Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 04:28 AM EDT

PDB ID	:	5LG6
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 (i) 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 (i)) were used in the production of this report:

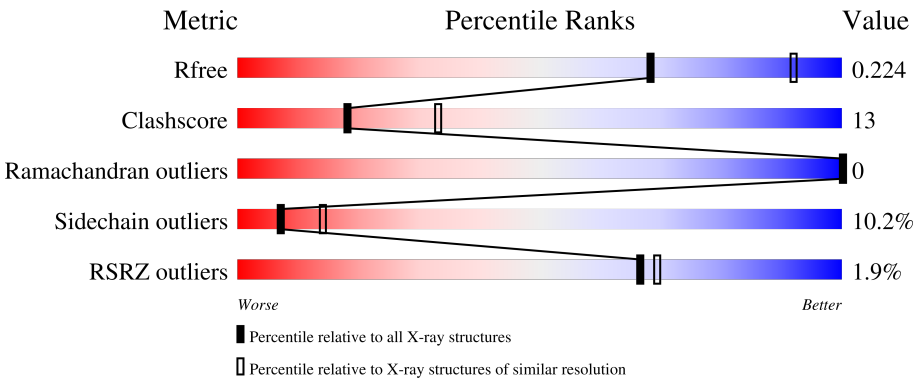
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	2% 67% 20% • 8%
1	B	968	2% 67% 20% • 8%

2 Entry composition (i)

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
			Total	C	N	O	S	Se			
1	A	889	7154	4578	1190	1356	6	24	0	0	0
1	B	887	7138	4564	1188	1356	6	24	0	0	0

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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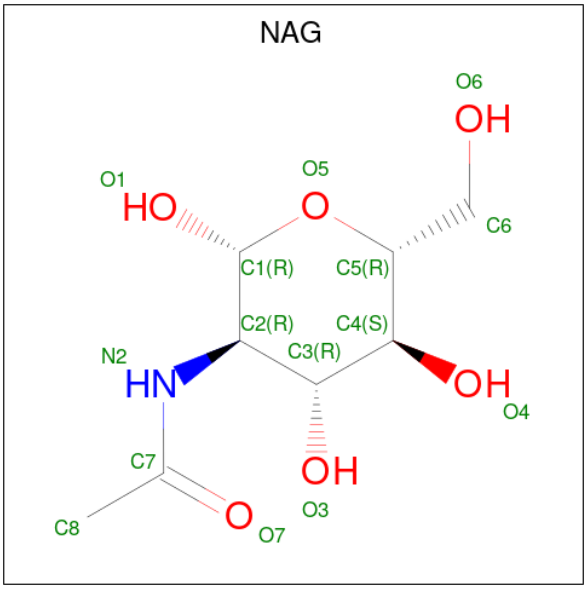
Chain	Residue	Modelled	Actual	Comment	Reference
B	970	GLU	-	expression tag	UNP P15145
B	971	HIS	-	expression tag	UNP P15145
B	972	SER	-	expression tag	UNP P15145
B	973	LEU	-	expression tag	UNP P15145
B	974	VAL	-	expression tag	UNP P15145
B	975	PRO	-	expression tag	UNP P15145
B	976	ARG	-	expression tag	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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

