Full wwPDB EM Validation Report ⓘ

Mar 31, 2024 – 12:51 AM JST

PDB ID	:	8W8Q
EMDB ID	:	EMD-37356
Title	:	Cryo-EM structure of the GPR101-Gs complex
Authors	:	Sun, J.P.; Gao, N.; Yu, X.; Wang, G.P.; Yang, F.; Wang, J.Y.; Yang, Z.; Guan, Y.
Deposited on	:	2023-09-04
Resolution	:	2.89 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:

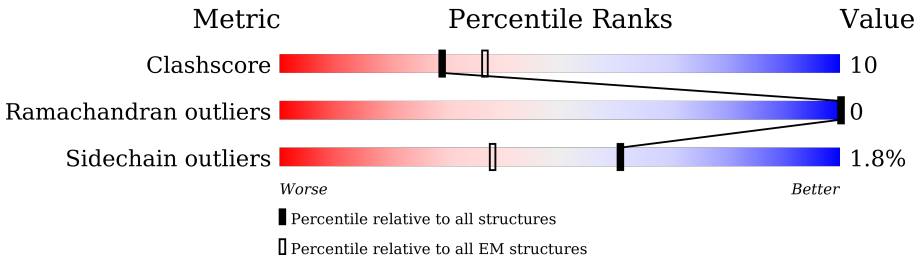
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.89 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	C	655	33% 10% • 56%
2	A	394	47% 11% 41%
3	B	339	74% 25% •
4	G	58	88% 12%
5	N	128	80% 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8168 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 Soluble cytochrome b562,Probable G-protein coupled receptor 101.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	287	Total	C	N	O	S	0	0
			2283	1536	365	369	13		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-146	MET	-	initiating methionine	UNP P0ABE7
C	-145	LYS	-	expression tag	UNP P0ABE7
C	-144	THR	-	expression tag	UNP P0ABE7
C	-143	ILE	-	expression tag	UNP P0ABE7
C	-142	ILE	-	expression tag	UNP P0ABE7
C	-141	ALA	-	expression tag	UNP P0ABE7
C	-140	LEU	-	expression tag	UNP P0ABE7
C	-139	SER	-	expression tag	UNP P0ABE7
C	-138	TYR	-	expression tag	UNP P0ABE7
C	-137	ILE	-	expression tag	UNP P0ABE7
C	-136	PHE	-	expression tag	UNP P0ABE7
C	-135	CYS	-	expression tag	UNP P0ABE7
C	-134	LEU	-	expression tag	UNP P0ABE7
C	-133	VAL	-	expression tag	UNP P0ABE7
C	-132	PHE	-	expression tag	UNP P0ABE7
C	-131	ALA	-	expression tag	UNP P0ABE7
C	-130	ASP	-	expression tag	UNP P0ABE7
C	-129	TYR	-	expression tag	UNP P0ABE7
C	-128	LYS	-	expression tag	UNP P0ABE7
C	-127	ASP	-	expression tag	UNP P0ABE7
C	-126	ASP	-	expression tag	UNP P0ABE7
C	-125	ASP	-	expression tag	UNP P0ABE7
C	-124	ASP	-	expression tag	UNP P0ABE7
C	-123	LYS	-	expression tag	UNP P0ABE7
C	-122	HIS	-	expression tag	UNP P0ABE7
C	-121	HIS	-	expression tag	UNP P0ABE7
C	-120	HIS	-	expression tag	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-119	HIS	-	expression tag	UNP P0ABE7
C	-118	HIS	-	expression tag	UNP P0ABE7
C	-117	HIS	-	expression tag	UNP P0ABE7
C	-116	HIS	-	expression tag	UNP P0ABE7
C	-115	HIS	-	expression tag	UNP P0ABE7
C	-114	HIS	-	expression tag	UNP P0ABE7
C	-113	HIS	-	expression tag	UNP P0ABE7
C	-112	GLU	-	expression tag	UNP P0ABE7
C	-111	ASN	-	expression tag	UNP P0ABE7
C	-110	LEU	-	expression tag	UNP P0ABE7
C	-109	TYR	-	expression tag	UNP P0ABE7
C	-108	PHE	-	expression tag	UNP P0ABE7
C	-107	GLN	-	expression tag	UNP P0ABE7
C	-106	GLY	-	expression tag	UNP P0ABE7
C	-99	TRP	MET	conflict	UNP P0ABE7
C	-4	ILE	HIS	conflict	UNP P0ABE7
C	0	LEU	ARG	conflict	UNP P0ABE7

