Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Jan 13, 2018 – 02:31 PM EST

PDB ID	:	6BO8
EMDB ID:	:	EMD-7120
Title	:	Cryo-EM structure of human TRPV6 in nanodiscs
Authors	:	McGoldrick, L.L.; Singh, A.K.; Saotome, K.; Yelshanskaya, M.V.; Twomey, E.C.; Grassucci, R.A.; Sobolevsky, A.I.
Deposited on	:	2017-11-18
Resolution	:	3.60 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

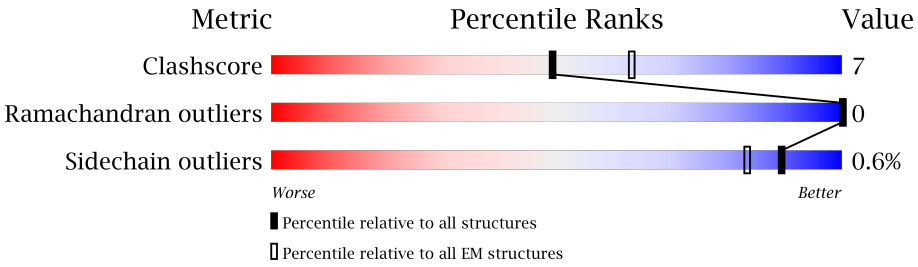
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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%

Mol	Chain	Length	Quality of chain
1	A	742	64% 16% 20%
1	B	742	64% 15% 20%
1	C	742	64% 16% 20%
1	D	742	64% 16% 20%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19048 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	593	Total 4762	C 3076	N 805	O 842	S 39	0	0
1	B	593	Total 4762	C 3076	N 805	O 842	S 39	0	0
1	C	593	Total 4762	C 3076	N 805	O 842	S 39	0	0
1	D	593	Total 4762	C 3076	N 805	O 842	S 39	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	726	LEU	-	expression tag	UNP Q9H1D0
A	727	VAL	-	expression tag	UNP Q9H1D0
A	728	PRO	-	expression tag	UNP Q9H1D0
A	729	ARG	-	expression tag	UNP Q9H1D0
A	730	GLY	-	expression tag	UNP Q9H1D0
A	731	SER	-	expression tag	UNP Q9H1D0
A	732	ALA	-	expression tag	UNP Q9H1D0
A	733	ALA	-	expression tag	UNP Q9H1D0
A	734	ALA	-	expression tag	UNP Q9H1D0
A	735	TRP	-	expression tag	UNP Q9H1D0
A	736	SER	-	expression tag	UNP Q9H1D0
A	737	HIS	-	expression tag	UNP Q9H1D0
A	738	PRO	-	expression tag	UNP Q9H1D0
A	739	GLN	-	expression tag	UNP Q9H1D0
A	740	PHE	-	expression tag	UNP Q9H1D0
A	741	GLU	-	expression tag	UNP Q9H1D0
A	742	LYS	-	expression tag	UNP Q9H1D0
B	726	LEU	-	expression tag	UNP Q9H1D0
B	727	VAL	-	expression tag	UNP Q9H1D0
B	728	PRO	-	expression tag	UNP Q9H1D0
B	729	ARG	-	expression tag	UNP Q9H1D0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	730	GLY	-	expression tag	UNP Q9H1D0
B	731	SER	-	expression tag	UNP Q9H1D0
B	732	ALA	-	expression tag	UNP Q9H1D0
B	733	ALA	-	expression tag	UNP Q9H1D0
B	734	ALA	-	expression tag	UNP Q9H1D0
B	735	TRP	-	expression tag	UNP Q9H1D0
B	736	SER	-	expression tag	UNP Q9H1D0
B	737	HIS	-	expression tag	UNP Q9H1D0
B	738	PRO	-	expression tag	UNP Q9H1D0
B	739	GLN	-	expression tag	UNP Q9H1D0
B	740	PHE	-	expression tag	UNP Q9H1D0
B	741	GLU	-	expression tag	UNP Q9H1D0
B	742	LYS	-	expression tag	UNP Q9H1D0
C	726	LEU	-	expression tag	UNP Q9H1D0
C	727	VAL	-	expression tag	UNP Q9H1D0
C	728	PRO	-	expression tag	UNP Q9H1D0
C	729	ARG	-	expression tag	UNP Q9H1D0
C	730	GLY	-	expression tag	UNP Q9H1D0
C	731	SER	-	expression tag	UNP Q9H1D0
C	732	ALA	-	expression tag	UNP Q9H1D0
C	733	ALA	-	expression tag	UNP Q9H1D0
C	734	ALA	-	expression tag	UNP Q9H1D0
C	735	TRP	-	expression tag	UNP Q9H1D0
C	736	SER	-	expression tag	UNP Q9H1D0
C	737	HIS	-	expression tag	UNP Q9H1D0
C	738	PRO	-	expression tag	UNP Q9H1D0
C	739	GLN	-	expression tag	UNP Q9H1D0
C	740	PHE	-	expression tag	UNP Q9H1D0
C	741	GLU	-	expression tag	UNP Q9H1D0
C	742	LYS	-	expression tag	UNP Q9H1D0
D	726	LEU	-	expression tag	UNP Q9H1D0
D	727	VAL	-	expression tag	UNP Q9H1D0
D	728	PRO	-	expression tag	UNP Q9H1D0
D	729	ARG	-	expression tag	UNP Q9H1D0
D	730	GLY	-	expression tag	UNP Q9H1D0
D	731	SER	-	expression tag	UNP Q9H1D0
D	732	ALA	-	expression tag	UNP Q9H1D0
D	733	ALA	-	expression tag	UNP Q9H1D0
D	734	ALA	-	expression tag	UNP Q9H1D0
D	735	TRP	-	expression tag	UNP Q9H1D0
D	736	SER	-	expression tag	UNP Q9H1D0
D	737	HIS	-	expression tag	UNP Q9H1D0

