Full wwPDB EM Validation Report ⓘ

Dec 15, 2024 – 12:08 AM JST

PDB ID	:	9IVG
EMDB ID	:	EMD-60927
Title	:	Cryo-EM structure of the GLP-1(9-36)-bound human GLP-1R-Gs complex
Authors	:	Li, J.; Li, G.; Mai, Y.; Liu, X.; Yang, D.; Zhou, Q.; Wang, M.-W.
Deposited on	:	2024-07-23
Resolution	:	3.00 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:

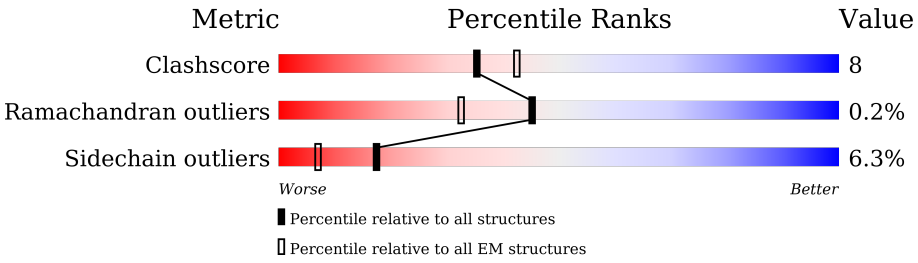
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	P	28	57% 18% 25%
2	R	440	65% 21% • 13%
3	A	361	52% 15% • 32%
4	B	345	74% 23% ••
5	G	70	76% • 20%
6	N	140	76% 11% • 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9325 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 GLP-1(9-36).

Mol	Chain	Residues	Atoms				AltConf	Trace
1	P	21	Total	C	N	O	0	0
			160	101	23	36		

- Molecule 2 is a protein called Glucagon-like peptide 1 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	384	Total	C	N	O	S	0	0
			3161	2086	517	540	18		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1,Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	245	Total	C	N	O	S	0	0
			2014	1271	361	374	8		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	ASP	GLY	conflict	UNP P63092
A	50	ASN	GLU	conflict	UNP P63092
A	63	TYR	LEU	conflict	UNP P63092
A	226	ALA	GLY	conflict	UNP P63092
A	249	ASP	ALA	conflict	UNP P63092
A	252	ASP	SER	conflict	UNP P63092
A	272	ASP	LEU	conflict	UNP P63092
A	366	SER	ALA	conflict	UNP P63092
A	372	ALA	ILE	conflict	UNP P63092
A	375	ILE	VAL	conflict	UNP P63092

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	338	Total	C	N	O	S	0	0
			2600	1604	467	508	21		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	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 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	56	Total	C	N	O	S	0	0
			429	269	76	81	3		

- Molecule 6 is a protein called Nanobody-35.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	126	Total	C	N	O	S	0	0
			961	599	168	188	6		

3 Residue-property plots (i)

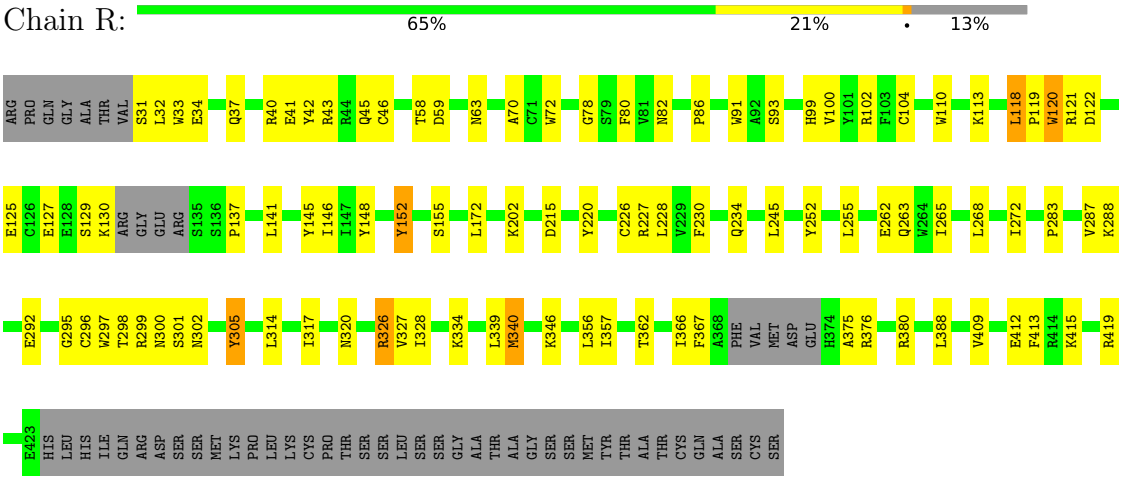
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: GLP-1(9-36)

