



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:43 am BST

PDB ID : 6JFL
Title : Nucleotide-free Mitofusin2 (MFN2)
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Deposited on : 2019-02-10
Resolution : 2.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

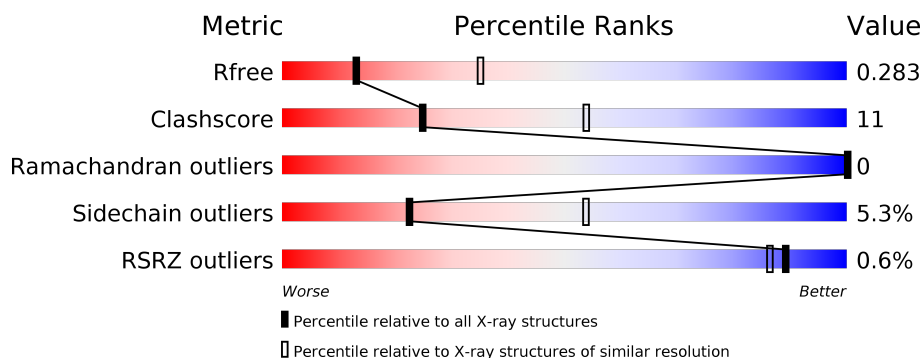
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	438	 69% 24% • 6%
1	B	438	 72% 20% • 6%
1	C	438	 64% 28% • 6%
1	D	438	 71% 23% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13486 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 Mitofusin-2,cDNA FLJ57997, highly similar to Transmembrane GTPase MFN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	1	0
			3328	2087	591	630	20			
1	B	413	Total	C	N	O	S	0	1	0
			3337	2094	591	633	19			
1	C	412	Total	C	N	O	S	0	1	0
			3332	2090	593	629	20			
1	D	415	Total	C	N	O	S	0	1	0
			3350	2102	593	634	21			

There are 28 discrepancies between the modelled and reference sequences:

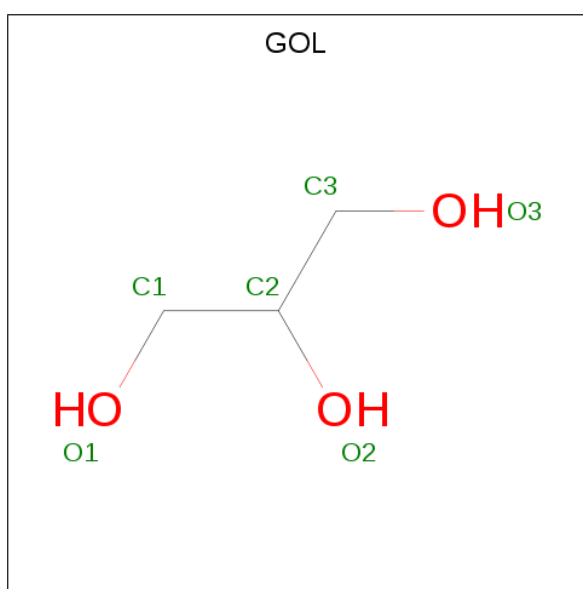
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP O95140
A	16	PRO	-	expression tag	UNP O95140
A	17	HIS	-	expression tag	UNP O95140
A	18	MET	-	expression tag	UNP O95140
A	19	GLY	-	expression tag	UNP O95140
A	20	GLY	-	expression tag	UNP O95140
A	21	SER	-	expression tag	UNP O95140
B	15	GLY	-	expression tag	UNP O95140
B	16	PRO	-	expression tag	UNP O95140
B	17	HIS	-	expression tag	UNP O95140
B	18	MET	-	expression tag	UNP O95140
B	19	GLY	-	expression tag	UNP O95140
B	20	GLY	-	expression tag	UNP O95140
B	21	SER	-	expression tag	UNP O95140
C	15	GLY	-	expression tag	UNP O95140
C	16	PRO	-	expression tag	UNP O95140
C	17	HIS	-	expression tag	UNP O95140
C	18	MET	-	expression tag	UNP O95140
C	19	GLY	-	expression tag	UNP O95140
C	20	GLY	-	expression tag	UNP O95140

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	SER	-	expression tag	UNP O95140
D	15	GLY	-	expression tag	UNP O95140
D	16	PRO	-	expression tag	UNP O95140
D	17	HIS	-	expression tag	UNP O95140
D	18	MET	-	expression tag	UNP O95140
D	19	GLY	-	expression tag	UNP O95140
D	20	GLY	-	expression tag	UNP O95140
D	21	SER	-	expression tag	UNP O95140

