



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:26 AM GMT

PDB ID : 3A7B
Title : Crystal structure of TLR2-Streptococcus Pneumoniae lipoteichoic acid complex
Authors : Kang, J.Y.; Jin, M.S.; Lee, J.-O.
Deposited on : 2009-09-20
Resolution : 2.53 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>

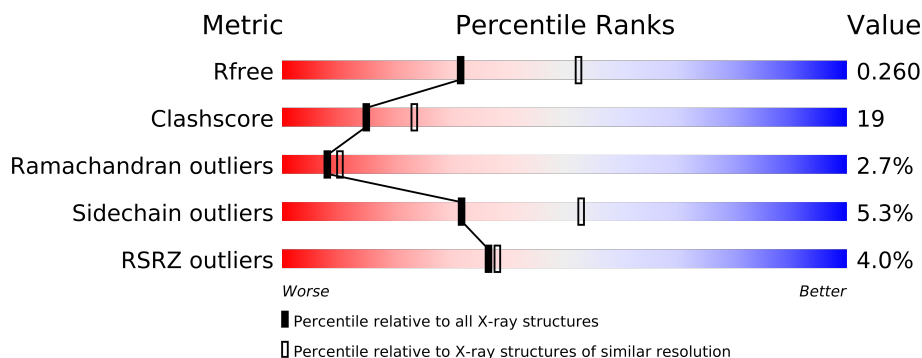
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.53 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	3240 (2.54-2.50)
Clashscore	79885	4080 (2.54-2.50)
Ramachandran outliers	78287	3990 (2.54-2.50)
Sidechain outliers	78261	3992 (2.54-2.50)
RSRZ outliers	66119	3241 (2.54-2.50)

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 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	580	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	NDG	A	821	-	X
4	LTC	A	581	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4720 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.

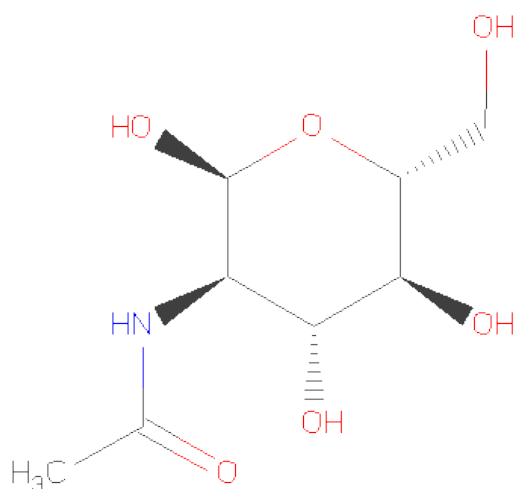
- Molecule 1 is a protein called Toll-like receptor 2, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	550	4355	2771	736	828	20	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	507	ALA	-	LINKER	UNP Q4G1L2
A	508	SER	-	LINKER	UNP Q4G1L2
A	577	LEU	-	EXPRESSION TAG	UNP Q4G1L2
A	578	VAL	-	EXPRESSION TAG	UNP Q4G1L2
A	579	PRO	-	EXPRESSION TAG	UNP Q4G1L2
A	580	ARG	-	EXPRESSION TAG	UNP Q4G1L2

- Molecule 2 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

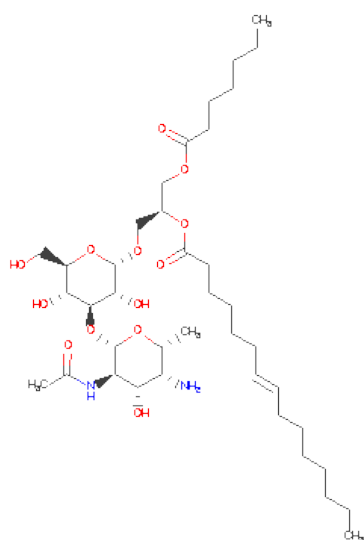
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	507	ALA	-	LINKER	UNP Q4G1L2
A	508	SER	-	LINKER	UNP Q4G1L2
A	577	LEU	-	EXPRESSION TAG	UNP Q4G1L2
A	578	VAL	-	EXPRESSION TAG	UNP Q4G1L2
A	579	PRO	-	EXPRESSION TAG	UNP Q4G1L2
A	580	ARG	-	EXPRESSION TAG	UNP Q4G1L2

