



Full wwPDB EM Validation Report ⓘ

May 6, 2026 – 12:10 AM JST

PDB ID : 9JKX / pdb_00009jkx
EMDB ID : EMD-61573
Title : acifran-HCAR3-Gi complex
Authors : Binghao, Z.; Fang, Y.
Deposited on : 2024-09-17
Resolution : 3.18 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

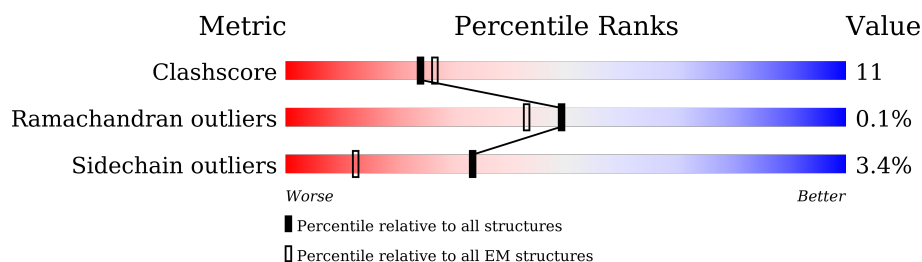
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	387	
2	C	351	
3	B	337	
4	G	56	
5	S	247	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8574 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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	285	Total	C	N	O	S	0	0
			2121	1401	360	343	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	215	Total	C	N	O	S	0	0
			1701	1083	288	318	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	203	ALA	GLY	engineered mutation	UNP P63096
C	326	SER	ALA	engineered mutation	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
3	B	337	Total	C	N	O	S	0	0
			2574	1589	460	504	21		

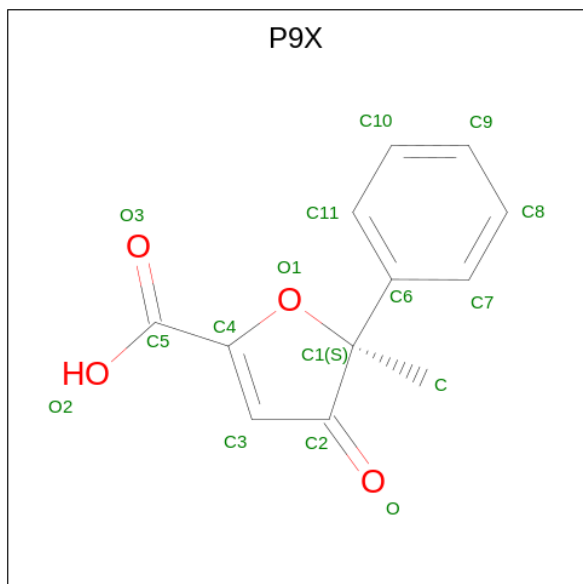
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	56	Total	C	N	O	S	0	0
			390	244	67	76	3		

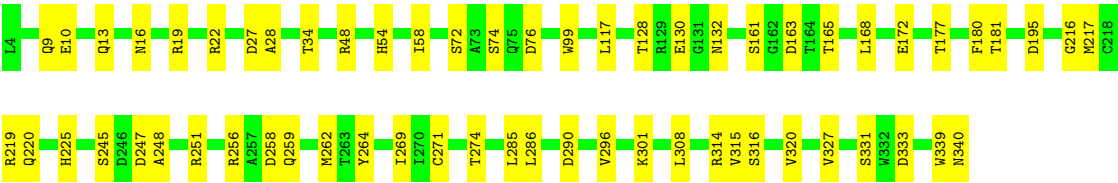
- Molecule 5 is a protein called ScFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	233	1772	1128	296	338	10	0	0

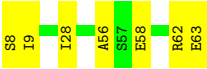
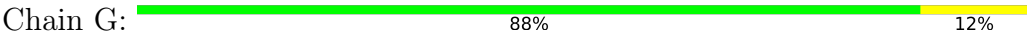
- Molecule 6 is (5 {S})-5-methyl-4-oxidanylidene-5-phenyl-furan-2-carboxylic acid (CCD ID: P9X) (formula: C₁₂H₁₀O₄) (labeled as "Ligand of Interest" by depositor).