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	232	Total	C	N	O	S	0	0
			1898	1201	345	346	6		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	engineered mutation	UNP P63092
A	60	PHE	MET	engineered mutation	UNP P63092
A	226	ALA	GLY	engineered mutation	UNP P63092
A	268	ALA	GLU	engineered mutation	UNP P63092
A	271	LYS	ASN	engineered mutation	UNP P63092
A	274	ASP	LYS	engineered mutation	UNP P63092
A	280	LYS	ARG	engineered mutation	UNP P63092
A	284	ASP	THR	engineered mutation	UNP P63092
A	285	THR	ILE	engineered mutation	UNP P63092

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	339	Total	C	N	O	S	0	0
			2579	1594	461	503	21		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	58	Total	C	N	O	S	0	0
			438	274	76	85	3		

- Molecule 5 is a protein called Nb35.

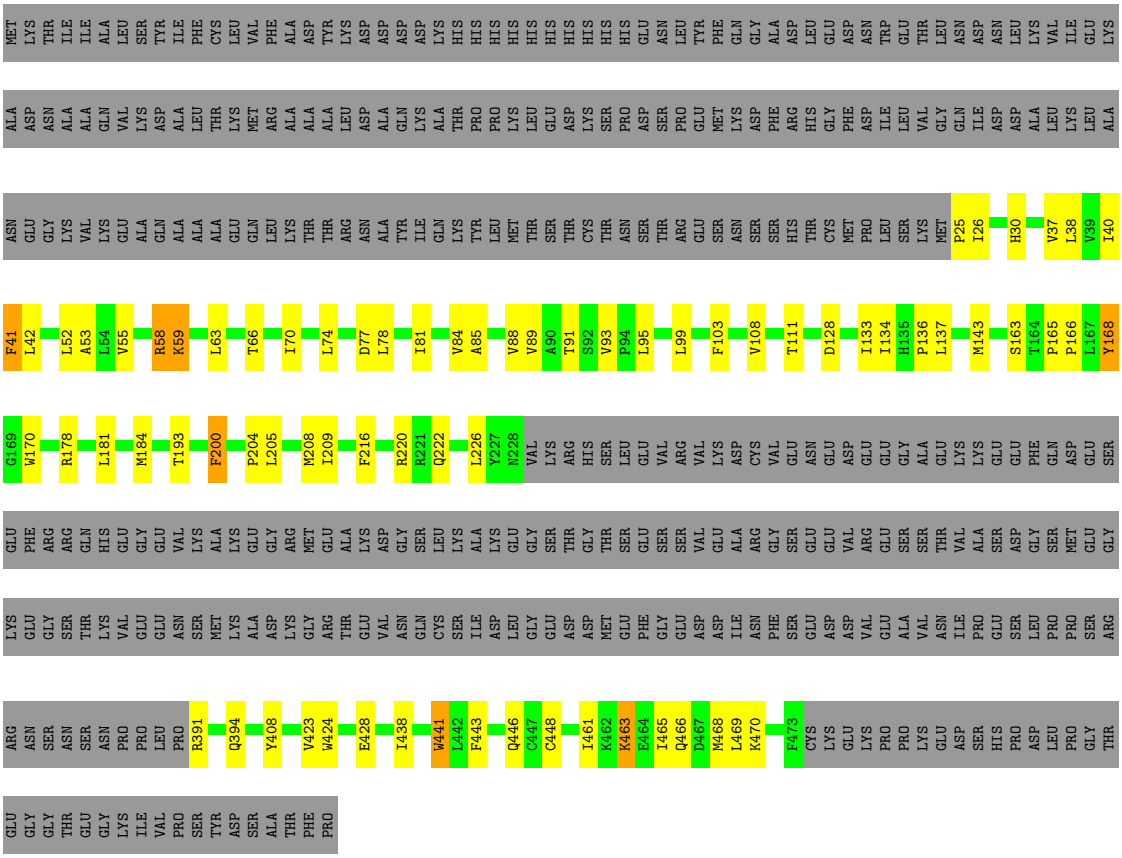
Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	128	Total	C	N	O	S	0	0
			970	604	170	190	6		

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.

