Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:01 AM GMT

PDB ID	:	2Z82
Title	:	Crystal structure of the TLR1-TLR2 heterodimer induced by binding of a tri-acylated lipopeptide
Authors	:	Lee, J.O.; Jin, M.S.; Kim, S.E.; Heo, J.Y.
Deposited on	:	2007-08-30
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

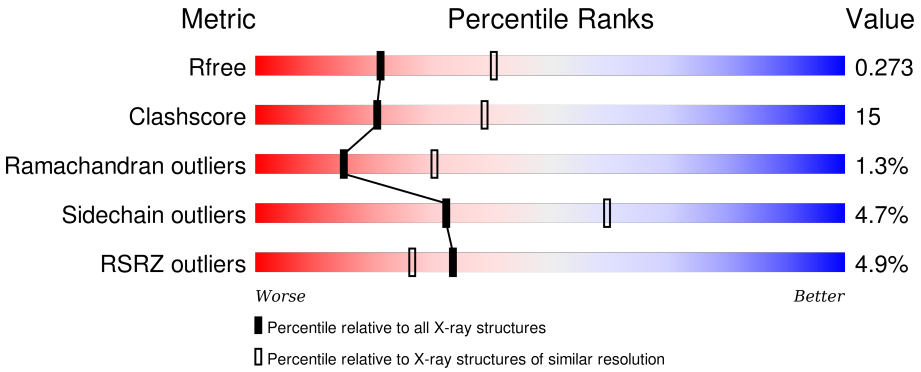
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	5% 67% 30% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PDJ	A	1	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4565 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 Toll-like receptor 2, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4353	2769	738	826	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	507	SER	-	LINKER	UNP Q9QUN7
A	508	ARG	-	LINKER	UNP Q9QUN7

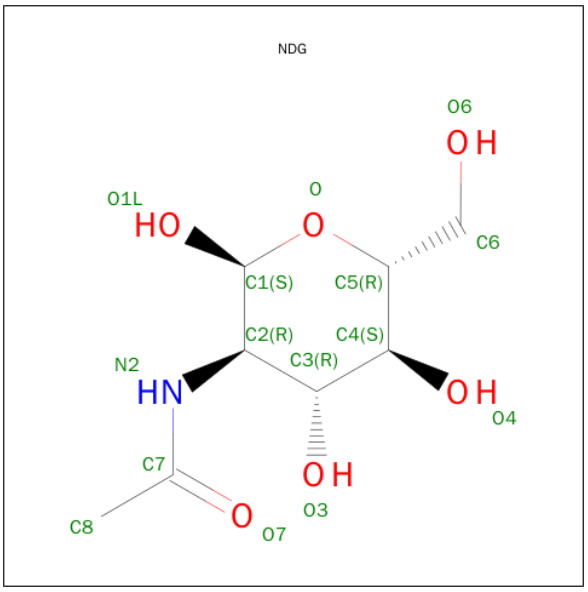
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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

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

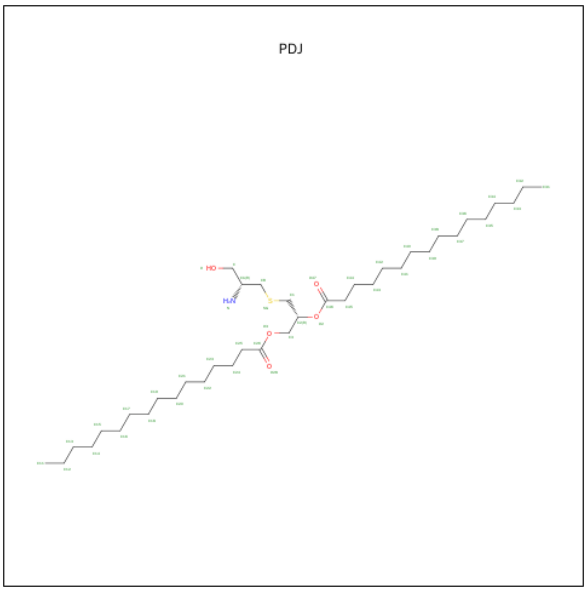
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is (2R)-3-{[(2R)-2-AMINO-3-HYDROXYPROPYL]THIO}PROPANE-1,2-DIYL DIHEXADECANOATE (three-letter code: PDJ) (formula: $C_{38}H_{75}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			45	38	1	5	1		

- Molecule 6 is water.

