Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:37 PM GMT

PDB ID	:	1L3W
Title	:	C-cadherin Ectodomain
Authors	:	Boggon, T.J.; Murray, J.; Chappuis-Flament, S.; Wong, E.; Gumbiner, B.M.; Shapiro, L.
Deposited on	:	2002-03-01
Resolution	:	3.08 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

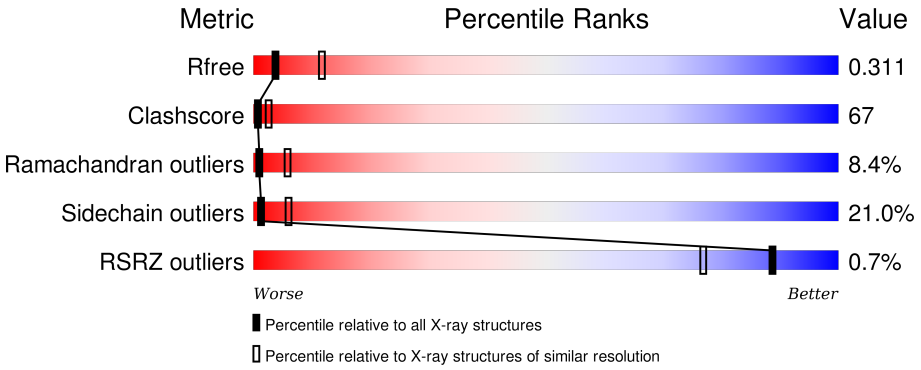
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	546	% 32% 45% 17% 5% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	801	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	803	-	-	-	X
2	NAG	A	805	X	-	X	X
2	NAG	A	806	X	-	X	X
2	NAG	A	807	-	-	X	X
2	NAG	A	808	-	-	-	X
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-
2	NAG	A	904	-	-	X	-
3	NDG	A	804	-	-	-	X
3	NDG	A	811	-	-	-	X
3	NDG	A	902	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4292 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.

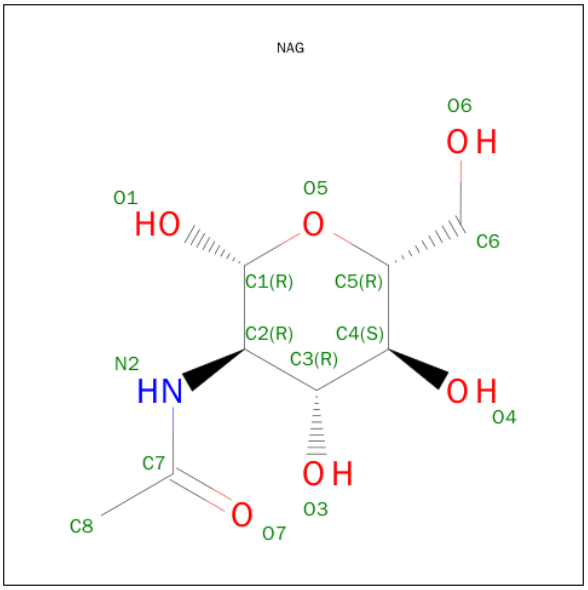
- Molecule 1 is a protein called EP-cadherin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	540	4032	2537	657	827	11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

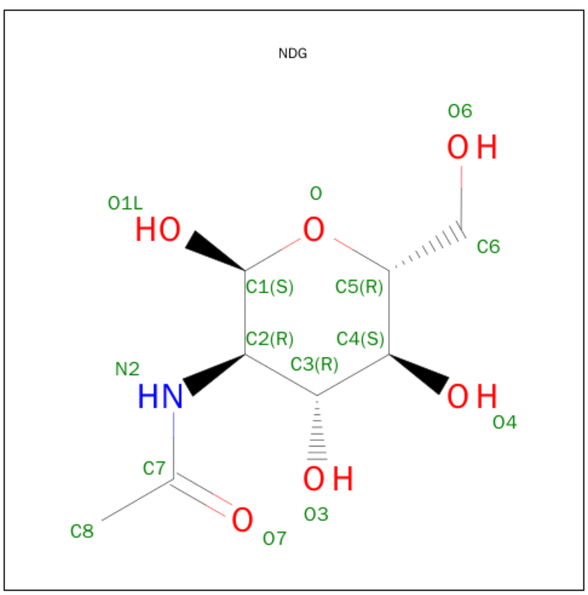
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP P33148
A	-4	HIS	-	EXPRESSION TAG	UNP P33148
A	-3	HIS	-	EXPRESSION TAG	UNP P33148
A	-2	HIS	-	EXPRESSION TAG	UNP P33148
A	-1	HIS	-	EXPRESSION TAG	UNP P33148
A	0	HIS	-	EXPRESSION TAG	UNP P33148

- 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 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total Ca 12 12	0	0

- Molecule 5 is water.

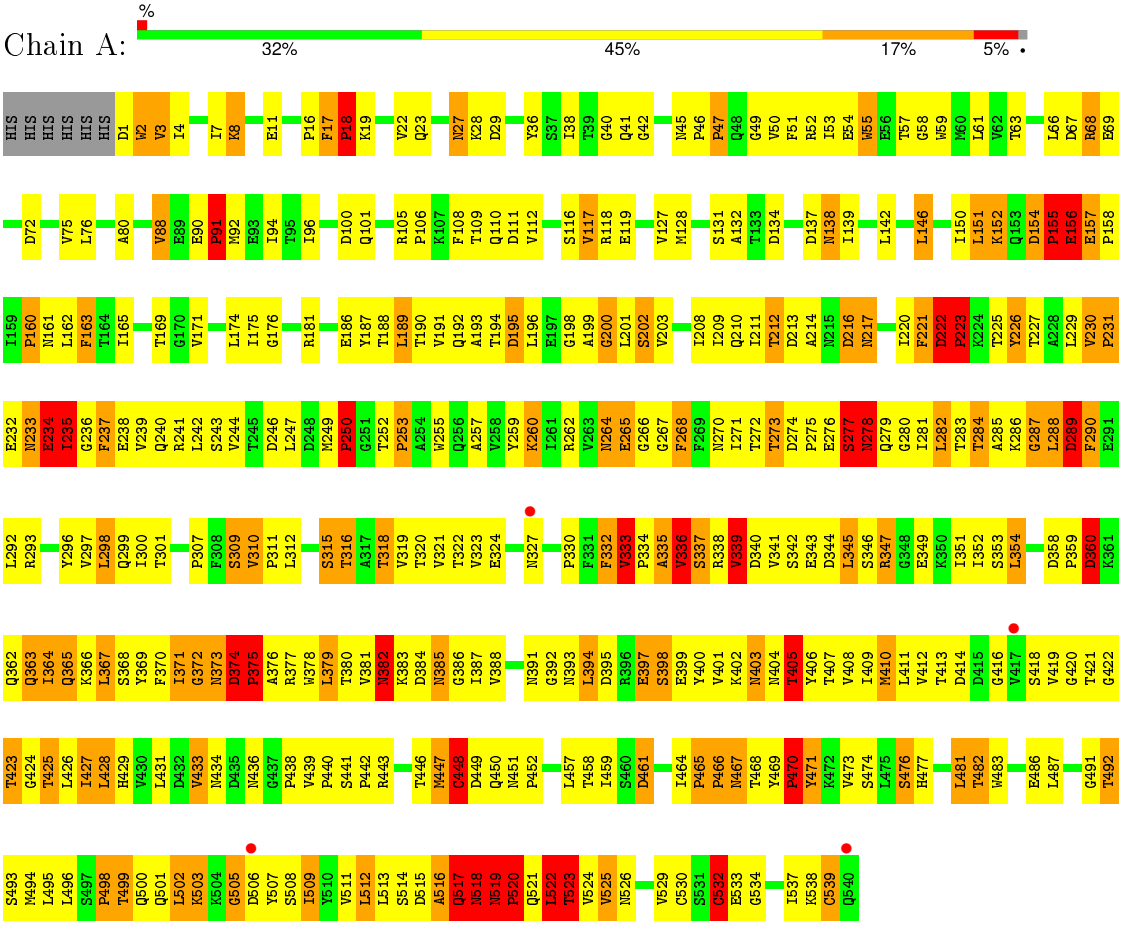
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	38	Total O 38 38	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: EP-cadherin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.17Å 75.14Å 129.81Å 90.00° 105.50° 90.00°	Depositor
Resolution (Å)	20.00 – 3.08 19.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	69.8 (20.00-3.08) 85.4 (19.88-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	0.71 (at 2.98Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.243 , 0.276 0.280 , 0.311	Depositor DCC
R_{free} test set	1049 reflections (5.68%)	DCC
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 75.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 23044 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4292	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, NDG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.70	8/4115 (0.2%)	1.37	76/5651 (1.3%)