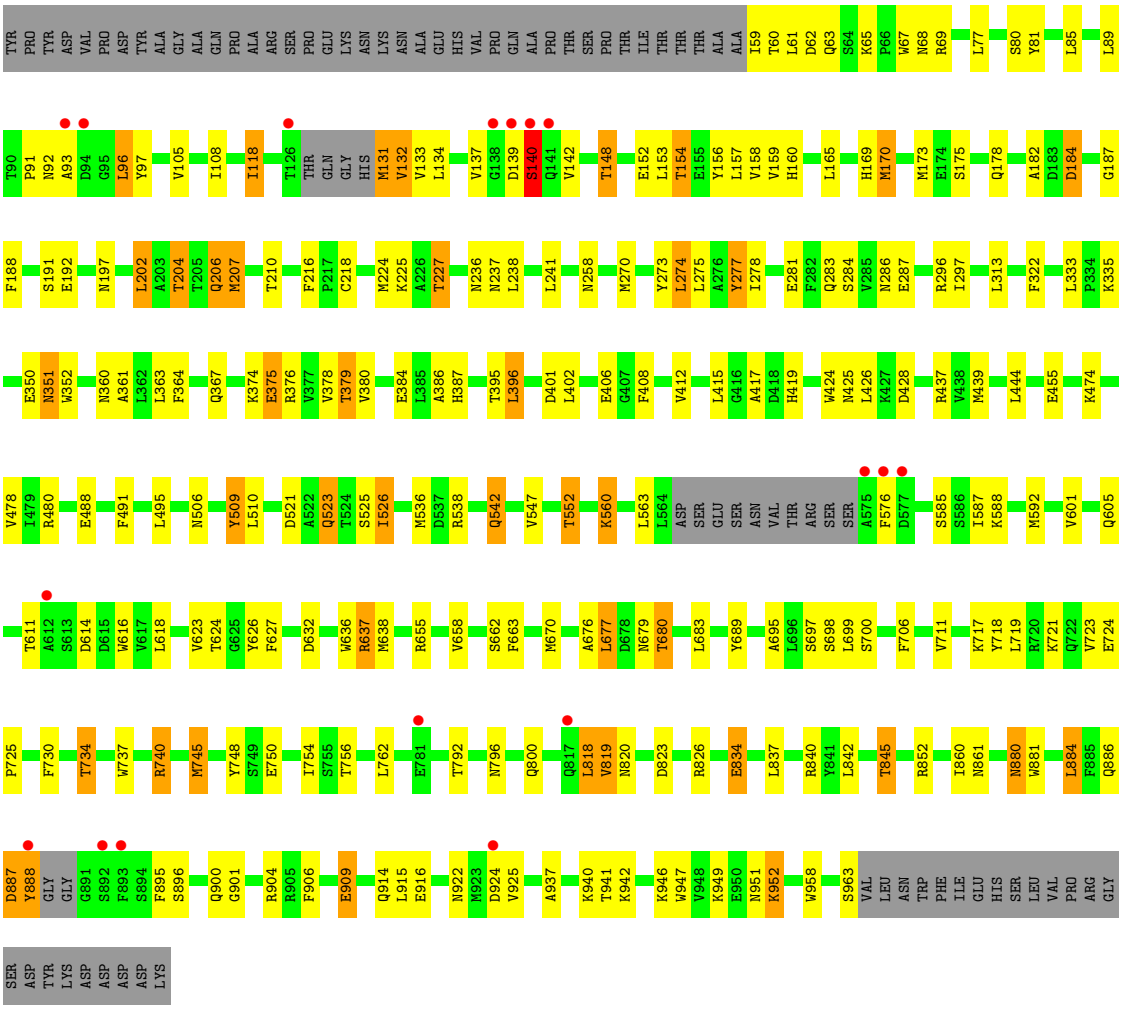
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	216	216	216	0	0
			Total	O		
4	B	165	165	165	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