- Molecule 4 is (2S)-1-({3-O-[2-(ACETYLAMINO)-4-AMINO-2,4,6-TRIDEOXY-BETA-D-GALACTOPYRANOSYL]-ALPHA-D-GLUCOPYRANOSYL}OXY)-3-(HEPTANOYLOXY)PROPAN-2-YL(7Z)-PENTADEC-7-ENOATE (three-letter code: LTC) (formula: C₃₉H₇₀N₂O₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			54	39	2	13		

- Molecule 5 is water.

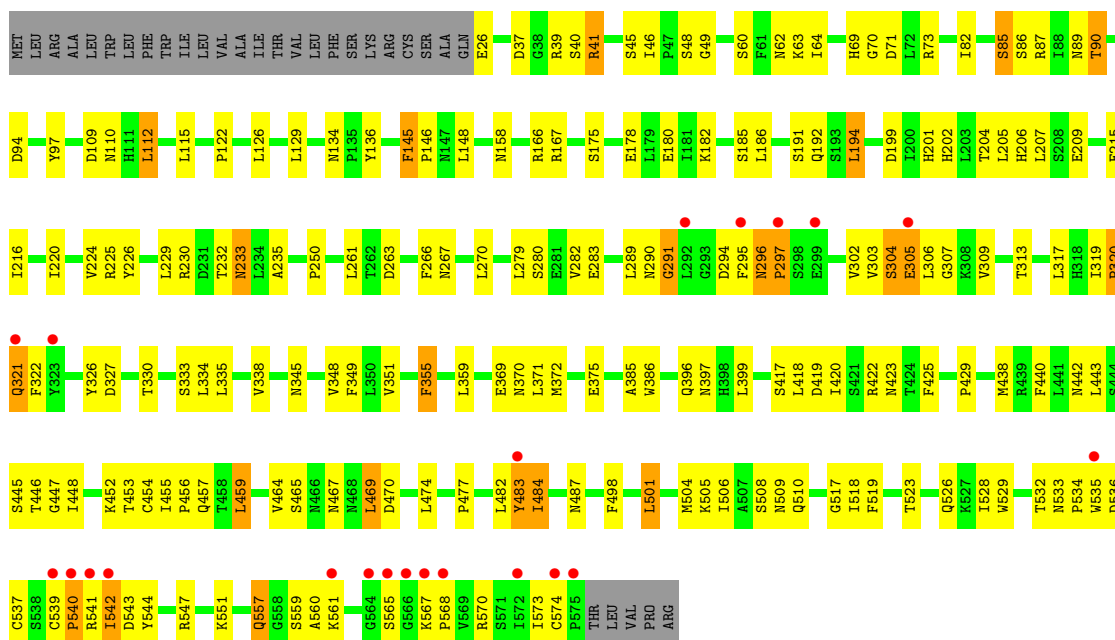
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	269	Total 269	O 269	0	0

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: Toll-like receptor 2, Variable lymphocyte receptor B

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.58Å 83.19Å 214.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.10 – 2.53 45.10 – 2.53	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.10-2.53) 95.5 (45.10-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.42 (at 2.54Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.270 0.228 , 0.260	Depositor DCC
R_{free} test set	4014 reflections (11.17%)	DCC
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 39965 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4720	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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: LTC, NAG, NDG

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	0.66	1/4439 (0.0%)	0.82	3/6013 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	540	PRO	C-N	5.47	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	351	VAL	N-CA-C	-5.21	96.92	111.00
1	A	86	SER	N-CA-C	-5.17	97.03	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4355	0	4400	169	0
2	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	25	2	0
4	A	54	0	70	7	0
5	A	269	0	0	2	0
All	All	4720	0	4508	171	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 19.

