Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 03:30 PM EDT

PDB ID	:	2NSX
Title	:	Structure of acid-beta-glucosidase with pharmacological chaperone provides insight into Gaucher disease
Authors	:	Lieberman, R.L.; Petsko, G.A.; Ringe, D.
Deposited on	:	2006-11-06
Resolution	:	2.11 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:

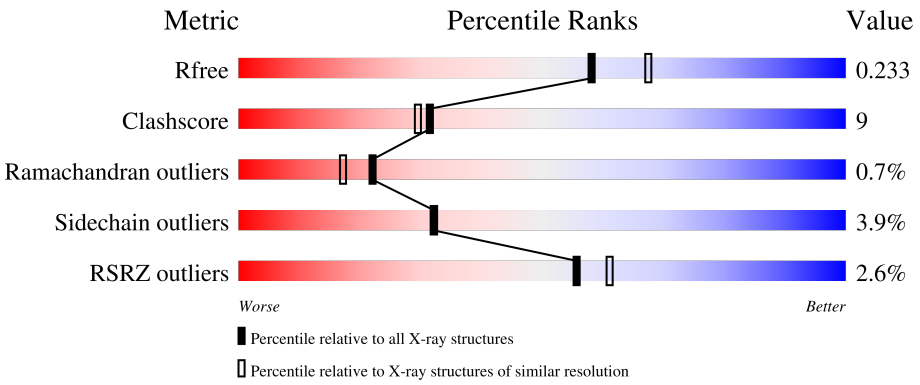
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	497	4% 85% 13% •
1	B	497	2% 84% 14% •
1	C	497	4% 82% 16% • •
1	D	497	% 81% 17% •

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	498	X	-	-	-
2	NAG	C	498	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16918 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.

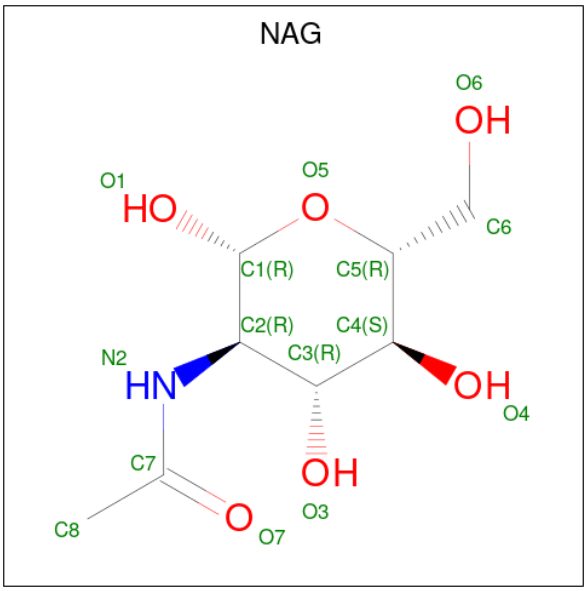
- Molecule 1 is a protein called Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3930	2532	671	711	16	0	0	0
1	B	497	3930	2532	671	711	16	0	0	0
1	C	497	3930	2532	671	711	16	0	0	0
1	D	497	3930	2532	671	711	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

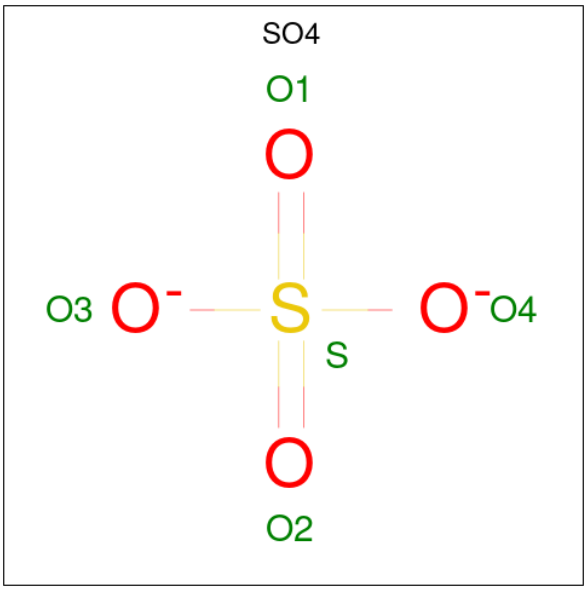
Chain	Residue	Modelled	Actual	Comment	Reference
A	495	HIS	ARG	conflict	UNP P04062
B	495	HIS	ARG	conflict	UNP P04062
C	495	HIS	ARG	conflict	UNP P04062
D	495	HIS	ARG	conflict	UNP P04062

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



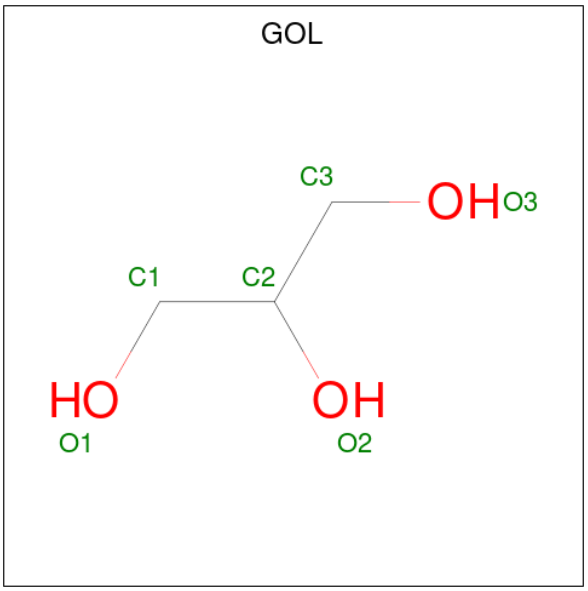
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0
2	D	1	14	8	1	5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



