Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:50 PM GMT

PDB ID	:	1MAL
Title	:	STRUCTURAL BASIS FOR SUGAR TRANSLOCATION THROUGH MALTOPORIN CHANNELS AT 3.1 ANGSTROMS RESOLUTION
Authors	:	Schirmer, T.
Deposited on	:	1994-11-24
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

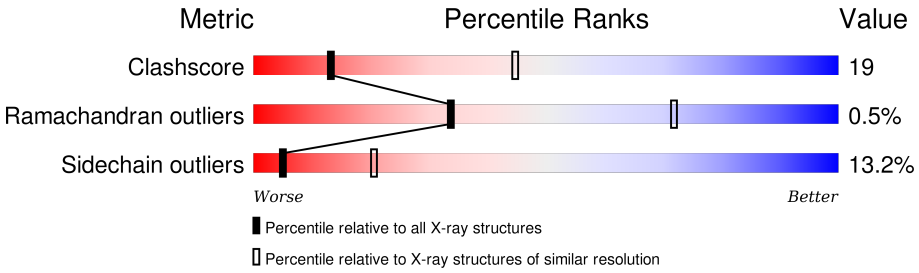
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	421	65% 29% 5% •
1	B	421	65% 30% 5% •
1	C	421	64% 30% 5% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10050 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 MALTOPORIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	73	0	0
			3350	2110	571	655	14			
1	B	421	Total	C	N	O	S	73	0	0
			3350	2110	571	655	14			
1	C	421	Total	C	N	O	S	73	0	0
			3350	2110	571	655	14			

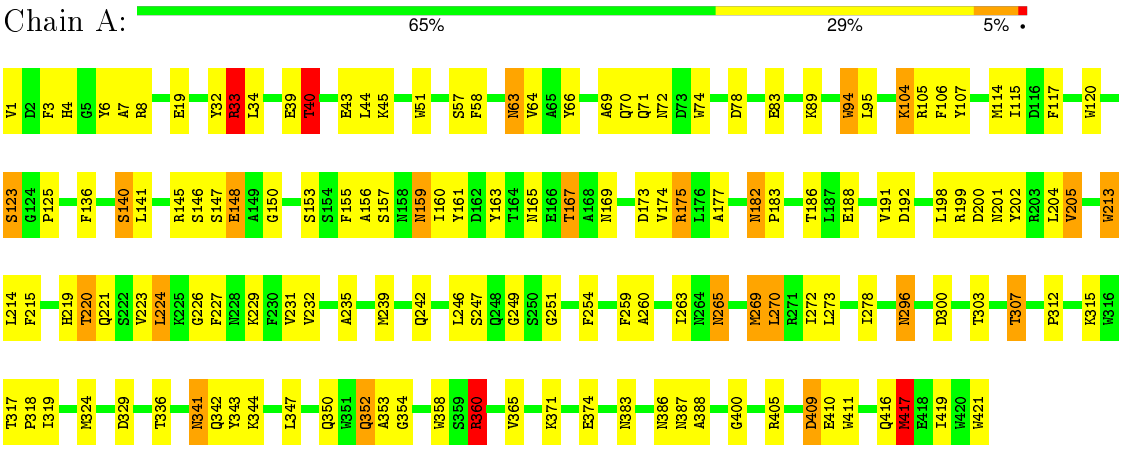
3 Residue-property plots (i)

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

Note EDS was not executed.

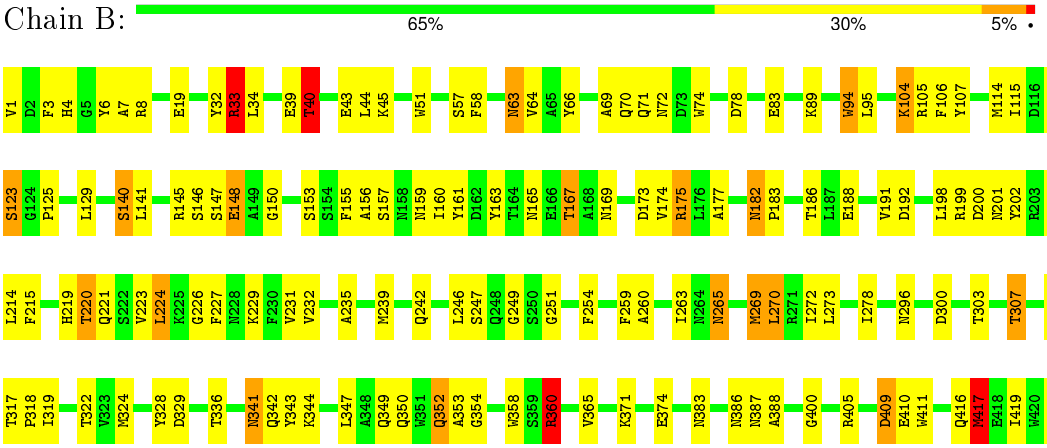
- Molecule 1: MALTOPORIN

Chain A:



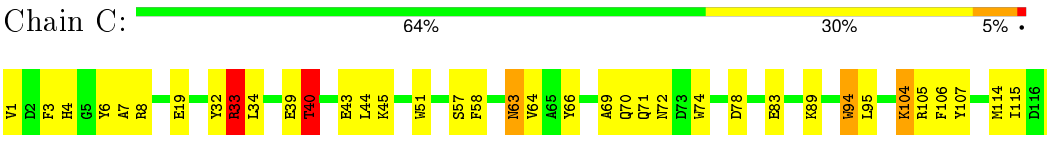
- Molecule 1: MALTOPORIN

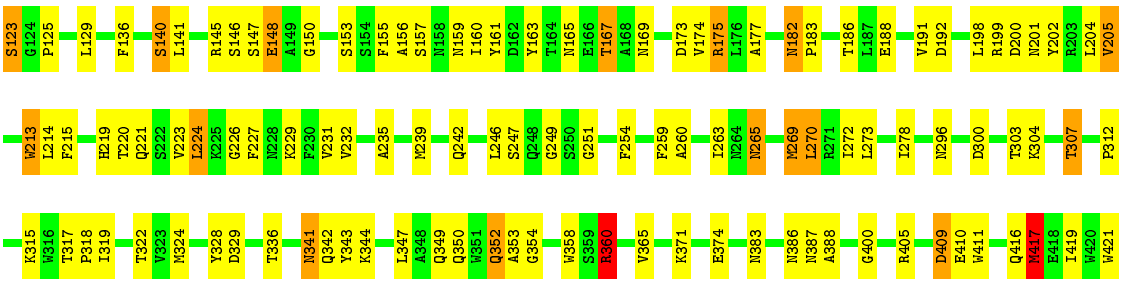
Chain B:



- Molecule 1: MALTOPORIN

Chain C:




S123 G124 P125 L129 F136 S140 L141 R145 S146 S147 E148 A149 G150 S153 S154 F155 A156 S157 N158 N159 I160 Y161 D162 Y163 T164 N165 E166 T167 A168 N169 D173 V174 R175 L176 A177 N182 P183 T186 L187 E188 V191 D192 L198 R199 D200 N201 Y202 R203 L204 V205
W213 L214 F215 H219 T220 Q221 S222 V223 L224 K225 G226 F227 M228 K229 F230 V231 V232 A235 M239 Q242 L246 S247 Q248 G249 S250 G251 F254 F259 A260 I263 N264 N265 M269 L270 R271 I272 L273 I278 M296 D300 T303 K304 T307 P312
K315 W316 T317 P318 I319 T322 V323 M324 Y328 D329 T336 N341 Q342 Y343 K344 L347 A348 Q349 Q350 W351 Q352 A353 G354 W358 S359 R360 V365 K371 E374 N383 N386 N387 A388 G400 R405 D409 E410 W411 Q416 M417 E418 I419 W420 W421

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	131.89Å 214.79Å 220.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.10	Depositor
% Data completeness (in resolution range)	95.5 (8.00-3.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.217 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10050	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.92	7/3443 (0.2%)	1.05	8/4668 (0.2%)
1	B	0.92	6/3443 (0.2%)	1.05	8/4668 (0.2%)
1	C	0.92	7/3443 (0.2%)	1.05	8/4668 (0.2%)
All	All	0.92	20/10329 (0.2%)	1.05	24/14004 (0.2%)

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	3
1	B	0	3
1	C	0	3
All	All	0	9

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	ASP	CB-CG	7.06	1.66	1.51
1	A	78	ASP	CB-CG	7.05	1.66	1.51
1	B	78	ASP	CB-CG	7.04	1.66	1.51
1	B	239	MET	SD-CE	-5.79	1.45	1.77
1	A	239	MET	SD-CE	-5.78	1.45	1.77
1	C	239	MET	SD-CE	-5.78	1.45	1.77
1	A	358	TRP	CB-CG	-5.67	1.40	1.50
1	C	358	TRP	CB-CG	-5.67	1.40	1.50
1	B	358	TRP	CB-CG	-5.66	1.40	1.50
1	B	365	VAL	CA-CB	-5.49	1.43	1.54
1	A	365	VAL	CA-CB	-5.49	1.43	1.54
1	C	365	VAL	CA-CB	-5.46	1.43	1.54
1	B	417	MET	CG-SD	-5.15	1.67	1.81
1	A	417	MET	CG-SD	-5.15	1.67	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	417	MET	CG-SD	-5.12	1.67	1.81
1	A	69	ALA	CA-CB	-5.11	1.41	1.52
1	C	69	ALA	CA-CB	-5.11	1.41	1.52
1	B	69	ALA	CA-CB	-5.09	1.41	1.52
1	A	213	TRP	CB-CG	-5.04	1.41	1.50
1	C	213	TRP	CB-CG	-5.03	1.41	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	78	ASP	CB-CG-OD1	11.22	128.40	118.30
1	A	78	ASP	CB-CG-OD1	11.21	128.39	118.30
1	C	78	ASP	CB-CG-OD1	11.20	128.38	118.30
1	A	239	MET	CG-SD-CE	7.22	111.76	100.20
1	C	239	MET	CG-SD-CE	7.22	111.76	100.20
1	B	239	MET	CG-SD-CE	7.20	111.73	100.20
1	B	33	ARG	N-CA-C	7.04	130.01	111.00
1	C	33	ARG	N-CA-C	7.04	130.00	111.00
1	A	33	ARG	N-CA-C	7.03	129.98	111.00
1	B	33	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	33	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	33	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	78	ASP	OD1-CG-OD2	-5.26	113.31	123.30
1	A	78	ASP	OD1-CG-OD2	-5.25	113.32	123.30
1	C	78	ASP	OD1-CG-OD2	-5.24	113.35	123.30
1	B	360	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	A	360	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	B	417	MET	CG-SD-CE	5.14	108.43	100.20
1	A	417	MET	CG-SD-CE	5.12	108.39	100.20
1	C	360	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	C	417	MET	CG-SD-CE	5.12	108.39	100.20
1	C	40	THR	N-CA-C	-5.06	97.34	111.00
1	A	40	THR	N-CA-C	-5.05	97.36	111.00
1	B	40	THR	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TYR	Sidechain
1	A	33	ARG	Sidechain
1	A	360	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	B	107	TYR	Sidechain
1	B	33	ARG	Sidechain
1	B	360	ARG	Mainchain
1	C	107	TYR	Sidechain
1	C	33	ARG	Sidechain
1	C	360	ARG	Mainchain

5.2 Too-close contacts

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	3350	0	3070	122	0
1	B	3350	0	3070	122	0
1	C	3350	0	3070	122	0
All	All	10050	0	9210	354	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 19.