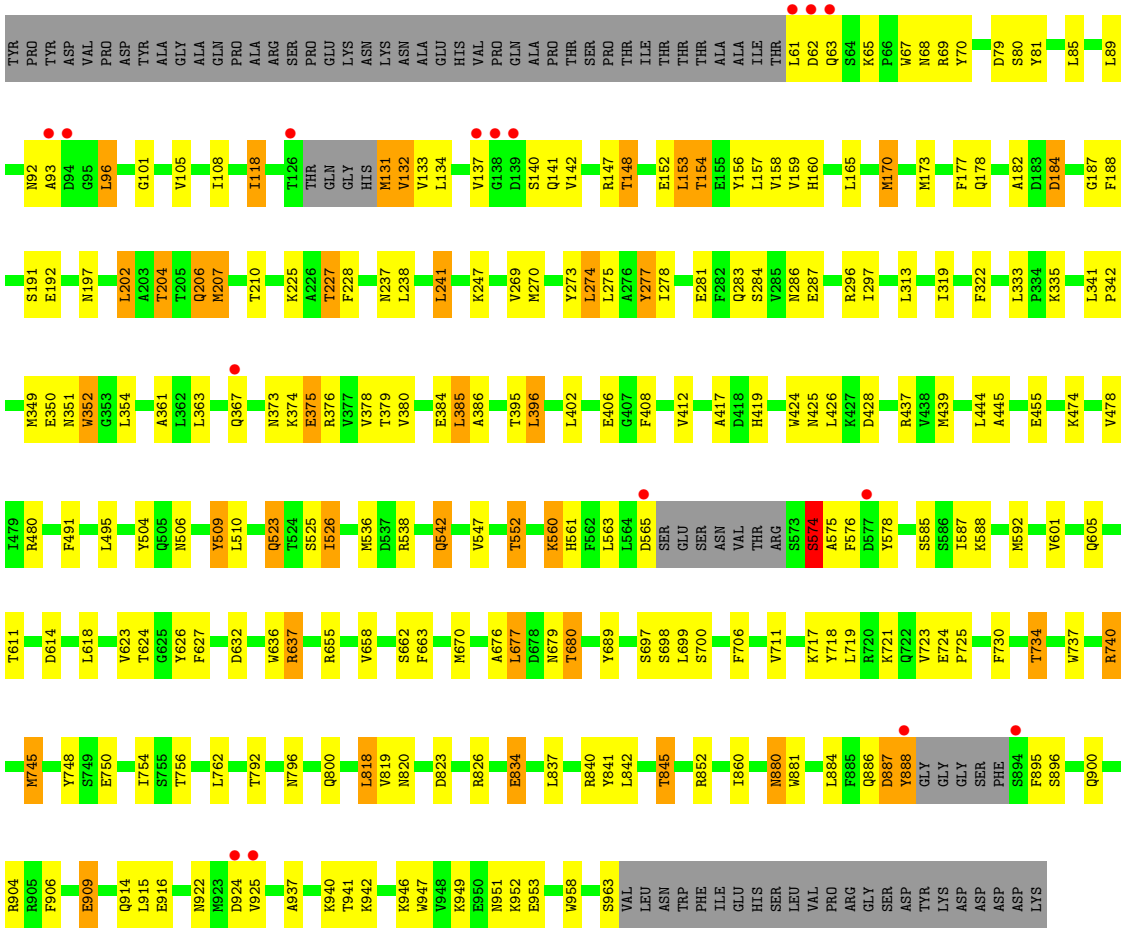
• Molecule 1: Aminopeptidase N

Chain A:



• Molecule 1: Aminopeptidase N

Chain B:


TYR PRO TYR ASP VAL PRO ASP TYR ALA GLY ALA GLN PRO ALA ARG SER PRO GLU LYS ASN LYS ASN ALA GLU HIS VAL PRO GLN ALA PRO THR SER PRO THR ILE THR THR THR ALA ALA ILE THR L61 D62 Q63 S64 K65 P66 W67 N68 R69 Y70 D79 S80 Y81 L85 L89
N92 A93 D94 G95 L96 G101 V105 I108 I118 T126 THR GLN GLY HIS M131 V132 V133 L134 V137 G138 D139 S140 Q141 V142 R147 T148 E152 L153 T154 E155 Y156 L157 V158 V159 H160 L165 M170 M173 F177 Q178 A182 D183 D184 G187 F188
S191 E192 N197 L202 A203 T204 T205 Q206 M207 T210 K225 A226 T227 F228 N237 L238 L241 K247 V269 M270 Y273 L274 L275 A276 Y277 I278 E281 F282 Q283 S284 V285 N286 E287 R296 I297 L313 I319 F322 L333 P334 K335 L341 P342
M349 E350 N351 W352 G353 L354 A361 L362 L363 Q367 N373 K374 E375 R376 V377 V378 T379 V380 E384 L385 A386 T395 L396 L402 E406 G407 F408 V412 A417 D418 H419 W424 N425 L426 K427 D428 R437 V438 M439 L444 A445 E455 K474 V478
I479 R480 F491 L495 Y504 Q505 N506 Y509 L510 Q523 T524 S525 I526 M536 D537 R538 Q542 V547 T552 K560 H561 F562 L563 L564 D565 SER GLU SER ASN VAL THR ARG S573 S574 A575 F576 D577 Y578 S585 S586 I587 K588 M592 V601 Q605
T611 D614 L618 V623 T624 G625 Y626 F627 D632 W636 R637 R655 V658 S662 F663 M670 A676 L677 D678 N679 T680 Y689 S697 S698 L699 S700 F706 V711 K717 Y718 L719 R720 K721 Q722 V723 E724 P725 F730 T734 W737 R740
M745 Y748 S749 E750 I754 S755 T756 L762 T792 N796 Q800 L818 V819 N820 D823 R826 E834 L837 R840 Y841 L842 T845 R852 I860 N880 W881 L884 F885 Q886 D887 Y888 GLY GLY GLY SER PHE S894 F895 S896 Q900
R904 R905 F906 E909 Q914 L915 E916 N922 M923 D924 V925 A937 K940 T941 K942 K946 W947 Y948 K949 E950 N951 K952 E953 W958 S963 VAL LEU ASN TRP PHE ILE GLU HIS SER LEU VAL PRO ARG GLY SER ASP TYR LYS ASP ASP ASP ASP LYS