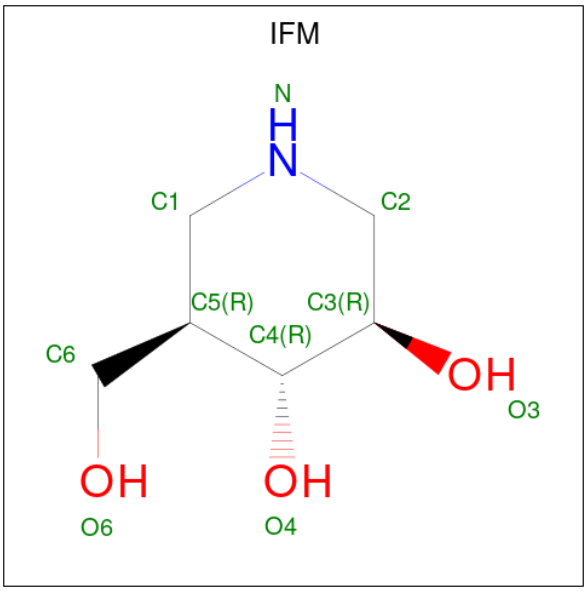
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	C	1	5	4	1	0	0
			Total	O	S		
3	C	1	5	4	1	0	0
			Total	O	S		
3	C	1	5	4	1	0	0
			Total	O	S		
3	D	1	5	4	1	0	0
			Total	O	S		
3	D	1	5	4	1	0	0
			Total	O	S		
3	D	1	5	4	1	0	0
			Total	O	S		
3	D	1	5	4	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	6	3	3		0	0
			Total	C	O			
4	C	1	6	3	3		0	0

- Molecule 5 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (three-letter code: IFM) (formula: $C_6H_{13}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	10	6	1	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	D	1	10	6	1	3	0	0

- Molecule 6 is water.

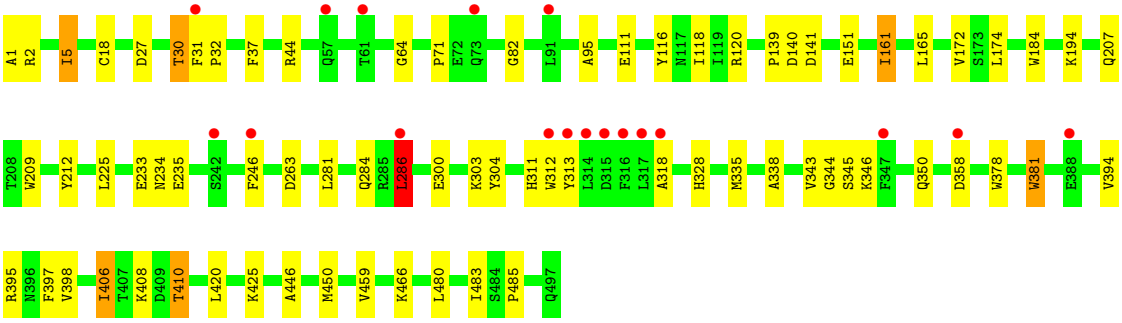
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	258	258	258	0	0
			Total	O		
6	B	246	246	246	0	0
			Total	O		
6	C	260	260	260	0	0
			Total	O		
6	D	242	242	242	0	0

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.

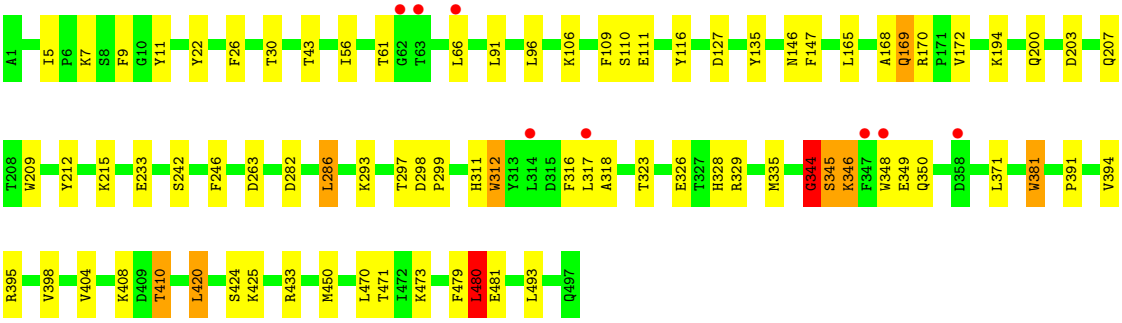
- Molecule 1: Glucosylceramidase

Chain A:



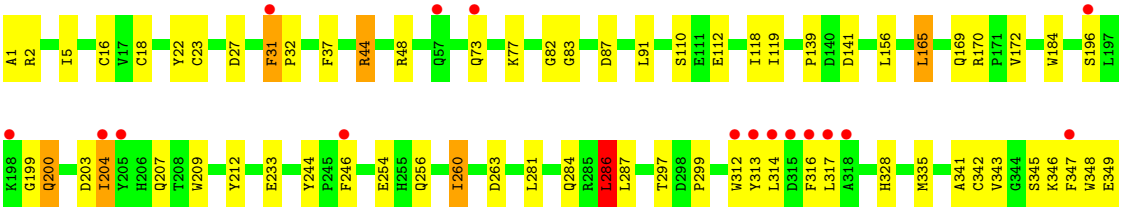
- Molecule 1: Glucosylceramidase

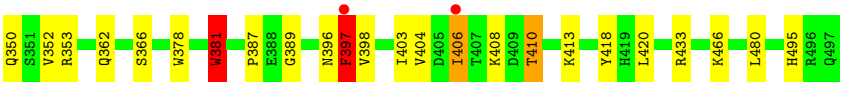
Chain B:



- Molecule 1: Glucosylceramidase

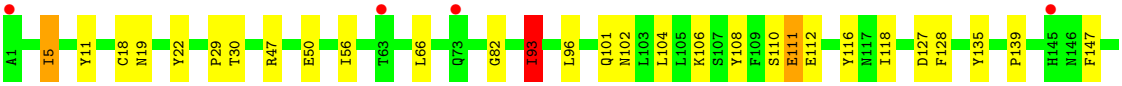
Chain C:

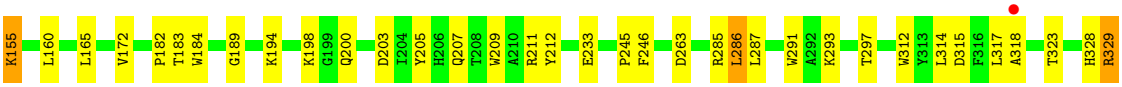


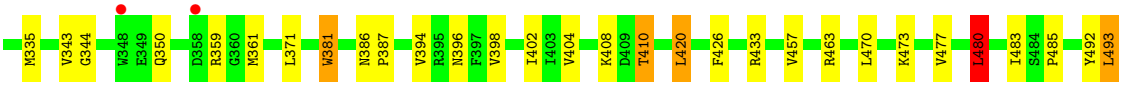


- Molecule 1: Glucosylceramidase

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.97Å 92.22Å 152.67Å 90.00° 110.94° 90.00°	Depositor
Resolution (Å)	50.00 – 2.11 46.91 – 2.11	Depositor EDS
% Data completeness (in resolution range)	91.3 (50.00-2.11) 91.2 (46.91-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.94 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.191 , 0.235 0.191 , 0.233	Depositor DCC
R_{free} test set	7501 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 28.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16918	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: SO4, GOL, NAG, IFM

