Full wwPDB EM Validation Report

Nov 18, 2024 – 12:59 PM JST

PDB ID	:	8WWH
EMDB ID	:	EMD-37888
Title	:	MCHR1-Gi complex,S1 state
Authors	:	Gong, W.; Ye, X.; Liu, G.
Deposited on	:	2023-10-25
Resolution	:	2.84 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

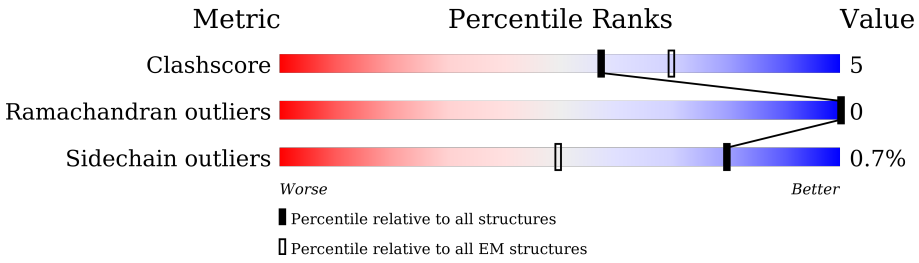
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	354	55% 8% 37%
2	B	376	74% 16% 9%
3	C	71	72% 8% 20%
4	E	255	82% 8% 9%
5	R	624	41% 5% 54%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8821 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	224	1749	1114	292	330	13	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	conflict	UNP P63096
A	203	ALA	GLY	conflict	UNP P63096
A	245	ALA	GLU	conflict	UNP P63096
A	326	SER	ALA	conflict	UNP P63096

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	342	2622	1615	471	515	21	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873
B	341	GLY	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	342	SER	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	SER	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	VAL	-	expression tag	UNP P62873
B	357	SER	-	expression tag	UNP P62873
B	358	GLY	-	expression tag	UNP P62873
B	359	TRP	-	expression tag	UNP P62873
B	360	ARG	-	expression tag	UNP P62873
B	361	LEU	-	expression tag	UNP P62873
B	362	PHE	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	LYS	-	expression tag	UNP P62873
B	365	ILE	-	expression tag	UNP P62873
B	366	SER	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	57	Total	C	N	O	S	0	0
			436	273	77	83	3		

- Molecule 4 is a protein called Antibody fragment ScFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	231	Total	C	N	O	S	0	0
			1779	1129	294	346	10		

- Molecule 5 is a protein called Fusion protein 1,Melanin-concentrating hormone receptor 1,Fusion protein 2.

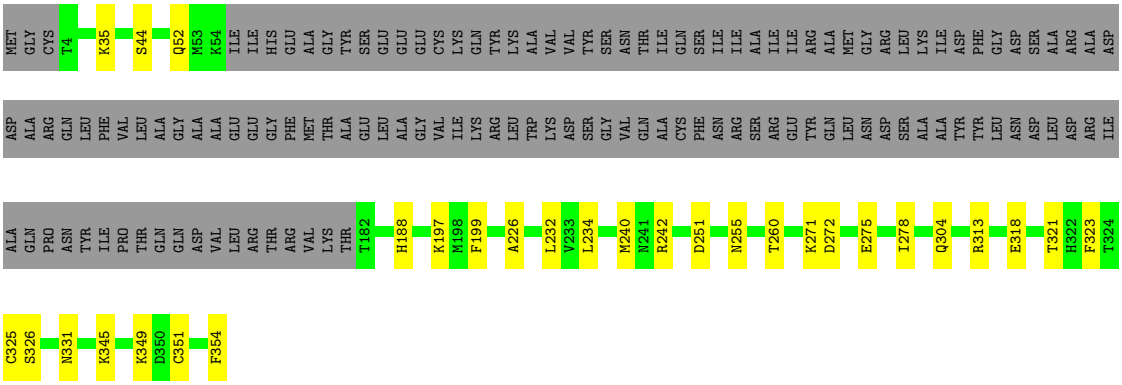
Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	289	Total	C	N	O	S	0	0
			2235	1487	357	374	17		

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. 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.