4 Data and refinement statistics (i)

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) 93.8 (24.98-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.10 (at 2.50Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.191 , 0.229 0.185 , 0.224	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 , 29.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	2/7315 (0.0%)	0.62	2/9929 (0.0%)
1	B	0.46	4/7298 (0.1%)	0.62	1/9906 (0.0%)
All	All	0.46	6/14613 (0.0%)	0.62	3/19835 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	350	GLU	CG-CD	-8.99	1.38	1.51
1	B	909	GLU	CD-OE2	-6.56	1.18	1.25
1	A	909	GLU	CD-OE2	-6.25	1.18	1.25
1	B	909	GLU	CD-OE1	-5.75	1.19	1.25
1	A	909	GLU	CD-OE1	-5.74	1.19	1.25
1	B	350	GLU	CB-CG	-5.19	1.42	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	909	GLU	CA-CB-CG	6.34	127.35	113.40
1	A	909	GLU	CA-CB-CG	6.13	126.88	113.40
1	A	140	SER	N-CA-C	-5.50	96.16	111.00

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 (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	7154	0	6924	184	1
1	B	7138	0	6904	193	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	383	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 13.

All (383) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:B:202:LEU:HD23	1:B:202:LEU:C	2.14	0.68
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:A:587:ILE:HG22	1:A:618:LEU:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:202:LEU:C	1:A:202:LEU:HD23	2.16	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
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: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:A:80:SER:HG	1:A:227:THR:HG22	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:LEU:O	1:B:680:THR:HB	2.09	0.53
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:B:80:SER:HG	1:B:227:THR:HG22	1.74	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:182:ALA:C	1:A:184:ASP:H	2.15	0.48
1:B:137:VAL:HG13	1:B:137:VAL:O	2.13	0.48
1:A:206:GLN:C	1:A:207:MSE:HE3	2.34	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:575:ALA:C	1:B:576:PHE:HD1	2.16	0.48
1:A:697:SER:O	1:A:700:SER:HB3	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLU:HB2	1:B:313:LEU:HD11	1.97	0.47
1:B:182:ALA:C	1:B:184:ASP:H	2.18	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:204:THR:HG23	1:B:278:ILE:HG23	1.99	0.43
1:B:351:ASN:ND2	1:B:351:ASN:N	2.65	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: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:445:ALA:HB2	1:B:565:ASP:CG	2.38	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:206:GLN:C	1:B:207:MSE:HE3	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:202:LEU:CD2	1:B:202:LEU:C	2.87	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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 (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	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 (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	787/830 (95%)	708 (90%)	79 (10%)	7 15
1	B	786/830 (95%)	705 (90%)	81 (10%)	7 14
All	All	1573/1660 (95%)	1413 (90%)	160 (10%)	7 14

All (160) 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	188	PHE
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
1	A	333	LEU
1	A	335	LYS
1	A	351	ASN
1	A	363	LEU
1	A	375	GLU
1	A	378	VAL
1	A	379	THR

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Mol	Chain	Res	Type
1	A	396	LEU
1	A	415	LEU
1	A	437	ARG
1	A	444	LEU
1	A	455	GLU
1	A	509	TYR
1	A	523	GLN
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	588	LYS
1	A	601	VAL
1	A	605	GLN
1	A	614	ASP
1	A	624	THR
1	A	637	ARG
1	A	677	LEU
1	A	680	THR
1	A	721	LYS
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
1	A	840	ARG
1	A	845	THR
1	A	880	ASN
1	A	884	LEU
1	A	886	GLN
1	A	887	ASP
1	A	888	TYR
1	A	896	SER
1	A	909	GLU
1	A	914	GLN
1	A	915	LEU
1	A	916	GLU
1	A	924	ASP