All (171) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:372:MET:H	1:A:397:ASN:HD22	1.03	0.93
1:A:63:LYS:HD3	1:A:87:ARG:HD2	1.52	0.91
1:A:283:GLU:HG2	1:A:313:THR:HB	1.53	0.90
1:A:537:CYS:HA	1:A:542:ILE:HG12	1.54	0.89
1:A:303:VAL:HG12	1:A:330:THR:HG23	1.57	0.85
1:A:469:LEU:H	1:A:487:ASN:HD22	1.24	0.84
1:A:539:CYS:SG	1:A:573:ILE:HG13	2.19	0.82
1:A:296:ASN:H	1:A:297:PRO:HD2	1.49	0.78
1:A:348:VAL:H	1:A:370:ASN:ND2	1.82	0.77
1:A:348:VAL:H	1:A:370:ASN:HD22	1.31	0.76
1:A:355:PHE:HE1	1:A:359:LEU:HD21	1.52	0.73
1:A:372:MET:H	1:A:397:ASN:ND2	1.84	0.73
1:A:446:THR:H	1:A:467:ASN:HD21	1.32	0.73
1:A:112:LEU:H	1:A:134:ASN:HD22	1.37	0.72
1:A:561:LYS:HA	1:A:568:PRO:HA	1.72	0.71
3:A:831:NAG:H61	3:A:832:NAG:H82	1.75	0.68
1:A:306:LEU:HD11	4:A:581:LTC:H11	1.75	0.68
1:A:417:SER:HB3	1:A:440:PHE:HB3	1.74	0.67
1:A:372:MET:N	1:A:397:ASN:HD22	1.87	0.67
1:A:279:LEU:HD12	1:A:309:VAL:HG22	1.77	0.67
1:A:446:THR:HG23	1:A:448:ILE:HG23	1.77	0.66
1:A:335:LEU:O	1:A:338:VAL:HG22	1.96	0.66
1:A:456:PRO:HG2	1:A:459:LEU:HD13	1.78	0.66
1:A:304:SER:HB2	1:A:333:SER:OG	1.96	0.65
1:A:63:LYS:NZ	1:A:87:ARG:NE	2.45	0.64
1:A:233:ASN:HD21	1:A:235:ALA:HB3	1.62	0.64
1:A:396:GLN:HG2	1:A:422:ARG:HB3	1.80	0.63
1:A:110:ASN:HB2	1:A:134:ASN:HD21	1.64	0.62
1:A:446:THR:HG22	1:A:467:ASN:HD21	1.63	0.62
1:A:70:GLY:HA2	1:A:73:ARG:HG2	1.82	0.62
1:A:201:HIS:HD2	1:A:225:ARG:HG3	1.64	0.61
1:A:37:ASP:OD1	1:A:39:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:455:ILE:HG23	1:A:459:LEU:HD22	1.82	0.61
1:A:482:LEU:HD23	1:A:504:MET:CE	2.32	0.59
1:A:467:ASN:HB2	1:A:487:ASN:HD21	1.68	0.58
1:A:509:ASN:O	1:A:510:GLN:HB2	2.04	0.58
1:A:559:SER:HB2	1:A:570:ARG:NH2	2.19	0.58
1:A:396:GLN:HG3	1:A:422:ARG:CZ	2.34	0.58
1:A:220:ILE:HB	1:A:224:VAL:HG23	1.85	0.57
1:A:321:GLN:CD	4:A:581:LTC:H4	2.25	0.57
1:A:447:GLY:H	1:A:467:ASN:ND2	2.02	0.56
1:A:69:HIS:HD2	1:A:94:ASP:OD1	1.87	0.56
