



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 10:15 AM JST

PDB ID : 21FO / pdb_000021fo
Title : CYMAL-7-bound MexB
Authors : Ueda, Y.; Yonehara, R.; Nakagawa, A.; Yamashita, E.
Deposited on : 2025-12-11
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

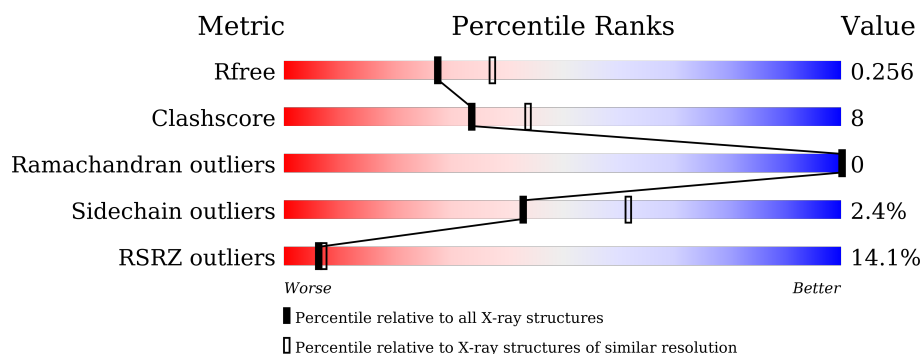
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1054	<div> <div>14%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	B	1054	<div> <div>19%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
1	C	1054	<div> <div>9%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23460 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 Multidrug resistance protein MexB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1024	Total	C	N	O	S	0	0	0
			7764	4998	1289	1437	40			
1	B	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	C	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			

There are 24 discrepancies between the modelled and reference sequences:

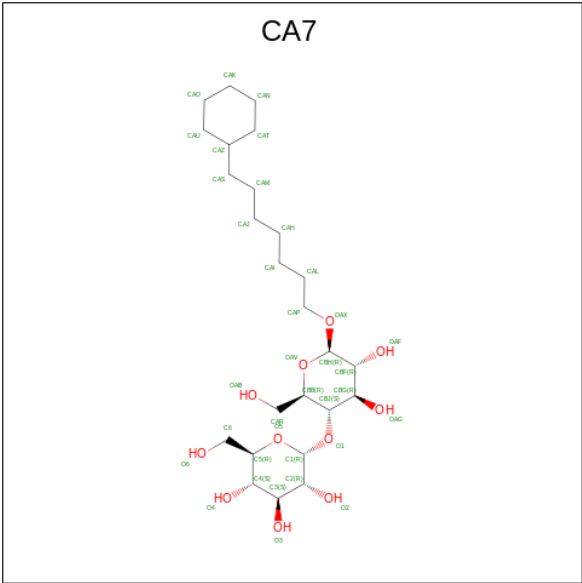
Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	LEU	-	expression tag	UNP P52002
A	1048	GLU	-	expression tag	UNP P52002
A	1049	HIS	-	expression tag	UNP P52002
A	1050	HIS	-	expression tag	UNP P52002
A	1051	HIS	-	expression tag	UNP P52002
A	1052	HIS	-	expression tag	UNP P52002
A	1053	HIS	-	expression tag	UNP P52002
A	1054	HIS	-	expression tag	UNP P52002
B	1047	LEU	-	expression tag	UNP P52002
B	1048	GLU	-	expression tag	UNP P52002
B	1049	HIS	-	expression tag	UNP P52002
B	1050	HIS	-	expression tag	UNP P52002
B	1051	HIS	-	expression tag	UNP P52002
B	1052	HIS	-	expression tag	UNP P52002
B	1053	HIS	-	expression tag	UNP P52002
B	1054	HIS	-	expression tag	UNP P52002
C	1047	LEU	-	expression tag	UNP P52002
C	1048	GLU	-	expression tag	UNP P52002
C	1049	HIS	-	expression tag	UNP P52002
C	1050	HIS	-	expression tag	UNP P52002
C	1051	HIS	-	expression tag	UNP P52002
C	1052	HIS	-	expression tag	UNP P52002
C	1053	HIS	-	expression tag	UNP P52002

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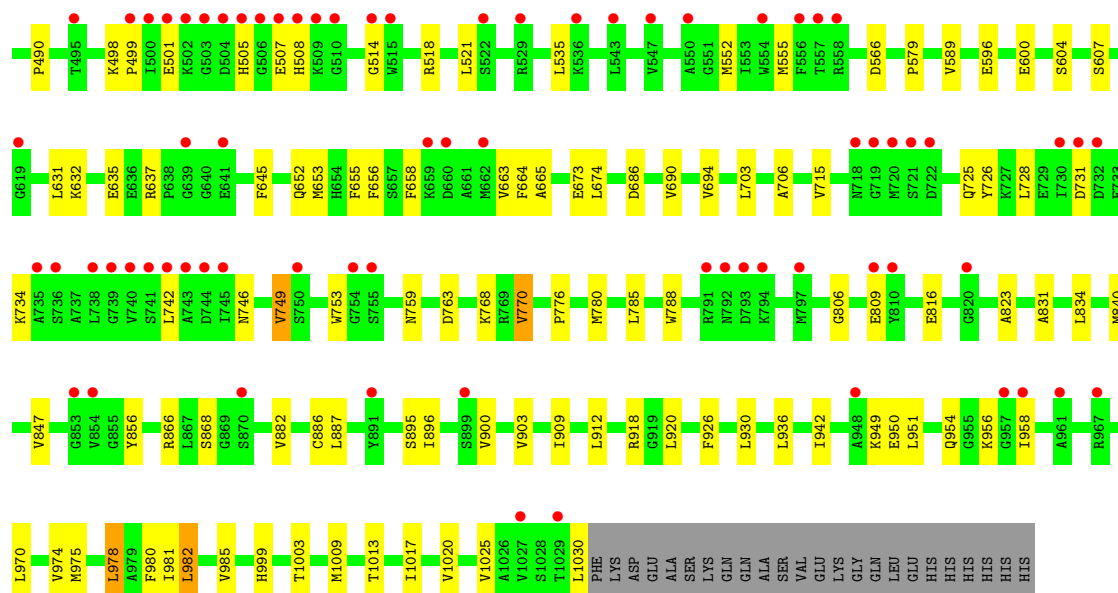
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P52002

- Molecule 2 is 7-cyclohexylheptyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (CCD ID: CA7) (formula: C₂₅H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			36	25	11		
2	C	1	Total	C	O	0	0
			36	25	11		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.04Å 168.87Å 172.21Å 90.00° 102.23° 90.00°	Depositor
Resolution (Å)	40.55 – 2.30 40.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.55-2.30) 98.6 (40.55-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419+SVN	Depositor
R, R_{free}	0.221 , 0.255 0.221 , 0.256	Depositor DCC
R_{free} test set	12429 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23460	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: CA7

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	0.42	0/7921	0.60	0/10765
1	B	0.32	0/7971	0.48	0/10833
1	C	0.37	1/7971 (0.0%)	0.55	4/10833 (0.0%)
All	All	0.37	1/23863 (0.0%)	0.54	4/32431 (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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	579	PRO	CA-C	7.42	1.55	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	579	PRO	O-C-N	5.23	123.71	121.31
1	C	982	LEU	CA-CB-CG	-5.07	98.55	116.30
1	C	84	SER	CA-C-N	5.06	131.21	121.54
1	C	84	SER	C-N-CA	5.06	131.21	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	766	ARG	Sidechain

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	7764	0	7899	120	0
1	B	7812	0	7944	135	0
1	C	7812	0	7944	124	0
2	B	36	0	46	0	0
2	C	36	0	46	1	0
All	All	23460	0	23879	364	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 8.