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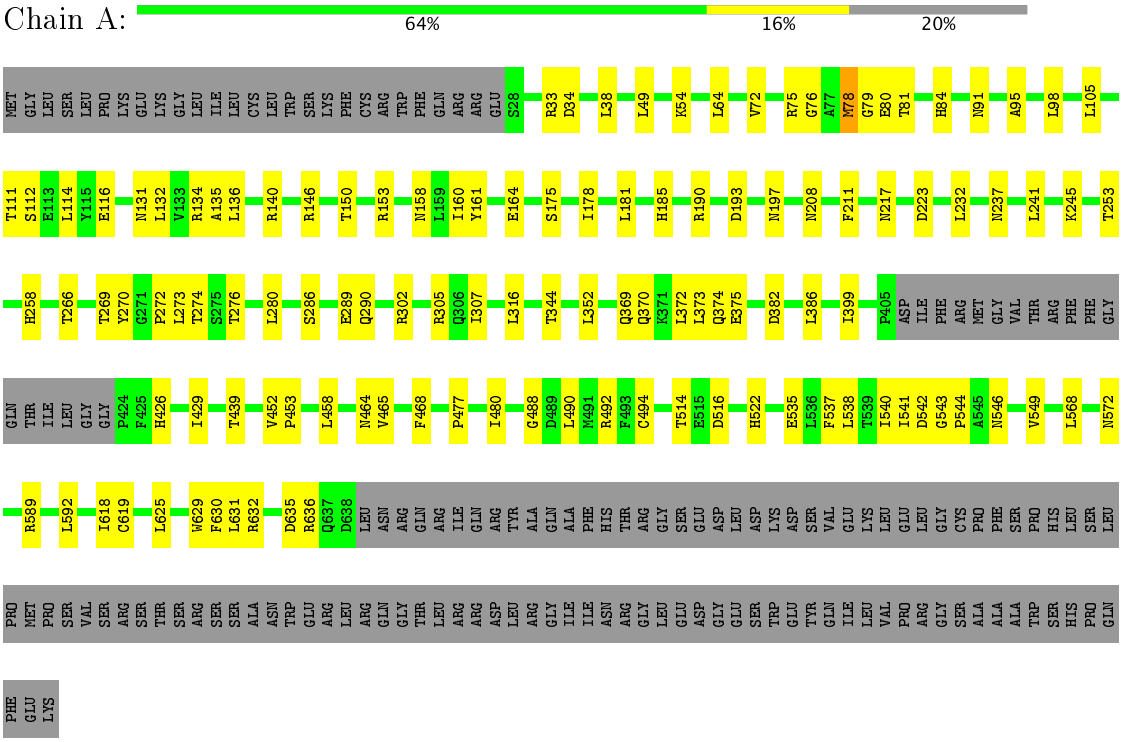
Chain	Residue	Modelled	Actual	Comment	Reference
D	738	PRO	-	expression tag	UNP Q9H1D0
D	739	GLN	-	expression tag	UNP Q9H1D0
D	740	PHE	-	expression tag	UNP Q9H1D0
D	741	GLU	-	expression tag	UNP Q9H1D0
D	742	LYS	-	expression tag	UNP Q9H1D0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

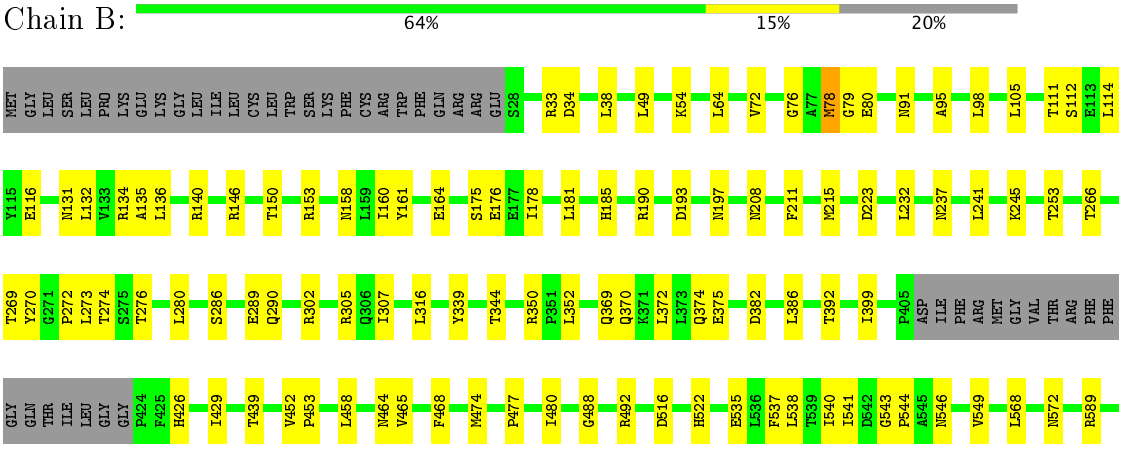
- Molecule 1: Transient receptor potential cation channel subfamily V member 6

