



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:02 AM GMT

PDB ID : 2Z7X
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 : 2007-08-29
Resolution : 2.10 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

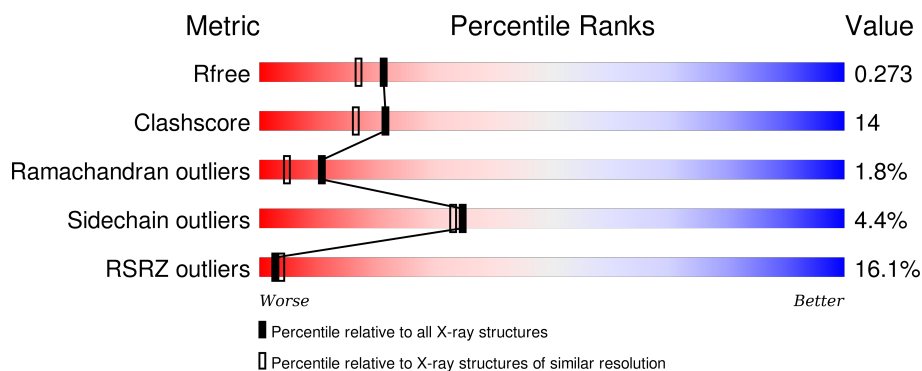
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 $\leq 5\%$. 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	549	<div> <div>29%</div> <div>59%</div> <div>37%</div> <div>.</div> </div>
2	B	520	<div> <div>2%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
3	C	5	<div> <div>20%</div> <div>80%</div> <div>20%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9088 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
			4366	2766	735	844	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	507	SER	-	LINKER	UNP O60603
A	508	ARG	-	LINKER	UNP O60603

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	520	Total	C	N	O	S	0	0	0
			4172	2671	697	784	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	476	ALA	-	LINKER	UNP Q15399
B	477	SER	-	LINKER	UNP Q15399

- Molecule 3 is a protein called Pam3CSK4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			43	27	9	7			

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

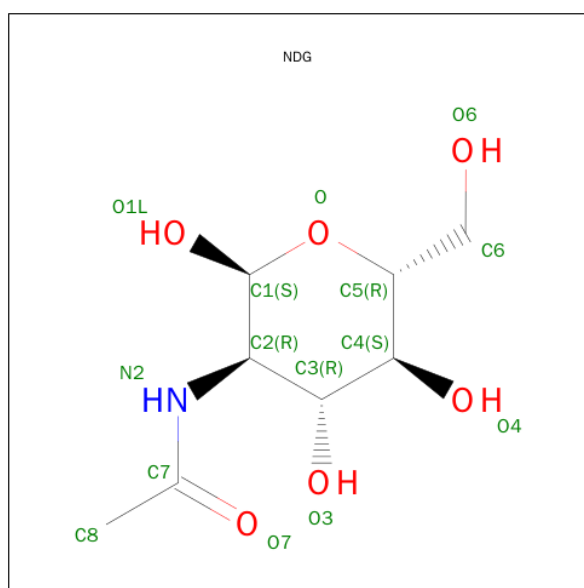
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 7 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
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

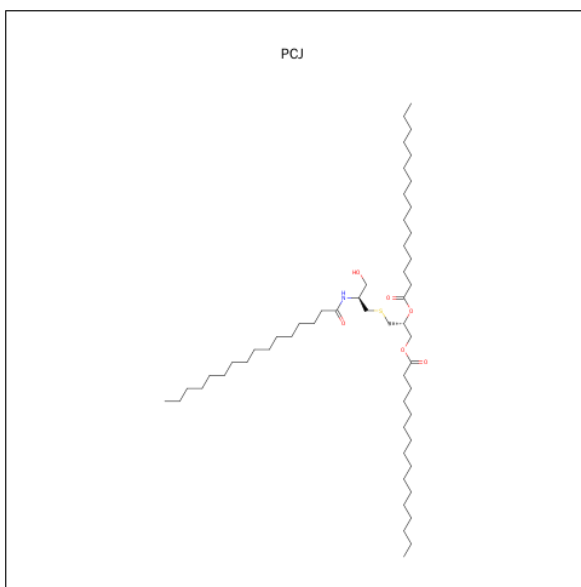


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	2	Total	C	N	O	0	0
			25	14	1	10		

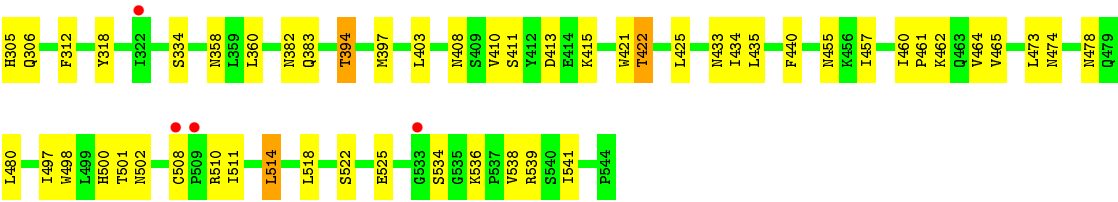
- Molecule 10 is (2R)-3-{[(2S)-3-HYDROXY-2-(PALMITOYLAMINO)PROPYL]THIO}PROPANE-1,2-DIYL DIHEXADECANOATE (three-letter code: PCJ) (formula: C₅₄H₁₀₅NO₆S).