All (354) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:MET:SD	1:A:417:MET:CE	2.03	1.47
1:B:417:MET:SD	1:B:417:MET:CE	2.03	1.45
1:C:417:MET:SD	1:C:417:MET:CE	2.03	1.44
1:B:317:THR:HG22	1:B:319:ILE:H	1.22	1.05
1:C:317:THR:HG22	1:C:319:ILE:H	1.22	1.03
1:A:317:THR:HG22	1:A:319:ILE:H	1.22	1.02
1:A:155:PHE:CE1	1:A:157:SER:HB3	2.10	0.87
1:C:155:PHE:HE1	1:C:157:SER:HB3	1.40	0.86
1:B:155:PHE:CE1	1:B:157:SER:HB3	2.10	0.86
1:C:155:PHE:CE1	1:C:157:SER:HB3	2.10	0.85
1:B:155:PHE:HE1	1:B:157:SER:HB3	1.40	0.85
1:A:155:PHE:HE1	1:A:157:SER:HB3	1.40	0.84
1:C:163:TYR:CD2	1:C:205:VAL:HG23	2.16	0.80
1:A:163:TYR:CD2	1:A:205:VAL:HG23	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:TYR:CD2	1:B:205:VAL:HG23	2.16	0.80
1:C:223:VAL:HG12	1:C:224:LEU:HG	1.68	0.76
1:A:223:VAL:HG12	1:A:224:LEU:HG	1.67	0.76
1:C:161:TYR:HE2	1:C:259:PHE:HD2	1.34	0.76
1:B:223:VAL:HG12	1:B:224:LEU:HG	1.68	0.75
1:A:161:TYR:HE2	1:A:259:PHE:HD2	1.34	0.75
1:C:94:TRP:CD1	1:C:95:LEU:HG	2.23	0.74
1:A:94:TRP:CD1	1:A:95:LEU:HG	2.23	0.74
1:B:94:TRP:CD1	1:B:95:LEU:HG	2.23	0.74
1:A:374:GLU:OE1	1:A:405:ARG:HB2	1.88	0.74
1:B:182:ASN:HB2	1:B:183:PRO:HD2	1.70	0.73
1:B:161:TYR:HE2	1:B:259:PHE:HD2	1.34	0.73
1:C:145:ARG:HG3	1:C:146:SER:N	2.04	0.73
1:C:374:GLU:OE1	1:C:405:ARG:HB2	1.88	0.72
1:B:374:GLU:OE1	1:B:405:ARG:HB2	1.88	0.72
1:A:182:ASN:HB2	1:A:183:PRO:HD2	1.70	0.72
1:B:145:ARG:HG3	1:B:146:SER:N	2.04	0.72
1:A:145:ARG:HG3	1:A:146:SER:N	2.04	0.72
1:C:182:ASN:HB2	1:C:183:PRO:HD2	1.70	0.71
1:B:63:ASN:HB3	1:B:83:GLU:CG	2.22	0.70
1:A:63:ASN:HB3	1:A:83:GLU:CG	2.22	0.70
1:C:63:ASN:HB3	1:C:83:GLU:CG	2.22	0.70
1:B:161:TYR:CE2	1:B:259:PHE:HD2	2.10	0.69
1:B:223:VAL:HG12	1:B:224:LEU:N	2.08	0.69
1:A:161:TYR:CE2	1:A:259:PHE:HD2	2.11	0.69
1:A:106:PHE:HA	1:A:123:SER:HB3	1.75	0.69
1:B:169:ASN:HD21	1:B:249:GLY:H	1.41	0.69
1:A:223:VAL:HG12	1:A:224:LEU:N	2.08	0.68
1:A:169:ASN:HD21	1:A:249:GLY:H	1.41	0.68
1:C:161:TYR:CE2	1:C:259:PHE:HD2	2.11	0.68
1:B:63:ASN:HB3	1:B:83:GLU:HG2	1.76	0.68
1:B:106:PHE:HA	1:B:123:SER:HB3	1.76	0.68
1:B:214:LEU:HD13	1:B:235:ALA:HB2	1.76	0.68
1:C:169:ASN:HD21	1:C:249:GLY:H	1.41	0.68
1:A:63:ASN:HB3	1:A:83:GLU:HG2	1.76	0.67
1:A:214:LEU:HD13	1:A:235:ALA:HB2	1.77	0.67
1:C:63:ASN:HB3	1:C:83:GLU:HG2	1.76	0.66
1:C:223:VAL:HG12	1:C:224:LEU:N	2.08	0.66
1:C:214:LEU:HD13	1:C:235:ALA:HB2	1.76	0.66
1:C:106:PHE:HA	1:C:123:SER:HB3	1.75	0.66
1:B:317:THR:HG23	1:B:318:PRO:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASP:OD1	1:A:175:ARG:HD2	1.97	0.65
1:C:317:THR:HG23	1:C:318:PRO:HD2	1.79	0.65
1:A:317:THR:HG23	1:A:318:PRO:HD2	1.79	0.65
1:B:173:ASP:OD1	1:B:175:ARG:HD2	1.97	0.64
1:C:342:GLN:HG2	1:C:343:TYR:N	2.11	0.64
1:B:342:GLN:HG2	1:B:343:TYR:N	2.11	0.64
1:B:63:ASN:HD22	1:B:64:VAL:N	1.96	0.64
1:A:342:GLN:HG2	1:A:343:TYR:N	2.11	0.64
1:C:173:ASP:OD1	1:C:175:ARG:HD2	1.97	0.64
1:C:63:ASN:HD22	1:C:64:VAL:N	1.96	0.63
1:A:63:ASN:HD22	1:A:64:VAL:N	1.96	0.62
1:C:63:ASN:C	1:C:63:ASN:HD22	2.02	0.62
1:A:63:ASN:C	1:A:63:ASN:HD22	2.02	0.62
1:C:153:SER:HB2	1:C:163:TYR:CD1	2.34	0.62
1:B:153:SER:HB2	1:B:163:TYR:CD1	2.34	0.62
1:A:219:HIS:CE1	1:A:221:GLN:HB2	2.35	0.62
1:C:341:ASN:C	1:C:341:ASN:HD22	2.03	0.62
1:B:341:ASN:HD22	1:B:341:ASN:C	2.03	0.62
1:A:153:SER:HB2	1:A:163:TYR:CD1	2.34	0.61
1:A:341:ASN:C	1:A:341:ASN:HD22	2.03	0.61
1:C:219:HIS:CE1	1:C:221:GLN:HB2	2.35	0.61
1:B:63:ASN:C	1:B:63:ASN:HD22	2.02	0.61
1:B:219:HIS:CE1	1:B:221:GLN:HB2	2.35	0.61
1:C:182:ASN:C	1:C:182:ASN:HD22	2.04	0.61
1:B:145:ARG:HG3	1:B:146:SER:H	1.65	0.60
1:A:145:ARG:HG3	1:A:146:SER:H	1.65	0.60
1:A:43:GLU:C	1:A:44:LEU:HD23	2.22	0.60
1:B:63:ASN:CB	1:B:83:GLU:HG3	2.32	0.59
1:C:63:ASN:CB	1:C:83:GLU:HG3	2.32	0.59
1:B:182:ASN:HD22	1:B:182:ASN:C	2.04	0.59
1:C:43:GLU:C	1:C:44:LEU:HD23	2.22	0.59
1:C:145:ARG:HG3	1:C:146:SER:H	1.65	0.59
1:A:182:ASN:HD22	1:A:182:ASN:C	2.04	0.59
1:B:43:GLU:C	1:B:44:LEU:HD23	2.22	0.59
