



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:00 PM GMT

PDB ID : 4HG6
Title : Structure of a cellulose synthase - cellulose translocation intermediate
Authors : Zimmer, J.
Deposited on : 2012-10-07
Resolution : 3.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

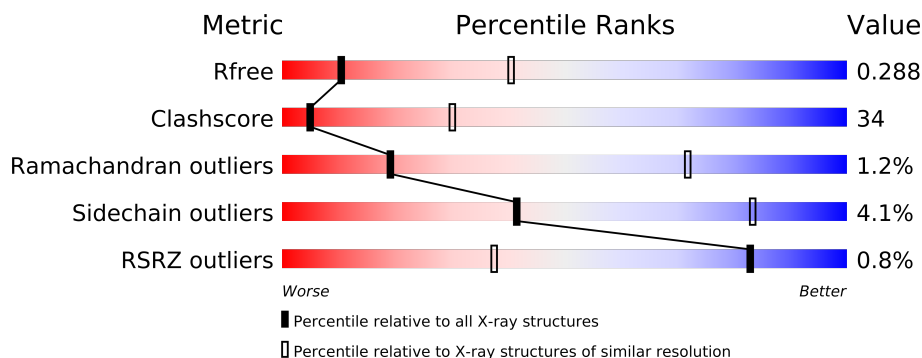
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.25 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}	66092	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (3.32-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	802	
2	B	707	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	UDP	A	919	-	X
5	LDA	A	920	-	X
5	LDA	A	921	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11029 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Cellulose Synthase Subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			5893	3822	1029	1011	31			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	789	HIS	-	EXPRESSION TAG	UNP Q3J125
A	790	HIS	-	EXPRESSION TAG	UNP Q3J125
A	791	HIS	-	EXPRESSION TAG	UNP Q3J125
A	792	HIS	-	EXPRESSION TAG	UNP Q3J125
A	793	HIS	-	EXPRESSION TAG	UNP Q3J125
A	794	HIS	-	EXPRESSION TAG	UNP Q3J125
A	795	LYS	-	EXPRESSION TAG	UNP Q3J125
A	796	LEU	-	EXPRESSION TAG	UNP Q3J125
A	797	HIS	-	EXPRESSION TAG	UNP Q3J125
A	798	HIS	-	EXPRESSION TAG	UNP Q3J125
A	799	HIS	-	EXPRESSION TAG	UNP Q3J125
A	800	HIS	-	EXPRESSION TAG	UNP Q3J125
A	801	HIS	-	EXPRESSION TAG	UNP Q3J125
A	802	HIS	-	EXPRESSION TAG	UNP Q3J125

- Molecule 2 is a protein called Cellulose Synthase Subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	655	Total	C	N	O	S	0	0	0
			4887	3100	864	907	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	MET	-	EXPRESSION TAG	UNP Q3J126
B	20	GLY	-	EXPRESSION TAG	UNP Q3J126

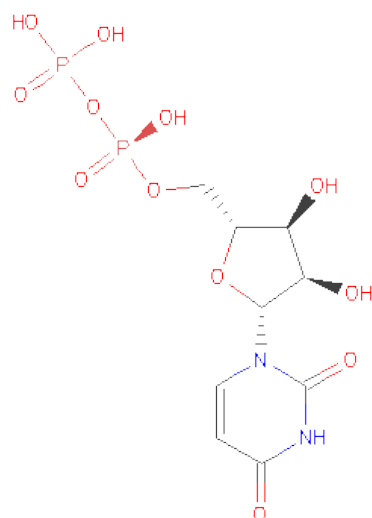
- Molecule 3 is a polymer of unknown type called SUGAR (18-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	18	Total	C	O	0	0
			199	108	91		

There are 14 discrepancies between the modelled and reference sequences:

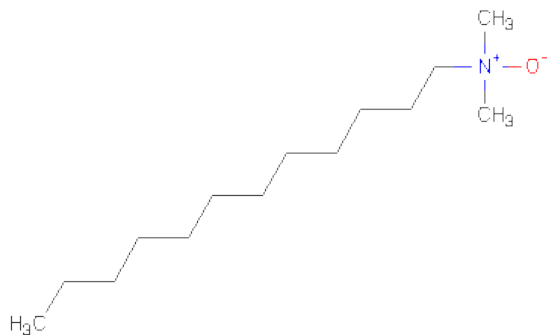
Chain	Residue	Modelled	Actual	Comment	Reference
A	789	HIS	-	EXPRESSION TAG	UNP Q3J125
A	790	HIS	-	EXPRESSION TAG	UNP Q3J125
A	791	HIS	-	EXPRESSION TAG	UNP Q3J125
A	792	HIS	-	EXPRESSION TAG	UNP Q3J125
A	793	HIS	-	EXPRESSION TAG	UNP Q3J125
A	794	HIS	-	EXPRESSION TAG	UNP Q3J125
A	795	LYS	-	EXPRESSION TAG	UNP Q3J125
A	796	LEU	-	EXPRESSION TAG	UNP Q3J125
A	797	HIS	-	EXPRESSION TAG	UNP Q3J125
A	798	HIS	-	EXPRESSION TAG	UNP Q3J125
A	799	HIS	-	EXPRESSION TAG	UNP Q3J125
A	800	HIS	-	EXPRESSION TAG	UNP Q3J125
A	801	HIS	-	EXPRESSION TAG	UNP Q3J125
A	802	HIS	-	EXPRESSION TAG	UNP Q3J125