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	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ALA	CA-CB	-8.34	1.34	1.52
1	A	539	CYS	CB-SG	8.16	1.96	1.82
1	A	223	PRO	CG-CD	7.01	1.73	1.50
1	A	523	THR	N-CA	-6.24	1.33	1.46
1	A	522	LEU	N-CA	-5.97	1.34	1.46
1	A	18	PRO	N-CD	5.93	1.56	1.47
1	A	530	CYS	CB-SG	5.50	1.91	1.82
1	A	499	THR	CA-CB	5.04	1.66	1.53

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	520	PRO	CA-C-N	-13.28	87.99	117.20
1	A	235	ILE	N-CA-C	12.73	145.36	111.00
1	A	290	PHE	N-CA-C	12.73	145.36	111.00
1	A	374	ASP	N-CA-C	11.61	142.34	111.00
1	A	17	PHE	C-N-CD	-11.54	95.22	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	398	SER	N-CA-C	11.37	141.69	111.00
1	A	465	PRO	C-N-CD	-11.03	96.34	120.60
1	A	222	ASP	CB-CG-OD2	10.03	127.33	118.30
1	A	236	GLY	N-CA-C	-9.98	88.14	113.10
1	A	230	VAL	C-N-CD	-9.94	98.72	120.60
1	A	376	ALA	N-CA-C	9.66	137.07	111.00
1	A	522	LEU	CA-CB-CG	-9.37	93.75	115.30
1	A	223	PRO	N-CA-C	-9.30	87.92	112.10
1	A	221	PHE	C-N-CA	-9.30	98.45	121.70
1	A	520	PRO	N-CA-C	9.30	136.27	112.10
1	A	481	LEU	N-CA-C	-9.28	85.94	111.00
1	A	481	LEU	CA-CB-CG	-8.76	95.16	115.30
1	A	289	ASP	C-N-CA	-8.42	100.64	121.70
1	A	516	ALA	N-CA-C	-8.36	88.44	111.00
1	A	222	ASP	C-N-CD	-8.20	102.55	120.60
1	A	290	PHE	CA-C-N	-8.19	99.19	117.20
1	A	46	PRO	C-N-CD	-8.03	102.93	120.60
1	A	233	ASN	N-CA-C	7.86	132.23	111.00
1	A	336	VAL	N-CA-C	7.80	132.07	111.00
1	A	522	LEU	C-N-CA	-7.79	102.22	121.70
1	A	362	GLN	N-CA-C	-7.71	90.17	111.00
1	A	234	GLU	N-CA-C	-7.58	90.53	111.00
1	A	234	GLU	C-N-CA	7.41	140.22	121.70
1	A	521	GLN	C-N-CA	-7.37	103.27	121.70
1	A	277	SER	N-CA-C	-7.20	91.56	111.00
1	A	337	SER	N-CA-C	-7.17	91.63	111.00
1	A	503	LYS	N-CA-C	7.01	129.92	111.00
1	A	523	THR	N-CA-CB	-6.94	97.11	110.30
1	A	492	THR	N-CA-C	6.78	129.30	111.00
1	A	448	CYS	CA-CB-SG	-6.69	101.96	114.00
1	A	476	SER	N-CA-C	6.57	128.74	111.00
1	A	398	SER	C-N-CA	-6.57	105.28	121.70
1	A	491	GLY	N-CA-C	6.53	129.42	113.10
1	A	525	VAL	N-CA-C	-6.50	93.44	111.00
1	A	335	ALA	N-CA-C	-6.32	93.92	111.00
1	A	532	CYS	N-CA-C	6.30	128.02	111.00
1	A	234	GLU	CA-C-N	-6.27	103.40	117.20
1	A	222	ASP	N-CA-C	6.16	127.62	111.00
1	A	235	ILE	CA-C-N	-6.14	103.92	116.20
1	A	397	GLU	C-N-CA	-6.13	106.37	121.70
1	A	18	PRO	CA-N-CD	-6.08	102.99	111.50
1	A	502	LEU	N-CA-C	6.05	127.34	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	TRP	N-CA-C	-6.03	94.73	111.00
1	A	374	ASP	C-N-CD	5.96	140.92	128.40
1	A	222	ASP	N-CA-CB	5.95	121.32	110.60
1	A	364	ILE	N-CA-C	-5.91	95.03	111.00
1	A	382	ASN	N-CA-C	-5.83	95.26	111.00
1	A	376	ALA	CA-C-N	-5.83	104.38	117.20
1	A	471	TYR	N-CA-C	5.73	126.48	111.00
1	A	481	LEU	CA-C-N	-5.69	104.68	117.20
1	A	374	ASP	C-N-CA	-5.66	98.21	122.00
1	A	403	ASN	N-CA-C	-5.63	95.80	111.00
1	A	221	PHE	CA-C-N	5.56	129.43	117.20
1	A	505	GLY	N-CA-C	5.55	126.99	113.10
1	A	157	GLU	C-N-CD	-5.47	108.57	120.60
1	A	519	ASN	N-CA-C	5.35	125.43	111.00
1	A	405	THR	N-CA-C	5.32	125.37	111.00
1	A	367	LEU	CA-CB-CG	-5.30	103.10	115.30
1	A	521	GLN	N-CA-C	-5.21	96.94	111.00
1	A	290	PHE	O-C-N	5.19	131.00	122.70
1	A	520	PRO	C-N-CA	5.16	134.59	121.70
1	A	532	CYS	N-CA-CB	-5.16	101.32	110.60
1	A	18	PRO	CA-CB-CG	-5.12	94.27	104.00
1	A	522	LEU	N-CA-C	-5.11	97.20	111.00
1	A	339	VAL	N-CA-C	5.11	124.79	111.00
1	A	16	PRO	C-N-CA	-5.07	109.02	121.70
1	A	332	PHE	N-CA-C	-5.03	97.41	111.00
1	A	470	PRO	N-CA-C	5.01	125.14	112.10
1	A	221	PHE	N-CA-C	5.01	124.53	111.00
1	A	539	CYS	N-CA-C	5.01	124.53	111.00
1	A	234	GLU	O-C-N	5.00	130.70	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	PHE	Sidechain
1	A	18	PRO	Mainchain
1	A	222	ASP	Mainchain
1	A	520	PRO	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4032	0	3772	538	0
2	A	154	0	143	81	0
3	A	56	0	52	16	0
4	A	12	0	0	0	0
5	A	38	0	0	3	0
All	All	4292	0	3967	553	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 67.

