



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:17 AM GMT

PDB ID : 3A79  
Title : Crystal structure of TLR2-TLR6-Pam2CSK4 complex  
Authors : Kang, J.Y.; Jin, M.S.; Lee, J.-O.  
Deposited on : 2009-09-20  
Resolution : 2.90 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](mailto: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.

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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

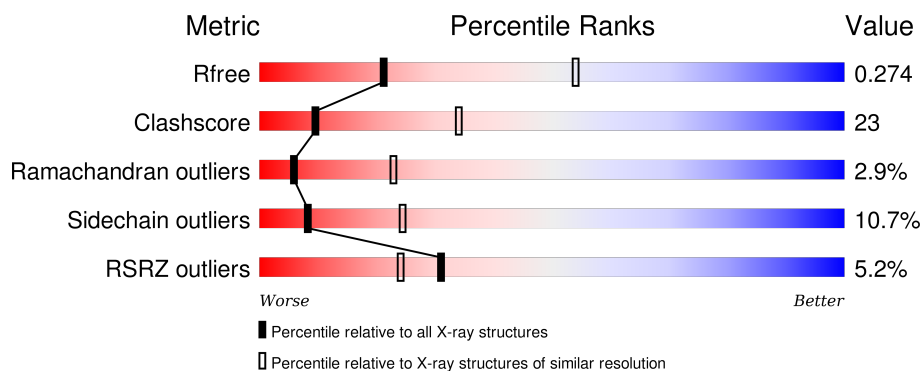
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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  $\geq 3$ , 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	580	<div> <div>5%</div> <div> <div>54%</div> <div>35%</div> <div>5% • 5%</div> </div> </div>
2	B	562	<div> <div>4%</div> <div> <div>52%</div> <div>35%</div> <div>6% 7%</div> </div> </div>
3	C	6	<div> <div>33%</div> <div> <div>33%</div> <div>50%</div> <div>17%</div> </div> </div>

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
4	PXS	C	581	-	-	-	X
5	NAG	A	811	-	-	-	X
5	NAG	B	981	-	-	-	X
8	NDG	B	971	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8906 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	550	Total	C	N	O	S	0	0	0
			4355	2771	736	828	20			

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 a protein called Toll-like receptor 6, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	525	Total	C	N	O	S	0	0	0
			4192	2675	721	769	27			

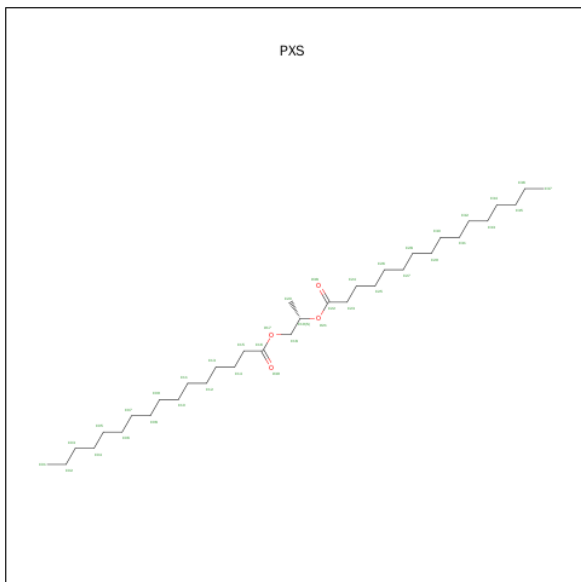
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	LEU	-	EXPRESSION TAG	UNP Q4G1L3
B	560	VAL	-	EXPRESSION TAG	UNP Q4G1L3
B	561	PRO	-	EXPRESSION TAG	UNP Q4G1L3
B	562	ARG	-	EXPRESSION TAG	UNP Q4G1L3

- Molecule 3 is a protein called Pam2CSK4.

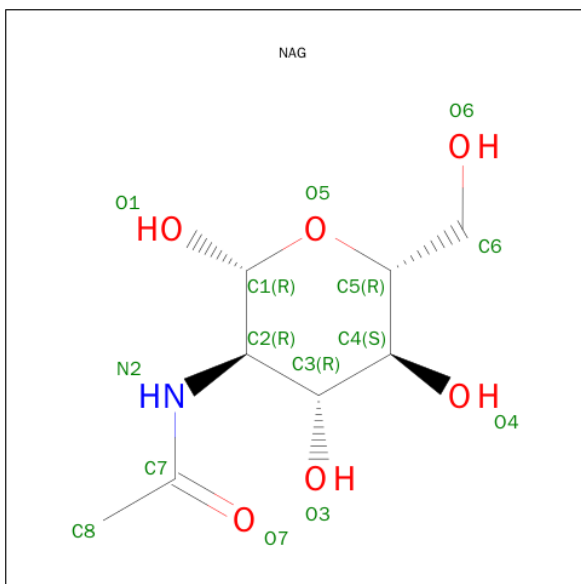
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	S	0	0	0
			49	30	10	8	1			

- Molecule 4 is (2S)-PROPANE-1,2-DIYL DIHEXADECANOATE (three-letter code: PXS) (formula:  $C_{35}H_{68}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			39	35	4		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

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

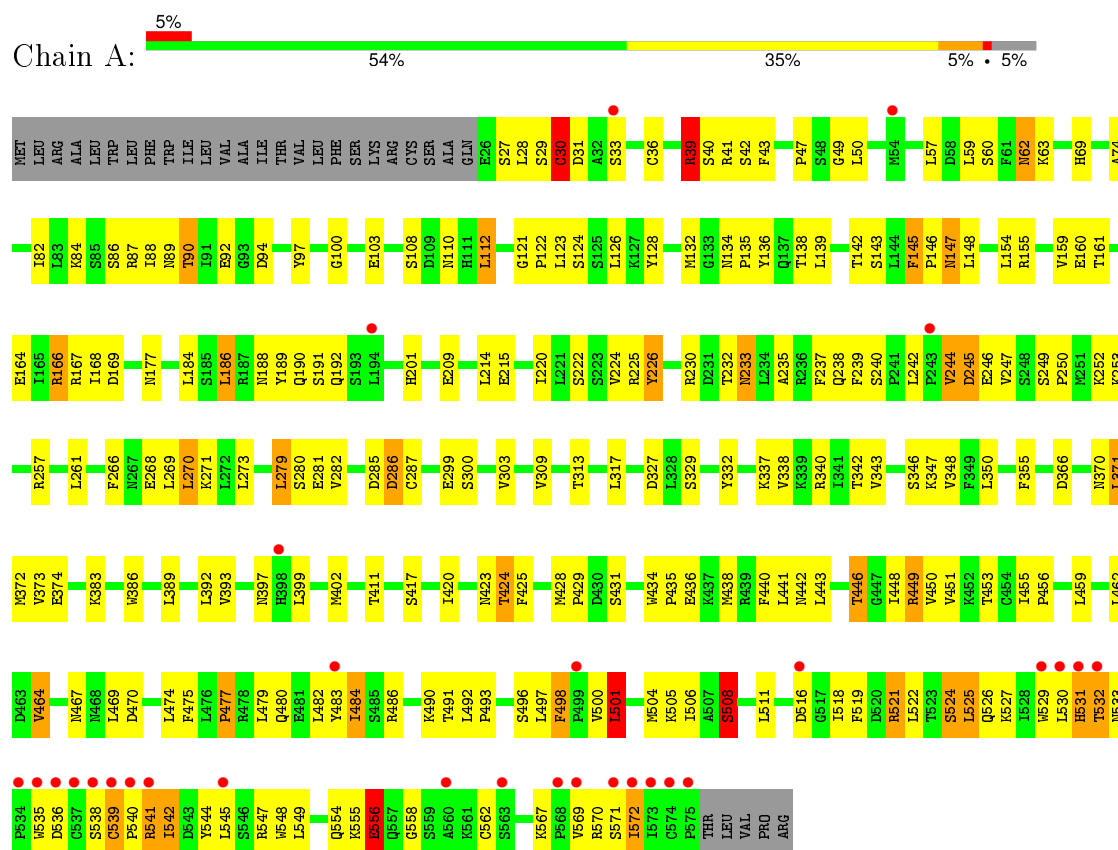
- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