All (364) 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:359:LEU:HD21	1:B:971:ARG:HH12	1.39	0.87
1:A:399:VAL:HG11	1:A:987:LEU:HD11	1.63	0.81
1:A:728:LEU:HD11	1:A:753:TRP:HZ3	1.47	0.79
1:B:330:THR:HA	1:B:333:VAL:HG12	1.71	0.72
1:C:728:LEU:HD11	1:C:753:TRP:HZ3	1.56	0.70
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.72	0.70
1:B:510:GLY:H	1:B:514:GLY:HA3	1.55	0.70
1:B:966:CYS:SG	1:B:1021:PRO:HG3	2.31	0.70
1:A:351:VAL:HG22	1:A:979:ALA:HB1	1.72	0.70
1:B:224:ALA:HB1	1:C:780:MET:HE1	1.74	0.69
1:B:792:ASN:HB2	1:B:796:GLU:H	1.58	0.69
1:B:493:CYS:HA	1:B:497:LEU:HD23	1.74	0.68
1:A:847:VAL:HG11	1:A:856:TYR:CD1	2.28	0.68
1:A:25:LEU:HD11	1:B:878:LEU:HD21	1.75	0.68
1:B:572:LEU:HB3	1:B:629:ILE:HB	1.76	0.68
1:C:218:GLN:NE2	1:C:231:ASN:HD21	1.93	0.67
1:A:355:MET:SD	1:A:368:PRO:HG2	2.34	0.67
1:C:652:GLN:HE22	1:C:664:PHE:HA	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:HD3	1:A:432:ARG:HE	1.60	0.66
1:C:218:GLN:HE21	1:C:231:ASN:HD21	1.44	0.65
1:C:690:VAL:HG22	1:C:694:VAL:HG21	1.78	0.65
1:C:435:MET:HE3	1:C:490:PRO:HB3	1.78	0.65
1:A:390:ILE:HG23	1:A:395:MET:HE3	1.77	0.65
1:A:728:LEU:HD11	1:A:753:TRP:CZ3	2.32	0.64
1:C:198:LEU:HD21	1:C:252:LYS:HD3	1.80	0.64
1:A:370:ILE:O	1:A:373:PRO:HD2	1.98	0.63
1:A:409:ALA:O	1:A:413:VAL:HG23	1.98	0.63
1:A:703:LEU:HD11	1:A:717:PRO:HG3	1.80	0.63
1:B:423:GLU:HB2	1:B:425:LEU:HD23	1.80	0.63
1:A:47:VAL:HG12	1:A:88:MET:HE3	1.79	0.63
1:A:414:GLU:HG3	1:A:975:MET:HE1	1.81	0.62
1:B:566:ASP:HB3	1:B:645:PHE:CZ	2.34	0.62
1:A:146:ASP:HB3	1:A:148:SER:H	1.64	0.62
1:B:204:SER:O	1:B:208:GLN:HG3	2.00	0.62
1:C:706:ALA:HB1	1:C:715:VAL:HG21	1.80	0.62
1:A:456:MET:HB3	1:A:875:LEU:HD13	1.82	0.62
1:B:900:VAL:O	1:B:903:VAL:HG12	1.99	0.62
1:A:400:LEU:HD11	1:A:1001:ILE:HD11	1.82	0.62
1:A:949:LYS:O	1:A:953:GLU:HG2	2.00	0.62
1:A:470:PHE:CE1	1:A:474:ILE:HG13	2.35	0.62
1:C:447:MET:CE	1:C:886:CYS:HB3	2.30	0.61
1:A:531:VAL:O	1:A:534:ILE:HG13	2.01	0.61
1:C:68:GLN:HG3	1:C:114:ALA:HB2	1.83	0.61
1:B:310:ILE:HG21	1:B:323:VAL:HG11	1.83	0.60
1:B:445:ILE:HG13	1:B:446:ALA:N	2.17	0.60
1:B:47:VAL:HG12	1:B:88:MET:HE3	1.83	0.60
1:C:376:LEU:HD11	1:C:402:ILE:HD11	1.84	0.60
1:C:632:LYS:O	1:C:637:ARG:HD3	2.01	0.59
1:B:574:ALA:HB3	1:B:627:ALA:HB3	1.82	0.59
1:B:792:ASN:HB3	1:B:794:LYS:H	1.65	0.59
1:C:903:VAL:HG21	1:C:1020:VAL:HG22	1.85	0.59
1:A:831:ALA:HB3	1:A:834:LEU:HD13	1.84	0.59
1:B:193:LEU:HG	1:B:265:VAL:HG13	1.85	0.59
1:A:140:VAL:HG11	1:A:310:ILE:CD1	2.33	0.58
1:A:534:ILE:HG22	1:A:541:TYR:CZ	2.37	0.58
1:C:428:ARG:NH2	1:C:432:ARG:HH11	2.02	0.58
1:B:749:VAL:HG22	1:B:753:TRP:CZ3	2.39	0.58
1:A:355:MET:HE1	1:A:410:ILE:HG12	1.84	0.58
1:C:332:VAL:O	1:C:336:SER:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:847:VAL:HG21	1:C:856:TYR:CD1	2.38	0.58
1:A:535:LEU:HD23	1:A:959:VAL:HG22	1.86	0.57
1:A:441:ALA:O	1:A:445:ILE:HD12	2.04	0.57
1:B:1009:MET:HE2	1:B:1009:MET:HA	1.87	0.57
1:C:2:SER:HB3	1:C:435:MET:HG3	1.86	0.57
1:C:56:THR:O	1:C:60:THR:HB	2.05	0.57
1:C:463:THR:HG21	1:C:868:SER:HB3	1.86	0.56
1:A:435:MET:HE2	1:A:435:MET:HA	1.87	0.56
1:C:427:PRO:HD3	1:C:499:PRO:HB3	1.87	0.56
1:B:637:ARG:O	1:B:637:ARG:HG2	2.05	0.56
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.88	0.56
1:C:412:VAL:HG13	1:C:435:MET:HE1	1.88	0.56
1:B:214:ILE:HA	1:C:746:ASN:ND2	2.21	0.55
1:B:149:MET:HE1	1:B:318:PRO:HG2	1.87	0.55
1:A:405:LEU:HD11	1:A:477:ALA:HB1	1.87	0.55
1:C:653:MET:HE3	1:C:656:PHE:HD2	1.70	0.55
1:C:655:PHE:HB3	1:C:663:VAL:HB	1.89	0.55
1:B:359:LEU:HD21	1:B:971:ARG:NH1	2.16	0.54
1:B:492:LEU:O	1:B:496:MET:HB2	2.07	0.54
1:B:831:ALA:HB3	1:B:834:LEU:HD13	1.88	0.54
1:A:456:MET:HE1	1:A:928:VAL:HG23	1.89	0.54
1:C:39:ALA:HB2	1:C:673:GLU:HG3	1.90	0.54
1:B:524:THR:HG22	1:B:967:ARG:HG2	1.88	0.54
1:B:930:LEU:O	1:B:934:ILE:HG13	2.07	0.54
1:A:876:TYR:O	1:A:880:LEU:HG	2.07	0.54
1:B:1011:THR:O	1:B:1015:LEU:HB2	2.08	0.54
1:A:355:MET:CE	1:A:410:ILE:HG12	2.37	0.54
1:A:339:GLU:O	1:A:343:THR:HG23	2.07	0.54
1:A:380:PHE:CE1	1:A:395:MET:HE1	2.42	0.54
1:B:910:GLY:H	1:B:1011:THR:HG21	1.73	0.54
1:B:186:ILE:HD13	1:B:262:LEU:HD21	1.91	0.53
1:C:958:ILE:H	1:C:958:ILE:HD12	1.73	0.53
1:A:36:PRO:HG3	1:A:469:GLN:HG3	1.88	0.53
1:B:501:GLU:HB3	1:B:504:ASP:HB2	1.91	0.53
1:C:38:ILE:HG23	1:C:462:SER:HB2	1.90	0.52
1:A:375:VAL:HG13	1:A:480:LEU:HB3	1.90	0.52
1:A:983:GLY:O	1:A:986:PRO:HD2	2.09	0.52
1:B:225:VAL:H	1:C:780:MET:HE2	1.73	0.52
1:B:534:ILE:HG23	1:B:541:TYR:CD2	2.44	0.52
1:B:1015:LEU:O	1:B:1019:TRP:HD1	1.93	0.52
1:C:363:ARG:HH12	1:C:498:LYS:HE3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.90	0.52
1:A:463:THR:HG22	1:A:563:PHE:CE1	2.45	0.52
1:C:419:VAL:HG12	1:C:425:LEU:HD23	1.91	0.52
1:C:753:TRP:CE2	1:C:785:LEU:HD22	2.45	0.52
1:B:528:GLU:CD	1:B:967:ARG:HG3	2.34	0.52
1:B:459:PHE:CE1	1:B:875:LEU:HD12	2.45	0.51
1:C:303:ALA:HB2	1:C:330:THR:HG21	1.92	0.51
1:A:594:MET:HE1	1:A:627:ALA:HB2	1.93	0.51
1:B:216:SER:HB2	1:B:234:ILE:O	2.10	0.51
1:A:450:SER:O	1:A:454:LEU:HB2	2.11	0.51
1:C:456:MET:HG3	1:C:467:TYR:HB3	1.93	0.51
1:A:899:SER:HA	1:A:1023:PHE:HB3	1.92	0.51
1:C:658:PHE:HD2	1:C:663:VAL:HG21	1.75	0.51
1:B:610:PHE:HB3	1:B:628:PHE:HB2	1.93	0.51
1:A:904:VAL:HG13	1:A:934:ILE:HG12	1.93	0.50
1:A:406:VAL:O	1:A:410:ILE:HG13	2.10	0.50
1:C:455:PRO:HG3	1:C:882:VAL:HG21	1.92	0.50
1:C:507:GLU:HG2	1:C:508:HIS:N	2.26	0.50
1:B:80:SER:OG	1:B:817:ARG:HB2	2.12	0.50
1:C:365:THR:O	1:C:368:PRO:HD2	2.11	0.50
1:A:26:SER:O	1:A:30:LEU:HG	2.12	0.50
1:B:228:GLN:CD	1:C:780:MET:HE3	2.36	0.50
1:C:981:ILE:O	1:C:985:VAL:HG23	2.11	0.50
1:C:887:LEU:HD13	1:C:900:VAL:HG21	1.92	0.50
