



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:41 PM UTC

PDB ID : 5LG6 / pdb_00005lg6
Title : Structure of the deglycosylated porcine aminopeptidase N ectodomain
Authors : Santiago, C.; Reguera, J.; Mudgal, G.; Casasnovas, J.M.
Deposited on : 2016-07-06
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

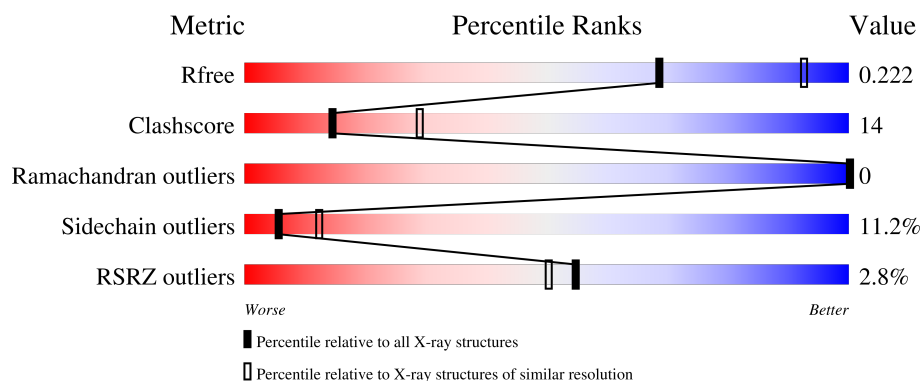
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	968	
1	B	968	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14927 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	889	Total	C	N	O	S	Se	0	0	0
			7154	4578	1190	1356	6	24			
1	B	887	Total	C	N	O	S	Se	0	0	0
			7138	4564	1188	1356	6	24			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	TYR	-	expression tag	UNP P15145
A	20	PRO	-	expression tag	UNP P15145
A	21	TYR	-	expression tag	UNP P15145
A	22	ASP	-	expression tag	UNP P15145
A	23	VAL	-	expression tag	UNP P15145
A	24	PRO	-	expression tag	UNP P15145
A	25	ASP	-	expression tag	UNP P15145
A	26	TYR	-	expression tag	UNP P15145
A	27	ALA	-	expression tag	UNP P15145
A	28	GLY	-	expression tag	UNP P15145
A	29	ALA	-	expression tag	UNP P15145
A	30	GLN	-	expression tag	UNP P15145
A	31	PRO	-	expression tag	UNP P15145
A	32	ALA	-	expression tag	UNP P15145
A	33	ARG	-	expression tag	UNP P15145
A	34	SER	-	expression tag	UNP P15145
A	35	PRO	-	expression tag	UNP P15145
A	107	PHE	LEU	conflict	UNP P15145
A	108	ILE	LEU	conflict	UNP P15145
A	964	VAL	-	expression tag	UNP P15145
A	965	LEU	-	expression tag	UNP P15145
A	966	ASN	-	expression tag	UNP P15145
A	967	TRP	-	expression tag	UNP P15145
A	968	PHE	-	expression tag	UNP P15145
A	969	ILE	-	expression tag	UNP P15145

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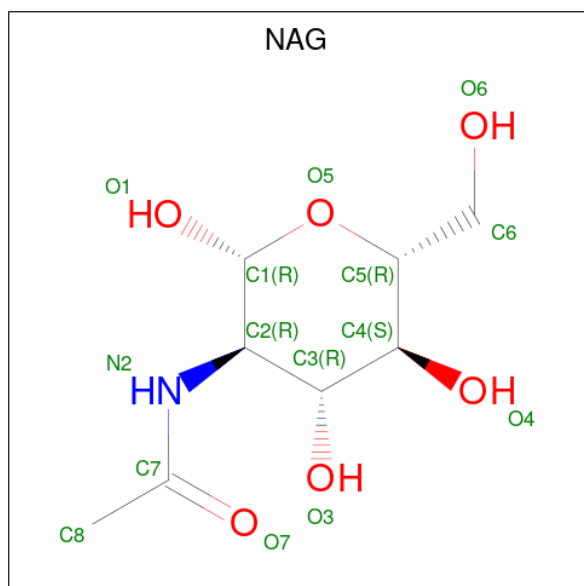
Chain	Residue	Modelled	Actual	Comment	Reference
A	970	GLU	-	expression tag	UNP P15145
A	971	HIS	-	expression tag	UNP P15145
A	972	SER	-	expression tag	UNP P15145
A	973	LEU	-	expression tag	UNP P15145
A	974	VAL	-	expression tag	UNP P15145
A	975	PRO	-	expression tag	UNP P15145
A	976	ARG	-	expression tag	UNP P15145
A	977	GLY	-	expression tag	UNP P15145
A	978	SER	-	expression tag	UNP P15145
A	979	ASP	-	expression tag	UNP P15145
A	980	TYR	-	expression tag	UNP P15145
A	981	LYS	-	expression tag	UNP P15145
A	982	ASP	-	expression tag	UNP P15145
A	983	ASP	-	expression tag	UNP P15145
A	984	ASP	-	expression tag	UNP P15145
A	985	ASP	-	expression tag	UNP P15145
A	986	LYS	-	expression tag	UNP P15145
B	19	TYR	-	expression tag	UNP P15145
B	20	PRO	-	expression tag	UNP P15145
B	21	TYR	-	expression tag	UNP P15145
B	22	ASP	-	expression tag	UNP P15145
B	23	VAL	-	expression tag	UNP P15145
B	24	PRO	-	expression tag	UNP P15145
B	25	ASP	-	expression tag	UNP P15145
B	26	TYR	-	expression tag	UNP P15145
B	27	ALA	-	expression tag	UNP P15145
B	28	GLY	-	expression tag	UNP P15145
B	29	ALA	-	expression tag	UNP P15145
B	30	GLN	-	expression tag	UNP P15145
B	31	PRO	-	expression tag	UNP P15145
B	32	ALA	-	expression tag	UNP P15145
B	33	ARG	-	expression tag	UNP P15145
B	34	SER	-	expression tag	UNP P15145
B	35	PRO	-	expression tag	UNP P15145
B	107	PHE	LEU	conflict	UNP P15145
B	108	ILE	LEU	conflict	UNP P15145
B	964	VAL	-	expression tag	UNP P15145
B	965	LEU	-	expression tag	UNP P15145
B	966	ASN	-	expression tag	UNP P15145
B	967	TRP	-	expression tag	UNP P15145
B	968	PHE	-	expression tag	UNP P15145
B	969	ILE	-	expression tag	UNP P15145

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Chain	Residue	Modelled	Actual	Comment	Reference
B	970	GLU	-	expression tag	UNP P15145
B	971	HIS	-	expression tag	UNP P15145
B	972	SER	-	expression tag	UNP P15145
B	973	LEU	-	expression tag	UNP P15145
B	974	VAL	-	expression tag	UNP P15145
B	975	PRO	-	expression tag	UNP P15145
B	976	ARG	-	expression tag	UNP P15145
B	977	GLY	-	expression tag	UNP P15145
B	978	SER	-	expression tag	UNP P15145
B	979	ASP	-	expression tag	UNP P15145
B	980	TYR	-	expression tag	UNP P15145
B	981	LYS	-	expression tag	UNP P15145
B	982	ASP	-	expression tag	UNP P15145
B	983	ASP	-	expression tag	UNP P15145
B	984	ASP	-	expression tag	UNP P15145
B	985	ASP	-	expression tag	UNP P15145
B	986	LYS	-	expression tag	UNP P15145