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

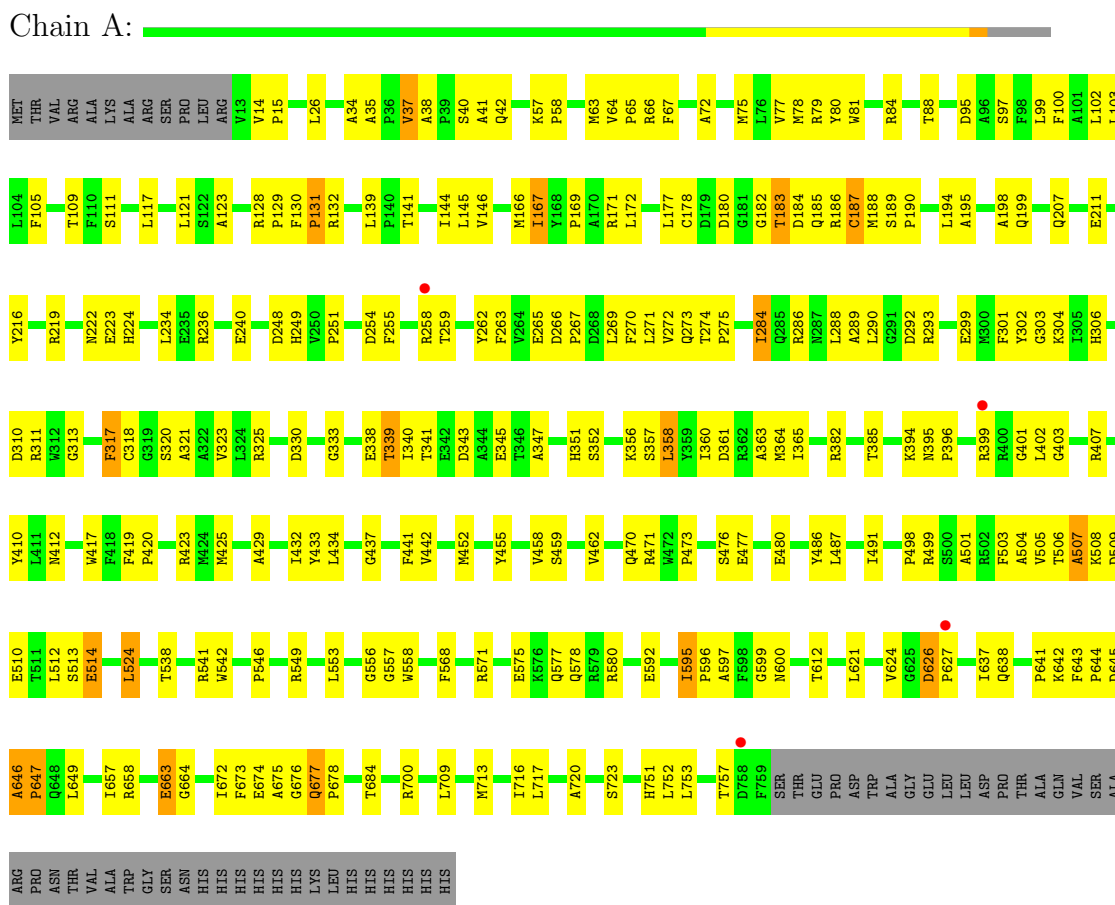


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	9	7	1	1	0	0
5	A	1	Total 16	14	1	1	0	0

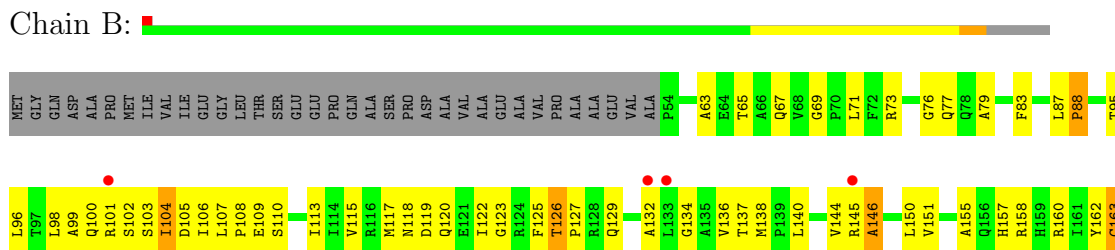
3 Residue-property plots

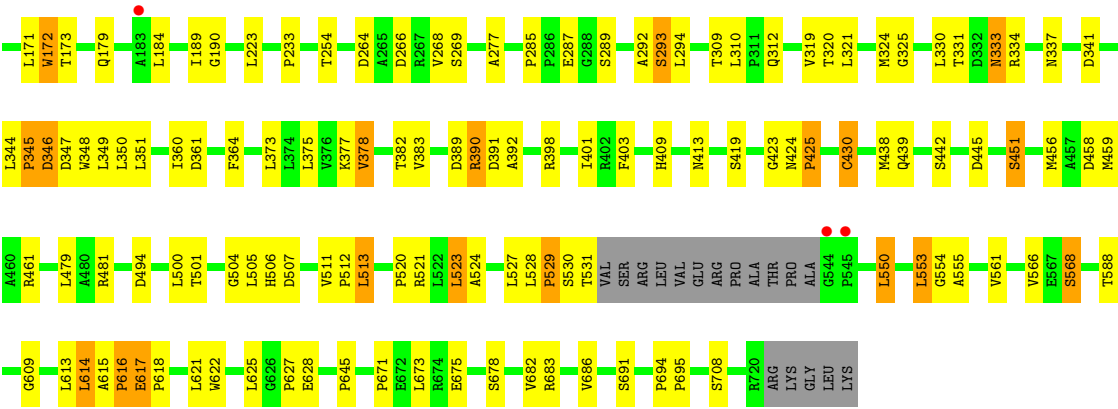
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Cellulose Synthase Subunit A



• Molecule 2: Cellulose Synthase Subunit B





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.12Å 103.12Å 468.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.81 – 3.25 34.81 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.81-3.25) 99.9 (34.81-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.213 , 0.282 0.232 , 0.288	Depositor DCC
R_{free} test set	2055 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	117.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 95.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 41092 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11029	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BGC, UDP

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	0.41	0/6044	0.63	2/8217 (0.0%)
2	B	0.39	1/5006 (0.0%)	0.63	2/6865 (0.0%)
All	All	0.40	1/11050 (0.0%)	0.63	4/15082 (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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	345	PRO	N-CD	-10.24	1.33	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	346	ASP	CB-CA-C	-7.15	96.10	110.40
2	B	345	PRO	CA-N-CD	6.14	120.30	111.70
1	A	646	ALA	C-N-CD	-6.03	107.33	120.60
1	A	663	GLU	N-CA-C	-5.53	96.06	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	390	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5893	0	0	212	0
2	B	4887	0	0	152	0
3	A	199	0	0	15	0
4	A	25	0	0	2	0
5	A	25	0	0	1	0
All	All	11029	0	0	372	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