1:B:330:THR:N	1:B:331:PRO:HD2	2.27	0.50
1:C:912:LEU:HD23	1:C:926:PHE:HZ	1.77	0.50
1:C:60:THR:HG23	1:C:119:PRO:HD3	1.94	0.49
1:A:685:GLN:O	1:A:854:VAL:HA	2.12	0.49
1:B:463:THR:HG22	1:B:563:PHE:CZ	2.47	0.49
1:A:355:MET:SD	1:A:368:PRO:CG	3.00	0.49
1:A:413:VAL:HA	1:A:416:VAL:HG12	1.93	0.49
1:B:965:ALA:HA	1:B:968:MET:HE3	1.94	0.49
1:A:164:ASP:HB2	1:A:165:PRO:HD3	1.94	0.49
1:C:362:PHE:CE2	1:C:366:LEU:HD22	2.47	0.49
1:B:407:ASP:OD2	1:B:976:THR:HG21	2.13	0.49
1:A:293:LEU:HG	1:A:297:ALA:HB3	1.95	0.49
1:B:44:ALA:HB3	1:B:130:THR:HG22	1.94	0.49
1:C:607:SER:HB2	1:C:632:LYS:HG3	1.95	0.49
1:B:300:LEU:HD11	1:B:334:SER:HB3	1.95	0.48
1:C:186:ILE:HD13	1:C:262:LEU:HD21	1.95	0.48
1:C:403:GLY:HA3	1:C:980:PHE:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:MET:HE1	1:A:866:ARG:HB2	1.96	0.48
1:C:420:MET:HE3	1:C:505:HIS:CE1	2.47	0.48
1:C:62:VAL:HG22	1:C:88:MET:HG2	1.95	0.48
1:C:447:MET:HE3	1:C:886:CYS:HB3	1.95	0.48
1:A:686:ASP:OD1	1:A:690:VAL:HG22	2.13	0.48
1:B:713:GLN:HG2	1:B:714:ARG:HG3	1.95	0.48
1:A:453:PHE:O	1:A:456:MET:HG2	2.13	0.48
1:A:478:MET:HB3	1:A:478:MET:HE2	1.71	0.48
1:A:726:TYR:CZ	1:A:806:GLY:HA3	2.49	0.48
1:C:887:LEU:CD1	1:C:900:VAL:HG21	2.44	0.48
1:A:400:LEU:HD12	1:A:470:PHE:HE2	1.78	0.48
1:B:17:LEU:O	1:B:21:LEU:HG	2.14	0.48
1:B:364:ALA:HB2	1:B:497:LEU:HD11	1.96	0.48
1:C:23:GLY:HA3	1:C:377:LEU:O	2.13	0.48
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.95	0.48
1:C:728:LEU:HD11	1:C:753:TRP:CZ3	2.44	0.48
1:C:759:ASN:O	1:C:770:VAL:HG13	2.13	0.48
1:C:753:TRP:HE1	1:C:788:TRP:CD1	2.32	0.48
1:A:468:ARG:HG3	1:A:472:ILE:HD13	1.95	0.47
1:C:428:ARG:O	1:C:432:ARG:HG3	2.14	0.47
1:A:317:MET:HE3	1:A:321:MET:SD	2.54	0.47
1:A:754:GLY:O	1:A:773:GLN:HG3	2.13	0.47
1:A:603:SER:O	1:A:632:LYS:HE2	2.14	0.47
1:B:569:GLN:NE2	1:B:670:SER:HA	2.29	0.47
1:C:981:ILE:HG13	1:C:1009:MET:HG2	1.96	0.47
1:A:274:ASP:OD2	1:A:276:SER:HB2	2.14	0.47
1:A:372:VAL:CG2	1:A:373:PRO:HD3	2.45	0.47
1:B:199:THR:HG22	1:B:202:ASP:CG	2.39	0.47
1:A:923:ASP:O	1:A:927:GLN:HG3	2.14	0.47
1:B:235:ILE:HD13	1:C:725:GLN:HB3	1.96	0.47
1:B:726:TYR:CZ	1:B:806:GLY:HA3	2.49	0.47
1:B:984:VAL:HG13	1:B:987:LEU:HD12	1.97	0.47
1:C:380:PHE:CZ	1:C:395:MET:HE1	2.50	0.47
1:C:418:ARG:O	1:C:422:GLU:HG3	2.15	0.47
1:C:731:ASP:HB3	1:C:734:LYS:HB2	1.96	0.47
1:B:214:ILE:HA	1:C:746:ASN:HD21	1.78	0.47
1:B:400:LEU:HA	1:B:400:LEU:HD23	1.72	0.47
1:A:137:LEU:HD13	1:A:293:LEU:HD13	1.97	0.46
1:B:626:MET:HG2	1:B:628:PHE:CE1	2.50	0.46
1:B:425:LEU:HD12	1:B:429:GLU:HB2	1.96	0.46
1:A:861:LEU:H	1:A:861:LEU:HD12	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:THR:OG1	1:B:245:GLN:HG3	2.16	0.46
1:B:273:GLN:HG3	1:B:771:TYR:CE1	2.50	0.46
1:B:480:LEU:HD23	1:B:480:LEU:HA	1.72	0.46
1:B:964:GLU:O	1:B:968:MET:HG3	2.15	0.46
1:B:971:ARG:O	1:B:975:MET:HG3	2.16	0.46
1:C:521:LEU:HD12	1:C:521:LEU:HA	1.71	0.46
1:B:337:ILE:O	1:B:341:VAL:HG12	2.16	0.46
1:B:441:ALA:O	1:B:445:ILE:HG23	2.15	0.46
1:C:652:GLN:NE2	1:C:665:ALA:H	2.13	0.46
1:A:915:THR:HG23	1:A:920:LEU:HB2	1.97	0.46
1:A:164:ASP:HB3	1:A:168:ARG:NH2	2.31	0.46
1:B:342:LYS:HE3	1:B:346:GLU:OE1	2.15	0.46
1:C:596:GLU:O	1:C:600:GLU:HG2	2.15	0.46
1:A:408:ASP:O	1:A:412:VAL:HG12	2.16	0.45
1:A:540:PRO:O	1:A:544:ILE:HG23	2.16	0.45
1:A:952:HIS:HD1	1:A:952:HIS:C	2.24	0.45
1:B:573:PHE:CE2	1:B:668:PRO:HB3	2.51	0.45
1:A:140:VAL:HG11	1:A:310:ILE:HD11	1.97	0.45
1:A:134:LYS:HD2	1:A:134:LYS:HA	1.71	0.45
1:B:545:TYR:HB2	1:B:1019:TRP:CZ3	2.51	0.45
1:A:704:MET:HE2	1:A:704:MET:HB3	1.74	0.45
1:A:156:ASN:HA	1:A:181:GLN:HA	1.98	0.45
1:A:544:ILE:HD11	1:A:1019:TRP:CZ2	2.51	0.45
1:A:936:LEU:HD23	1:A:936:LEU:HA	1.68	0.45
1:C:686:ASP:CG	1:C:690:VAL:HG12	2.42	0.45
1:A:792:ASN:ND2	1:A:796:GLU:HG3	2.32	0.45
1:B:58:GLN:HG2	1:B:59:ASP:OD1	2.16	0.45
1:B:887:LEU:HB2	1:B:897:PRO:HB3	1.99	0.45
1:C:16:ALA:O	1:C:20:MET:HG3	2.17	0.45
1:C:239:ARG:HG2	1:C:239:ARG:HH11	1.80	0.45
1:B:959:VAL:O	1:B:963:ILE:HG12	2.17	0.45
1:C:763:ASP:HB3	1:C:768:LYS:HD2	1.98	0.45
1:A:474:ILE:O	1:A:478:MET:HB2	2.16	0.45
1:B:187:TRP:HA	1:B:773:GLN:O	2.16	0.45
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.98	0.45
1:C:635:GLU:CD	1:C:635:GLU:H	2.25	0.45
1:B:451:ALA:HB3	1:B:883:VAL:HG12	1.99	0.45
1:B:535:LEU:HD22	1:B:959:VAL:HG13	1.99	0.45
1:B:986:PRO:HA	1:B:989:ILE:HD11	1.99	0.45
1:B:70:ASN:O	1:B:110:LYS:HE3	2.17	0.44
1:B:614:GLY:HA2	1:B:621:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:ARG:HD3	1:B:1003:THR:HG21	1.99	0.44
1:B:247:GLU:HG3	1:B:268:VAL:HB	1.99	0.44
1:B:493:CYS:O	1:B:497:LEU:HB2	2.18	0.44
1:C:33:ASN:O	1:C:391:ASN:HA	2.16	0.44
1:B:228:GLN:OE1	1:C:780:MET:HE3	2.16	0.44
1:A:506:GLY:HA2	1:A:509:LYS:HE3	1.99	0.44
1:A:1009:MET:HE2	1:A:1009:MET:HA	1.99	0.44
1:B:896:ILE:N	1:B:897:PRO:HD2	2.32	0.44
1:B:900:VAL:HG11	1:B:942:ILE:HG13	1.99	0.44
1:A:380:PHE:CZ	1:A:395:MET:HE1	2.53	0.44
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.82	0.44
1:C:451:ALA:HB1	1:C:882:VAL:HG12	1.98	0.44
1:C:555:MET:HA	1:C:555:MET:HE2	1.99	0.44
1:A:407:ASP:O	1:A:411:VAL:HG23	2.18	0.44
1:B:775:ARG:HD3	1:B:777:ASP:OD1	2.16	0.44
1:B:1007:GLY:O	1:B:1011:THR:HG22	2.18	0.44
1:B:303:ALA:HB2	1:B:330:THR:HG21	1.99	0.44
1:B:326:PRO:HB2	1:B:630:MET:HE2	1.99	0.44
1:B:185:ARG:HD3	1:B:272:GLY:O	2.17	0.44
1:A:414:GLU:HG3	1:A:975:MET:CE	2.48	0.44
1:B:876:TYR:HA	1:B:879:SER:HB3	2.00	0.44
1:C:63:GLN:O	1:C:67:GLN:HG2	2.18	0.44
1:A:80:SER:OG	1:A:817:ARG:HB2	2.17	0.43
1:A:496:MET:HE2	1:A:496:MET:HB3	1.87	0.43
1:C:1009:MET:HE3	1:C:1009:MET:HA	2.00	0.43
1:A:407:ASP:OD2	1:A:976:THR:HG21	2.18	0.43