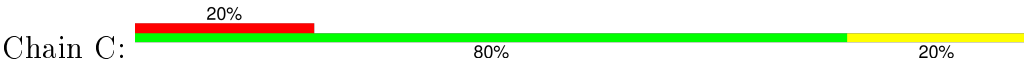
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	N	O	S	0	0
			62	54	1	6	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	70	Total	O	0	0
			70	70		
11	B	175	Total	O	0	0
			175	175		
11	C	2	Total	O	0	0
			2	2		



● Molecule 3: Pam3CSK4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	200.30 Å 120.14 Å 74.12 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.85 – 2.10 45.85 – 2.08	Depositor EDS
% Data completeness (in resolution range)	94.5 (45.85-2.10) 93.0 (45.85-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.08 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.244 , 0.270 0.250 , 0.273	Depositor DCC
R_{free} test set	5022 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 101143 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9088	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PCJ, BMA, 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	0.32	0/4442	0.60	2/6014 (0.0%)
2	B	0.38	0/4257	0.63	0/5766
3	C	0.38	0/42	0.50	0/49
All	All	0.35	0/8741	0.61	2/11829 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	PHE	N-CA-C	-5.74	95.51	111.00
1	A	351	VAL	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4366	0	4418	155	0
2	B	4172	0	4221	91	0
3	C	43	0	56	0	0
4	A	39	0	34	4	0
5	A	39	0	34	0	0
6	A	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	14	0	13	0	0
8	A	28	0	26	1	0
8	B	14	0	13	0	0
9	A	25	0	22	2	0
10	C	62	0	102	4	0
11	A	70	0	0	3	0
11	B	175	0	0	3	0
11	C	2	0	0	0	0
All	All	9088	0	8973	251	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 14.

