Full wwPDB EM Validation Report ⓘ

May 7, 2026 – 06:14 PM JST

PDB ID	:	8Z8A / pdb_00008z8a
EMDB ID	:	EMD-39843
Title	:	Cryo-EM structure of the Lactate-bound human HCAR1-Gi1 complex
Authors	:	Gao, M.; Zang, S.; Zhu, Y.; Mao, C.; Zhang, Y.; Ma, X.
Deposited on	:	2024-04-21
Resolution	:	2.82 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:

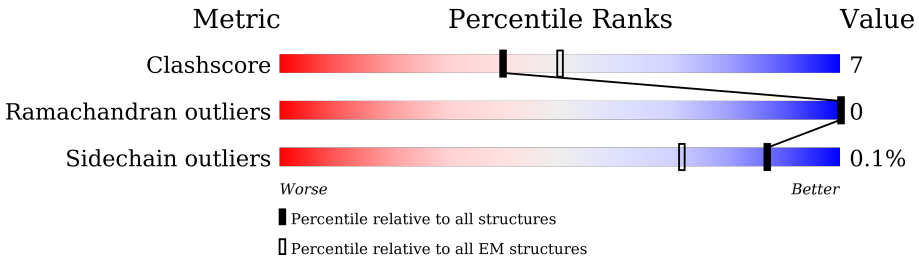
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	NOT EXECUTED
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.82 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	R	346	65% 16% 19%
2	A	354	51% 12% 36%
3	B	345	79% 19% .
4	G	70	77% 6% 17%
5	S	250	78% 16% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	2OP	R	401	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8881 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 Hydroxycarboxylic acid receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	281	2218	1462	372	362	22	0	0

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	225	1811	1150	301	346	14	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 3 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		
3	B	339	2607	1607	468	511	21	0	0

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

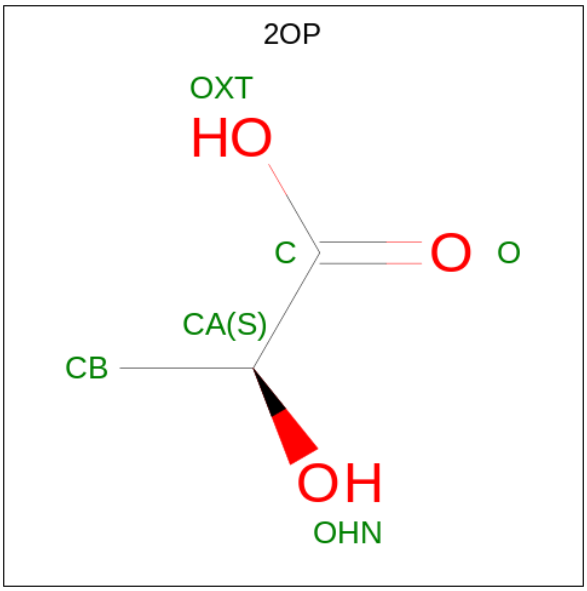
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	58	444	277	79	85	3	0	0

- Molecule 5 is a protein called single Fab chain (scFv16).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	234	1795	1137	297	351	10	0	0

- Molecule 6 is (2S)-2-HYDROXYPROPANOIC ACID (CCD ID: 2OP) (formula: $C_3H_6O_3$) (labeled as "Ligand of Interest" by depositor).



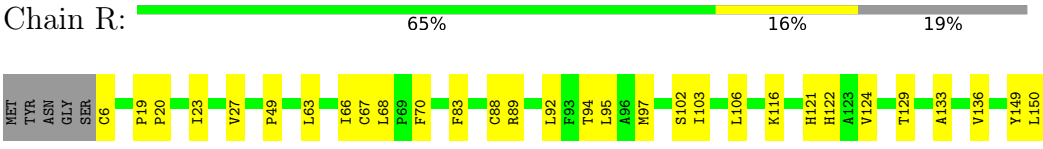
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	R	1	6	3	3	0