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	0.69	0/4051	0.74	1/5523 (0.0%)
1	B	0.70	0/4051	0.72	2/5523 (0.0%)
1	C	0.70	0/4051	0.74	4/5523 (0.1%)
1	D	0.71	0/4051	0.74	4/5523 (0.1%)
All	All	0.70	0/16204	0.74	11/22092 (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	B	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	286	LEU	CA-CB-CG	-10.55	91.03	115.30
1	C	286	LEU	CA-CB-CG	6.98	131.35	115.30
1	B	344	GLY	N-CA-C	6.75	129.99	113.10
1	D	317	LEU	CA-CB-CG	6.08	129.29	115.30
1	C	397	PHE	N-CA-C	5.93	127.00	111.00
1	D	480	LEU	CA-CB-CG	5.72	128.46	115.30
1	C	433	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	93	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	D	359	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	165	LEU	CA-CB-CG	5.21	127.27	115.30
1	B	480	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	344	GLY	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	3930	0	3843	63	0
1	B	3930	0	3843	57	0
1	C	3930	0	3843	95	0
1	D	3930	0	3846	73	0
2	A	14	0	13	1	0
2	B	28	0	26	0	0
2	C	14	0	13	1	0
2	D	14	0	13	3	0
3	A	25	0	0	1	0
3	B	30	0	0	0	0
3	C	15	0	0	1	0
3	D	20	0	0	0	0
4	A	6	0	8	0	0
4	C	6	0	8	3	0
5	B	10	0	13	0	0
5	D	10	0	13	0	0
6	A	258	0	0	12	0
6	B	246	0	0	6	0
6	C	260	0	0	17	0
6	D	242	0	0	13	0
All	All	16918	0	15482	278	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 9.