All (251) 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:511:LEU:H	1:A:533:ASN:HD22	1.01	0.95
2:B:229:LYS:HD2	2:B:263:ARG:HE	1.32	0.94
1:A:456:PRO:HG2	1:A:459:LEU:HD13	1.59	0.84
1:A:372:MET:H	1:A:397:ASN:HD22	1.25	0.84
2:B:81:ILE:H	2:B:103:ASN:HD22	1.27	0.81
1:A:170:PHE:HA	1:A:173:LEU:HD21	1.62	0.81
1:A:469:LEU:H	1:A:487:ASN:HD22	1.28	0.79
1:A:56:SER:HA	1:A:80:ALA:HB3	1.65	0.79
2:B:457:ILE:H	2:B:478:ASN:HD22	1.29	0.79
2:B:410:VAL:H	2:B:433:ASN:HD22	1.34	0.76
1:A:30:CYS:HA	1:A:36:CYS:HA	1.67	0.76
1:A:239:PHE:H	1:A:268:GLN:HE21	1.34	0.75
2:B:435:LEU:H	2:B:455:ASN:HD22	1.33	0.74
2:B:55:ASN:HB2	2:B:79:ASN:HD21	1.53	0.73
1:A:123:LEU:HD13	1:A:126:LEU:HD22	1.69	0.72
1:A:511:LEU:H	1:A:533:ASN:ND2	1.84	0.72
1:A:183:ALA:HB1	1:A:186:LEU:HB2	1.72	0.71
2:B:229:LYS:HD2	2:B:263:ARG:NE	2.04	0.71
4:A:803:NDG:H8C3	2:B:54:GLN:HE22	1.55	0.71
1:A:121:LYS:HB3	1:A:122:PRO:HD3	1.73	0.69
1:A:346:SER:H	1:A:370:ASN:HD21	1.38	0.69
2:B:103:ASN:HB2	2:B:124:ASN:HD21	1.57	0.69
2:B:410:VAL:H	2:B:433:ASN:ND2	1.89	0.69
1:A:571:SER:O	1:A:572:ILE:HG23	1.93	0.69
1:A:64:ILE:HB	1:A:86:ASN:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLN:HA	1:A:190:GLU:HB3	1.75	0.68
1:A:511:LEU:N	1:A:533:ASN:HD22	1.84	0.68
1:A:38:GLY:H	1:A:58:ASP:HB3	1.57	0.68
1:A:487:ASN:HB2	1:A:509:ASN:HD21	1.58	0.68
1:A:218:VAL:HG12	1:A:244:THR:HB	1.77	0.67
1:A:489:LEU:H	1:A:509:ASN:HD22	1.43	0.66
1:A:112:LEU:H	1:A:134:ASN:HD22	1.42	0.66
1:A:158:ASN:HD22	1:A:160:ASP:HB2	1.59	0.66
1:A:59:LEU:HD12	1:A:64:ILE:HD11	1.78	0.66
1:A:112:LEU:HD22	1:A:115:LEU:HD23	1.78	0.65
1:A:239:PHE:H	1:A:268:GLN:NE2	1.95	0.65
2:B:408:ASN:HB2	2:B:433:ASN:HD21	1.61	0.65
9:A:923:NAG:H62	9:A:924:BMA:O5	1.96	0.64
2:B:115:ASN:ND2	2:B:138:MET:HA	2.13	0.63
4:A:803:NDG:C8	2:B:54:GLN:HE22	2.12	0.63
1:A:110:ASN:HB2	1:A:134:ASN:HD21	1.64	0.63
1:A:310:GLU:HG3	1:A:311:THR:HG23	1.80	0.62
2:B:62:THR:HA	2:B:88:VAL:HG13	1.80	0.62
1:A:68:SER:HA	1:A:92:GLU:HB2	1.80	0.62
1:A:158:ASN:ND2	1:A:160:ASP:HB2	2.13	0.62
1:A:43:LEU:HD12	1:A:43:LEU:H	1.62	0.62
1:A:489:LEU:HB2	1:A:509:ASN:HD22	1.64	0.62
2:B:397:MET:O	2:B:422:THR:HG21	2.01	0.61
2:B:281:VAL:HG12	2:B:283:LEU:HD13	1.82	0.61
2:B:360:LEU:H	2:B:382:ASN:HD22	1.48	0.61
1:A:489:LEU:HB2	1:A:509:ASN:ND2	2.15	0.61
2:B:239:LYS:O	2:B:242:THR:HG22	2.00	0.60
2:B:57:ILE:H	2:B:79:ASN:HD22	1.49	0.60
1:A:270:MET:HB3	1:A:304:ILE:HD12	1.83	0.60
10:C:1:PCJ:H321	10:C:1:PCJ:H113	1.82	0.60
1:A:395:ARG:O	1:A:421:SER:O	2.20	0.60
2:B:455:ASN:HB2	2:B:478:ASN:HD21	1.66	0.60
1:A:113:SER:HB3	1:A:135:PRO:HB2	1.84	0.60
2:B:433:ASN:HB2	2:B:455:ASN:HD21	1.67	0.60
1:A:73:GLN:HA	1:A:98:SER:HB2	1.82	0.59
2:B:460:ILE:HG23	2:B:464:VAL:HG21	1.83	0.59
1:A:522:LEU:HD22	1:A:522:LEU:H	1.68	0.58
1:A:569:VAL:HA	1:A:572:ILE:HD11	1.85	0.58
1:A:78:LEU:HD23	1:A:99:LEU:HD22	1.84	0.58
1:A:234:LEU:HB3	1:A:261:ILE:HD12	1.86	0.57
1:A:52:GLU:OE1	1:A:76:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:LEU:HD13	2:B:40:PRO:HD3	1.86	0.57
1:A:146:SER:HA	1:A:172:GLY:HA3	1.86	0.57
1:A:346:SER:H	1:A:370:ASN:ND2	2.02	0.57
9:A:923:NAG:H4	9:A:924:BMA:O2	2.04	0.56
2:B:242:THR:O	2:B:244:PRO:HD3	2.04	0.56
1:A:446:THR:CG2	1:A:448:ILE:HG23	2.35	0.56
2:B:36:LEU:H	2:B:55:ASN:ND2	2.02	0.56
1:A:425:PHE:O	1:A:446:THR:O	2.23	0.56
1:A:537:CYS:HA	1:A:542:ILE:HG21	1.87	0.56
1:A:378:LYS:HA	1:A:408:THR:HG23	1.87	0.56
1:A:35:ILE:HG23	1:A:56:SER:HB2	1.87	0.56
2:B:358:ASN:HB2	2:B:382:ASN:HD21	1.70	0.56
1:A:481:GLU:HG2	1:A:503:VAL:HB	1.88	0.56
1:A:79:GLN:HA	1:A:102:LEU:HA	1.88	0.55
1:A:82:VAL:HA	1:A:106:ASP:HB3	1.89	0.55
1:A:85:SER:HA	1:A:109:TYR:O	2.07	0.55
2:B:80:ARG:HG2	2:B:80:ARG:HH11	1.72	0.55
1:A:335:THR:HB	1:A:359:LEU:HD23	1.89	0.55