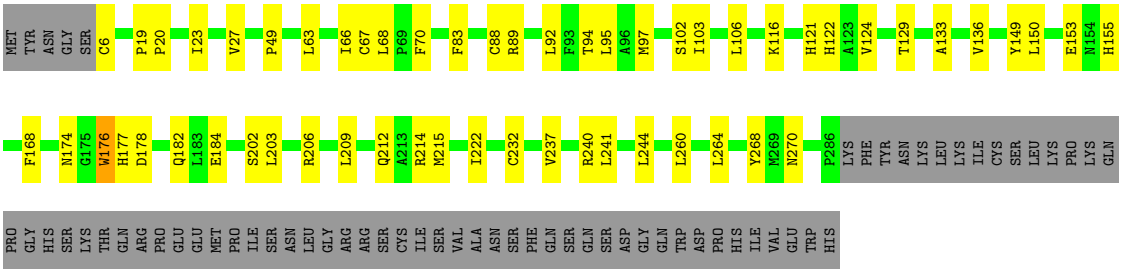
3 Residue-property plots (i)

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: Hydroxycarboxylic acid receptor 1

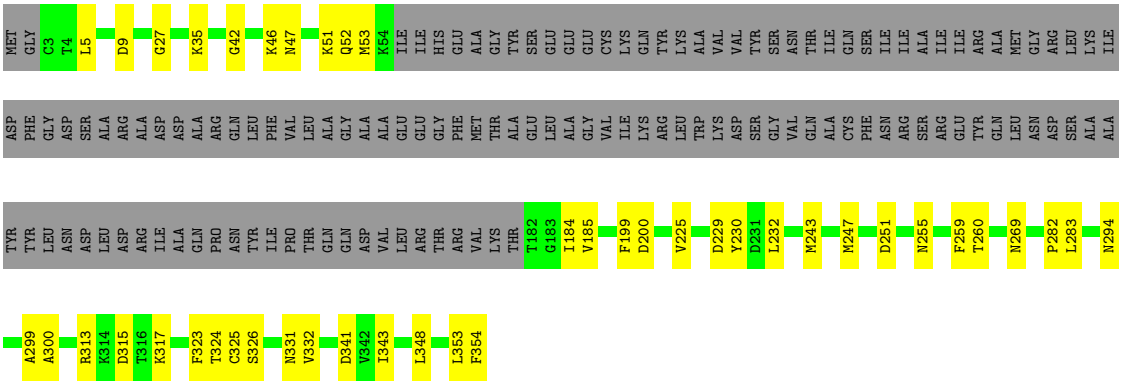
Chain R:





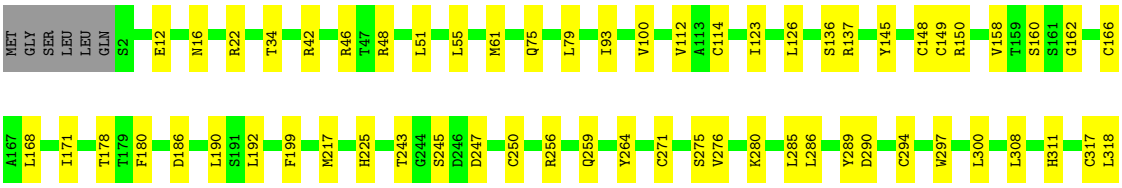
• Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-1

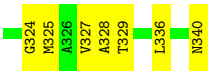
Chain A:



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

Chain B:



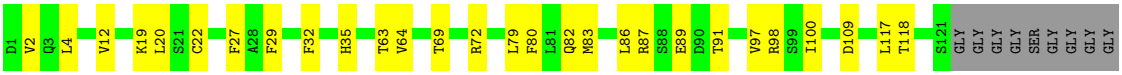


• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:

• Molecule 5: single Fab chain (scFv16)

Chain S:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	319661	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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2OP

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	R	0.31	0/2282	0.55	2/3109 (0.1%)
2	A	0.27	0/1841	0.47	0/2471
3	B	0.17	0/2654	0.38	0/3597
4	G	0.12	0/450	0.29	0/608
5	S	0.15	0/1839	0.36	0/2493
All	All	0.23	0/9066	0.44	2/12278 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	176	TRP	N-CA-C	-5.94	105.52	112.89
1	R	116	LYS	N-CA-CB	-5.55	101.68	110.28