Chain P:

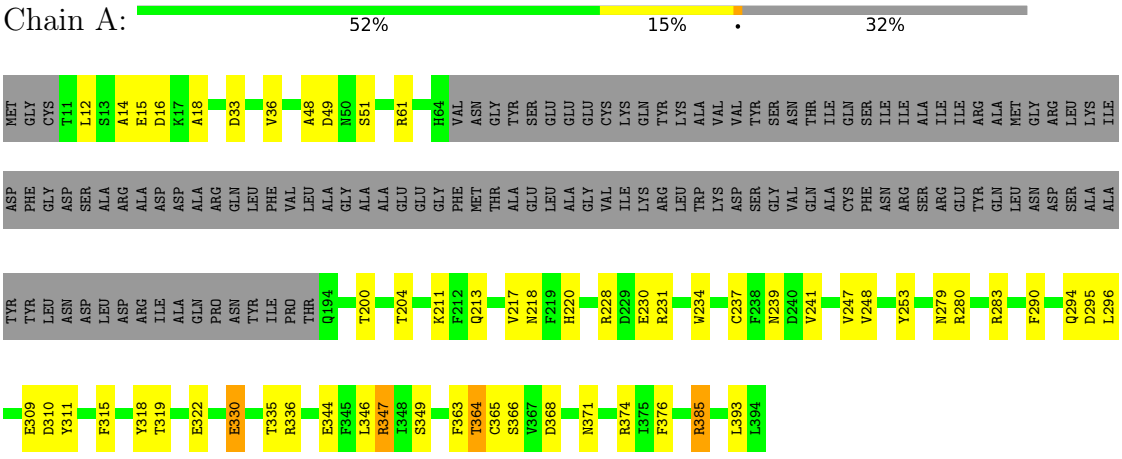
• Molecule 2: Glucagon-like peptide 1 receptor

Chain R:



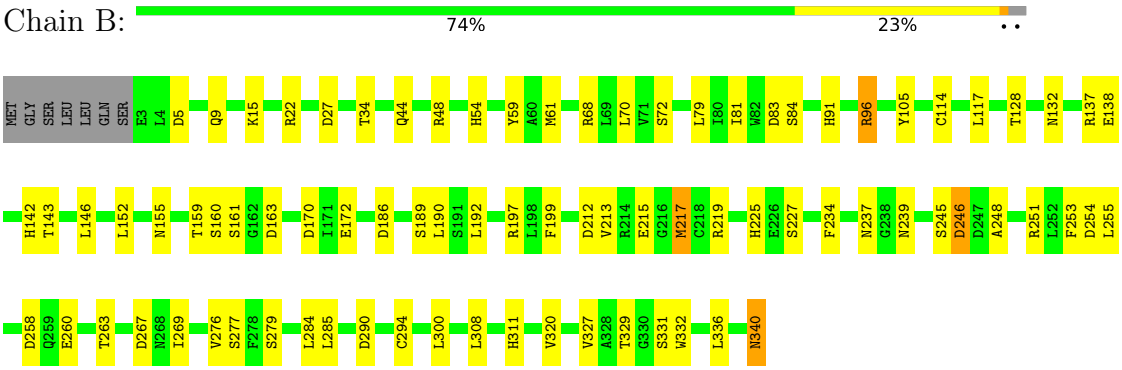
• Molecule 3: Guanine nucleotide-binding protein G(i) subunit alpha-1,Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain A:



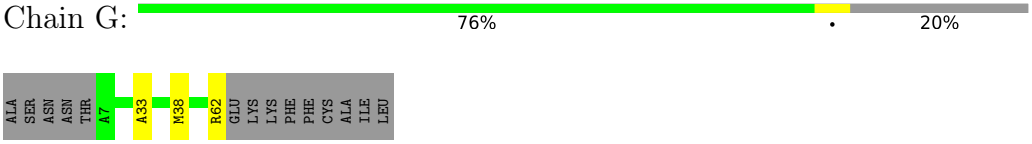
• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



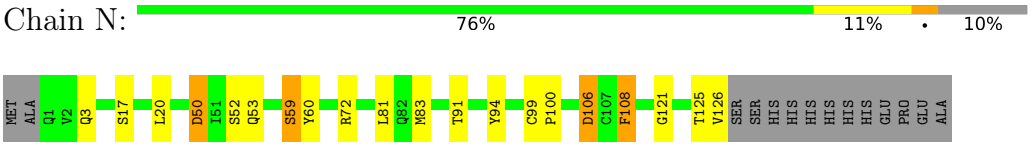
• Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:



• Molecule 6: Nanobody-35

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99120	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (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	P	0.24	0/162	0.36	0/217
2	R	0.26	0/3257	0.48	0/4437
3	A	0.29	0/2053	0.52	0/2769
4	B	0.27	0/2647	0.56	0/3589
5	G	0.24	0/435	0.43	0/587
6	N	0.28	0/981	0.51	0/1329
All	All	0.27	0/9535	0.51	0/12928

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	P	160	0	145	3	0
2	R	3161	0	3116	59	0
3	A	2014	0	1971	33	0
4	B	2600	0	2505	45	0
5	G	429	0	441	2	0
6	N	961	0	928	13	0
All	All	9325	0	9106	142	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 8.