1:A:448:VAL:HG22	1:A:886:CYS:HB3	2.00	0.43
1:B:452:VAL:CG1	1:B:931:LEU:HD12	2.48	0.43
1:B:569:GLN:HE21	1:B:670:SER:HA	1.83	0.43
1:C:840:MET:HE1	1:C:866:ARG:CG	2.48	0.43
1:B:212:VAL:HG22	1:C:742:LEU:HD23	2.00	0.43
1:C:154:LEU:HD23	1:C:321:MET:HE2	1.99	0.43
1:C:514:GLY:O	1:C:518:ARG:HG2	2.18	0.43
1:C:918:ARG:O	1:C:918:ARG:HG3	2.19	0.43
1:A:388:PHE:CE2	1:A:472:ILE:HG21	2.53	0.43
1:A:400:LEU:HD12	1:A:470:PHE:CE2	2.53	0.43
1:A:669:PRO:HB3	1:A:678:THR:HG22	2.00	0.43
1:B:902:LEU:O	1:B:905:PRO:HD2	2.18	0.43
1:C:974:VAL:O	1:C:978:LEU:HB2	2.18	0.43
1:A:3:LYS:O	1:A:6:ILE:HG13	2.19	0.43
1:A:410:ILE:HD12	1:A:976:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ASN:HD22	1:B:517:ASN:HA	1.66	0.43
1:A:419:VAL:HG11	1:A:433:LYS:HD2	2.00	0.43
1:A:836:SER:O	1:A:840:MET:HG3	2.19	0.43
1:B:216:SER:OG	1:C:51:GLY:HA2	2.19	0.43
1:B:435:MET:SD	1:B:490:PRO:HG3	2.58	0.43
1:C:370:ILE:O	1:C:374:VAL:HG23	2.19	0.43
1:A:187:TRP:HA	1:A:773:GLN:O	2.19	0.43
1:A:370:ILE:O	1:A:374:VAL:HG23	2.19	0.43
1:B:498:LYS:HD2	1:B:498:LYS:HA	1.44	0.43
1:A:972:PRO:HA	1:A:975:MET:HE3	2.01	0.42
1:B:359:LEU:HD23	1:B:359:LEU:HA	1.62	0.42
1:B:453:PHE:HE1	1:B:931:LEU:HB3	1.84	0.42
1:A:275:TYR:CD1	1:C:223:PRO:HD3	2.54	0.42
1:B:786:SER:HB3	1:B:801:ASN:HD22	1.84	0.42
1:A:655:PHE:HA	1:A:658:PHE:HD2	1.84	0.42
1:B:105:VAL:HA	1:B:108:GLN:HG2	2.00	0.42
1:B:359:LEU:CD2	1:B:971:ARG:HH12	2.23	0.42
1:C:139:VAL:O	1:C:326:PRO:HD2	2.20	0.42
1:C:776:PRO:O	1:C:780:MET:HG2	2.19	0.42
1:C:816:GLU:HB2	1:C:823:ALA:O	2.19	0.42
1:A:457:ALA:HB2	1:A:471:SER:OG	2.19	0.42
1:B:908:VAL:HG23	1:B:930:LEU:HD11	2.01	0.42
1:C:703:LEU:HD23	1:C:715:VAL:HG12	2.01	0.42
1:A:451:ALA:O	1:A:879:SER:HB2	2.18	0.42
1:B:33:ASN:HB3	1:B:293:LEU:HD23	2.01	0.42
1:A:112:GLN:HG3	1:B:112:GLN:CD	2.44	0.42
1:A:520:PHE:CZ	1:A:970:LEU:HD23	2.54	0.42
1:B:150:THR:HG23	1:B:153:ASP:H	1.84	0.42
1:A:599:LEU:HD23	1:A:599:LEU:HA	1.86	0.42
1:A:762:ILE:HD11	1:B:59:ASP:HB3	2.02	0.42
1:B:723:GLU:OE2	1:B:813:PRO:HB3	2.20	0.42
1:B:847:VAL:HG21	1:B:856:TYR:CE1	2.55	0.42
1:B:903:VAL:HG23	1:B:906:LEU:HD12	2.02	0.42
1:C:404:LEU:HD21	1:C:936:LEU:HD21	2.01	0.42
1:A:449:LEU:HB2	1:A:478:MET:SD	2.60	0.42
1:B:237:LYS:HD3	1:B:238:THR:O	2.20	0.42
1:B:791:ARG:HD3	1:B:797:MET:HE1	2.02	0.42
1:C:501:GLU:H	1:C:501:GLU:CD	2.27	0.42
1:C:566:ASP:HB3	1:C:645:PHE:CZ	2.54	0.42
1:A:534:ILE:HA	1:A:541:TYR:CE2	2.55	0.42
1:A:535:LEU:HD22	1:A:959:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:MET:SD	1:A:865:GLU:HG2	2.59	0.41
1:B:709:ASN:HA	1:B:710:PRO:HD3	1.94	0.41
1:C:242:THR:OG1	1:C:245:GLN:HG3	2.20	0.41
1:B:138:MET:HE2	1:B:138:MET:HB3	1.80	0.41
1:C:463:THR:CG2	1:C:868:SER:HB3	2.49	0.41
1:C:999:HIS:O	1:C:1003:THR:HG23	2.20	0.41
1:A:730:ILE:HB	1:C:237:LYS:HE2	2.02	0.41
1:B:975:MET:HE2	1:B:975:MET:HB3	1.87	0.41
1:C:552:MET:HA	1:C:909:ILE:HD13	2.02	0.41
1:C:951:LEU:HB3	1:C:956:LYS:HD3	2.01	0.41
1:A:753:TRP:C	1:A:754:GLY:O	2.61	0.41
1:B:542:LEU:HG	1:B:1022:LEU:HD21	2.01	0.41
1:B:668:PRO:HB2	1:B:672:LEU:HD21	2.02	0.41
1:A:456:MET:HG3	1:A:471:SER:HB2	2.02	0.41
1:C:746:ASN:HA	1:C:749:VAL:HG13	2.01	0.41
1:A:978:LEU:HD22	1:A:978:LEU:HA	1.86	0.41
1:C:293:LEU:HD22	1:C:297:ALA:HB3	2.03	0.41
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.79	0.41
1:A:544:ILE:O	1:A:548:ILE:HG13	2.21	0.41
1:B:225:VAL:N	1:C:780:MET:HE2	2.35	0.41
1:C:69:MET:O	1:C:72:ILE:HG13	2.21	0.41
1:C:831:ALA:HB3	1:C:834:LEU:HD12	2.03	0.41
1:C:950:GLU:O	1:C:954:GLN:HG3	2.21	0.41
1:B:399:VAL:HG11	1:B:987:LEU:HD11	2.02	0.41
1:B:918:ARG:HD3	1:B:1003:THR:CG2	2.51	0.41
1:C:631:LEU:HD23	1:C:637:ARG:CZ	2.51	0.41
1:A:131:LYS:HG3	1:A:131:LYS:O	2.19	0.41
1:B:355:MET:HE3	1:B:355:MET:HB3	1.96	0.41
1:C:363:ARG:NH1	1:C:498:LYS:HE3	2.36	0.41
1:C:447:MET:HE2	1:C:447:MET:HB3	1.69	0.41
1:C:674:LEU:HD23	1:C:674:LEU:HA	1.90	0.41
1:C:896:ILE:HD11	1:C:949:LYS:HD2	2.03	0.41
1:A:310:ILE:HG21	1:A:323:VAL:HG11	2.02	0.41
1:A:903:VAL:HG23	1:A:906:LEU:HD12	2.03	0.41
1:A:952:HIS:HD2	1:A:958:ILE:HG22	1.86	0.41
1:B:534:ILE:HG12	1:B:541:TYR:CE2	2.55	0.41
1:C:358:PHE:CD2	1:C:975:MET:HG2	2.56	0.41
1:C:726:TYR:CZ	1:C:806:GLY:HA3	2.56	0.41
1:B:150:THR:HG22	1:B:153:ASP:OD2	2.21	0.40
1:B:453:PHE:CE1	1:B:931:LEU:HB3	2.57	0.40
1:B:875:LEU:HD23	1:B:875:LEU:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE2	1:C:1:MET:HB3	1.80	0.40
1:C:60:THR:HG22	1:C:61:VAL:HG23	2.03	0.40
1:C:1013:THR:O	1:C:1017:ILE:HG12	2.22	0.40
1:A:410:ILE:HD12	1:A:976:THR:CG2	2.52	0.40
1:A:574:ALA:HB3	1:A:627:ALA:HB3	2.04	0.40
1:B:196:TYR:CD2	1:B:260:VAL:HG21	2.56	0.40
1:C:432:ARG:HE	1:C:432:ARG:HB3	1.40	0.40
1:A:329:THR:O	1:A:332:VAL:HG12	2.22	0.40
1:B:252:LYS:O	1:B:260:VAL:HG12	2.21	0.40
1:B:543:LEU:O	1:B:547:VAL:HG23	2.22	0.40
1:C:3:LYS:NZ	2:C:2001:CA7:H6	2.37	0.40
1:C:64:VAL:HG12	1:C:114:ALA:HB1	2.03	0.40
1:C:435:MET:HE3	1:C:490:PRO:CB	2.49	0.40
1:C:535:LEU:HD22	1:C:1025:VAL:HG21	2.03	0.40
1:B:88:MET:SD	1:B:88:MET:C	3.04	0.40
1:B:198:LEU:HD23	1:B:198:LEU:HA	1.72	0.40
1:B:542:LEU:O	1:B:546:VAL:HG23	2.21	0.40
1:C:887:LEU:HD23	1:C:887:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1020/1054 (97%)	1000 (98%)	20 (2%)	0	100	100
1	B	1028/1054 (98%)	1002 (98%)	26 (2%)	0	100	100
1	C	1028/1054 (98%)	1009 (98%)	19 (2%)	0	100	100
All	All	3076/3162 (97%)	3011 (98%)	65 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	836/862 (97%)	814 (97%)	22 (3%)	40	59
1	B	841/862 (98%)	825 (98%)	16 (2%)	50	69
1	C	841/862 (98%)	819 (97%)	22 (3%)	40	59
All	All	2518/2586 (97%)	2458 (98%)	60 (2%)	43	62