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		

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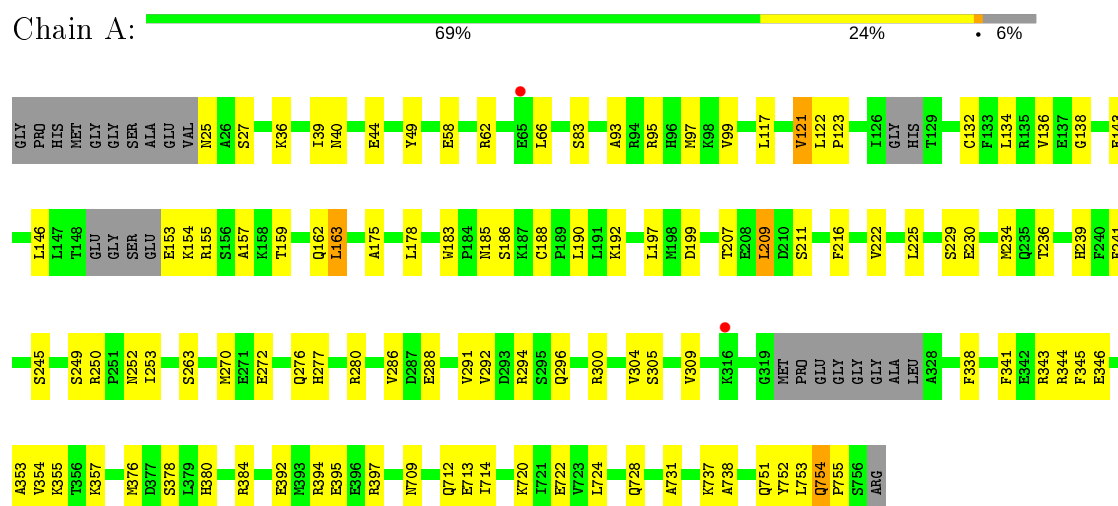
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	41	Total 41	O 41	0	0
4	C	29	Total 29	O 29	0	0
4	D	27	Total 27	O 27	0	0

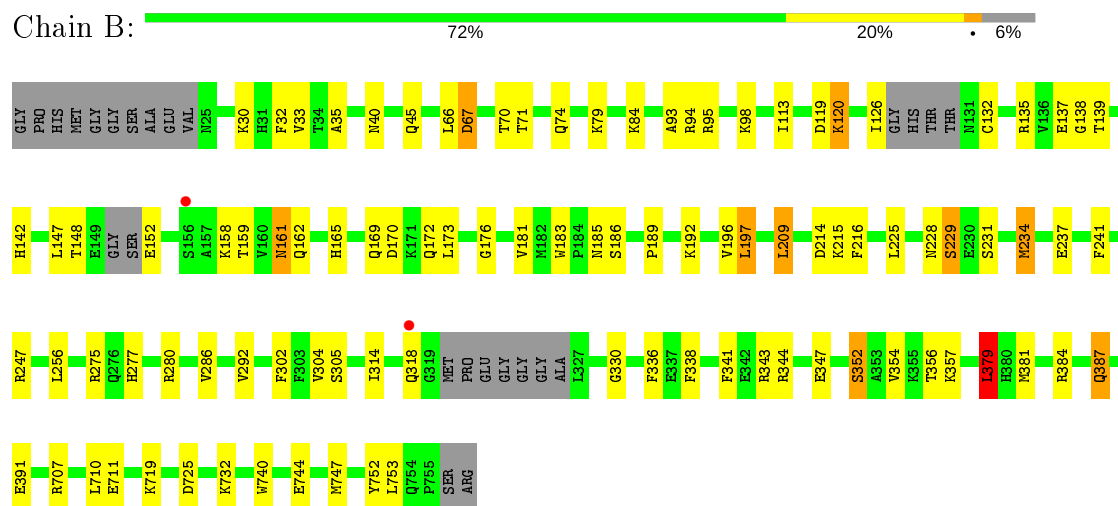
3 Residue-property plots

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 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: Mitofusin-2,cDNA FLJ57997, highly similar to Transmembrane GTPase MFN2

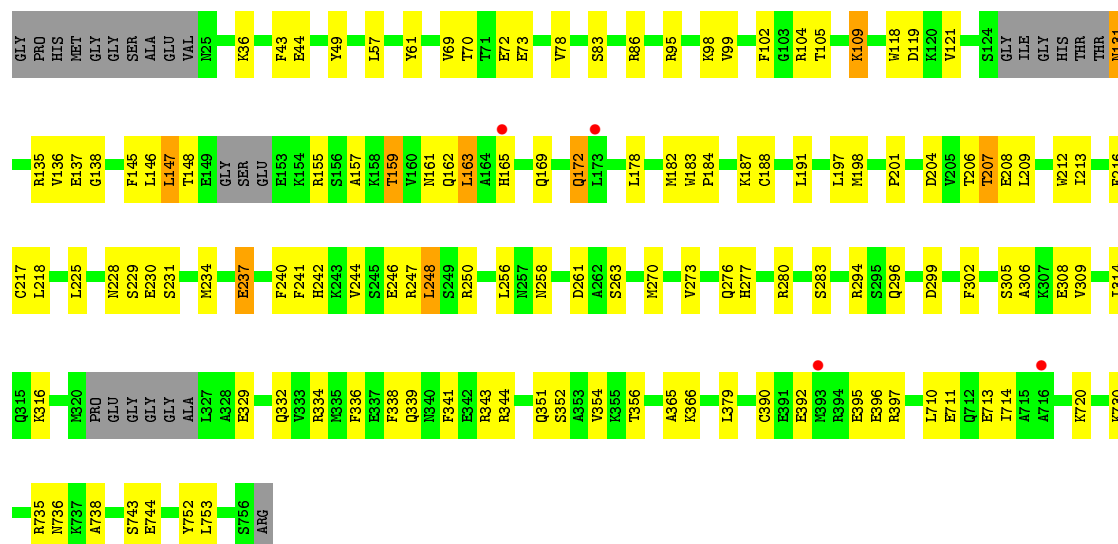


- Molecule 1: Mitofusin-2,cDNA FLJ57997, highly similar to Transmembrane GTPase MFN2