All (142) 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)
4:B:54:HIS:HE2	4:B:72:SER:HG	1.31	0.79
2:R:113:LYS:HG2	2:R:120:TRP:HA	1.70	0.72
2:R:118:LEU:HD22	2:R:119:PRO:HD2	1.73	0.70
3:A:228:ARG:NH1	4:B:186:ASP:OD1	2.26	0.69
2:R:82:ASN:ND2	2:R:99:HIS:ND1	2.37	0.69
2:R:34:GLU:HG2	2:R:299:ARG:HD3	1.75	0.68
3:A:247:VAL:HG12	3:A:290:PHE:HB2	1.76	0.67
4:B:161:SER:OG	4:B:163:ASP:OD1	2.13	0.67
4:B:34:THR:HG21	4:B:300:LEU:HB3	1.78	0.66
2:R:100:VAL:HG12	2:R:125:GLU:HB3	1.77	0.64
1:P:12:PHE:HZ	2:R:202:LYS:HD3	1.63	0.63
2:R:121:ARG:NH1	2:R:122:ASP:OD1	2.33	0.61
3:A:294:GLN:H	3:A:365:CYS:HA	1.64	0.61
4:B:128:THR:OG1	4:B:132:ASN:O	2.16	0.61
2:R:288:LYS:HD3	2:R:292:GLU:HB3	1.82	0.60
3:A:279:ASN:HD22	6:N:108:PHE:HE2	1.50	0.60
3:A:294:GLN:HB2	3:A:365:CYS:HB3	1.83	0.60
2:R:412:GLU:OE2	2:R:415:LYS:NZ	2.35	0.59
2:R:148:TYR:CE1	2:R:388:LEU:HD22	2.38	0.59
4:B:225:HIS:CE1	4:B:251:ARG:HG3	2.37	0.59
6:N:52:SER:OG	6:N:53:GLN:N	2.36	0.59
3:A:318:TYR:O	3:A:336:ARG:NH1	2.37	0.58
2:R:31:SER:OG	2:R:32:LEU:N	2.36	0.58
2:R:375:ALA:HB1	2:R:380:ARG:HD2	1.87	0.56
4:B:294:CYS:HB2	4:B:308:LEU:HB2	1.86	0.56
3:A:231:ARG:HH21	6:N:108:PHE:HE1	1.54	0.56
4:B:320:VAL:HG22	4:B:327:VAL:HG22	1.88	0.56
2:R:82:ASN:HB2	2:R:99:HIS:HB3	1.88	0.55
4:B:245:SER:OG	4:B:246:ASP:N	2.39	0.55
4:B:160:SER:HB3	4:B:190:LEU:HD23	1.88	0.55
3:A:365:CYS:SG	3:A:366:SER:N	2.79	0.55
3:A:234:TRP:HB2	4:B:117:LEU:HD21	1.88	0.55
6:N:52:SER:O	6:N:72:ARG:NH1	2.33	0.55
2:R:302:ASN:HB3	2:R:305:TYR:HB2	1.87	0.55
4:B:192:LEU:HD23	4:B:199:PHE:HB3	1.90	0.53
2:R:78:GLY:N	2:R:104:CYS:O	2.40	0.53
2:R:91:TRP:HZ3	2:R:129:SER:H	1.56	0.52
4:B:15:LYS:NZ	6:N:3:GLN:OE1	2.42	0.52
3:A:217:VAL:HG21	3:A:376:PHE:HE1	1.74	0.52
4:B:212:ASP:OD2	4:B:219:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:142:HIS:HD1	4:B:161:SER:HG	1.56	0.52
6:N:17:SER:HA	6:N:83:MET:O	2.10	0.52
2:R:148:TYR:CZ	2:R:152:TYR:HE2	2.27	0.51
2:R:41:GLU:O	2:R:45:GLN:NE2	2.43	0.51
2:R:119:PRO:O	2:R:121:ARG:N	2.44	0.50
4:B:227:SER:OG	6:N:100:PRO:O	2.26	0.50
6:N:106:ASP:OD1	6:N:106:ASP:N	2.37	0.50
3:A:49:ASP:OD1	3:A:49:ASP:N	2.45	0.50
2:R:63:ASN:H	2:R:110:TRP:HZ2	1.59	0.50
2:R:120:TRP:HD1	2:R:121:ARG:HG2	1.77	0.49
2:R:120:TRP:CD1	2:R:121:ARG:HG2	2.48	0.49
3:A:309:GLU:HG3	3:A:315:PHE:HB3	1.95	0.49
4:B:260:GLU:OE2	4:B:263:THR:OG1	2.30	0.49
2:R:58:THR:OG1	2:R:59:ASP:N	2.44	0.49
4:B:27:ASP:OD1	4:B:27:ASP:N	2.38	0.49
2:R:33:TRP:HA	2:R:220:TYR:OH	2.13	0.49
2:R:252:TYR:HE1	2:R:326:ARG:HG2	1.77	0.48
4:B:79:LEU:HD11	4:B:114:CYS:HB3	1.96	0.48
1:P:25:ALA:O	1:P:29:ILE:HG13	2.13	0.48
4:B:146:LEU:HD11	4:B:159:THR:HB	1.95	0.48
4:B:311:HIS:HE2	4:B:329:THR:HG1	1.59	0.48
6:N:20:LEU:HD12	6:N:81:LEU:HD23	1.94	0.48
2:R:245:LEU:HA	2:R:320:ASN:OD1	2.12	0.47
2:R:356:LEU:HD13	3:A:393:LEU:HD21	1.97	0.47
4:B:215:GLU:HB3	4:B:217:MET:SD	2.54	0.47
2:R:255:LEU:HD12	2:R:327:VAL:HG22	1.96	0.47
4:B:22:ARG:NH2	4:B:258:ASP:OD1	2.47	0.47
2:R:366:ILE:HG22	2:R:367:PHE:CD1	2.49	0.47
2:R:292:GLU:OE2	2:R:301:SER:OG	2.27	0.47
3:A:346:LEU:HA	3:A:349:SER:OG	2.15	0.47
2:R:346:LYS:HA	2:R:346:LYS:HD2	1.71	0.47
3:A:295:ASP:H	3:A:365:CYS:HB2	1.79	0.47
2:R:91:TRP:HH2	2:R:127:GLU:HA	1.80	0.47
2:R:172:LEU:HD13	2:R:409:VAL:HG12	1.97	0.47
2:R:113:LYS:HG3	2:R:118:LEU:HD12	1.96	0.46
4:B:48:ARG:HG3	4:B:340:ASN:HB2	1.97	0.46