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	R	2218	0	2221	36	0
2	A	1811	0	1799	32	0
3	B	2607	0	2510	39	0
4	G	444	0	454	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1795	0	1727	24	0
6	R	6	0	5	2	0
All	All	8881	0	8716	125	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 (125) 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:A:52:GLN:OE1	2:A:331:ASN:ND2	2.12	0.82
1:R:268:TYR:OH	6:R:401:2OP:HB3	1.91	0.70
1:R:209:LEU:O	1:R:215:MET:HG3	1.93	0.68
5:S:187:LEU:HD21	5:S:190:TYR:HB3	1.76	0.67
3:B:61:MET:HE1	3:B:328:ALA:HB3	1.77	0.64
3:B:51:LEU:HB2	3:B:336:LEU:HB2	1.80	0.64
1:R:209:LEU:HD13	2:A:341:ASP:HB3	1.80	0.64
1:R:222:ILE:HG12	2:A:353:LEU:HD21	1.79	0.64
5:S:180:ARG:NH2	5:S:222:GLU:OE2	2.31	0.64
2:A:53:MET:HG3	2:A:332:VAL:HG22	1.79	0.63
1:R:215:MET:SD	2:A:354:PHE:HE1	2.24	0.61
1:R:222:ILE:CG1	2:A:353:LEU:HD21	2.32	0.60
3:B:250:CYS:HB2	3:B:264:TYR:HB2	1.84	0.60
1:R:212:GLN:HG2	1:R:214:ARG:H	1.66	0.59
3:B:286:LEU:HD22	3:B:327:VAL:HG21	1.84	0.59
3:B:22:ARG:O	3:B:259:GLN:NE2	2.35	0.59
3:B:34:THR:HG21	3:B:300:LEU:HB3	1.85	0.58
5:S:91:THR:HG23	5:S:118:THR:HA	1.85	0.58
2:A:260:THR:HG22	2:A:313:ARG:HE	1.69	0.58
3:B:12:GLU:OE2	3:B:16:ASN:ND2	2.38	0.57
2:A:251:ASP:OD1	2:A:255:ASN:ND2	2.37	0.57
3:B:46:ARG:HE	3:B:48:ARG:HH22	1.54	0.56
3:B:137:ARG:NE	3:B:171:ILE:O	2.38	0.56
1:R:203:LEU:HD22	1:R:215:MET:HE1	1.88	0.56
3:B:168:LEU:HB3	3:B:178:THR:HB	1.88	0.56
3:B:325:MET:O	3:B:340:ASN:ND2	2.39	0.56
3:B:245:SER:OG	3:B:247:ASP:OD1	2.24	0.55
2:A:324:THR:HG22	2:A:331:ASN:OD1	2.06	0.55
2:A:348:LEU:HD22	2:A:353:LEU:HD23	1.87	0.55
3:B:217:MET:HE1	4:G:21:MET:HE3	1.89	0.55
1:R:215:MET:SD	2:A:354:PHE:CE1	3.00	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:348:LEU:CD2	2:A:353:LEU:HD23	2.38	0.54
3:B:79:LEU:HB2	3:B:93:ILE:HB	1.90	0.53
5:S:87:ARG:HG3	5:S:89:GLU:HG2	1.90	0.52
2:A:230:TYR:HA	2:A:243:MET:HB2	1.90	0.52
2:A:184:ILE:HD11	2:A:199:PHE:HB3	1.92	0.52
3:B:166:CYS:HB2	3:B:180:PHE:HB2	1.92	0.52
3:B:48:ARG:HE	3:B:340:ASN:HB2	1.75	0.51
3:B:271:CYS:HB2	3:B:290:ASP:HB2	1.91	0.51
1:R:121:HIS:HE1	2:A:343:ILE:HD12	1.74	0.51
5:S:22:CYS:HB3	5:S:79:LEU:HB3	1.92	0.51
2:A:42:GLY:O	2:A:46:LYS:NZ	2.42	0.51
2:A:282:PRO:HB3	2:A:294:ASN:HD21	1.75	0.51
1:R:202:SER:O	1:R:206:ARG:HG2	2.12	0.50
2:A:283:LEU:HD13	2:A:299:ALA:HB1	1.93	0.50