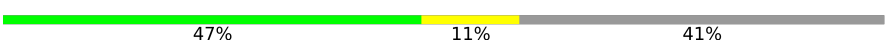
• Molecule 1: Soluble cytochrome b562,Probable G-protein coupled receptor 101

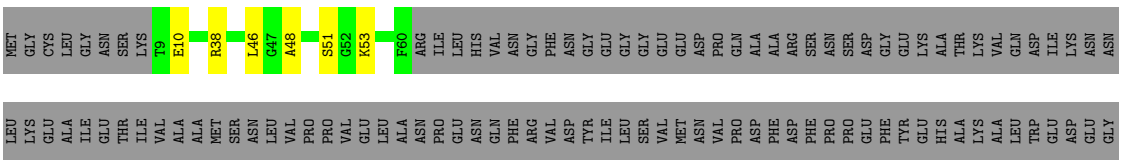
Chain C:

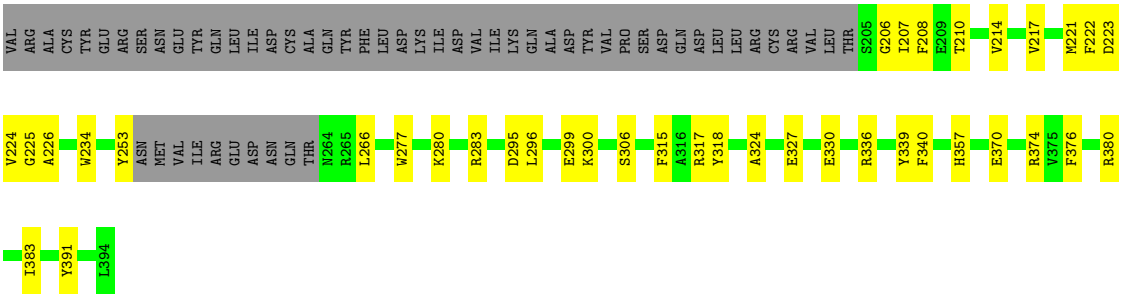


• Molecule 2: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain A:

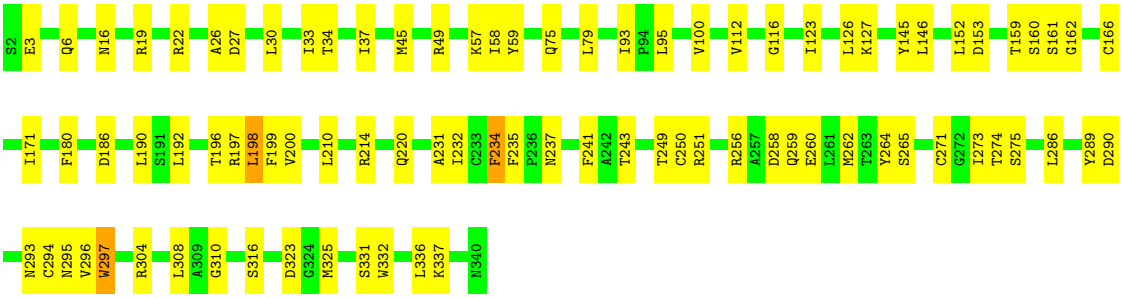






• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:

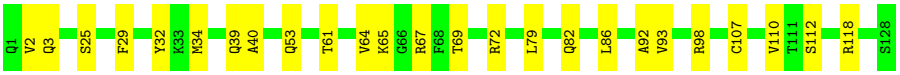


• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:

• Molecule 5: Nb35

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	166138	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (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	C	0.29	0/2349	0.45	0/3215
2	A	0.36	0/1933	0.51	0/2598
3	B	0.35	0/2626	0.57	0/3564
4	G	0.28	0/444	0.44	0/601
5	N	0.29	0/990	0.51	0/1341
All	All	0.32	0/8342	0.51	0/11319

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	C	2283	0	2373	58	0
2	A	1898	0	1871	29	0
3	B	2579	0	2471	65	0
4	G	438	0	443	7	0
5	N	970	0	930	16	0
All	All	8168	0	8088	167	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 10.