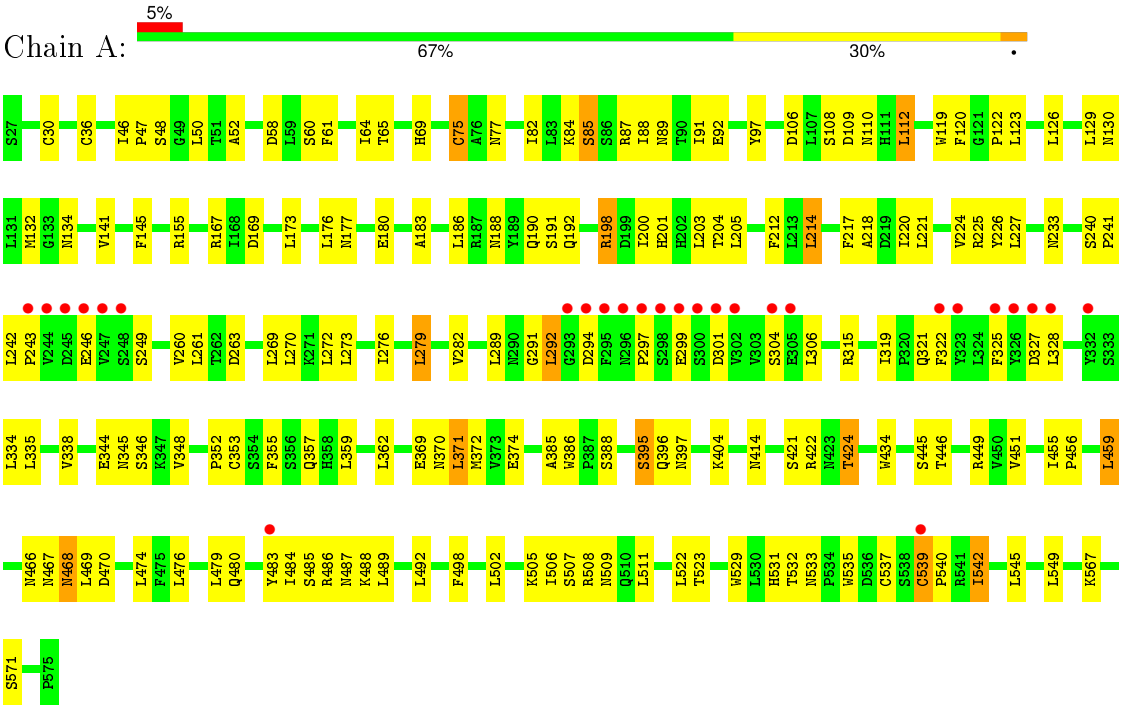
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	86	Total O 86 86	0	0

3 Residue-property plots (i)

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 (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.65Å 81.33Å 90.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.68 – 2.60 39.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.9 (39.68-2.60) 94.5 (39.68-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.95 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.277 0.221 , 0.273	Depositor DCC
R_{free} test set	921 reflections (4.87%)	DCC
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.9	EDS
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 18903 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4565	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PDJ, NAG, NDG, MAN

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	0.40	0/4437	0.69	0/6008

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4353	0	4402	129	0
2	A	28	0	25	1	0
3	A	39	0	34	0	0
4	A	14	0	13	2	0
5	A	45	0	74	5	0
6	A	86	0	0	8	0
All	All	4565	0	4548	131	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 15.

