



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:01 PM GMT

PDB ID : 4WJL
Title : Structure of human dipeptidyl peptidase 10 (DPPY): a modulator of neuronal Kv4 channels
Authors : Bezerra, G.A.; Dobrovetsky, E.; Seitova, A.; Fedosyuk, S.; Dhe-Paganon, S.; Gruber, K.
Deposited on : 2014-09-30
Resolution : 3.40 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

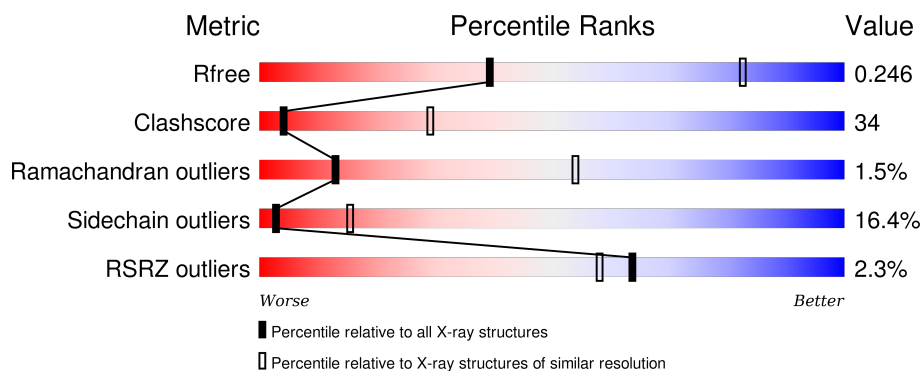
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	719	<div> <div>3%</div> <div>45%</div> <div>43%</div> <div>11%</div> <div>.</div> </div>
1	B	719	<div> <div>2%</div> <div>44%</div> <div>45%</div> <div>10%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11829 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 Inactive dipeptidyl peptidase 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	717	Total	C	N	O	S	0	0	0
			5794	3730	959	1080	25			
1	B	719	Total	C	N	O	S	0	0	0
			5806	3736	960	1085	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	MET	VAL	variant	UNP Q8N608
A	401	ILE	VAL	variant	UNP Q8N608
B	288	MET	VAL	variant	UNP Q8N608
B	401	ILE	VAL	variant	UNP Q8N608

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

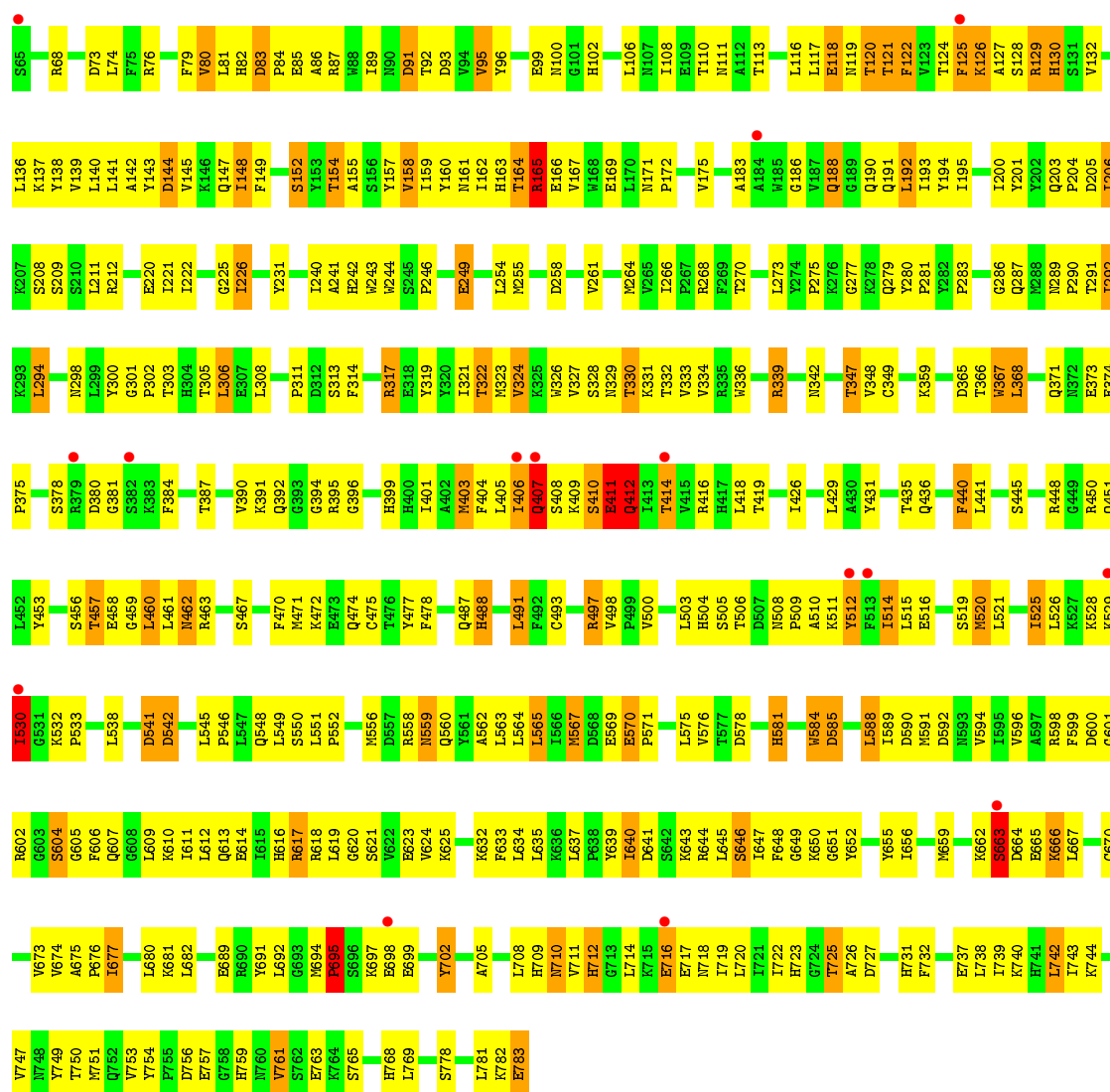
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

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 ($\text{RSRZ} > 2$). 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.

- Chain A:**

- Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.91Å 143.73Å 176.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.55 – 3.40 66.55 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.55-3.40) 99.9 (66.55-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.207 , 0.242 0.226 , 0.246	Depositor DCC
R_{free} test set	1476 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 28971 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11829	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	0.39	0/5940	0.63	1/8052 (0.0%)
1	B	0.41	0/5952	0.64	1/8069 (0.0%)
All	All	0.40	0/11892	0.63	2/16121 (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
1	A	0	2
1	B	0	5
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	585	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	714	LEU	N-CA-C	-5.20	96.95	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	412	GLN	Mainchain,Peptide
1	B	407	GLN	Peptide
1	B	412	GLN	Mainchain
1	B	695	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	B	710	ASN	Mainchain,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	5794	0	5719	404	0
1	B	5806	0	5720	392	0
2	A	28	0	26	1	0
2	B	28	0	26	6	0
3	A	50	0	43	4	0
4	A	28	0	25	4	0
4	B	56	0	50	7	0
5	B	39	0	34	4	0
All	All	11829	0	11643	794	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 34.