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		

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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	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	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		
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		
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		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	216	Total 216	O 216	0	0
4	B	165	Total 165	O 165	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.47Å 215.69Å 78.63Å 90.00° 91.90° 90.00°	Depositor
Resolution (Å)	24.98 – 2.50 24.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (24.98-2.50) 93.7 (24.98-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.50Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.191 , 0.229 0.185 , 0.222	Depositor DCC
R_{free} test set	1989 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14927	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NAG, ZN

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	0.56	0/7315	0.90	19/9929 (0.2%)
1	B	0.55	2/7298 (0.0%)	0.89	17/9906 (0.2%)
All	All	0.55	2/14613 (0.0%)	0.90	36/19835 (0.2%)

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	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	350	GLU	CG-CD	-5.44	1.38	1.52
1	B	351	ASN	CG-ND2	-5.15	1.22	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ASP	N-CA-C	8.59	121.72	111.33
1	A	140	SER	N-CA-C	-8.02	96.16	109.07
1	B	331	TYR	CA-C-N	7.23	126.86	119.19
1	B	331	TYR	C-N-CA	7.23	126.86	119.19
1	A	331	TYR	CA-C-N	7.10	126.72	119.19
1	A	331	TYR	C-N-CA	7.10	126.72	119.19
1	B	350	GLU	N-CA-C	6.79	121.01	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	909	GLU	CA-CB-CG	6.62	127.35	114.10
1	A	183	ASP	CA-C-N	6.58	129.40	120.38
1	A	183	ASP	C-N-CA	6.58	129.40	120.38
1	B	210	THR	N-CA-C	6.57	120.60	112.59
1	A	909	GLU	CA-CB-CG	6.39	126.88	114.10
1	A	210	THR	CB-CA-C	-6.22	102.50	111.70
1	B	706	PHE	N-CA-C	6.10	120.89	113.38
1	A	706	PHE	N-CA-C	5.96	120.71	113.38
1	A	350	GLU	N-CA-C	5.95	119.59	112.93
1	B	245	PRO	CA-C-N	5.81	125.75	119.76
1	B	245	PRO	C-N-CA	5.81	125.75	119.76
1	B	92	ASN	CA-C-N	-5.73	114.10	122.06
1	B	92	ASN	C-N-CA	-5.73	114.10	122.06
1	A	256	ASP	CA-C-N	5.68	125.38	119.82
1	A	256	ASP	C-N-CA	5.68	125.38	119.82
1	A	183	ASP	N-CA-C	-5.61	106.75	113.21
1	B	819	VAL	CB-CA-C	-5.61	103.17	112.26
1	B	256	ASP	CA-C-N	5.55	125.26	119.82
1	B	256	ASP	C-N-CA	5.55	125.26	119.82
1	A	892	SER	N-CA-C	5.54	117.40	110.91
1	A	341	LEU	CA-C-N	5.43	125.26	119.28
1	A	341	LEU	C-N-CA	5.43	125.26	119.28
1	A	881	TRP	N-CA-C	5.41	117.61	111.11
1	B	183	ASP	N-CA-C	-5.32	107.09	113.21
1	A	893	PHE	N-CA-C	5.11	121.68	110.80
1	B	184	ASP	N-CA-C	5.08	121.61	110.80
1	B	601	VAL	N-CA-C	-5.04	101.60	108.06
1	B	350	GLU	CB-CA-C	-5.03	101.81	110.72
1	A	584	ILE	N-CA-C	5.01	115.66	107.24