2:B:230:CYS:HA	11:B:858:HOH:O	2.06	0.54
1:A:506:ILE:HD12	1:A:511:LEU:HD11	1.88	0.54
1:A:356:SER:HB3	1:A:385:ALA:HB1	1.89	0.54
2:B:282:LYS:HG2	11:B:817:HOH:O	2.06	0.54
1:A:540:PRO:O	1:A:541:ARG:HG3	2.07	0.54
2:B:538:VAL:HA	2:B:541:ILE:HD13	1.88	0.54
2:B:66:LEU:HD12	2:B:67:SER:N	2.23	0.54
2:B:273:VAL:HG23	2:B:299:LEU:HD21	1.90	0.54
1:A:535:TRP:CD1	1:A:560:ALA:HB1	2.42	0.53
2:B:193:HIS:HD2	11:B:889:HOH:O	1.91	0.53
2:B:522:SER:HA	2:B:539:ARG:HH21	1.72	0.53
1:A:469:LEU:H	1:A:487:ASN:ND2	2.02	0.53
1:A:212:LEU:HD22	1:A:215:GLU:OE1	2.09	0.53
1:A:506:ILE:O	1:A:506:ILE:HG23	2.08	0.53
1:A:36:CYS:HB2	1:A:57:LEU:HD23	1.89	0.53
1:A:129:LEU:HG	1:A:131:LEU:HD21	1.91	0.53
1:A:369:GLU:HA	1:A:396:GLN:O	2.10	0.52
2:B:147:SER:O	2:B:148:THR:HG23	2.08	0.52
1:A:121:LYS:H	1:A:122:PRO:CD	2.23	0.52
2:B:113:THR:HG23	2:B:114:VAL:O	2.10	0.52
1:A:573:ILE:N	1:A:573:ILE:HD12	2.24	0.52
1:A:377:LEU:HG	1:A:408:THR:HG21	1.91	0.51
1:A:138:THR:HG22	1:A:139:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:GLU:OE1	1:A:559:SER:HA	2.10	0.51
1:A:65:THR:HG23	1:A:89:ASN:OD1	2.10	0.51
1:A:124:SER:O	1:A:150:LYS:HD3	2.11	0.51
2:B:34:ASN:H	2:B:55:ASN:HD21	1.59	0.51
1:A:467:ASN:HB2	1:A:487:ASN:HD21	1.75	0.51
1:A:370:ASN:HB2	1:A:397:ASN:HD21	1.76	0.50
1:A:137:LYS:HA	1:A:162:PHE:HA	1.94	0.50
1:A:446:THR:HG22	1:A:448:ILE:HG23	1.93	0.50
1:A:167:ARG:C	1:A:169:ASP:H	2.15	0.50
1:A:443:LEU:O	1:A:446:THR:HB	2.11	0.50
1:A:510:GLN:NE2	1:A:534:PRO:HG2	2.27	0.50
2:B:215:ASN:HD22	2:B:248:ASN:HB2	1.75	0.50
1:A:548:TRP:HE3	1:A:549:LEU:HD12	1.76	0.50
2:B:435:LEU:H	2:B:455:ASN:ND2	2.05	0.49
1:A:50:LEU:H	1:A:50:LEU:HD12	1.78	0.49
2:B:57:ILE:H	2:B:79:ASN:ND2	2.09	0.49
2:B:394:THR:CG2	2:B:422:THR:H	2.25	0.49
2:B:229:LYS:HB2	2:B:260:SER:OG	2.12	0.49
1:A:96:PHE:CE1	1:A:119:TRP:HB3	2.48	0.49
2:B:312:PHE:O	10:C:1:PCJ:H651	2.13	0.49
1:A:139:LEU:HB2	1:A:169:ASP:OD1	2.13	0.48
2:B:440:PHE:CD2	2:B:464:VAL:HG22	2.49	0.48
1:A:306:PRO:HG3	1:A:334:LEU:HA	1.96	0.48
1:A:218:VAL:HG13	1:A:242:LEU:HD22	1.95	0.48
2:B:480:LEU:H	2:B:502:ASN:HD22	1.62	0.48
1:A:198:GLN:HG2	1:A:199:ASN:OD1	2.13	0.48
2:B:500:HIS:HD2	2:B:501:THR:OG1	1.97	0.47
1:A:87:GLY:HA2	1:A:111:TYR:CD1	2.50	0.47
1:A:234:LEU:HD22	1:A:259:VAL:HG11	1.96	0.47
1:A:345:ASN:HA	1:A:369:GLU:O	2.15	0.47
1:A:512:LYS:HA	1:A:534:PRO:O	2.15	0.47
2:B:273:VAL:HG23	2:B:299:LEU:CD2	2.44	0.47
4:A:801:NAG:C6	2:B:33:LYS:HE3	2.45	0.47
2:B:129:LEU:HA	2:B:148:THR:CG2	2.44	0.47
1:A:298:SER:HB3	1:A:303:VAL:HG12	1.97	0.46
1:A:118:SER:O	1:A:122:PRO:HD3	2.14	0.46
2:B:129:LEU:HA	2:B:148:THR:HG23	1.98	0.46
1:A:158:ASN:OD1	1:A:162:PHE:HB2	2.16	0.46
2:B:462:LYS:O	2:B:465:VAL:HG22	2.16	0.46
1:A:161:THR:O	1:A:163:THR:HG23	2.16	0.46
2:B:518:LEU:HG	2:B:525:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ASN:HD21	2:B:138:MET:HA	1.77	0.45
2:B:474:ASN:HA	2:B:498:TRP:HB2	1.98	0.45
2:B:413:ASP:OD1	2:B:415:LYS:HG2	2.16	0.45
2:B:534:SER:OG	2:B:536:LYS:HG3	2.14	0.45
1:A:469:LEU:N	1:A:487:ASN:HD22	2.04	0.45
1:A:125:SER:HA	1:A:150:LYS:HD3	1.97	0.45
1:A:132:LEU:HD11	1:A:155:ARG:HB3	1.99	0.45
1:A:182:ASP:HA	1:A:206:HIS:HB2	1.97	0.45
1:A:173:LEU:N	1:A:173:LEU:HD23	2.31	0.45
1:A:385:ALA:O	1:A:386:TRP:C	2.55	0.45
1:A:328:LEU:HA	11:A:930:HOH:O	2.17	0.45
1:A:475:ASN:HA	1:A:497:LEU:HB3	1.99	0.45
2:B:28:LEU:HD22	2:B:29:VAL:N	2.30	0.45
2:B:37:ILE:HG13	2:B:38:HIS:CD2	2.52	0.45
1:A:398:HIS:ND1	2:B:383:GLN:NE2	2.64	0.44
2:B:305:HIS:CD2	2:B:334:SER:HB2	2.52	0.44
1:A:383:GLU:O	1:A:384:ASP:HB2	2.17	0.44
2:B:514:LEU:O	2:B:518:LEU:HB2	2.17	0.44
2:B:221:ILE:HD13	2:B:233:PHE:CZ	2.52	0.44
2:B:115:ASN:HA	2:B:115:ASN:HD22	1.58	0.44
2:B:541:ILE:HD12	2:B:541:ILE:N	2.33	0.44
1:A:28:LEU:HD13	1:A:36:CYS:HB3	2.00	0.44