5:S:20:LEU:HG	5:S:83:MET:HE2	1.93	0.50
2:A:325:CYS:SG	2:A:326:SER:N	2.85	0.50
5:S:2:VAL:HG22	5:S:27:PHE:HB3	1.92	0.50
5:S:29:PHE:O	5:S:72:ARG:NH2	2.45	0.49
3:B:294:CYS:HB3	3:B:308:LEU:HB2	1.94	0.49
2:A:353:LEU:O	2:A:353:LEU:HG	2.11	0.48
1:R:240:ARG:O	1:R:244:LEU:HG	2.13	0.48
5:S:83:MET:HB3	5:S:86:LEU:HD21	1.95	0.48
1:R:237:VAL:O	1:R:241:LEU:HG	2.14	0.48
5:S:83:MET:HE1	5:S:117:LEU:HD13	1.95	0.48
1:R:63:LEU:HA	1:R:66:ILE:HD12	1.95	0.47
3:B:158:VAL:HG12	3:B:190:LEU:HD21	1.96	0.47
1:R:168:PHE:O	1:R:240:ARG:NH1	2.48	0.47
2:A:229:ASP:HA	2:A:232:LEU:HD13	1.96	0.47
3:B:256:ARG:HB3	4:G:28:ILE:HG12	1.97	0.47
5:S:98:ARG:NH2	5:S:109:ASP:OD2	2.43	0.47
3:B:150:ARG:HD3	3:B:150:ARG:HA	1.76	0.47
3:B:192:LEU:HD23	3:B:199:PHE:HB3	1.97	0.47
3:B:225:HIS:NE2	3:B:243:THR:OG1	2.41	0.47
1:R:70:PHE:HD1	1:R:83:PHE:HE2	1.64	0.46
5:S:35:HIS:HB2	5:S:97:VAL:HB	1.97	0.46
3:B:149:CYS:O	3:B:150:ARG:NH1	2.48	0.46
1:R:174:ASN:HB2	1:R:177:HIS:HB3	1.97	0.46
1:R:260:LEU:O	1:R:264:LEU:HD23	2.16	0.46
3:B:79:LEU:HD11	3:B:114:CYS:HB3	1.98	0.45
2:A:324:THR:CG2	2:A:331:ASN:OD1	2.65	0.45
3:B:148:CYS:O	3:B:160:SER:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:4:LEU:HD11	5:S:98:ARG:HB2	1.97	0.45
2:A:185:VAL:HB	2:A:200:ASP:HB3	1.99	0.45
1:R:103:ILE:HG21	1:R:184:GLU:O	2.16	0.45
3:B:75:GLN:NE2	3:B:100:VAL:O	2.49	0.45
1:R:232:CYS:CB	1:R:270:ASN:HB2	2.47	0.44
3:B:276:VAL:HG13	3:B:285:LEU:HD11	1.99	0.44
2:A:247:MET:HE3	2:A:247:MET:HB3	1.91	0.44
5:S:63:THR:HG23	5:S:64:VAL:HG13	1.98	0.44
3:B:280:LYS:HB2	3:B:324:GLY:HA3	2.00	0.44
5:S:12:VAL:HG11	5:S:86:LEU:HD12	1.99	0.44
2:A:35:LYS:HD2	2:A:199:PHE:HZ	1.82	0.44
2:A:225:VAL:O	2:A:269:ASN:N	2.43	0.44
1:R:49:PRO:HD3	1:R:129:THR:HG22	2.00	0.44
5:S:149:VAL:HG21	5:S:219:LEU:HD13	1.99	0.44
5:S:191:ARG:C	5:S:193:SER:H	2.25	0.43
3:B:162:GLY:HA2	3:B:186:ASP:HB3	2.00	0.43
1:R:88:CYS:SG	1:R:155:HIS:HB2	2.57	0.43
2:A:5:LEU:HD22	2:A:9:ASP:HB3	2.01	0.43
1:R:97:MET:HE2	1:R:97:MET:HB3	1.90	0.43
1:R:95:LEU:HD13	6:R:401:2OP:HB3	2.01	0.43
1:R:176:TRP:O	1:R:177:HIS:C	2.62	0.43
3:B:311:HIS:NE2	3:B:329:THR:OG1	2.45	0.43
2:A:27:GLY:HA3	3:B:55:LEU:HD13	2.01	0.42
2:A:300:ALA:HB1	2:A:323:PHE:CE2	2.55	0.42
1:R:19:PRO:HB2	1:R:20:PRO:HD3	2.01	0.42
3:B:61:MET:HG2	3:B:317:CYS:HB2	2.02	0.42
1:R:23:ILE:O	1:R:27:VAL:HG12	2.19	0.42
2:A:47:ASN:O	2:A:51:LYS:HG3	2.20	0.42