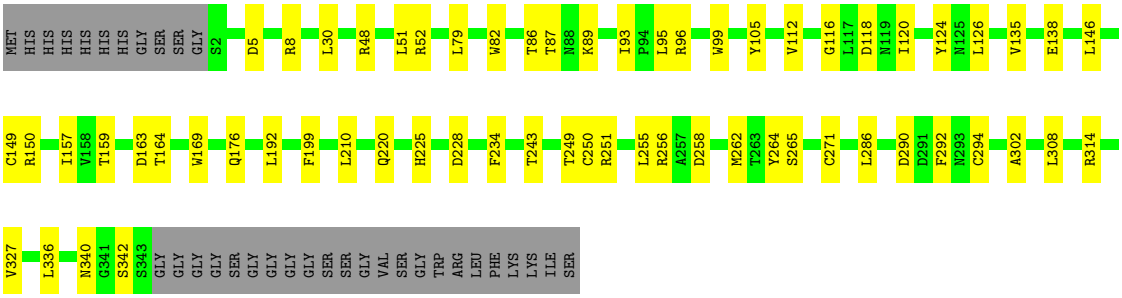
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



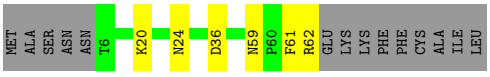
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



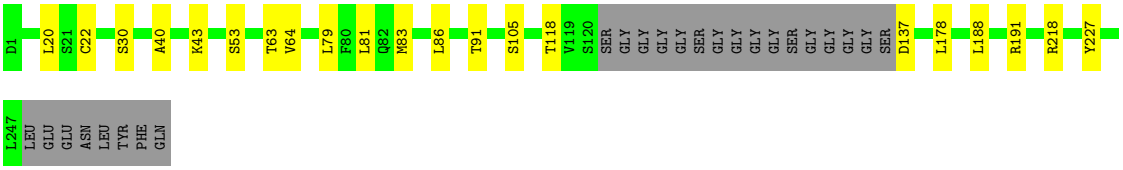
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:



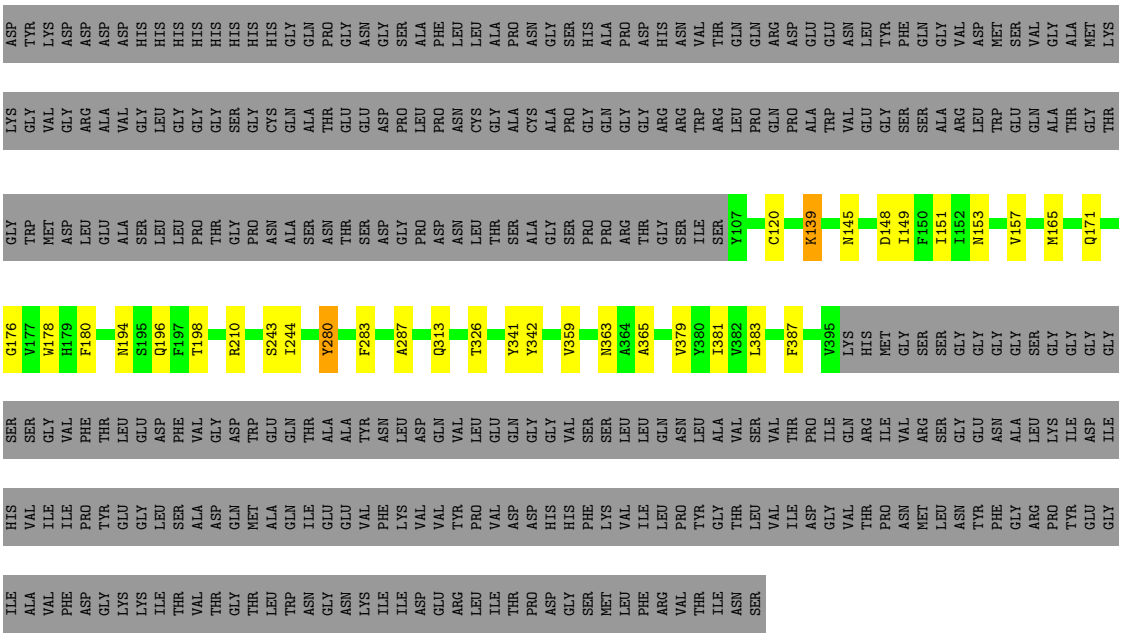
• Molecule 4: Antibody fragment ScFv16

Chain E:



• Molecule 5: Fusion protein 1,Melanin-concentrating hormone receptor 1,Fusion protein 2

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	247274	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/1779	0.43	0/2396
2	B	0.28	0/2669	0.53	0/3618
3	C	0.24	0/442	0.41	0/597
4	E	0.29	0/1823	0.49	0/2472
5	R	0.25	0/2297	0.42	0/3148
All	All	0.27	0/9010	0.47	0/12231

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1749	0	1692	16	0
2	B	2622	0	2523	36	0
3	C	436	0	448	4	0
4	E	1779	0	1714	11	0
5	R	2235	0	2270	19	0
All	All	8821	0	8647	81	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 5.