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

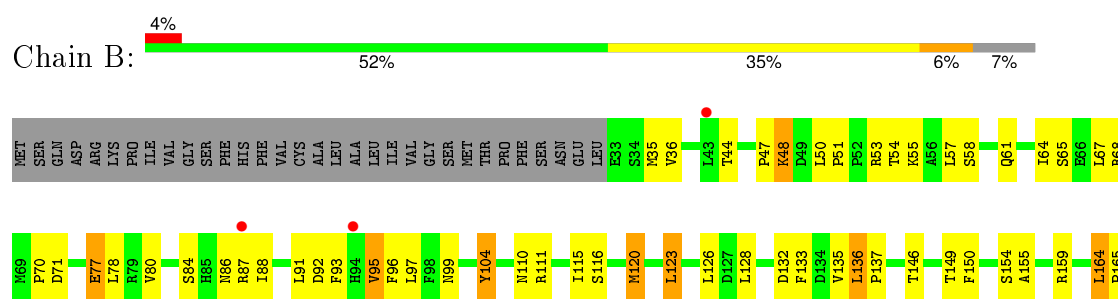
### 3 Residue-property plots

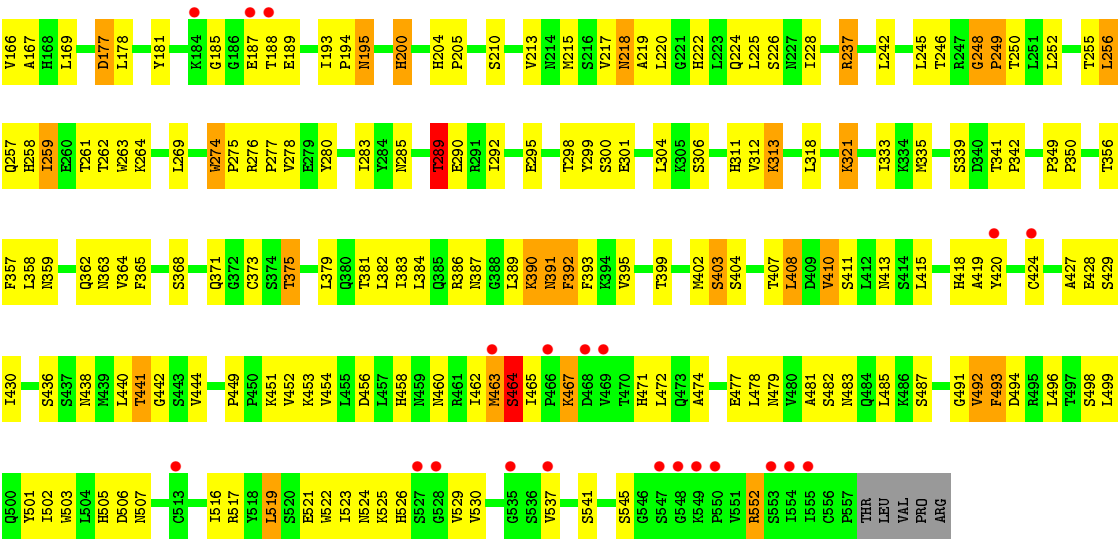
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



- Molecule 2: Toll-like receptor 6, Variable lymphocyte receptor B





● Molecule 3: Pam2CSK4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.90Å 168.90Å 231.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.11 – 2.90 34.11 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.11-2.90) 99.7 (34.11-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.73 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.208 , 0.280 0.206 , 0.274	Depositor DCC
$R_{free}$ test set	4433 reflections (11.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.0	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 43597 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8906	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PXS, BMA, 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	0.37	0/4439	0.58	0/6013
2	B	0.41	0/4286	0.60	2/5821 (0.0%)
3	C	0.44	0/48	0.47	0/57
All	All	0.39	0/8773	0.59	2/11891 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	313	LYS	CD-CE-NZ	5.86	125.18	111.70
2	B	289	THR	N-CA-C	5.10	124.78	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	248	GLY	Peptide

## 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	4355	0	4400	198	0
2	B	4192	0	4201	198	0
3	C	49	0	60	5	0
4	C	39	0	67	12	0
5	A	28	0	26	0	0
5	B	42	0	39	2	0
6	A	28	0	25	2	0
6	B	28	0	25	4	0
7	B	117	0	102	2	0
8	B	28	0	25	0	0
All	All	8906	0	8970	403	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 23.