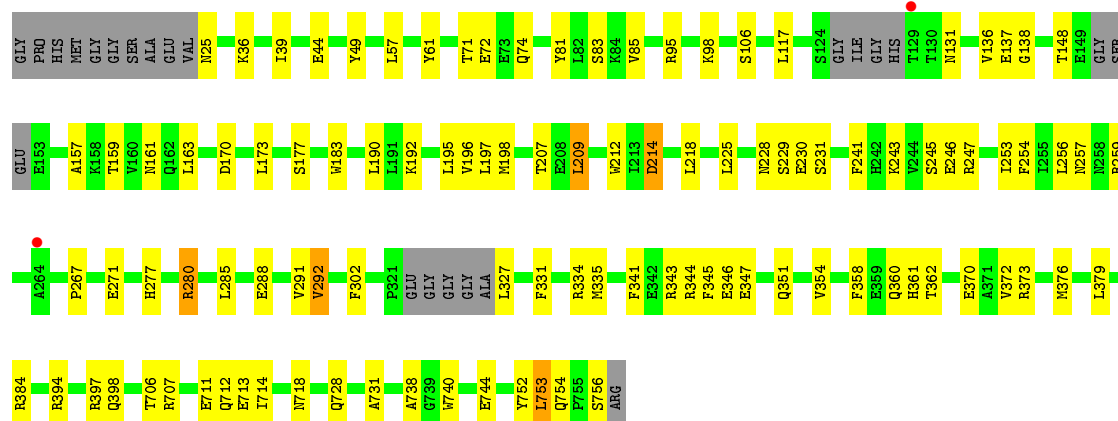
- Molecule 1: Mitofusin-2,cDNA FLJ57997, highly similar to Transmembrane GTPase MFN2





- Molecule 1: Mitofusin-2,cDNA FLJ57997, highly similar to Transmembrane GTPase MFN2

Chain D: 71% 23% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.48 Å 128.42 Å 91.33 Å 90.00° 106.27° 90.00°	Depositor
Resolution (Å)	36.34 – 2.81 48.70 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.1 (36.34-2.81) 98.2 (48.70-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.81 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.207 , 0.283 0.207 , 0.283	Depositor DCC
R_{free} test set	2206 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13486	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1451e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/3386	0.64	0/4555
1	B	0.48	1/3395 (0.0%)	0.66	2/4565 (0.0%)
1	C	0.47	0/3390	0.70	2/4557 (0.0%)
1	D	0.47	0/3409	0.65	1/4585 (0.0%)
All	All	0.47	1/13580 (0.0%)	0.66	5/18262 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	753	LEU	C-N	-5.75	1.20	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	379	LEU	CA-CB-CG	7.72	133.06	115.30
1	C	753	LEU	C-N-CA	-6.55	105.33	121.70
1	C	248	LEU	CA-CB-CG	6.49	130.23	115.30
1	B	209	LEU	CA-CB-CG	6.47	130.18	115.30
1	D	753	LEU	C-N-CA	-5.79	107.21	121.70

There are no chirality outliers.

There are no planarity outliers.

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	3328	0	3298	71	2
1	B	3337	0	3303	69	1
1	C	3332	0	3304	85	3
1	D	3350	0	3321	72	0
2	A	6	0	8	0	0
3	C	1	0	0	0	0
4	A	35	0	0	0	1
4	B	41	0	0	3	0
4	C	29	0	0	2	0
4	D	27	0	0	2	0
All	All	13486	0	13234	287	4

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 11.