2:A:315:ASP:OD1	2:A:315:ASP:N	2.52	0.42
5:S:19:LYS:HE2	5:S:80:PHE:CD1	2.54	0.42
3:B:123:ILE:O	3:B:136:SER:N	2.50	0.42
4:G:57:SER:O	4:G:62:ARG:NH2	2.52	0.42
3:B:275:SER:HB2	3:B:318:LEU:HB2	2.01	0.42
5:S:109:ASP:OD1	5:S:109:ASP:N	2.48	0.42
5:S:202:ARG:NH2	5:S:223:ASP:OD1	2.34	0.42
1:R:67:CYS:SG	1:R:94:THR:HG23	2.61	0.41
3:B:112:VAL:HG23	3:B:126:LEU:HD11	2.01	0.41
5:S:178:LEU:HD13	5:S:227:TYR:CZ	2.55	0.41
1:R:149:TYR:CE2	1:R:150:LEU:HD12	2.55	0.41
5:S:69:THR:O	5:S:82:GLN:N	2.52	0.41
1:R:133:ALA:HA	1:R:136:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:102:SER:O	1:R:106:LEU:HG	2.21	0.41
1:R:178:ASP:O	1:R:182:GLN:HG2	2.20	0.41
5:S:32:PHE:CE2	5:S:100:ILE:HB	2.56	0.41
1:R:68:LEU:HD23	1:R:68:LEU:HA	1.94	0.41
3:B:145:TYR:O	3:B:162:GLY:N	2.40	0.41
3:B:289:TYR:OH	3:B:297:TRP:NE1	2.53	0.41
1:R:92:LEU:HB3	1:R:150:LEU:HD23	2.03	0.41
1:R:122:HIS:ND1	1:R:124:VAL:HG23	2.35	0.41
3:B:42:ARG:HD2	3:B:42:ARG:HA	1.86	0.41
1:R:89:ARG:HD3	1:R:153:GLU:O	2.21	0.40
5:S:32:PHE:CD2	5:S:98:ARG:HG2	2.55	0.40
2:A:259:PHE:O	2:A:317:LYS:NZ	2.42	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	R	279/346 (81%)	267 (96%)	12 (4%)	0	100	100
2	A	221/354 (62%)	213 (96%)	8 (4%)	0	100	100
3	B	337/345 (98%)	326 (97%)	11 (3%)	0	100	100
4	G	56/70 (80%)	56 (100%)	0	0	100	100
5	S	230/250 (92%)	225 (98%)	5 (2%)	0	100	100
All	All	1123/1365 (82%)	1087 (97%)	36 (3%)	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	R	237/305 (78%)	236 (100%)	1 (0%)	84 94
2	A	200/305 (66%)	200 (100%)	0	100 100
3	B	282/287 (98%)	282 (100%)	0	100 100
4	G	47/57 (82%)	47 (100%)	0	100 100
5	S	198/202 (98%)	198 (100%)	0	100 100
All	All	964/1156 (83%)	963 (100%)	1 (0%)	87 96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	6	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	121	HIS
1	R	154	ASN
1	R	174	ASN
2	A	294	ASN
2	A	333	GLN
5	S	171	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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	2OP	R	401	-	5,5,5	1.93	2 (40%)	4,6,6	1.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	2OP	R	401	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	401	2OP	OHN-CA	3.23	1.53	1.42
6	R	401	2OP	CB-CA	-2.08	1.40	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	401	2OP	O-C-CA-CB
6	R	401	2OP	OXT-C-CA-CB
6	R	401	2OP	O-C-CA-OHN
6	R	401	2OP	OXT-C-CA-OHN