All (553) 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:482:THR:HG23	1:A:499:THR:CG2	1.75	1.17
1:A:234:GLU:H	1:A:235:ILE:HG23	1.08	1.15
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.15
1:A:8:LYS:H	1:A:8:LYS:HD2	1.04	1.14
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.12
1:A:154:ASP:C	2:A:801:NAG:H82	1.70	1.10
1:A:227:THR:HG21	2:A:807:NAG:C8	1.82	1.08
1:A:222:ASP:O	1:A:222:ASP:OD1	1.69	1.08
1:A:301:THR:HG21	2:A:805:NAG:H82	1.29	1.07
1:A:335:ALA:HB1	3:A:811:NDG:O6	1.54	1.07
1:A:482:THR:HG23	1:A:499:THR:HG22	1.09	1.07
1:A:290:PHE:HB2	1:A:292:LEU:N	1.69	1.06
1:A:337:SER:HA	1:A:427:ILE:HG23	1.38	1.05
1:A:482:THR:CG2	1:A:499:THR:N	2.22	1.02
1:A:290:PHE:HB2	1:A:292:LEU:H	0.88	1.02
1:A:482:THR:HG21	1:A:499:THR:H	1.23	1.01
1:A:403:ASN:HB2	3:A:902:NDG:C8	1.90	1.01
1:A:522:LEU:HD22	1:A:523:THR:HB	1.39	1.00
1:A:274:ASP:O	1:A:278:ASN:HA	1.61	1.00
1:A:188:THR:HG23	1:A:208:ILE:HG12	1.43	1.00
1:A:523:THR:HG23	1:A:524:VAL:H	1.27	0.99
1:A:320:THR:HG21	2:A:807:NAG:N2	1.78	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LYS:HG3	1:A:367:LEU:H	1.28	0.97
1:A:482:THR:CG2	1:A:499:THR:H	1.76	0.96
1:A:235:ILE:CG1	1:A:287:GLY:HA2	1.96	0.96
1:A:320:THR:HG21	2:A:807:NAG:HN2	1.31	0.95
1:A:290:PHE:CB	1:A:292:LEU:H	1.79	0.95
1:A:27:ASN:HD22	1:A:28:LYS:N	1.66	0.94
1:A:227:THR:HG21	2:A:807:NAG:H83	1.48	0.94
1:A:195:ASP:HB2	1:A:201:LEU:H	1.34	0.93
1:A:352:ILE:HG13	1:A:388:VAL:HB	1.51	0.93
1:A:227:THR:HG21	2:A:807:NAG:C7	1.99	0.93
1:A:403:ASN:HB2	3:A:902:NDG:C7	2.00	0.92
1:A:366:LYS:CG	1:A:367:LEU:H	1.80	0.92
1:A:446:THR:HG23	1:A:539:CYS:SG	2.10	0.92
1:A:482:THR:HG21	1:A:499:THR:N	1.81	0.92
2:A:805:NAG:H62	2:A:806:NAG:C7	2.00	0.92
1:A:289:ASP:O	1:A:290:PHE:HB3	1.67	0.92
1:A:335:ALA:CB	3:A:811:NDG:O6	2.18	0.91
2:A:805:NAG:O5	2:A:806:NAG:H83	1.71	0.91
1:A:234:GLU:N	1:A:235:ILE:HG23	1.86	0.91
1:A:517:GLN:O	1:A:519:ASN:N	2.03	0.90
1:A:340:ASP:HA	1:A:429:HIS:HB3	1.53	0.90
1:A:378:TRP:HB2	1:A:379:LEU:HD23	1.53	0.90
1:A:374:ASP:O	1:A:375:PRO:C	2.06	0.90
1:A:154:ASP:HB3	1:A:155:PRO:HD2	1.54	0.90
1:A:518:ASN:O	1:A:520:PRO:HD3	1.72	0.90
1:A:8:LYS:HD2	1:A:8:LYS:N	1.87	0.89
1:A:318:THR:HG21	2:A:806:NAG:H5	1.56	0.88
1:A:371:ILE:CD1	1:A:381:VAL:HG11	2.03	0.88
1:A:483:TRP:CZ3	1:A:498:PRO:HG3	2.09	0.88
1:A:523:THR:HG23	1:A:524:VAL:CG2	2.03	0.88
1:A:343:GLU:HB3	1:A:433:VAL:HG21	1.55	0.87
1:A:440:PRO:CD	1:A:522:LEU:HD12	2.05	0.87
1:A:8:LYS:H	1:A:8:LYS:CD	1.74	0.86
1:A:221:PHE:HE1	1:A:315:SER:O	1.56	0.86
1:A:441:SER:OG	1:A:442:PRO:HD3	1.75	0.86
1:A:449:ASP:H	1:A:532:CYS:HB3	1.37	0.86
1:A:423:THR:CB	2:A:810:NAG:C7	2.54	0.86
1:A:257:ALA:O	1:A:273:THR:HG21	1.74	0.86
1:A:333:VAL:HB	1:A:334:PRO:HD3	1.56	0.86
1:A:320:THR:HG21	2:A:807:NAG:C2	2.05	0.85
1:A:483:TRP:HZ2	1:A:507:TYR:CE1	1.95	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:THR:HG23	1:A:524:VAL:N	1.90	0.85
1:A:438:PRO:HB3	1:A:471:TYR:HE2	1.41	0.85
1:A:235:ILE:HG13	1:A:287:GLY:HA2	1.58	0.85
1:A:375:PRO:HB3	1:A:400:TYR:CE2	2.12	0.84
1:A:155:PRO:HB2	2:A:801:NAG:H81	1.59	0.84
1:A:483:TRP:HZ2	1:A:507:TYR:HE1	1.24	0.83
1:A:451:ASN:N	1:A:533:GLU:O	2.10	0.83
1:A:423:THR:HB	2:A:810:NAG:N2	1.93	0.83
1:A:230:VAL:O	1:A:324:GLU:N	2.11	0.83
1:A:28:LYS:HD3	1:A:88:VAL:HG12	1.61	0.83
1:A:423:THR:CB	2:A:810:NAG:N2	2.42	0.82
1:A:482:THR:HG21	1:A:500:GLN:N	1.95	0.82
1:A:154:ASP:HB3	2:A:801:NAG:N2	1.95	0.82
1:A:440:PRO:HD2	1:A:522:LEU:HD12	1.59	0.82
1:A:448:CYS:O	1:A:452:PRO:HG3	1.78	0.82
1:A:234:GLU:H	1:A:235:ILE:CG2	1.92	0.82
1:A:154:ASP:HB3	2:A:801:NAG:HN2	1.45	0.81
1:A:289:ASP:OD2	1:A:289:ASP:O	1.97	0.81
1:A:446:THR:HG21	1:A:537:ILE:O	1.79	0.81
1:A:486:GLU:O	1:A:494:MET:HA	1.81	0.81
1:A:299:GLN:HG2	1:A:318:THR:HG23	1.62	0.81
1:A:277:SER:C	1:A:278:ASN:HD22	1.83	0.80
1:A:290:PHE:CE2	1:A:293:ARG:HB2	2.16	0.80
1:A:517:GLN:C	1:A:519:ASN:H	1.84	0.80
1:A:127:VAL:HG13	1:A:128:MET:H	1.46	0.80
1:A:222:ASP:C	1:A:222:ASP:OD1	2.20	0.80
1:A:371:ILE:HD11	1:A:381:VAL:HG11	1.64	0.80
1:A:290:PHE:HD2	1:A:293:ARG:H	1.28	0.80
1:A:265:GLU:HB3	1:A:268:PHE:HE2	1.46	0.79
1:A:496:LEU:HD21	1:A:509:ILE:HD13	1.63	0.79
1:A:406:TYR:CD1	2:A:808:NAG:H83	2.17	0.79
1:A:232:GLU:HG3	1:A:290:PHE:N	1.98	0.79
1:A:449:ASP:HB3	1:A:532:CYS:H	1.47	0.79
1:A:301:THR:HG21	2:A:805:NAG:C8	2.12	0.78
2:A:904:NAG:O7	2:A:904:NAG:H3	1.82	0.78
2:A:809:NAG:H61	2:A:810:NAG:H62	1.65	0.78
1:A:154:ASP:CB	1:A:155:PRO:HD2	2.13	0.78
1:A:155:PRO:C	1:A:157:GLU:H	1.86	0.78
1:A:524:VAL:CG2	2:A:904:NAG:H81	2.14	0.77
1:A:194:THR:HB	1:A:198:GLY:HA2	1.67	0.77
1:A:365:GLN:O	1:A:365:GLN:HG3	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:GLN:HG2	1:A:501:GLN:O	1.84	0.77
1:A:290:PHE:HZ	1:A:296:TYR:HH	1.33	0.77
1:A:523:THR:HG23	1:A:524:VAL:HG22	1.67	0.77
1:A:156:GLU:HG3	1:A:160:PRO:HB3	1.66	0.77
1:A:195:ASP:HB3	1:A:200:GLY:HA3	1.65	0.77
1:A:440:PRO:HB3	1:A:457:LEU:HD21	1.67	0.76
1:A:238:GLU:HA	1:A:283:THR:HG22	1.66	0.76
1:A:223:PRO:HD2	1:A:226:TYR:OH	1.85	0.76
1:A:366:LYS:CG	1:A:367:LEU:N	2.48	0.76
1:A:196:LEU:HB2	1:A:199:ALA:HB3	1.67	0.75
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.75
1:A:272:THR:HG22	1:A:273:THR:H	1.51	0.75
1:A:448:CYS:SG	1:A:537:ILE:HG22	2.27	0.75
1:A:241:ARG:HE	1:A:281:ILE:HD12	1.51	0.75
1:A:449:ASP:HB3	1:A:532:CYS:N	2.02	0.75
1:A:290:PHE:CD2	1:A:293:ARG:N	2.55	0.74
1:A:188:THR:HG23	1:A:208:ILE:CG1	2.16	0.74
1:A:371:ILE:HD12	1:A:410:MET:HB3	1.68	0.74
1:A:451:ASN:O	1:A:534:GLY:HA2	1.88	0.74
1:A:290:PHE:HE2	1:A:293:ARG:HB2	1.52	0.74
1:A:27:ASN:HD22	1:A:27:ASN:C	1.85	0.73
1:A:333:VAL:CB	1:A:334:PRO:HD3	2.18	0.73
1:A:223:PRO:HB2	1:A:226:TYR:CE2	2.23	0.73
1:A:373:ASN:ND2	1:A:374:ASP:H	1.87	0.73
1:A:276:GLU:HG3	1:A:277:SER:H	1.54	0.73
1:A:511:VAL:HG23	1:A:523:THR:O	1.89	0.73
1:A:298:LEU:HD23	1:A:298:LEU:N	2.03	0.72
1:A:273:THR:O	2:A:803:NAG:H82	1.89	0.72
1:A:320:THR:CG2	2:A:807:NAG:N2	2.52	0.72
1:A:320:THR:CG2	2:A:807:NAG:HN2	2.01	0.72
1:A:366:LYS:HG3	1:A:367:LEU:N	2.04	0.72
1:A:394:LEU:HD12	1:A:394:LEU:N	2.05	0.71
1:A:482:THR:CG2	1:A:499:THR:CG2	2.62	0.71