All (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:THR:H	1:A:467:ASN:HD21	1.25	0.84
1:A:110:ASN:HB2	1:A:134:ASN:HD21	1.43	0.83
1:A:469:LEU:H	1:A:487:ASN:HD22	1.29	0.80
1:A:374:GLU:HG2	1:A:404:LYS:HD3	1.64	0.79
1:A:469:LEU:H	1:A:487:ASN:ND2	1.84	0.76
1:A:112:LEU:H	1:A:134:ASN:HD22	1.37	0.71
1:A:218:ALA:HB2	1:A:242:LEU:HD22	1.74	0.70
1:A:456:PRO:HG2	1:A:459:LEU:HD13	1.74	0.68
1:A:335:LEU:HD21	5:A:1:PDJ:H181	1.76	0.66
1:A:489:LEU:HB2	1:A:509:ASN:ND2	2.13	0.64
1:A:315:ARG:HD3	1:A:344:GLU:OE1	1.99	0.63
1:A:489:LEU:HB2	1:A:509:ASN:HD22	1.62	0.63
1:A:304:SER:HA	1:A:334:LEU:HD23	1.78	0.63
1:A:198:ARG:HH11	1:A:198:ARG:HB2	1.64	0.62
1:A:508:ARG:HG2	1:A:532:THR:HG21	1.80	0.61
1:A:449:ARG:HG2	1:A:468:ASN:HB3	1.83	0.61
4:A:821:NDG:H4	6:A:836:HOH:O	2.00	0.60
1:A:492:LEU:HD12	1:A:506:ILE:HD13	1.83	0.60
1:A:348:VAL:HA	5:A:1:PDJ:H452	1.82	0.60
1:A:372:MET:H	1:A:397:ASN:HD22	1.50	0.60
1:A:292:LEU:N	1:A:292:LEU:HD23	2.17	0.59
1:A:359:LEU:HD13	1:A:362:LEU:HD22	1.85	0.58
1:A:509:ASN:HB2	1:A:533:ASN:HD21	1.70	0.57
1:A:506:ILE:O	1:A:506:ILE:HG12	2.04	0.57
1:A:273:LEU:HD23	1:A:276:ILE:HD11	1.86	0.57
1:A:304:SER:HA	1:A:334:LEU:CD2	2.35	0.56
1:A:270:LEU:HD23	5:A:1:PDJ:H122	1.87	0.55
1:A:214:LEU:HD12	6:A:855:HOH:O	2.05	0.55
1:A:120:PHE:HA	1:A:123:LEU:HD12	1.89	0.55
1:A:241:PRO:O	1:A:243:PRO:HD3	2.07	0.54
1:A:466:ASN:HB2	1:A:486:ARG:CZ	2.38	0.53
1:A:446:THR:H	1:A:467:ASN:ND2	2.00	0.53
1:A:84:LYS:HB2	1:A:106:ASP:OD2	2.07	0.53
1:A:487:ASN:C	1:A:488:LYS:HD2	2.28	0.53
1:A:414:ASN:CG	2:A:801:NAG:H82	2.29	0.53
4:A:821:NDG:C4	6:A:836:HOH:O	2.55	0.52
1:A:269:LEU:O	1:A:272:LEU:HB2	2.09	0.52
1:A:126:LEU:HD21	1:A:129:LEU:HD13	1.92	0.52
1:A:201:HIS:HA	1:A:225:ARG:HD2	1.91	0.52
1:A:91:ILE:HB	1:A:119:TRP:CZ2	2.45	0.52
1:A:46:ILE:HD13	1:A:64:ILE:HD13	1.92	0.51
1:A:112:LEU:HB2	1:A:134:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:N	1:A:487:ASN:HD22	2.04	0.50
1:A:352:PRO:O	1:A:355:PHE:HB3	2.11	0.50
1:A:52:ALA:HB1	1:A:77:ASN:ND2	2.26	0.49