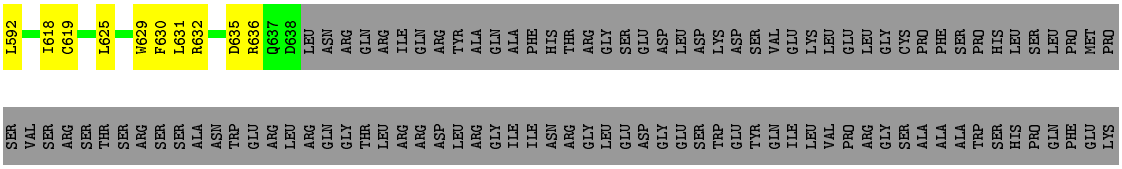
Chain A:



- Molecule 1: Transient receptor potential cation channel subfamily V member 6

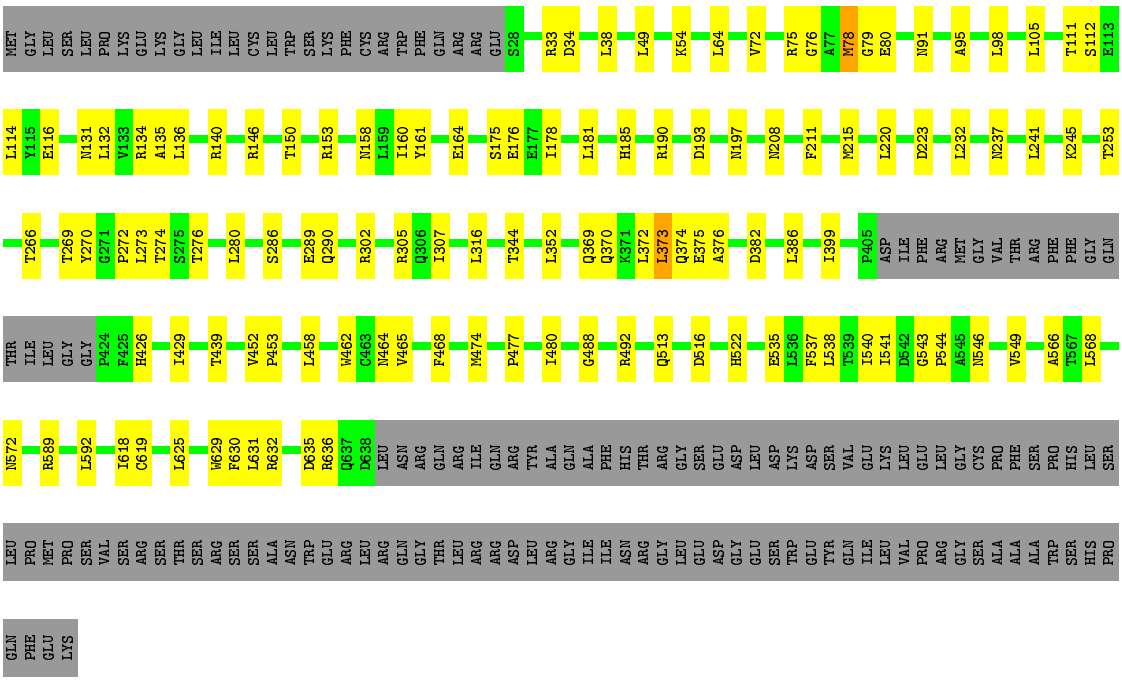
Chain B:





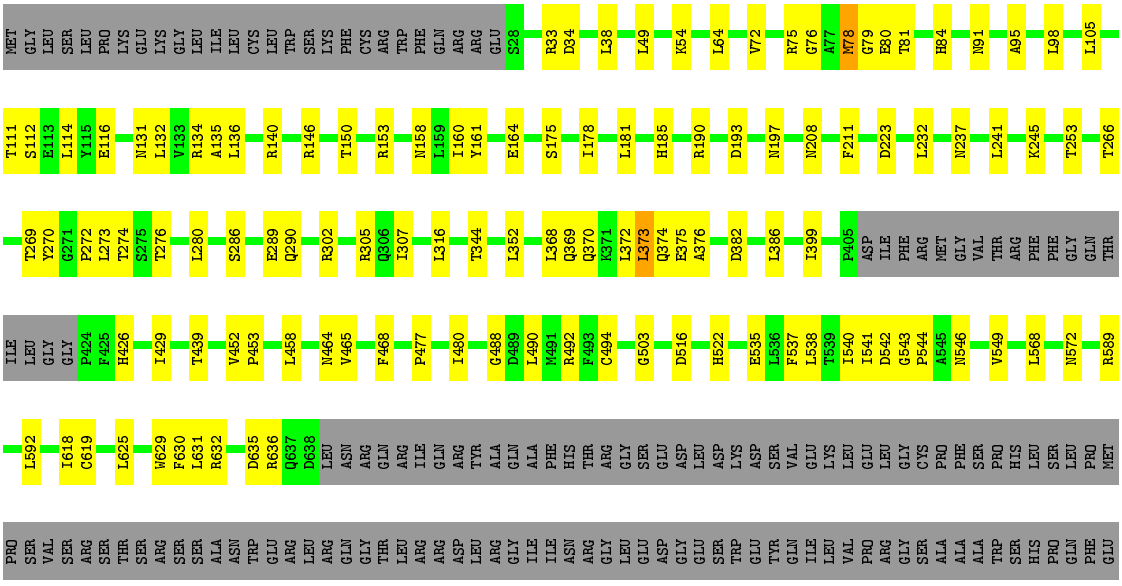
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