1:A:342:SER:HA	1:A:431:LEU:HB2	1.71	0.71
1:A:227:THR:O	2:A:812:NAG:O5	2.09	0.71
1:A:276:GLU:CG	1:A:277:SER:H	2.03	0.71
1:A:229:LEU:HD23	1:A:322:THR:HB	1.73	0.71
1:A:403:ASN:CB	3:A:902:NDG:N2	2.54	0.71
1:A:434:ASN:OD1	1:A:467:ASN:HB3	1.90	0.70
1:A:438:PRO:HB3	1:A:471:TYR:CE2	2.26	0.70
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:THR:O	2:A:806:NAG:H82	1.91	0.69
1:A:187:TYR:HA	2:A:801:NAG:C7	2.21	0.69
1:A:414:ASP:HB3	1:A:420:GLY:HA3	1.73	0.69
1:A:53:ILE:HG13	1:A:59:TRP:O	1.93	0.69
1:A:282:LEU:HD23	1:A:283:THR:H	1.58	0.68
1:A:242:LEU:HD12	1:A:280:GLY:O	1.93	0.68
1:A:290:PHE:HZ	1:A:296:TYR:OH	1.77	0.68
1:A:27:ASN:C	1:A:27:ASN:ND2	2.46	0.68
1:A:482:THR:HG21	1:A:500:GLN:H	1.58	0.68
1:A:155:PRO:HB2	2:A:801:NAG:C8	2.24	0.68
1:A:320:THR:HG21	2:A:807:NAG:H2	1.76	0.68
1:A:483:TRP:CZ2	1:A:507:TYR:HE1	2.09	0.68
1:A:337:SER:CA	1:A:427:ILE:HG23	2.20	0.68
1:A:221:PHE:CE1	1:A:315:SER:O	2.45	0.68
1:A:1:ASP:CG	1:A:2:TRP:H	1.96	0.68
1:A:137:ASP:OD2	1:A:139:ILE:HG22	1.94	0.68
1:A:272:THR:HG22	1:A:273:THR:N	2.09	0.68
1:A:289:ASP:CG	1:A:289:ASP:O	2.30	0.68
1:A:371:ILE:CG2	1:A:372:GLY:N	2.57	0.68
1:A:423:THR:HB	2:A:810:NAG:C8	2.24	0.67
1:A:440:PRO:HA	1:A:458:THR:O	1.94	0.67
1:A:186:GLU:OE1	2:A:801:NAG:H62	1.93	0.67
1:A:195:ASP:HB2	1:A:201:LEU:N	2.08	0.67
1:A:347:ARG:CD	1:A:392:GLY:H	2.07	0.67
1:A:282:LEU:HD23	1:A:283:THR:N	2.08	0.67
1:A:289:ASP:O	1:A:290:PHE:CB	2.25	0.67
1:A:347:ARG:CG	1:A:392:GLY:H	2.08	0.67
1:A:524:VAL:HG21	2:A:904:NAG:H81	1.76	0.67
1:A:474:SER:HB2	1:A:512:LEU:CG	2.15	0.66
1:A:333:VAL:HB	1:A:334:PRO:CD	2.24	0.66
1:A:373:ASN:ND2	1:A:374:ASP:N	2.43	0.66
1:A:446:THR:CG2	1:A:537:ILE:O	2.44	0.66
1:A:464:ILE:O	1:A:467:ASN:HB2	1.96	0.66
3:A:902:NDG:H3	3:A:902:NDG:O7	1.95	0.66
1:A:366:LYS:HG3	1:A:367:LEU:HG	1.77	0.66
2:A:805:NAG:C6	2:A:806:NAG:C7	2.74	0.66
1:A:403:ASN:HB2	3:A:902:NDG:H8C1	1.78	0.66
1:A:440:PRO:HD2	1:A:522:LEU:CD1	2.26	0.66
1:A:232:GLU:HG3	1:A:290:PHE:H	1.61	0.66
1:A:524:VAL:HG23	2:A:904:NAG:H81	1.78	0.66
2:A:809:NAG:C6	2:A:810:NAG:H62	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:VAL:HG13	1:A:405:THR:O	1.95	0.65
1:A:265:GLU:HB3	1:A:268:PHE:CE2	2.31	0.65
1:A:232:GLU:HG2	1:A:289:ASP:HA	1.77	0.65
1:A:187:TYR:HA	2:A:801:NAG:C8	2.25	0.65
1:A:405:THR:OG1	1:A:406:TYR:N	2.22	0.65
1:A:403:ASN:HB2	3:A:902:NDG:N2	2.10	0.65
1:A:406:TYR:CE1	2:A:808:NAG:H83	2.32	0.65
2:A:904:NAG:O7	2:A:904:NAG:C3	2.45	0.64
1:A:474:SER:CB	1:A:512:LEU:HG	2.14	0.64
1:A:347:ARG:HD2	1:A:392:GLY:H	1.60	0.64
1:A:409:ILE:HG12	1:A:425:THR:HG23	1.80	0.64
1:A:346:SER:OG	1:A:349:GLU:HG3	1.97	0.64
1:A:327:ASN:HA	1:A:360:ASP:OD2	1.97	0.64
1:A:222:ASP:CG	1:A:222:ASP:O	2.32	0.64
1:A:341:VAL:HG21	1:A:345:LEU:HD12	1.79	0.64
1:A:142:LEU:HB3	1:A:196:LEU:HA	1.81	0.63
1:A:482:THR:HG21	1:A:499:THR:CA	2.27	0.63
1:A:127:VAL:HG22	1:A:128:MET:N	2.14	0.63
1:A:368:SER:HG	1:A:370:PHE:HE1	1.45	0.63
1:A:486:GLU:O	1:A:494:MET:CA	2.46	0.63
1:A:343:GLU:HB3	1:A:433:VAL:CG2	2.28	0.63
1:A:212:THR:HG22	1:A:213:ASP:H	1.62	0.63
1:A:227:THR:CG2	2:A:807:NAG:C7	2.76	0.63
1:A:440:PRO:HD3	1:A:522:LEU:HD12	1.78	0.63
1:A:22:VAL:HG22	1:A:23:GLN:N	2.14	0.63
1:A:154:ASP:CA	2:A:801:NAG:H82	2.29	0.63
1:A:524:VAL:HG23	2:A:904:NAG:C8	2.29	0.63
1:A:446:THR:CG2	1:A:539:CYS:SG	2.86	0.63
1:A:411:LEU:HD22	1:A:421:THR:HG23	1.81	0.62
1:A:347:ARG:HG3	1:A:392:GLY:H	1.62	0.62
1:A:419:VAL:HG13	2:A:809:NAG:O7	1.98	0.62
1:A:375:PRO:HB3	1:A:400:TYR:CD2	2.33	0.62
1:A:403:ASN:CB	3:A:902:NDG:C7	2.76	0.62
1:A:3:VAL:O	5:A:1001:HOH:O	2.16	0.62
1:A:403:ASN:O	1:A:405:THR:N	2.33	0.62
1:A:154:ASP:O	1:A:155:PRO:C	2.36	0.62
1:A:508:SER:HB3	1:A:526:ASN:OD1	2.00	0.62
1:A:68:ARG:HD3	1:A:100:ASP:HA	1.82	0.62
1:A:524:VAL:CG2	2:A:904:NAG:C8	2.78	0.62
1:A:486:GLU:O	1:A:495:LEU:N	2.31	0.61
1:A:235:ILE:HG12	1:A:287:GLY:HA2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ASP:O	1:A:375:PRO:O	2.17	0.61
1:A:212:THR:HG22	1:A:213:ASP:N	2.15	0.61
1:A:154:ASP:O	2:A:801:NAG:H82	1.98	0.61
1:A:518:ASN:O	1:A:520:PRO:CD	2.46	0.61
1:A:449:ASP:H	1:A:532:CYS:CB	2.12	0.61
1:A:371:ILE:CG2	1:A:372:GLY:H	2.13	0.61
1:A:379:LEU:HD23	1:A:379:LEU:H	1.66	0.61
1:A:232:GLU:CG	1:A:290:PHE:N	2.64	0.60
1:A:181:ARG:NE	1:A:213:ASP:OD1	2.34	0.60
1:A:371:ILE:HG22	1:A:372:GLY:N	2.14	0.60
1:A:189:LEU:HD23	1:A:189:LEU:N	2.17	0.60
1:A:482:THR:HG22	1:A:499:THR:N	2.13	0.60
1:A:49:GLY:O	1:A:63:THR:HG21	2.02	0.59
1:A:336:VAL:HB	1:A:426:LEU:HD23	1.84	0.59
1:A:239:VAL:HG13	1:A:240:GLN:H	1.67	0.59
1:A:508:SER:HA	1:A:526:ASN:HA	1.84	0.59
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.67	0.59
1:A:458:THR:HG22	1:A:493:SER:CB	2.32	0.59
1:A:195:ASP:CB	1:A:200:GLY:HA3	2.33	0.59
1:A:268:PHE:HA	1:A:285:ALA:HB3	1.85	0.59
1:A:473:VAL:HA	1:A:513:LEU:HD23	1.85	0.59
1:A:514:SER:HA	1:A:517:GLN:O	2.02	0.58
1:A:367:LEU:CB	1:A:413:THR:O	2.51	0.58
1:A:38:ILE:HG22	1:A:53:ILE:HG22	1.85	0.58
1:A:443:ARG:HA	1:A:525:VAL:HG13	1.85	0.58
1:A:116:SER:HA	1:A:210:GLN:O	2.02	0.58
1:A:296:TYR:HB2	1:A:321:VAL:HB	1.86	0.58
1:A:447:MET:HB2	1:A:529:VAL:HG22	1.84	0.58
1:A:286:LYS:O	1:A:287:GLY:O	2.21	0.58
1:A:406:TYR:HB3	1:A:428:LEU:CD2	2.33	0.58
1:A:299:GLN:C	1:A:300:ILE:HD12	2.24	0.58
1:A:335:ALA:HB1	3:A:811:NDG:C6	2.33	0.58
1:A:221:PHE:HA	1:A:244:VAL:HG12	1.85	0.58
1:A:146:LEU:HA	1:A:194:THR:O	2.02	0.58
1:A:232:GLU:HG2	1:A:289:ASP:CA	2.33	0.58
1:A:155:PRO:C	1:A:157:GLU:N	2.56	0.58
1:A:309:SER:O	1:A:310:VAL:HG23	2.03	0.58
1:A:154:ASP:CB	2:A:801:NAG:HN2	2.16	0.57
1:A:332:PHE:CD2	1:A:424:GLY:HA3	2.39	0.57
1:A:154:ASP:CB	1:A:155:PRO:CD	2.82	0.57
1:A:330:PRO:HD3	1:A:414:ASP:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLY:HA2	1:A:47:PRO:O	2.04	0.57
1:A:226:TYR:CE2	1:A:242:LEU:HD23	2.39	0.57
1:A:406:TYR:HB3	1:A:428:LEU:HD21	1.87	0.57
1:A:259:TYR:O	1:A:260:LYS:HB3	2.05	0.57
1:A:108:PHE:CE1	1:A:203:VAL:HG23	2.40	0.57
1:A:523:THR:CG2	1:A:524:VAL:H	1.94	0.56
1:A:240:GLN:HG3	1:A:241:ARG:N	2.19	0.56
1:A:189:LEU:HD21	1:A:209:ILE:HD12	1.87	0.56
1:A:393:ASN:C	1:A:394:LEU:HD12	2.25	0.56