All (167) 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:C:66:THR:HG22	1:C:128:ASP:OD1	1.61	1.01
3:B:34:THR:O	3:B:37:ILE:HG22	1.75	0.86
1:C:38:LEU:HD12	1:C:41:PHE:HE2	1.40	0.86
1:C:438:ILE:HD13	1:C:441:TRP:HE1	1.45	0.79
5:N:107:CYS:SG	5:N:110:VAL:HG11	2.24	0.77
1:C:58:ARG:HB3	1:C:59:LYS:HD2	1.67	0.76
3:B:271:CYS:HB2	3:B:290:ASP:HB2	1.68	0.75
3:B:197:ARG:HH21	3:B:214:ARG:HG3	1.52	0.74
2:A:253:TYR:HB3	2:A:266:LEU:HD12	1.73	0.71
3:B:57:LYS:NZ	3:B:75:GLN:HG3	2.09	0.68
3:B:112:VAL:HG23	3:B:126:LEU:HD11	1.76	0.67
1:C:143:MET:O	2:A:38:ARG:NH2	2.28	0.67
1:C:93:VAL:HG12	1:C:95:LEU:H	1.59	0.66
1:C:78:LEU:HD12	1:C:81:ILE:HD11	1.78	0.65
1:C:63:LEU:HB3	1:C:66:THR:OG1	1.97	0.65
2:A:208:PHE:HB2	2:A:223:ASP:OD1	1.97	0.65
1:C:438:ILE:HA	1:C:441:TRP:NE1	2.11	0.65
1:C:438:ILE:HA	1:C:441:TRP:HE1	1.62	0.65
5:N:112:SER:O	5:N:118:ARG:NH2	2.26	0.64
3:B:232:ILE:HG13	3:B:243:THR:HG22	1.79	0.63
3:B:152:LEU:HD23	3:B:196:THR:HB	1.80	0.63
1:C:25:PRO:HA	1:C:178:ARG:HA	1.81	0.62
3:B:256:ARG:NH2	4:G:36:ASP:OD2	2.31	0.62
1:C:38:LEU:HD12	1:C:41:PHE:CE2	2.29	0.62
2:A:224:VAL:HG21	2:A:234:TRP:CH2	2.35	0.62
1:C:42:LEU:HD22	1:C:81:ILE:HG22	1.82	0.61
3:B:250:CYS:HB2	3:B:264:TYR:HB2	1.80	0.61
3:B:286:LEU:CD1	3:B:296:VAL:HG22	2.31	0.61
3:B:289:TYR:OH	3:B:297:TRP:CH2	2.52	0.61
1:C:38:LEU:HA	1:C:41:PHE:CD2	2.36	0.60
1:C:58:ARG:NH1	1:C:468:MET:CE	2.64	0.60
3:B:286:LEU:HD13	3:B:296:VAL:HG22	1.83	0.60
1:C:55:VAL:HG21	1:C:465:ILE:HG22	1.83	0.60
2:A:370:GLU:HG3	2:A:374:ARG:HG3	1.84	0.60
3:B:162:GLY:HA2	3:B:186:ASP:HB2	1.84	0.60
3:B:250:CYS:SG	3:B:273:ILE:HD13	2.41	0.59
5:N:40:ALA:HA	5:N:92:ALA:HB2	1.85	0.59
5:N:107:CYS:SG	5:N:110:VAL:CG1	2.90	0.59
3:B:57:LYS:HZ3	3:B:75:GLN:HG3	1.68	0.58
5:N:53:GLN:OE1	5:N:53:GLN:N	2.30	0.58
1:C:424:TRP:CE3	1:C:424:TRP:HA	2.38	0.58
5:N:39:GLN:O	5:N:92:ALA:HB1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LEU:HD11	1:C:461:ILE:HD11	1.87	0.57
2:A:214:VAL:O	2:A:217:VAL:HG12	2.05	0.57
3:B:289:TYR:OH	3:B:297:TRP:HH2	1.87	0.57
3:B:231:ALA:HB2	3:B:275:SER:HA	1.87	0.57
3:B:294:CYS:HB2	3:B:308:LEU:HB2	1.87	0.56