1:C:141:LEU:HD22	1:C:174:VAL:HG22	1.85	0.59
1:B:141:LEU:HD22	1:B:174:VAL:HG22	1.85	0.58
1:A:63:ASN:CB	1:A:83:GLU:HG3	2.32	0.58
1:C:182:ASN:HB2	1:C:183:PRO:CD	2.34	0.58
1:A:383:ASN:HB3	1:A:386:ASN:H	1.69	0.58
1:A:141:LEU:HD22	1:A:174:VAL:HG22	1.85	0.58
1:A:182:ASN:HB2	1:A:183:PRO:CD	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ASN:HB2	1:B:183:PRO:CD	2.34	0.57
1:C:383:ASN:HB3	1:C:386:ASN:H	1.69	0.57
1:B:383:ASN:HB3	1:B:386:ASN:H	1.69	0.57
1:B:145:ARG:HD2	1:C:71:GLN:OE1	2.05	0.56
1:A:145:ARG:HD2	1:B:71:GLN:OE1	2.05	0.56
1:A:145:ARG:CG	1:A:146:SER:N	2.68	0.56
1:C:94:TRP:HD1	1:C:95:LEU:HG	1.69	0.56
1:B:145:ARG:CG	1:B:146:SER:N	2.68	0.56
1:C:145:ARG:CG	1:C:146:SER:N	2.68	0.56
1:B:94:TRP:HD1	1:B:95:LEU:HG	1.69	0.56
1:A:148:GLU:HG3	1:A:167:THR:HG23	1.88	0.56
1:A:317:THR:HG22	1:A:319:ILE:N	2.06	0.55
1:B:219:HIS:HE1	1:B:221:GLN:HB2	1.71	0.55
1:C:317:THR:HG22	1:C:319:ILE:N	2.06	0.55
1:A:71:GLN:OE1	1:C:145:ARG:HD2	2.05	0.55
1:B:63:ASN:HB3	1:B:83:GLU:HG3	1.88	0.55
1:C:219:HIS:HE1	1:C:221:GLN:HB2	1.71	0.55
1:C:148:GLU:HG3	1:C:167:THR:HG23	1.88	0.55
1:B:148:GLU:HG3	1:B:167:THR:HG23	1.88	0.55
1:C:63:ASN:HB3	1:C:83:GLU:HG3	1.89	0.55
1:C:198:LEU:HD11	1:C:204:LEU:HG	1.89	0.54
1:B:317:THR:HG22	1:B:319:ILE:N	2.06	0.54
1:C:141:LEU:CD2	1:C:174:VAL:HG22	2.37	0.54
1:A:198:LEU:HD11	1:A:204:LEU:HG	1.89	0.54
1:B:141:LEU:CD2	1:B:174:VAL:HG22	2.37	0.54
1:A:163:TYR:CE2	1:A:205:VAL:HG23	2.42	0.54
1:B:163:TYR:CE2	1:B:205:VAL:HG23	2.42	0.54
1:B:115:ILE:HG13	1:B:117:PHE:HB2	1.90	0.54
1:C:383:ASN:HB3	1:C:386:ASN:HB2	1.90	0.54
1:A:141:LEU:CD2	1:A:174:VAL:HG22	2.37	0.53
1:A:202:TYR:N	1:A:202:TYR:CD1	2.76	0.53
1:A:94:TRP:HD1	1:A:95:LEU:HG	1.69	0.53
1:B:383:ASN:HB3	1:B:386:ASN:HB2	1.91	0.53
1:C:155:PHE:HD1	1:C:156:ALA:O	1.92	0.53
1:C:163:TYR:CE2	1:C:205:VAL:HG23	2.42	0.53
1:C:341:ASN:C	1:C:341:ASN:ND2	2.62	0.53
1:A:341:ASN:ND2	1:A:341:ASN:C	2.62	0.53
1:A:155:PHE:HD1	1:A:156:ALA:O	1.92	0.53
1:C:32:TYR:HB2	1:C:344:LYS:HE2	1.91	0.53
1:B:198:LEU:HD11	1:B:204:LEU:HG	1.89	0.53
1:A:115:ILE:HG13	1:A:117:PHE:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ILE:HG13	1:C:117:PHE:HB2	1.90	0.53
1:A:63:ASN:HB3	1:A:83:GLU:HG3	1.88	0.53
1:A:383:ASN:HB3	1:A:386:ASN:HB2	1.91	0.52
1:B:202:TYR:N	1:B:202:TYR:CD1	2.76	0.52
1:B:341:ASN:C	1:B:341:ASN:ND2	2.62	0.52
1:B:32:TYR:HB2	1:B:344:LYS:HE2	1.91	0.52
1:C:202:TYR:CD1	1:C:202:TYR:N	2.76	0.52
1:A:219:HIS:HE1	1:A:221:GLN:HB2	1.71	0.52
1:A:161:TYR:HE2	1:A:259:PHE:CD2	2.23	0.52
1:B:44:LEU:N	1:B:44:LEU:HD23	2.25	0.51
1:A:32:TYR:HB2	1:A:344:LYS:HE2	1.91	0.51
1:B:155:PHE:HD1	1:B:156:ALA:O	1.92	0.51
1:B:63:ASN:CB	1:B:83:GLU:CG	2.88	0.51
1:B:115:ILE:HG13	1:B:117:PHE:CB	2.41	0.51
1:A:115:ILE:HG13	1:A:117:PHE:CB	2.41	0.51
1:B:254:PHE:CE1	1:B:260:ALA:HB2	2.46	0.51
1:C:223:VAL:CG1	1:C:224:LEU:N	2.74	0.51
1:C:254:PHE:CE1	1:C:260:ALA:HB2	2.45	0.51
1:C:44:LEU:HD23	1:C:44:LEU:N	2.25	0.51
1:A:140:SER:O	1:A:141:LEU:HD23	2.10	0.51
1:A:44:LEU:HD23	1:A:44:LEU:N	2.25	0.51
1:A:4:HIS:HA	1:A:421:TRP:CD1	2.46	0.51
1:C:4:HIS:HA	1:C:421:TRP:CD1	2.46	0.51
1:B:140:SER:O	1:B:141:LEU:HD23	2.10	0.50
1:B:1:VAL:HG23	1:C:3:PHE:CD2	2.45	0.50
1:A:254:PHE:CE1	1:A:260:ALA:HB2	2.46	0.50
1:C:169:ASN:ND2	1:C:249:GLY:H	2.08	0.50
1:A:1:VAL:HG23	1:B:3:PHE:CD2	2.46	0.50
1:B:231:VAL:HG12	1:B:232:VAL:N	2.27	0.50
1:A:43:GLU:HB3	1:A:63:ASN:HD21	1.77	0.50
1:C:140:SER:O	1:C:141:LEU:HD23	2.10	0.50
1:B:40:THR:OG1	1:B:70:GLN:NE2	2.45	0.50
1:B:202:TYR:N	1:B:202:TYR:HD1	2.10	0.50
1:C:202:TYR:HD1	1:C:202:TYR:N	2.10	0.50
1:A:352:GLN:NE2	1:A:354:GLY:O	2.44	0.50
1:B:4:HIS:HA	1:B:421:TRP:CD1	2.46	0.50
1:B:161:TYR:HE2	1:B:259:PHE:CD2	2.23	0.50
1:C:40:THR:OG1	1:C:70:GLN:NE2	2.45	0.50
1:C:163:TYR:HE2	1:C:205:VAL:HA	1.77	0.50
1:A:202:TYR:N	1:A:202:TYR:HD1	2.10	0.50
1:A:40:THR:OG1	1:A:70:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:HG12	1:A:232:VAL:N	2.27	0.50