All (278) 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:D:19:ASN:HD21	2:D:498:NAG:C1	1.25	1.49
1:C:312:TRP:CZ3	1:C:314:LEU:HB2	1.57	1.39
1:D:329:ARG:HG2	1:D:329:ARG:HH11	1.04	1.11
1:A:286:LEU:HD22	1:B:317:LEU:HA	1.33	1.07
1:C:73:GLN:OE1	6:C:655:HOH:O	1.70	1.07
1:B:346:LYS:HD2	1:B:348:TRP:NE1	1.70	1.06
1:D:93:ILE:HB	6:D:742:HOH:O	1.58	1.03
1:B:345:SER:HB3	6:B:612:HOH:O	1.61	1.00
1:C:312:TRP:CE3	1:C:314:LEU:HB2	1.97	1.00
1:D:102:ASN:HB3	6:D:736:HOH:O	1.62	0.99
1:A:286:LEU:CD2	1:B:317:LEU:HA	1.94	0.97
1:A:286:LEU:HB3	6:A:761:HOH:O	1.63	0.97
1:D:56:ILE:HG21	1:D:477:VAL:HG12	1.47	0.95
1:C:328:HIS:HD2	6:C:544:HOH:O	1.53	0.90
1:D:329:ARG:HG2	1:D:329:ARG:NH1	1.85	0.88
1:C:312:TRP:CZ3	1:C:314:LEU:CB	2.53	0.84
1:A:286:LEU:HD12	1:A:318:ALA:HB1	1.59	0.84
1:C:5:ILE:HD12	1:C:22:TYR:CE2	2.14	0.82
1:B:346:LYS:HD2	1:B:348:TRP:HE1	1.43	0.81
1:D:329:ARG:HH11	1:D:329:ARG:CG	1.90	0.81
1:C:346:LYS:HG2	6:C:762:HOH:O	1.81	0.79
1:C:312:TRP:HZ3	1:C:314:LEU:HB2	1.47	0.77
1:A:286:LEU:CD1	1:A:318:ALA:HB1	2.15	0.77
1:C:396:ASN:O	6:C:588:HOH:O	2.01	0.77
1:A:328:HIS:HD2	6:A:532:HOH:O	1.67	0.76
1:B:66:LEU:HD11	1:B:473:LYS:HB2	1.69	0.74
1:B:345:SER:H	1:B:398:VAL:HG12	1.52	0.74
1:D:29:PRO:HD3	1:D:111:GLU:HG3	1.70	0.73
1:A:95:ALA:HB1	1:A:406:ILE:HG21	1.71	0.71
1:B:328:HIS:HD2	6:B:539:HOH:O	1.74	0.70
1:A:346:LYS:HA	6:A:576:HOH:O	1.91	0.70
1:C:381:TRP:NE1	4:C:502:GOL:H32	2.07	0.69
1:B:344:GLY:HA2	1:B:349:GLU:OE2	1.92	0.69
1:D:56:ILE:HG12	1:D:480:LEU:HD22	1.73	0.69
1:C:312:TRP:CD2	1:C:314:LEU:HD13	2.28	0.69
1:C:312:TRP:CE2	1:C:341:ALA:HB1	2.28	0.69
1:A:161:ILE:CD1	1:A:225:LEU:HD13	2.23	0.68
1:A:312:TRP:HB3	6:A:749:HOH:O	1.94	0.68
1:D:93:ILE:CB	6:D:742:HOH:O	2.28	0.68
1:B:207:GLN:NE2	1:B:263:ASP:OD1	2.22	0.68
1:C:312:TRP:CZ2	1:C:378:TRP:HZ2	2.13	0.67
1:A:161:ILE:HD13	1:A:225:LEU:HD13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:HIS:HD2	6:D:544:HOH:O	1.79	0.66
1:C:314:LEU:HD21	1:C:366:SER:HB2	1.78	0.65
1:C:381:TRP:HE1	4:C:502:GOL:H32	1.62	0.65
1:A:95:ALA:CB	1:A:406:ILE:HG21	2.27	0.65
1:C:31:PHE:CD1	1:C:31:PHE:N	2.64	0.64
1:D:211:ARG:HG2	6:D:745:HOH:O	1.97	0.64
1:A:161:ILE:HD11	1:A:174:LEU:HD11	1.80	0.63
1:D:102:ASN:CB	6:D:736:HOH:O	2.34	0.63
1:C:204:ILE:HG12	6:C:572:HOH:O	1.98	0.62
1:B:326:GLU:OE1	1:B:329:ARG:HD2	1.99	0.62
1:C:408:LYS:O	1:C:410:THR:HG23	2.00	0.62
1:C:312:TRP:CZ2	1:C:341:ALA:HB1	2.35	0.62
1:D:93:ILE:HG22	1:D:104:LEU:HD13	1.81	0.61
1:C:389:GLY:O	6:C:588:HOH:O	2.16	0.61
1:C:346:LYS:HA	6:C:648:HOH:O	2.01	0.61
1:D:198:LYS:HE2	1:D:205:TYR:CZ	2.36	0.61
1:B:345:SER:CB	6:B:612:HOH:O	2.31	0.60
1:B:5:ILE:CD1	1:B:22:TYR:CE2	2.84	0.60
1:C:312:TRP:NE1	1:C:378:TRP:CZ2	2.68	0.60
1:A:397:PHE:CD1	1:A:398:VAL:HG13	2.36	0.60
1:D:116:TYR:OH	1:D:420:LEU:HD13	2.01	0.60
1:C:312:TRP:CH2	1:C:314:LEU:HD22	2.37	0.60
1:C:314:LEU:HD21	6:C:752:HOH:O	2.01	0.60
1:C:410:THR:HG21	6:C:761:HOH:O	2.00	0.59
1:C:110:SER:HB2	6:C:747:HOH:O	2.03	0.59
1:A:151:GLU:CD	1:D:155:LYS:HZ2	2.04	0.59
1:A:313:TYR:OH	1:A:345:SER:N	2.30	0.59
1:A:30:THR:O	1:A:32:PRO:HD3	2.03	0.59
1:D:102:ASN:O	1:D:106:LYS:HG3	2.03	0.59
1:A:207:GLN:NE2	1:A:263:ASP:OD1	2.27	0.58
1:D:410:THR:HG21	6:D:708:HOH:O	2.02	0.58
1:B:408:LYS:O	1:B:410:THR:HG23	2.03	0.57
1:A:406:ILE:HG23	6:A:751:HOH:O	2.05	0.57
1:C:18:CYS:O	1:C:410:THR:HB	2.05	0.57
1:C:91:LEU:HD23	1:C:156:LEU:HD13	1.84	0.57
1:C:346:LYS:HG3	1:C:349:GLU:HB2	1.86	0.57
1:C:347:PHE:CZ	1:D:396:ASN:HB3	2.40	0.57
1:A:286:LEU:HD13	1:B:317:LEU:HD22	1.85	0.57
1:D:93:ILE:HG13	6:D:742:HOH:O	2.03	0.57
1:B:5:ILE:HD12	1:B:22:TYR:CE2	2.39	0.57
1:A:5:ILE:HD11	6:A:707:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:SER:N	1:B:398:VAL:HG12	2.20	0.56
1:B:56:ILE:HG12	1:B:480:LEU:HD22	1.86	0.56
1:D:93:ILE:O	1:D:101:GLN:HG2	2.06	0.56
1:B:371:LEU:O	1:B:433:ARG:HD2	2.07	0.55
1:C:312:TRP:CZ2	1:C:378:TRP:CZ2	2.93	0.55
1:A:82:GLY:HA3	1:A:118:ILE:O	2.06	0.55
1:B:194:LYS:HB2	1:B:242:SER:HA	1.88	0.55
1:D:343:VAL:HG12	1:D:344:GLY:N	2.21	0.55
1:A:1:ALA:HB1	6:A:743:HOH:O	2.07	0.55
1:C:254:GLU:OE2	6:C:756:HOH:O	2.18	0.54
1:D:286:LEU:HD12	1:D:314:LEU:HD13	1.89	0.54