All (81) 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)
2:B:220:GLN:NE2	2:B:258:ASP:OD1	2.26	0.68
4:E:20:LEU:HD12	4:E:81:LEU:HD23	1.77	0.66
1:A:44:SER:HA	1:A:226:ALA:HB2	1.78	0.66
4:E:22:CYS:HB3	4:E:79:LEU:HB3	1.78	0.64
5:R:243:SER:O	5:R:280:TYR:OH	2.16	0.63
5:R:196:GLN:NE2	5:R:342:TYR:OH	2.33	0.62
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.82	0.61
3:C:20:LYS:O	3:C:24:ASN:ND2	2.29	0.59
5:R:359:VAL:O	5:R:363:ASN:ND2	2.36	0.59
2:B:290:ASP:HA	2:B:314:ARG:HG3	1.85	0.59
2:B:146:LEU:HD11	2:B:159:THR:HB	1.85	0.58
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.37	0.57
2:B:79:LEU:HB3	2:B:93:ILE:HB	1.88	0.56
2:B:249:THR:HG22	2:B:265:SER:HB3	1.88	0.55
1:A:52:GLN:OE1	1:A:331:ASN:ND2	2.36	0.55
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.89	0.55
4:E:105:SER:O	4:E:191:ARG:NH2	2.38	0.55
2:B:192:LEU:HD23	2:B:199:PHE:HB3	1.89	0.55
2:B:225:HIS:NE2	2:B:243:THR:OG1	2.33	0.54
4:E:83:MET:HB3	4:E:86:LEU:HD21	1.88	0.54
2:B:52:ARG:HH12	5:R:139:LYS:HB3	1.73	0.53
2:B:30:LEU:HD23	2:B:262:MET:HB2	1.91	0.53
2:B:225:HIS:CE1	2:B:251:ARG:HG3	2.44	0.53
2:B:112:VAL:HG13	2:B:126:LEU:HD11	1.92	0.52
4:E:63:THR:HG23	4:E:64:VAL:HG13	1.92	0.52
5:R:283:PHE:HA	5:R:287:ALA:HB3	1.92	0.51
5:R:379:VAL:HG13	5:R:383:LEU:HD12	1.93	0.51
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.91	0.51
4:E:30:SER:O	4:E:53:SER:OG	2.25	0.51
5:R:381:ILE:HG12	5:R:387:PHE:HE2	1.75	0.51
5:R:326:THR:HA	5:R:383:LEU:HD13	1.92	0.50
5:R:149:ILE:O	5:R:153:ASN:ND2	2.34	0.50
1:A:35:LYS:HB3	1:A:199:PHE:HE2	1.76	0.50
2:B:294:CYS:HB3	2:B:308:LEU:HB2	1.93	0.50
1:A:345:LYS:HG2	1:A:349:LYS:HE3	1.92	0.50
1:A:325:CYS:SG	1:A:326:SER:N	2.85	0.49
2:B:79:LEU:HB2	2:B:95:LEU:HD21	1.94	0.49
2:B:149:CYS:O	2:B:150:ARG:NH1	2.45	0.49
2:B:99:TRP:O	2:B:116:GLY:HA3	2.12	0.49
2:B:96:ARG:NH1	2:B:138:GLU:OE2	2.46	0.48
2:B:286:LEU:HD22	2:B:327:VAL:HG21	1.95	0.48
5:R:194:ASN:HB2	5:R:244:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD12	1:A:240:MET:HB3	1.95	0.47
4:E:91:THR:HG23	4:E:118:THR:HA	1.96	0.47
1:A:304:GLN:HG3	1:A:321:THR:HG21	1.97	0.47
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.97	0.47
2:B:256:ARG:NH2	3:C:36:ASP:OD2	2.48	0.47
2:B:118:ASP:O	2:B:120:ILE:HG12	2.16	0.46
2:B:340:ASN:HD21	3:C:61:PHE:HB2	1.80	0.46
5:R:145:ASN:ND2	5:R:148:ASP:OD1	2.39	0.46