All (794) 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:165:ARG:H	1:A:165:ARG:CD	1.60	1.14
1:A:165:ARG:H	1:A:165:ARG:HD2	1.08	1.08
1:A:488:HIS:HB3	1:A:505:SER:HA	1.38	1.05
1:A:644:ARG:HD2	1:A:781:LEU:O	1.57	1.04
1:B:488:HIS:HB3	1:B:505:SER:HA	1.39	1.03
1:B:165:ARG:HD2	1:B:165:ARG:H	1.18	1.03
1:A:165:ARG:HD2	1:A:165:ARG:N	1.72	1.02
1:B:644:ARG:HD2	1:B:781:LEU:O	1.58	1.02
1:B:165:ARG:N	1:B:165:ARG:HD2	1.72	1.01
1:A:118:GLU:HG3	1:A:119:ASN:H	1.28	0.98
1:B:118:GLU:HG3	1:B:119:ASN:N	1.80	0.95
1:A:602:ARG:HD2	1:A:614:GLU:HG2	1.47	0.94
1:B:118:GLU:HG3	1:B:119:ASN:H	1.33	0.94
1:B:602:ARG:HD2	1:B:614:GLU:HG2	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:LYS:NZ	2:B:809:NAG:H62	1.83	0.93
1:A:118:GLU:HG3	1:A:119:ASN:N	1.82	0.92
1:B:710:ASN:O	1:B:712:HIS:N	2.01	0.91
1:A:201:TYR:CE1	1:A:212:ARG:HG3	2.05	0.91
1:A:570:GLU:HG3	1:A:571:PRO:HD2	1.52	0.91
1:B:201:TYR:CE1	1:B:212:ARG:HG3	2.10	0.87
1:A:409:LYS:HG2	1:A:410:SER:H	1.40	0.87
1:A:775:LYS:CE	2:B:809:NAG:H62	2.05	0.86
1:A:710:ASN:C	1:A:712:HIS:H	1.78	0.85
1:B:742:LEU:HD23	1:B:747:VAL:HB	1.58	0.85
1:B:570:GLU:HG3	1:B:571:PRO:HD2	1.57	0.85
1:A:399:HIS:CE1	1:A:609:LEU:HD21	2.12	0.85
1:A:742:LEU:HD23	1:A:747:VAL:HB	1.59	0.84
1:A:695:PRO:HA	1:A:702:TYR:CD2	2.13	0.84
1:A:440:PHE:HE1	1:A:453:TYR:HB3	1.43	0.83
1:B:399:HIS:HE1	1:B:609:LEU:HD21	1.43	0.83
1:B:195:ILE:HD12	1:B:226:ILE:HG23	1.61	0.83
1:B:440:PHE:HE1	1:B:453:TYR:HB3	1.43	0.82
1:B:440:PHE:CE1	1:B:453:TYR:CB	2.63	0.82
1:A:609:LEU:HB3	1:A:613:GLN:HE21	1.45	0.82
1:B:399:HIS:CE1	1:B:609:LEU:HD21	2.14	0.82
1:A:440:PHE:CE1	1:A:453:TYR:CB	2.63	0.82
1:A:195:ILE:HD12	1:A:226:ILE:HG23	1.63	0.81
1:A:399:HIS:HE1	1:A:609:LEU:HD21	1.44	0.81
1:A:753:VAL:HG11	1:B:753:VAL:HG11	1.63	0.81
1:B:411:GLU:O	1:B:412:GLN:HB2	1.80	0.80
1:B:673:VAL:HG11	1:B:676:PRO:HB3	1.64	0.80
1:A:460:LEU:H	1:A:460:LEU:HD13	1.47	0.79
1:B:609:LEU:HB3	1:B:613:GLN:HE21	1.46	0.78
1:B:644:ARG:HD3	1:B:783:GLU:OE2	1.83	0.78
1:B:460:LEU:H	1:B:460:LEU:HD13	1.47	0.78
1:B:448:ARG:HH11	1:B:448:ARG:HG3	1.48	0.78
1:B:695:PRO:HA	1:B:702:TYR:CD2	2.18	0.78
1:B:287:GLN:HE21	1:B:287:GLN:HA	1.49	0.78
1:B:440:PHE:HE1	1:B:453:TYR:CB	1.96	0.78
1:A:673:VAL:HG11	1:A:676:PRO:HB3	1.66	0.78
1:A:607:GLN:HG3	1:A:611:ILE:HD12	1.66	0.78
1:B:145:VAL:HA	1:B:155:ALA:HB2	1.64	0.78
1:A:145:VAL:HA	1:A:155:ALA:HB2	1.64	0.77
1:A:448:ARG:HG3	1:A:448:ARG:HH11	1.46	0.77
1:B:673:VAL:CG1	1:B:676:PRO:HB3	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:CE1	1:A:453:TYR:HB2	2.20	0.76
1:A:83:ASP:OD2	1:A:85:GLU:HG3	1.84	0.76
1:B:607:GLN:HG3	1:B:611:ILE:HD12	1.67	0.76
1:B:440:PHE:CE1	1:B:453:TYR:HB2	2.19	0.76
1:A:287:GLN:HA	1:A:287:GLN:HE21	1.49	0.76
1:A:260:LEU:HD11	3:A:803:NAG:H62	1.67	0.76
1:A:333:VAL:HG12	1:A:348:VAL:HG22	1.68	0.76
1:B:460:LEU:HD23	1:B:462:ASN:H	1.52	0.75
1:A:514:ILE:HD12	1:A:514:ILE:H	1.50	0.75
1:B:761:VAL:HG21	1:B:769:LEU:HD12	1.67	0.75
1:B:411:GLU:O	1:B:412:GLN:CB	2.28	0.75
1:A:270:THR:HG21	1:B:740:LYS:HD2	1.68	0.75
1:A:270:THR:CG2	1:B:740:LYS:HD2	2.17	0.74
1:B:514:ILE:H	1:B:514:ILE:HD12	1.52	0.74
1:A:440:PHE:HE1	1:A:453:TYR:CB	1.97	0.74
1:B:333:VAL:HG12	1:B:348:VAL:HG22	1.68	0.74
1:A:403:MET:HG3	1:A:418:LEU:HD21	1.70	0.74
1:A:761:VAL:HG21	1:A:769:LEU:HD12	1.68	0.74
1:A:460:LEU:HD23	1:A:462:ASN:H	1.53	0.73
1:B:562:ALA:HB1	1:B:781:LEU:HD13	1.71	0.73
1:B:83:ASP:OD2	1:B:85:GLU:HG3	1.88	0.73
1:B:403:MET:HG3	1:B:418:LEU:HD21	1.71	0.73
1:A:409:LYS:HG2	1:A:410:SER:N	2.02	0.72
1:B:695:PRO:HA	1:B:702:TYR:CE2	2.23	0.72
5:B:804:NAG:H62	5:B:805:NAG:C7	2.19	0.72
1:B:165:ARG:N	1:B:165:ARG:CD	2.49	0.72
1:A:673:VAL:CG1	1:A:676:PRO:HB3	2.17	0.72
1:B:390:VAL:HG23	1:B:392:GLN:HG2	1.71	0.71
1:A:562:ALA:HB1	1:A:781:LEU:HD13	1.72	0.71
1:A:662:LYS:HB3	1:A:712:HIS:HE1	1.56	0.71
1:B:710:ASN:C	1:B:712:HIS:N	2.44	0.71
1:B:477:TYR:O	1:B:493:CYS:O	2.08	0.71
1:A:160:TYR:HE1	1:A:162:ILE:HD12	1.56	0.70
1:A:493:CYS:HB3	1:A:500:VAL:H	1.56	0.70
1:A:440:PHE:CE1	1:A:453:TYR:HB3	2.24	0.70
1:B:478:PHE:CE1	1:B:491:LEU:HD11	2.27	0.70
1:A:201:TYR:HE1	1:A:212:ARG:HG3	1.53	0.70
1:A:695:PRO:HA	1:A:702:TYR:CE2	2.28	0.69
1:A:292:ILE:HD11	1:A:321:ILE:HG13	1.75	0.69
1:A:710:ASN:C	1:A:712:HIS:N	2.46	0.69
1:A:390:VAL:HG23	1:A:392:GLN:HG2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:MET:O	1:B:592:ASP:HB2	1.93	0.69
1:A:478:PHE:CE1	1:A:491:LEU:HD11	2.27	0.69
1:B:440:PHE:CE1	1:B:453:TYR:HB3	2.23	0.69
1:B:246:PRO:HD2	1:B:329:ASN:HA	1.73	0.69
1:A:695:PRO:HA	1:A:702:TYR:HD2	1.56	0.69
1:A:246:PRO:HD2	1:A:329:ASN:HA	1.74	0.69
1:B:287:GLN:NE2	1:B:287:GLN:HA	2.08	0.68
1:B:545:LEU:HD13	1:B:601:GLY:HA2	1.75	0.68
1:B:192:LEU:HD23	1:B:203:GLN:HB2	1.76	0.68
1:B:471:MET:HB2	1:B:475:CYS:N	2.09	0.68
1:B:662:LYS:HB3	1:B:712:HIS:HE1	1.59	0.68
1:B:493:CYS:HB3	1:B:500:VAL:H	1.58	0.68
1:A:220:GLU:HG3	1:A:281:PRO:HD3	1.76	0.68
1:A:169:GLU:HG2	1:A:171:ASN:HD21	1.57	0.68
1:A:775:LYS:NZ	2:B:809:NAG:C6	2.56	0.68
1:A:287:GLN:HA	1:A:287:GLN:NE2	2.07	0.68
1:A:192:LEU:HD23	1:A:203:GLN:HB2	1.76	0.68
3:A:804:NAG:O3	3:A:805:BMA:H2	1.94	0.68
1:B:148:ILE:HG13	1:B:154:THR:HG22	1.76	0.68
1:B:201:TYR:HE1	1:B:212:ARG:HG3	1.57	0.67
1:B:655:TYR:OH	1:B:705:ALA:HB1	1.95	0.67
1:B:677:ILE:O	1:B:677:ILE:HG13	1.93	0.67
1:A:139:VAL:HG23	1:A:162:ILE:HD13	1.75	0.67
1:A:581:HIS:C	1:A:581:HIS:ND1	2.47	0.67
1:A:148:ILE:HG13	1:A:154:THR:HG22	1.75	0.67
1:B:169:GLU:HG2	1:B:171:ASN:HD21	1.58	0.67
1:A:324:VAL:HB	1:A:334:VAL:HG22	1.75	0.67
1:A:477:TYR:O	1:A:493:CYS:O	2.11	0.67
1:B:139:VAL:HG23	1:B:162:ILE:HD13	1.77	0.67
1:A:270:THR:HG22	1:A:270:THR:O	1.95	0.66
1:A:73:ASP:HA	1:A:76:ARG:HG3	1.76	0.66
1:B:373:GLU:CD	1:B:387:THR:HG22	2.16	0.66
1:B:581:HIS:ND1	1:B:581:HIS:C	2.47	0.66
1:A:419:THR:HG21	1:A:440:PHE:HE2	1.61	0.66
1:B:160:TYR:HE1	1:B:162:ILE:HD12	1.59	0.66
1:A:373:GLU:CD	1:A:387:THR:HG22	2.16	0.66
1:B:407:GLN:HB3	1:B:408:SER:OG	1.95	0.66
1:A:129:ARG:HB3	1:A:142:ALA:HB3	1.77	0.66
4:A:807:NAG:H4	4:A:808:NAG:C7	2.24	0.66
1:B:84:PRO:HG3	1:B:516:GLU:CB	2.26	0.66
1:B:467:SER:HB2	1:B:478:PHE:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:MET:O	1:A:592:ASP:HB2	1.95	0.66
1:B:450:ARG:NH2	1:B:606:PHE:CD2	2.64	0.66
1:A:445:SER:OG	1:A:451:GLN:HG3	1.95	0.66
1:A:132:VAL:HG11	1:A:136:LEU:HD23	1.78	0.65
1:B:475:CYS:HB3	1:B:478:PHE:CZ	2.31	0.65
1:A:195:ILE:HG21	1:A:226:ILE:HG12	1.79	0.65
1:A:655:TYR:OH	1:A:705:ALA:HB1	1.97	0.65
1:A:84:PRO:HG3	1:A:516:GLU:CB	2.25	0.65
1:B:549:LEU:HD21	1:B:634:LEU:HD21	1.77	0.65
1:A:545:LEU:HD13	1:A:601:GLY:HA2	1.77	0.65
1:B:292:ILE:HD11	1:B:321:ILE:HG13	1.79	0.65
1:A:677:ILE:HG13	1:A:677:ILE:O	1.94	0.65
1:A:467:SER:HB2	1:A:478:PHE:CE2	2.32	0.65
1:B:220:GLU:HG3	1:B:281:PRO:HD3	1.78	0.65
1:A:68:ARG:HB2	1:A:590:ASP:OD2	1.96	0.65
1:A:674:VAL:HG22	1:A:722:ILE:HB	1.79	0.65
1:B:132:VAL:HG11	1:B:136:LEU:HD23	1.79	0.65
1:A:538:LEU:HD21	1:A:633:PHE:CD2	2.32	0.65
1:A:143:TYR:O	1:A:155:ALA:HB1	1.97	0.65
1:B:129:ARG:HB3	1:B:142:ALA:HB3	1.78	0.65