1:A:346:SER:H	1:A:370:ASN:HD21	1.59	0.49
1:A:545:LEU:O	1:A:549:LEU:HG	2.11	0.49
1:A:335:LEU:HA	1:A:338:VAL:HG23	1.94	0.49
1:A:348:VAL:O	1:A:370:ASN:HB3	2.12	0.49
1:A:289:LEU:HB3	1:A:319:ILE:HD13	1.95	0.49
1:A:489:LEU:H	1:A:509:ASN:HD22	1.59	0.49
1:A:388:SER:HA	1:A:414:ASN:HD22	1.77	0.49
1:A:434:TRP:CD1	1:A:456:PRO:HD3	2.48	0.49
1:A:567:LYS:HE2	1:A:571:SER:HB3	1.95	0.49
1:A:87:ARG:HD3	6:A:885:HOH:O	2.11	0.49
1:A:88:ILE:H	1:A:110:ASN:HD22	1.60	0.48
1:A:489:LEU:HD13	1:A:509:ASN:HD21	1.78	0.48
1:A:191:SER:O	1:A:192:GLN:HB2	2.13	0.48
1:A:539:CYS:HB2	6:A:888:HOH:O	2.13	0.48
1:A:273:LEU:CD2	1:A:279:LEU:HD12	2.43	0.48
1:A:60:SER:OG	1:A:82:ILE:HG22	2.13	0.48
1:A:292:LEU:HD12	1:A:294:ASP:OD1	2.14	0.47
1:A:61:PHE:HA	1:A:85:SER:O	2.14	0.47
1:A:282:VAL:HG11	5:A:1:PDJ:H132	1.96	0.47
1:A:369:GLU:HA	1:A:396:GLN:HB3	1.95	0.47
1:A:292:LEU:HD12	1:A:294:ASP:OD2	2.15	0.47
1:A:167:ARG:H	1:A:190:GLN:NE2	2.12	0.47
1:A:224:VAL:HG11	1:A:227:LEU:HB2	1.96	0.46
1:A:353:CYS:O	1:A:357:GLN:HG3	2.15	0.46
1:A:395:SER:O	1:A:421:SER:O	2.34	0.46
1:A:484:ILE:HD13	1:A:489:LEU:HD21	1.97	0.46
1:A:292:LEU:HD11	6:A:899:HOH:O	2.16	0.46
1:A:188:ASN:HA	1:A:212:PHE:CZ	2.51	0.46
1:A:315:ARG:HG2	1:A:344:GLU:HG2	1.98	0.46
1:A:369:GLU:HA	1:A:396:GLN:O	2.16	0.46
1:A:220:ILE:HB	1:A:224:VAL:CG2	2.46	0.46
1:A:345:ASN:HA	1:A:369:GLU:O	2.16	0.45
1:A:167:ARG:NH1	1:A:190:GLN:HB3	2.31	0.45
1:A:220:ILE:HB	1:A:224:VAL:HG23	1.98	0.45
1:A:299:GLU:HB3	6:A:898:HOH:O	2.16	0.45
1:A:217:PHE:O	1:A:221:LEU:HG	2.16	0.45
1:A:155:ARG:NH1	1:A:180:GLU:OE1	2.49	0.45
1:A:47:PRO:HG2	1:A:50:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TYR:HE2	1:A:485:SER:HB2	1.80	0.45
1:A:173:LEU:HD13	1:A:176:LEU:HD11	1.99	0.45
1:A:58:ASP:HA	1:A:82:ILE:HB	1.99	0.45
1:A:297:PRO:HB2	1:A:301:ASP:HB2	1.98	0.45
1:A:65:THR:HG23	1:A:89:ASN:ND2	2.32	0.45
1:A:370:ASN:C	1:A:371:LEU:HD13	2.37	0.44
1:A:505:LYS:HG2	1:A:529:TRP:CE3	2.51	0.44
1:A:306:LEU:HD22	1:A:334:LEU:O	2.17	0.44
1:A:451:VAL:O	1:A:451:VAL:HG23	2.17	0.44