2:B:181:PRO:HG3	2:B:205:ILE:HD12	2.00	0.44
8:A:911:NAG:C7	11:A:968:HOH:O	2.66	0.44
2:B:114:VAL:HG12	2:B:115:ASN:H	1.83	0.44
2:B:358:ASN:HB2	2:B:382:ASN:ND2	2.33	0.44
1:A:138:THR:HG22	1:A:139:LEU:N	2.32	0.44
1:A:460:GLU:HG3	1:A:480:LYS:HG2	2.00	0.44
1:A:176:LEU:HD11	1:A:200:VAL:HG22	1.99	0.43
2:B:394:THR:HG21	2:B:421:TRP:HE3	1.83	0.43
1:A:52:GLU:C	1:A:54:VAL:H	2.22	0.43
1:A:67:ILE:HB	1:A:91:ILE:HG12	2.00	0.43
2:B:411:SER:HB3	2:B:434:ILE:HG13	1.99	0.43
2:B:79:ASN:HB2	2:B:103:ASN:HD21	1.83	0.43
1:A:115:LEU:HA	1:A:119:TRP:HZ3	1.84	0.43
1:A:542:ILE:HD12	1:A:546:SER:OG	2.18	0.43
1:A:132:LEU:HA	1:A:157:GLY:O	2.19	0.43
1:A:142:THR:O	1:A:143:SER:C	2.56	0.43
2:B:457:ILE:H	2:B:478:ASN:ND2	2.06	0.43
1:A:43:LEU:HD12	1:A:43:LEU:N	2.30	0.43
4:A:801:NAG:H61	4:A:803:NDG:H8C3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:ARG:HD2	2:B:318:TYR:CE2	2.54	0.43
2:B:177:GLU:O	2:B:178:LYS:C	2.57	0.43
1:A:535:TRP:NE1	1:A:560:ALA:HB1	2.35	0.42
2:B:480:LEU:H	2:B:502:ASN:ND2	2.16	0.42
1:A:176:LEU:CD1	1:A:200:VAL:HG22	2.49	0.42
1:A:560:ALA:O	1:A:561:LYS:HD2	2.20	0.42
2:B:73:ILE:HG23	2:B:97:TYR:CD2	2.54	0.42
1:A:61:ASN:HA	1:A:85:SER:O	2.19	0.42
1:A:484:ILE:HG12	1:A:484:ILE:O	2.19	0.42
2:B:128:ALA:C	2:B:148:THR:HG22	2.40	0.42
2:B:39:VAL:HG11	2:B:64:ASP:HB3	2.02	0.42
1:A:402:LEU:HD12	1:A:428:MET:HB3	2.02	0.42
1:A:519:PHE:HB2	1:A:544:TYR:OH	2.20	0.42
1:A:505:LYS:HA	1:A:529:TRP:HB2	2.01	0.42
1:A:41:GLY:HA2	1:A:62:ASN:OD1	2.20	0.42
2:B:229:LYS:HE2	2:B:259:ASN:HB2	2.02	0.42
1:A:195:LYS:HB2	1:A:219:ASP:HB3	2.02	0.42
2:B:511:ILE:O	2:B:511:ILE:HG13	2.20	0.42
1:A:348:VAL:H	1:A:370:ASN:ND2	2.18	0.41
1:A:134:ASN:HA	1:A:135:PRO:HD3	1.89	0.41
2:B:394:THR:O	2:B:422:THR:HG23	2.19	0.41
1:A:82:VAL:HG13	1:A:82:VAL:O	2.20	0.41
1:A:446:THR:HG22	1:A:448:ILE:HG12	2.02	0.41
1:A:74:ARG:O	1:A:74:ARG:HG3	2.20	0.41
2:B:84:LEU:HD22	2:B:85:ASP:N	2.35	0.41
1:A:451:VAL:HG21	1:A:472:PHE:CD1	2.55	0.41
2:B:105:LEU:H	2:B:124:ASN:HD22	1.69	0.41
1:A:131:LEU:HD22	1:A:131:LEU:N	2.34	0.41
2:B:28:LEU:HD22	2:B:29:VAL:H	1.85	0.41
1:A:158:ASN:HD21	1:A:161:THR:H	1.68	0.41
1:A:78:LEU:HD23	1:A:99:LEU:CD2	2.50	0.41
2:B:73:ILE:HG12	2:B:97:TYR:HB3	2.03	0.41
1:A:290:ASN:HB2	11:A:932:HOH:O	2.19	0.41
1:A:506:ILE:HG22	1:A:529:TRP:O	2.21	0.41
1:A:139:LEU:HD21	1:A:156:VAL:HG21	2.02	0.41
2:B:35:GLY:N	2:B:55:ASN:ND2	2.69	0.41
1:A:58:ASP:HA	1:A:82:VAL:CG1	2.50	0.41
2:B:360:LEU:H	2:B:382:ASN:ND2	2.16	0.41
1:A:538:SER:O	1:A:542:ILE:HG12	2.20	0.41
1:A:418:ILE:HD12	1:A:438:MET:SD	2.61	0.41
1:A:141:GLU:HB3	1:A:168:LYS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:PRO:HB2	1:A:518:ILE:HB	2.02	0.41
1:A:565:SER:C	1:A:567:LYS:H	2.24	0.41
1:A:282:LEU:CD1	10:C:1:PCJ:H312	2.51	0.41
10:C:1:PCJ:HA	10:C:1:PCJ:H652	1.84	0.41
2:B:440:PHE:CD1	2:B:461:PRO:HD2	2.56	0.41
2:B:508:CYS:C	2:B:510:ARG:H	2.23	0.41
1:A:224:VAL:HG12	1:A:225:GLU:N	2.36	0.41
1:A:121:LYS:HA	1:A:147:HIS:HD2	1.86	0.41
2:B:113:THR:OG1	2:B:114:VAL:N	2.52	0.41
1:A:50:LEU:N	1:A:50:LEU:HD12	2.36	0.41
1:A:112:LEU:H	1:A:134:ASN:ND2	2.15	0.40
1:A:573:ILE:HG22	1:A:574:CYS:N	2.36	0.40
1:A:234:LEU:HD22	1:A:259:VAL:CG1	2.51	0.40
1:A:155:ARG:HG2	1:A:155:ARG:HH11	1.87	0.40
2:B:473:LEU:O	2:B:497:ILE:HA	2.21	0.40
1:A:159:MET:H	1:A:159:MET:HG3	1.65	0.40
2:B:237:LEU:HB3	2:B:267:LEU:HD22	2.03	0.40
1:A:103:GLU:HA	1:A:126:LEU:HA	2.02	0.40
1:A:145:PHE:HB3	1:A:148:LEU:HD11	2.02	0.40
1:A:230:ARG:HG2	1:A:257:ARG:HB3	2.03	0.40
1:A:84:THR:HG23	1:A:108:SER:HB2	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%)	458 (84%)	72 (13%)	17 (3%)	5 1
2	B	518/520 (100%)	480 (93%)	36 (7%)	2 (0%)	39 37
3	C	3/5 (60%)	3 (100%)	0	0	100 100
All	All	1068/1074 (99%)	941 (88%)	108 (10%)	19 (2%)	11 5