4:B:248:ALA:HB1	4:B:269:ILE:HG22	1.95	0.46
2:R:110:TRP:HE3	2:R:120:TRP:HH2	1.63	0.46
2:R:415:LYS:O	2:R:419:ARG:HG3	2.16	0.46
2:R:37:GLN:HA	2:R:40:ARG:HG3	1.97	0.46
2:R:262:GLU:HG2	2:R:263:GLN:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:371:ASN:OD1	3:A:374:ARG:NH1	2.49	0.46
2:R:227:ARG:HG2	2:R:297:TRP:CH2	2.51	0.45
2:R:314:LEU:HD23	2:R:314:LEU:HA	1.84	0.45
4:B:237:ASN:HD21	4:B:239:ASN:HB2	1.81	0.45
4:B:254:ASP:OD1	4:B:255:LEU:N	2.49	0.45
2:R:362:THR:HG22	2:R:366:ILE:HD13	1.97	0.45
3:A:364:THR:O	3:A:364:THR:OG1	2.33	0.45
4:B:276:VAL:HG13	4:B:285:LEU:HD11	1.99	0.45
3:A:228:ARG:NH2	3:A:230:GLU:OE2	2.44	0.45
2:R:314:LEU:HD23	2:R:317:ILE:HD12	1.98	0.44
2:R:70:ALA:HB2	2:R:86:PRO:HG3	1.99	0.44
2:R:268:LEU:O	2:R:272:ILE:HG23	2.18	0.44
3:A:294:GLN:HG3	3:A:363:PHE:HB3	1.99	0.44
3:A:213:GLN:NE2	3:A:218:ASN:OD1	2.51	0.44
3:A:330:GLU:OE1	3:A:335:THR:OG1	2.28	0.44
6:N:50:ASP:OD2	6:N:59:SER:OG	2.28	0.44
6:N:94:TYR:O	6:N:121:GLY:HA2	2.18	0.44
3:A:12:LEU:HB2	3:A:16:ASP:OD2	2.18	0.43
4:B:142:HIS:CE1	4:B:161:SER:HG	2.34	0.43
2:R:339:LEU:HD23	2:R:340:MET:N	2.32	0.43
2:R:288:LYS:HB3	2:R:297:TRP:CD1	2.52	0.43
3:A:14:ALA:O	3:A:18:ALA:N	2.51	0.43
2:R:283:PRO:O	2:R:287:VAL:HB	2.18	0.43
3:A:213:GLN:HE21	3:A:213:GLN:HB2	1.64	0.43
3:A:344:GLU:OE2	3:A:347:ARG:NH2	2.34	0.43
4:B:155:ASN:ND2	4:B:170:ASP:OD1	2.51	0.43
4:B:290:ASP:N	4:B:290:ASP:OD1	2.51	0.43
4:B:279:SER:HB2	4:B:284:LEU:HB2	2.01	0.43
1:P:11:THR:HG23	2:R:141:LEU:HB3	2.01	0.43
2:R:334:LYS:HD3	2:R:334:LYS:HA	1.84	0.43
4:B:68:ARG:O	4:B:84:SER:OG	2.35	0.43
4:B:253:PHE:CE2	4:B:260:GLU:HB2	2.54	0.43
4:B:254:ASP:OD2	5:G:33:ALA:HB1	2.19	0.43
2:R:110:TRP:HB3	2:R:120:TRP:HZ3	1.84	0.42
3:A:204:THR:HG21	4:B:143:THR:HG22	2.01	0.42
2:R:129:SER:O	2:R:129:SER:OG	2.34	0.42
3:A:48:ALA:O	3:A:51:SER:OG	2.31	0.42
4:B:81:ILE:HB	4:B:91:HIS:HB2	2.02	0.42
2:R:43:ARG:NE	2:R:43:ARG:HA	2.35	0.42
2:R:146:ILE:HD13	2:R:146:ILE:HA	1.89	0.42
4:B:137:ARG:HE	4:B:137:ARG:HB2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:311:HIS:CD2	4:B:329:THR:HG1	2.37	0.42
4:B:331:SER:OG	4:B:332:TRP:N	2.53	0.42
6:N:91:THR:HG23	6:N:125:THR:HA	2.01	0.41
2:R:328:ILE:HD13	2:R:328:ILE:HA	1.95	0.41
4:B:96:ARG:NH1	4:B:138:GLU:OE2	2.53	0.41
2:R:295:GLY:O	2:R:298:THR:HG23	2.20	0.41
4:B:300:LEU:HD13	5:G:38:MET:HG2	2.02	0.41
3:A:211:LYS:HG2	3:A:220:HIS:CD2	2.56	0.41
4:B:68:ARG:HE	4:B:83:ASP:CG	2.24	0.41
3:A:33:ASP:O	3:A:36:VAL:HG12	2.20	0.41
2:R:226:CYS:HB3	2:R:296:CYS:HB3	1.32	0.41
2:R:357:ILE:HD13	2:R:362:THR:HB	2.02	0.41
3:A:295:ASP:OD1	3:A:296:LEU:N	2.53	0.41
3:A:310:ASP:OD1	3:A:311:TYR:N	2.53	0.41
4:B:152:LEU:HD21	4:B:213:VAL:HG11	2.03	0.40
2:R:137:PRO:O	2:R:141:LEU:HB2	2.21	0.40
4:B:142:HIS:CG	4:B:161:SER:HG	2.34	0.40
3:A:15:GLU:HG2	3:A:16:ASP:N	2.35	0.40
6:N:91:THR:OG1	6:N:126:VAL:N	2.47	0.40
2:R:339:LEU:HD12	3:A:385:ARG:HH12	1.87	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	P	19/28 (68%)	19 (100%)	0	0	100	100
2	R	378/440 (86%)	348 (92%)	28 (7%)	2 (0%)	25	61
3	A	241/361 (67%)	224 (93%)	17 (7%)	0	100	100
4	B	336/345 (97%)	324 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	G	54/70 (77%)	52 (96%)	2 (4%)	0	100 100
6	N	124/140 (89%)	124 (100%)	0	0	100 100
All	All	1152/1384 (83%)	1091 (95%)	59 (5%)	2 (0%)	45 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	120	TRP
2	R	118	LEU

