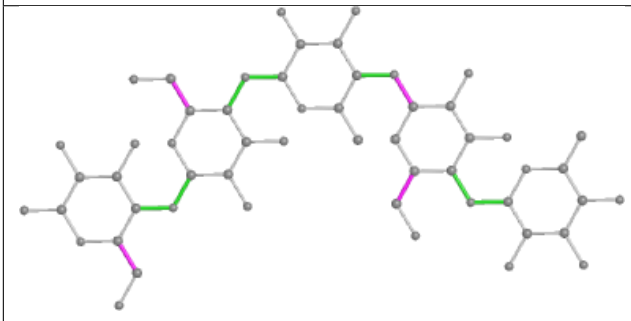
Ligand ACG B 988



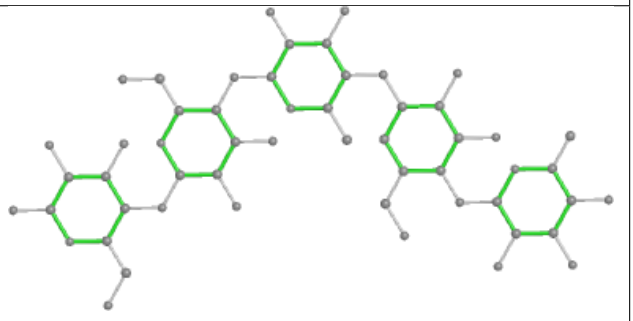
Bond lengths



Bond angles



Torsions



Rings

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.