All (372) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:262:TYR:CE1	1:A:360:ILE:CD1	2.17	1.28
1:A:317:PHE:CE2	1:A:347:ALA:CB	2.21	1.23
1:A:269:LEU:O	1:A:269:LEU:CD1	1.87	1.23
2:B:107:LEU:CD1	2:B:160:ARG:CA	2.24	1.14
2:B:377:LYS:CG	2:B:382:THR:CG2	2.27	1.12
2:B:330:LEU:CD2	2:B:439:GLN:CG	2.28	1.12
1:A:643:PHE:CB	1:A:646:ALA:CB	2.30	1.10
1:A:364:MET:O	1:A:365:ILE:CG2	2.08	1.02
2:B:73:ARG:CD	2:B:172:TRP:CE3	2.45	0.99
1:A:434:LEU:CD1	1:A:538:THR:CG2	2.41	0.99
1:A:317:PHE:CD2	1:A:347:ALA:CB	2.46	0.98
1:A:571:ARG:CD	1:A:723:SER:CB	2.45	0.94
2:B:122:ILE:CG2	2:B:140:LEU:CB	2.47	0.93
2:B:118:ASN:CG	2:B:144:VAL:CG1	2.37	0.92
1:A:399:ARG:NH2	1:A:410:TYR:CB	2.33	0.92
2:B:377:LYS:CD	2:B:382:THR:CG2	2.48	0.90
2:B:321:LEU:CA	2:B:324:MET:CG	2.48	0.90
2:B:505:LEU:CD2	2:B:523:LEU:CD2	2.51	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:178:CYS:SG	1:A:180:ASP:CB	2.61	0.89
3:A:907:BGC:O3	3:A:908:BGC:O5	1.93	0.87
3:A:905:BGC:C6	2:B:566:VAL:CG1	2.53	0.86
2:B:107:LEU:CD1	2:B:160:ARG:CB	2.52	0.86
2:B:398:ARG:NH2	2:B:445:ASP:CG	2.30	0.85
1:A:95:ASP:O	1:A:99:LEU:CD1	2.24	0.84
2:B:158:ARG:O	2:B:171:LEU:CD2	2.26	0.83
2:B:419:SER:CB	2:B:438:MET:CE	2.57	0.82
2:B:117:MET:SD	2:B:151:VAL:CG2	2.69	0.81
2:B:163:CYS:O	2:B:163:CYS:SG	2.37	0.81
2:B:615:ALA:CB	2:B:621:LEU:CG	2.58	0.81
1:A:103:LEU:CD1	1:A:425:MET:CE	2.60	0.81
1:A:751:HIS:ND1	1:A:752:LEU:N	2.30	0.80
2:B:321:LEU:CA	2:B:324:MET:CB	2.60	0.80
1:A:84:ARG:CA	1:A:88:THR:OG1	2.30	0.80
1:A:646:ALA:CB	1:A:647:PRO:CD	2.60	0.80
1:A:507:ALA:CB	1:A:509:ASP:OD1	2.30	0.80
1:A:503:PHE:O	1:A:503:PHE:CD1	2.35	0.79
2:B:346:ASP:O	2:B:346:ASP:OD1	1.99	0.79
2:B:345:PRO:O	2:B:346:ASP:CB	2.30	0.79
1:A:271:LEU:CD1	1:A:317:PHE:CB	2.62	0.78
2:B:96:LEU:CD2	2:B:137:THR:CG2	2.62	0.78
1:A:182:GLY:O	1:A:183:THR:C	2.20	0.77
2:B:145:ARG:O	2:B:146:ALA:CB	2.32	0.77
1:A:452:MET:CE	1:A:558:TRP:NE1	2.48	0.76
1:A:258:ARG:NH2	1:A:364:MET:CE	2.48	0.76
1:A:752:LEU:O	1:A:753:LEU:CB	2.31	0.76
1:A:182:GLY:O	1:A:185:GLN:N	2.20	0.75
2:B:107:LEU:CB	2:B:110:SER:CB	2.64	0.75
1:A:284:ILE:O	1:A:288:LEU:CD1	2.34	0.75
1:A:183:THR:O	1:A:187:CYS:N	2.19	0.75
4:A:919:UDP:O1B	4:A:919:UDP:O1A	2.05	0.74
1:A:262:TYR:CZ	1:A:360:ILE:CD1	2.69	0.74
2:B:118:ASN:OD1	2:B:144:VAL:CG1	2.36	0.74
1:A:658:ARG:CG	1:A:672:ILE:CD1	2.65	0.74
2:B:511:VAL:N	2:B:512:PRO:CD	2.51	0.73
1:A:637:ILE:CD1	1:A:657:ILE:CG2	2.66	0.73
2:B:350:LEU:CD1	2:B:451:SER:CB	2.66	0.73
1:A:304:LYS:CG	1:A:470:GLN:OE1	2.37	0.73
2:B:266:ASP:CB	2:B:285:PRO:CD	2.66	0.72
2:B:125:PHE:CZ	2:B:138:MET:CG	2.73	0.72
1:A:259:THR:CG2	1:A:323:VAL:CG2	2.67	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:163:CYS:O	2:B:423:GLY:CA	2.38	0.71
2:B:616:PRO:O	2:B:617:GLU:CG	2.38	0.71
1:A:675:ALA:CB	1:A:757:THR:O	2.38	0.71
1:A:288:LEU:CD1	1:A:288:LEU:N	2.51	0.70
1:A:66:ARG:NH1	1:A:123:ALA:O	2.25	0.70
1:A:507:ALA:O	1:A:508:LYS:C	2.30	0.70
2:B:390:ARG:C	2:B:391:ASP:OD1	2.30	0.70
2:B:344:LEU:CB	2:B:345:PRO:CD	2.70	0.69
1:A:676:GLY:C	1:A:678:PRO:CD	2.61	0.69
1:A:649:LEU:O	1:A:684:THR:CG2	2.40	0.69
2:B:616:PRO:C	2:B:617:GLU:CG	2.59	0.69
1:A:132:ARG:N	1:A:265:GLU:OE2	2.26	0.69
1:A:182:GLY:O	1:A:184:ASP:N	2.26	0.68
1:A:595:ILE:CG2	1:A:596:PRO:CD	2.71	0.68
1:A:169:PRO:O	1:A:171:ARG:N	2.26	0.68
3:A:911:BGC:O3	3:A:912:BGC:O5	2.12	0.68
2:B:118:ASN:CB	2:B:144:VAL:CG2	2.71	0.67
1:A:258:ARG:NE	1:A:364:MET:CE	2.58	0.67
1:A:455:TYR:OH	3:A:912:BGC:C6	2.43	0.67
1:A:121:LEU:CD2	1:A:412:ASN:ND2	2.58	0.66
2:B:122:ILE:CG2	2:B:140:LEU:CG	2.74	0.66
2:B:678:SER:O	2:B:682:VAL:CG2	2.44	0.66
1:A:35:ALA:O	1:A:79:ARG:NH2	2.29	0.65
1:A:592:GLU:OE2	1:A:642:LYS:CE	2.44	0.65
1:A:339:THR:CG2	1:A:345:GLU:CG	2.74	0.65
1:A:272:VAL:CG2	1:A:358:LEU:CD1	2.75	0.65
1:A:751:HIS:ND1	1:A:752:LEU:O	2.29	0.65
1:A:301:PHE:CZ	1:A:306:HIS:CD2	2.85	0.65
2:B:456:MET:SD	2:B:671:PRO:CB	2.84	0.65
2:B:117:MET:N	2:B:120:GLN:O	2.30	0.65
1:A:506:THR:O	1:A:507:ALA:CB	2.45	0.65
1:A:358:LEU:CD1	1:A:358:LEU:N	2.59	0.64
