



Full wwPDB EM Model Validation Report ⓘ

Mar 25, 2020 – 09:52 AM EDT

PDB ID : 6LML
EMDB ID : EMD-0918
Title : Cryo-EM structure of the human glucagon receptor in complex with Gi1
Authors : Qiao, A.; Han, S.; Li, X.; Sun, F.; Zhao, Q.; Wu, B.
Deposited on : 2019-12-26
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM 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

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

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
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

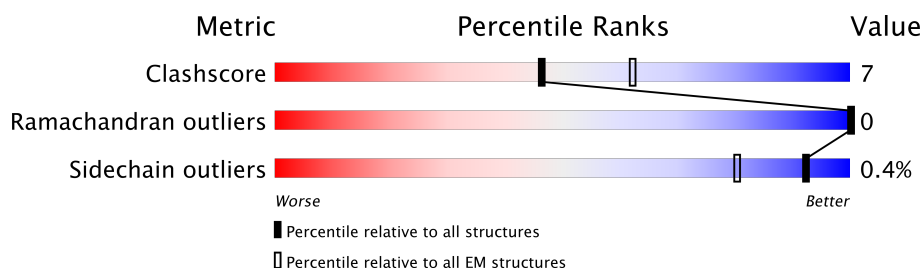
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	354	 57% 6% 37%
2	B	351	 65% 22% 13%
3	C	71	 45% . 54%
4	D	247	 75% 19% 6%
5	E	29	 83% 17%
6	R	422	 77% 16% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9438 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
1	A	224	Total	C	N	O	S	0	0
			1735	1106	293	326	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	245	ALA	GLU	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	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
2	B	306	Total	C	N	O	S	0	0
			2322	1441	413	450	18		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	expression tag	UNP P62873
B	-9	HIS	-	expression tag	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	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	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	33	Total	C	N	O	S	0	0
			241	153	38	48	2		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1742	1111	293	329	9		

- Molecule 5 is a protein called Glucagon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	29	Total	C	N	O	S	0	0
			245	153	43	48	1		

- Molecule 6 is a protein called Glucagon receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	395	Total	C	N	O	S	0	0
			3153	2072	545	517	19		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	126	ARG	GLU	engineered mutation	UNP P47871
R	200	TRP	THR	engineered mutation	UNP P47871
R	366	MET	ALA	engineered mutation	UNP P47871
R	433	GLY	-	expression tag	UNP P47871
R	434	SER	-	expression tag	UNP P47871
R	435	GLY	-	expression tag	UNP P47871
R	436	SER	-	expression tag	UNP P47871
R	437	GLU	-	expression tag	UNP P47871
R	438	ASP	-	expression tag	UNP P47871
R	439	GLN	-	expression tag	UNP P47871
R	440	VAL	-	expression tag	UNP P47871
R	441	ASP	-	expression tag	UNP P47871
R	442	PRO	-	expression tag	UNP P47871
R	443	ARG	-	expression tag	UNP P47871
R	444	LEU	-	expression tag	UNP P47871
R	445	ILE	-	expression tag	UNP P47871

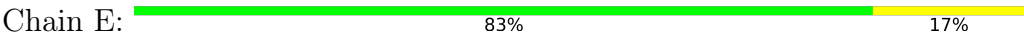
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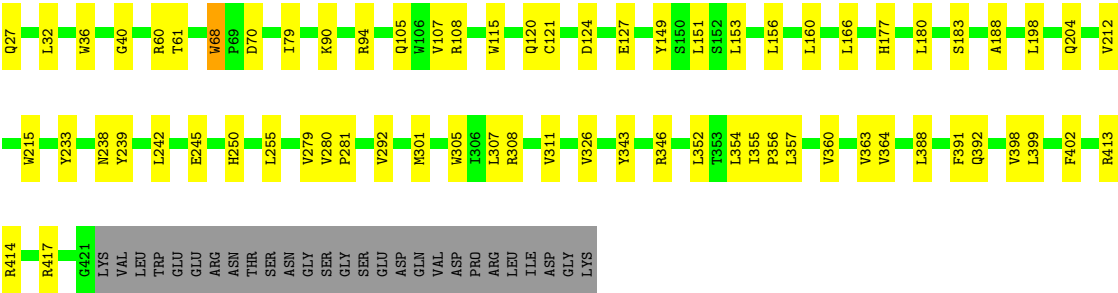
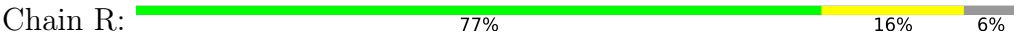
Chain	Residue	Modelled	Actual	Comment	Reference
R	446	ASP	-	expression tag	UNP P47871
R	447	GLY	-	expression tag	UNP P47871
R	448	LYS	-	expression tag	UNP P47871