1:B:419:THR:HG21	1:B:440:PHE:HE2	1.62	0.64
1:B:652:TYR:O	1:B:655:TYR:HB3	1.96	0.64
1:B:270:THR:O	1:B:270:THR:HG22	1.95	0.64
1:B:324:VAL:HB	1:B:334:VAL:HG22	1.80	0.64
1:A:775:LYS:HE2	2:B:809:NAG:H62	1.80	0.64
4:B:807:NAG:H4	4:B:808:NAG:C7	2.27	0.64
1:B:457:THR:HG23	1:B:458:GLU:H	1.63	0.64
1:A:450:ARG:NH2	1:A:606:PHE:CD2	2.66	0.64
1:B:445:SER:OG	1:B:451:GLN:HG3	1.97	0.63
1:B:102:HIS:HE2	4:B:802:NAG:HO6	1.45	0.63
1:A:775:LYS:HZ3	2:B:809:NAG:C6	2.09	0.63
1:A:775:LYS:HZ3	2:B:809:NAG:H62	1.63	0.63
1:A:457:THR:HG23	1:A:458:GLU:H	1.63	0.63
1:A:471:MET:HB2	1:A:475:CYS:N	2.13	0.63
1:B:609:LEU:HB3	1:B:613:GLN:NE2	2.14	0.63
1:A:475:CYS:HB3	1:A:478:PHE:CZ	2.33	0.63
1:B:73:ASP:HA	1:B:76:ARG:HG3	1.80	0.63
1:A:286:GLY:HA3	1:A:695:PRO:HG3	1.80	0.62
1:B:195:ILE:HG21	1:B:226:ILE:HG12	1.81	0.62
1:B:436:GLN:O	1:B:457:THR:HG22	1.99	0.62
1:A:652:TYR:O	1:A:655:TYR:HB3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:GLN:O	1:B:409:LYS:O	2.16	0.62
1:B:68:ARG:HB2	1:B:590:ASP:OD2	1.98	0.62
1:B:172:PRO:HG2	1:B:175:VAL:HB	1.82	0.62
1:A:530:ILE:O	1:A:530:ILE:HG23	2.00	0.62
1:A:694:MET:HB3	1:A:697:LYS:HB2	1.81	0.62
1:A:416:ARG:HH11	1:A:461:LEU:HD21	1.65	0.62
1:A:609:LEU:HB3	1:A:613:GLN:NE2	2.13	0.62
1:A:436:GLN:O	1:A:457:THR:HG22	2.00	0.62
1:A:401:ILE:HD11	1:A:440:PHE:CD2	2.35	0.62
1:B:530:ILE:HG23	1:B:530:ILE:O	1.98	0.62
1:A:549:LEU:HD21	1:A:634:LEU:HD21	1.81	0.61
1:A:504:HIS:ND1	1:A:511:LYS:HA	2.15	0.61
1:A:710:ASN:O	1:A:712:HIS:N	2.22	0.61
1:B:436:GLN:O	1:B:457:THR:N	2.32	0.61
1:B:530:ILE:CG2	1:B:530:ILE:O	2.48	0.61
1:B:674:VAL:HG22	1:B:722:ILE:HB	1.81	0.61
1:B:538:LEU:HD21	1:B:633:PHE:CD2	2.35	0.61
1:A:378:SER:HB3	1:A:381:GLY:H	1.65	0.61
1:A:220:GLU:HG2	1:A:279:GLN:O	2.01	0.61
1:B:86:ALA:HA	1:B:96:TYR:HA	1.81	0.61
1:A:172:PRO:HG2	1:A:175:VAL:HB	1.82	0.61
1:B:403:MET:HB2	1:B:416:ARG:O	2.00	0.61
1:B:694:MET:HB3	1:B:697:LYS:HB2	1.82	0.61
1:B:416:ARG:HH11	1:B:461:LEU:HD21	1.66	0.61
1:B:714:LEU:HD13	1:B:719:ILE:HD12	1.82	0.60
1:B:120:THR:O	1:B:122:PHE:N	2.32	0.60
1:A:121:THR:HG22	1:A:127:ALA:HB3	1.82	0.60
1:A:86:ALA:HA	1:A:96:TYR:HA	1.82	0.60
1:A:403:MET:HB2	1:A:416:ARG:O	2.00	0.60
1:A:448:ARG:HD3	1:A:576:VAL:HG12	1.83	0.60
1:B:616:HIS:NE2	1:B:617:ARG:HD2	2.16	0.60
1:A:342:ASN:HA	1:A:368:LEU:HD23	1.84	0.60
1:B:143:TYR:O	1:B:155:ALA:HB1	2.02	0.60
1:B:231:TYR:OH	1:B:292:ILE:HG21	2.01	0.60
1:A:585:ASP:OD2	1:A:598:ARG:NH2	2.35	0.60
1:A:294:LEU:HD23	1:A:308:LEU:HB2	1.84	0.60
1:A:436:GLN:O	1:A:457:THR:N	2.33	0.60
1:A:530:ILE:CG2	1:A:530:ILE:O	2.50	0.60
1:A:328:SER:HG	1:A:331:LYS:H	1.50	0.60
1:B:695:PRO:CA	1:B:702:TYR:CE2	2.85	0.60
1:A:448:ARG:HB3	1:A:578:ASP:OD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:MET:HG2	1:A:418:LEU:HD11	1.83	0.59
1:A:194:TYR:CE2	1:A:201:TYR:HD2	2.20	0.59
1:B:448:ARG:HD3	1:B:576:VAL:HG12	1.84	0.59
1:B:192:LEU:CD2	1:B:203:GLN:HB2	2.33	0.59
1:A:79:PHE:O	1:A:80:VAL:HB	2.00	0.59
1:A:317:ARG:O	1:A:319:TYR:HD1	1.85	0.59
4:A:807:NAG:H4	4:A:808:NAG:N2	2.16	0.59
1:B:279:GLN:O	1:B:279:GLN:HG3	2.02	0.59
1:A:342:ASN:C	1:A:368:LEU:HD23	2.23	0.59
1:B:125:PHE:O	1:B:126:LYS:C	2.42	0.59
1:A:331:LYS:HA	1:A:349:CYS:O	2.03	0.59
1:B:317:ARG:O	1:B:319:TYR:HD1	1.85	0.59
1:A:764:LYS:HD3	1:B:744:LYS:HD2	1.85	0.58
1:B:592:ASP:OD1	1:B:778:SER:HB2	2.04	0.58
1:B:339:ARG:HD2	1:B:689:GLU:OE1	2.03	0.58
1:B:342:ASN:HA	1:B:368:LEU:HD23	1.84	0.58
1:B:589:ILE:HG22	1:B:590:ASP:N	2.17	0.58
1:B:698:GLU:C	1:B:699:GLU:HG2	2.22	0.58
1:B:644:ARG:CD	1:B:783:GLU:OE2	2.52	0.58
1:B:450:ARG:HG3	1:B:450:ARG:HH11	1.69	0.58
1:A:641:ASP:OD1	1:A:643:LYS:HB2	2.04	0.58
1:A:563:LEU:HB3	1:A:645:LEU:HD22	1.85	0.58
1:B:563:LEU:HB3	1:B:645:LEU:HD22	1.85	0.58
1:B:448:ARG:HB3	1:B:578:ASP:OD1	2.04	0.57
1:B:270:THR:O	1:B:270:THR:CG2	2.52	0.57
1:A:192:LEU:CD2	1:A:203:GLN:HB2	2.34	0.57
1:B:121:THR:HG22	1:B:127:ALA:HB3	1.84	0.57
1:B:471:MET:HB3	1:B:474:GLN:HB2	1.85	0.57
1:A:616:HIS:NE2	1:A:617:ARG:HD2	2.20	0.57
1:B:401:ILE:HD11	1:B:440:PHE:CD2	2.40	0.57
1:A:714:LEU:HD13	1:A:719:ILE:HD12	1.86	0.57
5:B:805:NAG:H61	5:B:806:BMA:O2	2.05	0.57
1:A:698:GLU:C	1:A:699:GLU:HG2	2.23	0.57
1:B:504:HIS:ND1	1:B:511:LYS:HA	2.20	0.57
1:A:231:TYR:OH	1:A:292:ILE:HG21	2.05	0.57
1:B:342:ASN:C	1:B:368:LEU:HD23	2.25	0.57
1:A:165:ARG:H	1:A:165:ARG:HD3	1.61	0.56
1:A:270:THR:CG2	1:A:270:THR:O	2.52	0.56
1:A:450:ARG:HG3	1:A:450:ARG:HH11	1.70	0.56
1:B:220:GLU:HG2	1:B:279:GLN:O	2.05	0.56
1:A:538:LEU:HD12	1:A:599:PHE:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:LYS:C	1:A:717:GLU:H	2.08	0.56
1:B:694:MET:HE3	1:B:695:PRO:HD2	1.86	0.56
1:A:740:LYS:HD2	1:B:270:THR:CG2	2.35	0.56
1:A:739:ILE:HD13	1:A:751:MET:HE3	1.87	0.56
1:A:339:ARG:HD2	1:A:689:GLU:OE1	2.05	0.56
1:B:323:MET:HE2	1:B:373:GLU:O	2.05	0.56
1:B:79:PHE:O	1:B:80:VAL:HB	2.04	0.56
1:A:125:PHE:O	1:A:126:LYS:C	2.43	0.56
1:B:378:SER:HB3	1:B:381:GLY:H	1.70	0.56
1:B:488:HIS:ND1	1:B:488:HIS:N	2.53	0.56
1:B:448:ARG:NH1	1:B:448:ARG:HG3	2.20	0.56
1:A:89:ILE:HD11	1:A:95:VAL:HB	1.87	0.56
1:A:279:GLN:O	1:A:279:GLN:HG3	2.06	0.56
1:B:331:LYS:HA	1:B:349:CYS:O	2.06	0.56
1:A:471:MET:HB3	1:A:474:GLN:HB2	1.87	0.56
1:A:589:ILE:HG22	1:A:590:ASP:N	2.20	0.56
1:B:394:GLY:O	1:B:395:ARG:CB	2.52	0.56
1:B:225:GLY:C	1:B:241:ALA:HB3	2.25	0.56
1:A:394:GLY:O	1:A:395:ARG:CB	2.54	0.55
1:B:186:GLY:HA3	1:B:191:GLN:HG3	1.88	0.55
1:B:510:ALA:C	1:B:512:TYR:H	2.10	0.55
1:A:575:LEU:HD22	1:A:598:ARG:HD3	1.89	0.55
1:A:589:ILE:HG13	1:A:596:VAL:HG13	1.89	0.55
1:A:663:SER:HB3	1:A:712:HIS:CE1	2.41	0.55
1:B:695:PRO:CA	1:B:702:TYR:HE2	2.20	0.55
1:B:403:MET:HG2	1:B:418:LEU:HD11	1.88	0.55
1:B:96:TYR:CG	1:B:96:TYR:O	2.59	0.55
1:A:563:LEU:HB3	1:A:645:LEU:CD2	2.36	0.55
1:B:563:LEU:HB3	1:B:645:LEU:CD2	2.36	0.55
1:A:194:TYR:CE2	1:A:201:TYR:CD2	2.95	0.54
4:A:807:NAG:H2	4:A:808:NAG:O7	2.06	0.54
1:A:565:LEU:HD22	1:A:567:MET:CE	2.37	0.54
1:A:110:THR:O	1:A:111:ASN:HB2	2.07	0.54
1:B:89:ILE:HD11	1:B:95:VAL:HB	1.89	0.54
1:B:102:HIS:CD2	4:B:802:NAG:HO6	2.26	0.54
1:B:471:MET:HG3	1:B:475:CYS:SG	2.46	0.54
1:A:118:GLU:CG	1:A:119:ASN:N	2.64	0.54
1:B:194:TYR:CE2	1:B:201:TYR:HD2	2.25	0.54
1:B:84:PRO:HG3	1:B:516:GLU:HB2	1.89	0.54
1:A:592:ASP:OD1	1:A:778:SER:HB2	2.07	0.54
1:B:575:LEU:HD13	1:B:598:ARG:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:PRO:CA	1:A:702:TYR:CE2	2.91	0.54
1:B:431:TYR:HE1	1:B:457:THR:HG21	1.73	0.54
1:A:488:HIS:N	1:A:488:HIS:ND1	2.54	0.54
1:A:120:THR:O	1:A:122:PHE:N	2.41	0.54
1:A:575:LEU:HD13	1:A:598:ARG:HB3	1.90	0.54
1:A:694:MET:HE3	1:A:695:PRO:HD2	1.90	0.53
1:A:431:TYR:HE1	1:A:457:THR:HG21	1.73	0.53
1:A:225:GLY:C	1:A:241:ALA:HB3	2.27	0.53
1:B:538:LEU:HD12	1:B:599:PHE:CE1	2.43	0.53
1:A:84:PRO:HG3	1:A:516:GLU:HB2	1.90	0.53
1:B:725:THR:HG22	1:B:756:ASP:H	1.74	0.53
1:B:663:SER:HB3	1:B:712:HIS:CE1	2.43	0.53
1:B:739:ILE:HD13	1:B:751:MET:CE	2.38	0.53
1:A:448:ARG:NH1	1:A:448:ARG:HG3	2.18	0.53
1:B:110:THR:O	1:B:111:ASN:HB2	2.08	0.53
1:B:460:LEU:HD23	1:B:462:ASN:HB3	1.89	0.53
1:A:715:LYS:C	1:A:717:GLU:N	2.61	0.53