2:B:673:LEU:CD1	2:B:675:GLU:O	2.46	0.64
1:A:442:VAL:O	1:A:442:VAL:CG2	2.44	0.64
2:B:459:MET:SD	2:B:613:LEU:CD2	2.86	0.64
2:B:95:THR:CG2	2:B:96:LEU:N	2.61	0.64
1:A:514:GLU:CA	1:A:578:GLN:CB	2.76	0.64
2:B:361:ASP:OD2	2:B:398:ARG:NH1	2.30	0.63
1:A:146:VAL:O	1:A:177:LEU:N	2.31	0.63
3:A:910:BGC:O3	3:A:911:BGC:O5	2.15	0.63
2:B:360:ILE:CD1	2:B:401:ILE:CD1	2.78	0.62
1:A:599:GLY:O	1:A:600:ASN:CB	2.45	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:126:THR:N	2:B:127:PRO:CD	2.63	0.61
2:B:528:LEU:CB	2:B:529:PRO:CD	2.78	0.61
1:A:549:ARG:O	1:A:553:LEU:CD1	2.48	0.61
1:A:644:PRO:C	1:A:646:ALA:N	2.52	0.61
1:A:273:GLN:OE1	1:A:317:PHE:CA	2.49	0.61
1:A:382:ARG:NE	4:A:919:UDP:O2B	2.33	0.61
1:A:270:PHE:CD2	1:A:271:LEU:N	2.69	0.60
1:A:361:ASP:OD1	1:A:700:ARG:NH1	2.35	0.60
1:A:434:LEU:CD2	1:A:538:THR:CG2	2.80	0.60
2:B:481:ARG:NH1	2:B:504:GLY:CA	2.64	0.60
1:A:399:ARG:NH1	1:A:407:ARG:CA	2.65	0.60
2:B:144:VAL:C	2:B:145:ARG:CG	2.70	0.60
1:A:473:PRO:O	1:A:716:ILE:CD1	2.50	0.60
2:B:122:ILE:CG2	2:B:140:LEU:CD1	2.79	0.59
2:B:107:LEU:N	2:B:107:LEU:CD1	2.65	0.59
1:A:364:MET:C	1:A:365:ILE:CG2	2.71	0.59
2:B:419:SER:CB	2:B:438:MET:SD	2.90	0.59
1:A:270:PHE:CG	1:A:271:LEU:N	2.71	0.59
2:B:458:ASP:OD1	2:B:461:ARG:NH1	2.36	0.59
1:A:513:SER:O	1:A:514:GLU:CB	2.51	0.59
1:A:132:ARG:CB	1:A:265:GLU:OE2	2.51	0.58
1:A:486:TYR:OH	1:A:524:LEU:CD1	2.51	0.58
2:B:341:ASP:OD2	2:B:645:PRO:CG	2.50	0.58
1:A:510:GLU:N	1:A:510:GLU:OE1	2.36	0.58
1:A:663:GLU:O	1:A:664:GLY:C	2.40	0.57
2:B:383:VAL:O	2:B:383:VAL:CG1	2.51	0.57
1:A:503:PHE:CG	1:A:503:PHE:O	2.57	0.57
2:B:373:LEU:CD1	2:B:375:LEU:CD1	2.82	0.57
2:B:424:ASN:CB	2:B:425:PRO:CD	2.83	0.57
2:B:383:VAL:CG2	2:B:403:PHE:CB	2.82	0.57
1:A:487:LEU:N	1:A:487:LEU:CD1	2.68	0.57
1:A:269:LEU:CD1	1:A:269:LEU:C	2.68	0.57
2:B:320:THR:O	2:B:442:SER:O	2.23	0.57
1:A:144:ILE:CG1	1:A:144:ILE:O	2.52	0.57
1:A:612:THR:OG1	1:A:753:LEU:CA	2.53	0.56
2:B:682:VAL:O	2:B:686:VAL:CG2	2.53	0.56
1:A:273:GLN:OE1	1:A:318:CYS:N	2.38	0.56
1:A:271:LEU:O	1:A:358:LEU:CD1	2.53	0.56
2:B:351:LEU:CD1	2:B:691:SER:CB	2.83	0.56
2:B:501:THR:CG2	2:B:622:TRP:CD2	2.88	0.56
1:A:128:ARG:NH1	1:A:310:ASP:OD1	2.38	0.56
1:A:402:LEU:CG	1:A:403:GLY:N	2.68	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:105:ASP:O	2:B:105:ASP:OD2	2.24	0.56
1:A:676:GLY:O	1:A:678:PRO:CD	2.53	0.56
2:B:122:ILE:CG2	2:B:140:LEU:CD2	2.84	0.56
2:B:523:LEU:N	2:B:523:LEU:CD1	2.69	0.56
1:A:258:ARG:CZ	1:A:364:MET:CE	2.84	0.56
2:B:409:HIS:O	2:B:413:ASN:OD1	2.25	0.55
2:B:320:THR:O	2:B:321:LEU:CB	2.55	0.55
1:A:84:ARG:CD	1:A:88:THR:CG2	2.84	0.55
2:B:115:VAL:CG1	2:B:123:GLY:O	2.54	0.55
1:A:498:PRO:O	1:A:499:ARG:CB	2.54	0.55
2:B:264:ASP:N	2:B:264:ASP:OD1	2.40	0.55
2:B:105:ASP:O	2:B:105:ASP:CG	2.45	0.55
5:A:920:LDA:CM2	2:B:708:SER:OG	2.55	0.55
1:A:100:PHE:CG	1:A:432:ILE:CD1	2.89	0.55
1:A:471:ARG:NH1	1:A:476:SER:OG	2.40	0.54
1:A:394:LYS:O	1:A:395:ASN:C	2.44	0.54
2:B:350:LEU:CD1	2:B:350:LEU:N	2.71	0.54
2:B:292:ALA:O	2:B:294:LEU:N	2.41	0.54
1:A:423:ARG:NH1	1:A:480:GLU:OE1	2.41	0.54
2:B:347:ASP:C	2:B:347:ASP:OD1	2.47	0.53
1:A:37:VAL:CG1	1:A:38:ALA:N	2.70	0.53
2:B:375:LEU:CD1	2:B:375:LEU:N	2.71	0.53
1:A:292:ASP:OD1	1:A:293:ARG:N	2.42	0.53
1:A:188:MET:O	1:A:189:SER:C	2.44	0.53
1:A:310:ASP:O	1:A:313:GLY:N	2.41	0.53
1:A:338:GLU:OE2	1:A:499:ARG:NH2	2.42	0.53
2:B:383:VAL:CG1	2:B:401:ILE:CG2	2.86	0.53
1:A:330:ASP:O	1:A:333:GLY:N	2.41	0.53
2:B:346:ASP:O	2:B:346:ASP:CG	2.45	0.53
3:A:909:BGC:O3	3:A:910:BGC:O5	2.26	0.52
1:A:100:PHE:CD2	1:A:432:ILE:CD1	2.92	0.52
1:A:403:GLY:O	1:A:407:ARG:N	2.43	0.52
1:A:360:ILE:CG2	1:A:361:ASP:N	2.72	0.52
1:A:130:PHE:O	1:A:131:PRO:C	2.46	0.52
2:B:113:ILE:O	2:B:125:PHE:N	2.43	0.52
1:A:169:PRO:C	1:A:171:ARG:N	2.62	0.52
2:B:292:ALA:O	2:B:293:SER:C	2.48	0.52
2:B:553:LEU:O	2:B:555:ALA:N	2.42	0.52
1:A:647:PRO:CB	1:A:649:LEU:CB	2.88	0.51
2:B:614:LEU:CD1	2:B:614:LEU:N	2.72	0.51
1:A:77:VAL:CG2	1:A:78:MET:N	2.72	0.51
1:A:42:GLN:OE1	1:A:79:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:409:HIS:N	2:B:413:ASN:ND2	2.58	0.51