1:A:242:GLN:NE2	1:A:246:LEU:HD12	2.27	0.50
1:A:3:PHE:CD2	1:C:1:VAL:HG23	2.46	0.49
1:B:43:GLU:HB3	1:B:63:ASN:HD21	1.77	0.49
1:C:115:ILE:HG13	1:C:117:PHE:CB	2.41	0.49
1:C:352:GLN:NE2	1:C:354:GLY:O	2.44	0.49
1:C:231:VAL:HG12	1:C:232:VAL:N	2.27	0.49
1:B:169:ASN:ND2	1:B:249:GLY:H	2.07	0.49
1:A:150:GLY:HA2	1:A:165:ASN:O	2.13	0.49
1:B:242:GLN:NE2	1:B:246:LEU:HD12	2.27	0.49
1:C:242:GLN:NE2	1:C:246:LEU:HD12	2.27	0.49
1:B:352:GLN:NE2	1:B:354:GLY:O	2.44	0.49
1:B:417:MET:SD	1:B:417:MET:C	2.91	0.49
1:A:63:ASN:C	1:A:63:ASN:ND2	2.65	0.49
1:C:43:GLU:HB3	1:C:63:ASN:HD21	1.77	0.49
1:C:150:GLY:HA2	1:C:165:ASN:O	2.13	0.49
1:A:163:TYR:HE2	1:A:205:VAL:HA	1.77	0.49
1:B:150:GLY:HA2	1:B:165:ASN:O	2.13	0.49
1:A:417:MET:SD	1:A:417:MET:C	2.91	0.49
1:C:417:MET:C	1:C:417:MET:SD	2.91	0.49
1:A:136:PHE:N	1:A:136:PHE:CD1	2.72	0.49
1:B:317:THR:CG2	1:B:318:PRO:N	2.76	0.49
1:B:63:ASN:C	1:B:63:ASN:ND2	2.65	0.49
1:C:150:GLY:HA2	1:C:165:ASN:C	2.34	0.49
1:C:63:ASN:C	1:C:63:ASN:ND2	2.65	0.48
1:B:150:GLY:HA2	1:B:165:ASN:C	2.34	0.48
1:C:317:THR:CG2	1:C:318:PRO:N	2.76	0.48
1:A:223:VAL:CG1	1:A:224:LEU:N	2.74	0.48
1:C:163:TYR:N	1:C:163:TYR:CD1	2.81	0.48
1:A:163:TYR:HE2	1:A:205:VAL:CA	2.27	0.48
1:B:163:TYR:N	1:B:163:TYR:CD1	2.81	0.48
1:A:169:ASN:ND2	1:A:249:GLY:H	2.08	0.48
1:A:63:ASN:CB	1:A:83:GLU:CG	2.88	0.48
1:B:269:MET:HG2	1:B:270:LEU:N	2.29	0.48
1:B:223:VAL:CG1	1:B:224:LEU:N	2.74	0.48
1:A:410:GLU:HG3	1:A:411:TRP:N	2.29	0.48
1:C:163:TYR:HE2	1:C:205:VAL:CA	2.27	0.48
1:A:150:GLY:HA2	1:A:165:ASN:C	2.34	0.48
1:A:177:ALA:HB2	1:A:188:GLU:HG3	1.95	0.48
1:C:63:ASN:HB2	1:C:83:GLU:HG3	1.96	0.48
1:A:317:THR:CG2	1:A:318:PRO:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:TYR:HE2	1:B:205:VAL:CA	2.26	0.47
1:C:177:ALA:HB2	1:C:188:GLU:HG3	1.95	0.47
1:A:307:THR:HG23	1:A:329:ASP:OD1	2.14	0.47
1:C:269:MET:HG2	1:C:270:LEU:N	2.29	0.47
1:B:410:GLU:HG3	1:B:411:TRP:N	2.28	0.47
1:B:43:GLU:O	1:B:44:LEU:HD23	2.14	0.47
1:B:63:ASN:HB2	1:B:83:GLU:HG3	1.96	0.47
1:B:177:ALA:HB2	1:B:188:GLU:HG3	1.95	0.47
1:A:63:ASN:HB2	1:A:83:GLU:HG3	1.96	0.47
1:C:43:GLU:O	1:C:44:LEU:HD23	2.15	0.47
1:B:307:THR:HG23	1:B:329:ASP:OD1	2.14	0.47
1:A:269:MET:HG2	1:A:270:LEU:N	2.29	0.47
1:C:223:VAL:O	1:C:226:GLY:N	2.41	0.47
1:A:43:GLU:O	1:A:44:LEU:HD23	2.15	0.47
1:C:307:THR:HG23	1:C:329:ASP:OD1	2.14	0.47
1:C:312:PRO:HD2	1:C:324:MET:O	2.14	0.47
1:C:410:GLU:HG3	1:C:411:TRP:N	2.29	0.47
1:B:163:TYR:HE2	1:B:205:VAL:HA	1.77	0.47
1:C:63:ASN:CB	1:C:83:GLU:CG	2.88	0.47
1:B:312:PRO:HD2	1:B:324:MET:O	2.14	0.47
1:A:163:TYR:N	1:A:163:TYR:CD1	2.81	0.47
1:A:182:ASN:CB	1:A:183:PRO:HD2	2.44	0.46
1:B:198:LEU:HD21	1:B:204:LEU:HD21	1.98	0.46
1:A:312:PRO:HD2	1:A:324:MET:O	2.14	0.46
1:B:163:TYR:N	1:B:163:TYR:HD1	2.13	0.46
1:C:198:LEU:HD21	1:C:204:LEU:HD21	1.98	0.46
1:A:32:TYR:CB	1:A:344:LYS:HE2	2.46	0.46
1:B:32:TYR:CB	1:B:344:LYS:HE2	2.46	0.45
1:A:163:TYR:HD1	1:A:163:TYR:N	2.13	0.45
1:B:6:TYR:CD1	1:B:6:TYR:C	2.90	0.45
1:A:192:ASP:HB2	1:A:214:LEU:HB3	1.98	0.45
1:C:213:TRP:O	1:C:235:ALA:HA	2.16	0.45
1:A:191:VAL:HG22	1:A:215:PHE:HD1	1.82	0.45
1:A:198:LEU:HD21	1:A:204:LEU:HD21	1.98	0.45
1:C:6:TYR:CD1	1:C:6:TYR:C	2.90	0.45
1:C:192:ASP:HB2	1:C:214:LEU:HB3	1.98	0.45
1:B:191:VAL:HG22	1:B:215:PHE:HD1	1.82	0.45
1:C:163:TYR:N	1:C:163:TYR:HD1	2.14	0.45
1:C:182:ASN:CB	1:C:183:PRO:HD2	2.44	0.45
1:C:32:TYR:CB	1:C:344:LYS:HE2	2.46	0.45
1:A:409:ASP:O	1:A:410:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:ASP:O	1:B:410:GLU:HB2	2.17	0.44
1:C:136:PHE:CD1	1:C:136:PHE:N	2.72	0.44
1:B:213:TRP:O	1:B:235:ALA:HA	2.16	0.44
1:C:191:VAL:HG22	1:C:215:PHE:HD1	1.82	0.44
1:C:200:ASP:O	1:C:201:ASN:HB2	2.18	0.44
1:B:192:ASP:HB2	1:B:214:LEU:HB3	1.98	0.44
1:A:200:ASP:O	1:A:201:ASN:HB2	2.18	0.44
1:B:200:ASP:O	1:B:201:ASN:HB2	2.18	0.44
1:C:161:TYR:HE2	1:C:259:PHE:CD2	2.23	0.44
1:A:6:TYR:CD1	1:A:6:TYR:C	2.90	0.44
1:A:213:TRP:O	1:A:235:ALA:HA	2.16	0.44