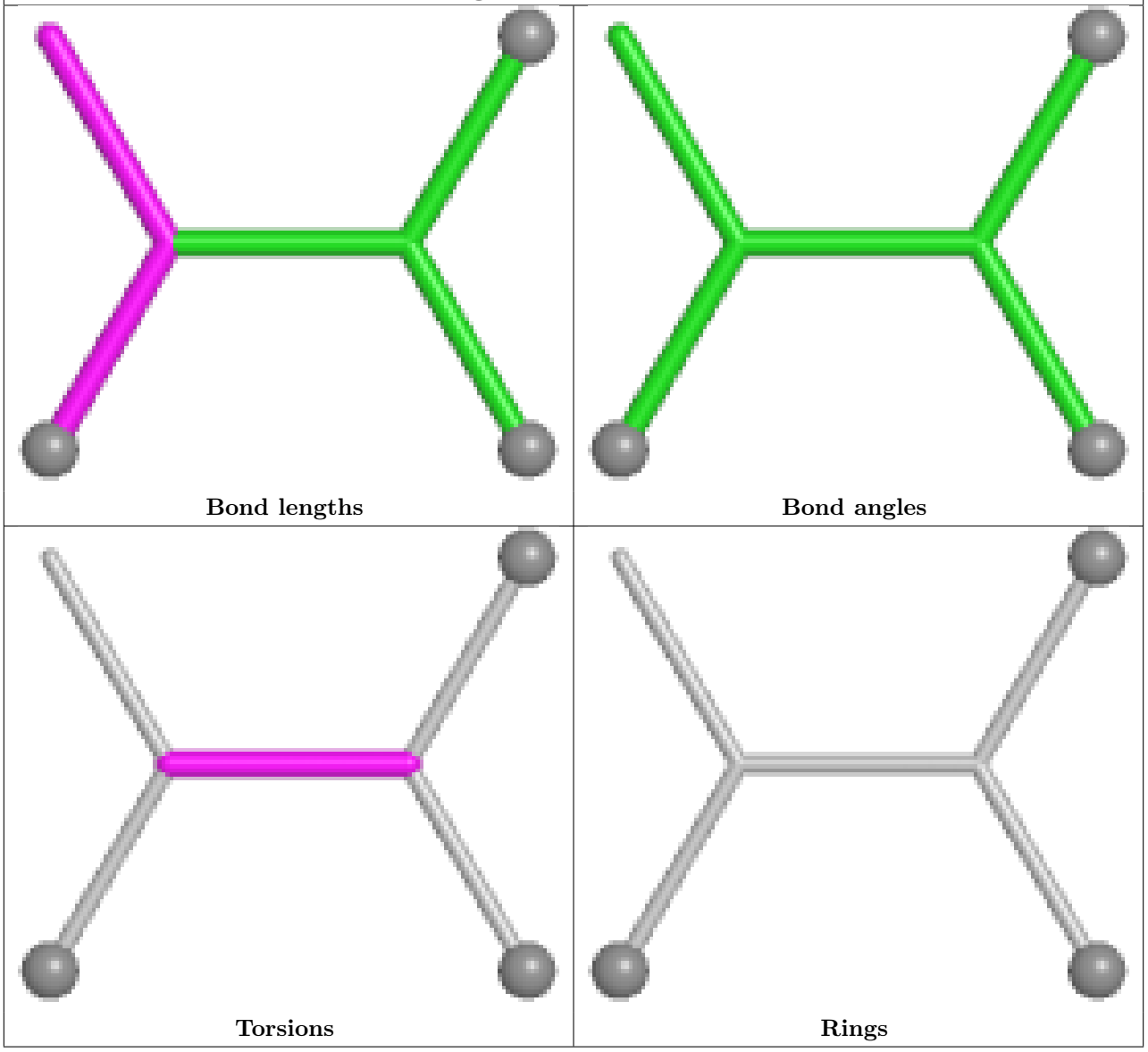
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	401	2OP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 2OP R 401



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.