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	143	SER
1	A	241	GLU
1	A	572	ILE
1	A	85	SER
1	A	395	ARG
1	A	494	ASP
1	A	40	SER
1	A	71	ASP
2	B	220	ASN
1	A	121	LYS
1	A	145	PHE
1	A	541	ARG
1	A	550	ASN
2	B	306	GLN
1	A	32	ARG
1	A	168	LYS
1	A	49	GLY
1	A	100	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	518/518 (100%)	492 (95%)	26 (5%)	30	27
2	B	494/494 (100%)	476 (96%)	18 (4%)	42	43
3	C	5/5 (100%)	4 (80%)	1 (20%)	1	0
All	All	1017/1017 (100%)	972 (96%)	45 (4%)	35	33

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	55	LYS

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Mol	Chain	Res	Type
1	A	148	LEU
1	A	159	MET
1	A	173	LEU
1	A	176	LEU
1	A	205	LEU
1	A	207	MET
1	A	227	LEU
1	A	229	LEU
1	A	234	LEU
1	A	242	LEU
1	A	254	PHE
1	A	270	MET
1	A	282	LEU
1	A	324	LEU
1	A	325	PHE
1	A	371	LEU
1	A	402	LEU
1	A	446	THR
1	A	459	LEU
1	A	470	ASN
1	A	490	MET
1	A	506	ILE
1	A	522	LEU
1	A	523	THR
2	B	41	LYS
2	B	60	LEU
2	B	80	ARG
2	B	84	LEU
2	B	115	ASN
2	B	116	LEU
2	B	157	LEU
2	B	188	ASN
2	B	189	THR
2	B	193	HIS
2	B	223	CYS
2	B	265	LEU
2	B	283	LEU
2	B	394	THR
2	B	403	LEU
2	B	422	THR
2	B	425	LEU
2	B	514	LEU

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Mol	Chain	Res	Type
3	C	3	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	62	ASN
1	A	73	GLN
1	A	86	ASN
1	A	134	ASN
1	A	147	HIS
1	A	158	ASN
1	A	202	HIS
1	A	258	ASN
1	A	268	GLN
1	A	290	ASN
1	A	370	ASN
1	A	397	ASN
1	A	417	ASN
1	A	423	ASN
1	A	470	ASN
1	A	475	ASN
1	A	478	GLN
1	A	487	ASN
1	A	509	ASN
1	A	510	GLN
1	A	526	GLN
1	A	531	HIS
1	A	533	ASN
1	A	557	GLN
2	B	38	HIS
2	B	54	GLN
2	B	55	ASN
2	B	79	ASN
2	B	82	GLN
2	B	92	ASN
2	B	103	ASN
2	B	115	ASN
2	B	118	HIS
2	B	124	ASN
2	B	188	ASN
2	B	193	HIS

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Mol	Chain	Res	Type
2	B	199	ASN
2	B	215	ASN
2	B	243	ASN
2	B	358	ASN
2	B	367	ASN
2	B	382	ASN
2	B	383	GLN
2	B	402	GLN
2	B	408	ASN
2	B	433	ASN
2	B	455	ASN
2	B	471	GLN
2	B	478	ASN
2	B	479	GLN
2	B	500	HIS
2	B	502	ASN
2	B	526	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 ⓘ