1:B:160:TYR:CE1	1:B:162:ILE:HD12	2.44	0.53
1:A:411:GLU:C	1:A:412:GLN:O	2.44	0.53
1:B:450:ARG:HG3	1:B:450:ARG:NH1	2.23	0.53
1:A:165:ARG:CD	1:A:165:ARG:N	2.37	0.53
1:A:739:ILE:HD13	1:A:751:MET:CE	2.38	0.53
1:B:725:THR:CG2	1:B:756:ASP:H	2.22	0.53
1:B:670:CYS:CB	1:B:718:ASN:HB3	2.39	0.53
1:A:169:GLU:HG2	1:A:171:ASN:ND2	2.24	0.53
1:A:141:LEU:HB2	1:A:158:VAL:HG12	1.91	0.53
1:A:694:MET:CE	1:A:697:LYS:HG3	2.39	0.53
1:B:193:ILE:HD11	1:B:242:HIS:CD2	2.44	0.53
1:B:589:ILE:HG13	1:B:596:VAL:HG13	1.90	0.53
1:A:258:ASP:OD1	1:A:290:PRO:HB3	2.09	0.53
1:B:714:LEU:HD13	1:B:719:ILE:CD1	2.38	0.52
1:B:322:THR:HG21	1:B:371:GLN:OE1	2.07	0.52
1:B:294:LEU:HD23	1:B:308:LEU:HB2	1.90	0.52
1:A:96:TYR:O	1:A:96:TYR:CG	2.62	0.52
1:B:709:HIS:O	1:B:710:ASN:HB2	2.09	0.52
1:A:73:ASP:OD1	1:A:76:ARG:NH1	2.43	0.52
1:A:584:TRP:HH2	1:A:648:PHE:CE1	2.28	0.52
1:B:584:TRP:HH2	1:B:648:PHE:CZ	2.27	0.52
1:B:584:TRP:HH2	1:B:648:PHE:CE1	2.27	0.52
1:B:339:ARG:NH1	1:B:689:GLU:OE2	2.43	0.52
1:A:725:THR:CG2	1:A:756:ASP:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:HIS:NE2	4:B:802:NAG:O6	2.38	0.52
1:A:725:THR:HG22	1:A:756:ASP:H	1.74	0.52
1:A:510:ALA:C	1:A:512:TYR:H	2.11	0.52
1:B:695:PRO:HA	1:B:702:TYR:HD2	1.69	0.52
1:B:328:SER:HG	1:B:331:LYS:H	1.58	0.52
1:B:739:ILE:HD13	1:B:751:MET:HE3	1.91	0.52
1:B:623:GLU:HG3	1:B:656:ILE:CD1	2.40	0.52
1:B:264:MET:HE2	1:B:264:MET:HA	1.92	0.52
1:B:677:ILE:HD11	1:B:680:LEU:HD22	1.90	0.52
1:A:193:ILE:HD11	1:A:242:HIS:CD2	2.44	0.52
1:A:186:GLY:HA3	1:A:191:GLN:HG3	1.90	0.52
1:B:641:ASP:OD1	1:B:643:LYS:HB2	2.09	0.52
1:B:511:LYS:O	1:B:512:TYR:C	2.49	0.51
1:B:694:MET:CE	1:B:697:LYS:HG3	2.41	0.51
4:B:807:NAG:H2	4:B:808:NAG:O7	2.10	0.51
1:A:623:GLU:HG3	1:A:656:ILE:CD1	2.40	0.51
1:A:520:MET:HG2	1:A:521:LEU:N	2.25	0.51
1:A:118:GLU:C	1:A:120:THR:H	2.14	0.51
1:A:188:GLN:O	1:A:191:GLN:HG2	2.09	0.51
1:B:520:MET:HG2	1:B:521:LEU:N	2.24	0.51
1:B:95:VAL:O	1:B:95:VAL:HG13	2.10	0.51
1:A:322:THR:HG21	1:A:371:GLN:OE1	2.10	0.51
1:A:426:ILE:HD12	1:A:450:ARG:HG2	1.93	0.51
1:A:132:VAL:HG22	1:A:139:VAL:HG22	1.93	0.51
1:A:670:CYS:CB	1:A:718:ASN:HB3	2.41	0.51
1:A:401:ILE:HD11	1:A:440:PHE:HD2	1.75	0.51
1:A:403:MET:O	1:A:405:LEU:HD22	2.11	0.51
1:B:169:GLU:HG2	1:B:171:ASN:ND2	2.26	0.51
1:B:584:TRP:CH2	1:B:648:PHE:CZ	2.99	0.51
1:A:193:ILE:HG23	1:A:244:TRP:CH2	2.45	0.51
1:A:588:LEU:HD22	1:A:594:VAL:HB	1.93	0.51
1:B:588:LEU:HD22	1:B:594:VAL:HB	1.93	0.50
1:A:644:ARG:CD	1:A:781:LEU:O	2.46	0.50
1:A:440:PHE:N	1:A:440:PHE:CD1	2.78	0.50
1:B:460:LEU:N	1:B:460:LEU:HD22	2.26	0.50
1:A:95:VAL:HG13	1:A:95:VAL:O	2.11	0.50
3:A:804:NAG:O3	3:A:806:MAN:H3	2.10	0.50
1:B:141:LEU:HB2	1:B:158:VAL:HG12	1.93	0.50
1:B:508:ASN:OD1	1:B:510:ALA:HB2	2.12	0.50
1:A:159:ILE:HG21	1:A:206:ILE:HD11	1.93	0.50
1:B:403:MET:O	1:B:405:LEU:HD22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:CE1	1:A:162:ILE:HD12	2.41	0.50
1:A:450:ARG:HG3	1:A:450:ARG:NH1	2.25	0.50
1:B:550:SER:HB2	1:B:596:VAL:HG22	1.92	0.50
1:A:567:MET:SD	1:A:647:ILE:HD11	2.51	0.50
1:B:73:ASP:OD2	1:B:528:LYS:NZ	2.45	0.50
1:A:460:LEU:HD22	1:A:460:LEU:N	2.26	0.50
1:A:513:PHE:HB3	2:A:801:NAG:H61	1.93	0.50
1:B:194:TYR:CE2	1:B:201:TYR:CD2	2.99	0.50
1:B:567:MET:SD	1:B:647:ILE:HD11	2.52	0.50
1:A:460:LEU:HD23	1:A:462:ASN:HB3	1.94	0.50
1:A:508:ASN:OD1	1:A:510:ALA:HB2	2.12	0.50
1:B:646:SER:HA	1:B:670:CYS:O	2.12	0.50
1:A:403:MET:CG	1:A:418:LEU:HD11	2.42	0.49
1:B:405:LEU:HB2	1:B:414:THR:HG23	1.94	0.49
1:B:188:GLN:O	1:B:191:GLN:HG2	2.12	0.49
1:A:264:MET:HG2	1:A:731:HIS:NE2	2.27	0.49
1:B:249:GLU:HG3	1:B:300:TYR:CE2	2.47	0.49
1:B:694:MET:HE2	1:B:697:LYS:HG3	1.94	0.49
1:B:73:ASP:OD1	1:B:76:ARG:NH1	2.44	0.49
1:B:367:TRP:C	1:B:367:TRP:CD1	2.85	0.49
1:B:410:SER:C	1:B:411:GLU:O	2.51	0.49
1:B:193:ILE:HG23	1:B:244:TRP:CH2	2.46	0.49
1:B:264:MET:HG2	1:B:731:HIS:NE2	2.28	0.49
1:B:488:HIS:HB2	1:B:504:HIS:O	2.11	0.49
1:A:373:GLU:OE2	1:A:387:THR:HG22	2.12	0.49
1:B:142:ALA:HB2	1:B:157:TYR:CE2	2.47	0.49
1:A:488:HIS:HB2	1:A:504:HIS:O	2.12	0.49
1:B:102:HIS:CE1	1:B:119:ASN:OD1	2.66	0.49
1:A:714:LEU:HD13	1:A:719:ILE:CD1	2.43	0.49
1:B:132:VAL:HG22	1:B:139:VAL:HG22	1.95	0.49
1:B:620:GLY:N	1:B:623:GLU:OE1	2.40	0.49
1:B:161:ASN:ND2	1:B:164:THR:HG23	2.28	0.49
1:A:511:LYS:O	1:A:512:TYR:C	2.50	0.49
1:A:550:SER:HB2	1:A:596:VAL:HG22	1.95	0.49
1:A:666:LYS:NZ	1:A:666:LYS:HB3	2.27	0.49
1:A:525:ILE:HD13	1:A:526:LEU:N	2.28	0.49
1:B:562:ALA:CB	1:B:781:LEU:HD13	2.41	0.49
1:A:677:ILE:HD11	1:A:680:LEU:HD22	1.95	0.49
1:B:286:GLY:HA3	1:B:695:PRO:HG3	1.93	0.49
1:A:121:THR:CG2	1:A:127:ALA:HB3	2.42	0.49
1:A:339:ARG:NH1	1:A:689:GLU:OE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:CYS:HB3	1:A:718:ASN:HB3	1.95	0.49
1:B:373:GLU:OE2	1:B:387:THR:HG22	2.13	0.48
1:A:695:PRO:CA	1:A:702:TYR:HE2	2.27	0.48
1:B:663:SER:O	1:B:664:ASP:C	2.50	0.48
1:B:710:ASN:O	1:B:712:HIS:CG	2.67	0.48
1:B:450:ARG:H	1:B:477:TYR:HA	1.78	0.48
5:B:804:NAG:H4	5:B:805:NAG:O7	2.14	0.48
1:A:669:LYS:HD2	1:A:780:CYS:O	2.13	0.48
1:B:159:ILE:HG21	1:B:206:ILE:HD11	1.95	0.48
1:A:409:LYS:CG	1:A:410:SER:H	2.10	0.48
1:A:694:MET:HE2	1:A:697:LYS:HG3	1.95	0.48
1:B:195:ILE:CD1	1:B:226:ILE:HG23	2.38	0.48
1:B:575:LEU:HD22	1:B:598:ARG:HD3	1.95	0.48
1:A:268:ARG:NH1	1:A:277:GLY:HA2	2.29	0.48
1:A:512:TYR:HB3	1:A:513:PHE:H	1.54	0.48
1:B:470:PHE:CE1	1:B:491:LEU:HD12	2.49	0.48
1:A:751:MET:HG2	1:A:751:MET:O	2.13	0.48
1:A:640:ILE:O	1:A:640:ILE:HD13	2.13	0.48
1:B:143:TYR:O	1:B:144:ASP:HB2	2.14	0.48
1:A:584:TRP:HH2	1:A:648:PHE:CZ	2.32	0.48
1:A:378:SER:C	1:A:380:ASP:H	2.17	0.48
1:B:666:LYS:HB3	1:B:666:LYS:NZ	2.29	0.48
1:B:429:LEU:HD11	1:B:441:LEU:CD2	2.44	0.48
1:A:646:SER:HA	1:A:670:CYS:O	2.13	0.48
1:B:159:ILE:HD13	1:B:206:ILE:HD11	1.96	0.48
1:B:666:LYS:HB3	1:B:666:LYS:HZ2	1.79	0.48
1:B:440:PHE:N	1:B:440:PHE:CD1	2.81	0.48
1:A:471:MET:HG3	1:A:475:CYS:SG	2.54	0.48
1:B:602:ARG:HA	1:B:611:ILE:HG23	1.96	0.47
1:A:243:TRP:HH2	1:A:254:LEU:HG	1.78	0.47
1:B:670:CYS:HB3	1:B:718:ASN:HB3	1.96	0.47
1:A:695:PRO:C	1:A:697:LYS:N	2.68	0.47
1:B:637:LEU:HD13	1:B:639:TYR:CZ	2.49	0.47
1:A:166:GLU:H	1:A:166:GLU:HG3	1.47	0.47
1:A:562:ALA:CB	1:A:781:LEU:HD13	2.43	0.47
1:B:525:ILE:HD13	1:B:526:LEU:N	2.29	0.47
1:B:118:GLU:CG	1:B:119:ASN:N	2.64	0.47
4:A:807:NAG:H4	4:A:808:NAG:O7	2.14	0.47
1:A:488:HIS:CB	1:A:504:HIS:O	2.62	0.47
1:B:460:LEU:HD23	1:B:462:ASN:N	2.23	0.47
1:B:738:LEU:HG	1:B:742:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HB2	1:A:414:THR:HG23	1.97	0.47
1:B:648:PHE:CD1	1:B:648:PHE:C	2.87	0.47
1:B:121:THR:CG2	1:B:127:ALA:HB3	2.44	0.47
1:B:488:HIS:CB	1:B:504:HIS:O	2.63	0.47
1:B:571:PRO:HD3	1:B:652:TYR:CD2	2.50	0.47
1:B:426:ILE:HD12	1:B:450:ARG:HG2	1.96	0.47
1:B:585:ASP:HB2	1:B:596:VAL:HG11	1.97	0.47
1:B:605:GLY:HA2	1:B:612:LEU:HD13	1.97	0.47
1:A:138:TYR:CD1	1:A:161:ASN:HA	2.50	0.47
1:A:431:TYR:CE1	1:A:457:THR:HG21	2.50	0.47
1:B:158:VAL:HG13	1:B:167:VAL:HG13	1.97	0.47
1:B:268:ARG:NH1	1:B:277:GLY:HA2	2.29	0.47
1:A:301:GLY:HA3	1:A:302:PRO:HD3	1.80	0.47