1:C:312:TRP:CE3	1:C:314:LEU:CB	2.81	0.54
1:C:209:TRP:O	1:C:212:TYR:HB3	2.08	0.54
1:A:151:GLU:CD	1:D:155:LYS:NZ	2.62	0.54
1:C:346:LYS:CG	6:C:762:HOH:O	2.47	0.53
1:C:312:TRP:CE3	1:C:314:LEU:HD13	2.43	0.53
1:C:352:VAL:HG11	1:C:403:ILE:HD13	1.89	0.53
1:D:408:LYS:O	1:D:410:THR:HG23	2.09	0.53
1:A:286:LEU:HD21	1:B:317:LEU:HA	1.89	0.53
1:A:286:LEU:CD1	1:A:318:ALA:CB	2.87	0.53
1:B:346:LYS:HD2	1:B:348:TRP:CD1	2.43	0.52
1:D:102:ASN:CG	6:D:736:HOH:O	2.47	0.52
1:C:284:GLN:HB2	1:C:286:LEU:HD13	1.92	0.52
1:B:96:LEU:HD21	1:B:404:VAL:HG13	1.91	0.52
1:B:116:TYR:OH	1:B:420:LEU:HD13	2.09	0.52
1:D:165:LEU:HD22	1:D:172:VAL:HB	1.92	0.52
1:C:82:GLY:HA3	1:C:118:ILE:O	2.10	0.51
1:C:207:GLN:NE2	1:C:263:ASP:OD1	2.31	0.51
1:D:106:LYS:O	1:D:110:SER:HB3	2.10	0.51
1:C:165:LEU:HD22	1:C:172:VAL:HB	1.92	0.51
1:D:96:LEU:HD21	1:D:404:VAL:HG13	1.91	0.51
1:D:207:GLN:NE2	1:D:263:ASP:OD1	2.29	0.51
1:D:112:GLU:HB3	6:D:735:HOH:O	2.08	0.51
1:C:352:VAL:CG1	1:C:403:ILE:HD13	2.40	0.51
1:C:256:GLN:O	1:C:260:ILE:HG12	2.10	0.51
1:C:312:TRP:CE2	1:C:378:TRP:HZ2	2.29	0.51
1:C:397:PHE:CD2	1:C:398:VAL:HG13	2.46	0.51
1:D:93:ILE:HG13	1:D:160:LEU:CD1	2.41	0.50
1:A:1:ALA:HB2	1:A:27:ASP:OD1	2.11	0.50
1:A:446:ALA:HA	1:A:459:VAL:O	2.12	0.50
1:A:286:LEU:CD2	1:B:317:LEU:CA	2.82	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:THR:O	1:C:299:PRO:HD3	2.11	0.50
1:A:161:ILE:HD11	1:A:225:LEU:HD13	1.93	0.50
1:C:349:GLU:HG2	1:C:353:ARG:HH21	1.76	0.50
1:B:5:ILE:HD11	1:B:22:TYR:CE2	2.45	0.50
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.94	0.50
1:C:313:TYR:HD2	1:C:316:PHE:HE1	1.58	0.50
1:B:91:LEU:HD23	1:B:391:PRO:HG3	1.92	0.50
1:C:396:ASN:O	1:C:398:VAL:N	2.39	0.49
1:C:312:TRP:CE2	1:C:341:ALA:CB	2.95	0.49
1:D:11:TYR:OH	1:D:350:GLN:NE2	2.35	0.49
1:D:318:ALA:HB1	1:D:323:THR:HG21	1.95	0.49
1:B:293:LYS:O	1:B:297:THR:HG23	2.12	0.49
1:C:209:TRP:CZ3	1:C:212:TYR:CD2	3.00	0.49
1:C:404:VAL:HG12	1:C:406:ILE:HG22	1.95	0.49
1:B:286:LEU:HD12	1:B:318:ALA:HB2	1.95	0.48
1:D:5:ILE:HD13	1:D:22:TYR:CE2	2.47	0.48
1:D:371:LEU:O	1:D:433:ARG:HD2	2.13	0.48
1:A:161:ILE:HD11	1:A:174:LEU:CD1	2.43	0.48
1:C:196:SER:HB3	6:C:671:HOH:O	2.14	0.48
1:C:200:GLN:N	1:C:203:ASP:OD2	2.34	0.48
1:C:312:TRP:HZ2	1:C:378:TRP:HZ2	1.59	0.48
1:D:293:LYS:O	1:D:297:THR:HG23	2.14	0.48
1:C:91:LEU:HD23	1:C:156:LEU:CD1	2.44	0.48
1:C:313:TYR:HE1	1:C:342:CYS:SG	2.37	0.48
1:A:116:TYR:OH	1:A:420:LEU:HD13	2.14	0.48
1:C:1:ALA:HB2	1:C:27:ASP:OD1	2.13	0.48
1:C:139:PRO:HA	1:C:184:TRP:CD1	2.49	0.47
1:D:135:TYR:O	1:D:147:PHE:HA	2.14	0.47
1:B:43:THR:HB	6:B:533:HOH:O	2.14	0.47
1:B:408:LYS:O	1:B:410:THR:CG2	2.63	0.47
1:D:82:GLY:HA3	1:D:118:ILE:O	2.14	0.47
1:B:170:ARG:NH2	1:B:425:LYS:O	2.46	0.47
1:C:381:TRP:HE1	4:C:502:GOL:C3	2.26	0.47
2:C:498:NAG:H82	6:C:627:HOH:O	2.15	0.47
1:A:312:TRP:HD1	6:A:722:HOH:O	1.97	0.47
1:D:93:ILE:HG13	1:D:160:LEU:HD13	1.97	0.47
1:B:11:TYR:OH	1:B:350:GLN:NE2	2.29	0.47
1:A:394:VAL:O	1:A:395:ARG:HB2	2.15	0.47
1:C:37:PHE:CD2	1:C:480:LEU:HG	2.51	0.47
1:A:151:GLU:OE1	1:D:155:LYS:NZ	2.48	0.46
1:A:161:ILE:HD13	1:A:225:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ARG:NH1	3:C:501:SO4:O2	2.41	0.46
1:A:30:THR:O	1:A:32:PRO:CD	2.63	0.46
1:A:140:ASP:HB3	6:A:731:HOH:O	2.15	0.46
1:D:483:ILE:O	1:D:485:PRO:HD3	2.15	0.46
1:B:209:TRP:O	1:B:212:TYR:HB3	2.15	0.46
1:C:87:ASP:O	1:C:91:LEU:HG	2.15	0.46
1:C:312:TRP:HZ2	1:C:378:TRP:CZ2	2.31	0.46
1:D:5:ILE:HD12	2:D:498:NAG:O6	2.15	0.46
1:B:109:PHE:O	1:B:168:ALA:HA	2.16	0.46
1:D:93:ILE:CG1	6:D:742:HOH:O	2.52	0.46
1:D:328:HIS:CD2	6:D:544:HOH:O	2.60	0.46
1:C:169:GLN:HG2	1:C:170:ARG:HG3	1.97	0.46
1:C:23:CYS:SG	1:C:413:LYS:HE3	2.55	0.46
1:B:111:GLU:HG2	1:B:169:GLN:HB2	1.98	0.46
1:A:71:PRO:HB3	1:A:450:MET:HE1	1.98	0.46
1:A:37:PHE:CD2	1:A:480:LEU:HG	2.51	0.45
1:A:346:LYS:HB2	6:A:524:HOH:O	2.15	0.45
1:C:312:TRP:NE1	1:C:378:TRP:HZ2	2.12	0.45
1:D:329:ARG:NH1	1:D:329:ARG:CG	2.60	0.45
1:C:199:GLY:HA3	1:C:203:ASP:OD2	2.17	0.45
1:A:286:LEU:CD2	1:B:316:PHE:O	2.64	0.45
1:D:457:VAL:HA	1:D:492:TYR:O	2.17	0.45
1:C:408:LYS:O	1:C:410:THR:CG2	2.63	0.45
1:A:343:VAL:HG22	1:A:344:GLY:N	2.32	0.45