4:E:20:LEU:HB2	4:E:81:LEU:HB3	1.98	0.46
4:E:178:LEU:HB2	4:E:188:LEU:HD11	1.97	0.45
2:B:228:ASP:N	2:B:228:ASP:OD1	2.49	0.45
4:E:178:LEU:HD13	4:E:227:TYR:CZ	2.51	0.45
2:B:5:ASP:OD1	2:B:8:ARG:NH1	2.50	0.44
2:B:82:TRP:CH2	2:B:89:LYS:HE3	2.52	0.44
2:B:124:TYR:CE1	2:B:135:VAL:HG22	2.52	0.44
3:C:59:ASN:O	3:C:62:ARG:HG3	2.17	0.44
1:A:271:LYS:HZ1	1:A:323:PHE:HB3	1.83	0.44
2:B:48:ARG:HH22	2:B:342:SER:HB3	1.83	0.44
5:R:157:VAL:HG11	5:R:198:THR:HB	2.00	0.44
4:E:40:ALA:HB3	4:E:43:LYS:HB2	1.99	0.43
1:A:318:GLU:HA	5:R:313:GLN:HE22	1.84	0.43
5:R:171:GLN:O	5:R:176:GLY:HA2	2.19	0.42
2:B:163:ASP:O	2:B:164:THR:OG1	2.34	0.42
5:R:148:ASP:HA	5:R:151:ILE:HG22	2.02	0.42
1:A:275:GLU:O	1:A:278:ILE:HG22	2.18	0.42
2:B:149:CYS:HB2	2:B:157:ILE:HD11	2.02	0.41
2:B:86:THR:O	2:B:87:THR:OG1	2.36	0.41
2:B:262:MET:SD	2:B:302:ALA:HB2	2.60	0.41
5:R:120:CYS:HB2	5:R:165:MET:SD	2.60	0.41
1:A:188:HIS:CD2	1:A:197:LYS:HG2	2.56	0.41
5:R:178:TRP:CE2	5:R:180:PHE:HB2	2.56	0.41
1:A:272:ASP:OD1	1:A:272:ASP:N	2.53	0.41
1:A:351:CYS:HB3	5:R:210:ARG:HG2	2.02	0.41
1:A:232:LEU:HB2	1:A:242:ARG:HG3	2.02	0.41
1:A:260:THR:HA	1:A:313:ARG:HH11	1.85	0.41
5:R:341:TYR:HA	5:R:365:ALA:HB1	2.02	0.40
2:B:48:ARG:HG3	2:B:340:ASN:HD21	1.86	0.40
2:B:292:PHE:N	2:B:292:PHE:CD1	2.90	0.40
2:B:169:TRP:HA	2:B:176:GLN:HA	2.02	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	220/354 (62%)	218 (99%)	2 (1%)	0	100	100
2	B	340/376 (90%)	332 (98%)	8 (2%)	0	100	100
3	C	55/71 (78%)	55 (100%)	0	0	100	100
4	E	227/255 (89%)	222 (98%)	5 (2%)	0	100	100
5	R	287/624 (46%)	282 (98%)	5 (2%)	0	100	100
All	All	1129/1680 (67%)	1109 (98%)	20 (2%)	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	184/305 (60%)	183 (100%)	1 (0%)	86	94
2	B	284/306 (93%)	282 (99%)	2 (1%)	81	91
3	C	46/58 (79%)	46 (100%)	0	100	100
4	E	196/208 (94%)	194 (99%)	2 (1%)	73	87
5	R	242/522 (46%)	240 (99%)	2 (1%)	79	90
All	All	952/1399 (68%)	945 (99%)	7 (1%)	80	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	PHE
2	B	105	TYR
2	B	234	PHE
4	E	137	ASP
4	E	218	ARG
5	R	139	LYS
5	R	280	TYR

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	188	HIS
1	A	322	HIS
2	B	91	HIS
2	B	259	GLN
2	B	340	ASN
3	C	59	ASN
4	E	113	GLN
4	E	183	GLN
5	R	194	ASN
5	R	196	GLN
5	R	281	GLN
5	R	345	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.