All (403) 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)
2:B:48:LYS:HD3	2:B:48:LYS:H	1.13	1.08
1:A:269:LEU:HB3	4:C:581:PXS:H01	1.39	1.05
2:B:389:LEU:H	2:B:413:ASN:HD22	1.03	1.02
2:B:218:ASN:OD1	5:B:981:NAG:O6	1.79	1.00
1:A:112:LEU:H	1:A:134:ASN:HD22	1.06	0.96
2:B:442:GLY:HA3	2:B:464:SER:O	1.66	0.96
2:B:246:THR:HG21	2:B:276:ARG:HD3	1.48	0.94
2:B:258:HIS:HD2	2:B:285:ASN:HD22	1.07	0.94
1:A:350:LEU:O	4:C:581:PXS:H18	1.70	0.91
2:B:246:THR:HG22	2:B:276:ARG:HH11	1.35	0.90
1:A:29:SER:O	1:A:30:CYS:HB2	1.70	0.89
2:B:259:ILE:HD12	2:B:259:ILE:H	1.39	0.86
2:B:467:LYS:H	2:B:467:LYS:HD3	1.39	0.86
1:A:348:VAL:HG22	4:C:581:PXS:H25	1.62	0.82
1:A:446:THR:H	1:A:467:ASN:HD21	1.25	0.82
2:B:462:ILE:H	2:B:483:ASN:HD22	1.28	0.80
2:B:246:THR:CG2	2:B:276:ARG:HD3	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:MET:HG2	2:B:123:LEU:HD22	1.62	0.80
1:A:112:LEU:HB2	1:A:134:ASN:ND2	1.97	0.79
2:B:224:GLN:HG3	2:B:255:THR:HB	1.63	0.79
2:B:262:THR:HG22	2:B:264:LYS:N	1.96	0.79
1:A:57:LEU:HD11	1:A:59:LEU:HD21	1.66	0.77
2:B:349:PRO:O	2:B:375:THR:HG21	1.85	0.77
1:A:39:ARG:HH11	1:A:39:ARG:HB2	1.49	0.76
2:B:485:LEU:HB2	2:B:507:ASN:ND2	2.01	0.76
2:B:193:ILE:HB	2:B:217:VAL:HG22	1.68	0.75
2:B:427:ALA:HB3	2:B:430:ILE:HD11	1.68	0.75
2:B:218:ASN:ND2	2:B:218:ASN:H	1.84	0.75
2:B:389:LEU:H	2:B:413:ASN:ND2	1.83	0.75
2:B:48:LYS:HD3	2:B:48:LYS:N	1.97	0.74
1:A:112:LEU:N	1:A:134:ASN:HD22	1.85	0.73
2:B:258:HIS:CD2	2:B:285:ASN:HD22	1.99	0.73
2:B:418:HIS:CE1	2:B:441:THR:HG21	2.24	0.73
1:A:399:LEU:HB2	1:A:423:ASN:HD22	1.53	0.73
1:A:531:HIS:HD2	1:A:558:GLY:HA3	1.52	0.73
1:A:112:LEU:H	1:A:134:ASN:ND2	1.84	0.72
1:A:110:ASN:HB2	1:A:134:ASN:HD21	1.55	0.71
1:A:529:TRP:O	1:A:530:LEU:HD12	1.91	0.70
1:A:555:LYS:O	1:A:556:GLU:HB2	1.90	0.70
2:B:88:ILE:H	2:B:110:ASN:HD22	1.39	0.70
2:B:502:ILE:HG22	2:B:529:VAL:HG12	1.73	0.70
2:B:257:GLN:HE21	2:B:258:HIS:CE1	2.08	0.70
1:A:30:CYS:HA	1:A:36:CYS:HA	1.73	0.70
2:B:449:PRO:O	2:B:452:VAL:HG23	1.91	0.70
1:A:521:ARG:H	1:A:521:ARG:HD3	1.55	0.70
2:B:248:GLY:HA3	2:B:277:PRO:HG2	1.73	0.69
1:A:518:ILE:HG23	1:A:519:PHE:CD2	2.28	0.69
1:A:88:ILE:H	1:A:110:ASN:HD22	1.41	0.68
1:A:446:THR:HG23	1:A:448:ILE:HG23	1.74	0.68
2:B:467:LYS:N	2:B:467:LYS:HD3	2.07	0.68
2:B:289:THR:HG22	2:B:290:GLU:HG3	1.76	0.67
2:B:393:PHE:HD1	2:B:419:ALA:HB3	1.59	0.67
1:A:29:SER:OG	1:A:30:CYS:N	2.28	0.67
2:B:493:PHE:HB3	2:B:522:TRP:CZ2	2.30	0.66
2:B:391:ASN:HD22	2:B:391:ASN:C	1.96	0.66
1:A:372:MET:H	1:A:397:ASN:HD22	1.43	0.66
1:A:505:LYS:HA	1:A:529:TRP:HB2	1.78	0.66
2:B:449:PRO:HB2	2:B:452:VAL:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TRP:CD1	1:A:456:PRO:HG3	2.30	0.66
2:B:492:VAL:HG23	2:B:493:PHE:H	1.61	0.65
2:B:154:SER:HB3	2:B:177:ASP:OD1	1.96	0.65
1:A:63:LYS:HG2	1:A:87:ARG:HG3	1.79	0.64
2:B:262:THR:HG22	2:B:264:LYS:H	1.61	0.64
1:A:121:GLY:N	1:A:122:PRO:HD2	2.11	0.64
1:A:506:ILE:HG12	1:A:506:ILE:O	1.98	0.64
1:A:492:LEU:HG	1:A:493:PRO:HD2	1.80	0.64
1:A:313:THR:HG23	1:A:342:THR:HB	1.79	0.64
2:B:428:GLU:CD	2:B:428:GLU:H	2.00	0.64
2:B:218:ASN:H	2:B:218:ASN:HD22	1.46	0.64
2:B:92:ASP:O	2:B:95:VAL:HB	1.98	0.63
2:B:289:THR:CG2	2:B:290:GLU:HG3	2.28	0.63
1:A:222:SER:HB3	1:A:247:VAL:HG11	1.80	0.63
1:A:441:LEU:HB3	1:A:459:LEU:HD21	1.80	0.63
1:A:386:TRP:HB3	1:A:389:LEU:HB2	1.79	0.63
2:B:53:ARG:HD2	2:B:77:GLU:OE1	1.99	0.63
1:A:50:LEU:O	1:A:74:ALA:HB1	1.99	0.63
2:B:154:SER:CB	2:B:177:ASP:OD1	2.47	0.63
6:B:931:NAG:H61	6:B:932:NAG:H2	1.81	0.63
1:A:147:ASN:C	1:A:148:LEU:HD12	2.19	0.63
1:A:480:GLN:O	1:A:501:LEU:HD22	1.99	0.62
1:A:346:SER:H	1:A:370:ASN:HD21	1.47	0.62
1:A:280:SER:HA	1:A:309:VAL:HA	1.82	0.62
1:A:268:GLU:O	1:A:271:LYS:HB2	1.99	0.62
1:A:530:LEU:HD23	1:A:535:TRP:CZ2	2.35	0.62
1:A:89:ASN:OD1	1:A:90:THR:HG22	1.99	0.62
2:B:485:LEU:H	2:B:507:ASN:ND2	1.97	0.61
1:A:531:HIS:CD2	1:A:558:GLY:HA3	2.33	0.61
1:A:554:GLN:HG3	1:A:555:LYS:H	1.65	0.61
1:A:484:ILE:HG12	1:A:484:ILE:O	1.99	0.61
2:B:387:ASN:HB2	2:B:413:ASN:HD21	1.65	0.61
1:A:455:ILE:H	1:A:455:ILE:HD12	1.66	0.60
1:A:145:PHE:N	1:A:146:PRO:HD3	2.16	0.60
2:B:189:GLU:HB2	2:B:213:VAL:HG22	1.82	0.60
2:B:391:ASN:ND2	2:B:393:PHE:H	1.99	0.60
2:B:311:HIS:NE2	2:B:313:LYS:HE2	2.17	0.60
1:A:538:SER:HB2	1:A:541:ARG:HD3	1.84	0.60
1:A:103:GLU:HA	1:A:126:LEU:HA	1.84	0.60
2:B:395:VAL:HG21	2:B:415:LEU:HD21	1.84	0.59
1:A:186:LEU:HD21	1:A:189:TYR:HB2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:THR:CG2	2:B:276:ARG:HH11	2.11	0.59
2:B:393:PHE:CD1	2:B:419:ALA:HB3	2.37	0.59
1:A:443:LEU:O	1:A:446:THR:HB	2.03	0.59
2:B:349:PRO:HB2	2:B:375:THR:HG23	1.85	0.58
1:A:483:TYR:CD2	1:A:505:LYS:HD3	2.38	0.58
1:A:518:ILE:HG23	1:A:519:PHE:CE2	2.38	0.58
1:A:138:THR:HG22	1:A:164:GLU:HB2	1.85	0.58
2:B:93:PHE:H	2:B:116:SER:HB3	1.68	0.58
1:A:159:VAL:HA	1:A:184:LEU:HD12	1.85	0.58
1:A:451:VAL:HG12	1:A:474:LEU:HD22	1.84	0.58
2:B:451:LYS:O	2:B:453:LYS:HE3	2.03	0.58
2:B:465:ILE:HG13	2:B:485:LEU:HD21	1.85	0.58
2:B:218:ASN:ND2	2:B:218:ASN:N	2.52	0.57
2:B:259:ILE:HD13	2:B:283:ILE:HG23	1.86	0.57
1:A:329:SER:HA	1:A:332:TYR:CE1	2.39	0.57
1:A:167:ARG:NH2	1:A:190:GLN:HE21	2.01	0.57
2:B:217:VAL:HG11	2:B:220:LEU:HB2	1.86	0.57
2:B:210:SER:HB2	2:B:237:ARG:NH2	2.19	0.57
2:B:505:HIS:HD2	2:B:506:ASP:OD2	1.88	0.57
2:B:55:LYS:O	2:B:78:LEU:HD12	2.05	0.57
2:B:35:MET:HG3	2:B:36:VAL:N	2.18	0.56
2:B:312:VAL:O	2:B:342:PRO:HD3	2.05	0.56
2:B:478:LEU:HD12	2:B:479:ASN:H	1.69	0.56
2:B:478:LEU:O	2:B:503:TRP:HE3	1.88	0.56
1:A:455:ILE:HD12	1:A:455:ILE:N	2.21	0.56
1:A:220:ILE:HB	1:A:224:VAL:HG23	1.86	0.56
1:A:266:PHE:N	4:C:581:PXS:H37	2.20	0.56
2:B:523:ILE:HG23	2:B:530:VAL:HG21	1.87	0.56
1:A:266:PHE:CA	4:C:581:PXS:H37	2.36	0.56
2:B:120:MET:HG2	2:B:123:LEU:CD2	2.35	0.56
1:A:383:LYS:HA	1:A:411:THR:HG22	1.88	0.56
2:B:363:ASN:HB2	2:B:387:ASN:HD21	1.69	0.55
1:A:43:PHE:CE1	1:A:47:PRO:HG3	2.41	0.55
1:A:526:GLN:HA	1:A:555:LYS:HE3	1.89	0.55
2:B:391:ASN:ND2	2:B:391:ASN:C	2.60	0.55