All (287) 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:304:VAL:HG21	1:B:338:PHE:HD2	1.21	1.02
1:B:98:LYS:NZ	1:B:216:PHE:O	2.01	0.93
1:A:222:VAL:HG21	1:A:345:PHE:HE1	1.42	0.84
1:B:304:VAL:HG21	1:B:338:PHE:CD2	2.12	0.83
1:B:277:HIS:HA	1:B:280:ARG:HD3	1.64	0.78
1:A:40:ASN:HD21	1:A:93:ALA:HB2	1.48	0.77
1:D:209:LEU:HD22	1:D:212:TRP:CZ2	2.20	0.76
1:A:222:VAL:HG12	1:A:252:ASN:HB2	1.69	0.74
1:D:214:ASP:OD1	1:D:247:ARG:NH2	2.22	0.72
1:C:209:LEU:HD23	1:C:240:PHE:HB2	1.72	0.72
1:A:304:VAL:HG21	1:A:338:PHE:HB2	1.70	0.72
1:C:250:ARG:HE	1:C:356:THR:HG22	1.55	0.69
1:B:159:THR:HG23	1:B:162:GLN:H	1.57	0.69
1:D:384:ARG:HD3	1:D:728:GLN:HE22	1.58	0.69
1:D:394:ARG:NH1	1:D:718:ASN:OD1	2.19	0.69
1:C:70:THR:HB	1:C:379:LEU:HD11	1.75	0.68
1:A:159:THR:HG23	1:A:162:GLN:H	1.58	0.68
1:D:106:SER:O	1:D:259:ARG:NH2	2.28	0.67
1:B:176:GLY:O	1:B:215:LYS:NZ	2.23	0.67
1:B:387:GLN:NE2	1:B:391:GLU:OE2	2.27	0.67
1:B:139:THR:O	1:B:185:ASN:ND2	2.25	0.66
1:C:296:GLN:HG2	1:C:299:ASP:HB2	1.77	0.66
1:B:119:ASP:HA	1:B:314:ILE:HD11	1.77	0.66
1:D:209:LEU:HB3	1:D:212:TRP:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:TRP:HE1	1:C:187:LYS:HD2	1.59	0.65
1:A:397:ARG:NE	1:A:713:GLU:OE2	2.29	0.65
1:D:190:LEU:HD21	1:D:346:GLU:OE2	1.97	0.64
1:B:161:ASN:N	1:B:161:ASN:OD1	2.27	0.64
1:C:234:MET:HB2	1:C:237:GLU:HG2	1.80	0.64
1:B:113:ILE:HG12	1:B:197:LEU:HD23	1.79	0.63
1:C:157:ALA:HB1	1:C:163:LEU:HB2	1.80	0.63
1:B:740:TRP:CZ3	1:B:744:GLU:HG3	2.33	0.63
1:C:201:PRO:HG2	1:C:212:TRP:CZ2	2.33	0.63
1:B:45:GLN:OE1	1:D:25:ASN:ND2	2.22	0.62
1:B:158:LYS:H	1:B:162:GLN:NE2	1.97	0.61
1:C:263:SER:HB3	1:C:270:MET:HG3	1.82	0.61
1:D:343:ARG:HG2	1:D:344:ARG:NH1	2.14	0.61
1:A:222:VAL:HG21	1:A:345:PHE:CE1	2.31	0.61
1:A:354:VAL:HG11	1:A:752:TYR:HB3	1.83	0.61
1:A:49:TYR:OH	1:A:738:ALA:HB2	2.01	0.61
1:D:98:LYS:NZ	1:D:198:MET:SD	2.72	0.60
1:B:384:ARG:NH1	4:B:803:HOH:O	2.34	0.60
1:B:214:ASP:OD1	1:B:247:ARG:NH1	2.32	0.60
1:C:250:ARG:NE	1:C:356:THR:HG22	2.16	0.60
1:D:117:LEU:HD11	1:D:136:VAL:HG11	1.84	0.59
1:D:253:ILE:HD12	1:D:291:VAL:HG21	1.83	0.59
1:C:36:LYS:NZ	1:C:95:ARG:O	2.35	0.59
1:B:286:VAL:HG22	1:B:292:VAL:HG23	1.84	0.59
1:C:204:ASP:N	1:C:207:THR:OG1	2.29	0.58
1:C:244:VAL:O	1:C:248:LEU:HD23	2.02	0.58
1:C:159:THR:HG23	1:C:162:GLN:HB3	1.85	0.58
1:C:102:PHE:C	1:C:109:LYS:HD3	2.24	0.58
1:A:134:LEU:HB2	1:A:199:ASP:HB3	1.86	0.57
1:D:207:THR:HB	1:D:209:LEU:HD21	1.87	0.57
1:D:257:ASN:ND2	1:D:277:HIS:CE1	2.72	0.57
1:D:327:LEU:HD22	1:D:331:PHE:CE2	2.40	0.56
1:C:308:GLU:OE2	1:C:334:ARG:NH1	2.35	0.56
1:B:225:LEU:HB2	1:B:241:PHE:CZ	2.40	0.56
1:A:207:THR:HG22	1:A:209:LEU:HD13	1.89	0.55
1:A:304:VAL:HG22	1:A:305:SER:H	1.72	0.55
1:C:258:ASN:HD21	1:C:306:ALA:HB3	1.70	0.55
1:A:117:LEU:HD12	1:A:121:VAL:HG11	1.87	0.55
1:B:170:ASP:OD2	1:B:173:LEU:HG	2.07	0.55
1:C:118:TRP:HZ3	1:C:316:LYS:HD2	1.72	0.55
1:D:285:LEU:HB3	1:D:292:VAL:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:VAL:HG22	1:A:305:SER:N	2.23	0.54
1:D:61:TYR:CZ	1:D:72:GLU:HG3	2.43	0.54
1:D:190:LEU:HB3	1:D:195:LEU:HD23	1.88	0.54
1:B:135:ARG:O	1:B:181:VAL:N	2.37	0.54
1:C:258:ASN:HD21	1:C:306:ALA:CB	2.20	0.54
1:C:354:VAL:HG11	1:C:752:TYR:HB3	1.89	0.54
1:C:165:HIS:O	1:C:169:GLN:HG2	2.08	0.54
1:A:132:CYS:HA	1:A:175:ALA:HA	1.90	0.54
1:B:275:ARG:NH2	4:B:805:HOH:O	2.40	0.54
1:D:209:LEU:HD22	1:D:212:TRP:CE2	2.43	0.53
1:B:71:THR:OG1	1:B:74:GLN:HG3	2.09	0.53
1:D:397:ARG:NE	1:D:713:GLU:OE1	2.40	0.53
1:D:49:TYR:OH	1:D:738:ALA:HB2	2.09	0.53
1:C:146:LEU:HB2	1:C:155:ARG:HB2	1.91	0.53
1:B:256:LEU:HD23	1:B:302:PHE:HB2	1.91	0.52
1:A:309:VAL:HG11	1:A:338:PHE:CD2	2.45	0.52
1:B:113:ILE:HG23	1:B:197:LEU:HD22	1.91	0.52
1:A:58:GLU:OE2	1:A:62:ARG:NH2	2.42	0.52
1:C:343:ARG:HG3	1:C:344:ARG:NH1	2.25	0.52
1:A:263:SER:HB3	1:A:270:MET:HG3	1.90	0.52
1:A:239:HIS:HA	1:B:142:HIS:HD2	1.75	0.52
1:C:118:TRP:CZ3	1:C:316:LYS:HD2	2.45	0.52
1:D:397:ARG:NH1	1:D:397:ARG:O	2.42	0.51
1:D:95:ARG:NH2	1:D:361:HIS:HE1	2.09	0.51
1:D:354:VAL:HG11	1:D:752:TYR:HB3	1.92	0.51
1:B:98:LYS:HE3	1:B:135:ARG:HH12	1.76	0.51
1:C:135:ARG:HD2	1:C:178:LEU:HD11	1.93	0.51
1:B:228:ASN:HB3	1:B:231:SER:HB3	1.93	0.51
1:B:158:LYS:HG3	1:B:162:GLN:HE22	1.76	0.51