1:A:60:SER:OG	1:A:82:ILE:HG22	2.05	0.56
1:A:537:CYS:HA	1:A:542:ILE:CG1	2.31	0.56
1:A:97:TYR:HA	1:A:122:PRO:HG3	1.87	0.56
1:A:306:LEU:HB3	1:A:309:VAL:HB	1.88	0.56
1:A:469:LEU:HD23	1:A:484:ILE:HD11	1.87	0.56
1:A:529:TRP:CZ2	1:A:557:GLN:HG2	2.41	0.56
1:A:205:LEU:HD11	1:A:216:ILE:HG21	1.88	0.55
1:A:498:PHE:HB3	1:A:501:LEU:HG	1.86	0.55
1:A:417:SER:CB	1:A:440:PHE:HB3	2.36	0.55
1:A:349:PHE:CE2	4:A:581:LTC:H28	2.42	0.54
1:A:539:CYS:H	1:A:540:PRO:HD2	1.72	0.54
1:A:469:LEU:H	1:A:487:ASN:ND2	1.99	0.54
1:A:510:GLN:HA	1:A:534:PRO:CD	2.38	0.54
1:A:233:ASN:HD22	1:A:233:ASN:C	2.10	0.54
1:A:542:ILE:O	1:A:542:ILE:HD12	2.08	0.53
3:A:831:NAG:H61	3:A:832:NAG:C8	2.39	0.53
1:A:455:ILE:HB	1:A:474:LEU:HD21	1.90	0.53
1:A:279:LEU:HD12	1:A:309:VAL:CG2	2.39	0.53
1:A:446:THR:HG22	1:A:467:ASN:ND2	2.24	0.53
1:A:532:THR:HG22	1:A:532:THR:O	2.08	0.52
1:A:355:PHE:CE1	1:A:359:LEU:HD21	2.40	0.52
1:A:375:GLU:HB2	5:A:612:HOH:O	2.09	0.52
1:A:464:VAL:HG23	1:A:484:ILE:HG12	1.92	0.52
1:A:175:SER:HA	1:A:199:ASP:O	2.09	0.51
1:A:60:SER:HG	1:A:82:ILE:HG22	1.76	0.51
1:A:518:ILE:HG23	1:A:519:PHE:N	2.25	0.51
1:A:45:SER:HA	1:A:64:ILE:HG23	1.92	0.51
1:A:303:VAL:O	1:A:304:SER:C	2.48	0.51
1:A:399:LEU:H	1:A:423:ASN:ND2	2.07	0.51
1:A:317:LEU:CD2	1:A:319:ILE:HD11	2.41	0.51
1:A:425:PHE:HD1	1:A:446:THR:OG1	1.94	0.51
1:A:399:LEU:H	1:A:423:ASN:HD22	1.59	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:535:TRP:CD1	1:A:560:ALA:HB1	2.47	0.50
1:A:85:SER:HA	1:A:109:ASP:O	2.12	0.50
1:A:26:GLU:CD	5:A:659:HOH:O	2.49	0.50
1:A:510:GLN:HA	1:A:534:PRO:HD2	1.94	0.50
1:A:220:ILE:HB	1:A:224:VAL:CG2	2.41	0.50
1:A:446:THR:H	1:A:467:ASN:ND2	2.06	0.49
1:A:372:MET:HG2	1:A:397:ASN:ND2	2.27	0.49
1:A:280:SER:HA	1:A:309:VAL:HA	1.95	0.49
1:A:385:ALA:O	1:A:386:TRP:C	2.50	0.49
1:A:369:GLU:HA	1:A:396:GLN:O	2.12	0.49
1:A:115:LEU:HD21	1:A:136:TYR:CD2	2.48	0.49