Chain C:



• Molecule 1: Transient receptor potential cation channel subfamily V member 6

Chain D:



LYS

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	46124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
1	A	0.39	0/4871	0.60	2/6610 (0.0%)
1	B	0.39	0/4871	0.60	1/6610 (0.0%)
1	C	0.39	0/4871	0.60	2/6610 (0.0%)
1	D	0.39	0/4871	0.60	2/6610 (0.0%)
All	All	0.39	0/19484	0.60	7/26440 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	372	LEU	CA-CB-CG	8.40	134.63	115.30
1	D	372	LEU	CA-CB-CG	8.40	134.62	115.30
1	A	372	LEU	CA-CB-CG	8.40	134.62	115.30
1	C	372	LEU	CA-CB-CG	8.40	134.62	115.30
1	A	373	LEU	CA-CB-CG	5.01	126.82	115.30
1	D	373	LEU	CA-CB-CG	5.01	126.82	115.30
1	C	373	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	ASP	Peptide
1	B	223	ASP	Peptide
1	C	223	ASP	Peptide
1	D	223	ASP	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	4762	0	4816	72	0
1	B	4762	0	4816	70	0
1	C	4762	0	4816	75	0
1	D	4762	0	4816	74	0
All	All	19048	0	19264	269	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 7.

All (269) 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:B:273:LEU:HD11	1:C:160:ILE:HG12	1.69	0.73
1:A:160:ILE:HG12	1:D:273:LEU:HD11	1.76	0.67
1:A:208:ASN:HB3	1:A:211:PHE:HB3	1.78	0.66
1:D:208:ASN:HB3	1:D:211:PHE:HB3	1.78	0.66
1:C:208:ASN:HB3	1:C:211:PHE:HB3	1.78	0.66
1:B:208:ASN:HB3	1:B:211:PHE:HB3	1.78	0.65
1:C:79:GLY:HA3	1:C:111:THR:H	1.62	0.65
1:B:79:GLY:HA3	1:B:111:THR:H	1.62	0.64
1:A:79:GLY:HA3	1:A:111:THR:H	1.61	0.64
1:D:79:GLY:HA3	1:D:111:THR:H	1.62	0.64
1:C:541:ILE:HG22	1:C:543:GLY:H	1.63	0.64
1:D:541:ILE:HG22	1:D:543:GLY:H	1.63	0.63
1:B:541:ILE:HG22	1:B:543:GLY:H	1.63	0.63
1:C:273:LEU:HD11	1:D:160:ILE:HG12	1.81	0.63
1:A:541:ILE:HG22	1:A:543:GLY:H	1.63	0.62
1:D:131:ASN:OD1	1:D:134:ARG:NH1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ASN:OD1	1:A:134:ARG:NH1	2.33	0.62
1:C:369:GLN:HE22	1:D:516:ASP:HA	1.63	0.61
1:B:131:ASN:OD1	1:B:134:ARG:NH1	2.33	0.61
1:C:131:ASN:OD1	1:C:134:ARG:NH1	2.33	0.61
1:D:344:THR:HG22	1:D:458:LEU:HD11	1.83	0.61
1:C:54:LYS:O	1:C:91:ASN:ND2	2.34	0.61
1:B:369:GLN:HE22	1:C:516:ASP:HA	1.65	0.61
1:A:344:THR:HG22	1:A:458:LEU:HD11	1.83	0.61
1:A:38:LEU:HD11	1:D:618:ILE:HD12	1.81	0.61
1:B:54:LYS:O	1:B:91:ASN:ND2	2.34	0.61
1:B:190:ARG:HG2	1:B:232:LEU:HD13	1.83	0.60
1:A:190:ARG:HG2	1:A:232:LEU:HD13	1.83	0.60
1:C:344:THR:HG22	1:C:458:LEU:HD11	1.83	0.60
1:D:54:LYS:O	1:D:91:ASN:ND2	2.34	0.60
1:B:344:THR:HG22	1:B:458:LEU:HD11	1.83	0.60
1:A:54:LYS:O	1:A:91:ASN:ND2	2.34	0.59
1:A:618:ILE:HD12	1:B:38:LEU:HD11	1.83	0.59
1:A:273:LEU:HD11	1:B:160:ILE:HG12	1.84	0.59
1:D:190:ARG:HG2	1:D:232:LEU:HD13	1.83	0.59
1:D:546:ASN:HD22	1:D:549:VAL:HG22	1.68	0.59
1:C:190:ARG:HG2	1:C:232:LEU:HD13	1.83	0.59
1:C:193:ASP:OD1	1:C:197:ASN:N	2.37	0.58
1:B:632:ARG:NH1	1:C:34:ASP:OD1	2.36	0.58
1:C:546:ASN:HD22	1:C:549:VAL:HG22	1.68	0.58
1:A:546:ASN:HD22	1:A:549:VAL:HG22	1.68	0.58
1:D:146:ARG:NH1	1:D:164:GLU:OE1	2.36	0.58
1:A:34:ASP:OD1	1:D:632:ARG:NH1	2.36	0.58
1:B:618:ILE:HD12	1:C:38:LEU:HD11	1.86	0.57
1:B:546:ASN:HD22	1:B:549:VAL:HG22	1.68	0.57
1:C:618:ILE:HD12	1:D:38:LEU:HD11	1.87	0.57
1:C:146:ARG:NH1	1:C:164:GLU:OE1	2.36	0.56
1:B:193:ASP:OD1	1:B:197:ASN:N	2.37	0.56