1:C:409:ASP:O	1:C:410:GLU:HB2	2.17	0.44
1:C:350:GLN:HG3	1:C:352:GLN:HG3	2.00	0.44
1:A:51:TRP:O	1:A:57:SER:HA	2.17	0.44
1:A:104:LYS:HA	1:A:125:PRO:HA	2.00	0.44
1:A:182:ASN:CB	1:A:183:PRO:CD	2.96	0.44
1:C:4:HIS:O	1:C:45:LYS:HB2	2.18	0.44
1:A:350:GLN:HG3	1:A:352:GLN:HG3	2.00	0.44
1:C:51:TRP:O	1:C:57:SER:HA	2.17	0.44
1:A:4:HIS:O	1:A:45:LYS:HB2	2.18	0.43
1:B:223:VAL:O	1:B:226:GLY:N	2.41	0.43
1:C:129:LEU:HA	1:C:129:LEU:HD12	1.70	0.43
1:B:214:LEU:CD1	1:B:235:ALA:HB2	2.47	0.43
1:C:419:ILE:O	1:C:419:ILE:HG23	2.18	0.43
1:B:4:HIS:O	1:B:45:LYS:HB2	2.18	0.43
1:B:51:TRP:O	1:B:57:SER:HA	2.17	0.43
1:B:265:ASN:HD22	1:B:265:ASN:C	2.21	0.43
1:A:419:ILE:O	1:A:419:ILE:HG23	2.18	0.43
1:C:74:TRP:CD1	1:C:74:TRP:C	2.92	0.43
1:B:104:LYS:HA	1:B:125:PRO:HA	2.00	0.43
1:A:74:TRP:C	1:A:74:TRP:CD1	2.92	0.43
1:C:104:LYS:HA	1:C:125:PRO:HA	2.00	0.43
1:A:214:LEU:CD1	1:A:235:ALA:HB2	2.47	0.43
1:A:224:LEU:HB2	1:A:278:ILE:HB	2.01	0.43
1:C:214:LEU:CD1	1:C:235:ALA:HB2	2.47	0.43
1:B:74:TRP:CD1	1:B:74:TRP:C	2.92	0.43
1:B:182:ASN:CB	1:B:183:PRO:CD	2.96	0.43
1:B:350:GLN:HG3	1:B:352:GLN:HG3	2.00	0.43
1:B:419:ILE:HG23	1:B:419:ILE:O	2.18	0.42
1:B:224:LEU:HB2	1:B:278:ILE:HB	2.01	0.42
1:B:64:VAL:HG12	1:B:66:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ARG:HH11	1:B:360:ARG:HD2	1.66	0.42
1:A:265:ASN:C	1:A:265:ASN:HD22	2.21	0.42
1:B:317:THR:HG23	1:B:318:PRO:CD	2.48	0.42
1:A:227:PHE:HE2	1:A:229:LYS:HG3	1.85	0.42
1:A:251:GLY:O	1:A:263:ILE:N	2.52	0.42
1:C:317:THR:HG23	1:C:318:PRO:CD	2.48	0.42
1:C:64:VAL:HG12	1:C:66:TYR:CE1	2.55	0.42
1:B:120:TRP:CH2	1:B:175:ARG:HG2	2.55	0.42
1:B:387:ASN:OD1	1:B:388:ALA:N	2.53	0.42
1:A:64:VAL:HG12	1:A:66:TYR:CE1	2.54	0.42
1:B:6:TYR:CD1	1:B:7:ALA:N	2.88	0.42
1:B:227:PHE:HE2	1:B:229:LYS:HG3	1.85	0.42
1:C:387:ASN:OD1	1:C:388:ALA:N	2.53	0.42
1:B:129:LEU:HD12	1:B:129:LEU:HA	1.70	0.42
1:A:120:TRP:CH2	1:A:175:ARG:HG2	2.55	0.41
1:B:104:LYS:NZ	1:C:72:ASN:O	2.53	0.41
1:A:387:ASN:OD1	1:A:388:ALA:N	2.53	0.41
1:C:265:ASN:C	1:C:265:ASN:HD22	2.21	0.41
1:C:328:TYR:HD1	1:C:343:TYR:HB3	1.85	0.41
1:C:120:TRP:CH2	1:C:175:ARG:HG2	2.55	0.41
1:A:104:LYS:NZ	1:B:72:ASN:O	2.53	0.41
1:C:227:PHE:HE2	1:C:229:LYS:HG3	1.85	0.41
1:B:328:TYR:HD1	1:B:343:TYR:HB3	1.85	0.41
1:B:251:GLY:O	1:B:263:ILE:N	2.52	0.41
1:A:317:THR:HG23	1:A:318:PRO:CD	2.48	0.41
1:C:224:LEU:HB2	1:C:278:ILE:HB	2.01	0.41
1:A:350:GLN:HE21	1:A:352:GLN:HG2	1.85	0.41
1:C:6:TYR:CD1	1:C:7:ALA:N	2.88	0.41
1:A:6:TYR:CD1	1:A:7:ALA:N	2.88	0.41
1:B:74:TRP:CD1	1:B:74:TRP:O	2.74	0.41
1:C:304:LYS:HE3	1:C:304:LYS:HB2	1.89	0.41
1:A:353:ALA:HB2	1:C:58:PHE:CD2	2.55	0.41
1:A:74:TRP:O	1:A:74:TRP:CD1	2.74	0.41
1:C:251:GLY:O	1:C:263:ILE:N	2.52	0.41
1:B:58:PHE:CD2	1:C:353:ALA:HB2	2.55	0.41
1:A:223:VAL:O	1:A:226:GLY:N	2.41	0.41
1:A:72:ASN:O	1:C:104:LYS:NZ	2.53	0.41
1:A:159:ASN:HA	1:A:159:ASN:HD22	1.60	0.41
1:B:322:THR:OG1	1:B:349:GLN:NE2	2.52	0.41
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.78	0.41
1:C:182:ASN:CB	1:C:183:PRO:CD	2.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:GLN:HE21	1:B:352:GLN:HG2	1.85	0.41
1:A:220:THR:HG23	1:A:229:LYS:HD3	2.03	0.41
1:B:182:ASN:CB	1:B:183:PRO:HD2	2.44	0.40
1:C:214:LEU:HD12	1:C:214:LEU:HA	1.73	0.40
1:A:374:GLU:CD	1:A:405:ARG:HB2	2.42	0.40
1:B:220:THR:HG23	1:B:229:LYS:HD3	2.03	0.40
1:A:296:ASN:HD22	1:A:296:ASN:C	2.25	0.40
1:C:322:THR:OG1	1:C:349:GLN:NE2	2.52	0.40
1:A:58:PHE:CD2	1:B:353:ALA:HB2	2.56	0.40
1:B:223:VAL:CG1	1:B:224:LEU:HG	2.46	0.40
1:C:374:GLU:CD	1:C:405:ARG:HB2	2.42	0.40
1:C:350:GLN:HE21	1:C:352:GLN:HG2	1.85	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	419/421 (100%)	383 (91%)	34 (8%)	2 (0%)	34	72
1	B	419/421 (100%)	383 (91%)	34 (8%)	2 (0%)	34	72
1	C	419/421 (100%)	383 (91%)	34 (8%)	2 (0%)	34	72
All	All	1257/1263 (100%)	1149 (91%)	102 (8%)	6 (0%)	34	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LEU
1	B	224	LEU
1	C	224	LEU
1	A	400	GLY
1	B	400	GLY