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ASP	Peptide
1	A	93	ALA	Peptide
1	B	574	SER	Peptide
1	B	93	ALA	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	7154	0	6924	192	1
1	B	7138	0	6904	202	1
2	A	126	0	117	5	0
2	B	126	0	117	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	216	0	0	3	0
4	B	165	0	0	10	0
All	All	14927	0	14062	400	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (400) 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:542:GLN:NE2	1:A:576:PHE:HB2	1.58	1.17
1:B:947:TRP:O	1:B:951:ASN:ND2	1.81	1.14
1:A:947:TRP:O	1:A:951:ASN:ND2	1.84	1.08
1:B:187:GLY:HA2	1:B:207:MSE:HE1	1.34	1.06
1:A:187:GLY:HA2	1:A:207:MSE:HE1	1.35	1.05
1:A:140:SER:HB3	1:A:169:HIS:HD2	1.26	1.01
1:A:542:GLN:HE21	1:A:576:PHE:HB2	1.20	0.97
1:A:636:TRP:HZ3	1:A:658:VAL:HG23	1.30	0.95
1:B:636:TRP:HZ3	1:B:658:VAL:HG23	1.32	0.94
1:B:187:GLY:HA2	1:B:207:MSE:CE	2.02	0.89
1:A:191:SER:HB3	1:A:202:LEU:HD22	1.58	0.86
1:B:680:THR:HG22	1:B:718:TYR:OH	1.77	0.85
1:B:191:SER:HB3	1:B:202:LEU:CD2	2.06	0.85
1:B:637:ARG:HG3	1:B:637:ARG:HH11	1.42	0.85
1:A:680:THR:HG22	1:A:718:TYR:OH	1.77	0.85
1:A:187:GLY:HA2	1:A:207:MSE:CE	2.06	0.84
1:A:191:SER:HB3	1:A:202:LEU:CD2	2.06	0.84
1:B:132:VAL:HG11	1:B:173:MSE:HE3	1.62	0.82
1:B:270:MSE:HE1	1:B:275:LEU:HD23	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:GLU:OE2	4:A:1101:HOH:O	1.99	0.80
1:A:132:VAL:HG11	1:A:173:MSE:HE3	1.62	0.80
1:A:178:GLN:OE1	2:A:1001:NAG:H81	1.81	0.80
1:B:574:SER:HA	1:B:575:ALA:HB3	1.65	0.79
1:B:888:TYR:OH	4:B:1101:HOH:O	2.00	0.79
1:B:796:ASN:OD1	1:B:800:GLN:NE2	2.17	0.78
1:A:140:SER:HB3	1:A:169:HIS:CD2	2.16	0.78
1:B:734:THR:HG23	1:B:737:TRP:H	1.47	0.77
1:A:637:ARG:HG3	1:A:637:ARG:HH11	1.47	0.77
1:A:796:ASN:OD1	1:A:800:GLN:NE2	2.17	0.76
1:A:270:MSE:HE1	1:A:275:LEU:HD23	1.65	0.76
1:B:61:LEU:HD21	1:B:153:LEU:HD13	1.68	0.75
1:B:191:SER:HB3	1:B:202:LEU:HD22	1.67	0.75
1:A:734:THR:HG23	1:A:737:TRP:H	1.49	0.75
1:B:80:SER:OG	1:B:227:THR:HG22	1.89	0.73
1:B:202:LEU:HD23	1:B:202:LEU:C	2.14	0.73
1:A:154:THR:HG23	1:A:156:TYR:CD2	2.24	0.72
2:B:1002:NAG:H81	2:B:1009:NAG:HN2	1.54	0.72
1:A:80:SER:OG	1:A:227:THR:HG22	1.89	0.71
1:A:158:VAL:HG12	1:A:160:HIS:CD2	2.26	0.71
1:B:154:THR:HG23	1:B:156:TYR:CD2	2.24	0.71
1:A:202:LEU:C	1:A:202:LEU:HD23	2.16	0.71
1:B:192:GLU:O	1:B:852:ARG:NH2	2.23	0.71
1:A:887:ASP:HB2	1:A:888:TYR:CD2	2.26	0.70
1:A:192:GLU:O	1:A:852:ARG:NH2	2.24	0.70
1:B:887:ASP:HB2	1:B:888:TYR:CD2	2.27	0.70
1:A:108:ILE:HB	1:A:170:MSE:HE3	1.76	0.68
1:A:480:ARG:NH2	1:A:623:VAL:O	2.26	0.68
1:B:108:ILE:HB	1:B:170:MSE:HE3	1.75	0.67
1:B:367:GLN:OE1	1:B:367:GLN:HA	1.93	0.67
1:B:408:PHE:O	1:B:412:VAL:HG22	1.95	0.67
1:B:80:SER:HG	1:B:227:THR:HG22	1.59	0.67
1:A:587:ILE:HG22	1:A:618:LEU:HB2	1.78	0.66
1:B:538:ARG:HG2	1:B:576:PHE:HD2	1.60	0.66
1:B:734:THR:HG23	1:B:737:TRP:N	2.10	0.66
1:A:367:GLN:HA	1:A:367:GLN:OE1	1.95	0.66
1:A:734:THR:HG23	1:A:737:TRP:N	2.10	0.66
2:A:1002:NAG:H81	2:A:1009:NAG:HN2	1.60	0.66
1:B:480:ARG:NH2	1:B:623:VAL:O	2.28	0.66
1:A:547:VAL:HG11	1:A:670:MSE:HE1	1.76	0.66
1:B:662:SER:OG	1:B:679:ASN:ND2	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:SER:OG	1:A:679:ASN:ND2	2.28	0.65
1:A:182:ALA:HB3	1:A:184:ASP:HB2	1.79	0.65
1:B:547:VAL:HG11	1:B:670:MSE:HE1	1.79	0.65
1:A:734:THR:HG23	1:A:737:TRP:HA	1.78	0.64
1:B:574:SER:O	1:B:574:SER:OG	2.12	0.64
1:B:637:ARG:HG3	1:B:637:ARG:NH1	2.10	0.64
1:A:880:ASN:N	1:A:880:ASN:HD22	1.96	0.64
1:A:946:LYS:HA	1:A:949:LYS:HE2	1.79	0.63
1:A:439:MSE:HE3	1:A:626:TYR:CD1	2.33	0.63
1:B:946:LYS:HA	1:B:949:LYS:HE2	1.81	0.63
1:B:937:ALA:O	1:B:941:THR:OG1	2.15	0.63
1:A:408:PHE:O	1:A:412:VAL:HG22	1.99	0.63
1:B:182:ALA:HB3	1:B:184:ASP:HB2	1.80	0.63
1:B:587:ILE:HG22	1:B:618:LEU:HB2	1.80	0.63
1:A:937:ALA:O	1:A:941:THR:OG1	2.16	0.62
1:A:636:TRP:CZ3	1:A:658:VAL:HG23	2.22	0.62
1:A:737:TRP:CH2	1:A:754:ILE:HD11	2.34	0.62
1:B:118:ILE:CD1	1:B:157:LEU:HD23	2.30	0.62
1:A:717:LYS:HG2	1:A:963:SER:HB2	1.81	0.62
1:A:67:TRP:O	1:A:154:THR:HG21	1.99	0.62
1:A:80:SER:HG	1:A:227:THR:HG22	1.64	0.61
1:A:637:ARG:HG3	1:A:637:ARG:NH1	2.15	0.61
1:A:118:ILE:HD12	1:A:157:LEU:HB3	1.83	0.61
1:B:118:ILE:HD11	1:B:157:LEU:HD23	1.83	0.61
1:B:118:ILE:HD12	1:B:157:LEU:HB3	1.83	0.61
1:B:538:ARG:CG	1:B:576:PHE:HD2	2.14	0.61
1:A:552:THR:HB	1:A:632:ASP:OD1	2.01	0.61
1:A:734:THR:HG21	1:A:737:TRP:CE3	2.36	0.61
1:B:623:VAL:O	1:B:623:VAL:HG12	1.99	0.61
1:B:191:SER:HB3	1:B:202:LEU:HD21	1.81	0.61
1:B:247:LYS:HD3	4:B:1115:HOH:O	2.00	0.61
1:A:118:ILE:CD1	1:A:157:LEU:HD23	2.31	0.61
1:A:754:ILE:HG22	1:A:792:THR:HG21	1.83	0.60
1:B:445:ALA:HB2	1:B:565:ASP:OD1	2.01	0.60
1:B:574:SER:HA	1:B:575:ALA:CB	2.30	0.60
1:A:210:THR:O	1:A:210:THR:OG1	2.12	0.60
1:B:737:TRP:CH2	1:B:754:ILE:HD11	2.36	0.60
1:B:67:TRP:O	1:B:154:THR:HG21	2.01	0.60
1:B:147:ARG:CZ	1:B:160:HIS:ND1	2.64	0.60
2:B:1002:NAG:C8	2:B:1009:NAG:HN2	2.13	0.59
1:B:717:LYS:HG2	1:B:963:SER:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASN:ND2	1:A:351:ASN:H	1.98	0.59
1:A:623:VAL:O	1:A:623:VAL:HG12	2.02	0.59
1:B:734:THR:HG23	1:B:737:TRP:HA	1.85	0.59
1:A:542:GLN:NE2	1:A:576:PHE:CB	2.50	0.59
1:B:734:THR:CG2	1:B:737:TRP:H	2.15	0.59
1:A:207:MSE:HE2	1:A:207:MSE:HA	1.85	0.58
1:A:375:GLU:HG2	1:A:748:TYR:OH	2.03	0.58
1:B:61:LEU:HB3	1:B:68:ASN:HB3	1.85	0.58
1:A:834:GLU:HG3	1:A:837:LEU:HD12	1.86	0.58
1:A:734:THR:HG23	1:A:737:TRP:CA	2.33	0.58
1:A:61:LEU:HB3	1:A:68:ASN:HB3	1.85	0.58
1:B:677:LEU:HB3	1:B:958:TRP:CE2	2.38	0.58
1:B:158:VAL:HG12	1:B:160:HIS:CD2	2.39	0.58
1:A:677:LEU:HB3	1:A:958:TRP:CE2	2.39	0.57
1:A:677:LEU:HB3	1:A:958:TRP:CZ2	2.38	0.57
1:B:880:ASN:N	1:B:880:ASN:HD22	2.01	0.57
1:A:542:GLN:HE22	1:A:576:PHE:HB2	1.63	0.57
1:A:677:LEU:O	1:A:680:THR:HB	2.05	0.57
1:B:754:ILE:HG22	1:B:792:THR:HG21	1.85	0.57
1:B:538:ARG:HG2	1:B:576:PHE:CD2	2.39	0.57
1:B:723:VAL:HG21	1:B:756:THR:CG2	2.35	0.57
1:A:734:THR:CG2	1:A:737:TRP:HA	2.35	0.57
1:A:207:MSE:CE	1:A:207:MSE:HA	2.34	0.57
1:A:734:THR:CG2	1:A:737:TRP:H	2.18	0.56
1:B:734:THR:HG21	1:B:737:TRP:CE3	2.39	0.56