1:B:751:MET:HG2	1:B:751:MET:O	2.14	0.47
1:B:410:SER:O	1:B:411:GLU:O	2.32	0.47
1:A:591:MET:O	1:A:592:ASP:CB	2.63	0.47
1:A:584:TRP:CH2	1:A:648:PHE:CZ	3.03	0.47
1:A:273:LEU:HA	1:A:273:LEU:HD23	1.80	0.47
1:A:163:HIS:ND1	1:A:163:HIS:C	2.68	0.47
1:B:92:THR:O	1:B:108:ILE:HG12	2.15	0.47
1:A:738:LEU:HG	1:A:742:LEU:HD12	1.97	0.47
1:A:753:VAL:HG13	1:B:751:MET:HE2	1.97	0.47
1:A:648:PHE:C	1:A:648:PHE:CD1	2.87	0.47
1:B:645:LEU:HD12	1:B:667:LEU:O	2.15	0.47
1:A:666:LYS:HB3	1:A:666:LYS:HZ2	1.79	0.47
1:B:431:TYR:CE1	1:B:457:THR:HG21	2.50	0.46
1:A:126:LYS:HA	1:A:126:LYS:HE3	1.98	0.46
1:A:740:LYS:HD2	1:B:270:THR:HG21	1.96	0.46
1:B:80:VAL:O	1:B:80:VAL:HG12	2.15	0.46
1:B:258:ASP:OD1	1:B:290:PRO:HB3	2.14	0.46
1:B:163:HIS:C	1:B:163:HIS:ND1	2.68	0.46
1:A:249:GLU:HG3	1:A:300:TYR:CE2	2.51	0.46
1:B:754:TYR:HB3	1:B:757:GLU:HG3	1.98	0.46
1:A:470:PHE:HE2	1:A:511:LYS:HG3	1.80	0.46
1:A:292:ILE:HD11	1:A:321:ILE:CG1	2.45	0.46
1:A:450:ARG:H	1:A:477:TYR:HA	1.80	0.46
1:B:617:ARG:NH2	1:B:699:GLU:OE2	2.48	0.46
1:B:328:SER:HG	1:B:331:LYS:N	2.13	0.46
1:A:158:VAL:HG13	1:A:167:VAL:HG13	1.98	0.46
1:A:367:TRP:C	1:A:367:TRP:CD1	2.89	0.46
1:B:640:ILE:O	1:B:640:ILE:HD13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:MET:O	1:A:404:PHE:C	2.54	0.46
1:A:142:ALA:HB2	1:A:157:TYR:CE2	2.51	0.46
1:A:328:SER:OG	1:A:330:THR:HG23	2.15	0.46
1:A:80:VAL:HG12	1:A:80:VAL:O	2.14	0.46
1:A:541:ASP:HB3	1:A:542:ASP:H	1.38	0.46
1:A:602:ARG:HA	1:A:611:ILE:HG23	1.98	0.46
1:A:195:ILE:CD1	1:A:226:ILE:HG23	2.40	0.46
1:A:73:ASP:OD2	1:A:528:LYS:NZ	2.49	0.46
1:A:409:LYS:CG	1:A:410:SER:N	2.67	0.46
1:B:609:LEU:HD13	1:B:613:GLN:NE2	2.31	0.46
1:A:753:VAL:HG11	1:B:753:VAL:CG1	2.41	0.46
1:A:436:GLN:HG2	1:A:458:GLU:HB2	1.97	0.46
1:B:644:ARG:NH1	1:B:781:LEU:O	2.49	0.46
1:B:126:LYS:HE3	1:B:126:LYS:HA	1.98	0.46
1:B:161:ASN:C	1:B:161:ASN:OD1	2.55	0.46
1:A:719:ILE:O	1:A:750:THR:HG23	2.16	0.46
1:B:436:GLN:HG2	1:B:458:GLU:HB2	1.97	0.46
1:A:273:LEU:HD23	1:B:682:LEU:HD23	1.97	0.46
1:B:714:LEU:HD12	1:B:747:VAL:HG11	1.97	0.45
1:A:460:LEU:HD23	1:A:462:ASN:N	2.26	0.45
4:B:807:NAG:O3	4:B:808:NAG:N2	2.49	0.45
1:A:268:ARG:HH12	1:A:277:GLY:HA2	1.81	0.45
1:A:301:GLY:O	1:A:303:THR:HG23	2.16	0.45
1:A:644:ARG:NH1	1:A:781:LEU:O	2.49	0.45
1:A:545:LEU:HB3	1:A:600:ASP:O	2.17	0.45
1:A:172:PRO:HG2	1:A:175:VAL:CB	2.45	0.45
1:B:172:PRO:HG2	1:B:175:VAL:CB	2.46	0.45
1:A:548:GLN:HB2	1:A:576:VAL:HG22	1.99	0.45
1:B:82:HIS:HB3	1:B:516:GLU:OE2	2.16	0.45
1:B:591:MET:O	1:B:592:ASP:CB	2.61	0.45
1:A:497:ARG:HD3	1:A:498:VAL:O	2.16	0.45
1:A:564:LEU:HD22	1:A:588:LEU:HD12	1.99	0.45
1:A:411:GLU:O	1:A:412:GLN:O	2.34	0.45
1:A:147:GLN:HA	1:A:147:GLN:OE1	2.17	0.45
1:A:569:GLU:O	1:A:652:TYR:HB3	2.17	0.45
1:B:548:GLN:HB2	1:B:576:VAL:HG22	1.99	0.45
1:A:82:HIS:HB3	1:A:516:GLU:OE2	2.15	0.45
1:B:545:LEU:HB3	1:B:600:ASP:O	2.17	0.45
4:B:807:NAG:H4	4:B:808:NAG:N2	2.31	0.45
1:B:124:THR:O	1:B:125:PHE:C	2.55	0.45
1:B:268:ARG:O	1:B:275:PRO:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ILE:HG22	1:A:222:ILE:HG13	1.98	0.45
1:B:403:MET:CG	1:B:418:LEU:HD11	2.46	0.45
1:B:471:MET:O	1:B:472:LYS:HB2	2.17	0.45
1:A:92:THR:O	1:A:108:ILE:HG12	2.17	0.45
1:B:691:TYR:CD1	1:B:691:TYR:N	2.85	0.45
1:B:403:MET:O	1:B:404:PHE:C	2.53	0.45
1:A:157:TYR:CE2	1:A:183:ALA:HB3	2.52	0.45
1:A:193:ILE:HG12	1:A:244:TRP:HZ2	1.81	0.45
1:A:327:VAL:HG23	1:A:328:SER:H	1.81	0.45
1:A:645:LEU:HD12	1:A:667:LEU:O	2.17	0.45
1:B:541:ASP:HB3	1:B:542:ASP:H	1.37	0.45
1:A:143:TYR:O	1:A:144:ASP:HB2	2.17	0.45
1:A:268:ARG:O	1:A:275:PRO:HB2	2.17	0.45
1:A:161:ASN:ND2	1:A:164:THR:HG23	2.32	0.45
1:A:637:LEU:HD13	1:A:639:TYR:CZ	2.52	0.45
1:A:754:TYR:HB3	1:A:757:GLU:HG3	1.97	0.45
1:A:691:TYR:N	1:A:691:TYR:CD1	2.85	0.45
1:B:564:LEU:HD22	1:B:588:LEU:HD12	1.99	0.45
1:A:264:MET:HG2	1:A:731:HIS:CD2	2.52	0.45
1:B:401:ILE:HD11	1:B:440:PHE:HD2	1.80	0.44
1:A:762:SER:O	1:A:766:LYS:HB2	2.16	0.44
1:B:147:GLN:OE1	1:B:147:GLN:HA	2.17	0.44
1:A:102:HIS:HD1	1:A:118:GLU:HA	1.82	0.44
1:A:460:LEU:H	1:A:460:LEU:CD1	2.16	0.44
1:A:450:ARG:HD2	1:A:477:TYR:CZ	2.52	0.44
1:A:666:LYS:HD2	1:A:717:GLU:HG3	2.00	0.44
1:A:498:VAL:CG1	1:A:521:LEU:HD22	2.47	0.44
1:B:488:HIS:HB3	1:B:505:SER:CA	2.29	0.44
1:A:709:HIS:O	1:A:710:ASN:HB2	2.17	0.44
1:A:584:TRP:CD1	1:A:585:ASP:N	2.86	0.44
1:B:193:ILE:HD11	1:B:242:HIS:NE2	2.32	0.44
1:A:617:ARG:NH2	1:A:699:GLU:OE2	2.50	0.44
1:A:126:LYS:HG3	1:A:126:LYS:O	2.17	0.44
1:B:624:VAL:HG21	1:B:659:MET:HB2	1.99	0.44
1:A:255:MET:C	1:A:255:MET:SD	2.95	0.44
1:B:749:TYR:CD1	1:B:749:TYR:C	2.91	0.44
1:A:609:LEU:HD13	1:A:613:GLN:NE2	2.33	0.44
1:A:714:LEU:HD12	1:A:747:VAL:HG11	1.99	0.44
1:A:193:ILE:HD11	1:A:242:HIS:NE2	2.32	0.44
1:A:666:LYS:HE2	1:A:716:GLU:HG2	2.00	0.44
1:A:739:ILE:O	1:A:743:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ALA:HB1	1:A:254:LEU:HB2	1.98	0.44
1:B:498:VAL:CG1	1:B:521:LEU:HD22	2.47	0.44
1:B:565:LEU:HD22	1:B:567:MET:CE	2.48	0.44
1:B:204:PRO:HG2	1:B:208:SER:HB2	2.00	0.44
1:B:301:GLY:O	1:B:303:THR:HG23	2.17	0.44
1:B:662:LYS:HB3	1:B:712:HIS:CE1	2.47	0.44
1:B:695:PRO:CA	1:B:702:TYR:CD2	2.97	0.44
1:B:648:PHE:CD1	1:B:649:GLY:N	2.85	0.44
1:B:497:ARG:HD3	1:B:498:VAL:O	2.17	0.44
1:B:666:LYS:HE2	1:B:716:GLU:HG2	1.99	0.44
1:A:506:THR:O	1:A:509:PRO:HD3	2.18	0.44
1:A:165:ARG:O	1:A:166:GLU:C	2.55	0.44
1:B:366:THR:OG1	1:B:367:TRP:N	2.50	0.44
1:B:450:ARG:HD2	1:B:477:TYR:CZ	2.53	0.44
1:A:620:GLY:N	1:A:623:GLU:OE1	2.42	0.44
1:B:551:LEU:HA	1:B:552:PRO:HD3	1.89	0.44
1:A:172:PRO:HA	1:A:194:TYR:OH	2.17	0.44
1:B:183:ALA:O	1:B:193:ILE:O	2.36	0.44
1:A:739:ILE:CD1	1:A:751:MET:HE3	2.48	0.44
1:A:159:ILE:HD13	1:A:206:ILE:HD11	1.98	0.44
1:A:161:ASN:OD1	1:A:161:ASN:C	2.57	0.44
1:A:315:LYS:O	1:A:316:SER:OG	2.27	0.44
1:A:87:ARG:HB3	1:A:95:VAL:HG12	2.00	0.44
1:A:648:PHE:CD1	1:A:649:GLY:N	2.86	0.44
1:B:243:TRP:HH2	1:B:254:LEU:HG	1.82	0.44
1:B:666:LYS:CE	1:B:716:GLU:HG2	2.48	0.44
1:B:190:GLN:HG3	1:B:205:ASP:HA	2.00	0.44
1:B:292:ILE:HD13	1:B:292:ILE:O	2.17	0.43
1:B:394:GLY:O	1:B:395:ARG:HB2	2.17	0.43
1:B:138:TYR:CD1	1:B:161:ASN:HA	2.53	0.43
1:B:268:ARG:HH12	1:B:277:GLY:HA2	1.82	0.43
1:B:396:GLY:HA3	1:B:610:LYS:HB2	2.00	0.43
1:B:532:LYS:HA	1:B:533:PRO:HD3	1.55	0.43
1:B:681:LYS:HE3	1:B:681:LYS:HB2	1.70	0.43
1:B:221:ILE:HG22	1:B:222:ILE:HG13	2.00	0.43
1:B:157:TYR:CE2	1:B:183:ALA:HB3	2.53	0.43
1:B:172:PRO:HA	1:B:194:TYR:OH	2.17	0.43
1:B:193:ILE:HG12	1:B:244:TRP:HZ2	1.83	0.43
1:B:126:LYS:O	1:B:126:LYS:HG3	2.17	0.43
1:B:366:THR:OG1	1:B:613:GLN:OE1	2.30	0.43
1:A:584:TRP:CG	1:A:585:ASP:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:THR:C	1:B:122:PHE:N	2.72	0.43
1:A:183:ALA:O	1:A:193:ILE:O	2.36	0.43
1:A:328:SER:HG	1:A:331:LYS:N	2.15	0.43
1:A:311:PRO:HG2	1:A:314:PHE:HB2	2.00	0.43
1:B:194:TYR:CZ	1:B:201:TYR:HD2	2.37	0.43
1:B:460:LEU:H	1:B:460:LEU:CD1	2.16	0.43
1:B:545:LEU:HA	1:B:546:PRO:HD3	1.74	0.43
1:B:148:ILE:HG13	1:B:154:THR:CG2	2.47	0.43
1:A:148:ILE:HB	1:A:152:SER:HB3	2.00	0.43