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Mol	Chain	Res	Type
1	A	940	LYS
1	A	952	LYS
1	B	62	ASP
1	B	89	LEU
1	B	96	LEU
1	B	118	ILE
1	B	131	MSE
1	B	132	VAL
1	B	134	LEU
1	B	140	SER
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	188	PHE
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
1	B	241	LEU
1	B	274	LEU
1	B	277	TYR
1	B	283	GLN
1	B	333	LEU
1	B	335	LYS
1	B	352	TRP
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	444	LEU
1	B	455	GLU

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Mol	Chain	Res	Type
1	B	509	TYR
1	B	523	GLN
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	588	LYS
1	B	601	VAL
1	B	605	GLN
1	B	614	ASP
1	B	624	THR
1	B	637	ARG
1	B	677	LEU
1	B	680	THR
1	B	721	LYS
1	B	734	THR
1	B	740	ARG
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	841	TYR
1	B	845	THR
1	B	880	ASN
1	B	884	LEU
1	B	886	GLN
1	B	887	ASP
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	952	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	351	ASN
1	A	542	GLN
1	A	880	ASN
1	B	351	ASN
1	B	880	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 monosaccharides 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	B	1009	1	14,14,15	0.57	0	17,19,21	1.24	1 (5%)
2	NAG	B	1004	1	14,14,15	0.50	0	17,19,21	0.63	0
2	NAG	A	1001	1	14,14,15	0.67	0	17,19,21	1.09	2 (11%)
2	NAG	A	1004	1	14,14,15	0.50	0	17,19,21	1.31	3 (17%)
2	NAG	A	1008	1	14,14,15	0.56	0	17,19,21	0.85	0
2	NAG	B	1008	1	14,14,15	0.68	0	17,19,21	1.48	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	1006	1	14,14,15	0.46	0	17,19,21	1.28	1 (5%)
2	NAG	A	1005	1	14,14,15	0.60	0	17,19,21	1.33	3 (17%)
2	NAG	A	1009	1	14,14,15	0.53	0	17,19,21	1.42	1 (5%)
2	NAG	A	1003	1	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
2	NAG	B	1001	1	14,14,15	0.63	0	17,19,21	0.79	0
2	NAG	B	1007	1	14,14,15	0.48	0	17,19,21	1.36	1 (5%)
2	NAG	B	1005	1	14,14,15	0.48	0	17,19,21	0.89	0
2	NAG	B	1002	1	14,14,15	0.62	0	17,19,21	1.21	3 (17%)
2	NAG	B	1006	1	14,14,15	0.41	0	17,19,21	1.59	3 (17%)
2	NAG	A	1007	1	14,14,15	0.52	0	17,19,21	1.43	1 (5%)
2	NAG	A	1002	1	14,14,15	0.57	0	17,19,21	0.92	0
2	NAG	B	1003	1	14,14,15	0.58	0	17,19,21	0.74	1 (5%)

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

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1009	NAG	C1-O5-C5	4.95	118.90	112.19
2	A	1007	NAG	C1-O5-C5	4.67	118.52	112.19
2	B	1007	NAG	C1-O5-C5	4.26	117.96	112.19
2	B	1006	NAG	C2-N2-C7	-4.12	117.03	122.90
2	B	1009	NAG	C1-O5-C5	4.01	117.63	112.19
2	A	1006	NAG	C2-N2-C7	-3.46	117.97	122.90
2	B	1006	NAG	C1-O5-C5	3.06	116.34	112.19
2	B	1008	NAG	C3-C4-C5	3.05	115.68	110.24
2	A	1001	NAG	C2-N2-C7	-3.04	118.58	122.90
2	B	1008	NAG	O5-C1-C2	-2.89	106.73	111.29
2	B	1002	NAG	C3-C4-C5	-2.70	105.43	110.24
2	A	1005	NAG	C3-C4-C5	2.64	114.94	110.24
2	A	1003	NAG	C2-N2-C7	-2.56	119.25	122.90
2	A	1004	NAG	C1-O5-C5	2.54	115.63	112.19
2	B	1008	NAG	C6-C5-C4	-2.53	107.08	113.00
2	B	1003	NAG	O5-C5-C6	2.43	111.01	107.20
2	A	1005	NAG	O5-C5-C6	2.33	110.85	107.20
2	A	1004	NAG	C3-C4-C5	2.31	114.36	110.24
2	B	1002	NAG	O5-C5-C6	2.27	110.76	107.20
2	A	1001	NAG	O5-C1-C2	-2.13	107.93	111.29
2	B	1002	NAG	O4-C4-C5	2.06	114.41	109.30
2	A	1005	NAG	C6-C5-C4	-2.03	108.25	113.00
2	B	1006	NAG	C4-C3-C2	-2.01	108.08	111.02
2	A	1004	NAG	C6-C5-C4	-2.01	108.31	113.00