1:A:64:GLY:HA2	3:A:501:SO4:O2	2.17	0.45
1:A:338:ALA:HB3	1:A:378:TRP:HA	1.99	0.45
1:B:395:ARG:NH1	6:B:624:HOH:O	2.50	0.44
1:A:141:ASP:O	1:A:184:TRP:HH2	2.01	0.44
1:D:56:ILE:HD13	1:D:477:VAL:HG11	2.00	0.44
1:D:194:LYS:HE3	6:D:741:HOH:O	2.16	0.44
1:D:183:THR:O	1:D:189:GLY:HA2	2.18	0.44
1:A:120:ARG:HD3	6:A:507:HOH:O	2.16	0.44
1:C:5:ILE:HD12	1:C:22:TYR:CZ	2.53	0.44
2:A:498:NAG:H82	6:A:683:HOH:O	2.17	0.44
1:C:406:ILE:HG23	6:C:577:HOH:O	2.18	0.44
1:B:215:LYS:HA	1:B:215:LYS:HD2	1.79	0.43
1:C:244:TYR:HA	6:C:758:HOH:O	2.18	0.43
1:B:203:ASP:OD1	1:B:203:ASP:C	2.55	0.43
1:D:127:ASP:HB3	1:D:246:PHE:CG	2.53	0.43
1:D:203:ASP:OD1	1:D:203:ASP:C	2.57	0.43
1:D:426:PHE:HB3	1:D:493:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:PHE:H	1:C:31:PHE:HD1	1.57	0.43
1:C:352:VAL:HG13	1:C:403:ILE:HD11	2.00	0.43
1:D:128:PHE:CZ	1:D:398:VAL:HG22	2.53	0.43
1:D:66:LEU:HD11	1:D:473:LYS:HB2	2.00	0.43
1:B:471:THR:CG2	1:B:479:PHE:HB3	2.48	0.43
1:A:165:LEU:HD22	1:A:172:VAL:HB	2.01	0.43
1:A:313:TYR:HE2	1:A:345:SER:HG	1.65	0.43
1:B:106:LYS:O	1:B:110:SER:HB3	2.19	0.43
1:C:91:LEU:CD2	1:C:156:LEU:CD1	2.97	0.43
1:C:317:LEU:O	1:D:286:LEU:HD11	2.18	0.43
1:D:18:CYS:O	1:D:410:THR:HB	2.19	0.43
1:D:209:TRP:O	1:D:212:TYR:HB3	2.19	0.43
1:A:111:GLU:O	1:A:425:LYS:NZ	2.52	0.43
1:A:139:PRO:HA	1:A:184:TRP:CD1	2.54	0.43
1:A:345:SER:HB2	1:A:397:PHE:HB2	2.01	0.43
1:C:312:TRP:CE2	1:C:378:TRP:CZ2	3.07	0.43
1:B:480:LEU:HD23	1:B:480:LEU:N	2.34	0.42
1:A:209:TRP:O	1:A:212:TYR:HB3	2.19	0.42
1:D:285:ARG:HG2	1:D:315:ASP:OD1	2.19	0.42
1:B:146:ASN:ND2	6:B:748:HOH:O	2.50	0.42
1:C:352:VAL:HG13	1:C:403:ILE:CD1	2.49	0.42
1:D:209:TRP:CZ3	1:D:212:TYR:CD2	3.07	0.42
1:D:287:LEU:HB3	1:D:291:TRP:CD1	2.54	0.42
1:B:5:ILE:CD1	1:B:22:TYR:CD2	3.03	0.42
1:A:284:GLN:OE1	1:A:312:TRP:HE3	2.03	0.42
1:A:350:GLN:H	1:A:350:GLN:CD	2.23	0.42
1:C:352:VAL:CG1	1:C:403:ILE:CD1	2.98	0.42
1:B:318:ALA:HB1	1:B:323:THR:HG21	2.01	0.42
1:C:209:TRP:HA	1:C:209:TRP:CE3	2.55	0.42
1:C:387:PRO:HD3	1:C:404:VAL:O	2.20	0.42
1:A:234:ASN:OD1	1:A:311:HIS:HE1	2.02	0.42
1:A:313:TYR:CD1	1:A:313:TYR:C	2.90	0.42
1:B:312:TRP:CD1	1:B:312:TRP:C	2.93	0.42
1:D:386:ASN:HB2	1:D:387:PRO:CD	2.49	0.42
1:B:282:ASP:OD1	1:B:311:HIS:NE2	2.50	0.42
1:C:91:LEU:CD2	1:C:156:LEU:HD13	2.49	0.42
1:D:198:LYS:HE2	1:D:205:TYR:CE2	2.54	0.42
1:C:16:CYS:SG	1:C:48:ARG:HG3	2.60	0.41
1:C:83:GLY:O	1:C:119:ILE:HA	2.19	0.41
1:A:408:LYS:O	1:A:410:THR:HG23	2.19	0.41
1:C:348:TRP:CD2	1:D:245:PRO:HD3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:GLU:HG3	6:C:630:HOH:O	2.20	0.41
1:C:313:TYR:CD2	1:C:316:PHE:HE1	2.37	0.41
1:D:19:ASN:CG	2:D:498:NAG:C1	2.84	0.41
1:D:182:PRO:HB3	1:D:184:TRP:NE1	2.36	0.41
1:A:18:CYS:O	1:A:410:THR:HB	2.20	0.41
1:B:135:TYR:O	1:B:147:PHE:HA	2.20	0.41
1:C:312:TRP:CZ2	1:C:314:LEU:HD22	2.55	0.41
1:B:450:MET:HB2	1:B:450:MET:HE3	1.78	0.41
1:C:31:PHE:HA	1:C:32:PRO:HD2	1.72	0.41
1:C:314:LEU:HD23	1:C:362:GLN:HB3	2.02	0.41
1:B:5:ILE:HD12	1:B:22:TYR:CD2	2.56	0.41
1:C:284:GLN:CB	1:C:286:LEU:HD13	2.51	0.41
1:D:47:ARG:HB3	1:D:50:GLU:HG3	2.02	0.41
1:B:26:PHE:CG	1:B:425:LYS:HE2	2.56	0.41
1:B:170:ARG:NH1	1:B:424:SER:O	2.45	0.41
1:C:286:LEU:HD22	1:C:287:LEU:HG	2.03	0.41
1:B:7:LYS:HE3	1:B:9:PHE:CZ	2.56	0.40
1:B:298:ASP:HA	1:B:299:PRO:HD3	1.92	0.40
1:C:350:GLN:CD	1:C:350:GLN:H	2.24	0.40
1:D:5:ILE:CD1	1:D:22:TYR:CD2	3.04	0.40
1:D:108:TYR:CE1	1:D:402:ILE:HD12	2.56	0.40
1:A:286:LEU:HD13	1:A:318:ALA:CB	2.51	0.40
1:D:139:PRO:HA	1:D:184:TRP:CD1	2.56	0.40
1:B:127:ASP:HB3	1:B:246:PHE:CG	2.57	0.40
1:C:48:ARG:HD2	1:C:418:TYR:CD1	2.56	0.40
1:C:141:ASP:O	1:C:184:TRP:HH2	2.04	0.40
1:D:361:MET:SD	1:D:463:ARG:HG2	2.62	0.40
1:A:234:ASN:O	1:A:235:GLU:C	2.59	0.40
1:A:483:ILE:O	1:A:485:PRO:HD3	2.21	0.40
1:D:207:GLN:HE22	1:D:263:ASP:HA	1.86	0.40
1:A:303:LYS:HE3	1:A:304:TYR:CZ	2.57	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	495/497 (100%)	467 (94%)	23 (5%)	5 (1%)	15	10
1	B	495/497 (100%)	471 (95%)	21 (4%)	3 (1%)	25	20
1	C	495/497 (100%)	470 (95%)	21 (4%)	4 (1%)	19	14
1	D	495/497 (100%)	476 (96%)	17 (3%)	2 (0%)	34	32
All	All	1980/1988 (100%)	1884 (95%)	82 (4%)	14 (1%)	22	17