1:B:344:ARG:HH11	1:B:347:GLU:CD	2.14	0.51
1:B:95:ARG:NH2	1:B:357:LYS:O	2.44	0.51
1:B:732:LYS:HE2	4:B:829:HOH:O	2.11	0.50
1:C:213:ILE:HA	1:C:217:CYS:HB2	1.92	0.50
1:D:360:GLN:OE1	4:D:801:HOH:O	2.19	0.50
1:D:81:TYR:O	1:D:85:VAL:HG13	2.11	0.50
1:B:354:VAL:HG11	1:B:752:TYR:HB3	1.93	0.50
1:C:70:THR:HB	1:C:379:LEU:CD1	2.41	0.50
1:B:158:LYS:H	1:B:162:GLN:HE21	1.59	0.50
1:C:36:LYS:HD3	4:C:919:HOH:O	2.11	0.50
1:B:747:MET:HG3	1:D:347:GLU:CD	2.32	0.50
1:C:711:GLU:HA	1:C:714:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:GLU:HG3	1:D:196:VAL:HG22	1.94	0.50
1:D:159:THR:HG22	1:D:161:ASN:H	1.78	0.49
1:D:117:LEU:HD21	1:D:197:LEU:HD13	1.93	0.49
1:B:165:HIS:O	1:B:169:GLN:N	2.35	0.49
1:C:131:ASN:OD1	1:C:131:ASN:N	2.45	0.49
1:A:394:ARG:HG3	1:A:714:ILE:HD12	1.93	0.49
1:C:138:GLY:HA2	1:C:183:TRP:O	2.12	0.49
1:A:751:GLN:HE21	1:C:351:GLN:NE2	2.10	0.49
1:A:97:MET:HG2	1:A:353:ALA:CB	2.43	0.49
1:D:131:ASN:N	1:D:131:ASN:OD1	2.45	0.49
1:D:267:PRO:O	1:D:271:GLU:HG3	2.12	0.49
1:A:209:LEU:CD2	1:A:236:THR:HG22	2.42	0.48
1:D:370:GLU:HG3	1:D:373:ARG:HH11	1.76	0.48
1:C:145:PHE:CE2	1:C:182:MET:HG3	2.48	0.48
1:C:183:TRP:HB3	1:C:191:LEU:CD1	2.43	0.48
1:C:390:CYS:SG	1:C:720:LYS:HD2	2.53	0.48
1:A:724:LEU:O	1:A:728:GLN:HG3	2.13	0.48
1:C:256:LEU:HD23	1:C:302:PHE:HB2	1.94	0.48
1:A:27:SER:OG	1:A:346:GLU:OE1	2.31	0.48
1:D:228:ASN:ND2	1:D:230:GLU:H	2.11	0.48
1:A:66:LEU:HD23	1:A:720:LYS:HE3	1.96	0.48
1:C:119:ASP:OD2	1:C:187:LYS:HD3	2.13	0.48
1:C:270:MET:HA	1:C:273:VAL:HB	1.95	0.48
1:D:209:LEU:HB3	1:D:212:TRP:CG	2.49	0.48
1:A:157:ALA:HB1	1:A:163:LEU:HD12	1.96	0.48
1:A:343:ARG:HG3	1:A:344:ARG:NH2	2.29	0.48
1:C:146:LEU:HD21	1:C:163:LEU:HD23	1.95	0.48
1:C:61:TYR:OH	1:C:72:GLU:HB2	2.14	0.48
1:A:146:LEU:HB2	1:A:155:ARG:HB3	1.96	0.48
1:A:95:ARG:HD2	1:A:357:LYS:HB3	1.96	0.47
1:C:336:PHE:HA	1:C:339:GLN:HE21	1.77	0.47
1:C:242:HIS:O	1:C:246:GLU:HG3	2.14	0.47
1:C:735:ARG:NH1	1:C:736:ASN:OD1	2.47	0.47
1:D:71:THR:OG1	1:D:74:GLN:HG3	2.14	0.47
1:C:99:VAL:CG1	1:C:197:LEU:HD22	2.44	0.47
1:C:225:LEU:HB2	1:C:241:PHE:CZ	2.49	0.47
1:D:257:ASN:HD21	1:D:277:HIS:CE1	2.32	0.47
1:D:358:PHE:O	1:D:362:THR:HG23	2.14	0.47
1:A:185:ASN:HB2	1:A:192:LYS:HG3	1.95	0.47
1:C:352:SER:O	1:C:356:THR:HG23	2.15	0.47
1:D:707:ARG:O	1:D:707:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:GLU:N	1:C:208:GLU:OE1	2.48	0.47
1:C:86:ARG:NH1	4:C:903:HOH:O	2.45	0.47
1:A:157:ALA:CB	1:A:163:LEU:HD12	2.46	0.46
1:C:244:VAL:HG13	1:C:248:LEU:HD21	1.96	0.46
1:D:209:LEU:HD13	1:D:212:TRP:CZ3	2.51	0.46
1:A:277:HIS:HD2	1:A:280:ARG:HE	1.64	0.46
1:D:225:LEU:HB2	1:D:241:PHE:CZ	2.50	0.46
1:D:362:THR:HG21	1:D:753:LEU:HD11	1.96	0.46
1:A:384:ARG:HB2	1:A:728:GLN:NE2	2.30	0.46
1:B:189:PRO:HA	1:B:192:LYS:HB2	1.98	0.46
1:C:161:ASN:O	1:C:165:HIS:N	2.43	0.46
1:A:277:HIS:CD2	1:A:280:ARG:HE	2.34	0.46
1:B:302:PHE:CG	1:B:341:PHE:HB2	2.51	0.46
1:D:243:LYS:O	1:D:247:ARG:HG2	2.16	0.46
1:A:153:GLU:HG3	1:A:154:LYS:H	1.80	0.45
1:A:138:GLY:HA2	1:A:183:TRP:O	2.17	0.45
1:C:43:PHE:CZ	1:C:365:ALA:HB2	2.52	0.45
1:C:49:TYR:OH	1:C:738:ALA:HB2	2.17	0.45
1:C:276:GLN:HG3	1:C:277:HIS:N	2.32	0.45
1:D:39:ILE:HD11	1:D:362:THR:HG22	1.98	0.45
1:A:376:MET:HE2	1:A:731:ALA:HA	1.97	0.45
1:B:304:VAL:HG22	1:B:305:SER:N	2.31	0.45
1:C:231:SER:O	1:C:280:ARG:NH1	2.50	0.45
1:D:138:GLY:HA2	1:D:183:TRP:O	2.17	0.45
1:B:707:ARG:HA	1:B:710:LEU:HB2	1.99	0.45
1:D:157:ALA:HB1	1:D:163:LEU:HD12	1.98	0.45
1:B:352:SER:O	1:B:356:THR:HG23	2.17	0.45
1:C:121:VAL:HG22	1:C:183:TRP:CH2	2.52	0.45
1:C:234:MET:HB2	1:C:237:GLU:CG	2.46	0.45
1:B:185:ASN:HD22	1:B:185:ASN:H	1.65	0.44
1:B:35:ALA:HB2	1:B:752:TYR:CE1	2.52	0.44
1:C:183:TRP:NE1	1:C:187:LYS:HD2	2.31	0.44
1:B:354:VAL:CG1	1:B:752:TYR:HB3	2.47	0.44
1:B:70:THR:HB	1:B:379:LEU:CD2	2.48	0.44
1:C:135:ARG:HA	1:C:198:MET:HA	1.99	0.44
1:C:309:VAL:HG11	1:C:338:PHE:CD2	2.52	0.44
1:A:737:LYS:HE2	1:A:737:LYS:HB3	1.76	0.44
1:C:146:LEU:N	1:C:155:ARG:O	2.37	0.44
1:D:711:GLU:HG2	1:D:712:GLN:H	1.82	0.44
1:A:40:ASN:HD21	1:A:93:ALA:CB	2.24	0.44
1:C:308:GLU:CD	1:C:334:ARG:HH11	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:754:GLN:O	1:D:756:SER:N	2.50	0.44
1:B:229:SER:HA	1:B:277:HIS:ND1	2.33	0.44