1:A:68:ARG:HG3	1:A:69:GLU:N	2.19	0.56
1:A:537:ILE:HG12	1:A:538:LYS:N	2.19	0.56
1:A:369:TYR:HD1	1:A:383:LYS:O	1.88	0.56
1:A:222:ASP:N	1:A:243:SER:O	2.38	0.56
1:A:118:ARG:HA	1:A:212:THR:HB	1.87	0.56
1:A:272:THR:CG2	1:A:273:THR:H	2.19	0.56
1:A:162:LEU:O	1:A:174:LEU:HD12	2.06	0.56
1:A:505:GLY:HA2	1:A:529:VAL:H	1.69	0.56
1:A:439:VAL:HG13	1:A:522:LEU:HD11	1.88	0.56
1:A:378:TRP:O	1:A:391:ASN:HB2	2.06	0.55
1:A:394:LEU:N	1:A:394:LEU:CD1	2.69	0.55
1:A:155:PRO:N	2:A:801:NAG:H82	2.20	0.55
1:A:482:THR:HG21	1:A:499:THR:C	2.27	0.55
1:A:482:THR:HG22	1:A:499:THR:H	1.70	0.55
1:A:450:GLN:CB	1:A:533:GLU:HA	2.37	0.55
1:A:339:VAL:HG21	1:A:351:ILE:CG2	2.36	0.55
1:A:333:VAL:CG2	1:A:334:PRO:HD3	2.36	0.55
1:A:278:ASN:N	1:A:278:ASN:HD22	2.05	0.55
1:A:154:ASP:CG	1:A:155:PRO:CD	2.75	0.55
1:A:268:PHE:N	1:A:268:PHE:CD2	2.75	0.55
1:A:419:VAL:CG1	1:A:420:GLY:N	2.70	0.54
1:A:75:VAL:O	1:A:76:LEU:HD23	2.07	0.54
1:A:117:VAL:O	1:A:211:ILE:HA	2.07	0.54
1:A:320:THR:CG2	2:A:807:NAG:C2	2.76	0.54
1:A:155:PRO:HG2	2:A:801:NAG:O7	2.07	0.54
1:A:438:PRO:HB2	1:A:513:LEU:HD12	1.89	0.54
1:A:371:ILE:HG23	1:A:372:GLY:H	1.73	0.54
1:A:169:THR:OG1	1:A:171:VAL:HG23	2.08	0.54
1:A:226:TYR:O	1:A:227:THR:CG2	2.55	0.53
1:A:226:TYR:HB2	1:A:319:VAL:HG22	1.89	0.53
1:A:249:MET:O	1:A:252:THR:HB	2.09	0.53
1:A:367:LEU:HD12	1:A:367:LEU:C	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:HG21	1:A:471:TYR:CE2	2.42	0.53
1:A:28:LYS:HB3	1:A:88:VAL:HG11	1.89	0.53
1:A:332:PHE:HD2	1:A:424:GLY:HA3	1.73	0.53
1:A:241:ARG:NE	1:A:281:ILE:HD12	2.22	0.53
1:A:22:VAL:HG22	1:A:23:GLN:H	1.73	0.53
1:A:217:ASN:N	1:A:217:ASN:ND2	2.56	0.53
1:A:330:PRO:HB3	1:A:358:ASP:HB2	1.89	0.53
1:A:522:LEU:CD2	1:A:523:THR:HB	2.26	0.53
1:A:276:GLU:CG	1:A:277:SER:N	2.71	0.53
1:A:466:PRO:O	1:A:468:THR:N	2.40	0.53
1:A:373:ASN:HB3	1:A:409:ILE:H	1.74	0.53
1:A:252:THR:HG23	1:A:253:PRO:HD2	1.90	0.53
1:A:347:ARG:HG3	1:A:391:ASN:HA	1.91	0.53
1:A:242:LEU:O	1:A:279:GLN:HB3	2.09	0.53
1:A:482:THR:CG2	1:A:499:THR:CA	2.87	0.52
1:A:426:LEU:O	1:A:426:LEU:HD13	2.10	0.52
1:A:312:LEU:O	3:A:804:NDG:C8	2.57	0.52
1:A:352:ILE:HG13	1:A:388:VAL:CB	2.33	0.52
1:A:379:LEU:H	1:A:379:LEU:CD2	2.22	0.52
1:A:272:THR:CG2	2:A:803:NAG:HN2	2.23	0.52
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.23	0.52
1:A:227:THR:CG2	2:A:807:NAG:H83	2.32	0.52
1:A:367:LEU:HD13	1:A:412:VAL:HG23	1.91	0.52
1:A:28:LYS:CD	1:A:88:VAL:HG12	2.38	0.52
1:A:533:GLU:HA	1:A:533:GLU:OE2	2.09	0.52
1:A:450:GLN:CB	1:A:532:CYS:O	2.58	0.52
1:A:268:PHE:C	1:A:285:ALA:HB3	2.30	0.52
1:A:336:VAL:O	1:A:426:LEU:HD22	2.10	0.52
1:A:221:PHE:HB3	1:A:223:PRO:O	2.10	0.52
1:A:514:SER:HB3	1:A:517:GLN:O	2.10	0.52
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.91	0.51
1:A:482:THR:HG22	1:A:482:THR:O	2.09	0.51
1:A:403:ASN:C	1:A:405:THR:H	2.12	0.51
1:A:471:TYR:CD1	1:A:471:TYR:N	2.79	0.51
1:A:458:THR:HA	1:A:493:SER:HA	1.93	0.51
1:A:155:PRO:CD	2:A:801:NAG:H82	2.40	0.51
2:A:807:NAG:H3	2:A:807:NAG:O7	2.11	0.51
1:A:347:ARG:HD2	1:A:392:GLY:N	2.25	0.51
1:A:517:GLN:C	1:A:519:ASN:N	2.47	0.51
1:A:80:ALA:O	1:A:88:VAL:HG23	2.11	0.51
1:A:194:THR:HG22	1:A:195:ASP:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:THR:HB	2:A:810:NAG:H83	1.94	0.50
1:A:142:LEU:O	1:A:196:LEU:HD23	2.11	0.50
1:A:327:ASN:OD1	1:A:360:ASP:OD1	2.30	0.50
1:A:419:VAL:HG22	2:A:809:NAG:H81	1.93	0.50
1:A:428:LEU:O	1:A:428:LEU:HD23	2.11	0.50
1:A:151:LEU:HD12	1:A:190:THR:O	2.11	0.50
1:A:217:ASN:N	1:A:217:ASN:HD22	2.09	0.50
1:A:234:GLU:HB2	1:A:235:ILE:HG22	1.93	0.50
1:A:297:VAL:CG2	2:A:807:NAG:H62	2.41	0.50
1:A:72:ASP:OD2	5:A:1016:HOH:O	2.19	0.50
1:A:457:LEU:HD23	1:A:494:MET:SD	2.52	0.49
1:A:109:THR:HG22	1:A:110:GLN:CG	2.42	0.49
1:A:496:LEU:HD21	1:A:509:ILE:CD1	2.38	0.49
1:A:68:ARG:HD3	1:A:100:ASP:CA	2.43	0.49
1:A:382:ASN:OD1	1:A:385:ASN:N	2.45	0.49
1:A:138:ASN:HD22	1:A:138:ASN:C	2.13	0.49
1:A:155:PRO:HG2	2:A:801:NAG:C7	2.42	0.49
1:A:154:ASP:O	2:A:801:NAG:C8	2.60	0.49
1:A:449:ASP:CB	1:A:532:CYS:N	2.74	0.49
1:A:252:THR:CG2	1:A:253:PRO:HD2	2.43	0.49
1:A:216:ASP:HB2	1:A:217:ASN:ND2	2.27	0.49
1:A:109:THR:HG22	1:A:110:GLN:HG3	1.94	0.49
1:A:397:GLU:OE1	1:A:397:GLU:N	2.45	0.49
1:A:273:THR:H	2:A:803:NAG:HN2	1.60	0.49
1:A:11:GLU:OE2	1:A:69:GLU:OE1	2.30	0.49
1:A:368:SER:OG	1:A:370:PHE:HE1	1.94	0.49
1:A:27:ASN:C	1:A:29:ASP:H	2.15	0.49
1:A:76:LEU:O	1:A:94:ILE:N	2.44	0.49
2:A:809:NAG:H61	2:A:810:NAG:C6	2.39	0.48
1:A:367:LEU:HD13	1:A:412:VAL:CG2	2.43	0.48
2:A:809:NAG:H62	2:A:810:NAG:O6	2.13	0.48
1:A:154:ASP:CG	1:A:155:PRO:HD2	2.33	0.48
1:A:67:ASP:OD2	1:A:69:GLU:HB2	2.13	0.48
1:A:318:THR:CG2	2:A:806:NAG:H5	2.34	0.48
1:A:367:LEU:HB2	1:A:413:THR:O	2.12	0.48
1:A:151:LEU:O	1:A:152:LYS:HB2	2.13	0.48
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.32	0.48
1:A:226:TYR:C	1:A:227:THR:HG23	2.33	0.48
1:A:481:LEU:HA	1:A:481:LEU:HD12	1.50	0.48
1:A:250:PRO:O	1:A:255:TRP:CE3	2.66	0.48
2:A:809:NAG:C6	2:A:810:NAG:C6	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:O	1:A:212:THR:N	2.46	0.48
1:A:281:ILE:O	1:A:281:ILE:HG23	2.13	0.48
1:A:151:LEU:H	1:A:151:LEU:HD12	1.78	0.48
1:A:150:ILE:HD11	1:A:165:ILE:HB	1.96	0.48
1:A:418:SER:O	1:A:419:VAL:HG23	2.14	0.48
1:A:449:ASP:CB	1:A:532:CYS:H	2.22	0.48
1:A:192:GLN:HA	1:A:203:VAL:O	2.13	0.48
1:A:537:ILE:CG1	1:A:538:LYS:N	2.77	0.48
1:A:290:PHE:CE2	1:A:293:ARG:CB	2.92	0.48
1:A:402:LYS:C	1:A:403:ASN:O	2.46	0.48
1:A:403:ASN:HB2	3:A:902:NDG:H8C2	1.87	0.48
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.95	0.48
1:A:186:GLU:OE1	2:A:801:NAG:C6	2.59	0.47
1:A:365:GLN:HA	1:A:416:GLY:HA3	1.95	0.47
1:A:300:ILE:HD12	1:A:300:ILE:N	2.30	0.47
1:A:282:LEU:CD2	1:A:283:THR:N	2.76	0.47
1:A:50:VAL:HB	1:A:51:PHE:CD1	2.50	0.47
1:A:373:ASN:CG	1:A:374:ASP:H	2.18	0.47
1:A:333:VAL:CB	1:A:334:PRO:CD	2.88	0.47
1:A:335:ALA:CB	3:A:811:NDG:C6	2.90	0.47
1:A:225:THR:HA	1:A:318:THR:O	2.14	0.47
1:A:268:PHE:CA	1:A:285:ALA:HB3	2.45	0.47
1:A:241:ARG:HE	1:A:281:ILE:CD1	2.24	0.47
1:A:36:TYR:O	1:A:55:TRP:HA	2.15	0.47
1:A:41:GLN:HA	1:A:45:ASN:HB2	1.95	0.47
1:A:320:THR:CB	2:A:807:NAG:N2	2.78	0.47