1:A:532:LYS:HA	1:A:533:PRO:HD3	1.57	0.43
1:A:289:ASN:HA	1:A:289:ASN:HD22	1.57	0.43
1:A:663:SER:O	1:A:664:ASP:C	2.56	0.43
1:A:624:VAL:HG21	1:A:659:MET:HB2	2.01	0.43
1:A:498:VAL:HA	1:A:499:PRO:HD3	1.92	0.43
1:A:429:LEU:HD11	1:A:441:LEU:CD2	2.48	0.43
1:A:194:TYR:CZ	1:A:201:TYR:HD2	2.36	0.43
1:A:270:THR:HG23	1:B:740:LYS:HD2	1.98	0.43
1:B:292:ILE:HD11	1:B:321:ILE:CG1	2.48	0.43
1:A:764:LYS:CE	1:B:744:LYS:HD2	2.49	0.43
1:B:121:THR:HG23	1:B:141:LEU:HD12	2.00	0.43
1:A:124:THR:O	1:A:125:PHE:C	2.57	0.43
1:B:328:SER:OG	1:B:330:THR:HG23	2.18	0.43
1:B:650:LYS:HG2	1:B:651:GLY:N	2.34	0.43
1:B:515:LEU:HA	1:B:515:LEU:HD12	1.70	0.43
1:A:662:LYS:HB3	1:A:712:HIS:CE1	2.45	0.43
1:B:692:LEU:HD12	1:B:702:TYR:CE1	2.54	0.43
1:A:605:GLY:HA2	1:A:612:LEU:HD13	2.00	0.43
1:A:740:LYS:HD2	1:B:270:THR:HG23	2.00	0.42
1:A:342:ASN:CA	1:A:368:LEU:HD23	2.49	0.42
1:B:670:CYS:HB2	1:B:718:ASN:HB3	2.01	0.42
1:B:374:GLU:HA	1:B:375:PRO:HD2	1.90	0.42
1:A:775:LYS:HE3	1:A:775:LYS:HB2	1.71	0.42
1:B:569:GLU:O	1:B:652:TYR:HB3	2.19	0.42
1:A:440:PHE:N	1:A:440:PHE:HD1	2.15	0.42
1:A:83:ASP:HA	1:A:84:PRO:HD3	1.81	0.42
1:A:116:LEU:C	1:A:162:ILE:HD11	2.40	0.42
1:A:585:ASP:HB2	1:A:596:VAL:HG11	2.01	0.42
1:A:436:GLN:C	1:A:457:THR:HG22	2.40	0.42
1:B:520:MET:HG2	1:B:521:LEU:H	1.84	0.42
1:A:749:TYR:C	1:A:749:TYR:CD1	2.92	0.42
1:A:222:ILE:HD11	3:A:803:NAG:HN2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:MET:HG2	1:B:731:HIS:CD2	2.54	0.42
1:A:419:THR:HG22	1:A:463:ARG:HD3	2.01	0.42
1:B:616:HIS:CD2	1:B:617:ARG:HD2	2.55	0.42
1:A:666:LYS:CE	1:A:716:GLU:HG2	2.49	0.42
1:A:266:ILE:HG23	1:A:726:ALA:HA	2.02	0.42
1:A:396:GLY:HA3	1:A:610:LYS:HB2	2.01	0.42
1:A:584:TRP:C	1:A:584:TRP:CD1	2.92	0.42
1:B:79:PHE:N	1:B:79:PHE:CD1	2.87	0.42
1:B:87:ARG:HB3	1:B:95:VAL:HG12	2.01	0.42
1:A:385:PHE:CG	1:A:438:ILE:HD12	2.53	0.42
1:A:511:LYS:O	1:A:511:LYS:HG2	2.20	0.42
1:B:74:LEU:N	1:B:74:LEU:HD12	2.34	0.42
1:B:116:LEU:C	1:B:162:ILE:HD11	2.40	0.42
1:B:436:GLN:C	1:B:457:THR:HG22	2.39	0.42
1:A:650:LYS:HG2	1:A:651:GLY:N	2.34	0.42
1:A:782:LYS:HE3	1:A:782:LYS:HB2	1.22	0.42
1:A:323:MET:HE2	1:A:375:PRO:HD2	2.01	0.42
1:B:727:ASP:OD1	1:B:759:HIS:HB2	2.19	0.42
1:A:116:LEU:HB3	1:A:162:ILE:HD11	2.02	0.42
1:A:148:ILE:HG22	1:A:149:PHE:N	2.35	0.42
1:B:378:SER:C	1:B:380:ASP:H	2.23	0.42
1:A:650:LYS:CG	1:A:651:GLY:N	2.83	0.42
1:A:720:LEU:HA	1:A:750:THR:O	2.19	0.42
1:B:419:THR:HG22	1:B:463:ARG:HD3	2.02	0.42
1:B:584:TRP:C	1:B:584:TRP:CD1	2.92	0.42
1:B:584:TRP:CD1	1:B:585:ASP:N	2.88	0.42
1:A:669:LYS:HG3	1:A:670:CYS:N	2.34	0.42
1:B:130:HIS:ND1	1:B:130:HIS:C	2.73	0.42
1:B:222:ILE:HD11	5:B:804:NAG:HN2	1.85	0.42
1:A:95:VAL:O	1:A:96:TYR:C	2.58	0.42
1:B:116:LEU:HB3	1:B:162:ILE:HD11	2.02	0.42
1:A:620:GLY:H	1:A:623:GLU:CD	2.22	0.42
1:B:666:LYS:HD2	1:B:717:GLU:HG3	2.02	0.42
1:A:366:THR:OG1	1:A:367:TRP:N	2.49	0.42
1:A:443:THR:HB	1:A:447:PRO:HA	2.02	0.42
1:B:575:LEU:HD23	1:B:575:LEU:HA	1.78	0.41
1:A:91:ASP:O	1:A:108:ILE:HD11	2.19	0.41
1:B:298:ASN:OD1	1:B:303:THR:HA	2.20	0.41
1:B:301:GLY:HA3	1:B:302:PRO:HD3	1.78	0.41
1:B:712:HIS:N	1:B:712:HIS:ND1	2.68	0.41
1:B:619:LEU:HB2	1:B:692:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:HH22	1:A:132:VAL:H	1.68	0.41
1:A:575:LEU:HA	1:A:575:LEU:HD23	1.82	0.41
1:B:241:ALA:HB1	1:B:254:LEU:HB2	2.02	0.41
1:A:498:VAL:HG13	1:A:521:LEU:HD22	2.03	0.41
1:B:306:LEU:HD12	1:B:306:LEU:N	2.35	0.41
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.79	0.41
1:A:692:LEU:HD12	1:A:702:TYR:CE1	2.55	0.41
1:A:448:ARG:NH1	1:A:448:ARG:CG	2.82	0.41
1:B:162:ILE:HA	1:B:162:ILE:HD12	1.93	0.41
1:B:327:VAL:HG23	1:B:328:SER:H	1.84	0.41
1:A:765:SER:HA	1:B:743:ILE:HG21	2.01	0.41
1:B:644:ARG:HB3	1:B:781:LEU:HD22	2.03	0.41
1:B:287:GLN:HE21	1:B:287:GLN:CA	2.28	0.41
1:B:601:GLY:O	1:B:604:SER:HB3	2.19	0.41
1:A:269:PHE:CD1	1:B:732:PHE:HD2	2.39	0.41
1:B:93:ASP:HA	1:B:106:LEU:O	2.20	0.41
1:A:515:LEU:HA	1:A:515:LEU:HD12	1.72	0.41
1:B:559:ASN:N	1:B:559:ASN:OD1	2.52	0.41
1:B:675:ALA:HA	1:B:723:HIS:CE1	2.55	0.41
1:A:460:LEU:O	1:A:461:LEU:HB2	2.21	0.41
1:B:148:ILE:HG22	1:B:149:PHE:N	2.35	0.41
1:B:81:LEU:HA	1:B:521:LEU:HD13	2.01	0.41
1:A:726:ALA:HB3	1:A:757:GLU:O	2.21	0.41
1:A:476:THR:H	1:A:496:PRO:HD3	1.85	0.41
1:B:761:VAL:CG1	1:B:765:SER:HB2	2.50	0.41
1:B:584:TRP:CG	1:B:585:ASP:N	2.88	0.41
1:B:620:GLY:H	1:B:623:GLU:CD	2.22	0.41
1:A:204:PRO:HG2	1:A:208:SER:HB2	2.03	0.41
1:A:74:LEU:HD12	1:A:74:LEU:N	2.34	0.41
1:B:137:LYS:HE3	1:B:137:LYS:HB2	1.92	0.41
1:A:416:ARG:HH11	1:A:461:LEU:CD2	2.31	0.41
1:A:436:GLN:O	1:A:456:SER:HA	2.20	0.41
1:A:620:GLY:O	1:A:624:VAL:HB	2.19	0.41
1:B:782:LYS:HE3	1:B:782:LYS:HB2	1.08	0.41
1:A:240:ILE:HG12	1:A:240:ILE:H	1.60	0.41
1:B:409:LYS:O	1:B:410:SER:C	2.58	0.41
1:A:459:GLY:O	1:A:461:LEU:HD12	2.21	0.41
1:B:416:ARG:HH11	1:B:461:LEU:CD2	2.31	0.41
1:B:148:ILE:HB	1:B:152:SER:HB3	2.03	0.41
1:B:621:SER:O	1:B:625:LYS:HG3	2.21	0.41
1:A:190:GLN:HG3	1:A:205:ASP:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:TRP:HE1	1:B:347:THR:HB	1.85	0.41
1:A:644:ARG:HB3	1:A:781:LEU:HD22	2.03	0.41
1:B:411:GLU:O	1:B:412:GLN:CG	2.68	0.41
1:B:231:TYR:CZ	1:B:292:ILE:HG21	2.55	0.41
1:B:73:ASP:O	1:B:76:ARG:HB2	2.21	0.41
1:A:294:LEU:CD2	1:A:308:LEU:HB2	2.50	0.41
1:B:91:ASP:O	1:B:108:ILE:HD11	2.21	0.41
1:A:137:LYS:HE3	1:A:137:LYS:HB2	1.92	0.41
1:A:261:VAL:HG11	1:A:283:PRO:HD3	2.03	0.41
1:A:306:LEU:N	1:A:306:LEU:HD12	2.36	0.41
1:B:708:LEU:HD23	1:B:708:LEU:HA	1.87	0.41
1:A:200:ILE:C	1:A:201:TYR:HD1	2.25	0.41
1:B:200:ILE:O	1:B:201:TYR:HD1	2.04	0.41
1:B:765:SER:O	1:B:768:HIS:N	2.54	0.41
1:B:83:ASP:HA	1:B:84:PRO:HD3	1.80	0.41
1:A:148:ILE:HG13	1:A:154:THR:CG2	2.46	0.41
1:A:92:THR:HG22	1:A:109:GLU:HG3	2.03	0.41
1:B:650:LYS:CG	1:B:651:GLY:N	2.84	0.41
1:B:384:PHE:HD2	1:B:406:ILE:HG13	1.86	0.41
1:A:615:ILE:CG2	1:A:615:ILE:O	2.70	0.41
1:B:506:THR:O	1:B:509:PRO:HD3	2.21	0.41
1:B:326:TRP:HA	1:B:332:THR:HG22	2.03	0.41
1:A:652:TYR:HA	1:A:677:ILE:HG23	2.03	0.40
1:A:394:GLY:O	1:A:395:ARG:HB2	2.20	0.40
1:B:261:VAL:HG11	1:B:283:PRO:HD3	2.03	0.40
1:A:571:PRO:HD3	1:A:652:TYR:CD2	2.57	0.40
1:B:459:GLY:O	1:B:461:LEU:HD12	2.20	0.40
1:A:542:ASP:OD1	1:A:542:ASP:N	2.48	0.40
1:A:93:ASP:HA	1:A:106:LEU:O	2.21	0.40
1:A:130:HIS:ND1	1:A:130:HIS:C	2.74	0.40
1:A:270:THR:HG23	1:B:737:GLU:OE2	2.21	0.40
1:B:266:ILE:HG23	1:B:726:ALA:HA	2.03	0.40
1:B:436:GLN:O	1:B:456:SER:HA	2.21	0.40
1:A:79:PHE:CD1	1:A:79:PHE:N	2.88	0.40
1:B:342:ASN:CA	1:B:368:LEU:HD23	2.50	0.40
1:B:311:PRO:HG2	1:B:314:PHE:HB2	2.03	0.40
1:A:231:TYR:HA	1:A:235:LEU:HB2	2.04	0.40
1:A:291:THR:C	1:A:292:ILE:HG22	2.42	0.40
1:A:73:ASP:O	1:A:76:ARG:HB2	2.21	0.40
1:A:264:MET:HA	1:A:264:MET:CE	2.51	0.40
1:B:359:LYS:HG3	1:B:406:ILE:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LYS:HG3	1:A:406:ILE:CD1	2.52	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	715/719 (99%)	632 (88%)	71 (10%)	12 (2%)	11	51
1	B	717/719 (100%)	635 (89%)	72 (10%)	10 (1%)	14	55
All	All	1432/1438 (100%)	1267 (88%)	143 (10%)	22 (2%)	13	54