2:B:389:LEU:HG	2:B:413:ASN:ND2	2.22	0.55
1:A:143:SER:HB2	1:A:146:PRO:HG3	1.89	0.55
2:B:87:ARG:HD2	2:B:111:ARG:NH2	2.22	0.55
2:B:166:VAL:HB	2:B:169:LEU:HD12	1.88	0.55
1:A:479:LEU:HD21	1:A:482:LEU:HD13	1.88	0.55
1:A:542:ILE:O	1:A:542:ILE:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:HD12	2:B:97:LEU:O	2.06	0.55
2:B:477:GLU:HA	2:B:501:TYR:HB2	1.88	0.54
2:B:449:PRO:O	2:B:452:VAL:CG2	2.56	0.54
1:A:462:LEU:HG	1:A:464:VAL:CG2	2.37	0.54
2:B:349:PRO:HB2	2:B:375:THR:CG2	2.38	0.54
1:A:226:TYR:CE2	1:A:253:LYS:HD3	2.42	0.54
1:A:69:HIS:CD2	1:A:94:ASP:OD1	2.62	0.53
1:A:504:MET:HG2	1:A:506:ILE:HG22	1.90	0.53
1:A:492:LEU:HD23	1:A:493:PRO:O	2.07	0.53
6:B:931:NAG:O4	6:B:932:NAG:H4	2.07	0.53
2:B:321:LYS:HD2	2:B:321:LYS:N	2.24	0.53
2:B:262:THR:HG22	2:B:263:TRP:N	2.22	0.53
2:B:280:TYR:CE2	6:B:931:NAG:H62	2.43	0.53
1:A:483:TYR:CE2	1:A:505:LYS:HD3	2.42	0.53
1:A:501:LEU:O	1:A:524:SER:HB2	2.09	0.53
2:B:64:ILE:H	2:B:86:ASN:ND2	2.07	0.53
2:B:258:HIS:HD2	2:B:285:ASN:ND2	1.91	0.53
2:B:335:MET:HG2	2:B:357:PHE:HB3	1.91	0.53
3:C:14:LYS:HD2	3:C:15:LYS:HG2	1.90	0.52
2:B:365:PHE:H	2:B:387:ASN:HD22	1.55	0.52
2:B:136:LEU:HD13	2:B:155:ALA:HB2	1.92	0.52
2:B:485:LEU:H	2:B:507:ASN:HD22	1.57	0.52
1:A:525:LEU:HD12	1:A:527:LYS:H	1.74	0.52
2:B:491:GLY:HA2	2:B:494:ASP:OD2	2.09	0.52
2:B:358:LEU:HD12	2:B:379:LEU:HD22	1.92	0.52
1:A:455:ILE:H	1:A:455:ILE:CD1	2.23	0.52
2:B:133:PHE:CG	2:B:137:PRO:HG3	2.46	0.51
2:B:65:SER:O	2:B:88:ILE:HA	2.11	0.51
2:B:218:ASN:O	2:B:249:PRO:HG2	2.10	0.51
2:B:64:ILE:H	2:B:86:ASN:HD22	1.58	0.51
1:A:273:LEU:HD22	1:A:279:LEU:HD12	1.93	0.51
1:A:112:LEU:HB2	1:A:134:ASN:HD22	1.71	0.51
2:B:356:THR:HA	2:B:379:LEU:HA	1.93	0.51
2:B:262:THR:CG2	2:B:263:TRP:N	2.73	0.51
2:B:64:ILE:N	2:B:86:ASN:HD22	2.09	0.51
1:A:159:VAL:HG12	1:A:160:GLU:HG3	1.93	0.50
1:A:522:LEU:C	1:A:524:SER:H	2.14	0.50
2:B:415:LEU:H	2:B:438:ASN:HD22	1.59	0.50
1:A:299:GLU:O	1:A:303:VAL:HG23	2.11	0.50
1:A:134:ASN:HB2	1:A:136:TYR:CE2	2.46	0.50
1:A:446:THR:N	1:A:467:ASN:HD21	2.03	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:TRP:C	1:A:530:LEU:HD12	2.31	0.50
1:A:529:TRP:HD1	1:A:531:HIS:HE2	1.59	0.50
2:B:68:ARG:O	2:B:71:ASP:HB2	2.11	0.50
2:B:471:HIS:C	2:B:472:LEU:HG	2.31	0.50
1:A:233:ASN:HD21	1:A:235:ALA:HB2	1.76	0.50
2:B:402:MET:O	2:B:404:SER:N	2.44	0.50
2:B:492:VAL:O	2:B:494:ASP:N	2.45	0.50
1:A:285:ASP:O	1:A:287:CYS:N	2.45	0.50
1:A:399:LEU:CB	1:A:423:ASN:HD22	2.23	0.50
1:A:89:ASN:OD1	1:A:90:THR:CG2	2.60	0.50
2:B:259:ILE:CD1	2:B:283:ILE:HG23	2.42	0.49
2:B:264:LYS:HG3	2:B:295:GLU:OE1	2.13	0.49
2:B:359:ASN:HA	2:B:383:ILE:HB	1.94	0.49
2:B:462:ILE:H	2:B:483:ASN:ND2	2.04	0.49
2:B:120:MET:HE3	2:B:120:MET:H	1.77	0.49
1:A:371:LEU:HG	2:B:364:VAL:HG12	1.93	0.49
1:A:525:LEU:HD12	1:A:526:GLN:N	2.27	0.49
1:A:402:MET:HE3	1:A:428:MET:HB3	1.95	0.49
2:B:318:LEU:HA	3:C:11:CYS:O	2.11	0.49
2:B:492:VAL:C	2:B:494:ASP:H	2.16	0.49
1:A:139:LEU:HD12	1:A:169:ASP:HB3	1.95	0.49
2:B:51:PRO:O	2:B:54:THR:OG1	2.27	0.49
1:A:186:LEU:HD11	1:A:188:ASN:O	2.13	0.49
2:B:411:SER:HB2	2:B:436:SER:O	2.13	0.49
1:A:348:VAL:H	1:A:370:ASN:ND2	2.11	0.48
1:A:237:PHE:O	1:A:268:GLU:HG3	2.13	0.48
2:B:274:TRP:CE2	2:B:299:TYR:CD2	3.01	0.48
1:A:201:HIS:HD2	1:A:225:ARG:HD2	1.78	0.48
1:A:346:SER:O	1:A:347:LYS:HB2	2.13	0.48
2:B:519:LEU:O	2:B:523:ILE:HG12	2.14	0.48
2:B:375:THR:HG23	2:B:375:THR:O	2.12	0.48
1:A:159:VAL:HG12	1:A:160:GLU:CG	2.43	0.48
2:B:200:HIS:HE1	2:B:226:SER:OG	1.96	0.48
2:B:341:THR:H	2:B:363:ASN:HD22	1.62	0.48
2:B:195:ASN:N	2:B:195:ASN:OD1	2.45	0.48
2:B:321:LYS:HD2	2:B:321:LYS:H	1.79	0.48
2:B:368:SER:HA	2:B:371:GLN:HG2	1.95	0.48
1:A:214:LEU:HD22	1:A:242:LEU:HD21	1.94	0.48
2:B:225:LEU:HB2	2:B:228:ILE:HD11	1.96	0.47
1:A:538:SER:HB2	1:A:541:ARG:CD	2.43	0.47
2:B:278:VAL:O	2:B:304:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:C	1:A:440:PHE:CD2	2.87	0.47
2:B:78:LEU:HD11	2:B:80:VAL:O	2.15	0.47
1:A:279:LEU:HD22	1:A:281:GLU:H	1.79	0.47
1:A:270:LEU:HD22	1:A:270:LEU:O	2.14	0.47
1:A:346:SER:H	1:A:370:ASN:ND2	2.13	0.47
1:A:372:MET:N	1:A:397:ASN:HD22	2.12	0.47
2:B:389:LEU:N	2:B:413:ASN:HD22	1.89	0.47
2:B:120:MET:HE3	2:B:120:MET:N	2.29	0.47
2:B:96:PHE:HD1	2:B:120:MET:HE1	1.80	0.47
1:A:63:LYS:HG2	1:A:87:ARG:NH1	2.30	0.47
1:A:562:CYS:SG	1:A:567:LYS:O	2.73	0.47
1:A:249:SER:HA	1:A:250:PRO:HD3	1.65	0.47
2:B:478:LEU:HD12	2:B:479:ASN:N	2.30	0.46
1:A:521:ARG:N	1:A:521:ARG:HD3	2.24	0.46
1:A:490:LYS:O	1:A:511:LEU:HD23	2.15	0.46
1:A:529:TRP:HD1	1:A:531:HIS:NE2	2.14	0.46
1:A:538:SER:HB2	1:A:541:ARG:HG2	1.96	0.46
2:B:150:PHE:C	2:B:150:PHE:CD2	2.88	0.46
1:A:455:ILE:HA	1:A:456:PRO:HD3	1.75	0.46
1:A:252:LYS:O	1:A:279:LEU:HD23	2.16	0.46
1:A:69:HIS:HD2	1:A:94:ASP:OD1	1.98	0.46
1:A:128:TYR:CD2	1:A:128:TYR:C	2.89	0.46
4:C:581:PXS:H09	4:C:581:PXS:C31	2.46	0.46
2:B:442:GLY:C	2:B:444:VAL:N	2.69	0.46
1:A:167:ARG:CZ	1:A:190:GLN:HE21	2.28	0.46
1:A:533:ASN:HB3	1:A:535:TRP:NE1	2.30	0.46
2:B:456:ASP:OD1	2:B:458:HIS:ND1	2.47	0.46
1:A:486:ARG:NH1	6:A:832:NAG:H81	2.31	0.46
1:A:392:LEU:HD12	1:A:393:VAL:N	2.31	0.46
1:A:531:HIS:O	1:A:532:THR:C	2.55	0.46
2:B:67:LEU:O	2:B:95:VAL:HG21	2.16	0.46
1:A:145:PHE:CE2	1:A:154:LEU:HD21	2.51	0.46
1:A:329:SER:HA	1:A:332:TYR:CD1	2.51	0.46
2:B:362:GLN:HA	2:B:386:ARG:O	2.15	0.46
1:A:449:ARG:O	1:A:450:VAL:HG23	2.16	0.46
3:C:14:LYS:HG3	3:C:15:LYS:H	1.79	0.45
2:B:57:LEU:HD12	2:B:58:SER:N	2.31	0.45
1:A:497:LEU:HB2	1:A:498:PHE:CE2	2.51	0.45
2:B:215:MET:HB3	2:B:245:LEU:HD21	1.97	0.45
2:B:246:THR:HG22	2:B:276:ARG:NH1	2.17	0.45
2:B:485:LEU:HB2	2:B:507:ASN:HD22	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:525:LYS:HE2	2:B:526:HIS:CE1	2.51	0.45
6:B:931:NAG:C6	6:B:932:NAG:H2	2.44	0.45
1:A:159:VAL:HG22	1:A:184:LEU:CD1	2.47	0.45
1:A:462:LEU:HG	1:A:464:VAL:HG22	1.98	0.45
2:B:505:HIS:HB3	2:B:541:SER:HB3	1.98	0.45
1:A:440:PHE:HE2	1:A:442:ASN:HB2	1.80	0.45
1:A:508:SER:HA	1:A:532:THR:O	2.15	0.45
1:A:420:ILE:HD12	1:A:425:PHE:CZ	2.51	0.45