2:A:812:NAG:C1	2:A:812:NAG:O7	2.60	0.47
1:A:266:GLY:N	1:A:268:PHE:CE2	2.76	0.47
1:A:522:LEU:HA	1:A:522:LEU:HD23	1.36	0.46
1:A:511:VAL:N	1:A:523:THR:O	2.46	0.46
1:A:23:GLN:HB2	1:A:59:TRP:CE3	2.50	0.46
1:A:3:VAL:HB	1:A:4:ILE:H	1.51	0.46
1:A:227:THR:N	2:A:812:NAG:H2	2.31	0.46
1:A:270:ASN:OD1	1:A:271:ILE:N	2.49	0.46
1:A:301:THR:CG2	1:A:316:THR:HG23	2.45	0.46
1:A:272:THR:HG23	2:A:803:NAG:HN2	1.80	0.46
1:A:421:THR:HG21	2:A:809:NAG:H61	1.98	0.46
1:A:374:ASP:C	1:A:375:PRO:O	2.54	0.46
1:A:514:SER:CA	1:A:517:GLN:O	2.62	0.46
1:A:246:ASP:C	1:A:247:LEU:HD12	2.35	0.46
1:A:100:ASP:OD1	1:A:101:GLN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TYR:O	1:A:227:THR:HG23	2.15	0.46
1:A:451:ASN:O	1:A:534:GLY:CA	2.60	0.46
1:A:461:ASP:HB3	1:A:468:THR:CG2	2.46	0.46
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.16	0.46
1:A:381:VAL:HA	1:A:387:ILE:O	2.17	0.45
1:A:298:LEU:CD2	1:A:298:LEU:N	2.75	0.45
1:A:155:PRO:O	1:A:157:GLU:N	2.43	0.45
1:A:459:ILE:N	1:A:459:ILE:HD12	2.31	0.45
1:A:473:VAL:CG2	1:A:487:LEU:HD21	2.47	0.45
1:A:187:TYR:HE1	1:A:211:ILE:HD11	1.81	0.45
1:A:1:ASP:CG	5:A:1000:HOH:O	2.55	0.45
1:A:271:ILE:O	1:A:271:ILE:HG23	2.15	0.45
1:A:482:THR:O	1:A:483:TRP:CD2	2.70	0.45
1:A:194:THR:CG2	1:A:195:ASP:N	2.79	0.45
1:A:109:THR:CB	1:A:131:SER:HB2	2.46	0.45
1:A:262:ARG:HG3	1:A:299:GLN:HB2	1.98	0.45
1:A:448:CYS:SG	1:A:537:ILE:CG2	3.01	0.45
1:A:380:THR:CG2	1:A:381:VAL:N	2.79	0.45
1:A:187:TYR:CE1	1:A:211:ILE:HD11	2.52	0.45
1:A:152:LYS:O	1:A:189:LEU:HA	2.17	0.45
1:A:408:VAL:O	1:A:426:LEU:N	2.49	0.45
1:A:312:LEU:O	3:A:804:NDG:H8C1	2.17	0.45
1:A:299:GLN:CG	1:A:318:THR:HG23	2.42	0.45
1:A:339:VAL:HG11	1:A:351:ILE:HG23	1.98	0.45
1:A:109:THR:HB	1:A:131:SER:HB2	1.99	0.45
2:A:805:NAG:H62	2:A:806:NAG:N2	2.31	0.44
1:A:352:ILE:CG1	1:A:388:VAL:HB	2.33	0.44
1:A:310:VAL:HG12	1:A:311:PRO:O	2.15	0.44
1:A:227:THR:HG22	1:A:320:THR:HB	1.98	0.44
1:A:365:GLN:CG	1:A:365:GLN:O	2.54	0.44
1:A:380:THR:HG22	1:A:381:VAL:N	2.32	0.44
1:A:22:VAL:CG2	1:A:23:GLN:N	2.81	0.44
1:A:336:VAL:HG12	1:A:338:ARG:CB	2.47	0.44
1:A:108:PHE:HE1	1:A:203:VAL:HG23	1.80	0.44
1:A:286:LYS:C	1:A:287:GLY:O	2.55	0.44
1:A:155:PRO:CB	2:A:801:NAG:C8	2.94	0.44
1:A:276:GLU:HG3	1:A:277:SER:N	2.25	0.44
1:A:194:THR:HG23	1:A:201:LEU:O	2.18	0.44
1:A:450:GLN:CB	1:A:533:GLU:OE2	2.65	0.44
1:A:162:LEU:HB2	1:A:163:PHE:CE1	2.52	0.44
1:A:442:PRO:HD2	1:A:457:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:LEU:C	1:A:426:LEU:HD13	2.37	0.44
1:A:468:THR:C	1:A:469:TYR:O	2.54	0.44
1:A:220:ILE:HG22	1:A:220:ILE:O	2.18	0.44
1:A:513:LEU:C	1:A:514:SER:HG	2.22	0.44
1:A:368:SER:CB	1:A:370:PHE:HE1	2.31	0.43
1:A:247:LEU:HD12	1:A:247:LEU:N	2.33	0.43
1:A:90:GLU:O	1:A:91:PRO:O	2.37	0.43
1:A:232:GLU:HA	1:A:288:LEU:HD12	1.99	0.43
1:A:290:PHE:CD2	1:A:293:ARG:O	2.71	0.43
1:A:518:ASN:C	1:A:520:PRO:CD	2.87	0.43
1:A:421:THR:CG2	1:A:422:GLY:N	2.81	0.43
1:A:151:LEU:N	1:A:151:LEU:HD12	2.33	0.43
1:A:483:TRP:CZ2	1:A:507:TYR:CE1	2.87	0.43
2:A:805:NAG:C5	2:A:806:NAG:H83	2.46	0.43
1:A:449:ASP:N	1:A:532:CYS:HB3	2.19	0.43
1:A:354:LEU:HD12	1:A:386:GLY:O	2.18	0.43
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.81	0.43
1:A:441:SER:CB	1:A:442:PRO:HD3	2.47	0.43
1:A:134:ASP:HB2	1:A:146:LEU:HD11	1.99	0.43
1:A:260:LYS:HE3	1:A:260:LYS:HB3	1.81	0.43
1:A:188:THR:H	2:A:801:NAG:H83	1.84	0.43
1:A:371:ILE:HA	1:A:371:ILE:HD12	1.65	0.43
1:A:138:ASN:ND2	1:A:138:ASN:C	2.73	0.43
1:A:371:ILE:HG13	1:A:410:MET:SD	2.59	0.42
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.42
1:A:409:ILE:HD13	3:A:811:NDG:H8C3	2.01	0.42
1:A:339:VAL:HG21	1:A:351:ILE:HG22	2.01	0.42
1:A:250:PRO:HA	1:A:255:TRP:CG	2.54	0.42
1:A:524:VAL:HG21	2:A:904:NAG:C8	2.44	0.42
1:A:40:GLY:O	1:A:45:ASN:HB2	2.19	0.42
1:A:175:ILE:CG2	1:A:176:GLY:N	2.82	0.42
1:A:419:VAL:HG13	1:A:420:GLY:N	2.33	0.42
1:A:195:ASP:HB3	1:A:196:LEU:HG	2.01	0.42
1:A:461:ASP:HB3	1:A:468:THR:HG22	2.00	0.42
1:A:7:ILE:O	1:A:96:ILE:HG23	2.20	0.42
1:A:333:VAL:HG23	1:A:334:PRO:HD3	2.01	0.42
1:A:108:PHE:HA	1:A:132:ALA:CB	2.50	0.42
1:A:264:ASN:HB3	1:A:267:GLY:HA2	2.01	0.42
1:A:344:ASP:CG	1:A:344:ASP:O	2.57	0.42
1:A:373:ASN:O	1:A:374:ASP:CB	2.64	0.42
1:A:154:ASP:C	2:A:801:NAG:C8	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ARG:HD2	1:A:392:GLY:CA	2.50	0.42
1:A:371:ILE:HA	1:A:410:MET:HB3	2.02	0.42
1:A:515:ASP:OD1	1:A:516:ALA:N	2.53	0.42
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.93	0.41
1:A:347:ARG:HG3	1:A:392:GLY:N	2.33	0.41
1:A:474:SER:N	1:A:512:LEU:O	2.53	0.41
1:A:23:GLN:HA	1:A:58:GLY:O	2.21	0.41
1:A:230:VAL:O	1:A:323:VAL:HA	2.20	0.41
1:A:297:VAL:HG21	2:A:807:NAG:H62	2.01	0.41
1:A:154:ASP:HB3	2:A:801:NAG:C7	2.48	0.41
1:A:239:VAL:HG11	1:A:282:LEU:HD22	2.02	0.41
1:A:67:ASP:CG	1:A:69:GLU:HB2	2.40	0.41
1:A:119:GLU:CG	1:A:214:ALA:HB3	2.51	0.41
1:A:231:PRO:O	1:A:288:LEU:HD12	2.20	0.41
1:A:297:VAL:HG22	2:A:807:NAG:H62	2.03	0.41
1:A:400:TYR:O	1:A:401:VAL:C	2.59	0.41
1:A:440:PRO:HB3	1:A:457:LEU:CD2	2.43	0.41
1:A:367:LEU:HG	1:A:367:LEU:H	1.41	0.41
1:A:237:PHE:N	1:A:284:THR:OG1	2.42	0.41
1:A:118:ARG:CA	1:A:212:THR:HB	2.51	0.41
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.51	0.41
1:A:42:GLY:CA	1:A:47:PRO:O	2.69	0.41
1:A:108:PHE:HA	1:A:132:ALA:HB2	2.03	0.41
1:A:316:THR:OG1	2:A:806:NAG:H83	2.21	0.40
1:A:371:ILE:HD13	1:A:381:VAL:HG11	1.95	0.40
1:A:193:ALA:O	1:A:202:SER:HA	2.21	0.40
1:A:522:LEU:HB3	1:A:523:THR:H	1.57	0.40
1:A:438:PRO:HB2	1:A:513:LEU:CD1	2.51	0.40
1:A:239:VAL:HG13	1:A:240:GLN:N	2.33	0.40
1:A:23:GLN:HB2	1:A:59:TRP:CD2	2.55	0.40
1:A:108:PHE:CZ	1:A:191:VAL:HG23	2.56	0.40
1:A:231:PRO:O	1:A:235:ILE:HD13	2.21	0.40
1:A:409:ILE:HD13	3:A:811:NDG:C8	2.52	0.40
1:A:505:GLY:H	1:A:529:VAL:HB	1.85	0.40
1:A:111:ASP:O	1:A:112:VAL:HG13	2.21	0.40
1:A:290:PHE:CG	1:A:292:LEU:HB2	2.56	0.40
1:A:423:THR:CG2	2:A:810:NAG:N2	2.84	0.40
1:A:223:PRO:HB2	1:A:226:TYR:CZ	2.56	0.40
1:A:127:VAL:HG22	1:A:128:MET:HG3	2.03	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	538/546 (98%)	401 (74%)	92 (17%)	45 (8%)	1 6