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	GLN
1	A	413	ILE
1	A	663	SER
1	A	711	VAL
1	B	165	ARG
1	B	711	VAL
1	A	695	PRO
1	A	766	LYS
1	B	411	GLU
1	B	663	SER
1	B	695	PRO
1	A	715	LYS
1	A	716	GLU
1	A	529	LYS
1	A	697	LYS
1	B	410	SER
1	B	412	GLN

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Mol	Chain	Res	Type
1	B	529	LYS
1	A	80	VAL
1	B	80	VAL
1	A	530	ILE
1	B	530	ILE

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	645/650 (99%)	540 (84%)	105 (16%)	3	16
1	B	646/650 (99%)	539 (83%)	107 (17%)	3	15
All	All	1291/1300 (99%)	1079 (84%)	212 (16%)	3	15

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	A	91	ASP
1	A	95	VAL
1	A	99	GLU
1	A	100	ASN
1	A	113	THR
1	A	117	LEU
1	A	118	GLU
1	A	120	THR
1	A	121	THR
1	A	122	PHE
1	A	125	PHE
1	A	126	LYS
1	A	128	SER
1	A	129	ARG
1	A	130	HIS
1	A	140	LEU
1	A	144	ASP

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Mol	Chain	Res	Type
1	A	152	SER
1	A	154	THR
1	A	158	VAL
1	A	164	THR
1	A	165	ARG
1	A	166	GLU
1	A	188	GLN
1	A	192	LEU
1	A	209	SER
1	A	211	LEU
1	A	226	ILE
1	A	240	ILE
1	A	249	GLU
1	A	255	MET
1	A	280	TYR
1	A	289	ASN
1	A	291	THR
1	A	292	ILE
1	A	294	LEU
1	A	305	THR
1	A	306	LEU
1	A	313	SER
1	A	317	ARG
1	A	324	VAL
1	A	330	THR
1	A	339	ARG
1	A	347	THR
1	A	365	ASP
1	A	367	TRP
1	A	368	LEU
1	A	391	LYS
1	A	403	MET
1	A	406	ILE
1	A	407	GLN
1	A	412	GLN
1	A	414	THR
1	A	435	THR
1	A	440	PHE
1	A	457	THR
1	A	460	LEU
1	A	462	ASN
1	A	487	GLN

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Mol	Chain	Res	Type
1	A	488	HIS
1	A	491	LEU
1	A	497	ARG
1	A	503	LEU
1	A	512	TYR
1	A	514	ILE
1	A	519	SER
1	A	520	MET
1	A	525	ILE
1	A	528	LYS
1	A	530	ILE
1	A	541	ASP
1	A	542	ASP
1	A	556	MET
1	A	559	ASN
1	A	560	GLN
1	A	565	LEU
1	A	567	MET
1	A	570	GLU
1	A	581	HIS
1	A	584	TRP
1	A	588	LEU
1	A	596	VAL
1	A	604	SER
1	A	617	ARG
1	A	618	ARG
1	A	632	LYS
1	A	635	LEU
1	A	640	ILE
1	A	646	SER
1	A	663	SER
1	A	666	LYS
1	A	669	LYS
1	A	677	ILE
1	A	702	TYR
1	A	711	VAL
1	A	712	HIS
1	A	716	GLU
1	A	720	LEU
1	A	725	THR
1	A	742	LEU
1	A	750	THR