1:A:280:LEU:HD22	1:A:631:LEU:HD23	1.88	0.56
1:B:280:LEU:HD22	1:B:631:LEU:HD23	1.88	0.56
1:A:477:PRO:HG3	1:A:589:ARG:HB2	1.88	0.55
1:D:193:ASP:OD1	1:D:197:ASN:N	2.37	0.55
1:D:477:PRO:HG3	1:D:589:ARG:HB2	1.89	0.55
1:A:193:ASP:OD1	1:A:197:ASN:N	2.37	0.55
1:D:49:LEU:HA	1:D:64:LEU:HD21	1.88	0.55
1:B:146:ARG:NH1	1:B:164:GLU:OE1	2.36	0.55
1:B:477:PRO:HG3	1:B:589:ARG:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:LEU:HD22	1:D:631:LEU:HD23	1.88	0.55
1:A:49:LEU:HA	1:A:64:LEU:HD21	1.88	0.55
1:A:369:GLN:HE22	1:B:516:ASP:HA	1.72	0.55
1:C:280:LEU:HD22	1:C:631:LEU:HD23	1.88	0.55
1:C:477:PRO:HG3	1:C:589:ARG:HB2	1.88	0.55
1:C:175:SER:HB3	1:C:178:ILE:HD13	1.90	0.54
1:C:49:LEU:HA	1:C:64:LEU:HD21	1.88	0.54
1:B:480:ILE:HG21	1:B:592:LEU:HD23	1.90	0.54
1:D:175:SER:HB3	1:D:178:ILE:HD13	1.90	0.54
1:C:480:ILE:HG21	1:C:592:LEU:HD23	1.90	0.53
1:A:480:ILE:HG21	1:A:592:LEU:HD23	1.90	0.53
1:A:619:CYS:SG	1:A:629:TRP:NE1	2.81	0.53
1:D:480:ILE:HG21	1:D:592:LEU:HD23	1.90	0.53
1:A:146:ARG:NH1	1:A:164:GLU:OE1	2.36	0.53
1:C:619:CYS:SG	1:C:629:TRP:NE1	2.81	0.53
1:B:49:LEU:HA	1:B:64:LEU:HD21	1.88	0.53
1:D:619:CYS:SG	1:D:629:TRP:NE1	2.81	0.53
1:A:175:SER:HB3	1:A:178:ILE:HD13	1.90	0.53
1:B:452:VAL:HG13	1:B:453:PRO:HD3	1.91	0.53
1:A:132:LEU:HD12	1:A:135:ALA:HB3	1.91	0.53
1:B:175:SER:HB3	1:B:178:ILE:HD13	1.90	0.53
1:C:452:VAL:HG13	1:C:453:PRO:HD3	1.91	0.53
1:B:619:CYS:SG	1:B:629:TRP:NE1	2.81	0.53
1:D:452:VAL:HG13	1:D:453:PRO:HD3	1.91	0.53
1:A:452:VAL:HG13	1:A:453:PRO:HD3	1.91	0.53
1:C:632:ARG:NH1	1:D:34:ASP:OD1	2.41	0.52
1:A:568:LEU:O	1:A:572:ASN:ND2	2.43	0.52
1:D:568:LEU:O	1:D:572:ASN:ND2	2.43	0.52
1:C:374:GLN:HG3	1:C:375:GLU:HG2	1.92	0.52
1:B:568:LEU:O	1:B:572:ASN:ND2	2.43	0.52
1:A:632:ARG:NH1	1:B:34:ASP:OD1	2.39	0.52
1:B:374:GLN:HG3	1:B:375:GLU:HG2	1.92	0.52
1:C:439:THR:HB	1:C:453:PRO:HB2	1.92	0.52
1:B:33:ARG:HG3	1:B:114:LEU:HD21	1.93	0.51
1:B:635:ASP:N	1:B:635:ASP:OD1	2.43	0.51
1:D:132:LEU:HD12	1:D:135:ALA:HB3	1.91	0.51
1:B:245:LYS:NZ	1:B:290:GLN:O	2.41	0.51
1:C:132:LEU:HD12	1:C:135:ALA:HB3	1.91	0.51
1:C:568:LEU:O	1:C:572:ASN:ND2	2.43	0.51
1:C:635:ASP:OD1	1:C:635:ASP:N	2.43	0.51
1:B:132:LEU:HD12	1:B:135:ALA:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:THR:HB	1:B:453:PRO:HB2	1.92	0.51
1:D:374:GLN:HG3	1:D:375:GLU:HG2	1.92	0.51
1:A:33:ARG:HG3	1:A:114:LEU:HD21	1.92	0.51
1:A:439:THR:HB	1:A:453:PRO:HB2	1.92	0.51
1:A:635:ASP:OD1	1:A:635:ASP:N	2.43	0.51
1:C:33:ARG:HG3	1:C:114:LEU:HD21	1.92	0.51
1:D:33:ARG:HG3	1:D:114:LEU:HD21	1.92	0.51
1:D:245:LYS:NZ	1:D:290:GLN:O	2.41	0.51
1:D:382:ASP:O	1:D:386:LEU:N	2.44	0.51
1:B:272:PRO:HB2	1:B:636:ARG:HG3	1.93	0.51
1:A:374:GLN:HG3	1:A:375:GLU:HG2	1.92	0.50
1:A:272:PRO:HB2	1:A:636:ARG:HG3	1.93	0.50
1:A:382:ASP:O	1:A:386:LEU:N	2.44	0.50
1:D:439:THR:HB	1:D:453:PRO:HB2	1.92	0.50
1:C:161:TYR:OH	1:C:193:ASP:OD2	2.29	0.50
1:C:245:LYS:NZ	1:C:290:GLN:O	2.41	0.50
1:A:516:ASP:HA	1:D:369:GLN:HE22	1.76	0.50
1:C:266:THR:HA	1:C:276:THR:HA	1.94	0.50
1:C:153:ARG:O	1:C:158:ASN:ND2	2.45	0.50
1:C:272:PRO:HB2	1:C:636:ARG:HG3	1.93	0.50
1:D:635:ASP:N	1:D:635:ASP:OD1	2.43	0.50
1:D:161:TYR:OH	1:D:193:ASP:OD2	2.29	0.49
1:A:153:ARG:O	1:A:158:ASN:ND2	2.45	0.49
1:A:161:TYR:OH	1:A:193:ASP:OD2	2.29	0.49
1:C:619:CYS:HG	1:C:629:TRP:HE1	1.60	0.49