2:B:506:HIS:O	2:B:507:ASP:C	2.47	0.51
1:A:145:LEU:O	1:A:145:LEU:CD1	2.58	0.51
1:A:542:TRP:NE1	1:A:549:ARG:NH1	2.58	0.51
2:B:391:ASP:O	2:B:392:ALA:C	2.46	0.51
1:A:271:LEU:CD1	1:A:317:PHE:CD2	2.94	0.51
1:A:184:ASP:OD1	1:A:188:MET:CG	2.59	0.51
1:A:647:PRO:O	1:A:647:PRO:CD	2.59	0.51
2:B:345:PRO:CG	2:B:348:TRP:CB	2.89	0.51
1:A:290:LEU:CD2	1:A:290:LEU:N	2.70	0.51
1:A:166:MET:CE	1:A:251:PRO:CB	2.89	0.51
3:A:917:BGC:O3	3:A:918:BGC:O5	2.28	0.51
2:B:118:ASN:O	2:B:119:ASP:CB	2.59	0.50
2:B:292:ALA:C	2:B:294:LEU:N	2.63	0.50
2:B:101:ARG:NE	2:B:173:THR:OG1	2.43	0.50
1:A:14:VAL:CG1	1:A:15:PRO:CD	2.89	0.50
1:A:677:GLN:N	1:A:678:PRO:CD	2.74	0.50
1:A:63:MET:CE	1:A:67:PHE:CE2	2.94	0.50
2:B:390:ARG:O	2:B:391:ASP:OD1	2.30	0.50
2:B:223:LEU:CD1	2:B:479:LEU:CD2	2.90	0.50
2:B:524:ALA:O	2:B:528:LEU:CB	2.60	0.50
1:A:84:ARG:O	1:A:88:THR:OG1	2.30	0.49
1:A:77:VAL:O	1:A:81:TRP:N	2.45	0.49
2:B:103:SER:O	2:B:104:ILE:CB	2.57	0.49
2:B:364:PHE:CE1	2:B:391:ASP:C	2.86	0.49
1:A:580:ARG:NH2	1:A:751:HIS:O	2.46	0.49
1:A:505:VAL:CG1	1:A:505:VAL:O	2.61	0.49
2:B:627:PRO:O	2:B:628:GLU:CB	2.60	0.49
2:B:378:VAL:CG2	2:B:378:VAL:O	2.61	0.49
1:A:219:ARG:NH1	1:A:223:GLU:N	2.62	0.48
1:A:351:HIS:CE1	1:A:357:SER:OG	2.66	0.48
1:A:351:HIS:NE2	1:A:357:SER:OG	2.46	0.48
1:A:275:PRO:CG	1:A:363:ALA:N	2.76	0.48
1:A:330:ASP:O	1:A:333:GLY:CA	2.62	0.48
2:B:360:ILE:CG2	2:B:361:ASP:N	2.77	0.48
1:A:288:LEU:CD2	1:A:568:PHE:CD2	2.96	0.48
1:A:396:PRO:O	1:A:399:ARG:NE	2.46	0.48
1:A:612:THR:O	1:A:673:PHE:CD1	2.66	0.48
1:A:64:VAL:CB	1:A:65:PRO:CD	2.91	0.48
1:A:84:ARG:O	1:A:88:THR:CB	2.62	0.48
2:B:349:LEU:C	2:B:350:LEU:CD1	2.81	0.48
1:A:595:ILE:O	1:A:599:GLY:CA	2.62	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:477:GLU:OE2	3:A:913:BGC:O6	2.32	0.48
2:B:69:GLY:O	2:B:71:LEU:N	2.47	0.48
2:B:144:VAL:O	2:B:145:ARG:CG	2.61	0.48
1:A:288:LEU:O	1:A:289:ALA:C	2.51	0.48
1:A:128:ARG:NH1	1:A:310:ASP:OD2	2.46	0.48
1:A:270:PHE:CD2	1:A:356:LYS:O	2.66	0.48
2:B:107:LEU:CD1	2:B:160:ARG:CG	2.92	0.48
1:A:568:PHE:CD1	1:A:720:ALA:CA	2.97	0.48
1:A:674:GLU:O	1:A:675:ALA:CB	2.62	0.48
1:A:121:LEU:CD1	1:A:121:LEU:N	2.77	0.48
1:A:186:ARG:CG	1:A:199:GLN:CG	2.92	0.48
3:A:905:BGC:O6	2:B:568:SER:OG	2.31	0.47
2:B:501:THR:CG2	2:B:622:TRP:CG	2.97	0.47
2:B:63:ALA:CB	2:B:67:GLN:NE2	2.77	0.47
1:A:145:LEU:C	1:A:145:LEU:CD1	2.82	0.47
2:B:100:GLN:NE2	2:B:132:ALA:O	2.48	0.47
2:B:99:ALA:CB	2:B:129:GLN:OE1	2.62	0.47
2:B:527:LEU:CB	2:B:609:GLY:O	2.63	0.47
1:A:274:THR:OG1	1:A:321:ALA:O	2.32	0.47
1:A:504:ALA:O	1:A:506:THR:CG2	2.63	0.47
1:A:223:GLU:O	1:A:224:HIS:CB	2.63	0.47
2:B:69:GLY:C	2:B:71:LEU:N	2.67	0.47
1:A:597:ALA:C	1:A:599:GLY:N	2.68	0.47
1:A:37:VAL:CG1	1:A:41:ALA:CB	2.93	0.47
3:A:914:BGC:O3	3:A:915:BGC:O5	2.33	0.47
1:A:216:TYR:C	1:A:216:TYR:CD2	2.88	0.47
2:B:321:LEU:O	2:B:325:GLY:N	2.48	0.47
1:A:433:TYR:O	1:A:437:GLY:N	2.48	0.47
1:A:184:ASP:C	1:A:184:ASP:OD1	2.53	0.47
1:A:658:ARG:CD	1:A:672:ILE:CD1	2.93	0.47
1:A:57:LYS:N	1:A:58:PRO:CD	2.77	0.47
2:B:79:ALA:O	2:B:155:ALA:N	2.48	0.46
1:A:429:ALA:O	1:A:432:ILE:CG2	2.63	0.46
2:B:102:SER:CB	2:B:172:TRP:CD1	2.99	0.46
2:B:513:LEU:O	2:B:513:LEU:CD1	2.64	0.46
2:B:107:LEU:CB	2:B:110:SER:OG	2.64	0.46
2:B:113:ILE:N	2:B:125:PHE:O	2.49	0.46
2:B:76:GLY:O	2:B:77:GLN:CB	2.64	0.46
1:A:219:ARG:NH1	1:A:223:GLU:O	2.49	0.46
2:B:98:LEU:CD1	2:B:179:GLN:CB	2.93	0.46
1:A:182:GLY:C	1:A:184:ASP:N	2.69	0.46
1:A:195:ALA:O	1:A:199:GLN:N	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:194:LEU:O	1:A:198:ALA:CB	2.64	0.46
1:A:341:THR:CG2	1:A:341:THR:O	2.64	0.45
2:B:321:LEU:CD2	2:B:324:MET:CG	2.94	0.45
1:A:189:SER:O	1:A:190:PRO:C	2.54	0.45
1:A:130:PHE:O	1:A:131:PRO:O	2.35	0.45
3:A:911:BGC:C3	3:A:912:BGC:O5	2.63	0.45
2:B:456:MET:O	2:B:461:ARG:NH2	2.50	0.45
1:A:299:GLU:O	1:A:303:GLY:N	2.50	0.45
3:A:905:BGC:O6	2:B:566:VAL:CG1	2.64	0.45
1:A:644:PRO:O	1:A:645:ASP:CB	2.65	0.45
2:B:125:PHE:CZ	2:B:138:MET:SD	3.10	0.45
2:B:65:THR:OG1	2:B:67:GLN:NE2	2.49	0.45