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

Mol	Chain	Res	Type
1	A	134	LYS
1	A	158	ILE
1	A	265	VAL
1	A	291	ILE
1	A	310	ILE
1	A	324	VAL
1	A	334	SER
1	A	405	LEU
1	A	412	VAL
1	A	480	LEU
1	A	495	THR
1	A	533	SER
1	A	535	LEU
1	A	603	SER
1	A	854	VAL
1	A	861	LEU
1	A	862	SER
1	A	924	VAL
1	A	928	VAL
1	A	978	LEU
1	A	1022	LEU
1	A	1027	VAL
1	B	130	THR
1	B	214	ILE
1	B	258	SER
1	B	265	VAL

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Mol	Chain	Res	Type
1	B	349	LEU
1	B	498	LYS
1	B	556	PHE
1	B	591	VAL
1	B	605	SER
1	B	637	ARG
1	B	705	LEU
1	B	857	SER
1	B	964	GLU
1	B	967	ARG
1	B	978	LEU
1	B	1014	VAL
1	C	8	ARG
1	C	47	VAL
1	C	60	THR
1	C	125	GLN
1	C	195	SER
1	C	238	THR
1	C	265	VAL
1	C	295	THR
1	C	336	SER
1	C	589	VAL
1	C	604	SER
1	C	749	VAL
1	C	770	VAL
1	C	809	GLU
1	C	895	SER
1	C	920	LEU
1	C	930	LEU
1	C	942	ILE
1	C	970	LEU
1	C	978	LEU
1	C	982	LEU
1	C	1030	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	181	GLN
1	A	254	ASN
1	A	308	GLN

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Mol	Chain	Res	Type
1	A	781	ASN
1	A	954	GLN
1	B	120	GLN
1	B	229	GLN
1	B	517	ASN
1	B	525	HIS
1	B	569	GLN
1	B	676	ASN
1	B	773	GLN
1	C	83	ASN
1	C	218	GLN
1	C	231	ASN
1	C	248	ASN
1	C	360	GLN
1	C	415	ASN
1	C	437	GLN
1	C	505	HIS
1	C	569	GLN
1	C	652	GLN
1	C	654	HIS
1	C	708	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	CA7	C	2001	-	38,38,38	0.48	0	51,51,51	1.14	6 (11%)
2	CA7	B	2001	-	38,38,38	0.50	0	51,51,51	0.78	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	CA7	C	2001	-	-	10/19/67/67	0/3/3/3
2	CA7	B	2001	-	-	5/19/67/67	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	CA7	C1-O1-CBJ	2.89	125.12	117.96
2	C	2001	CA7	O1-CBJ-CBG	-2.81	99.81	107.28
2	C	2001	CA7	CAP-OAX-CBH	2.40	117.82	113.84
2	C	2001	CA7	CBF-CBG-CBJ	2.33	115.01	109.68
2	C	2001	CA7	O1-CBJ-CBB	2.24	115.59	109.45
2	C	2001	CA7	OAF-CBF-CBG	-2.07	105.56	110.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2001	CA7	OAV-CBH-OAX-CAP
2	B	2001	CA7	CBF-CBH-OAX-CAP
2	C	2001	CA7	C2-C1-O1-CBJ
2	C	2001	CA7	O5-C1-O1-CBJ
2	B	2001	CA7	CAI-CAL-CAP-OAX
2	C	2001	CA7	CAJ-CAM-CAS-CAZ
2	B	2001	CA7	CAL-CAP-OAX-CBH
2	C	2001	CA7	CBG-CBJ-O1-C1
2	B	2001	CA7	CAH-CAI-CAL-CAP