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Mol	Chain	Res	Type
1	C	400	GLY

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	340/340 (100%)	295 (87%)	45 (13%)	5 20
1	B	340/340 (100%)	295 (87%)	45 (13%)	5 20
1	C	340/340 (100%)	295 (87%)	45 (13%)	5 20
All	All	1020/1020 (100%)	885 (87%)	135 (13%)	5 20

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	19	GLU
1	A	33	ARG
1	A	34	LEU
1	A	39	GLU
1	A	40	THR
1	A	63	ASN
1	A	89	LYS
1	A	94	TRP
1	A	104	LYS
1	A	105	ARG
1	A	114	MET
1	A	123	SER
1	A	140	SER
1	A	147	SER
1	A	148	GLU
1	A	159	ASN
1	A	160	ILE
1	A	167	THR
1	A	175	ARG
1	A	182	ASN

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Mol	Chain	Res	Type
1	A	186	THR
1	A	199	ARG
1	A	205	VAL
1	A	220	THR
1	A	247	SER
1	A	265	ASN
1	A	269	MET
1	A	270	LEU
1	A	272	ILE
1	A	273	LEU
1	A	296	ASN
1	A	300	ASP
1	A	303	THR
1	A	307	THR
1	A	315	LYS
1	A	336	THR
1	A	341	ASN
1	A	347	LEU
1	A	352	GLN
1	A	360	ARG
1	A	371	LYS
1	A	409	ASP
1	A	416	GLN
1	A	417	MET
1	B	8	ARG
1	B	19	GLU
1	B	33	ARG
1	B	34	LEU
1	B	39	GLU
1	B	40	THR
1	B	63	ASN
1	B	89	LYS
1	B	94	TRP
1	B	104	LYS
1	B	105	ARG
1	B	114	MET
1	B	123	SER
1	B	140	SER
1	B	147	SER
1	B	148	GLU
1	B	159	ASN
1	B	160	ILE