2:B:136:LEU:HD13	2:B:155:ALA:CB	2.47	0.45
1:A:28:LEU:HD23	1:A:29:SER:N	2.32	0.45
1:A:486:ARG:HH12	6:A:832:NAG:H81	1.82	0.45
1:A:134:ASN:HA	1:A:135:PRO:HD3	1.65	0.45
2:B:427:ALA:O	2:B:430:ILE:HG12	2.17	0.45
1:A:440:PHE:CE2	1:A:442:ASN:HB2	2.52	0.45
2:B:167:ALA:HA	2:B:194:PRO:HB3	1.97	0.45
1:A:539:CYS:N	1:A:540:PRO:CD	2.80	0.45
2:B:195:ASN:HD22	5:B:981:NAG:H83	1.82	0.44
1:A:434:TRP:HE3	1:A:438:MET:HE1	1.81	0.44
1:A:285:ASP:HB3	1:A:286:ASP:H	1.49	0.44
2:B:516:ILE:O	2:B:516:ILE:HG13	2.16	0.44
1:A:348:VAL:HA	4:C:581:PXS:H24	1.99	0.44
1:A:27:SER:O	1:A:41:ARG:HG2	2.18	0.44
1:A:343:VAL:HG21	4:C:581:PXS:H13A	2.00	0.44
2:B:193:ILE:CB	2:B:217:VAL:HG22	2.44	0.44
2:B:522:TRP:CE2	2:B:526:HIS:CD2	3.06	0.44
1:A:220:ILE:HB	1:A:224:VAL:CG2	2.46	0.44
2:B:64:ILE:HB	2:B:86:ASN:ND2	2.32	0.44
1:A:525:LEU:O	1:A:555:LYS:HE3	2.17	0.44
2:B:154:SER:HB2	2:B:177:ASP:OD1	2.16	0.44
1:A:189:TYR:O	1:A:189:TYR:CD2	2.70	0.44
2:B:68:ARG:HB3	2:B:70:PRO:HD2	1.99	0.44
2:B:164:LEU:HA	2:B:164:LEU:HD23	1.77	0.44
2:B:263:TRP:CD1	2:B:292:ILE:HG23	2.53	0.44
1:A:530:LEU:O	1:A:531:HIS:O	2.36	0.44
1:A:554:GLN:HG3	1:A:555:LYS:N	2.32	0.44
1:A:504:MET:HG2	1:A:506:ILE:CG2	2.48	0.44
2:B:442:GLY:C	2:B:444:VAL:H	2.19	0.44
2:B:454:VAL:HG13	2:B:477:GLU:HB2	1.99	0.44
2:B:228:ILE:HB	2:B:259:ILE:HG23	2.00	0.44
2:B:373:CYS:SG	2:B:375:THR:HG22	2.58	0.44
1:A:123:LEU:HD12	1:A:126:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASN:N	1:A:62:ASN:OD1	2.51	0.44
2:B:496:LEU:HD12	2:B:499:LEU:HD22	2.00	0.44
1:A:569:VAL:O	1:A:569:VAL:HG12	2.17	0.44
2:B:195:ASN:HB3	2:B:219:ALA:HB3	1.99	0.44
2:B:222:HIS:CE1	2:B:255:THR:OG1	2.71	0.44
1:A:538:SER:HB2	1:A:541:ARG:CG	2.48	0.44
2:B:478:LEU:O	2:B:502:ILE:HA	2.18	0.43
2:B:185:GLY:O	2:B:187:GLU:HG3	2.19	0.43
2:B:408:LEU:HD13	2:B:410:VAL:HG22	1.99	0.43
2:B:438:ASN:C	2:B:460:ASN:ND2	2.72	0.43
1:A:451:VAL:CG1	1:A:474:LEU:HD22	2.46	0.43
2:B:390:LYS:O	2:B:415:LEU:HA	2.17	0.43
1:A:164:GLU:HB3	1:A:166:ARG:HD2	1.99	0.43
1:A:108:SER:HA	1:A:132:MET:O	2.17	0.43
1:A:92:GLU:HA	1:A:92:GLU:OE1	2.17	0.43
1:A:134:ASN:HB2	1:A:136:TYR:HE2	1.83	0.43
1:A:525:LEU:C	1:A:525:LEU:HD12	2.38	0.43
2:B:392:PHE:HA	2:B:415:LEU:HD22	2.00	0.43
1:A:373:VAL:O	1:A:374:GLU:C	2.57	0.43
1:A:266:PHE:HD1	4:C:581:PXS:H36	1.83	0.43
1:A:47:PRO:HD2	1:A:59:LEU:HD13	2.00	0.43
2:B:36:VAL:HG11	2:B:50:LEU:CD2	2.48	0.43
2:B:136:LEU:HA	2:B:137:PRO:HD3	1.75	0.43
1:A:366:ASP:HA	1:A:393:VAL:HB	2.01	0.43
2:B:181:TYR:CD2	2:B:181:TYR:C	2.91	0.43
1:A:435:PRO:HD2	1:A:438:MET:CE	2.49	0.43
1:A:549:LEU:HB3	1:A:570:ARG:HG2	2.01	0.43
2:B:126:LEU:HD11	2:B:128:LEU:HD21	2.00	0.43
1:A:266:PHE:HB2	4:C:581:PXS:H37	2.01	0.43
2:B:246:THR:CG2	2:B:246:THR:O	2.64	0.43
2:B:399:THR:HA	2:B:402:MET:HG3	1.98	0.43
2:B:339:SER:CB	7:B:951:NAG:H62	2.48	0.43
1:A:88:ILE:N	1:A:110:ASN:HD22	2.13	0.43
2:B:441:THR:OG1	2:B:442:GLY:N	2.50	0.43
2:B:256:LEU:HB3	2:B:259:ILE:HG12	2.01	0.43
1:A:428:MET:HA	1:A:429:PRO:HD3	1.83	0.43
1:A:317:LEU:HD23	4:C:581:PXS:H28A	2.01	0.42
1:A:97:TYR:CD1	1:A:122:PRO:HG3	2.54	0.42
2:B:363:ASN:HB2	2:B:387:ASN:ND2	2.33	0.42
2:B:86:ASN:HB3	2:B:87:ARG:H	1.64	0.42
2:B:274:TRP:N	2:B:275:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ASP:OD1	1:A:544:TYR:HB3	2.19	0.42
2:B:485:LEU:N	2:B:507:ASN:HD22	2.17	0.42
1:A:428:MET:SD	1:A:455:ILE:CD1	3.08	0.42
2:B:517:ARG:NH1	2:B:521:GLU:HG3	2.34	0.42
1:A:535:TRP:HB3	1:A:536:ASP:H	1.63	0.42
1:A:168:ILE:HG13	1:A:169:ASP:N	2.34	0.42
1:A:327:ASP:N	3:C:12:SER:O	2.52	0.42
1:A:261:LEU:HD13	4:C:581:PXS:H35	2.02	0.42
1:A:230:ARG:HG2	1:A:257:ARG:HB2	2.00	0.42
2:B:225:LEU:HD11	2:B:242:LEU:HD21	2.01	0.42
1:A:84:LYS:HG3	1:A:108:SER:OG	2.20	0.42
1:A:475:PHE:CZ	1:A:477:PRO:HG3	2.54	0.42
2:B:104:TYR:C	2:B:104:TYR:CD2	2.93	0.42
2:B:427:ALA:HB3	2:B:430:ILE:CD1	2.44	0.42
2:B:492:VAL:C	2:B:494:ASP:N	2.73	0.42
1:A:242:LEU:HB2	1:A:244:VAL:HG22	2.02	0.42
1:A:544:TYR:O	1:A:545:LEU:C	2.58	0.42
1:A:29:SER:O	1:A:30:CYS:CB	2.53	0.41
1:A:459:LEU:HD12	1:A:459:LEU:HA	1.84	0.41
3:C:14:LYS:CD	3:C:15:LYS:HG2	2.50	0.41
1:A:571:SER:O	1:A:572:ILE:O	2.37	0.41
1:A:239:PHE:CG	1:A:240:SER:N	2.87	0.41
2:B:467:LYS:CD	2:B:467:LYS:H	2.16	0.41
2:B:393:PHE:HD1	2:B:419:ALA:CB	2.31	0.41
2:B:222:HIS:HE1	2:B:255:THR:OG1	2.03	0.41
1:A:455:ILE:HG23	1:A:459:LEU:HD22	2.02	0.41
2:B:463:MET:HE2	2:B:463:MET:HB2	1.93	0.41
1:A:60:SER:OG	1:A:82:ILE:HG22	2.20	0.41
2:B:304:LEU:HA	2:B:304:LEU:HD23	1.85	0.41
2:B:289:THR:HG22	2:B:290:GLU:N	2.34	0.41
2:B:349:PRO:HA	2:B:350:PRO:HD3	1.92	0.41
1:A:177:ASN:O	1:A:201:HIS:HB2	2.20	0.41
1:A:329:SER:HA	1:A:332:TYR:CZ	2.55	0.41
2:B:382:LEU:HD21	2:B:384:LEU:HD11	2.03	0.41
2:B:427:ALA:C	2:B:429:SER:H	2.24	0.41
2:B:252:LEU:HD23	2:B:277:PRO:O	2.20	0.41
2:B:492:VAL:HG23	2:B:493:PHE:CD1	2.56	0.41
1:A:474:LEU:HA	1:A:474:LEU:HD12	1.89	0.41
2:B:362:GLN:HA	2:B:386:ARG:HB3	2.03	0.41
1:A:544:TYR:CE1	1:A:548:TRP:HB2	2.56	0.41
2:B:440:LEU:HD23	2:B:440:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:SER:O	2:B:301:GLU:C	2.58	0.41
1:A:370:ASN:HB2	1:A:397:ASN:HD21	1.86	0.41
1:A:434:TRP:HB3	1:A:435:PRO:HD2	2.02	0.41
1:A:63:LYS:HA	1:A:87:ARG:HB2	2.02	0.40
1:A:63:LYS:HA	1:A:87:ARG:CG	2.51	0.40
1:A:167:ARG:HH11	1:A:192:GLN:HB2	1.86	0.40
2:B:499:LEU:HD11	2:B:501:TYR:O	2.22	0.40
1:A:155:ARG:HG2	1:A:155:ARG:HH11	1.86	0.40
1:A:31:ASP:C	1:A:31:ASP:OD2	2.60	0.40
7:B:961:NAG:H61	7:B:962:NAG:C1	2.50	0.40
2:B:164:LEU:N	2:B:165:PRO:CD	2.84	0.40
2:B:381:THR:HG23	2:B:407:THR:HB	2.03	0.40
2:B:524:ASN:OD1	2:B:552:ARG:HB2	2.22	0.40
1:A:239:PHE:CD2	1:A:240:SER:N	2.89	0.40
2:B:204:HIS:HA	2:B:205:PRO:HD3	1.78	0.40
1:A:245:ASP:OD1	1:A:245:ASP:N	2.55	0.40
2:B:428:GLU:N	2:B:428:GLU:CD	2.72	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%)	449 (82%)	79 (14%)	20 (4%)	4	18
2	B	523/562 (93%)	430 (82%)	83 (16%)	10 (2%)	10	35
3	C	4/6 (67%)	3 (75%)	0	1 (25%)	0	0
All	All	1075/1148 (94%)	882 (82%)	162 (15%)	31 (3%)	6	23