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	155	PRO
1	A	235	ILE
1	A	347	ARG
1	A	363	GLN
1	A	364	ILE
1	A	374	ASP
1	A	404	ASN
1	A	467	ASN
1	A	476	SER
1	A	502	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	A	3	VAL
1	A	156	GLU
1	A	260	LYS
1	A	287	GLY
1	A	470	PRO
1	A	503	LYS
1	A	55	TRP
1	A	212	THR
1	A	250	PRO
1	A	333	VAL
1	A	360	ASP
1	A	372	GLY
1	A	377	ARG
1	A	506	ASP

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Mol	Chain	Res	Type
1	A	152	LYS
1	A	223	PRO
1	A	359	PRO
1	A	375	PRO
1	A	160	PRO
1	A	265	GLU
1	A	278	ASN
1	A	289	ASP
1	A	482	THR
1	A	498	PRO
1	A	523	THR
1	A	154	ASP
1	A	307	PRO
1	A	222	ASP
1	A	200	GLY
1	A	47	PRO
1	A	158	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	438/486 (90%)	346 (79%)	92 (21%)	1 6

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	18	PRO
1	A	19	LYS
1	A	27	ASN
1	A	52	ARG
1	A	61	LEU
1	A	66	LEU
1	A	68	ARG
1	A	88	VAL