1:D:272:PRO:HB2	1:D:636:ARG:HG3	1.93	0.49
1:D:266:THR:HA	1:D:276:THR:HA	1.94	0.49
1:A:132:LEU:O	1:A:136:LEU:N	2.35	0.49
1:B:72:VAL:HB	1:B:105:LEU:HD11	1.95	0.49
1:A:72:VAL:HB	1:A:105:LEU:HD11	1.95	0.49
1:C:72:VAL:HB	1:C:105:LEU:HD11	1.95	0.49
1:C:112:SER:HA	1:C:116:GLU:HG2	1.95	0.49
1:D:619:CYS:HG	1:D:629:TRP:HE1	1.57	0.49
1:C:382:ASP:O	1:C:386:LEU:N	2.44	0.49
1:C:132:LEU:HG	1:C:136:LEU:HG	1.95	0.48
1:B:112:SER:HA	1:B:116:GLU:HG2	1.95	0.48
1:B:161:TYR:OH	1:B:193:ASP:OD2	2.29	0.48
1:B:619:CYS:HG	1:B:629:TRP:HE1	1.60	0.48
1:D:72:VAL:HB	1:D:105:LEU:HD11	1.95	0.48
1:B:382:ASP:O	1:B:386:LEU:N	2.43	0.48
1:C:280:LEU:HD11	1:C:316:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:O	1:B:136:LEU:N	2.35	0.48
1:B:132:LEU:HG	1:B:136:LEU:HG	1.95	0.48
1:A:266:THR:HA	1:A:276:THR:HA	1.94	0.48
1:C:537:PHE:HD2	1:C:538:LEU:HD12	1.78	0.48
1:D:132:LEU:HG	1:D:136:LEU:HG	1.95	0.48
1:D:280:LEU:HD11	1:D:316:LEU:HD22	1.95	0.48
1:D:537:PHE:HD2	1:D:538:LEU:HD12	1.78	0.48
1:A:112:SER:HA	1:A:116:GLU:HG2	1.95	0.48
1:A:537:PHE:HD2	1:A:538:LEU:HD12	1.78	0.48
1:A:352:LEU:HG	1:A:370:GLN:HB3	1.96	0.48
1:B:266:THR:HA	1:B:276:THR:HA	1.94	0.47
1:A:132:LEU:HG	1:A:136:LEU:HG	1.95	0.47
1:B:153:ARG:O	1:B:158:ASN:ND2	2.45	0.47
1:D:112:SER:HA	1:D:116:GLU:HG2	1.95	0.47
1:C:352:LEU:HG	1:C:370:GLN:HB3	1.96	0.47
1:C:535:GLU:HB3	1:C:540:ILE:HB	1.97	0.47
1:D:153:ARG:O	1:D:158:ASN:ND2	2.45	0.47
1:D:352:LEU:HG	1:D:370:GLN:HB3	1.96	0.47
1:D:76:GLY:HA3	1:D:80:GLU:HB2	1.97	0.47
1:A:280:LEU:HD11	1:A:316:LEU:HD22	1.95	0.47
1:A:535:GLU:HB3	1:A:540:ILE:HB	1.97	0.47
1:A:76:GLY:HA3	1:A:80:GLU:HB2	1.96	0.47
1:B:280:LEU:HD11	1:B:316:LEU:HD22	1.95	0.47
1:B:537:PHE:HD2	1:B:538:LEU:HD12	1.78	0.47
1:D:535:GLU:HB3	1:D:540:ILE:HB	1.97	0.46
1:A:369:GLN:HG2	1:A:370:GLN:HE21	1.80	0.46
1:B:369:GLN:HG2	1:B:370:GLN:HE21	1.80	0.46
1:B:535:GLU:HB3	1:B:540:ILE:HB	1.97	0.46
1:C:76:GLY:HA3	1:C:80:GLU:HB2	1.97	0.46
1:C:369:GLN:HG2	1:C:370:GLN:HE21	1.80	0.46
1:B:352:LEU:HG	1:B:370:GLN:HB3	1.96	0.46
1:B:76:GLY:HA3	1:B:80:GLU:HB2	1.97	0.46
1:C:75:ARG:NH2	1:C:111:THR:OG1	2.38	0.46
1:A:522:HIS:CD2	1:A:544:PRO:HB3	2.51	0.45
1:C:132:LEU:O	1:C:136:LEU:N	2.35	0.45
1:C:522:HIS:CD2	1:C:544:PRO:HB3	2.51	0.45
1:D:522:HIS:CD2	1:D:544:PRO:HB3	2.51	0.45
1:A:237:ASN:HD21	1:A:241:LEU:HD12	1.82	0.45
1:C:237:ASN:HD21	1:C:241:LEU:HD12	1.82	0.45
1:D:369:GLN:HG2	1:D:370:GLN:HE21	1.80	0.45
1:B:522:HIS:CD2	1:B:544:PRO:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ASN:HD21	1:D:241:LEU:HD12	1.82	0.45
1:D:237:ASN:OD1	1:D:241:LEU:N	2.44	0.45
1:D:81:THR:OG1	1:D:84:HIS:ND1	2.42	0.44
1:B:286:SER:HB2	1:B:289:GLU:HB2	1.99	0.44
1:C:181:LEU:O	1:C:185:HIS:ND1	2.39	0.44
1:A:399:ILE:HG21	1:A:429:ILE:HG13	1.99	0.44
1:B:399:ILE:HG21	1:B:429:ILE:HG13	1.99	0.44
1:B:237:ASN:OD1	1:B:241:LEU:N	2.44	0.44
1:A:150:THR:HG23	1:A:153:ARG:HH11	1.83	0.44
1:C:474:MET:HB3	1:D:492:ARG:HD2	2.00	0.44
1:D:286:SER:HB2	1:D:289:GLU:HB2	1.99	0.44
1:D:75:ARG:HH21	1:D:111:THR:HG1	1.60	0.44
1:C:286:SER:HB2	1:C:289:GLU:HB2	1.99	0.44
1:A:286:SER:HB2	1:A:289:GLU:HB2	1.99	0.43
1:D:426:HIS:HA	1:D:429:ILE:HG22	2.00	0.43
1:B:150:THR:HG23	1:B:153:ARG:HH11	1.83	0.43
1:C:462:TRP:CD1	1:D:503:GLY:HA2	2.53	0.43