● Molecule 5: Glucagon



● Molecule 6: Glucagon receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	312974	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 ($e^-/\text{\AA}^2$)	1.875	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 >5	RMSZ	# Z >5
1	A	0.34	0/1765	0.57	3/2379 (0.1%)
2	B	0.39	0/2369	0.61	0/3218
3	C	0.28	0/247	0.44	0/338
4	D	0.34	0/1786	0.56	0/2429
5	E	0.36	0/251	0.44	0/338
6	R	0.34	0/3248	0.54	0/4422
All	All	0.35	0/9666	0.56	3/13124 (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
6	R	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	LEU	CA-CB-CG	6.36	129.94	115.30
1	A	38	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	36	LEU	CA-CB-CG	5.92	128.92	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	R	292	VAL	Peptide
6	R	356	PRO	Peptide

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	1735	0	1669	12	0
2	B	2322	0	2210	50	0
3	C	241	0	229	1	0
4	D	1742	0	1654	27	0
5	E	245	0	225	5	0
6	R	3153	0	3110	41	0
All	All	9438	0	9097	131	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 (131) 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:311:HIS:HE2	2:B:329:THR:HG1	1.28	0.79
2:B:62:HIS:HD2	2:B:105:TYR:H	1.37	0.73
2:B:159:THR:HG1	2:B:169:TRP:HE1	1.37	0.71
2:B:80:ILE:HG22	2:B:92:ALA:HA	1.78	0.66
6:R:363:VAL:HG23	6:R:364:VAL:HG23	1.83	0.61
2:B:294:CYS:HB2	2:B:308:LEU:HB2	1.82	0.60
6:R:326:VAL:HG12	6:R:352:LEU:HD11	1.84	0.60
4:D:51:ILE:HD11	4:D:70:ILE:HG12	1.84	0.60
2:B:74:SER:OG	2:B:75:GLN:N	2.33	0.59
6:R:120:GLN:NE2	6:R:121:CYS:SG	2.76	0.58
2:B:285:LEU:HD23	2:B:297:TRP:HB2	1.85	0.58
4:D:20:LEU:HB2	4:D:81:LEU:HB3	1.85	0.58
5:E:3:GLN:NE2	6:R:149:TYR:OH	2.37	0.57
2:B:99:TRP:HB2	2:B:117:LEU:HD22	1.87	0.57
5:E:18:ARG:NH2	6:R:204:GLN:O	2.38	0.57
2:B:161:SER:OG	2:B:162:GLY:N	2.40	0.55
4:D:93:MET:HA	4:D:116:THR:HA	1.86	0.55
2:B:210:LEU:HD12	2:B:220:GLN:HB2	1.88	0.55
1:A:271:LYS:H	1:A:325:CYS:HB3	1.71	0.55
4:D:105:SER:OG	4:D:106:SER:N	2.39	0.55
2:B:187:VAL:HA	2:B:203:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:360:VAL:HG22	6:R:388:LEU:HD13	1.88	0.55
1:A:251:ASP:HB3	1:A:310:LEU:HD23	1.89	0.54
4:D:202:ARG:NH2	4:D:223:ASP:OD2	2.39	0.54
6:R:105:GLN:OE1	6:R:108:ARG:NH2	2.40	0.54
6:R:180:LEU:HD11	6:R:242:LEU:HD23	1.90	0.54
2:B:119:ASN:HA	2:B:146:LEU:HD23	1.90	0.53
4:D:19:LYS:HA	4:D:82:GLN:HA	1.90	0.53
6:R:107:VAL:HG23	6:R:115:TRP:HB3	1.91	0.53
2:B:245:SER:OG	2:B:246:ASP:N	2.42	0.52
6:R:183:SER:O	6:R:238:ASN:ND2	2.42	0.52
1:A:186:GLU:OE2	1:A:197:LYS:NZ	2.43	0.52
2:B:283:ARG:NH1	2:B:298:ASP:OD1	2.43	0.52
2:B:71:VAL:HG21	2:B:112:VAL:HG21	1.92	0.52