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	233	GLU
1	C	397	PHE
1	B	233	GLU
1	B	381	TRP
1	D	233	GLU
1	D	381	TRP
1	A	233	GLU
1	A	281	LEU
1	A	381	TRP
1	B	345	SER
1	C	281	LEU
1	C	381	TRP
1	A	194	LYS
1	A	31	PHE

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	424/424 (100%)	410 (97%)	14 (3%)	38	39
1	B	424/424 (100%)	408 (96%)	16 (4%)	33	33
1	C	424/424 (100%)	406 (96%)	18 (4%)	30	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	424/424 (100%)	406 (96%)	18 (4%)	30	29
All	All	1696/1696 (100%)	1630 (96%)	66 (4%)	32	32

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	5	ILE
1	A	30	THR
1	A	44	ARG
1	A	161	ILE
1	A	246	PHE
1	A	286	LEU
1	A	300	GLU
1	A	335	MET
1	A	358	ASP
1	A	381	TRP
1	A	406	ILE
1	A	410	THR
1	A	466	LYS
1	B	30	THR
1	B	61	THR
1	B	169	GLN
1	B	200	GLN
1	B	286	LEU
1	B	312	TRP
1	B	335	MET
1	B	346	LYS
1	B	381	TRP
1	B	394	VAL
1	B	410	THR
1	B	420	LEU
1	B	470	LEU
1	B	480	LEU
1	B	481	GLU
1	B	493	LEU
1	C	2	ARG
1	C	31	PHE
1	C	44	ARG
1	C	77	LYS
1	C	200	GLN
1	C	204	ILE

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Mol	Chain	Res	Type
1	C	246	PHE
1	C	260	ILE
1	C	286	LEU
1	C	335	MET
1	C	343	VAL
1	C	345	SER
1	C	381	TRP
1	C	406	ILE
1	C	410	THR
1	C	420	LEU
1	C	466	LYS
1	C	495	HIS
1	D	5	ILE
1	D	30	THR
1	D	93	ILE
1	D	111	GLU
1	D	155	LYS
1	D	200	GLN
1	D	286	LEU
1	D	312	TRP
1	D	329	ARG
1	D	335	MET
1	D	381	TRP
1	D	394	VAL
1	D	410	THR
1	D	420	LEU
1	D	470	LEU
1	D	480	LEU
1	D	493	LEU
1	D	495	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	200	GLN
1	A	328	HIS
1	B	328	HIS
1	B	350	GLN
1	B	396	ASN
1	B	495	HIS
1	C	146	ASN

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Mol	Chain	Res	Type
1	C	328	HIS
1	C	495	HIS
1	D	328	HIS
1	D	350	GLN

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)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	B	501	-	4,4,4	0.13	0	6,6,6	0.32	0
3	SO4	D	501	-	4,4,4	0.19	0	6,6,6	0.70	0
3	SO4	C	499	-	4,4,4	0.07	0	6,6,6	0.51	0
2	NAG	A	498	1	14,14,15	0.61	0	17,19,21	2.15	6 (35%)
3	SO4	D	500	-	4,4,4	0.15	0	6,6,6	0.35	0
2	NAG	D	498	1	14,14,15	0.66	0	17,19,21	1.13	1 (5%)
3	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.15	0
3	SO4	D	499	-	4,4,4	0.23	0	6,6,6	0.40	0
3	SO4	A	502	-	4,4,4	0.16	0	6,6,6	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.17	0
3	SO4	A	500	-	4,4,4	0.13	0	6,6,6	0.33	0
2	NAG	C	498	1	14,14,15	0.57	0	17,19,21	2.24	6 (35%)
5	IFM	B	506	-	9,10,10	0.54	0	9,13,13	3.51	1 (11%)
3	SO4	B	504	-	4,4,4	0.16	0	6,6,6	0.34	0
3	SO4	B	505	-	4,4,4	0.13	0	6,6,6	0.21	0
3	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	A	501	-	4,4,4	0.16	0	6,6,6	0.34	0
2	NAG	B	499	1	14,14,15	0.65	0	17,19,21	1.22	2 (11%)
3	SO4	A	503	-	4,4,4	0.19	0	6,6,6	0.31	0
4	GOL	A	504	-	5,5,5	0.60	0	5,5,5	0.43	0
3	SO4	B	500	-	4,4,4	0.30	0	6,6,6	0.21	0
3	SO4	B	502	-	4,4,4	0.20	0	6,6,6	0.65	0
3	SO4	A	499	-	4,4,4	0.25	0	6,6,6	0.54	0
4	GOL	C	502	-	5,5,5	0.43	0	5,5,5	0.33	0
2	NAG	B	498	1	14,14,15	0.70	0	17,19,21	0.77	0
3	SO4	C	500	-	4,4,4	0.18	0	6,6,6	0.51	0
5	IFM	D	503	-	9,10,10	0.53	0	9,13,13	3.17	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IFM	B	506	-	-	0/2/16/16	0/1/1/1
4	GOL	C	502	-	-	2/4/4/4	-
2	NAG	B	498	1	-	2/6/23/26	0/1/1/1
2	NAG	A	498	1	1/1/5/7	6/6/23/26	0/1/1/1
2	NAG	D	498	1	-	0/6/23/26	0/1/1/1
2	NAG	C	498	1	1/1/5/7	6/6/23/26	0/1/1/1
2	NAG	B	499	1	-	0/6/23/26	0/1/1/1
5	IFM	D	503	-	-	0/2/16/16	0/1/1/1
4	GOL	A	504	-	-	4/4/4/4	-