1:B:552:THR:HB	1:B:632:ASP:OD1	2.05	0.56
1:A:131:MSE:HE2	1:A:148:THR:OG1	2.05	0.56
1:A:396:LEU:HD23	1:A:402:LEU:HA	1.87	0.56
1:B:178:GLN:OE1	2:B:1001:NAG:H81	2.05	0.56
1:B:286:ASN:ND2	4:B:1104:HOH:O	2.27	0.56
1:B:439:MSE:HE3	1:B:626:TYR:CD1	2.40	0.56
1:B:818:LEU:HD13	1:B:820:ASN:HB2	1.86	0.56
1:A:587:ILE:HD12	1:A:592:MSE:HA	1.88	0.56
1:B:523:GLN:OE1	1:B:526:ILE:HG12	2.04	0.56
1:B:834:GLU:HG3	1:B:837:LEU:HD12	1.87	0.56
1:B:147:ARG:NH2	1:B:160:HIS:CE1	2.74	0.56
1:B:538:ARG:CG	1:B:576:PHE:CD2	2.89	0.56
1:A:118:ILE:HD11	1:A:157:LEU:HD23	1.87	0.56
1:B:349:MSE:HG3	1:B:351:ASN:HD21	1.70	0.56
1:B:396:LEU:HD23	1:B:402:LEU:HA	1.88	0.56
1:A:63:GLN:HB3	1:A:69:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:LEU:HB3	1:B:958:TRP:CZ2	2.41	0.55
1:A:65:LYS:HD2	1:A:67:TRP:CZ2	2.42	0.55
1:A:154:THR:CG2	1:A:156:TYR:CD2	2.90	0.55
1:B:131:MSE:O	1:B:132:VAL:HG23	2.06	0.55
1:A:206:GLN:O	1:A:207:MSE:HE3	2.06	0.55
1:B:636:TRP:CZ3	1:B:658:VAL:HG23	2.25	0.55
1:B:662:SER:HB3	1:B:676:ALA:HA	1.89	0.55
1:B:154:THR:CG2	1:B:156:TYR:CD2	2.89	0.55
1:B:881:TRP:CH2	1:B:895:PHE:CZ	2.95	0.55
1:B:207:MSE:HA	1:B:207:MSE:HE2	1.88	0.54
1:B:207:MSE:CE	1:B:207:MSE:HA	2.36	0.54
1:B:131:MSE:HE2	1:B:148:THR:OG1	2.07	0.54
1:B:734:THR:HG23	1:B:737:TRP:CA	2.37	0.54
1:B:552:THR:HG23	1:B:611:THR:OG1	2.08	0.54
1:B:730:PHE:O	1:B:734:THR:HB	2.07	0.54
1:B:63:GLN:HB3	1:B:69:ARG:HD2	1.89	0.54
1:B:375:GLU:HG2	1:B:748:TYR:OH	2.07	0.54
1:A:85:LEU:HD13	1:A:277:TYR:CE2	2.43	0.54
1:B:373:ASN:HB3	4:B:1193:HOH:O	2.08	0.54
1:B:478:VAL:CG1	1:B:536:MSE:HE1	2.37	0.54
1:B:585:SER:HB3	1:B:592:MSE:HE1	1.90	0.53
1:A:61:LEU:HD21	1:A:153:LEU:HD23	1.89	0.53
1:A:737:TRP:CZ3	1:A:754:ILE:HD11	2.43	0.53
1:B:406:GLU:HA	1:B:406:GLU:OE1	2.08	0.53
1:B:587:ILE:HD12	1:B:592:MSE:HA	1.89	0.53
1:A:478:VAL:CG1	1:A:536:MSE:HE1	2.38	0.53
1:B:396:LEU:CD2	1:B:402:LEU:HA	2.39	0.53
1:A:206:GLN:C	1:A:207:MSE:HE3	2.34	0.53
1:A:552:THR:HG23	1:A:611:THR:OG1	2.07	0.53
1:A:845:THR:HG21	1:A:860:ILE:HD11	1.89	0.53
1:B:734:THR:CG2	1:B:737:TRP:HA	2.39	0.53
1:A:723:VAL:HG21	1:A:756:THR:CG2	2.39	0.53
1:B:273:TYR:CD1	1:B:274:LEU:HD13	2.44	0.53
1:A:182:ALA:C	1:A:184:ASP:H	2.15	0.53
1:B:677:LEU:O	1:B:680:THR:HB	2.09	0.53
1:B:575:ALA:C	1:B:576:PHE:HD1	2.16	0.52
1:A:159:VAL:HG21	1:A:173:MSE:CE	2.39	0.52
1:A:662:SER:HB3	1:A:676:ALA:HA	1.91	0.52
1:A:237:ASN:HD22	2:A:1003:NAG:H83	1.75	0.52
1:B:63:GLN:O	1:B:69:ARG:NH1	2.33	0.52
1:A:523:GLN:OE1	1:A:526:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD23	1:A:202:LEU:O	2.09	0.52
1:B:65:LYS:HD2	1:B:67:TRP:CZ2	2.44	0.52
1:B:202:LEU:HD23	1:B:202:LEU:O	2.09	0.52
1:A:730:PHE:O	1:A:734:THR:HB	2.09	0.52
1:B:187:GLY:CA	1:B:207:MSE:HE1	2.25	0.52
1:B:159:VAL:HG21	1:B:173:MSE:CE	2.40	0.52
1:A:474:LYS:HE3	1:A:626:TYR:CE2	2.45	0.52
1:B:206:GLN:O	1:B:207:MSE:HE3	2.09	0.52
1:B:182:ALA:C	1:B:184:ASP:H	2.18	0.51
1:A:818:LEU:HD13	1:A:820:ASN:HB2	1.90	0.51
1:A:396:LEU:CD2	1:A:402:LEU:HA	2.40	0.51
1:A:842:LEU:O	1:A:845:THR:HB	2.10	0.51
1:A:80:SER:CB	1:A:227:THR:HG22	2.41	0.51
1:B:85:LEU:HD13	1:B:277:TYR:CE2	2.46	0.51
1:B:349:MSE:HG3	1:B:351:ASN:ND2	2.26	0.51
1:A:270:MSE:HG3	1:A:352:TRP:HE3	1.77	0.50
1:A:284:SER:HA	1:A:297:ILE:O	2.11	0.50
1:B:237:ASN:HD22	2:B:1003:NAG:H83	1.76	0.50
1:A:680:THR:CG2	1:A:718:TYR:OH	2.54	0.50
1:B:845:THR:HG21	1:B:860:ILE:HD11	1.93	0.50
1:B:375:GLU:HG3	1:B:376:ARG:N	2.25	0.50
1:B:888:TYR:CD2	1:B:888:TYR:N	2.80	0.50
1:A:131:MSE:O	1:A:132:VAL:HG23	2.12	0.50
1:B:737:TRP:CZ3	1:B:754:ILE:HD11	2.46	0.50
1:B:270:MSE:HG3	1:B:352:TRP:HE3	1.75	0.50
1:B:906:PHE:HB2	1:B:941:THR:HG23	1.92	0.50
1:A:396:LEU:HD12	1:A:396:LEU:O	2.11	0.50
1:A:887:ASP:HB2	1:A:888:TYR:CE2	2.47	0.50
1:A:137:VAL:HG13	1:A:137:VAL:O	2.11	0.49
1:A:888:TYR:CD2	1:A:888:TYR:N	2.79	0.49
1:B:80:SER:CB	1:B:227:THR:HG22	2.42	0.49
1:B:206:GLN:HG3	4:B:1192:HOH:O	2.11	0.49
1:A:375:GLU:HG3	1:A:376:ARG:N	2.26	0.49
1:A:900:GLN:O	1:A:904:ARG:HG3	2.12	0.49
1:A:401:ASP:HB2	4:A:1128:HOH:O	2.13	0.49
1:A:881:TRP:CH2	1:A:895:PHE:CZ	3.01	0.49
1:A:906:PHE:HB2	1:A:941:THR:HG23	1.93	0.49
1:A:273:TYR:CD1	1:A:274:LEU:HD13	2.48	0.49
1:B:62:ASP:OD1	1:B:64:SER:OG	2.27	0.49
1:B:351:ASN:HB2	1:B:354:LEU:O	2.12	0.49
1:B:887:ASP:HB2	1:B:888:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ASN:OD1	1:B:96:LEU:CB	2.61	0.48
1:B:386:ALA:HB1	1:B:412:VAL:CG2	2.42	0.48
1:A:62:ASP:OD1	1:A:64:SER:OG	2.32	0.48
1:A:947:TRP:CG	1:A:951:ASN:ND2	2.82	0.48
1:B:225:LYS:HE2	4:B:1185:HOH:O	2.13	0.48
1:B:474:LYS:HE3	1:B:626:TYR:CE2	2.48	0.48
1:B:361:ALA:HB1	1:B:380:VAL:HG11	1.95	0.48
1:B:842:LEU:O	1:B:845:THR:HB	2.12	0.48
1:A:322:PHE:HB2	1:A:419:HIS:ND1	2.29	0.48
1:A:386:ALA:HB1	1:A:412:VAL:CG2	2.43	0.48
1:B:706:PHE:HB3	1:B:711:VAL:HB	1.94	0.48
1:A:63:GLN:O	1:A:69:ARG:NH1	2.37	0.48
1:B:137:VAL:HG13	1:B:137:VAL:O	2.13	0.48
1:A:92:ASN:OD1	1:A:96:LEU:CB	2.61	0.48
1:B:386:ALA:HB1	1:B:412:VAL:HG21	1.96	0.48
1:B:322:PHE:HB2	1:B:419:HIS:ND1	2.28	0.48
1:B:680:THR:CG2	1:B:718:TYR:OH	2.54	0.48
1:A:406:GLU:HA	1:A:406:GLU:OE1	2.13	0.48
2:A:1005:NAG:O4	2:B:1008:NAG:C6	2.62	0.48
1:B:273:TYR:CE1	1:B:274:LEU:HD13	2.49	0.48
1:B:445:ALA:HB2	1:B:565:ASP:CG	2.38	0.48
1:A:697:SER:O	1:A:700:SER:HB3	2.14	0.47
1:B:206:GLN:C	1:B:207:MSE:HE3	2.38	0.47
1:B:697:SER:O	1:B:700:SER:HB3	2.14	0.47
1:A:92:ASN:OD1	1:A:96:LEU:HB2	2.14	0.47
1:A:740:ARG:NH1	1:A:750:GLU:OE2	2.47	0.47
2:A:1005:NAG:O4	2:B:1008:NAG:H61	2.13	0.47
1:A:191:SER:HB3	1:A:202:LEU:HD21	1.89	0.47
1:A:491:PHE:CZ	1:A:495:LEU:HD11	2.49	0.47
1:A:952:LYS:HE2	1:A:952:LYS:HB2	1.55	0.47
1:A:286:ASN:HB3	1:A:296:ARG:HG2	1.96	0.47
1:A:361:ALA:HB1	1:A:380:VAL:HG11	1.95	0.47
1:A:364:PHE:CE1	1:A:374:LYS:HB2	2.50	0.47
1:A:386:ALA:HB1	1:A:412:VAL:HG21	1.96	0.47
1:A:439:MSE:HE1	1:A:627:PHE:N	2.30	0.47
1:A:187:GLY:CA	1:A:207:MSE:HE1	2.25	0.47
1:B:287:GLU:HB2	1:B:313:LEU:HD11	1.97	0.47
1:A:131:MSE:HB3	1:A:148:THR:HG21	1.97	0.47
1:A:706:PHE:HB3	1:A:711:VAL:HB	1.96	0.47
1:B:131:MSE:HB3	1:B:148:THR:HG21	1.97	0.46