1:C:98:LYS:NZ	1:C:216:PHE:O	2.50	0.44
1:D:331:PHE:CZ	1:D:335:MET:HE3	2.52	0.44
1:A:178:LEU:HB2	1:A:216:PHE:HE1	1.81	0.44
1:C:261:ASP:OD1	1:C:305:SER:OG	2.30	0.44
1:C:218:LEU:HD23	1:C:218:LEU:HA	1.69	0.44
1:A:99:VAL:HG23	1:A:222:VAL:HG23	1.99	0.44
1:A:304:VAL:HG11	1:A:338:PHE:HD1	1.82	0.44
1:A:380:HIS:HD2	1:A:728:GLN:O	2.01	0.44
1:A:276:GLN:O	1:A:280:ARG:HG3	2.18	0.43
1:A:304:VAL:HG21	1:A:338:PHE:CD1	2.53	0.43
1:B:137:GLU:HG3	1:B:196:VAL:HG22	2.00	0.43
1:B:67:ASP:OD2	1:B:67:ASP:N	2.50	0.43
1:C:273:VAL:HA	1:C:276:GLN:HG2	1.99	0.43
1:A:121:VAL:HG13	1:A:122:LEU:HG	2.00	0.43
1:D:256:LEU:HD23	1:D:256:LEU:HA	1.84	0.43
1:D:277:HIS:HD2	1:D:280:ARG:HB3	1.83	0.43
1:D:57:LEU:HD11	1:D:379:LEU:HD13	2.01	0.43
1:B:139:THR:C	1:B:185:ASN:ND2	2.72	0.43
1:B:344:ARG:NH1	1:B:347:GLU:OE2	2.37	0.43
1:A:136:VAL:HB	1:A:197:LEU:HB2	2.01	0.43
1:B:185:ASN:HB3	1:B:192:LYS:HG3	2.01	0.43
1:B:40:ASN:HD21	1:B:93:ALA:HA	1.83	0.43
1:C:710:LEU:O	1:C:714:ILE:N	2.46	0.43
1:C:397:ARG:NE	1:C:713:GLU:OE1	2.42	0.43
1:B:148:THR:O	1:B:152:GLU:N	2.52	0.43
1:A:250:ARG:HA	1:A:250:ARG:HD2	1.52	0.43
1:A:288:GLU:CD	1:B:186:SER:HB3	2.39	0.43
1:B:234:MET:HB2	1:B:237:GLU:OE2	2.18	0.43
1:C:228:ASN:ND2	1:C:230:GLU:H	2.17	0.43
1:D:95:ARG:HH21	1:D:361:HIS:HE1	1.65	0.43
1:A:286:VAL:HG11	1:A:294:ARG:HG2	2.01	0.43
1:D:57:LEU:HA	1:D:57:LEU:HD12	1.62	0.43
1:C:136:VAL:N	1:C:197:LEU:O	2.40	0.43
1:B:120:LYS:HE3	1:B:120:LYS:HB3	1.73	0.42
1:C:366:LYS:HB3	1:C:366:LYS:HE2	1.87	0.42
1:A:123:PRO:CG	1:A:163:LEU:HD23	2.48	0.42
1:A:751:GLN:NE2	1:C:351:GLN:NE2	2.67	0.42
1:C:162:GLN:O	1:C:165:HIS:HB2	2.20	0.42
1:B:343:ARG:HG2	1:B:344:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ASP:OD2	1:D:173:LEU:HG	2.19	0.42
1:A:25:ASN:ND2	1:C:744:GLU:OE2	2.52	0.42
1:A:712:GLN:HE21	1:A:712:GLN:HB3	1.58	0.42
1:B:225:LEU:HB2	1:B:241:PHE:CE2	2.54	0.42
1:D:254:PHE:CZ	1:D:345:PHE:HA	2.54	0.42
1:D:398:GLN:HE21	1:D:714:ILE:HG12	1.85	0.42
1:A:153:GLU:HG3	1:A:154:LYS:N	2.34	0.42
1:B:343:ARG:HG2	1:B:344:ARG:NH1	2.34	0.42
1:D:228:ASN:HB3	1:D:231:SER:HB2	2.02	0.42
1:C:183:TRP:CG	1:C:184:PRO:HD2	2.54	0.42
1:C:247:ARG:HD2	1:C:247:ARG:O	2.19	0.42
1:D:331:PHE:HA	1:D:334:ARG:NH1	2.34	0.42
1:D:36:LYS:NZ	1:D:95:ARG:O	2.33	0.42
1:A:249:SER:OG	1:A:249:SER:O	2.37	0.42
1:B:30:LYS:O	1:B:33:VAL:HG22	2.20	0.42
1:B:336:PHE:HZ	1:D:740:TRP:HB2	1.85	0.42
1:A:752:TYR:O	1:A:753:LEU:HD23	2.20	0.42
1:D:207:THR:CB	1:D:209:LEU:HD21	2.48	0.42
1:C:354:VAL:CG1	1:C:752:TYR:HB3	2.48	0.41
1:D:370:GLU:HG3	1:D:373:ARG:NH1	2.35	0.41
1:A:292:VAL:HG11	1:A:300:ARG:HG3	2.02	0.41
1:B:170:ASP:OD2	1:B:172:GLN:HG2	2.20	0.41
1:D:379:LEU:HD23	1:D:731:ALA:HB2	2.02	0.41
1:A:122:LEU:HD22	1:A:134:LEU:HD13	2.03	0.41
1:B:32:PHE:HD2	1:B:354:VAL:HG23	1.84	0.41
1:C:162:GLN:HA	1:C:165:HIS:ND1	2.35	0.41
1:C:710:LEU:O	1:C:714:ILE:HG13	2.20	0.41
1:D:372:VAL:O	1:D:376:MET:HG2	2.20	0.41
1:C:161:ASN:O	1:C:165:HIS:CD2	2.73	0.41
1:C:332:GLN:H	1:C:332:GLN:CD	2.24	0.41
1:A:159:THR:CG2	1:A:162:GLN:HB2	2.50	0.41
1:A:253:ILE:HD12	1:A:291:VAL:HG11	2.02	0.41
1:B:147:LEU:HD12	1:B:147:LEU:HA	1.84	0.41
1:C:147:LEU:HD13	1:C:148:THR:H	1.85	0.41
1:A:209:LEU:HD21	1:A:236:THR:HG22	2.03	0.41
1:C:169:GLN:OE1	1:C:169:GLN:HA	2.21	0.41
1:A:354:VAL:CG1	1:A:752:TYR:HB3	2.49	0.41
1:A:188[B]:CYS:SG	1:A:190:LEU:HB2	2.61	0.41
1:B:98:LYS:HE3	1:B:135:ARG:NH1	2.35	0.41
1:B:137:GLU:HG2	1:B:138:GLY:N	2.37	0.40
1:B:744:GLU:OE1	1:D:343:ARG:HD3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:VAL:HG22	1:A:292:VAL:O	2.22	0.40
1:B:138:GLY:HA2	1:B:183:TRP:O	2.20	0.40
1:C:188:CYS:SG	1:C:191:LEU:HG	2.60	0.40
1:A:225:LEU:HB2	1:A:241:PHE:CZ	2.56	0.40
1:C:57:LEU:CD1	1:C:78:VAL:HG21	2.51	0.40
1:B:343:ARG:HD3	1:D:744:GLU:OE1	2.21	0.40
1:B:330:GLY:HA2	4:D:803:HOH:O	2.22	0.40
1:C:137:GLU:HG2	1:C:138:GLY:N	2.37	0.40
1:D:190:LEU:HD23	1:D:190:LEU:HA	1.83	0.40
1:D:256:LEU:CD2	1:D:302:PHE:HB2	2.51	0.40
1:D:257:ASN:ND2	1:D:277:HIS:HE1	2.19	0.40
1:D:398:GLN:NE2	1:D:714:ILE:HG12	2.36	0.40
1:A:186:SER:HA	1:A:192:LYS:HE3	2.04	0.40
1:A:355:LYS:HD2	1:A:355:LYS:O	2.21	0.40
1:A:36:LYS:HA	1:A:39:ILE:HG22	2.02	0.40
1:A:754:GLN:HA	1:A:755:PRO:HD3	1.94	0.40
1:D:218:LEU:HD23	1:D:218:LEU:HA	1.89	0.40