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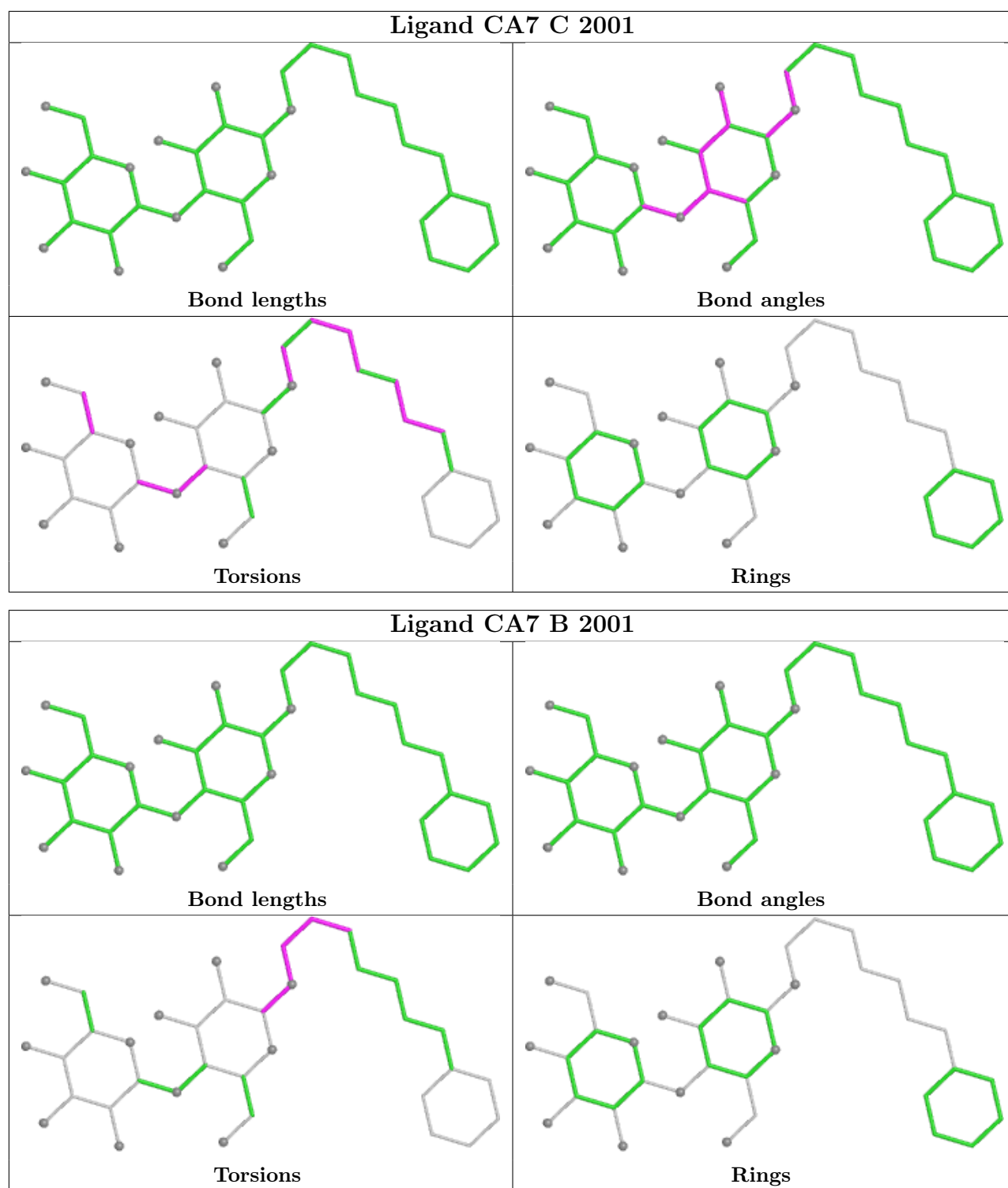
Mol	Chain	Res	Type	Atoms
2	C	2001	CA7	CAJ-CAH-CAI-CAL
2	C	2001	CA7	O5-C5-C6-O6
2	C	2001	CA7	CBB-CBJ-O1-C1
2	C	2001	CA7	CAH-CAJ-CAM-CAS
2	C	2001	CA7	CAH-CAI-CAL-CAP
2	C	2001	CA7	CAL-CAP-OAX-CBH

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	CA7	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

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, 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	1024/1054 (97%)	0.78	146 (14%) 6 7	37, 67, 114, 135	0
1	B	1030/1054 (97%)	1.20	195 (18%) 3 4	41, 93, 133, 166	0
1	C	1030/1054 (97%)	0.71	94 (9%) 15 16	42, 75, 115, 145	0
All	All	3084/3162 (97%)	0.90	435 (14%) 6 7	37, 80, 122, 166	0