1:A:204:THR:HG23	1:A:278:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLU:HG3	1:A:387:HIS:HB3	1.98	0.46
1:B:153:LEU:HB2	4:B:1211:HOH:O	2.15	0.46
1:B:286:ASN:HB3	1:B:296:ARG:HG2	1.98	0.46
1:A:270:MSE:HG3	1:A:352:TRP:CE3	2.50	0.46
1:B:823:ASP:OD1	1:B:826:ARG:NH2	2.47	0.46
1:B:270:MSE:HG3	1:B:352:TRP:CE3	2.50	0.46
1:A:526:ILE:HG12	1:A:526:ILE:H	1.66	0.46
1:A:538:ARG:CG	1:A:576:PHE:CD2	2.98	0.46
1:B:538:ARG:O	1:B:542:GLN:HG3	2.15	0.46
1:B:947:TRP:CG	1:B:951:ASN:ND2	2.84	0.46
1:B:80:SER:OG	1:B:227:THR:CG2	2.63	0.46
1:B:953:GLU:HB2	4:B:1172:HOH:O	2.16	0.45
1:A:360:ASN:HB3	1:A:819:VAL:HG13	1.99	0.45
1:B:284:SER:HA	1:B:297:ILE:O	2.16	0.45
1:B:906:PHE:CB	1:B:941:THR:HG23	2.46	0.45
1:A:861:ASN:OD1	1:A:901:GLY:HA3	2.17	0.45
1:A:350:GLU:OE1	1:A:350:GLU:N	2.47	0.45
1:A:509:TYR:CE2	1:A:510:LEU:HG	2.52	0.45
1:B:538:ARG:HG3	1:B:576:PHE:CD2	2.51	0.45
1:A:942:LYS:HE3	1:A:942:LYS:HB2	1.85	0.45
1:A:225:LYS:HE2	4:A:1240:HOH:O	2.17	0.45
1:A:286:ASN:CB	1:A:296:ARG:HG2	2.47	0.45
1:B:92:ASN:OD1	1:B:96:LEU:HB2	2.17	0.45
1:B:396:LEU:HD12	1:B:396:LEU:O	2.16	0.45
1:B:509:TYR:CE2	1:B:510:LEU:HG	2.52	0.45
1:B:947:TRP:CD1	1:B:951:ASN:HD21	2.35	0.45
1:B:947:TRP:CD2	1:B:951:ASN:ND2	2.85	0.45
1:A:238:LEU:CD2	1:A:281:GLU:HG3	2.47	0.44
1:A:497:SER:OG	1:A:515:HIS:ND1	2.47	0.44
1:B:238:LEU:CD2	1:B:281:GLU:HG3	2.47	0.44
1:B:576:PHE:N	1:B:576:PHE:CD1	2.84	0.44
1:A:428:ASP:HB2	1:A:745:MSE:HE1	2.00	0.44
1:A:655:ARG:O	1:A:658:VAL:HG12	2.17	0.44
1:B:374:LYS:HG2	1:B:424:TRP:HH2	1.82	0.44
1:B:439:MSE:HE1	1:B:627:PHE:N	2.32	0.44
1:A:159:VAL:HG21	1:A:173:MSE:HE1	1.99	0.44
1:B:241:LEU:HD22	4:B:1151:HOH:O	2.17	0.44
1:B:238:LEU:HD22	1:B:281:GLU:HG3	1.99	0.44
1:B:561:HIS:HB2	1:B:578:TYR:HB3	1.99	0.44
1:A:160:HIS:CD2	1:A:160:HIS:N	2.85	0.44
1:A:947:TRP:CD2	1:A:951:ASN:ND2	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:723:VAL:HG21	1:B:756:THR:HG21	2.00	0.44
1:B:491:PHE:CZ	1:B:495:LEU:HD11	2.53	0.44
1:B:542:GLN:OE1	1:B:578:TYR:HA	2.17	0.44
1:B:740:ARG:NH1	1:B:750:GLU:OE2	2.50	0.44
1:B:900:GLN:O	1:B:904:ARG:HG3	2.18	0.44
1:B:574:SER:CA	1:B:575:ALA:CB	2.94	0.44
1:A:374:LYS:HG2	1:A:424:TRP:HH2	1.82	0.43
1:A:478:VAL:HG13	1:A:536:MSE:HE1	2.00	0.43
1:A:538:ARG:HG2	1:A:576:PHE:CD2	2.53	0.43
1:A:560:LYS:NZ	1:A:670:MSE:HE3	2.33	0.43
1:B:504:TYR:HA	4:B:1126:HOH:O	2.18	0.43
1:B:426:LEU:O	1:B:427:LYS:C	2.62	0.43
1:A:947:TRP:CD1	1:A:951:ASN:HD21	2.36	0.43
1:B:204:THR:HG23	1:B:278:ILE:HG23	1.99	0.43
1:B:380:VAL:O	1:B:384:GLU:HG2	2.18	0.43
1:B:417:ALA:HB1	1:B:426:LEU:HD13	2.00	0.43
1:B:428:ASP:HB2	1:B:745:MSE:HE1	2.01	0.43
1:A:538:ARG:O	1:A:542:GLN:HG3	2.18	0.43
1:B:947:TRP:C	1:B:951:ASN:ND2	2.70	0.43
1:B:286:ASN:CB	1:B:296:ARG:HG2	2.48	0.43
1:A:91:PRO:HD3	1:A:97:TYR:CE1	2.54	0.43
1:A:395:THR:O	1:A:506:ASN:HA	2.18	0.43
1:A:724:GLU:HB3	1:A:725:PRO:HD3	2.00	0.43
1:B:225:LYS:HB3	1:B:269:VAL:HG12	2.01	0.43
1:B:478:VAL:HG13	1:B:536:MSE:HE1	2.01	0.43
1:A:538:ARG:HG2	1:A:576:PHE:HD2	1.84	0.43
1:A:740:ARG:HA	1:A:740:ARG:HD3	1.63	0.43
1:B:351:ASN:ND2	1:B:351:ASN:H	2.15	0.43
1:B:395:THR:O	1:B:506:ASN:HA	2.19	0.43
1:B:526:ILE:HG12	1:B:526:ILE:H	1.62	0.43
1:A:287:GLU:HB2	1:A:313:LEU:HD11	1.99	0.43
1:A:823:ASP:OD1	1:A:826:ARG:NH2	2.47	0.42
1:A:576:PHE:CD1	1:A:576:PHE:N	2.87	0.42
1:A:585:SER:HB3	1:A:592:MSE:HE1	2.01	0.42
1:B:62:ASP:O	1:B:62:ASP:CG	2.61	0.42
1:B:655:ARG:O	1:B:658:VAL:HG12	2.20	0.42
1:B:699:LEU:HD13	1:B:719:LEU:HD21	2.02	0.42
1:A:417:ALA:HB1	1:A:426:LEU:HD13	2.01	0.42
1:B:341:LEU:HA	1:B:342:PRO:HD3	1.83	0.42
1:B:663:PHE:CG	1:B:698:SER:HB3	2.54	0.42
1:B:351:ASN:ND2	1:B:351:ASN:N	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:CD2	1:B:202:LEU:C	2.87	0.42
1:B:724:GLU:HB3	1:B:725:PRO:HD3	2.00	0.42
2:B:1002:NAG:H83	2:B:1009:NAG:C1	2.50	0.42
1:A:538:ARG:CG	1:A:576:PHE:HD2	2.33	0.42
1:A:947:TRP:CG	1:A:951:ASN:HD21	2.38	0.42
1:B:81:TYR:CD1	1:B:105:VAL:HG22	2.54	0.42
1:B:101:GLY:HA3	1:B:177:PHE:CE2	2.54	0.42
1:B:132:VAL:CG1	1:B:133:VAL:N	2.80	0.42
1:A:380:VAL:O	1:A:384:GLU:HG2	2.20	0.41
1:A:689:TYR:CD1	1:A:748:TYR:HB3	2.55	0.41
1:B:386:ALA:CB	1:B:412:VAL:HG23	2.50	0.41
1:B:70:TYR:OH	1:B:153:LEU:HD22	2.20	0.41
1:B:689:TYR:CD1	1:B:748:TYR:HB3	2.55	0.41
1:A:663:PHE:CG	1:A:698:SER:HB3	2.55	0.41
1:A:922:ASN:O	1:A:925:VAL:O	2.38	0.41
1:B:79:ASP:HB2	1:B:170:MSE:HE2	2.02	0.41
1:B:947:TRP:CG	1:B:951:ASN:HD21	2.38	0.41
1:A:132:VAL:HG22	1:A:175:SER:HB3	2.03	0.41
1:A:538:ARG:HG3	1:A:576:PHE:CD2	2.56	0.41
1:A:682:PHE:C	1:A:684:ASN:N	2.78	0.41
1:B:158:VAL:HG11	1:B:160:HIS:HE2	1.85	0.41
1:B:424:TRP:O	1:B:425:ASN:HB2	2.20	0.41
1:B:942:LYS:HE3	1:B:942:LYS:HB2	1.84	0.41
1:A:216:PHE:CE2	1:A:218:CYS:HB3	2.56	0.41
1:A:236:ASN:OD1	1:A:258:ASN:O	2.39	0.41
1:A:375:GLU:O	1:A:379:THR:HB	2.21	0.41
1:B:228:PHE:CD1	1:B:275:LEU:HD11	2.55	0.41
1:A:132:VAL:CG1	1:A:133:VAL:N	2.84	0.41
1:A:386:ALA:CB	1:A:412:VAL:HG23	2.51	0.41
1:A:424:TRP:O	1:A:425:ASN:HB2	2.21	0.41
1:A:455:GLU:H	1:A:455:GLU:CD	2.28	0.41
1:A:699:LEU:HD13	1:A:719:LEU:HD21	2.02	0.41
1:A:884:LEU:HD12	1:A:884:LEU:HA	1.91	0.41
1:A:906:PHE:CB	1:A:941:THR:HG23	2.49	0.41
1:B:236:ASN:OD1	1:B:258:ASN:C	2.64	0.41
1:B:682:PHE:C	1:B:684:ASN:N	2.76	0.41
1:A:411:TYR:OH	1:A:488:GLU:OE1	2.38	0.41
1:A:616:TRP:HB3	1:A:638:MSE:HB3	2.02	0.41
1:A:683:LEU:HD11	1:A:695:ALA:HB2	2.02	0.41
1:A:238:LEU:HD22	1:A:281:GLU:HG3	2.03	0.40
1:A:273:TYR:CE1	1:A:274:LEU:HD13	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:TRP:C	1:A:951:ASN:ND2	2.71	0.40
1:B:922:ASN:O	1:B:925:VAL:O	2.39	0.40
1:A:80:SER:OG	1:A:227:THR:CG2	2.64	0.40
1:B:147:ARG:NH1	1:B:160:HIS:ND1	2.69	0.40
1:A:81:TYR:CD1	1:A:105:VAL:HG22	2.57	0.40
1:B:740:ARG:HA	1:B:740:ARG:HD3	1.61	0.40
1:A:158:VAL:HG12	1:A:160:HIS:HD2	1.78	0.40
1:B:319:ILE:HG22	1:B:385:LEU:HD23	2.03	0.40
1:B:455:GLU:H	1:B:455:GLU:CD	2.29	0.40
1:B:637:ARG:NH1	1:B:637:ARG:CG	2.77	0.40
1:A:77:LEU:HD23	1:A:224:MSE:HE2	2.03	0.40
1:B:560:LYS:NZ	1:B:670:MSE:HE3	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ASP:O	1:B:141:GLN:OE1[1_656]	2.02	0.18