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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

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Mol	Chain	Res	Type	Atoms
2	B	1001	NAG	O7-C7-N2-C2
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	O5-C5-C6-O6
2	B	1005	NAG	O5-C5-C6-O6
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	B	1009	NAG	3	0
2	A	1001	NAG	1	0
2	B	1008	NAG	2	0
2	A	1005	NAG	2	0
2	A	1009	NAG	1	0
2	A	1003	NAG	1	0
2	B	1001	NAG	1	0
2	B	1002	NAG	3	0
2	A	1002	NAG	1	0
2	B	1003	NAG	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.35	17 (1%)	65	68	4, 16, 43, 84	1 (0%)
1	B	863/968 (89%)	-0.32	16 (1%)	66	69	4, 16, 44, 83	1 (0%)
All	All	1728/1936 (89%)	-0.34	33 (1%)	66	69	4, 16, 44, 84	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	LEU	7.2
1	A	93	ALA	5.7
1	B	925	VAL	5.2
1	B	137	VAL	5.0
1	A	94	ASP	4.5
1	A	893	PHE	4.3
1	B	924	ASP	4.1
1	A	888	TYR	4.0
1	B	138	GLY	4.0
1	B	888	TYR	3.9
1	B	93	ALA	3.7
1	B	565	ASP	3.7
1	B	126	THR	3.5
1	B	894	SER	3.4
1	A	575	ALA	3.2
1	A	892	SER	3.0
1	A	612	ALA	2.8
1	A	138	GLY	2.8
1	A	141	GLN	2.8
1	A	140	SER	2.7
1	B	63	GLN	2.7
1	A	139	ASP	2.6
1	B	139	ASP	2.6
1	A	126	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	924	ASP	2.5
1	A	577	ASP	2.5
1	B	94	ASP	2.4
1	B	577	ASP	2.4
1	B	367	GLN	2.4
1	A	781	GLU	2.3
1	A	576	PHE	2.3
1	A	817	GLN	2.2
1	B	62	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å^2)	Q<0.9
2	NAG	B	1004	14/15	0.82	0.27	30,56,62,62	0
2	NAG	B	1003	14/15	0.87	0.23	38,49,59,61	0
2	NAG	B	1005	14/15	0.87	0.28	44,62,72,74	0
2	NAG	B	1001	14/15	0.88	0.28	30,50,62,64	0
2	NAG	A	1001	14/15	0.88	0.18	38,46,54,57	0
2	NAG	A	1003	14/15	0.88	0.20	32,43,52,55	0
2	NAG	A	1008	14/15	0.88	0.22	37,48,57,67	0
2	NAG	A	1004	14/15	0.89	0.19	26,41,50,53	0
2	NAG	B	1008	14/15	0.90	0.20	28,38,48,51	0
2	NAG	A	1005	14/15	0.92	0.19	13,27,44,47	0
2	NAG	B	1002	14/15	0.92	0.18	12,18,26,26	0
2	NAG	A	1009	14/15	0.92	0.23	25,34,43,54	0
2	NAG	B	1009	14/15	0.92	0.23	27,40,56,59	0
2	NAG	B	1007	14/15	0.93	0.16	24,29,40,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	1006	14/15	0.94	0.12	18,24,29,49	0
2	NAG	A	1007	14/15	0.95	0.18	19,26,35,37	0
2	NAG	A	1006	14/15	0.95	0.10	14,18,24,26	0
2	NAG	A	1002	14/15	0.96	0.11	9,14,19,24	0
3	ZN	B	1010	1/1	0.99	0.04	18,18,18,18	0
3	ZN	A	1010	1/1	1.00	0.03	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.