All (435) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	872	ALA	10.7
1	C	503	GLY	5.7
1	B	656	PHE	5.7
1	A	536	LYS	5.7
1	A	463	THR	5.6
1	C	505	HIS	5.6
1	C	500	ILE	5.5
1	B	664	PHE	5.4
1	B	870	SER	5.2
1	A	869	GLY	5.1
1	B	958	ILE	5.0
1	A	349	LEU	5.0
1	A	506	GLY	4.9
1	A	438	ILE	4.9
1	A	874	ALA	4.9
1	C	126	GLY	4.8
1	C	719	GLY	4.8
1	B	677	ALA	4.8
1	A	957	GLY	4.7
1	C	255	PRO	4.6
1	B	536	LYS	4.6
1	B	236	GLY	4.6
1	B	658	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	508	HIS	4.5
1	B	352	PHE	4.5
1	B	557	THR	4.5
1	B	675	GLY	4.5
1	B	793	ASP	4.5
1	C	730	ILE	4.4
1	B	909	ILE	4.4
1	C	458	PHE	4.2
1	A	523	THR	4.2
1	A	875	LEU	4.2
1	A	1025	VAL	4.1
1	A	499	PRO	4.1
1	C	515	TRP	4.1
1	A	525	HIS	4.1
1	A	434	SER	4.1
1	B	653	MET	4.1
1	A	867	LEU	4.0
1	A	419	VAL	4.0
1	B	599	LEU	4.0
1	A	754	GLY	4.0
1	B	362	PHE	4.0
1	B	537	HIS	3.9
1	C	732	ASP	3.9
1	A	878	LEU	3.9
1	A	656	PHE	3.9
1	B	338	HIS	3.9
1	B	633	PRO	3.9
1	A	425	LEU	3.9
1	B	543	LEU	3.9
1	A	6	ILE	3.9
1	B	255	PRO	3.9
1	B	544	ILE	3.9
1	C	547	VAL	3.9
1	B	357	LEU	3.8
1	C	504	ASP	3.8
1	B	515	TRP	3.8
1	B	1014	VAL	3.8
1	B	596	GLU	3.8
1	C	720	MET	3.8
1	B	634	TRP	3.7
1	C	740	VAL	3.7
1	A	230	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	560	PRO	3.7
1	A	458	PHE	3.7
1	B	508	HIS	3.7
1	A	443	VAL	3.6
1	B	1013	THR	3.6
1	B	349	LEU	3.6
1	C	250	LEU	3.6
1	B	554	TRP	3.6
1	B	215	SER	3.6
1	B	21	LEU	3.6
1	B	3	LYS	3.6
1	B	601	LYS	3.6
1	B	332	VAL	3.6
1	A	367	ILE	3.5
1	B	257	GLY	3.5
1	B	754	GLY	3.5
1	A	543	LEU	3.5
1	B	516	PHE	3.5
1	A	861	LEU	3.5
1	B	509	LYS	3.5
1	B	214	ILE	3.5
1	C	556	PHE	3.5
1	B	678	THR	3.4
1	A	522	SER	3.4
1	B	657	SER	3.4
1	B	868	SER	3.4
1	A	871	GLN	3.4
1	A	435	MET	3.4
1	B	341	VAL	3.4
1	B	739	GLY	3.4
1	B	610	PHE	3.4
1	B	603	SER	3.4
1	B	640	GLY	3.4
1	A	405	LEU	3.3
1	B	810	TYR	3.3
1	C	739	GLY	3.3
1	B	1001	ILE	3.3
1	B	253	VAL	3.3
1	A	436	GLY	3.3
1	C	810	TYR	3.3
1	B	607	SER	3.3
1	A	1000	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	877	ALA	3.3
1	B	25	LEU	3.3
1	B	316	PHE	3.3
1	B	216	SER	3.3
1	B	605	SER	3.3
1	B	237	LYS	3.2
1	B	740	VAL	3.2
1	C	735	ALA	3.2
1	B	923	ASP	3.2
1	A	429	GLU	3.2
1	A	561	THR	3.2
1	A	416	VAL	3.2
1	A	1027	VAL	3.2
1	C	253	VAL	3.2
1	B	500	ILE	3.2
1	A	362	PHE	3.2
1	A	870	SER	3.2
1	C	721	SER	3.2
1	A	956	LYS	3.2
1	C	509	LYS	3.2
1	A	991	THR	3.2
1	A	1	MET	3.2
1	A	965	ALA	3.1
1	C	743	ALA	3.1
1	A	488	LEU	3.1
1	A	410	ILE	3.1
1	B	503	GLY	3.1
1	C	957	GLY	3.1
1	B	143	VAL	3.1
1	A	558	ARG	3.1
1	A	445	ILE	3.1
1	C	741	SER	3.1
1	A	655	PHE	3.1
1	A	409	ALA	3.1
1	A	495	THR	3.1
1	B	669	PRO	3.1
1	B	513	PHE	3.0
1	B	17	LEU	3.0
1	B	606	VAL	3.0
1	B	659	LYS	3.0
1	C	754	GLY	3.0
1	A	984	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	547	VAL	3.0
1	C	501	GLU	3.0
1	B	238	THR	3.0
1	C	502	LYS	3.0
1	B	320	GLY	3.0
1	A	255	PRO	3.0
1	A	422	GLU	3.0
1	A	508	HIS	3.0
1	C	745	ILE	3.0
1	A	868	SER	3.0
1	C	258	SER	3.0
1	C	755	SER	3.0
1	A	440	GLY	3.0
1	C	639	GLY	3.0
1	A	1014	VAL	2.9
1	B	342	LYS	2.9
1	B	197	GLN	2.9
1	A	983	GLY	2.9
1	A	9	PRO	2.9
1	A	880	LEU	2.9
1	B	421	ALA	2.9
1	B	518	ARG	2.9
1	B	546	VAL	2.9
1	A	450	SER	2.9
1	B	527	TYR	2.9
1	C	820	GLY	2.9
1	A	970	LEU	2.9
1	B	511	GLY	2.9
1	A	459	PHE	2.9
1	A	962	ALA	2.9
1	B	512	PHE	2.9
1	B	1000	ALA	2.9
1	A	257	GLY	2.8
1	B	345	GLY	2.8
1	A	943	LEU	2.8
1	B	867	LEU	2.8
1	B	1005	VAL	2.8
1	A	960	GLU	2.8
1	B	991	THR	2.8
1	A	8	ARG	2.8
1	B	992	GLY	2.8
1	B	563	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	807	LYS	2.8
1	A	1029	THR	2.8
1	A	195	SER	2.8
1	B	525	HIS	2.8
1	B	1004	GLY	2.8
1	C	84	SER	2.8
1	C	257	GLY	2.8
1	A	437	GLN	2.8
1	B	987	LEU	2.8
1	A	457	ALA	2.8
1	A	961	ALA	2.8
1	B	1027	VAL	2.8
1	B	836	SER	2.8
1	B	333	VAL	2.8
1	B	952	HIS	2.7
1	B	335	ALA	2.7
1	A	413	VAL	2.7
1	C	722	ASP	2.7
1	B	637	ARG	2.7
1	B	918	ARG	2.7
1	A	441	ALA	2.7
1	B	999	HIS	2.7
1	B	655	PHE	2.7
1	B	360	GLN	2.7
1	C	1027	VAL	2.7
1	B	676	ASN	2.7
1	B	346	GLU	2.7
1	B	540	PRO	2.7
1	C	662	MET	2.7
1	C	744	ASP	2.7
1	B	913	LEU	2.7
1	C	550	ALA	2.6
1	A	433	LYS	2.6
1	B	417	GLU	2.6
1	A	253	VAL	2.6
1	C	854	VAL	2.6
1	A	534	ILE	2.6
1	B	570	GLY	2.6
1	A	1030	LEU	2.6
1	B	874	ALA	2.6
1	B	792	ASN	2.6
1	C	660	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	133	VAL	2.6
1	B	260	VAL	2.6
1	B	639	GLY	2.6
1	B	956	LYS	2.6
1	B	984	VAL	2.6
1	C	619	GLY	2.6
1	A	879	SER	2.6
1	B	258	SER	2.6
1	C	958	ILE	2.6
1	C	67	GLN	2.6
1	B	742	LEU	2.6
1	B	920	LEU	2.6
1	C	791	ARG	2.6
1	C	421	ALA	2.6
1	B	781	ASN	2.6
1	B	506	GLY	2.6
1	B	638	PRO	2.6
1	B	666	PHE	2.6
1	B	1029	THR	2.6
1	C	50	PRO	2.6
1	C	437	GLN	2.5
1	A	28	LEU	2.5
1	B	198	LEU	2.5
1	A	421	ALA	2.5
1	B	914	ALA	2.5
1	B	801	ASN	2.5
1	C	506	GLY	2.5
1	C	510	GLY	2.5
1	B	767	VAL	2.5
1	C	522	SER	2.5
1	B	521	LEU	2.5
1	A	456	MET	2.5
1	A	258	SER	2.5
1	C	354	VAL	2.5
1	C	543	LEU	2.5
1	C	738	LEU	2.5
1	B	496	MET	2.5
1	A	485	ALA	2.5
1	A	532	ALA	2.5
1	C	495	THR	2.5
1	A	635	GLU	2.5
1	A	544	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	963	ILE	2.5
1	B	168	ARG	2.5
1	B	348	ILE	2.5
1	B	904	VAL	2.5
1	B	325	TYR	2.5
1	C	742	LEU	2.5
1	A	447	MET	2.5
1	A	460	GLY	2.5
1	B	1030	LEU	2.4
1	B	649	LYS	2.4
1	B	794	LYS	2.4
1	C	536	LYS	2.4
1	A	529	ARG	2.4
1	B	994	GLY	2.4
1	C	507	GLU	2.4
1	B	593	SER	2.4
1	B	483	ILE	2.4
1	A	467	TYR	2.4
1	A	964	GLU	2.4
1	C	387	GLY	2.4
1	A	947	PHE	2.4
1	B	589	VAL	2.4
1	C	793	ASP	2.4
1	A	533	SER	2.4
1	B	1009	MET	2.4
1	A	492	LEU	2.4
1	B	213	GLN	2.4
1	A	356	TYR	2.3
1	B	356	TYR	2.3
1	B	499	PRO	2.3
1	B	632	LYS	2.3
1	A	4	PHE	2.3
1	A	411	VAL	2.3
1	A	412	VAL	2.3
1	B	1010	VAL	2.3
1	A	442	LEU	2.3
1	A	542	LEU	2.3
1	B	350	LEU	2.3
1	B	564	LEU	2.3
1	B	693	GLU	2.3
1	B	498	LYS	2.3
1	B	996	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	451	ALA	2.3
1	B	604	SER	2.3
1	A	866	ARG	2.3
1	C	967	ARG	2.3
1	B	359	LEU	2.3
1	B	597	TYR	2.3
1	B	957	GLY	2.3
1	C	797	MET	2.3
1	C	899	SER	2.3
1	A	423	GLU	2.3
1	B	259	GLN	2.3
1	C	259	GLN	2.3
1	A	944	ILE	2.3
1	B	559	ILE	2.3
1	B	924	VAL	2.3
1	B	510	GLY	2.3
1	A	496	MET	2.3
1	A	541	TYR	2.3
1	A	877	ALA	2.3
1	B	995	SER	2.3
1	B	411	VAL	2.3
1	B	951	LEU	2.2
1	A	966	CYS	2.2
1	C	264	ASP	2.2
1	A	662	MET	2.2
1	C	558	ARG	2.2
1	C	641	GLU	2.2
1	C	870	SER	2.2
1	A	386	PHE	2.2
1	A	945	VAL	2.2
1	B	254	ASN	2.2
1	C	853	GLY	2.2
1	C	809	GLU	2.2
1	C	961	ALA	2.2
1	B	863	TYR	2.2
1	A	515	TRP	2.2
1	B	553	ILE	2.2
1	A	951	LEU	2.2
1	A	1022	LEU	2.2
1	A	470	PHE	2.2
1	C	459	PHE	2.2
1	A	967	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	529	ARG	2.2
1	C	731	ASP	2.2
1	A	514	GLY	2.2
1	B	960	GLU	2.2
1	A	557	THR	2.2
1	A	17	LEU	2.2
1	B	989	ILE	2.2
1	B	529	ARG	2.2
1	A	520	PHE	2.2
1	A	700	ASN	2.2
1	B	519	MET	2.2
1	B	800	PHE	2.2
1	B	873	PRO	2.2
1	B	23	GLY	2.2
1	C	457	ALA	2.2
1	C	891	TYR	2.1
1	B	474	ILE	2.1
1	A	519	MET	2.1
1	B	520	PHE	2.1
1	B	646	GLU	2.1
1	C	659	LYS	2.1
1	C	794	LYS	2.1
1	A	424	GLY	2.1
1	A	426	SER	2.1
1	A	431	ALA	2.1
1	B	1003	THR	2.1
1	C	750	SER	2.1
1	A	521	LEU	2.1
1	A	231	ASN	2.1
1	A	248	ASN	2.1
1	B	732	ASP	2.1
1	C	429	GLU	2.1
1	A	448	VAL	2.1
1	C	416	VAL	2.1
1	A	511	GLY	2.1
1	C	514	GLY	2.1
1	B	130	THR	2.1
1	B	446	ALA	2.1
1	A	982	LEU	2.1
1	B	880	LEU	2.1
1	A	876	TYR	2.1
1	C	254	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	718	ASN	2.1
1	A	148	SER	2.1
1	A	916	SER	2.1
1	B	997	SER	2.1
1	B	1028	SER	2.1
1	B	735	ALA	2.1
1	B	841	ALA	2.1
1	C	948	ALA	2.1
1	B	600	GLU	2.1
1	A	19	ILE	2.1
1	A	958	ILE	2.1
1	C	487	ILE	2.1
1	C	499	PRO	2.1
1	B	416	VAL	2.1
1	A	227	GLY	2.1
1	B	281	PHE	2.1
1	B	837	GLY	2.1
1	A	342	LYS	2.0
1	B	561	THR	2.0
1	C	736	SER	2.0
1	A	948	ALA	2.0
1	B	979	ALA	2.0
1	B	674	LEU	2.0
1	C	792	ASN	2.0
1	A	466	ILE	2.0
1	A	418	ARG	2.0
1	B	265	VAL	2.0
1	B	884	PHE	2.0
1	C	554	TRP	2.0
1	C	557	THR	2.0
1	C	1029	THR	2.0
1	A	446	ALA	2.0
1	B	344	LEU	2.0
1	B	642	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