2:B:215:GLU:OE2	2:B:219:ARG:NH2	2.43	0.52
2:B:298:ASP:HB3	2:B:302:ALA:H	1.73	0.52
4:D:82:GLN:NE2	4:D:83:MET:O	2.43	0.52
2:B:68:ARG:O	2:B:84:SER:OG	2.26	0.51
1:A:206:SER:OG	1:A:207:GLU:N	2.40	0.51
4:D:74:ASP:O	4:D:77:ASN:ND2	2.44	0.51
4:D:158:SER:HA	4:D:213:THR:HA	1.92	0.51
6:R:36:TRP:O	6:R:40:GLY:N	2.43	0.51
6:R:183:SER:OG	6:R:183:SER:O	2.30	0.50
6:R:355:ILE:O	6:R:357:LEU:N	2.39	0.50
6:R:343:TYR:HA	6:R:346:ARG:HB3	1.92	0.50
1:A:39:LEU:HD23	1:A:253:ILE:HD13	1.94	0.50
2:B:51:LEU:HD11	2:B:338:ILE:HD11	1.92	0.50
2:B:119:ASN:ND2	2:B:144:GLY:O	2.40	0.50
5:E:1:HIS:O	6:R:308:ARG:NH1	2.43	0.50
2:B:328:ALA:HB2	2:B:338:ILE:HG23	1.94	0.49
4:D:171:ASN:OD1	4:D:171:ASN:N	2.44	0.49
2:B:229:ILE:HA	2:B:245:SER:HA	1.94	0.49
2:B:110:ASN:OD1	2:B:110:ASN:N	2.44	0.49
6:R:166:LEU:HD21	6:R:414:ARG:HH11	1.77	0.48
1:A:311:ASN:OD1	1:A:311:ASN:N	2.46	0.48
2:B:320:VAL:HG22	2:B:327:VAL:HG22	1.95	0.48
6:R:250:HIS:HD2	6:R:255:LEU:HD12	1.79	0.48
4:D:178:LEU:HD22	4:D:180:ARG:HH11	1.79	0.48
2:B:35:ASN:O	2:B:301:LYS:NZ	2.47	0.48
2:B:213:VAL:HG23	2:B:214:ARG:HE	1.79	0.48
2:B:321:THR:OG1	2:B:324:GLY:N	2.37	0.48
4:D:71:SER:OG	4:D:72:ARG:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:ASP:O	4:D:77:ASN:N	2.46	0.47
2:B:321:THR:HG1	2:B:324:GLY:H	1.60	0.47
4:D:7:SER:HG	4:D:21:SER:HG	1.60	0.47
6:R:212:VAL:HA	6:R:215:TRP:HB3	1.96	0.47
1:A:343:ILE:O	1:A:347:ASN:N	2.48	0.47
2:B:54:HIS:NE2	2:B:72:SER:OG	2.37	0.47
2:B:54:HIS:CE1	2:B:74:SER:HB2	2.49	0.47
6:R:32:LEU:O	6:R:36:TRP:N	2.46	0.47
2:B:176:GLN:OE1	2:B:179:THR:OG1	2.33	0.46
4:D:175:TYR:OH	4:D:191:ARG:NH1	2.48	0.46
6:R:90:LYS:NZ	6:R:124:ASP:OD2	2.43	0.46
1:A:183:GLY:HA3	2:B:118:ASP:HA	1.97	0.46
6:R:301:MET:O	6:R:305:TRP:N	2.48	0.46
2:B:290:ASP:OD2	2:B:314:ARG:NH1	2.49	0.46
4:D:224:VAL:HA	4:D:245:LEU:HD23	1.96	0.46
6:R:61:THR:H	6:R:68:TRP:HE1	1.64	0.46
6:R:233:TYR:HA	6:R:279:VAL:HG11	1.97	0.46
6:R:280:VAL:HG23	6:R:281:PRO:HD3	1.97	0.46
6:R:151:LEU:HD23	6:R:391:PHE:HE1	1.80	0.46
2:B:163:ASP:OD1	2:B:165:THR:OG1	2.35	0.45
4:D:67:ARG:NH1	4:D:85:SER:O	2.49	0.45
6:R:156:LEU:O	6:R:160:LEU:N	2.45	0.45
6:R:398:VAL:HA	6:R:402:PHE:HD2	1.80	0.45
2:B:227:SER:OG	2:B:228:ASP:N	2.48	0.45
4:D:169:ASN:OD1	4:D:169:ASN:N	2.49	0.45
6:R:68:TRP:HB3	6:R:79:ILE:HD13	1.99	0.45
1:A:49:ILE:HD12	1:A:52:GLN:HB3	2.00	0.44
4:D:5:VAL:HG23	4:D:23:SER:HB3	2.00	0.44
6:R:413:ARG:O	6:R:417:ARG:N	2.48	0.44
2:B:209:LYS:HZ1	2:B:218:CYS:HA	1.83	0.44
2:B:95:LEU:HD11	2:B:100:VAL:HG22	1.98	0.44
1:A:9:ASP:OD1	1:A:9:ASP:N	2.45	0.43
2:B:202:GLY:HA2	2:B:229:ILE:HD11	2.00	0.43
2:B:228:ASP:OD1	2:B:228:ASP:N	2.51	0.43
6:R:177:HIS:NE2	6:R:245:GLU:OE2	2.52	0.43