1:A:182:LYS:HA	1:A:206:HIS:HB2	1.94	0.48
1:A:145:PHE:N	1:A:146:PRO:HD2	2.28	0.48
1:A:178:GLU:HG3	1:A:202:HIS:HB3	1.94	0.48
1:A:320:PRO:O	1:A:321:GLN:HG2	2.14	0.48
1:A:506:ILE:O	1:A:506:ILE:HG12	2.13	0.48
1:A:89:ASN:ND2	1:A:90:THR:HG22	2.28	0.48
1:A:505:LYS:HG2	1:A:529:TRP:CE3	2.48	0.48
1:A:225:ARG:HD3	1:A:250:PRO:HB2	1.95	0.48
1:A:483:TYR:HA	1:A:505:LYS:HB2	1.95	0.48
1:A:535:TRP:NE1	1:A:560:ALA:HB1	2.29	0.48
1:A:63:LYS:CD	1:A:87:ARG:HD2	2.33	0.48
1:A:335:LEU:HD21	4:A:581:LTC:H11A	1.96	0.47
1:A:469:LEU:HB2	1:A:487:ASN:ND2	2.29	0.47
1:A:484:ILE:HG23	1:A:484:ILE:O	2.15	0.47
1:A:447:GLY:H	1:A:467:ASN:HD22	1.61	0.47
1:A:233:ASN:ND2	1:A:235:ALA:H	2.13	0.47
1:A:180:GLU:HG3	1:A:204:THR:HB	1.97	0.47
1:A:191:SER:O	1:A:192:GLN:CB	2.63	0.47
1:A:63:LYS:HZ1	1:A:87:ARG:NE	2.11	0.47
1:A:296:ASN:N	1:A:297:PRO:HD2	2.26	0.47
1:A:547:ARG:O	1:A:551:LYS:HG2	2.15	0.47
1:A:71:ASP:N	1:A:71:ASP:OD2	2.48	0.47
1:A:306:LEU:HD11	4:A:581:LTC:C11	2.43	0.47
1:A:191:SER:O	1:A:192:GLN:HB2	2.16	0.46
1:A:452:LYS:C	1:A:454:CYS:H	2.18	0.46
1:A:263:ASP:H	1:A:291:GLY:CA	2.28	0.46
1:A:303:VAL:O	1:A:305:GLU:N	2.48	0.45
1:A:305:GLU:C	1:A:307:GLY:H	2.19	0.45
1:A:420:ILE:HG13	1:A:443:LEU:HD23	1.97	0.45
1:A:541:ARG:O	1:A:542:ILE:HG13	2.16	0.45
1:A:504:MET:O	1:A:528:ILE:HA	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:457:GLN:HG2	1:A:477:PRO:HD2	1.97	0.45
1:A:206:HIS:CE1	1:A:230:ARG:HD2	2.51	0.45
1:A:263:ASP:HB2	1:A:291:GLY:HA3	1.98	0.45
1:A:536:ASP:O	1:A:542:ILE:HG12	2.17	0.45
1:A:319:ILE:N	1:A:319:ILE:HD12	2.32	0.45
1:A:419:ASP:HA	1:A:442:ASN:HB3	1.99	0.44
1:A:509:ASN:O	1:A:510:GLN:CB	2.65	0.44
1:A:112:LEU:H	1:A:134:ASN:ND2	2.08	0.44
1:A:321:GLN:HE22	4:A:581:LTC:H2	1.83	0.44
1:A:145:PHE:N	1:A:146:PRO:CD	2.81	0.44
1:A:63:LYS:HZ3	1:A:87:ARG:NE	2.14	0.44
1:A:541:ARG:C	1:A:542:ILE:HG13	2.38	0.44
1:A:207:LEU:O	1:A:232:THR:HA	2.18	0.43