3:B:160:SER:HB3	3:B:190:LEU:HD23	1.88	0.56
1:C:38:LEU:HA	1:C:41:PHE:CE2	2.41	0.56
3:B:295:ASN:OD1	3:B:304:ARG:HD3	2.05	0.56
4:G:58:GLU:OE2	4:G:58:GLU:N	2.26	0.56
3:B:200:VAL:HG13	3:B:234:PHE:CE2	2.41	0.56
1:C:137:LEU:HD12	2:A:383:ILE:HD12	1.88	0.55
3:B:198:LEU:HD12	3:B:198:LEU:O	2.07	0.55
2:A:206:GLY:HA2	2:A:226:ALA:HB3	1.89	0.55
5:N:69:THR:HG22	5:N:82:GLN:HB3	1.89	0.55
3:B:251:ARG:HD3	3:B:260:GLU:OE2	2.07	0.55
1:C:41:PHE:HD1	1:C:448:CYS:HG	1.55	0.54
2:A:318:TYR:O	2:A:336:ARG:NE	2.30	0.54
2:A:295:ASP:N	2:A:295:ASP:OD1	2.40	0.54
3:B:27:ASP:HB2	4:G:29:LYS:HZ1	1.73	0.54
1:C:200:PHE:O	1:C:408:TYR:OH	2.22	0.53
4:G:47:GLU:N	4:G:47:GLU:OE2	2.42	0.53
3:B:197:ARG:NH2	3:B:214:ARG:HG3	2.24	0.53
1:C:466:GLN:O	1:C:470:LYS:HD2	2.09	0.53
2:A:283:ARG:O	2:A:357:HIS:CD2	2.62	0.53
5:N:3:GLN:NE2	5:N:25:SER:OG	2.39	0.53
1:C:391:ARG:N	1:C:394:GLN:OE1	2.42	0.52
1:C:443:PHE:O	1:C:446:GLN:HG2	2.10	0.52
3:B:198:LEU:HD22	3:B:210:LEU:HD11	1.91	0.52
2:A:210:THR:HG21	2:A:221:MET:HE3	1.90	0.52
3:B:100:VAL:HA	3:B:116:GLY:HA3	1.91	0.52
1:C:77:ASP:O	1:C:81:ILE:HG12	2.09	0.52
1:C:66:THR:O	1:C:70:ILE:HG12	2.10	0.52
1:C:53:ALA:HB2	1:C:74:LEU:HD21	1.93	0.51
2:A:208:PHE:HE2	2:A:225:GLY:HA3	1.75	0.51
1:C:193:THR:HG21	1:C:423:VAL:HG21	1.93	0.51
1:C:204:PRO:O	1:C:208:MET:HG3	2.11	0.50
3:B:49:ARG:HH21	4:G:61:PHE:HA	1.75	0.50
1:C:163:SER:O	1:C:166:PRO:HD2	2.12	0.50
3:B:33:ILE:HD12	4:G:34:ALA:HB3	1.92	0.50
2:A:277:TRP:CE2	2:A:357:HIS:CE1	3.01	0.49
3:B:3:GLU:O	3:B:6:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:TRP:HA	1:C:424:TRP:HE3	1.78	0.49
1:C:108:VAL:HG11	1:C:184:MET:HG2	1.93	0.48
3:B:22:ARG:NE	3:B:258:ASP:O	2.45	0.48
3:B:58:ILE:HD13	3:B:336:LEU:HG	1.95	0.48
3:B:231:ALA:HB2	3:B:274:THR:O	2.14	0.48
2:A:48:ALA:HB3	2:A:51:SER:HB3	1.95	0.48
3:B:153:ASP:N	3:B:153:ASP:OD1	2.44	0.48
1:C:84:VAL:HG11	1:C:111:THR:HG23	1.95	0.48
2:A:315:PHE:HB2	2:A:340:PHE:CE2	2.49	0.48
1:C:37:VAL:O	1:C:40:ILE:HG13	2.14	0.47
1:C:58:ARG:HH12	1:C:468:MET:HE2	1.79	0.47
1:C:165:PRO:HB3	1:C:170:TRP:HB3	1.95	0.47
3:B:310:GLY:O	3:B:337:LYS:HE2	2.15	0.47