1:A:75:ARG:NH2	1:A:111:THR:OG1	2.38	0.43
1:A:269:THR:HG22	1:A:274:THR:HG23	2.00	0.43
1:A:245:LYS:NZ	1:A:290:GLN:O	2.41	0.43
1:B:237:ASN:HD21	1:B:241:LEU:HD12	1.82	0.43
1:C:302:ARG:HG3	1:C:305:ARG:HH21	1.84	0.43
1:A:426:HIS:HA	1:A:429:ILE:HG22	2.00	0.43
1:C:272:PRO:HG2	1:C:273:LEU:HD12	2.01	0.43
1:B:474:MET:HB3	1:C:492:ARG:HD2	1.99	0.43
1:D:150:THR:HG23	1:D:153:ARG:HH11	1.83	0.43
1:C:399:ILE:HG21	1:C:429:ILE:HG13	1.99	0.43
1:C:426:HIS:HA	1:C:429:ILE:HG22	2.00	0.43
1:D:399:ILE:HG21	1:D:429:ILE:HG13	1.99	0.43
1:D:302:ARG:HG3	1:D:305:ARG:HH21	1.84	0.43
1:B:339:TYR:OH	1:B:392:THR:O	2.31	0.43
1:D:181:LEU:O	1:D:185:HIS:ND1	2.39	0.43
1:D:253:THR:HG22	1:D:307:ILE:HD13	2.01	0.43
1:B:272:PRO:HG2	1:B:273:LEU:HD12	2.01	0.42
1:B:302:ARG:HG3	1:B:305:ARG:HH21	1.84	0.42
1:D:269:THR:HG22	1:D:274:THR:HG23	2.00	0.42
1:A:270:TYR:HB3	1:A:273:LEU:HB2	2.01	0.42
1:C:150:THR:HG23	1:C:153:ARG:HH11	1.83	0.42
1:D:488:GLY:O	1:D:492:ARG:NE	2.52	0.42
1:A:302:ARG:HG3	1:A:305:ARG:HH21	1.84	0.42
1:A:488:GLY:O	1:A:492:ARG:NE	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:HIS:HA	1:B:429:ILE:HG22	2.00	0.42
1:C:253:THR:HG22	1:C:307:ILE:HD13	2.01	0.42
1:A:619:CYS:HG	1:A:629:TRP:HE1	1.67	0.42
1:A:81:THR:OG1	1:A:84:HIS:ND1	2.42	0.42
1:B:95:ALA:HA	1:B:98:LEU:HD12	2.02	0.42
1:C:237:ASN:OD1	1:C:241:LEU:N	2.44	0.42
1:D:272:PRO:HG2	1:D:273:LEU:HD12	2.01	0.42
1:A:253:THR:HG22	1:A:307:ILE:HD13	2.01	0.42
1:A:95:ALA:HA	1:A:98:LEU:HD12	2.02	0.42
1:B:253:THR:HG22	1:B:307:ILE:HD13	2.01	0.42
1:B:350:ARG:HD3	1:C:513:GLN:OE1	2.19	0.42
1:A:625:LEU:HB3	1:A:630:PHE:HE2	1.85	0.42
1:D:95:ALA:HA	1:D:98:LEU:HD12	2.02	0.42
1:C:270:TYR:HB3	1:C:273:LEU:HB2	2.01	0.42
1:A:272:PRO:HG2	1:A:273:LEU:HD12	2.01	0.41
1:B:269:THR:HG22	1:B:274:THR:HG23	2.00	0.41
1:B:78:MET:N	1:B:78:MET:SD	2.93	0.41
1:A:514:THR:HG22	1:D:368:LEU:HB2	2.01	0.41
1:B:176:GLU:HA	1:B:215:MET:HE1	2.02	0.41
1:C:269:THR:HG22	1:C:274:THR:HG23	2.00	0.41
1:C:78:MET:SD	1:C:78:MET:N	2.93	0.41
1:D:78:MET:N	1:D:78:MET:SD	2.93	0.41
1:C:488:GLY:O	1:C:492:ARG:NE	2.52	0.41
1:D:465:VAL:HA	1:D:468:PHE:HD2	1.85	0.41
1:A:465:VAL:HA	1:A:468:PHE:HD2	1.85	0.41
1:B:181:LEU:O	1:B:185:HIS:ND1	2.39	0.41
1:B:465:VAL:HA	1:B:468:PHE:HD2	1.85	0.41
1:B:625:LEU:HB3	1:B:630:PHE:HE2	1.85	0.41
1:A:78:MET:N	1:A:78:MET:SD	2.93	0.41
1:A:217:ASN:OD1	1:A:258:HIS:NE2	2.41	0.41
1:B:270:TYR:HB3	1:B:273:LEU:HB2	2.01	0.41
1:A:241:LEU:HA	1:A:241:LEU:HD23	1.93	0.41
1:A:490:LEU:O	1:A:494:CYS:N	2.47	0.41
1:C:176:GLU:HA	1:C:215:MET:HE1	2.03	0.41
1:C:220:LEU:HD23	1:C:220:LEU:HA	1.94	0.41
1:C:465:VAL:HA	1:C:468:PHE:HD2	1.85	0.41
1:C:625:LEU:HB3	1:C:630:PHE:HE2	1.85	0.41
1:C:95:ALA:HA	1:C:98:LEU:HD12	2.02	0.41
1:B:488:GLY:O	1:B:492:ARG:NE	2.53	0.41
1:C:373:LEU:HD13	1:C:376:ALA:HB3	2.03	0.41
1:D:132:LEU:O	1:D:136:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:O	1:A:185:HIS:ND1	2.39	0.40
1:D:270:TYR:HB3	1:D:273:LEU:HB2	2.01	0.40
1:D:625:LEU:HB3	1:D:630:PHE:HE2	1.85	0.40
1:D:373:LEU:HD13	1:D:376:ALA:HB3	2.03	0.40
1:A:542:ASP:OD1	1:D:542:ASP:HB2	2.21	0.40
1:C:537:PHE:CD1	1:C:566:ALA:HB1	2.57	0.40
1:D:490:LEU:O	1:D:494:CYS:N	2.47	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 PDB entries followed by that with respect to all EM entries.