1:A:317:LEU:HG	1:A:319:ILE:HD12	2.00	0.43
1:A:348:VAL:HG22	4:A:581:LTC:H24A	2.00	0.43
1:A:447:GLY:N	1:A:467:ASN:ND2	2.65	0.43
1:A:565:SER:C	1:A:567:LYS:H	2.22	0.43
1:A:48:SER:OG	1:A:49:GLY:N	2.52	0.43
1:A:429:PRO:O	1:A:454:CYS:HB2	2.18	0.43
1:A:457:GLN:HG2	1:A:477:PRO:CD	2.48	0.43
1:A:370:ASN:HB2	1:A:397:ASN:HD21	1.84	0.43
1:A:263:ASP:H	1:A:291:GLY:HA2	1.84	0.43
1:A:279:LEU:CD1	1:A:309:VAL:HG22	2.48	0.42
1:A:482:LEU:HD23	1:A:504:MET:HE1	2.01	0.42
1:A:418:LEU:HB2	1:A:438:MET:HE2	2.01	0.42
1:A:39:ARG:O	1:A:41:ARG:HD2	2.20	0.42
1:A:62:ASN:HB3	1:A:63:LYS:H	1.67	0.42
1:A:270:LEU:HB2	1:A:302:VAL:HG11	2.02	0.42
1:A:63:LYS:HD3	1:A:87:ARG:CD	2.37	0.42
1:A:319:ILE:HG21	1:A:322:PHE:CE1	2.55	0.42
1:A:422:ARG:HA	1:A:445:SER:O	2.20	0.41
1:A:452:LYS:O	1:A:454:CYS:N	2.53	0.41
1:A:505:LYS:HA	1:A:529:TRP:HB2	2.01	0.41
1:A:517:GLY:HA2	1:A:544:TYR:CZ	2.54	0.41
1:A:267:ASN:ND2	1:A:302:VAL:CG1	2.83	0.41
1:A:559:SER:HB2	1:A:570:ARG:HH22	1.82	0.41
1:A:465:SER:HB3	1:A:483:TYR:CD1	2.55	0.41
1:A:46:ILE:HG12	1:A:46:ILE:H	1.73	0.41
1:A:498:PHE:HB3	1:A:501:LEU:HB2	2.02	0.41
1:A:508:SER:HA	1:A:532:THR:O	2.21	0.41
1:A:510:GLN:N	1:A:533:ASN:OD1	2.54	0.41
1:A:158:ASN:C	1:A:182:LYS:HG2	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:541:ARG:O	1:A:543:ASP:N	2.54	0.41
1:A:469:LEU:HD23	1:A:484:ILE:CD1	2.51	0.41
1:A:345:ASN:HA	1:A:369:GLU:O	2.20	0.41
1:A:185:SER:O	1:A:186:LEU:C	2.58	0.41
1:A:518:ILE:CG2	1:A:519:PHE:N	2.84	0.40
1:A:302:VAL:HG23	1:A:305:GLU:CB	2.50	0.40
1:A:539:CYS:N	1:A:540:PRO:HD2	2.35	0.40
1:A:279:LEU:HD11	1:A:282:VAL:HG22	2.02	0.40
1:A:305:GLU:C	1:A:307:GLY:N	2.73	0.40
1:A:261:LEU:HD13	1:A:266:PHE:HD1	1.87	0.40
1:A:126:LEU:HD21	1:A:129:LEU:HB2	2.03	0.40
1:A:567:LYS:HA	1:A:568:PRO:HD3	1.97	0.40
1:A:289:LEU:O	1:A:320:PRO:HD2	2.21	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	548/580 (94%)	483 (88%)	50 (9%)	15 (3%)	8 10