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	506	IFM	C1-N-C2	10.19	122.88	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	503	IFM	C1-N-C2	9.21	121.81	111.70
2	C	498	NAG	C2-N2-C7	-5.15	115.58	122.90
2	A	498	NAG	C2-N2-C7	-4.07	117.10	122.90
2	A	498	NAG	C3-C4-C5	-3.88	103.31	110.24
2	A	498	NAG	O5-C5-C6	3.64	112.90	107.20
2	A	498	NAG	O5-C5-C4	-3.30	102.81	110.83
2	C	498	NAG	O5-C1-C2	3.18	116.31	111.29
2	C	498	NAG	C8-C7-N2	3.07	121.29	116.10
2	D	498	NAG	C2-N2-C7	-3.03	118.58	122.90
2	B	499	NAG	O5-C1-C2	-2.88	106.74	111.29
2	C	498	NAG	O5-C5-C4	-2.73	104.18	110.83
2	C	498	NAG	O5-C5-C6	2.65	111.35	107.20
2	C	498	NAG	C3-C4-C5	-2.34	106.07	110.24
2	A	498	NAG	C8-C7-N2	2.18	119.80	116.10
2	A	498	NAG	C6-C5-C4	2.14	118.02	113.00
2	B	499	NAG	O4-C4-C5	2.03	114.34	109.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	498	NAG	C1
2	C	498	NAG	C1

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	498	NAG	C1-C2-N2-C7
2	A	498	NAG	C8-C7-N2-C2
2	A	498	NAG	O7-C7-N2-C2
2	C	498	NAG	C1-C2-N2-C7
2	C	498	NAG	O7-C7-N2-C2
4	A	504	GOL	O1-C1-C2-C3
4	A	504	GOL	C1-C2-C3-O3
4	C	502	GOL	O1-C1-C2-C3
2	C	498	NAG	C8-C7-N2-C2
2	A	498	NAG	O5-C5-C6-O6
2	C	498	NAG	O5-C5-C6-O6
2	C	498	NAG	C4-C5-C6-O6
2	A	498	NAG	C4-C5-C6-O6
4	C	502	GOL	O1-C1-C2-O2
4	A	504	GOL	O1-C1-C2-O2
4	A	504	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	498	NAG	C4-C5-C6-O6
2	C	498	NAG	C3-C2-N2-C7
2	B	498	NAG	O5-C5-C6-O6
2	A	498	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	498	NAG	1	0
2	D	498	NAG	3	0
2	C	498	NAG	1	0
3	C	501	SO4	1	0
3	A	501	SO4	1	0
4	C	502	GOL	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	497/497 (100%)	0.15	18 (3%)	42	49	23, 35, 52, 73	5 (1%)
1	B	497/497 (100%)	0.06	8 (1%)	72	76	23, 33, 48, 64	5 (1%)
1	C	497/497 (100%)	0.10	18 (3%)	42	49	24, 34, 53, 74	5 (1%)
1	D	497/497 (100%)	0.08	7 (1%)	75	78	22, 33, 48, 61	5 (1%)
All	All	1988/1988 (100%)	0.10	51 (2%)	56	61	22, 34, 50, 74	20 (1%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	317	LEU	8.1
1	A	313	TYR	8.1
1	A	317	LEU	7.0
1	A	347	PHE	6.4
1	C	312	TRP	5.8
1	A	316	PHE	4.9
1	B	317	LEU	4.3
1	D	348	TRP	4.3
1	B	347	PHE	4.1
1	C	31	PHE	4.1
1	C	315	ASP	3.8
1	D	1	ALA	3.6
1	B	62	GLY	3.6
1	C	316	PHE	3.6
1	C	314	LEU	3.5
1	A	315	ASP	3.4
1	C	57	GLN	3.2
1	C	406	ILE	3.1
1	A	73	GLN	2.8
1	C	318	ALA	2.8
1	C	313	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	242	SER	2.8
1	D	358	ASP	2.8
1	A	31	PHE	2.7
1	B	314	LEU	2.7
1	C	205	TYR	2.7
1	B	358	ASP	2.7
1	C	246	PHE	2.6
1	A	286	LEU	2.6
1	A	312	TRP	2.5
1	C	347	PHE	2.5
1	A	388	GLU	2.5
1	A	57	GLN	2.5
1	A	314	LEU	2.3
1	C	198	LYS	2.3
1	D	145	HIS	2.3
1	C	73	GLN	2.3
1	B	63	THR	2.2
1	D	63	THR	2.2
1	C	204	ILE	2.2
1	B	66	LEU	2.1
1	C	397	PHE	2.1
1	A	358	ASP	2.1
1	A	91	LEU	2.1
1	C	196	SER	2.1
1	A	318	ALA	2.1
1	D	318	ALA	2.1
1	A	246	PHE	2.1
1	A	61	THR	2.0
1	B	348	TRP	2.0
1	D	73	GLN	2.0

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

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

6.3 Carbohydrates (i)

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	498	14/15	0.78	0.16	64,66,67,67	0
2	NAG	A	498	14/15	0.80	0.16	49,55,56,56	0
2	NAG	C	498	14/15	0.87	0.14	45,53,55,56	0
3	SO4	D	500	5/5	0.88	0.18	73,74,76,76	0
2	NAG	D	498	14/15	0.89	0.14	38,48,51,51	0
5	IFM	B	506	10/10	0.89	0.15	26,28,33,33	0
2	NAG	B	499	14/15	0.90	0.12	40,43,45,46	0
4	GOL	C	502	6/6	0.91	0.17	44,47,48,49	0
4	GOL	A	504	6/6	0.91	0.20	51,52,53,54	0
3	SO4	B	504	5/5	0.93	0.14	83,83,84,85	0
3	SO4	B	505	5/5	0.93	0.10	81,81,82,82	0
3	SO4	B	503	5/5	0.94	0.11	66,67,67,68	0
3	SO4	C	501	5/5	0.94	0.10	85,86,86,86	0
3	SO4	A	503	5/5	0.95	0.13	60,60,61,62	0
3	SO4	B	501	5/5	0.95	0.11	71,73,74,74	0
5	IFM	D	503	10/10	0.95	0.11	27,32,35,37	0
3	SO4	A	502	5/5	0.96	0.11	47,48,50,51	0
3	SO4	A	500	5/5	0.96	0.15	79,79,80,80	0
3	SO4	C	499	5/5	0.96	0.12	49,52,53,54	0
3	SO4	D	501	5/5	0.97	0.11	48,48,49,50	0
3	SO4	D	502	5/5	0.97	0.07	71,72,72,72	0
3	SO4	B	502	5/5	0.97	0.12	51,51,51,52	0
3	SO4	A	499	5/5	0.98	0.14	41,44,45,45	0
3	SO4	D	499	5/5	0.98	0.14	40,42,44,45	0
3	SO4	A	501	5/5	0.98	0.13	64,65,66,67	0
3	SO4	C	500	5/5	0.99	0.09	39,40,41,42	0
3	SO4	B	500	5/5	0.99	0.13	46,47,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.