1:A:221:LEU:HD11	1:A:242:LEU:HD13	2.00	0.44
1:A:537:CYS:HA	1:A:542:ILE:HB	1.99	0.44
1:A:292:LEU:HD21	6:A:899:HOH:O	2.17	0.43
1:A:177:ASN:O	1:A:201:HIS:HB2	2.17	0.43
1:A:483:TYR:CE2	1:A:485:SER:HB2	2.52	0.43
1:A:291:GLY:HA3	1:A:325:PHE:CE1	2.53	0.43
1:A:180:GLU:HG3	1:A:204:THR:HB	2.01	0.43
1:A:292:LEU:HB2	1:A:294:ASP:OD1	2.18	0.43
1:A:507:SER:HB2	1:A:531:HIS:O	2.20	0.42
1:A:200:ILE:O	1:A:224:VAL:HA	2.19	0.42
1:A:97:TYR:HA	1:A:122:PRO:HG3	2.02	0.42
1:A:108:SER:HA	1:A:132:MET:O	2.19	0.42
1:A:221:LEU:O	1:A:249:SER:HA	2.19	0.42
1:A:424:THR:O	1:A:424:THR:OG1	2.30	0.42
1:A:249:SER:HB3	1:A:276:ILE:HA	2.02	0.42
1:A:233:ASN:HA	1:A:260:VAL:HB	2.01	0.42
1:A:483:TYR:HA	1:A:505:LYS:HB2	2.02	0.41
1:A:306:LEU:HD13	1:A:334:LEU:HB3	2.02	0.41
1:A:69:HIS:CE1	1:A:92:GLU:HG3	2.54	0.41
1:A:108:SER:HB3	1:A:130:ASN:OD1	2.21	0.41
1:A:480:GLN:HB3	1:A:502:LEU:HG	2.02	0.41
1:A:455:ILE:HG23	1:A:459:LEU:HD22	2.03	0.41
1:A:85:SER:HA	1:A:109:ASP:O	2.19	0.41
1:A:30:CYS:HA	1:A:36:CYS:HA	2.03	0.41
1:A:385:ALA:O	1:A:386:TRP:C	2.58	0.41
1:A:214:LEU:HD11	1:A:240:SER:OG	2.21	0.41
1:A:183:ALA:HB1	1:A:186:LEU:HB2	2.02	0.41
1:A:467:ASN:HD22	1:A:467:ASN:HA	1.69	0.41
1:A:112:LEU:O	1:A:134:ASN:HB3	2.20	0.41
1:A:65:THR:HG23	1:A:89:ASN:HD21	1.86	0.41
1:A:422:ARG:HA	1:A:445:SER:O	2.21	0.41
1:A:322:PHE:HE2	5:A:1:PDJ:H12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ILE:CD1	1:A:511:LEU:HD11	2.51	0.41
1:A:533:ASN:HB2	1:A:535:TRP:NE1	2.36	0.40
1:A:249:SER:OG	1:A:276:ILE:HG22	2.22	0.40
1:A:476:LEU:HD12	1:A:479:LEU:HD22	2.02	0.40
1:A:492:LEU:CD1	1:A:506:ILE:HD13	2.51	0.40
1:A:539:CYS:O	1:A:540:PRO:C	2.54	0.40
1:A:203:LEU:HD11	1:A:205:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	547/549 (100%)	486 (89%)	54 (10%)	7 (1%)	15 30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	395	SER
1	A	542	ILE
1	A	75	CYS
1	A	246	GLU
1	A	327	ASP
1	A	328	LEU
1	A	145	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	510/510 (100%)	486 (95%)	24 (5%)	32 59