6:R:60:ARG:HD3	6:R:70:ASP:HB3	1.99	0.43
2:B:86:THR:O	2:B:86:THR:OG1	2.35	0.43
2:B:158:VAL:HG22	2:B:168:LEU:HG	1.99	0.43
6:R:94:ARG:NH1	6:R:120:GLN:O	2.47	0.43
4:D:226:VAL:HA	4:D:244:LYS:HA	2.00	0.43
2:B:145:TYR:OH	2:B:188:MET:SD	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:SER:OG	2:B:228:ASP:OD1	2.36	0.42
1:A:231:ASP:OD1	1:A:231:ASP:N	2.48	0.42
5:E:15:ASP:OD2	6:R:27:GLN:N	2.52	0.42
3:C:37:LEU:HA	3:C:37:LEU:HD12	1.94	0.42
6:R:388:LEU:O	6:R:392:GLN:N	2.52	0.42
2:B:160:SER:HB3	2:B:190:LEU:HD22	2.01	0.42
6:R:94:ARG:HB3	6:R:120:GLN:HE22	1.84	0.42
6:R:307:LEU:HA	6:R:307:LEU:HD12	1.87	0.42
2:B:118:ASP:N	2:B:118:ASP:OD1	2.36	0.41
5:E:18:ARG:O	5:E:22:PHE:N	2.52	0.41
2:B:213:VAL:HG23	2:B:214:ARG:HG2	2.02	0.41
6:R:198:LEU:HD23	6:R:198:LEU:HA	1.92	0.41
4:D:157:ILE:HD12	4:D:157:ILE:HA	1.96	0.41
4:D:165:LEU:N	4:D:209:GLY:O	2.46	0.41
6:R:354:LEU:HD12	6:R:399:LEU:HD13	2.03	0.41
2:B:59:TYR:HD2	2:B:101:MET:HA	1.85	0.41
2:B:150:ARG:HB2	2:B:192:LEU:HD13	2.01	0.41
4:D:117:LEU:HA	4:D:117:LEU:HD12	1.85	0.41
1:A:200:ASP:OD1	1:A:200:ASP:N	2.54	0.41
2:B:254:ASP:OD2	2:B:257:ALA:N	2.53	0.41
6:R:239:TYR:HD2	6:R:311:VAL:HB	1.86	0.41
4:D:2:VAL:HG12	4:D:26:GLY:HA3	2.03	0.41
4:D:85:SER:O	4:D:85:SER:OG	2.39	0.41
2:B:62:HIS:CD2	2:B:105:TYR:H	2.27	0.40
6:R:90:LYS:NZ	6:R:127:GLU:OE1	2.52	0.40
4:D:188:LEU:HA	4:D:199:VAL:HG11	2.04	0.40
4:D:47:TRP:CG	4:D:237:LEU:HD12	2.57	0.40
6:R:153:LEU:HD12	6:R:188:ALA:HB3	2.04	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%)	204 (93%)	16 (7%)	0	100	100
2	B	304/351 (87%)	271 (89%)	33 (11%)	0	100	100
3	C	31/71 (44%)	29 (94%)	2 (6%)	0	100	100
4	D	228/247 (92%)	208 (91%)	20 (9%)	0	100	100
5	E	27/29 (93%)	27 (100%)	0	0	100	100
6	R	393/422 (93%)	358 (91%)	35 (9%)	0	100	100
All	All	1203/1474 (82%)	1097 (91%)	106 (9%)	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 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	179/305 (59%)	178 (99%)	1 (1%)	87	94
2	B	247/293 (84%)	245 (99%)	2 (1%)	83	91
3	C	25/58 (43%)	25 (100%)	0	100	100
4	D	183/200 (92%)	183 (100%)	0	100	100
5	E	27/27 (100%)	27 (100%)	0	100	100
6	R	326/368 (89%)	325 (100%)	1 (0%)	93	96
All	All	987/1251 (79%)	983 (100%)	4 (0%)	92	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ASP
2	B	105	TYR
2	B	295	ASN
6	R	68	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	GLN
2	B	35	ASN
2	B	62	HIS
2	B	266	HIS
4	D	3	GLN
4	D	77	ASN
4	D	183	GLN
5	E	1	HIS
5	E	3	GLN
6	R	120	GLN
6	R	250	HIS

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 carbohydrates 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.