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	881/968 (91%)	850 (96%)	31 (4%)	0	100	100
1	B	879/968 (91%)	848 (96%)	31 (4%)	0	100	100
All	All	1760/1936 (91%)	1698 (96%)	62 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	787/830 (95%)	701 (89%)	86 (11%)	6	13
1	B	786/830 (95%)	696 (88%)	90 (12%)	5	11
All	All	1573/1660 (95%)	1397 (89%)	176 (11%)	6	12

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	60	THR
1	A	62	ASP
1	A	89	LEU
1	A	96	LEU
1	A	118	ILE
1	A	131	MSE
1	A	132	VAL
1	A	134	LEU
1	A	140	SER
1	A	142	VAL
1	A	148	THR
1	A	152	GLU
1	A	154	THR
1	A	165	LEU
1	A	170	MSE
1	A	184	ASP
1	A	197	ASN
1	A	202	LEU
1	A	204	THR
1	A	206	GLN
1	A	207	MSE
1	A	227	THR
1	A	241	LEU
1	A	274	LEU
1	A	277	TYR
1	A	283	GLN

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Mol	Chain	Res	Type
1	A	333	LEU
1	A	351	ASN
1	A	363	LEU
1	A	375	GLU
1	A	378	VAL
1	A	379	THR
1	A	396	LEU
1	A	415	LEU
1	A	437	ARG
1	A	441	VAL
1	A	444	LEU
1	A	455	GLU
1	A	509	TYR
1	A	518	LYS
1	A	523	GLN
1	A	524	THR
1	A	525	SER
1	A	526	ILE
1	A	542	GLN
1	A	552	THR
1	A	560	LYS
1	A	563	LEU
1	A	587	ILE
1	A	588	LYS
1	A	591	VAL
1	A	601	VAL
1	A	605	GLN
1	A	614	ASP
1	A	624	THR
1	A	637	ARG
1	A	667	THR
1	A	677	LEU
1	A	680	THR
1	A	721	LYS
1	A	723	VAL
1	A	734	THR
1	A	740	ARG
1	A	745	MSE
1	A	762	LEU
1	A	818	LEU
1	A	819	VAL
1	A	834	GLU