11 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	$\# Z > 2$
4	NAG	A	801	2,4	14,14,15	0.76	0	15,19,21	0.77	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NDG	A	803	4	14,14,15	0.86	0	15,19,21	0.81	0
4	MAN	A	804	4	11,11,12	0.74	0	14,15,17	0.85	0
5	NAG	A	821	2,5	14,14,15	0.58	0	15,19,21	1.06	1 (6%)
5	NAG	A	823	5	14,14,15	0.67	0	15,19,21	0.78	1 (6%)
5	MAN	A	824	5	11,11,12	0.69	0	14,15,17	0.74	0
6	NAG	A	831	2,6	14,14,15	0.60	0	15,19,21	0.73	0
6	NAG	A	833	6	14,14,15	0.63	0	15,19,21	0.67	0
6	BMA	A	834	6	11,11,12	0.52	0	14,15,17	0.29	0
9	NAG	A	923	9	14,14,15	0.72	0	15,19,21	0.85	0
9	BMA	A	924	9	11,11,12	0.68	0	14,15,17	0.33	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
4	NAG	A	801	2,4	-	0/6/23/26	0/1/1/1
4	NDG	A	803	4	-	0/6/23/26	0/1/1/1
4	MAN	A	804	4	-	0/2/19/22	0/1/1/1
5	NAG	A	821	2,5	-	0/6/23/26	0/1/1/1
5	NAG	A	823	5	-	0/6/23/26	0/1/1/1
5	MAN	A	824	5	-	0/2/19/22	0/1/1/1
6	NAG	A	831	2,6	-	0/6/23/26	0/1/1/1
6	NAG	A	833	6	-	0/6/23/26	0/1/1/1
6	BMA	A	834	6	-	0/2/19/22	0/1/1/1
9	NAG	A	923	9	-	0/6/23/26	0/1/1/1
9	BMA	A	924	9	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	821	NAG	C2-N2-C7	-3.01	119.17	123.04
5	A	823	NAG	C2-N2-C7	-2.37	120.00	123.04
4	A	801	NAG	C2-N2-C7	-2.28	120.11	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	NAG	2	0
4	A	803	NDG	3	0
9	A	923	NAG	2	0
9	A	924	BMA	2	0

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
7	NDG	A	901	1	14,14,15	0.59	0	15,19,21	0.71	1 (6%)
8	NAG	A	911	1	14,14,15	0.64	0	15,19,21	0.64	0
8	NAG	A	921	1	14,14,15	0.55	0	15,19,21	0.63	0
8	NAG	B	811	2	14,14,15	0.55	0	15,19,21	0.76	1 (6%)
10	PCJ	C	1	3	60,61,61	0.76	1 (1%)	61,65,65	1.08	5 (8%)

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
7	NDG	A	901	1	-	0/6/23/26	0/1/1/1
8	NAG	A	911	1	-	0/6/23/26	0/1/1/1
8	NAG	A	921	1	-	0/6/23/26	0/1/1/1
8	NAG	B	811	2	-	0/6/23/26	0/1/1/1
10	PCJ	C	1	3	-	0/66/66/66	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1	PCJ	O-C	-4.56	1.22	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1	PCJ	C2-O2-C46	-2.91	110.91	117.89
8	B	811	NAG	C2-N2-C7	-2.49	119.84	123.04
10	C	1	PCJ	C3-O3-C26	-2.33	110.33	116.85
7	A	901	NDG	C2-N2-C7	-2.13	120.30	123.04
10	C	1	PCJ	O3-C26-C25	2.65	119.97	111.90
10	C	1	PCJ	O-C-CA	3.10	120.54	112.19
10	C	1	PCJ	O2-C46-C45	3.54	119.22	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	911	NAG	1	0
10	C	1	PCJ	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	549/549 (100%)	1.65	160 (29%) 1 1	22, 59, 130, 137	0
2	B	520/520 (100%)	0.21	12 (2%) 64 70	20, 35, 60, 83	0
3	C	5/5 (100%)	1.31	1 (20%) 1 2	41, 57, 74, 83	0
All	All	1074/1074 (100%)	0.95	173 (16%) 3 4	20, 43, 125, 137	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	THR	11.7
1	A	28	LEU	11.7
1	A	67	ILE	11.6
1	A	46	ILE	11.1
1	A	35	ILE	11.1
1	A	99	LEU	10.5
1	A	83	LEU	9.9
1	A	48	SER	9.8
1	A	573	ILE	9.7
1	A	247	THR	9.5
1	A	59	LEU	9.3
1	A	96	PHE	9.0
1	A	57	LEU	8.9
1	A	76	VAL	8.8
1	A	31	ASP	8.3
1	A	38	GLY	8.3
1	A	53	ALA	8.2
1	A	50	LEU	8.2
1	A	572	ILE	8.2
1	A	39	SER	8.1
1	A	33	ASN	8.1
1	A	47	PRO	8.0
1	A	27	SER	8.0