All (4) 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:230:GLU:OE1	1:C:104:ARG:NH1[1_455]	2.08	0.12
1:C:172:GLN:NE2	1:C:711:GLU:OE1[1_655]	2.08	0.12
1:A:392:GLU:OE2	4:A:926:HOH:O[1_655]	2.14	0.06
1:B:84:LYS:NZ	1:C:396:GLU:OE2[2_546]	2.16	0.04

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	406/438 (93%)	397 (98%)	9 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	406/438 (93%)	396 (98%)	10 (2%)	0	100	100
1	C	405/438 (92%)	394 (97%)	11 (3%)	0	100	100
1	D	408/438 (93%)	398 (98%)	10 (2%)	0	100	100
All	All	1625/1752 (93%)	1585 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/380 (96%)	348 (95%)	18 (5%)	25	57
1	B	366/380 (96%)	346 (94%)	20 (6%)	21	52
1	C	366/380 (96%)	342 (93%)	24 (7%)	16	44
1	D	369/380 (97%)	353 (96%)	16 (4%)	29	62
All	All	1467/1520 (96%)	1389 (95%)	78 (5%)	22	54

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	83	SER
1	A	121	VAL
1	A	143	GLU
1	A	163	LEU
1	A	209	LEU
1	A	211	SER
1	A	229	SER
1	A	234	MET
1	A	245	SER
1	A	272	GLU
1	A	296	GLN
1	A	341	PHE