2:B:125:PHE:CE1	2:B:136:VAL:CG2	2.99	0.45
1:A:286:ARG:NH2	1:A:575:GLU:OE1	2.50	0.45
1:A:129:PRO:O	1:A:130:PHE:C	2.54	0.45
1:A:207:GLN:O	1:A:211:GLU:CG	2.65	0.45
2:B:106:ILE:CB	2:B:160:ARG:CD	2.95	0.45
1:A:254:ASP:OD1	1:A:364:MET:SD	2.75	0.45
2:B:348:TRP:C	2:B:348:TRP:CE3	2.90	0.45
2:B:83:PHE:O	2:B:151:VAL:N	2.50	0.45
1:A:510:GLU:CG	1:A:512:LEU:CD1	2.95	0.45
2:B:122:ILE:CD1	2:B:140:LEU:O	2.65	0.44
1:A:128:ARG:NH1	1:A:310:ASP:CG	2.71	0.44
1:A:271:LEU:CD1	1:A:317:PHE:CG	3.00	0.44
1:A:751:HIS:CG	1:A:752:LEU:N	2.84	0.44
2:B:456:MET:O	2:B:461:ARG:NH1	2.51	0.44
1:A:263:PHE:O	1:A:325:ARG:NH1	2.51	0.44
2:B:118:ASN:OD1	2:B:144:VAL:CB	2.65	0.44
1:A:80:TYR:C	1:A:80:TYR:CD2	2.91	0.44
1:A:501:ALA:CB	1:A:503:PHE:CE2	3.00	0.44
2:B:345:PRO:CG	2:B:346:ASP:N	2.78	0.44
1:A:263:PHE:CE1	1:A:270:PHE:O	2.71	0.44
1:A:185:GLN:CG	1:A:222:ASN:ND2	2.80	0.44
2:B:254:THR:O	2:B:277:ALA:CB	2.65	0.44
1:A:641:PRO:CB	1:A:643:PHE:CE1	3.01	0.44
2:B:389:ASP:OD1	2:B:390:ARG:CG	2.65	0.44
1:A:302:TYR:OH	3:A:917:BGC:C6	2.66	0.44
2:B:99:ALA:O	2:B:134:GLY:CA	2.66	0.44
1:A:419:PHE:O	1:A:420:PRO:C	2.54	0.44
1:A:649:LEU:CG	1:A:649:LEU:O	2.66	0.43
2:B:189:ILE:CG1	2:B:190:GLY:N	2.82	0.43
1:A:310:ASP:O	1:A:311:ARG:C	2.56	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:PHE:O	1:A:109:THR:OG1	2.37	0.43
1:A:340:ILE:CD1	1:A:501:ALA:CB	2.97	0.43
1:A:343:ASP:N	1:A:343:ASP:OD1	2.51	0.43
2:B:87:LEU:CD1	2:B:88:PRO:O	2.66	0.43
2:B:77:GLN:OE1	2:B:337:ASN:ND2	2.52	0.43
2:B:333:ASN:OD1	2:B:333:ASN:N	2.51	0.43
1:A:249:HIS:CD2	1:A:320:SER:OG	2.72	0.43
2:B:330:LEU:CD2	2:B:439:GLN:CB	2.94	0.43
1:A:434:LEU:O	1:A:541:ARG:NH2	2.52	0.43
2:B:616:PRO:O	2:B:617:GLU:CB	2.63	0.43
1:A:78:MET:CE	1:A:78:MET:CA	2.96	0.43
1:A:423:ARG:NH2	3:A:913:BGC:O6	2.52	0.43
2:B:118:ASN:ND2	2:B:144:VAL:CG1	2.82	0.42
1:A:571:ARG:NH1	1:A:723:SER:CB	2.82	0.42
1:A:504:ALA:O	1:A:505:VAL:C	2.58	0.42
1:A:417:TRP:O	1:A:491:ILE:CD1	2.67	0.42
2:B:530:SER:O	2:B:531:THR:O	2.38	0.42
1:A:141:THR:O	1:A:240:GLU:CB	2.67	0.42
2:B:108:PRO:O	2:B:109:GLU:CB	2.66	0.42
1:A:117:LEU:O	1:A:121:LEU:CD1	2.68	0.42
1:A:88:THR:CG2	1:A:441:PHE:CZ	3.02	0.42
1:A:131:PRO:C	1:A:265:GLU:OE2	2.58	0.42
1:A:266:ASP:C	1:A:267:PRO:O	2.57	0.42
2:B:398:ARG:NH2	2:B:445:ASP:OD2	2.52	0.42
2:B:96:LEU:CD1	2:B:96:LEU:C	2.87	0.42
1:A:637:ILE:CG2	1:A:638:GLN:N	2.83	0.42
2:B:521:ARG:O	2:B:524:ALA:N	2.53	0.42
1:A:172:LEU:C	1:A:172:LEU:CD1	2.88	0.42
1:A:643:PHE:CB	1:A:647:PRO:CD	2.98	0.42
1:A:352:SER:O	1:A:401:GLY:CA	2.67	0.42
1:A:458:VAL:O	1:A:462:VAL:N	2.53	0.42
1:A:255:PHE:C	1:A:255:PHE:CD1	2.93	0.41
1:A:234:LEU:C	1:A:236:ARG:N	2.72	0.41
1:A:139:LEU:O	1:A:171:ARG:NH1	2.53	0.41
1:A:577:GLN:O	1:A:577:GLN:CG	2.68	0.41
1:A:546:PRO:CA	1:A:549:ARG:NE	2.83	0.41
1:A:709:LEU:CD1	1:A:709:LEU:C	2.89	0.41
1:A:167:ILE:N	1:A:167:ILE:CD1	2.83	0.41
2:B:83:PHE:N	2:B:151:VAL:O	2.52	0.41
2:B:285:PRO:C	2:B:287:GLU:N	2.74	0.41
2:B:162:TYR:N	2:B:162:TYR:CD2	2.89	0.41
1:A:84:ARG:C	1:A:88:THR:OG1	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:550:LEU:O	2:B:550:LEU:CG	2.68	0.41
2:B:266:ASP:O	2:B:268:VAL:N	2.54	0.41
2:B:617:GLU:CB	2:B:618:PRO:CD	2.98	0.41
3:A:910:BGC:C3	3:A:911:BGC:O5	2.69	0.41
2:B:694:PRO:N	2:B:695:PRO:CD	2.83	0.41
1:A:339:THR:OG1	1:A:340:ILE:O	2.38	0.40
1:A:34:ALA:O	2:B:683:ARG:NH1	2.54	0.40
1:A:592:GLU:OE2	1:A:642:LYS:NZ	2.54	0.40
1:A:626:ASP:N	1:A:627:PRO:CD	2.83	0.40
1:A:361:ASP:C	1:A:361:ASP:OD1	2.58	0.40
1:A:395:ASN:N	1:A:396:PRO:CD	2.84	0.40
1:A:72:ALA:O	1:A:75:MET:CG	2.70	0.40
2:B:625:LEU:CD1	2:B:625:LEU:N	2.84	0.40
1:A:713:MET:O	1:A:717:LEU:CD1	2.70	0.40
1:A:263:PHE:CZ	1:A:270:PHE:O	2.73	0.40
2:B:391:ASP:N	2:B:391:ASP:OD1	2.49	0.40
1:A:556:GLY:O	1:A:557:GLY:C	2.60	0.40
2:B:334:ARG:NH1	2:B:430:CYS:CB	2.85	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	745/802 (93%)	674 (90%)	64 (9%)	7 (1%)	25	77
2	B	651/707 (92%)	574 (88%)	67 (10%)	10 (2%)	15	66
All	All	1396/1509 (92%)	1248 (89%)	131 (9%)	17 (1%)	19	72