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	P	17/22 (77%)	16 (94%)	1 (6%)	16 47
2	R	341/392 (87%)	320 (94%)	21 (6%)	15 45
3	A	217/315 (69%)	201 (93%)	16 (7%)	11 38
4	B	281/287 (98%)	263 (94%)	18 (6%)	14 44
5	G	45/57 (79%)	44 (98%)	1 (2%)	47 76
6	N	104/116 (90%)	98 (94%)	6 (6%)	17 48
All	All	1005/1189 (84%)	942 (94%)	63 (6%)	17 45

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	19	TYR
2	R	42	TYR
2	R	46	CYS
2	R	72	TRP
2	R	80	PHE
2	R	93	SER
2	R	102	ARG
2	R	130	LYS

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Mol	Chain	Res	Type
2	R	145	TYR
2	R	152	TYR
2	R	155	SER
2	R	215	ASP
2	R	228	LEU
2	R	230	PHE
2	R	234	GLN
2	R	265	ILE
2	R	300	ASN
2	R	305	TYR
2	R	326	ARG
2	R	340	MET
2	R	376	ARG
2	R	413	PHE
3	A	61	ARG
3	A	200	THR
3	A	237	CYS
3	A	239	ASN
3	A	241	VAL
3	A	248	VAL
3	A	253	TYR
3	A	280	ARG
3	A	283	ARG
3	A	319	THR
3	A	322	GLU
3	A	330	GLU
3	A	347	ARG
3	A	364	THR
3	A	368	ASP
3	A	385	ARG
4	B	5	ASP
4	B	9	GLN
4	B	44	GLN
4	B	59	TYR
4	B	61	MET
4	B	70	LEU
4	B	96	ARG
4	B	105	TYR
4	B	172	GLU
4	B	189	SER
4	B	197	ARG
4	B	217	MET

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Mol	Chain	Res	Type
4	B	234	PHE
4	B	246	ASP
4	B	267	ASP
4	B	277	SER
4	B	336	LEU
4	B	340	ASN
5	G	62	ARG
6	N	50	ASP
6	N	59	SER
6	N	60	TYR
6	N	99	CYS
6	N	106	ASP
6	N	108	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	213	GLN
4	B	237	ASN
4	B	239	ASN

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.