2:A:324:ALA:HB1	2:A:339:TYR:CZ	2.49	0.47
2:A:210:THR:HG23	2:A:221:MET:HB3	1.96	0.47
3:B:57:LYS:HG3	3:B:75:GLN:HG3	1.95	0.47
3:B:235:PHE:CD2	3:B:237:ASN:HB3	2.50	0.47
3:B:231:ALA:CB	3:B:275:SER:HA	2.44	0.47
3:B:146:LEU:HD11	3:B:159:THR:HB	1.97	0.47
3:B:331:SER:OG	3:B:332:TRP:N	2.47	0.47
1:C:133:ILE:HD11	2:A:391:TYR:HD2	1.80	0.46
2:A:207:ILE:HD11	2:A:222:PHE:HB3	1.98	0.46
5:N:39:GLN:C	5:N:92:ALA:HB1	2.36	0.46
2:A:376:PHE:CE2	2:A:380:ARG:HD2	2.51	0.46
3:B:251:ARG:CD	3:B:260:GLU:OE2	2.64	0.45
2:A:223:ASP:OD1	2:A:223:ASP:N	2.50	0.45
3:B:260:GLU:O	3:B:260:GLU:HG3	2.16	0.45
5:N:65:LYS:HE3	5:N:65:LYS:HB2	1.50	0.45
1:C:178:ARG:HD3	1:C:428:GLU:OE1	2.17	0.44
3:B:123:ILE:HG13	3:B:171:ILE:HD12	1.98	0.44
3:B:220:GLN:HA	4:G:22:GLU:HG3	1.99	0.44
3:B:250:CYS:SG	3:B:273:ILE:CD1	3.05	0.44
1:C:58:ARG:HH12	1:C:468:MET:CE	2.29	0.44
1:C:165:PRO:HA	1:C:168:TYR:CE1	2.53	0.44
3:B:145:TYR:O	3:B:145:TYR:CD1	2.70	0.44
1:C:85:ALA:O	1:C:89:VAL:HG22	2.18	0.44
2:A:46:LEU:HD23	2:A:46:LEU:HA	1.79	0.44
3:B:235:PHE:HD2	3:B:237:ASN:HB3	1.82	0.44
5:N:2:VAL:HG11	5:N:98:ARG:HH21	1.83	0.44
3:B:58:ILE:O	3:B:316:SER:OG	2.29	0.44
1:C:99:LEU:HD22	1:C:103:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:112:VAL:CG2	3:B:126:LEU:HD11	2.46	0.44
3:B:16:ASN:OD1	3:B:19:ARG:NH2	2.52	0.43
3:B:95:LEU:HD13	3:B:100:VAL:HG11	2.01	0.43
1:C:184:MET:HE3	1:C:184:MET:HB3	1.84	0.43
1:C:26:ILE:HG13	1:C:30:HIS:HB3	2.00	0.43
1:C:42:LEU:HD22	1:C:81:ILE:CG2	2.49	0.43
3:B:57:LYS:HZ2	3:B:75:GLN:HG3	1.82	0.43
3:B:161:SER:OG	3:B:162:GLY:N	2.50	0.43
1:C:216:PHE:CE2	1:C:220:ARG:HD2	2.54	0.43
3:B:22:ARG:HB3	3:B:259:GLN:OE1	2.19	0.43
3:B:45:MET:HB2	3:B:308:LEU:HD11	2.00	0.42
5:N:67:ARG:NH1	5:N:86:LEU:HA	2.34	0.42
1:C:209:ILE:HD13	1:C:209:ILE:HA	1.92	0.42
3:B:323:ASP:OD2	3:B:325:MET:HB2	2.19	0.42
5:N:61:THR:HG22	5:N:64:VAL:HG22	2.01	0.42
3:B:232:ILE:HD11	3:B:241:PHE:CE2	2.55	0.42
1:C:42:LEU:HD23	1:C:42:LEU:HA	1.91	0.42
1:C:134:ILE:O	1:C:136:PRO:HD3	2.20	0.42
1:C:58:ARG:NH1	1:C:468:MET:HE1	2.34	0.42
2:A:10:GLU:H	2:A:10:GLU:HG3	1.70	0.42
5:N:29:PHE:O	5:N:72:ARG:NH2	2.52	0.42
5:N:32:TYR:CG	5:N:98:ARG:HD2	2.55	0.42