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	PRO
1	A	514	GLU

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Mol	Chain	Res	Type
1	A	647	PRO
2	B	146	ALA
2	B	529	PRO
2	B	104	ILE
2	B	425	PRO
1	A	677	GLN
2	B	293	SER
2	B	554	GLY
1	A	183	THR
2	B	520	PRO
1	A	507	ALA
2	B	88	PRO
1	A	624	VAL
2	B	126	THR
2	B	616	PRO

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	614/661 (93%)	595 (97%)	19 (3%)	52	88
2	B	520/559 (93%)	492 (95%)	28 (5%)	31	76
All	All	1134/1220 (93%)	1087 (96%)	47 (4%)	41	83

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	37	VAL
1	A	40	SER
1	A	97	SER
1	A	102	LEU
1	A	111	SER
1	A	167	ILE
1	A	187	CYS
1	A	248	ASP
1	A	284	ILE

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Mol	Chain	Res	Type
1	A	317	PHE
1	A	339	THR
1	A	358	LEU
1	A	385	THR
1	A	459	SER
1	A	524	LEU
1	A	595	ILE
1	A	621	LEU
1	A	626	ASP
2	B	150	LEU
2	B	157	HIS
2	B	163	CYS
2	B	172	TRP
2	B	184	LEU
2	B	233	PRO
2	B	269	SER
2	B	289	SER
2	B	309	THR
2	B	310	LEU
2	B	312	GLN
2	B	319	VAL
2	B	331	THR
2	B	333	ASN
2	B	378	VAL
2	B	430	CYS
2	B	451	SER
2	B	494	ASP
2	B	500	LEU
2	B	513	LEU
2	B	523	LEU
2	B	550	LEU
2	B	553	LEU
2	B	561	VAL
2	B	568	SER
2	B	588	THR
2	B	614	LEU
2	B	617	GLU

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

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

18 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BGC	A	901	3	12,12,12	0.47	0	17,17,17	1.87	3 (17%)
3	BGC	A	902	3	10,11,12	0.80	0	11,15,17	2.10	3 (27%)
3	BGC	A	903	3	10,11,12	0.78	0	11,15,17	1.48	1 (9%)
3	BGC	A	904	3	10,11,12	0.72	0	11,15,17	1.25	1 (9%)
3	BGC	A	905	3	10,11,12	0.78	0	11,15,17	1.08	1 (9%)
3	BGC	A	906	3	10,11,12	0.81	0	11,15,17	2.47	4 (36%)
3	BGC	A	907	3	10,11,12	0.79	0	11,15,17	1.52	2 (18%)
3	BGC	A	908	3	10,11,12	0.71	0	11,15,17	1.33	2 (18%)
3	BGC	A	909	3	10,11,12	0.73	0	11,15,17	1.79	3 (27%)
3	BGC	A	910	3	10,11,12	0.83	1 (10%)	11,15,17	1.24	3 (27%)
3	BGC	A	911	3	10,11,12	0.98	1 (10%)	11,15,17	1.47	2 (18%)
3	BGC	A	912	3	10,11,12	1.18	1 (10%)	11,15,17	1.75	3 (27%)
3	BGC	A	913	3	10,11,12	0.93	0	11,15,17	2.03	3 (27%)
3	BGC	A	914	3	10,11,12	0.78	0	11,15,17	2.52	4 (36%)
3	BGC	A	915	3	10,11,12	0.72	0	11,15,17	1.77	2 (18%)
3	BGC	A	916	3	10,11,12	0.69	0	11,15,17	1.80	2 (18%)
3	BGC	A	917	3	10,11,12	0.71	0	11,15,17	2.39	3 (27%)
3	BGC	A	918	3	10,11,12	0.86	1 (10%)	11,15,17	1.68	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	A	901	3	-	0/2/22/22	0/1/1/1
3	BGC	A	902	3	-	0/2/19/22	0/1/1/1
3	BGC	A	903	3	-	0/2/19/22	0/1/1/1
3	BGC	A	904	3	-	0/2/19/22	0/1/1/1
3	BGC	A	905	3	-	0/2/19/22	0/1/1/1
3	BGC	A	906	3	-	0/2/19/22	0/1/1/1
3	BGC	A	907	3	-	0/2/19/22	0/1/1/1
3	BGC	A	908	3	-	0/2/19/22	0/1/1/1
3	BGC	A	909	3	-	0/2/19/22	0/1/1/1
3	BGC	A	910	3	-	0/2/19/22	0/1/1/1
3	BGC	A	911	3	-	0/2/19/22	0/1/1/1
3	BGC	A	912	3	-	0/2/19/22	0/1/1/1
3	BGC	A	913	3	-	0/2/19/22	0/1/1/1
3	BGC	A	914	3	-	0/2/19/22	0/1/1/1
3	BGC	A	915	3	-	0/2/19/22	0/1/1/1
3	BGC	A	916	3	-	0/2/19/22	0/1/1/1
3	BGC	A	917	3	-	0/2/19/22	0/1/1/1
3	BGC	A	918	3	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	912	BGC	O5-C5	-3.18	1.39	1.45
3	A	911	BGC	O5-C5	-2.66	1.40	1.45
3	A	918	BGC	O5-C5	-2.20	1.41	1.45
3	A	910	BGC	O5-C5	-2.15	1.41	1.45