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Mol	Chain	Res	Type
1	A	845	THR
1	A	857	THR
1	A	868	ILE
1	A	880	ASN
1	A	884	LEU
1	A	886	GLN
1	A	896	SER
1	A	909	GLU
1	A	914	GLN
1	A	915	LEU
1	A	916	GLU
1	A	924	ASP
1	A	940	LYS
1	A	941	THR
1	A	942	LYS
1	A	951	ASN
1	A	952	LYS
1	B	62	ASP
1	B	89	LEU
1	B	96	LEU
1	B	118	ILE
1	B	126	THR
1	B	131	MSE
1	B	132	VAL
1	B	134	LEU
1	B	140	SER
1	B	141	GLN
1	B	142	VAL
1	B	148	THR
1	B	152	GLU
1	B	153	LEU
1	B	154	THR
1	B	165	LEU
1	B	170	MSE
1	B	184	ASP
1	B	197	ASN
1	B	202	LEU
1	B	204	THR
1	B	206	GLN
1	B	207	MSE
1	B	210	THR
1	B	227	THR

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Mol	Chain	Res	Type
1	B	241	LEU
1	B	274	LEU
1	B	283	GLN
1	B	333	LEU
1	B	351	ASN
1	B	363	LEU
1	B	375	GLU
1	B	378	VAL
1	B	379	THR
1	B	385	LEU
1	B	396	LEU
1	B	437	ARG
1	B	441	VAL
1	B	444	LEU
1	B	455	GLU
1	B	509	TYR
1	B	518	LYS
1	B	523	GLN
1	B	524	THR
1	B	525	SER
1	B	526	ILE
1	B	542	GLN
1	B	552	THR
1	B	560	LYS
1	B	563	LEU
1	B	574	SER
1	B	585	SER
1	B	587	ILE
1	B	588	LYS
1	B	591	VAL
1	B	601	VAL
1	B	605	GLN
1	B	614	ASP
1	B	624	THR
1	B	637	ARG
1	B	667	THR
1	B	677	LEU
1	B	680	THR
1	B	721	LYS
1	B	723	VAL
1	B	734	THR
1	B	740	ARG

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Mol	Chain	Res	Type
1	B	745	MSE
1	B	762	LEU
1	B	818	LEU
1	B	819	VAL
1	B	834	GLU
1	B	840	ARG
1	B	845	THR
1	B	857	THR
1	B	880	ASN
1	B	884	LEU
1	B	886	GLN
1	B	888	TYR
1	B	896	SER
1	B	909	GLU
1	B	914	GLN
1	B	915	LEU
1	B	916	GLU
1	B	924	ASP
1	B	940	LYS
1	B	941	THR
1	B	942	LYS
1	B	951	ASN
1	B	952	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	302	ASN
1	A	321	ASN
1	A	351	ASN
1	A	458	ASN
1	A	542	GLN
1	A	641	HIS
1	A	743	ASN
1	A	775	GLN
1	A	814	GLN
1	A	880	ASN
1	A	897	ASN
1	B	302	ASN
1	B	351	ASN
1	B	556	ASN

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Mol	Chain	Res	Type
1	B	641	HIS
1	B	743	ASN
1	B	767	ASN
1	B	775	GLN
1	B	814	GLN
1	B	878	GLN
1	B	880	ASN
1	B	951	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 for Mogul analysis.

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	1004	1	14,14,15	0.49	0	17,19,21	1.32	3 (17%)
2	NAG	A	1007	1	14,14,15	0.50	0	17,19,21	1.45	2 (11%)
2	NAG	A	1003	1	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
2	NAG	A	1008	1	14,14,15	0.55	0	17,19,21	0.84	0
2	NAG	A	1002	1	14,14,15	0.56	0	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1001	1	14,14,15	0.61	0	17,19,21	0.79	0
2	NAG	B	1003	1	14,14,15	0.57	0	17,19,21	0.63	0
2	NAG	B	1007	1	14,14,15	0.47	0	17,19,21	1.37	1 (5%)
2	NAG	A	1006	1	14,14,15	0.45	0	17,19,21	1.29	1 (5%)
2	NAG	B	1008	1	14,14,15	0.66	0	17,19,21	1.45	3 (17%)
2	NAG	A	1009	1	14,14,15	0.51	0	17,19,21	1.43	1 (5%)
2	NAG	B	1009	1	14,14,15	0.56	0	17,19,21	1.24	1 (5%)
2	NAG	B	1006	1	14,14,15	0.39	0	17,19,21	1.62	3 (17%)
2	NAG	B	1004	1	14,14,15	0.49	0	17,19,21	0.65	0
2	NAG	A	1005	1	14,14,15	0.59	0	17,19,21	1.27	1 (5%)
2	NAG	A	1001	1	14,14,15	0.66	0	17,19,21	1.13	2 (11%)
2	NAG	B	1005	1	14,14,15	0.47	0	17,19,21	0.86	0
2	NAG	B	1002	1	14,14,15	0.61	0	17,19,21	1.14	2 (11%)