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	304	SER
1	A	327	ASP
1	A	296	ASN
1	A	320	PRO
1	A	453	THR
1	A	574	CYS
1	A	294	ASP
1	A	297	PRO
1	A	326	TYR

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Mol	Chain	Res	Type
1	A	523	THR
1	A	41	ARG
1	A	542	ILE
1	A	145	PHE
1	A	291	GLY

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	510/537 (95%)	483 (95%)	27 (5%)	32 53

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	SER
1	A	90	THR
1	A	112	LEU
1	A	148	LEU
1	A	166	ARG
1	A	167	ARG
1	A	194	LEU
1	A	209	GLU
1	A	215	GLU
1	A	226	TYR
1	A	229	LEU
1	A	233	ASN
1	A	290	ASN
1	A	295	PHE
1	A	305	GLU
1	A	321	GLN
1	A	334	LEU
1	A	355	PHE
1	A	371	LEU
1	A	459	LEU
1	A	469	LEU
1	A	470	ASP
1	A	483	TYR

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Mol	Chain	Res	Type
1	A	484	ILE
1	A	501	LEU
1	A	526	GLN
1	A	557	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	69	HIS
1	A	89	ASN
1	A	104	HIS
1	A	110	ASN
1	A	134	ASN
1	A	177	ASN
1	A	201	HIS
1	A	233	ASN
1	A	267	ASN
1	A	290	ASN
1	A	321	GLN
1	A	370	ASN
1	A	397	ASN
1	A	423	ASN
1	A	457	GLN
1	A	467	ASN
1	A	487	ASN
1	A	526	GLN
1	A	552	ASN
1	A	554	GLN

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

2 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	NAG	A	831	1,3	12,14,15	0.75	0	15,19,21	0.97	0
3	NAG	A	832	3	12,14,15	0.61	0	15,19,21	0.87	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
3	NAG	A	831	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	832	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

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
4	LTC	A	581	-	55,55,55	0.81	1 (1%)	70,70,70	1.24	9 (12%)
2	NDG	A	821	1	12,14,15	0.65	0	15,19,21	1.26	2 (13%)

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	LTC	A	581	-	-	0/44/84/84	0/2/2/2
2	NDG	A	821	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	581	LTC	C19-C18	3.98	1.53	1.31

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	581	LTC	O10-C25-C24	3.86	120.02	111.56
4	A	581	LTC	C26-O10-C25	-3.32	109.73	117.92
2	A	821	NDG	C2-N2-C7	-2.98	118.08	123.09
4	A	581	LTC	C20-C19-C18	-2.63	110.53	125.43
4	A	581	LTC	C45-O2-C3	-2.59	111.39	117.99
4	A	581	LTC	C17-C18-C19	-2.54	111.02	125.43
4	A	581	LTC	C5-O1-C1	-2.52	108.83	113.73
4	A	581	LTC	C47-C41-C42	-2.50	109.41	113.87
4	A	581	LTC	O12-C29-C30	2.37	119.40	111.94
4	A	581	LTC	C28-O12-C29	-2.22	110.64	117.13
2	A	821	NDG	C3-C4-C5	-2.06	106.53	110.20

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	550/580 (94%)	0.09	22 (4%) 36 38	34, 53, 100, 123	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	PHE	7.2
1	A	483	TYR	6.4
1	A	539	CYS	6.0
1	A	540	PRO	5.5
1	A	566	GLY	5.4
1	A	541	ARG	4.9
1	A	564	GLY	4.5
1	A	567	LYS	3.8
1	A	535	TRP	3.5
1	A	542	ILE	3.4
1	A	299	GLU	3.4
1	A	575	PRO	3.1
1	A	568	PRO	3.1
1	A	572	ILE	3.0
1	A	305	GLU	2.6
1	A	561	LYS	2.6
1	A	574	CYS	2.6
1	A	565	SER	2.4
1	A	292	LEU	2.3
1	A	323	TYR	2.2
1	A	321	GLN	2.0
1	A	297	PRO	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 ⓘ

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	NAG	A	832	14/15	0.20	1.61	69,75,78,80	0
3	NAG	A	831	14/15	0.14	-0.40	50,54,56,63	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
2	NDG	A	821	14/15	0.20	7.03	65,67,69,69	0
4	LTC	A	581	54/54	0.35	3.77	81,91,97,101	0

6.5 Other polymers ⓘ

There are no such residues in this entry.