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	917	BGC	O5-C5-C4	6.45	118.84	110.65
3	A	914	BGC	O5-C5-C4	6.14	118.45	110.65
3	A	902	BGC	O5-C5-C4	5.31	117.39	110.65
3	A	901	BGC	O5-C5-C4	5.22	119.42	109.76
3	A	906	BGC	C4-C3-C2	5.13	117.39	110.50
3	A	913	BGC	O5-C5-C6	4.64	111.85	106.98
3	A	901	BGC	O5-C5-C6	4.51	117.41	106.34
3	A	916	BGC	O5-C5-C4	4.46	116.31	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	915	BGC	O5-C5-C6	4.03	111.22	106.98
3	A	906	BGC	O5-C5-C4	4.02	115.76	110.65
3	A	918	BGC	C4-C3-C2	3.74	115.52	110.50
3	A	914	BGC	O4-C4-C5	-3.72	99.49	109.28
3	A	911	BGC	O4-C4-C5	-3.62	99.74	109.28
3	A	913	BGC	C4-C3-C2	-3.58	105.70	110.50
3	A	903	BGC	O5-C5-C6	3.54	110.70	106.98
3	A	909	BGC	C4-C3-C2	3.31	114.94	110.50
3	A	904	BGC	O5-C5-C6	3.29	110.43	106.98
3	A	912	BGC	O4-C4-C5	-3.17	100.93	109.28
3	A	915	BGC	O4-C4-C3	-3.15	103.29	110.35
3	A	902	BGC	C3-C4-C5	2.94	115.45	110.20
3	A	917	BGC	O3-C3-C2	-2.93	104.58	109.94
3	A	906	BGC	C3-C4-C5	2.92	115.42	110.20
3	A	912	BGC	O5-C5-C6	2.81	109.93	106.98
3	A	912	BGC	C4-C3-C2	2.77	114.22	110.50
3	A	916	BGC	C3-C4-C5	-2.71	105.36	110.20
3	A	907	BGC	O5-C5-C4	2.69	114.06	110.65
3	A	918	BGC	O5-C5-C4	-2.62	107.32	110.65
3	A	917	BGC	O2-C2-C3	-2.53	104.71	110.18
3	A	914	BGC	O3-C3-C2	-2.52	105.33	109.94
3	A	909	BGC	O5-C5-C6	2.47	109.58	106.98
3	A	901	BGC	C6-C5-C4	2.35	118.68	113.00
3	A	911	BGC	O5-C5-C6	2.35	109.45	106.98
3	A	907	BGC	O2-C2-C3	-2.30	105.22	110.18
3	A	905	BGC	C4-C3-C2	2.22	113.49	110.50
3	A	908	BGC	O5-C5-C6	2.21	109.30	106.98
3	A	909	BGC	C6-C5-C4	-2.13	107.86	113.00
3	A	913	BGC	C6-C5-C4	-2.12	107.88	113.00
3	A	908	BGC	C3-C4-C5	-2.11	106.44	110.20
3	A	906	BGC	O4-C4-C3	-2.10	105.64	110.35
3	A	910	BGC	O4-C4-C5	-2.10	103.75	109.28
3	A	910	BGC	O4-C4-C3	2.04	114.94	110.35
3	A	902	BGC	O5-C5-C6	-2.04	104.84	106.98
3	A	910	BGC	O5-C5-C6	2.04	109.12	106.98
3	A	914	BGC	O4-C4-C3	2.02	114.89	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	UDP	A	919	-	26,26,26	0.90	1 (3%)	36,40,40	1.50	2 (5%)
5	LDA	A	920	-	8,8,15	5.55	3 (37%)	10,10,17	1.36	1 (10%)
5	LDA	A	921	-	15,15,15	3.56	2 (13%)	17,17,17	1.06	1 (5%)

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
4	UDP	A	919	-	-	0/14/32/32	0/2/2/2
5	LDA	A	920	-	-	0/6/6/13	0/0/0/0
5	LDA	A	921	-	-	0/13/13/13	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	920	LDA	O1-N1	-14.74	1.25	1.39
5	A	921	LDA	O1-N1	-13.52	1.26	1.39
5	A	920	LDA	C5-C4	-4.33	1.53	1.55
5	A	920	LDA	C1-N1	-2.74	1.46	1.51
5	A	921	LDA	C1-N1	-2.26	1.47	1.51
4	A	919	UDP	C6-C5	2.00	1.39	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	919	UDP	PA-O3A-PB	-5.44	115.74	131.68
4	A	919	UDP	N3-C2-N1	5.24	120.35	115.97
5	A	920	LDA	C2-C1-N1	-4.06	106.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	921	LDA	C2-C1-N1	-3.94	107.01	113.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	747/802 (93%)	-0.09	4 (0%)	88 48	77, 127, 205, 236	0
2	B	655/707 (92%)	-0.10	7 (1%)	77 30	82, 143, 210, 235	0
All	All	1402/1509 (92%)	-0.10	11 (0%)	83 37	77, 135, 208, 236	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	544	GLY	4.2
2	B	545	PRO	3.4
2	B	145	ARG	2.9
1	A	399	ARG	2.5
1	A	258	ARG	2.5
2	B	183	ALA	2.4
1	A	627	PRO	2.3
2	B	101	ARG	2.3
1	A	758	ASP	2.2
2	B	133	LEU	2.1
2	B	132	ALA	2.1

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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	BGC	A	913	11/12	0.41	6.36	88,107,120,127	0
3	BGC	A	914	11/12	0.35	3.57	97,114,126,129	0
3	BGC	A	912	11/12	0.34	3.03	86,103,140,157	0
3	BGC	A	915	11/12	0.34	1.48	108,116,170,173	0
3	BGC	A	917	11/12	0.33	1.37	97,106,119,140	0
3	BGC	A	918	11/12	0.35	1.08	116,121,136,142	0
3	BGC	A	907	11/12	0.18	0.71	79,109,137,143	0
3	BGC	A	911	11/12	0.21	0.43	83,93,108,111	0
3	BGC	A	916	11/12	0.26	0.24	90,104,129,158	0
3	BGC	A	906	11/12	0.16	-0.12	77,96,110,146	0
3	BGC	A	909	11/12	0.19	-0.46	70,96,103,127	0
3	BGC	A	910	11/12	0.17	-0.46	82,97,109,114	0
3	BGC	A	905	11/12	0.15	-0.50	95,114,142,143	0
3	BGC	A	908	11/12	0.15	-0.64	78,92,104,118	0
3	BGC	A	904	11/12	0.10	-2.05	97,115,128,142	0
3	BGC	A	901	12/12	0.39	-	176,192,196,198	0
3	BGC	A	902	11/12	0.23	-	149,170,193,198	0
3	BGC	A	903	11/12	0.10	-	100,112,144,154	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	UDP	A	919	25/25	0.71	4.81	57,85,113,131	25
5	LDA	A	921	16/16	0.34	2.70	105,128,177,182	0
5	LDA	A	920	9/16	0.32	2.11	92,109,143,144	0

6.5 Other polymers ⓘ

There are no such residues in this entry.