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Mol	Chain	Res	Type
1	A	91	PRO
1	A	92	MET
1	A	117	VAL
1	A	138	ASN
1	A	146	LEU
1	A	151	LEU
1	A	155	PRO
1	A	156	GLU
1	A	161	ASN
1	A	163	PHE
1	A	189	LEU
1	A	195	ASP
1	A	202	SER
1	A	216	ASP
1	A	217	ASN
1	A	223	PRO
1	A	226	TYR
1	A	231	PRO
1	A	233	ASN
1	A	234	GLU
1	A	235	ILE
1	A	237	PHE
1	A	250	PRO
1	A	253	PRO
1	A	264	ASN
1	A	268	PHE
1	A	273	THR
1	A	277	SER
1	A	278	ASN
1	A	282	LEU
1	A	284	THR
1	A	288	LEU
1	A	298	LEU
1	A	309	SER
1	A	310	VAL
1	A	315	SER
1	A	316	THR
1	A	318	THR
1	A	333	VAL
1	A	336	VAL
1	A	339	VAL
1	A	345	LEU

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Mol	Chain	Res	Type
1	A	353	SER
1	A	354	LEU
1	A	360	ASP
1	A	363	GLN
1	A	365	GLN
1	A	371	ILE
1	A	373	ASN
1	A	375	PRO
1	A	379	LEU
1	A	382	ASN
1	A	384	ASP
1	A	385	ASN
1	A	394	LEU
1	A	395	ASP
1	A	398	SER
1	A	399	GLU
1	A	405	THR
1	A	407	THR
1	A	410	MET
1	A	423	THR
1	A	425	THR
1	A	427	ILE
1	A	428	LEU
1	A	433	VAL
1	A	436	ASN
1	A	447	MET
1	A	448	CYS
1	A	461	ASP
1	A	465	PRO
1	A	466	PRO
1	A	470	PRO
1	A	477	HIS
1	A	492	THR
1	A	509	ILE
1	A	512	LEU
1	A	517	GLN
1	A	518	ASN
1	A	520	PRO
1	A	522	LEU
1	A	523	THR
1	A	532	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	27	ASN
1	A	45	ASN
1	A	104	ASN
1	A	110	GLN
1	A	122	GLN
1	A	138	ASN
1	A	217	ASN
1	A	233	ASN
1	A	240	GLN
1	A	278	ASN
1	A	299	GLN
1	A	373	ASN
1	A	385	ASN
1	A	391	ASN
1	A	455	GLN
1	A	467	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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	801	1	14,14,15	0.65	0	15,19,21	0.92	0
2	NAG	A	802	1	14,14,15	0.73	0	15,19,21	0.81	1 (6%)
2	NAG	A	803	1	14,14,15	0.93	1 (7%)	15,19,21	1.27	2 (13%)
3	NDG	A	804	1	14,14,15	0.64	0	15,19,21	0.82	0
2	NAG	A	805	1	14,14,15	0.70	0	15,19,21	1.17	1 (6%)
2	NAG	A	806	1	14,14,15	0.56	0	15,19,21	1.44	2 (13%)
2	NAG	A	807	1	14,14,15	0.64	0	15,19,21	1.15	1 (6%)
2	NAG	A	808	1	14,14,15	0.67	0	15,19,21	0.69	0
2	NAG	A	809	1	14,14,15	0.78	1 (7%)	15,19,21	0.83	0
2	NAG	A	810	1	14,14,15	0.63	0	15,19,21	1.13	2 (13%)
3	NDG	A	811	1	14,14,15	0.83	0	15,19,21	2.16	1 (6%)
2	NAG	A	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	A	902	1	14,14,15	1.10	1 (7%)	15,19,21	0.96	1 (6%)
3	NDG	A	903	1	14,14,15	0.52	0	15,19,21	0.62	0
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.73	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
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	A	803	1	-	0/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	807	1	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1	-	0/6/23/26	0/1/1/1
2	NAG	A	809	1	-	0/6/23/26	0/1/1/1
2	NAG	A	810	1	-	0/6/23/26	0/1/1/1
3	NDG	A	811	1	-	0/6/23/26	0/1/1/1
2	NAG	A	812	1	-	0/6/23/26	0/1/1/1
3	NDG	A	902	1	-	0/6/23/26	0/1/1/1
3	NDG	A	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	904	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	904	NAG	C1-C2	-2.45	1.49	1.52
2	A	812	NAG	C1-C2	-2.36	1.49	1.52
2	A	809	NAG	C1-C2	-2.07	1.49	1.52
2	A	803	NAG	O5-C5	2.33	1.48	1.43
3	A	902	NDG	C1-C2	3.26	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	811	NDG	C2-N2-C7	-7.85	112.95	123.04
2	A	806	NAG	C2-N2-C7	-3.89	118.04	123.04
2	A	805	NAG	C2-N2-C7	-3.41	118.66	123.04
2	A	807	NAG	C2-N2-C7	-3.30	118.80	123.04
2	A	803	NAG	C2-N2-C7	-3.23	118.88	123.04
2	A	810	NAG	C4-C3-C2	-2.45	107.42	111.23
2	A	806	NAG	C4-C3-C2	-2.44	107.44	111.23
2	A	810	NAG	C1-O5-C5	-2.41	109.19	112.25
2	A	812	NAG	C2-N2-C7	-2.36	120.00	123.04
2	A	904	NAG	C2-N2-C7	-2.23	120.17	123.04
2	A	802	NAG	C2-N2-C7	-2.15	120.28	123.04
3	A	902	NDG	C1-O-C5	2.09	114.90	112.25
2	A	803	NAG	C1-O5-C5	2.54	115.47	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	806	NAG	C1
2	A	805	NAG	C1

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	21	0
2	A	803	NAG	4	0
3	A	804	NDG	2	0
2	A	805	NAG	7	0
2	A	806	NAG	9	0
2	A	807	NAG	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	808	NAG	2	0
2	A	809	NAG	8	0
2	A	810	NAG	12	0
3	A	811	NDG	6	0
2	A	812	NAG	3	0
3	A	902	NDG	8	0
2	A	904	NAG	8	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	540/546 (98%)	-0.42	4 (0%)	89	77	6, 68, 100, 100	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	GLN	2.5
1	A	506	ASP	2.4
1	A	327	ASN	2.1
1	A	417	VAL	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	807	14/15	0.79	0.43	15.53	62,62,62,62	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	801	14/15	0.69	0.36	7.78	39,39,39,39	14
3	NDG	A	811	14/15	0.73	0.37	7.59	100,100,100,100	14
2	NAG	A	803	14/15	0.74	0.45	7.32	63,63,63,63	14
2	NAG	A	806	14/15	0.80	0.30	4.40	64,64,64,64	14
2	NAG	A	805	14/15	0.77	0.31	3.52	89,89,89,89	0
2	NAG	A	808	14/15	0.76	0.45	2.62	83,83,83,83	14
3	NDG	A	804	14/15	0.79	0.28	2.37	51,51,51,51	14
4	CA	A	604	1/1	0.98	0.14	-1.02	12,12,12,12	0
4	CA	A	603	1/1	0.98	0.12	-1.26	10,10,10,10	0
4	CA	A	610	1/1	0.85	0.06	-1.42	70,70,70,70	0
4	CA	A	607	1/1	0.85	0.11	-1.57	90,90,90,90	0
4	CA	A	602	1/1	0.93	0.13	-1.60	15,15,15,15	0
4	CA	A	605	1/1	0.97	0.11	-1.67	10,10,10,10	0
4	CA	A	601	1/1	0.99	0.11	-2.75	5,5,5,5	0
4	CA	A	611	1/1	0.92	0.08	-2.85	85,85,85,85	0
4	CA	A	609	1/1	0.92	0.05	-4.00	69,69,69,69	0
4	CA	A	600	1/1	0.99	0.04	-4.80	22,22,22,22	0
2	NAG	A	904	14/15	0.64	0.28	-	27,27,27,27	14
2	NAG	A	812	14/15	0.73	0.42	-	67,67,67,67	14
2	NAG	A	810	14/15	0.55	0.62	-	78,78,78,78	14
2	NAG	A	802	14/15	0.74	0.38	-	99,99,99,99	14
2	NAG	A	809	14/15	0.88	0.26	-	100,100,100,100	0
3	NDG	A	903	14/15	0.67	0.25	-	56,56,56,56	14
4	CA	A	608	1/1	0.98	0.05	-	34,34,34,34	0
4	CA	A	606	1/1	0.97	0.08	-	37,37,37,37	0
3	NDG	A	902	14/15	0.81	0.29	-	37,37,37,37	14

6.5 Other polymers (i)

There are no such residues in this entry.