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	CYS
1	A	39	ARG
1	A	531	HIS
1	A	572	ILE
2	B	249	PRO
2	B	464	SER
1	A	49	GLY
1	A	100	GLY
1	A	244	VAL
1	A	246	GLU
1	A	424	THR
1	A	532	THR
1	A	556	GLU
2	B	403	SER
2	B	481	ALA
2	B	493	PHE
3	C	14	LYS
2	B	250	THR
2	B	474	ALA
2	B	482	SER
1	A	124	SER
1	A	186	LEU
1	A	286	ASP
1	A	501	LEU
2	B	47	PRO
2	B	392	PHE
1	A	86	SER
1	A	508	SER
1	A	542	ILE
1	A	145	PHE
1	A	477	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	510/537 (95%)	457 (90%)	53 (10%)	9 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	492/525 (94%)	437 (89%)	55 (11%)	7	22
3	C	6/6 (100%)	6 (100%)	0	100	100
All	All	1008/1068 (94%)	900 (89%)	108 (11%)	8	24

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	CYS
1	A	33	SER
1	A	39	ARG
1	A	40	SER
1	A	42	SER
1	A	62	ASN
1	A	90	THR
1	A	112	LEU
1	A	142	THR
1	A	147	ASN
1	A	161	THR
1	A	166	ARG
1	A	191	SER
1	A	209	GLU
1	A	215	GLU
1	A	226	TYR
1	A	232	THR
1	A	233	ASN
1	A	238	GLN
1	A	245	ASP
1	A	270	LEU
1	A	279	LEU
1	A	282	VAL
1	A	300	SER
1	A	337	LYS
1	A	338	VAL
1	A	340	ARG
1	A	355	PHE
1	A	371	LEU
1	A	417	SER
1	A	424	THR
1	A	431	SER
1	A	436	GLU
1	A	446	THR