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Mol	Chain	Res	Type
1	B	167	THR
1	B	175	ARG
1	B	182	ASN
1	B	186	THR
1	B	199	ARG
1	B	205	VAL
1	B	220	THR
1	B	247	SER
1	B	265	ASN
1	B	269	MET
1	B	270	LEU
1	B	272	ILE
1	B	273	LEU
1	B	296	ASN
1	B	300	ASP
1	B	303	THR
1	B	307	THR
1	B	315	LYS
1	B	336	THR
1	B	341	ASN
1	B	347	LEU
1	B	352	GLN
1	B	360	ARG
1	B	371	LYS
1	B	409	ASP
1	B	416	GLN
1	B	417	MET
1	C	8	ARG
1	C	19	GLU
1	C	33	ARG
1	C	34	LEU
1	C	39	GLU
1	C	40	THR
1	C	63	ASN
1	C	89	LYS
1	C	94	TRP
1	C	104	LYS
1	C	105	ARG
1	C	114	MET
1	C	123	SER
1	C	140	SER
1	C	147	SER

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Mol	Chain	Res	Type
1	C	148	GLU
1	C	159	ASN
1	C	160	ILE
1	C	167	THR
1	C	175	ARG
1	C	182	ASN
1	C	186	THR
1	C	199	ARG
1	C	205	VAL
1	C	220	THR
1	C	247	SER
1	C	265	ASN
1	C	269	MET
1	C	270	LEU
1	C	272	ILE
1	C	273	LEU
1	C	296	ASN
1	C	300	ASP
1	C	303	THR
1	C	307	THR
1	C	315	LYS
1	C	336	THR
1	C	341	ASN
1	C	347	LEU
1	C	352	GLN
1	C	360	ARG
1	C	371	LYS
1	C	409	ASP
1	C	416	GLN
1	C	417	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	70	GLN
1	A	159	ASN
1	A	182	ASN
1	A	219	HIS
1	A	221	GLN
1	A	248	GLN
1	A	265	ASN

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Mol	Chain	Res	Type
1	A	266	ASN
1	A	268	HIS
1	A	275	HIS
1	A	296	ASN
1	A	341	ASN
1	A	349	GLN
1	B	63	ASN
1	B	70	GLN
1	B	159	ASN
1	B	182	ASN
1	B	219	HIS
1	B	221	GLN
1	B	248	GLN
1	B	265	ASN
1	B	266	ASN
1	B	268	HIS
1	B	275	HIS
1	B	296	ASN
1	B	341	ASN
1	B	349	GLN
1	C	63	ASN
1	C	70	GLN
1	C	159	ASN
1	C	182	ASN
1	C	219	HIS
1	C	221	GLN
1	C	248	GLN
1	C	265	ASN
1	C	266	ASN
1	C	268	HIS
1	C	275	HIS
1	C	296	ASN
1	C	341	ASN
1	C	349	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

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.