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

Mol	Chain	Res	Type
1	A	48	SER
1	A	75	CYS
1	A	85	SER
1	A	112	LEU
1	A	141	VAL
1	A	169	ASP
1	A	198	ARG
1	A	214	LEU
1	A	226	TYR
1	A	261	LEU
1	A	263	ASP
1	A	279	LEU
1	A	292	LEU
1	A	321	GLN
1	A	371	LEU
1	A	424	THR
1	A	459	LEU
1	A	468	ASN
1	A	470	ASP
1	A	474	LEU
1	A	498	PHE
1	A	522	LEU
1	A	523	THR
1	A	539	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	104	HIS
1	A	110	ASN
1	A	111	HIS
1	A	134	ASN
1	A	190	GLN

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Mol	Chain	Res	Type
1	A	267	ASN
1	A	290	ASN
1	A	370	ASN
1	A	397	ASN
1	A	423	ASN
1	A	433	GLN
1	A	467	ASN
1	A	468	ASN
1	A	487	ASN
1	A	509	ASN
1	A	526	GLN
1	A	533	ASN
1	A	557	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

5 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	$\#\|Z\| > 2$
2	NAG	A	801	1,2	14,14,15	0.62	0	15,19,21	0.84	1 (6%)
2	NAG	A	802	2	14,14,15	0.73	1 (7%)	15,19,21	0.74	0
3	NAG	A	811	1,3	14,14,15	0.67	0	15,19,21	0.79	1 (6%)
3	NAG	A	812	3	14,14,15	0.76	0	15,19,21	0.85	0
3	MAN	A	813	3	11,11,12	0.75	0	14,15,17	0.78	1 (7%)

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	NAG	A	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
3	NAG	A	811	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	812	3	-	0/6/23/26	0/1/1/1
3	MAN	A	813	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	NAG	C1-C2	2.06	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	NAG	C2-N2-C7	-2.42	119.92	123.04
3	A	811	NAG	C2-N2-C7	-2.25	120.14	123.04
3	A	813	MAN	C1-C2-C3	2.19	112.13	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	1	0

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	$\#\|Z\|>2$
5	PDJ	A	1	-	44,44,44	0.85	1 (2%)	41,47,47	1.24	5 (12%)
4	NDG	A	821	1	14,14,15	0.75	0	15,19,21	1.04	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
5	PDJ	A	1	-	-	0/47/47/47	0/0/0/0
4	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)
5	A	1	PDJ	O-C	-4.33	1.23	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1	PDJ	C2-O2-C46	-3.02	110.66	117.89
5	A	1	PDJ	C3-O3-C26	-2.48	109.92	116.85
4	A	821	NDG	C2-N2-C7	-2.03	120.43	123.04
4	A	821	NDG	C3-C4-C5	2.45	114.46	110.20
5	A	1	PDJ	O3-C26-C25	2.79	120.40	111.90
5	A	1	PDJ	O-C-CA	3.46	120.91	111.84
5	A	1	PDJ	O2-C46-C45	3.82	119.83	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	PDJ	5	0
4	A	821	NDG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	549/549 (100%)	-0.21	27 (4%) 33 26	11, 32, 78, 113	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	VAL	9.2
1	A	293	GLY	7.5
1	A	326	TYR	6.7
1	A	327	ASP	6.4
1	A	299	GLU	5.8
1	A	245	ASP	5.2
1	A	297	PRO	5.1
1	A	539	CYS	4.8
1	A	296	ASN	4.6
1	A	323	TYR	4.4
1	A	295	PHE	4.1
1	A	304	SER	4.1
1	A	298	SER	4.1
1	A	301	ASP	4.0
1	A	244	VAL	3.9
1	A	483	TYR	3.7
1	A	294	ASP	3.6
1	A	322	PHE	3.4
1	A	328	LEU	3.2
1	A	246	GLU	3.1
1	A	302	VAL	2.9
1	A	305	GLU	2.6
1	A	248	SER	2.6
1	A	243	PRO	2.4
1	A	332	TYR	2.3
1	A	300	SER	2.1
1	A	325	PHE	2.0

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

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

6.3 Carbohydrates (i)

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	801	14/15	0.84	0.20	1.65	50,56,60,65	0
3	NAG	A	811	14/15	0.95	0.13	-0.37	25,29,33,40	0
2	NAG	A	802	14/15	0.67	0.31	-	69,71,72,74	0
3	MAN	A	813	11/12	0.78	0.30	-	68,70,72,72	0
3	NAG	A	812	14/15	0.82	0.29	-	47,54,58,64	0

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. 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	PDJ	A	1	45/45	0.77	0.40	4.24	71,79,87,88	0
4	NDG	A	821	14/15	0.73	0.29	-	63,65,66,68	0

6.5 Other polymers (i)

There are no such residues in this entry.