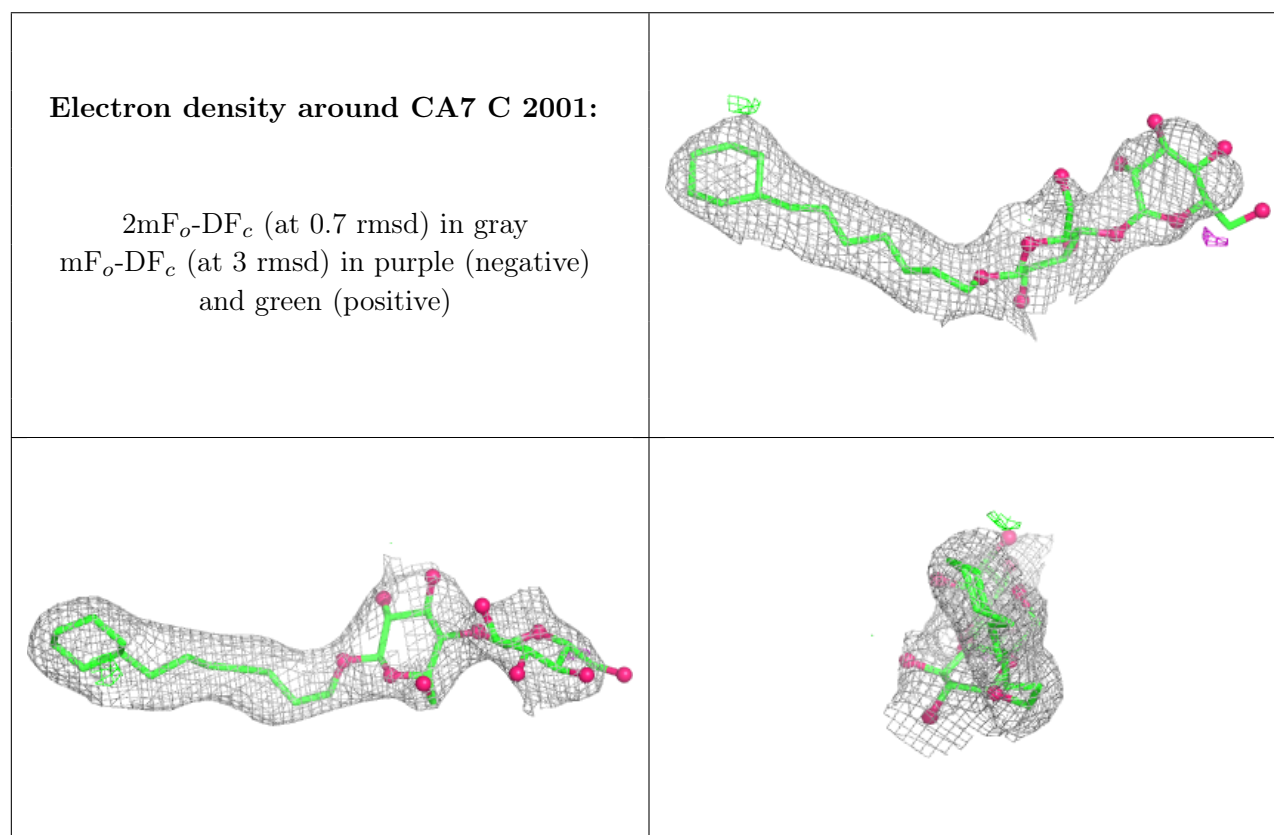
There are no oligosaccharides in this entry.

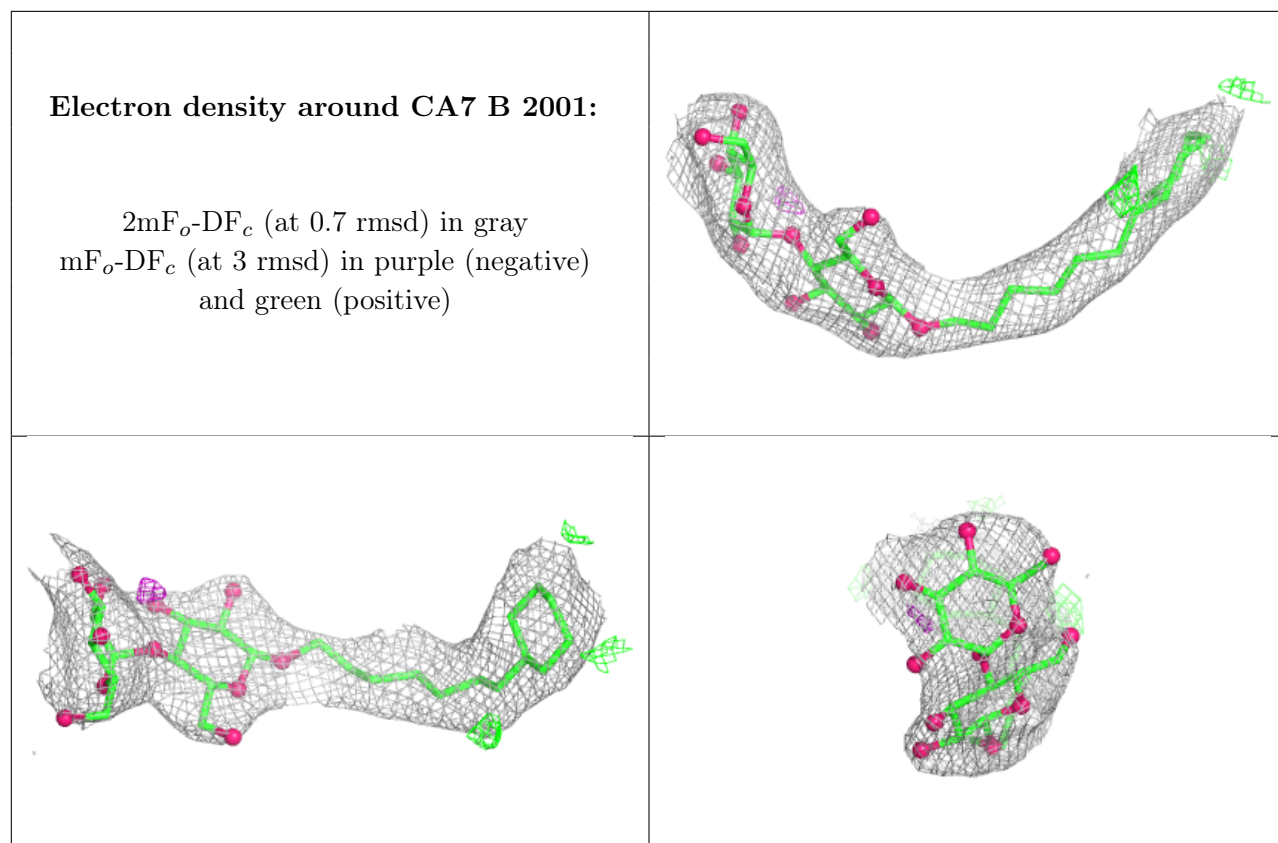
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA7	C	2001	36/36	0.84	0.14	85,105,124,134	0
2	CA7	B	2001	36/36	0.88	0.13	85,96,104,111	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.