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Mol	Chain	Res	Type
1	A	449	ARG
1	A	453	THR
1	A	464	VAL
1	A	469	LEU
1	A	470	ASP
1	A	484	ILE
1	A	491	THR
1	A	496	SER
1	A	498	PHE
1	A	500	VAL
1	A	501	LEU
1	A	508	SER
1	A	521	ARG
1	A	524	SER
1	A	525	LEU
1	A	539	CYS
1	A	541	ARG
1	A	547	ARG
1	A	556	GLU
2	B	44	THR
2	B	48	LYS
2	B	61	GLN
2	B	77	GLU
2	B	84	SER
2	B	91	LEU
2	B	95	VAL
2	B	99	ASN
2	B	104	TYR
2	B	115	ILE
2	B	120	MET
2	B	123	LEU
2	B	132	ASP
2	B	135	VAL
2	B	136	LEU
2	B	146	THR
2	B	149	THR
2	B	159	ARG
2	B	164	LEU
2	B	177	ASP
2	B	178	LEU
2	B	188	THR
2	B	195	ASN

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Mol	Chain	Res	Type
2	B	200	HIS
2	B	218	ASN
2	B	237	ARG
2	B	256	LEU
2	B	259	ILE
2	B	261	THR
2	B	269	LEU
2	B	274	TRP
2	B	289	THR
2	B	298	THR
2	B	306	SER
2	B	321	LYS
2	B	333	ILE
2	B	375	THR
2	B	390	LYS
2	B	391	ASN
2	B	403	SER
2	B	408	LEU
2	B	410	VAL
2	B	420	TYR
2	B	424	CYS
2	B	441	THR
2	B	463	MET
2	B	464	SER
2	B	467	LYS
2	B	487	SER
2	B	492	VAL
2	B	498	SER
2	B	519	LEU
2	B	537	VAL
2	B	545	SER
2	B	552	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	79	GLN
1	A	110	ASN
1	A	134	ASN
1	A	177	ASN
1	A	190	GLN

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Mol	Chain	Res	Type
1	A	201	HIS
1	A	233	ASN
1	A	370	ASN
1	A	397	ASN
1	A	426	HIS
1	A	457	GLN
1	A	467	ASN
1	A	487	ASN
1	A	526	GLN
1	A	531	HIS
2	B	62	ASN
2	B	86	ASN
2	B	110	ASN
2	B	125	HIS
2	B	131	ASN
2	B	200	HIS
2	B	204	HIS
2	B	222	HIS
2	B	224	GLN
2	B	258	HIS
2	B	363	ASN
2	B	387	ASN
2	B	391	ASN
2	B	413	ASN
2	B	416	ASN
2	B	418	HIS
2	B	438	ASN
2	B	460	ASN
2	B	483	ASN
2	B	505	HIS
2	B	507	ASN
2	B	526	HIS

### 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 ⓘ

15 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$
6	NAG	A	831	1,6	14,14,15	0.51	0	15,19,21	1.45	1 (6%)
6	NAG	A	832	6	14,14,15	0.59	0	15,19,21	1.08	1 (6%)
6	NAG	B	931	2,6	14,14,15	0.67	0	15,19,21	2.01	6 (40%)
6	NAG	B	932	6	14,14,15	0.59	0	15,19,21	0.80	0
7	NAG	B	941	2,7	14,14,15	0.48	0	15,19,21	1.44	2 (13%)
7	NAG	B	942	7	14,14,15	0.60	0	15,19,21	1.19	2 (13%)
7	BMA	B	943	7	11,11,12	0.63	0	14,15,17	0.77	0
7	NAG	B	951	2,7	14,14,15	0.55	0	15,19,21	1.09	1 (6%)
7	NAG	B	952	7	14,14,15	0.59	0	15,19,21	1.66	1 (6%)
7	BMA	B	953	7	11,11,12	0.53	0	14,15,17	1.02	1 (7%)
7	NAG	B	961	2,7	14,14,15	0.44	0	15,19,21	1.68	2 (13%)
7	NAG	B	962	7	14,14,15	0.69	0	15,19,21	0.88	1 (6%)
7	BMA	B	963	7	11,11,12	0.57	0	14,15,17	0.99	1 (7%)
8	NDG	B	971	8,2	14,14,15	0.40	0	15,19,21	2.20	4 (26%)
8	NAG	B	972	8	14,14,15	0.46	0	15,19,21	0.90	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
6	NAG	A	831	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	832	6	-	0/6/23/26	0/1/1/1
6	NAG	B	931	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	932	6	-	0/6/23/26	0/1/1/1
7	NAG	B	941	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	942	7	-	0/6/23/26	0/1/1/1
7	BMA	B	943	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	951	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	952	7	-	0/6/23/26	0/1/1/1
7	BMA	B	953	7	-	0/2/19/22	0/1/1/1
7	NAG	B	961	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	962	7	-	0/6/23/26	0/1/1/1
7	BMA	B	963	7	-	0/2/19/22	0/1/1/1
8	NDG	B	971	8,2	-	0/6/23/26	0/1/1/1
8	NAG	B	972	8	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	961	NAG	C2-N2-C7	-3.98	117.93	123.04
6	A	832	NAG	C2-N2-C7	-3.02	119.16	123.04
6	B	931	NAG	C6-C5-C4	-2.88	105.90	113.02
7	B	942	NAG	C2-N2-C7	-2.18	120.23	123.04
8	B	971	NDG	C6-C5-C4	-2.10	107.84	113.02
6	B	931	NAG	C3-C2-N2	-2.08	105.58	110.56
6	B	931	NAG	C3-C4-C5	2.01	113.70	110.20
7	B	942	NAG	O3-C3-C2	2.05	113.17	109.11
6	B	931	NAG	C2-N2-C7	2.09	125.72	123.04
7	B	953	BMA	C1-C2-C3	2.33	112.29	109.54
7	B	963	BMA	C1-O5-C5	2.34	115.22	112.25
7	B	962	NAG	C4-C3-C2	2.58	115.24	111.23
7	B	941	NAG	C1-O5-C5	2.63	115.58	112.25
7	B	941	NAG	C3-C4-C5	2.67	114.85	110.20
8	B	971	NDG	C4-C3-C2	2.71	115.44	111.23
7	B	951	NAG	C1-O5-C5	2.79	115.79	112.25
8	B	971	NDG	C3-C4-C5	2.97	115.38	110.20
6	B	931	NAG	C4-C3-C2	3.15	116.13	111.23
7	B	961	NAG	C1-O5-C5	4.24	117.63	112.25
6	A	831	NAG	C1-O5-C5	4.43	117.87	112.25
6	B	931	NAG	C1-O5-C5	4.89	118.46	112.25
7	B	952	NAG	C1-O5-C5	5.62	119.38	112.25
8	B	971	NDG	C1-O-C5	6.85	120.94	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	832	NAG	2	0
6	B	931	NAG	4	0
6	B	932	NAG	3	0
7	B	951	NAG	1	0
7	B	961	NAG	1	0
7	B	962	NAG	1	0