3:B:79:LEU:HB3	3:B:93:ILE:HB	2.02	0.41
3:B:289:TYR:HB2	3:B:293:ASN:O	2.20	0.41
2:A:300:LYS:HD3	2:A:306:SER:OG	2.21	0.41
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.84	0.41
3:B:166:CYS:HB2	3:B:180:PHE:HB2	2.02	0.41
1:C:88:VAL:O	1:C:91:THR:OG1	2.29	0.41
1:C:463:LYS:NZ	1:C:466:GLN:OE1	2.51	0.41
2:A:280:LYS:HA	2:A:283:ARG:HG3	2.01	0.41
1:C:41:PHE:O	1:C:448:CYS:SG	2.78	0.41
1:C:52:LEU:HD23	1:C:74:LEU:HD12	2.02	0.41
1:C:469:LEU:HD23	1:C:469:LEU:HA	1.89	0.41
2:A:327:GLU:HB3	2:A:330:GLU:HG2	2.01	0.41
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.92	0.41
3:B:26:ALA:HB2	3:B:259:GLN:NE2	2.36	0.41
3:B:127:LYS:HA	3:B:127:LYS:HD3	1.78	0.41
3:B:192:LEU:HD23	3:B:199:PHE:HB3	2.03	0.41
2:A:296:LEU:O	2:A:299:GLU:HG3	2.20	0.41
2:A:357:HIS:CD2	2:A:357:HIS:N	2.89	0.40
3:B:30:LEU:HD23	3:B:262:MET:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:34:MET:HB3	5:N:79:LEU:HD22	2.02	0.40
3:B:249:THR:HG22	3:B:265:SER:CB	2.51	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	C	283/655 (43%)	277 (98%)	6 (2%)	0	100	100
2	A	226/394 (57%)	223 (99%)	3 (1%)	0	100	100
3	B	337/339 (99%)	332 (98%)	5 (2%)	0	100	100
4	G	56/58 (97%)	56 (100%)	0	0	100	100
5	N	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
All	All	1028/1574 (65%)	1012 (98%)	16 (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	C	252/575 (44%)	243 (96%)	9 (4%)	35	69
2	A	200/349 (57%)	198 (99%)	2 (1%)	76	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	B	276/282 (98%)	272 (99%)	4 (1%)	67 89
4	G	46/47 (98%)	46 (100%)	0	100 100
5	N	104/106 (98%)	103 (99%)	1 (1%)	76 92
All	All	878/1359 (65%)	862 (98%)	16 (2%)	61 85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	41	PHE
1	C	58	ARG
1	C	59	LYS
1	C	168	TYR
1	C	181	LEU
1	C	200	PHE
1	C	222	GLN
1	C	441	TRP
1	C	463	LYS
2	A	53	LYS
2	A	317	ARG
3	B	59	TYR
3	B	198	LEU
3	B	234	PHE
3	B	297	TRP
5	N	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	GLN
2	A	357	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 monosaccharides 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.