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	589/742 (79%)	523 (89%)	66 (11%)	0	100	100
1	B	589/742 (79%)	524 (89%)	65 (11%)	0	100	100
1	C	589/742 (79%)	524 (89%)	65 (11%)	0	100	100
1	D	589/742 (79%)	525 (89%)	64 (11%)	0	100	100
All	All	2356/2968 (79%)	2096 (89%)	260 (11%)	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 PDB entries followed by that with respect to all EM entries.

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	516/646 (80%)	513 (99%)	3 (1%)	89 96
1	B	516/646 (80%)	513 (99%)	3 (1%)	89 96
1	C	516/646 (80%)	513 (99%)	3 (1%)	89 96
1	D	516/646 (80%)	513 (99%)	3 (1%)	89 96
All	All	2064/2584 (80%)	2052 (99%)	12 (1%)	89 96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	MET
1	A	140	ARG
1	A	464	ASN
1	B	78	MET
1	B	140	ARG
1	B	464	ASN
1	C	78	MET
1	C	140	ARG
1	C	464	ASN
1	D	78	MET
1	D	140	ARG
1	D	464	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	118	GLN
1	A	165	HIS
1	A	206	GLN
1	A	357	ASN
1	A	370	GLN
1	A	426	HIS
1	A	522	HIS
1	A	546	ASN
1	B	62	ASN
1	B	118	GLN
1	B	165	HIS
1	B	206	GLN
1	B	357	ASN
1	B	370	GLN

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Mol	Chain	Res	Type
1	B	426	HIS
1	B	546	ASN
1	C	62	ASN
1	C	118	GLN
1	C	165	HIS
1	C	206	GLN
1	C	357	ASN
1	C	370	GLN
1	C	426	HIS
1	C	522	HIS
1	C	546	ASN
1	D	62	ASN
1	D	165	HIS
1	D	206	GLN
1	D	357	ASN
1	D	370	GLN
1	D	426	HIS
1	D	546	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.