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Mol	Chain	Res	Type	RSRZ
1	A	40	SER	8.0
1	A	43	LEU	7.9
1	A	66	TYR	7.9
1	A	36	CYS	7.7
1	A	32	ARG	7.6
1	A	242	LEU	7.5
1	A	105	LEU	7.2
1	A	107	LEU	7.2
1	A	78	LEU	7.1
1	A	141	GLU	7.1
1	A	245	GLY	6.9
1	A	51	THR	6.9
1	A	74	ARG	6.5
1	A	30	CYS	6.4
1	A	29	SER	6.3
1	A	55	LYS	6.3
1	A	115	LEU	6.2
1	A	68	SER	6.2
1	A	574	CYS	6.2
1	A	243	SER	6.1
1	A	175	PHE	5.9
1	A	81	LEU	5.9
1	A	117	SER	5.9
1	A	72	LEU	5.8
2	B	228	ASN	5.8
1	A	61	ASN	5.7
1	A	90	THR	5.7
1	A	102	LEU	5.6
1	A	302	ARG	5.6
1	A	112	LEU	5.5
2	B	227	ASP	5.4
1	A	164	LYS	5.4
1	A	91	ILE	5.3
1	A	120	PHE	5.2
1	A	86	ASN	5.1
1	A	63	ARG	5.1
1	A	575	PRO	5.1
1	A	145	PHE	5.1
1	A	129	LEU	5.1
1	A	56	SER	5.0
1	A	88	ILE	4.9
1	A	49	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	140	GLY	4.7
1	A	77	ASN	4.7
1	A	170	PHE	4.6
1	A	564	GLY	4.6
1	A	151	LEU	4.6
2	B	25	SER	4.6
1	A	37	LYS	4.5
1	A	114	ASN	4.4
1	A	126	LEU	4.4
1	A	75	CYS	4.4
1	A	44	ASN	4.4
1	A	300	ASN	4.4
1	A	87	GLY	4.3
1	A	148	LEU	4.3
1	A	123	LEU	4.3
1	A	159	MET	4.3
1	A	176	LEU	4.3
1	A	103	GLU	4.3
1	A	135	PRO	4.2
1	A	143	SER	4.2
1	A	111	TYR	4.2
1	A	144	LEU	4.2
1	A	551	LYS	4.2
1	A	58	ASP	4.1
1	A	248	ASN	4.1
1	A	34	GLY	4.1
1	A	519	PHE	4.0
1	A	137	LYS	4.0
3	C	6	LYS	3.9
1	A	198	GLN	3.8
1	A	301	ASP	3.8
1	A	62	ASN	3.8
2	B	508	CYS	3.8
1	A	569	VAL	3.7
1	A	73	GLN	3.7
1	A	160	ASP	3.6
1	A	121	LYS	3.6
1	A	570	ARG	3.6
1	A	547	ARG	3.6
1	A	246	GLU	3.5
2	B	533	GLY	3.5
1	A	42	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	84	THR	3.4
1	A	65	THR	3.3
1	A	54	VAL	3.3
1	A	571	SER	3.3
1	A	82	VAL	3.3
1	A	539	CYS	3.3
1	A	168	LYS	3.2
1	A	558	GLY	3.1
2	B	226	GLU	3.1
1	A	89	ASN	3.1
1	A	41	GLY	3.1
1	A	94	ASP	3.1
1	A	70	SER	3.0
1	A	541	ARG	3.0
1	A	104	HIS	3.0
1	A	125	SER	3.0
1	A	173	LEU	2.9
1	A	147	HIS	2.9
1	A	109	TYR	2.9
1	A	542	ILE	2.8
1	A	92	GLU	2.8
1	A	298	SER	2.8
1	A	128	PHE	2.8
1	A	119	TRP	2.8
1	A	150	LYS	2.7
1	A	52	GLU	2.7
1	A	79	GLN	2.7
1	A	261	ILE	2.7
2	B	219	SER	2.7
1	A	211	ILE	2.6
1	A	139	LEU	2.6
1	A	156	VAL	2.6
2	B	114	VAL	2.6
1	A	136	TYR	2.6
1	A	45	SER	2.6
1	A	71	ASP	2.6
1	A	153	ILE	2.5
2	B	229	LYS	2.5
1	A	152	GLN	2.5
1	A	490	MET	2.4
1	A	187	GLN	2.4
1	A	540	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	510	GLN	2.4
1	A	172	GLY	2.4
1	A	118	SER	2.4
2	B	509	PRO	2.3
1	A	93	GLU	2.3
1	A	543	ASP	2.3
2	B	242	THR	2.3
1	A	535	TRP	2.3
1	A	64	ILE	2.3
1	A	60	SER	2.3
1	A	549	LEU	2.3
1	A	69	ASN	2.2
1	A	167	ARG	2.2
1	A	565	SER	2.2
1	A	516	ASP	2.2
1	A	544	TYR	2.2
1	A	124	SER	2.1
2	B	322	ILE	2.1
1	A	520	ASP	2.1
1	A	85	SER	2.1
1	A	546	SER	2.1
1	A	106	ASP	2.1
1	A	215	GLU	2.0
1	A	98	SER	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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	821	14/15	0.90	0.11	-0.61	41,46,52,56	0
4	NAG	A	801	14/15	0.93	0.09	-1.02	53,58,62,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	A	831	14/15	0.95	0.10	-1.18	24,30,33,40	0
9	NAG	A	923	14/15	0.43	0.28	-	90,93,96,96	0
6	BMA	A	834	11/12	0.79	0.18	-	68,72,74,77	0
4	MAN	A	804	11/12	0.36	0.71	-	98,100,102,102	0
5	MAN	A	824	11/12	0.74	0.46	-	81,84,86,88	0
6	NAG	A	833	14/15	0.93	0.10	-	35,48,54,62	0
4	NDG	A	803	14/15	0.61	0.29	-	80,85,89,94	0
9	BMA	A	924	11/12	0.48	0.31	-	96,98,99,99	0
5	NAG	A	823	14/15	0.84	0.19	-	55,65,71,75	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
10	PCJ	C	1	62/62	0.93	0.20	1.76	28,37,53,56	0
8	NAG	A	921	14/15	0.94	0.08	-1.51	31,34,37,37	0
8	NAG	B	811	14/15	0.70	0.29	-	74,78,80,81	0
7	NDG	A	901	14/15	0.67	0.46	-	104,106,107,107	0
8	NAG	A	911	14/15	0.55	0.22	-	71,74,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.