## 5.6 Ligand geometry [i](#)

6 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	NAG	A	811	1	14,14,15	0.43	0	15,19,21	1.60	1 (6%)
5	NAG	A	821	1	14,14,15	0.48	0	15,19,21	1.10	1 (6%)
5	NAG	B	911	2	14,14,15	0.65	0	15,19,21	1.98	3 (20%)
5	NAG	B	921	2	14,14,15	0.51	0	15,19,21	2.35	2 (13%)
5	NAG	B	981	2	14,14,15	0.50	0	15,19,21	2.34	2 (13%)
4	PXS	C	581	3	38,38,38	1.77	4 (10%)	40,40,40	0.98	3 (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
5	NAG	A	811	1	-	0/6/23/26	0/1/1/1
5	NAG	A	821	1	-	0/6/23/26	0/1/1/1
5	NAG	B	911	2	-	0/6/23/26	0/1/1/1
5	NAG	B	921	2	-	1/6/23/26	0/1/1/1
5	NAG	B	981	2	-	1/6/23/26	0/1/1/1
4	PXS	C	581	3	-	0/39/39/39	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	581	PXS	O21-C19	-8.86	1.30	1.47
4	C	581	PXS	C20-C19	-3.04	1.39	1.51
4	C	581	PXS	O21-C22	2.11	1.40	1.34
4	C	581	PXS	O17-C16	2.69	1.41	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	911	NAG	C2-N2-C7	-2.89	119.32	123.04
5	B	911	NAG	O3-C3-C2	2.35	113.77	109.11
4	C	581	PXS	O17-C16-C15	2.46	119.41	111.90
4	C	581	PXS	O21-C22-C23	2.56	117.09	111.53
4	C	581	PXS	O17-C18-C19	3.24	117.28	108.61
5	A	821	NAG	C1-O5-C5	3.29	116.42	112.25
5	B	921	NAG	C2-N2-C7	3.66	127.75	123.04
5	B	981	NAG	C2-N2-C7	3.67	127.76	123.04
5	A	811	NAG	C1-O5-C5	4.60	118.09	112.25
5	B	911	NAG	C1-O5-C5	5.82	119.64	112.25
5	B	981	NAG	C1-O5-C5	7.37	121.60	112.25
5	B	921	NAG	C1-O5-C5	7.41	121.65	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	981	NAG	O7-C7-N2-C2
5	B	921	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	981	NAG	2	0
4	C	581	PXS	12	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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	550/580 (94%)	-0.07	30 (5%)	29 22	43, 78, 165, 240	0
2	B	525/562 (93%)	0.01	24 (4%)	36 30	48, 78, 137, 202	0
3	C	6/6 (100%)	1.63	2 (33%)	0 0	67, 99, 139, 143	0
All	All	1081/1148 (94%)	-0.02	56 (5%)	31 24	43, 78, 151, 240	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	573	ILE	6.9
1	A	572	ILE	6.0
3	C	16	LYS	5.5
2	B	469	VAL	5.0
1	A	538	SER	4.9
2	B	537	VAL	4.8
1	A	539	CYS	4.6
2	B	554	ILE	4.3
1	A	540	PRO	4.0
2	B	547	SER	4.0
1	A	537	CYS	3.8
1	A	532	THR	3.8
2	B	187	GLU	3.7
1	A	569	VAL	3.7
2	B	555	ILE	3.6
2	B	94	HIS	3.5
2	B	43	LEU	3.5
2	B	527	SER	3.3
2	B	420	TYR	3.2
3	C	15	LYS	3.1
1	A	33	SER	3.1
1	A	574	CYS	3.1
2	B	466	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	87	ARG	2.9
1	A	563	SER	2.9
1	A	535	TRP	2.9
2	B	188	THR	2.9
1	A	568	PRO	2.8
2	B	553	SER	2.8
1	A	541	ARG	2.8
1	A	536	ASP	2.8
1	A	483	TYR	2.7
2	B	468	ASP	2.7
1	A	545	LEU	2.7
2	B	548	GLY	2.7
2	B	549	LYS	2.6
1	A	243	PRO	2.6
2	B	184	LYS	2.5
1	A	571	SER	2.5
1	A	531	HIS	2.5
1	A	54	MET	2.5
2	B	424	CYS	2.5
1	A	575	PRO	2.4
1	A	516	ASP	2.4
2	B	463	MET	2.4
1	A	530	LEU	2.3
1	A	560	ALA	2.3
2	B	535	GLY	2.3
2	B	550	PRO	2.3
1	A	529	TRP	2.3
2	B	513	CYS	2.3
2	B	528	GLY	2.2
1	A	534	PRO	2.1
1	A	398	HIS	2.1
1	A	194	LEU	2.0
1	A	499	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
8	NDG	B	971	14/15	0.90	0.28	3.06	89,104,118,119	0
7	NAG	B	951	14/15	0.95	0.19	0.21	57,64,76,81	0
6	NAG	A	831	14/15	0.97	0.15	0.02	71,84,92,97	0
6	NAG	B	931	14/15	0.92	0.18	-0.21	89,104,121,124	0
7	NAG	B	941	14/15	0.97	0.14	-0.85	58,67,79,80	0
7	BMA	B	943	11/12	0.79	0.27	-	86,104,110,112	0
6	NAG	A	832	14/15	0.94	0.28	-	93,111,122,126	0
7	BMA	B	963	11/12	0.72	0.40	-	154,164,174,175	0
7	NAG	B	942	14/15	0.97	0.22	-	63,76,86,89	0
7	NAG	B	962	14/15	0.80	0.32	-	94,147,165,175	0
7	BMA	B	953	11/12	0.83	0.39	-	95,124,136,138	0
7	NAG	B	961	14/15	0.86	0.26	-	98,116,136,148	0
8	NAG	B	972	14/15	0.83	0.39	-	104,126,137,139	0
7	NAG	B	952	14/15	0.96	0.30	-	61,71,91,101	0
6	NAG	B	932	14/15	0.89	0.23	-	87,135,145,145	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	B	981	14/15	0.54	0.52	15.07	117,139,157,157	0
4	PXS	C	581	39/39	0.95	0.25	2.58	52,64,96,120	0
5	NAG	A	811	14/15	0.71	0.27	2.33	96,140,149,153	0
5	NAG	B	921	14/15	0.85	0.34	1.29	91,132,147,149	0
5	NAG	B	911	14/15	0.92	0.17	0.64	64,80,99,110	0
5	NAG	A	821	14/15	0.89	0.23	-	95,109,122,122	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.