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Mol	Chain	Res	Type
1	A	761	VAL
1	A	763	GLU
1	A	769	LEU
1	B	83	ASP
1	B	91	ASP
1	B	95	VAL
1	B	99	GLU
1	B	100	ASN
1	B	113	THR
1	B	117	LEU
1	B	118	GLU
1	B	120	THR
1	B	121	THR
1	B	122	PHE
1	B	125	PHE
1	B	126	LYS
1	B	128	SER
1	B	129	ARG
1	B	130	HIS
1	B	140	LEU
1	B	144	ASP
1	B	148	ILE
1	B	152	SER
1	B	154	THR
1	B	158	VAL
1	B	164	THR
1	B	165	ARG
1	B	166	GLU
1	B	188	GLN
1	B	192	LEU
1	B	206	ILE
1	B	209	SER
1	B	211	LEU
1	B	226	ILE
1	B	240	ILE
1	B	249	GLU
1	B	255	MET
1	B	280	TYR
1	B	289	ASN
1	B	291	THR
1	B	292	ILE
1	B	294	LEU

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Mol	Chain	Res	Type
1	B	305	THR
1	B	306	LEU
1	B	313	SER
1	B	317	ARG
1	B	322	THR
1	B	324	VAL
1	B	330	THR
1	B	339	ARG
1	B	347	THR
1	B	365	ASP
1	B	367	TRP
1	B	368	LEU
1	B	391	LYS
1	B	403	MET
1	B	406	ILE
1	B	407	GLN
1	B	411	GLU
1	B	412	GLN
1	B	414	THR
1	B	435	THR
1	B	440	PHE
1	B	457	THR
1	B	460	LEU
1	B	462	ASN
1	B	487	GLN
1	B	488	HIS
1	B	491	LEU
1	B	497	ARG
1	B	503	LEU
1	B	512	TYR
1	B	514	ILE
1	B	519	SER
1	B	520	MET
1	B	525	ILE
1	B	530	ILE
1	B	541	ASP
1	B	542	ASP
1	B	556	MET
1	B	558	ARG
1	B	559	ASN
1	B	560	GLN
1	B	565	LEU

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Mol	Chain	Res	Type
1	B	567	MET
1	B	570	GLU
1	B	581	HIS
1	B	584	TRP
1	B	588	LEU
1	B	604	SER
1	B	617	ARG
1	B	618	ARG
1	B	632	LYS
1	B	635	LEU
1	B	640	ILE
1	B	646	SER
1	B	663	SER
1	B	665	GLU
1	B	666	LYS
1	B	677	ILE
1	B	702	TYR
1	B	712	HIS
1	B	716	GLU
1	B	720	LEU
1	B	725	THR
1	B	742	LEU
1	B	750	THR
1	B	761	VAL
1	B	763	GLU
1	B	783	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	B	287	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 ⓘ

13 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	A	803	1,3	14,14,15	0.47	0	15,19,21	1.72	2 (13%)
3	NAG	A	804	3	14,14,15	0.61	0	15,19,21	1.52	2 (13%)
3	BMA	A	805	3	11,11,12	0.67	0	14,15,17	2.83	5 (35%)
3	MAN	A	806	3	11,11,12	0.45	0	14,15,17	1.71	3 (21%)
4	NAG	A	807	1,4	14,14,15	0.60	0	15,19,21	0.97	1 (6%)
4	NAG	A	808	4	14,14,15	0.54	0	15,19,21	1.52	1 (6%)
4	NAG	B	802	1,4	14,14,15	0.75	1 (7%)	15,19,21	1.12	1 (6%)
4	NAG	B	803	4	14,14,15	0.53	0	15,19,21	0.76	0
5	NAG	B	804	1,5	14,14,15	0.71	0	15,19,21	0.98	1 (6%)
5	NAG	B	805	5	14,14,15	0.63	0	15,19,21	0.73	0
5	BMA	B	806	5	11,11,12	0.52	0	14,15,17	1.39	1 (7%)
4	NAG	B	807	1,4	14,14,15	0.62	0	15,19,21	1.56	4 (26%)
4	NAG	B	808	4	14,14,15	0.45	0	15,19,21	1.63	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	803	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	804	3	-	0/6/23/26	0/1/1/1
3	BMA	A	805	3	-	0/2/19/22	0/1/1/1
3	MAN	A	806	3	-	0/2/19/22	1/1/1/1
4	NAG	A	807	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	808	4	-	2/6/23/26	0/1/1/1
4	NAG	B	802	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	803	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	804	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	805	5	-	0/6/23/26	0/1/1/1
5	BMA	B	806	5	-	0/2/19/22	0/1/1/1
4	NAG	B	807	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	808	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	NAG	C1-C2	2.07	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	805	BMA	C1-C2-C3	-8.47	99.52	109.54
3	A	803	NAG	C2-N2-C7	-5.89	115.47	123.04
4	B	807	NAG	C4-C3-C2	-2.50	107.34	111.23
5	B	804	NAG	C2-N2-C7	-2.26	120.14	123.04
3	A	806	MAN	C2-C3-C4	-2.21	107.29	111.04
4	B	807	NAG	C3-C4-C5	-2.05	106.63	110.20
3	A	805	BMA	O3-C3-C4	2.01	114.87	110.34
4	B	807	NAG	O3-C3-C4	2.08	115.01	110.34
3	A	806	MAN	O5-C5-C6	2.18	112.06	107.35
3	A	803	NAG	C1-O5-C5	2.24	115.09	112.25
4	B	802	NAG	C3-C4-C5	2.24	114.11	110.20
3	A	805	BMA	O2-C2-C1	2.31	113.84	109.21
3	A	804	NAG	C3-C4-C5	2.34	114.27	110.20
4	A	807	NAG	C1-O5-C5	2.69	115.66	112.25
4	B	807	NAG	O4-C4-C3	2.80	116.65	110.34
3	A	805	BMA	C1-O5-C5	3.21	116.32	112.25
3	A	804	NAG	C1-O5-C5	3.61	116.83	112.25
3	A	805	BMA	C3-C4-C5	3.81	116.84	110.20
5	B	806	BMA	C1-O5-C5	4.29	117.69	112.25
3	A	806	MAN	C1-O5-C5	4.33	117.74	112.25
4	A	808	NAG	C1-O5-C5	4.88	118.44	112.25
4	B	808	NAG	C1-O5-C5	5.63	119.40	112.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	808	NAG	C8-C7-N2-C2
4	B	802	NAG	C8-C7-N2-C2
4	B	802	NAG	O7-C7-N2-C2
4	A	808	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	806	MAN	C1-C2-C3-C4-C5-O5

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	NAG	2	0
3	A	804	NAG	2	0
3	A	805	BMA	1	0
3	A	806	MAN	1	0
4	A	807	NAG	4	0
4	A	808	NAG	4	0
4	B	802	NAG	3	0
5	B	804	NAG	3	0
5	B	805	NAG	3	0
5	B	806	BMA	1	0
4	B	807	NAG	4	0
4	B	808	NAG	4	0

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	NAG	A	801	1	14,14,15	0.62	0	15,19,21	0.90	0
2	NAG	A	802	1	14,14,15	0.55	0	15,19,21	1.46	3 (20%)
2	NAG	B	801	1	14,14,15	0.41	0	15,19,21	1.93	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	809	1	14,14,15	0.59	0	15,19,21	1.50	3 (20%)

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	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1	-	2/6/23/26	0/1/1/1
2	NAG	B	809	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	809	NAG	C6-C5-C4	-3.36	104.74	113.02
2	A	802	NAG	C3-C2-N2	2.22	115.89	110.56
2	B	801	NAG	C2-N2-C7	2.27	125.95	123.04
2	A	802	NAG	O5-C5-C6	2.30	112.33	107.35
2	B	809	NAG	C3-C4-C5	2.45	114.47	110.20
2	B	809	NAG	C1-O5-C5	3.01	116.07	112.25
2	A	802	NAG	C2-N2-C7	3.49	127.53	123.04
2	B	801	NAG	C1-O5-C5	6.58	120.59	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	NAG	C8-C7-N2-C2
2	B	801	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	1	0
2	B	809	NAG	6	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	717/719 (99%)	0.24	18 (2%) 61 55	33, 69, 138, 251	19 (2%)
1	B	719/719 (100%)	0.28	15 (2%) 67 61	32, 67, 129, 227	11 (1%)
All	All	1436/1438 (99%)	0.26	33 (2%) 64 58	32, 68, 131, 251	30 (2%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	GLN	6.3
1	A	411	GLU	4.9
1	B	716	GLU	4.8
1	B	65	SER	4.6
1	A	408	SER	4.5
1	B	512	TYR	3.9
1	B	513	PHE	3.6
1	A	410	SER	3.6
1	B	406	ILE	3.4
1	A	406	ILE	3.4
1	B	382	SER	3.2
1	A	78	ASP	3.2
1	A	512	TYR	3.1
1	A	780	CYS	2.9
1	B	184	ALA	2.8
1	A	412	GLN	2.6
1	A	513	PHE	2.4
1	B	698	GLU	2.4
1	A	109	GLU	2.4
1	A	708	LEU	2.4
1	A	82	HIS	2.3
1	A	125	PHE	2.2
1	A	473	GLU	2.2
1	B	379	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	407	GLN	2.2
1	B	663	SER	2.1
1	B	530	ILE	2.1
1	A	524	ALA	2.1
1	B	529	LYS	2.1
1	A	525	ILE	2.1
1	B	125	PHE	2.1
1	B	414	THR	2.1
1	A	121	THR	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
4	NAG	B	807	14/15	0.93	0.22	0.68	71,71,71,71	0
5	NAG	B	804	14/15	0.87	0.26	-0.03	83,83,83,83	0
4	NAG	A	807	14/15	0.92	0.21	-0.41	77,77,77,77	0
3	NAG	A	803	14/15	0.92	0.15	-1.90	74,74,74,74	0
3	MAN	A	806	11/12	0.72	0.28	-	113,113,113,113	0
4	NAG	B	803	14/15	0.80	0.34	-	128,128,128,128	0
3	BMA	A	805	11/12	0.83	0.22	-	135,135,135,135	0
5	NAG	B	805	14/15	0.87	0.31	-	113,113,113,113	0
5	BMA	B	806	11/12	0.81	0.24	-	127,127,127,127	0
4	NAG	B	802	14/15	0.93	0.19	-	69,69,69,69	0
4	NAG	A	808	14/15	0.73	0.27	-	131,131,131,131	0
4	NAG	B	808	14/15	0.84	0.26	-	128,128,128,128	0
3	NAG	A	804	14/15	0.88	0.20	-	88,88,88,88	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(Å ²)	Q<0.9
2	NAG	A	801	14/15	0.83	0.27	-	109,109,109,109	0
2	NAG	A	802	14/15	0.89	0.26	-	84,84,84,84	0
2	NAG	B	809	14/15	0.73	0.48	-	189,189,189,189	0
2	NAG	B	801	14/15	0.84	0.25	-	106,106,106,106	0

6.5 Other polymers [i](#)

There are no such residues in this entry.