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Mol	Chain	Res	Type
1	A	378	SER
1	A	395	GLU
1	A	709	ASN
1	A	722	GLU
1	A	754	GLN
1	B	66	LEU
1	B	67	ASP
1	B	79	LYS
1	B	94	ARG
1	B	120	LYS
1	B	126	ILE
1	B	132	CYS
1	B	161	ASN
1	B	197	LEU
1	B	209	LEU
1	B	229	SER
1	B	234	MET
1	B	318	GLN
1	B	352	SER
1	B	379	LEU
1	B	381	MET
1	B	387	GLN
1	B	711	GLU
1	B	719	LYS
1	B	725	ASP
1	C	44	GLU
1	C	69	VAL
1	C	73	GLU
1	C	83	SER
1	C	105	THR
1	C	109	LYS
1	C	131	ASN
1	C	147	LEU
1	C	159	THR
1	C	163	LEU
1	C	172	GLN
1	C	206	THR
1	C	207	THR
1	C	229	SER
1	C	237	GLU
1	C	283	SER
1	C	294	ARG

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Mol	Chain	Res	Type
1	C	314	ILE
1	C	329	GLU
1	C	341	PHE
1	C	392	GLU
1	C	395	GLU
1	C	730	LYS
1	C	743	SER
1	D	44	GLU
1	D	83	SER
1	D	148	THR
1	D	177	SER
1	D	192	LYS
1	D	209	LEU
1	D	214	ASP
1	D	229	SER
1	D	245	SER
1	D	246	GLU
1	D	280	ARG
1	D	288	GLU
1	D	292	VAL
1	D	341	PHE
1	D	351	GLN
1	D	706	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	131	ASN
1	A	169	GLN
1	A	174	HIS
1	A	277	HIS
1	A	380	HIS
1	A	398	GLN
1	A	712	GLN
1	A	728	GLN
1	A	736	ASN
1	A	754	GLN
1	B	25	ASN
1	B	142	HIS
1	B	162	GLN
1	B	169	GLN

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Mol	Chain	Res	Type
1	B	242	HIS
1	B	276	GLN
1	B	315	GLN
1	B	398	GLN
1	B	709	ASN
1	B	728	GLN
1	B	750	HIS
1	C	74	GLN
1	C	96	HIS
1	C	131	ASN
1	C	142	HIS
1	C	228	ASN
1	C	276	GLN
1	C	277	HIS
1	C	339	GLN
1	C	351	GLN
1	C	361	HIS
1	C	751	GLN
1	C	754	GLN
1	D	31	HIS
1	D	96	HIS
1	D	228	ASN
1	D	257	ASN
1	D	277	HIS
1	D	351	GLN
1	D	361	HIS
1	D	712	GLN
1	D	728	GLN
1	D	751	GLN
1	D	754	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	GOL	A	801	-	5,5,5	0.35	0	5,5,5	0.23	0

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	GOL	A	801	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-O2
2	A	801	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	413/438 (94%)	-0.28	2 (0%) 91 88	29, 48, 89, 123	0
1	B	413/438 (94%)	-0.34	2 (0%) 91 88	27, 47, 91, 114	0
1	C	412/438 (94%)	-0.28	4 (0%) 82 77	28, 48, 86, 124	0
1	D	415/438 (94%)	-0.33	2 (0%) 91 88	27, 47, 82, 101	0
All	All	1653/1752 (94%)	-0.31	10 (0%) 89 86	27, 48, 87, 124	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	716	ALA	2.9
1	B	156	SER	2.8
1	D	264	ALA	2.5
1	B	318	GLN	2.5
1	C	393	MET	2.4
1	C	165	HIS	2.4
1	A	65	GLU	2.3
1	D	129	THR	2.2
1	A	316	LYS	2.1
1	C	173	LEU	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 carbohydrates 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(\AA^2)	Q<0.9
2	GOL	A	801	6/6	0.81	0.23	51,71,76,78	0
3	CA	C	801	1/1	0.84	0.12	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.