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	1004	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1003	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1003	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1008	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1009	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1009	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1006	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1004	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1001	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1005	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1002	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1009	NAG	C1-O5-C5	5.01	118.90	112.19
2	A	1007	NAG	C1-O5-C5	4.72	118.52	112.19
2	B	1006	NAG	C2-N2-C7	-4.38	117.03	122.90
2	B	1007	NAG	C1-O5-C5	4.31	117.96	112.19
2	B	1009	NAG	C1-O5-C5	4.06	117.63	112.19
2	A	1006	NAG	C2-N2-C7	-3.68	117.97	122.90
2	A	1001	NAG	C2-N2-C7	-3.23	118.58	122.90
2	B	1006	NAG	C1-O5-C5	3.10	116.34	112.19
2	B	1008	NAG	C3-C4-C5	3.00	115.68	110.23
2	B	1008	NAG	O5-C1-C2	-2.95	106.73	111.29
2	A	1003	NAG	C2-N2-C7	-2.72	119.25	122.90
2	B	1002	NAG	C3-C4-C5	-2.65	105.43	110.23
2	A	1005	NAG	C3-C4-C5	2.60	114.94	110.23
2	A	1004	NAG	C1-O5-C5	2.57	115.63	112.19
2	B	1008	NAG	C6-C5-C4	-2.42	107.08	113.02
2	A	1004	NAG	C3-C4-C5	2.28	114.36	110.23
2	A	1001	NAG	O5-C1-C2	-2.17	107.93	111.29
2	A	1004	NAG	C2-N2-C7	-2.07	120.13	122.90
2	B	1002	NAG	O4-C4-C5	2.07	114.41	109.32
2	A	1007	NAG	C2-N2-C7	-2.02	120.20	122.90
2	B	1006	NAG	C4-C3-C2	-2.01	108.08	111.02

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	NAG	O5-C5-C6-O6
2	B	1005	NAG	O5-C5-C6-O6
2	A	1001	NAG	C8-C7-N2-C2
2	A	1001	NAG	O7-C7-N2-C2
2	A	1002	NAG	C8-C7-N2-C2
2	A	1002	NAG	O7-C7-N2-C2
2	A	1003	NAG	C8-C7-N2-C2
2	A	1003	NAG	O7-C7-N2-C2
2	A	1004	NAG	C8-C7-N2-C2
2	A	1004	NAG	O7-C7-N2-C2
2	A	1009	NAG	C8-C7-N2-C2
2	A	1009	NAG	O7-C7-N2-C2
2	B	1001	NAG	C8-C7-N2-C2
2	B	1001	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	B	1002	NAG	C8-C7-N2-C2
2	B	1002	NAG	O7-C7-N2-C2
2	B	1003	NAG	C8-C7-N2-C2
2	B	1003	NAG	O7-C7-N2-C2
2	B	1004	NAG	C8-C7-N2-C2
2	B	1004	NAG	O7-C7-N2-C2
2	B	1005	NAG	C8-C7-N2-C2
2	B	1005	NAG	O7-C7-N2-C2
2	B	1009	NAG	C8-C7-N2-C2
2	B	1009	NAG	O7-C7-N2-C2
2	A	1001	NAG	C4-C5-C6-O6
2	B	1005	NAG	C4-C5-C6-O6
2	B	1003	NAG	C4-C5-C6-O6
2	B	1003	NAG	O5-C5-C6-O6
2	B	1002	NAG	C4-C5-C6-O6
2	B	1004	NAG	C4-C5-C6-O6
2	B	1002	NAG	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1003	NAG	1	0
2	A	1002	NAG	1	0
2	B	1001	NAG	1	0
2	B	1003	NAG	1	0
2	B	1008	NAG	2	0
2	A	1009	NAG	1	0
2	B	1009	NAG	3	0
2	A	1005	NAG	2	0
2	A	1001	NAG	1	0
2	B	1002	NAG	3	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	865/968 (89%)	-0.16	27 (3%)	51 47	4, 16, 43, 84	0
1	B	863/968 (89%)	-0.15	22 (2%)	58 54	4, 16, 44, 83	1 (0%)
All	All	1728/1936 (89%)	-0.15	49 (2%)	55 50	4, 16, 44, 84	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	565	ASP	5.4
1	A	888	TYR	4.9
1	A	93	ALA	4.7
1	A	893	PHE	4.5
1	B	61	LEU	4.2
1	B	925	VAL	4.2
1	B	888	TYR	3.8
1	B	367	GLN	3.6
1	B	126	THR	3.5
1	B	137	VAL	3.4
1	A	141	GLN	3.2
1	A	925	VAL	3.2
1	A	94	ASP	3.1
1	B	924	ASP	3.1
1	B	141	GLN	3.0
1	A	140	SER	2.9
1	A	139	ASP	2.9
1	A	892	SER	2.8
1	A	61	LEU	2.8
1	A	290	GLN	2.7
1	A	891	GLY	2.7
1	B	138	GLY	2.7
1	A	924	ASP	2.7
1	B	63	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	137	VAL	2.6
1	B	94	ASP	2.6
1	B	576	PHE	2.6
1	A	817	GLN	2.6
1	A	138	GLY	2.5
1	B	62	ASP	2.5
1	A	126	THR	2.5
1	A	613	SER	2.4
1	A	684	ASN	2.4
1	A	895	PHE	2.3
1	A	941	THR	2.3
1	A	576	PHE	2.3
1	B	895	PHE	2.3
1	B	93	ALA	2.3
1	B	684	ASN	2.3
1	A	62	ASP	2.2
1	B	577	ASP	2.2
1	B	894	SER	2.2
1	A	92	ASN	2.1
1	B	210	THR	2.1
1	A	886	GLN	2.1
1	A	887	ASP	2.0
1	B	909	GLU	2.0
1	B	926	GLY	2.0
1	A	210	THR	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 ⓘ

There are no oligosaccharides in this entry.

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	1005	14/15	0.65	0.19	44,62,72,74	0
2	NAG	B	1004	14/15	0.70	0.16	30,56,62,62	0
2	NAG	B	1003	14/15	0.76	0.14	38,49,59,61	0
2	NAG	A	1003	14/15	0.81	0.12	32,43,52,55	0
2	NAG	A	1004	14/15	0.81	0.12	26,41,50,53	0
2	NAG	A	1008	14/15	0.81	0.14	37,48,57,67	0
2	NAG	B	1008	14/15	0.83	0.14	28,38,48,51	0
2	NAG	B	1007	14/15	0.84	0.12	24,29,40,42	0
2	NAG	B	1001	14/15	0.85	0.11	30,50,62,64	0
2	NAG	A	1001	14/15	0.87	0.10	38,46,54,57	0
2	NAG	A	1009	14/15	0.87	0.10	25,34,43,54	0
2	NAG	B	1009	14/15	0.87	0.12	27,40,56,59	0
2	NAG	A	1005	14/15	0.89	0.10	13,27,44,47	0
2	NAG	A	1007	14/15	0.91	0.08	19,26,35,37	0
2	NAG	B	1002	14/15	0.91	0.09	12,18,26,26	0
2	NAG	A	1002	14/15	0.92	0.08	9,14,19,24	0
2	NAG	B	1006	14/15	0.93	0.07	18,24,29,49	0
2	NAG	A	1006	14/15	0.94	0.07	14,18,24,26	0
3	ZN	A	1010	1/1	0.99	0.02	17,17,17,17	0
3	ZN	B	1010	1/1	0.99	0.02	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.