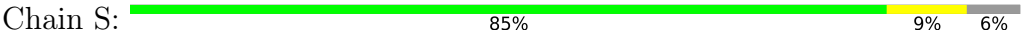
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	A	1	16	12	4	0



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



- Molecule 5: ScFv16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	375522	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 ($e^-/\text{\AA}^2$)	3.19	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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: P9X

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	0.53	0/2181	1.11	23/2983 (0.8%)
2	C	0.11	0/1729	0.30	0/2321
3	B	0.11	0/2621	0.27	0/3555
4	G	0.12	0/396	0.31	0/541
5	S	0.13	0/1816	0.91	6/2465 (0.2%)
All	All	0.28	0/8743	0.73	29/11865 (0.2%)

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
1	A	0	2

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	221	ALA	N-CA-C	36.21	149.81	111.07
1	A	284	TYR	N-CA-C	15.59	131.56	112.54
1	A	283	THR	CB-CA-C	12.75	131.90	110.74
5	S	221	ALA	CB-CA-C	-11.73	92.47	110.88
1	A	107	PHE	CB-CA-C	-11.34	93.50	110.96
5	S	223	ASP	N-CA-C	9.76	124.73	113.02
1	A	285	MET	N-CA-C	-8.59	100.94	111.33
1	A	180	PHE	N-CA-C	-8.41	96.02	109.39
1	A	36	LEU	N-CA-C	-8.38	102.23	111.36
1	A	181	SER	N-CA-C	-8.00	96.24	108.96
5	S	222	GLU	N-CA-CB	-8.00	96.39	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	LEU	N-CA-C	-7.80	102.77	111.82
1	A	89	ARG	CB-CA-C	-7.32	98.15	110.81
5	S	223	ASP	N-CA-CB	-7.23	99.99	110.47
1	A	284	TYR	N-CA-CB	-7.00	98.78	110.39
1	A	180	PHE	CB-CA-C	-6.96	100.80	112.00
1	A	198	PHE	CA-CB-CG	-6.02	107.78	113.80
5	S	222	GLU	CB-CA-C	5.96	122.32	110.17
1	A	87	TYR	N-CA-C	-5.95	104.73	112.23
1	A	107	PHE	N-CA-C	5.94	117.45	110.97
1	A	281	SER	CB-CA-C	5.78	121.66	110.46
1	A	105	PHE	CB-CA-C	-5.71	101.88	110.90
1	A	193	PHE	CB-CA-C	-5.44	101.76	110.79
1	A	109	MET	CB-CA-C	-5.39	101.52	110.68
1	A	281	SER	N-CA-C	-5.31	104.96	111.75
1	A	82	PHE	N-CA-C	5.22	117.38	111.11
1	A	192	MET	CB-CA-C	-5.17	102.54	110.81
1	A	110	ASN	N-CA-C	-5.07	105.40	111.03
1	A	182	ILE	CB-CA-C	5.04	119.56	111.29

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	89	ARG	Sidechain

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	2121	0	1972	111	0
2	C	1701	0	1671	25	0
3	B	2574	0	2466	36	0
4	G	390	0	354	4	0
5	S	1772	0	1698	11	0
6	A	16	0	0	0	0
All	All	8574	0	8161	181	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 11.

All (181) 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:A:100:CYS:O	1:A:104:LEU:HD22	1.59	1.02
1:A:275:ALA:O	1:A:279:THR:HG23	1.67	0.95
1:A:89:ARG:O	1:A:92:ASP:CG	2.10	0.94
1:A:250:VAL:HG21	1:A:279:THR:HG21	1.55	0.87
1:A:281:SER:O	1:A:284:TYR:HD2	1.59	0.85
1:A:281:SER:O	1:A:284:TYR:CD2	2.32	0.82
1:A:184:HIS:CE1	1:A:258:LEU:HG	2.15	0.81
1:A:274:LEU:HA	1:A:277:PHE:CD2	2.15	0.81
1:A:89:ARG:O	1:A:92:ASP:OD1	1.98	0.80
1:A:35:GLY:O	1:A:38:PHE:HB2	1.84	0.77
1:A:75:LEU:HD23	1:A:109:MET:HE1	1.67	0.77
1:A:285:MET:HA	1:A:288:MET:HE2	1.67	0.74
1:A:89:ARG:O	1:A:92:ASP:OD2	2.05	0.74
2:C:271:LYS:HD3	2:C:323:PHE:HB3	1.71	0.73
1:A:161:HIS:HB3	1:A:189:HIS:CE1	2.28	0.69
1:A:31:PRO:HB2	1:A:32:PRO:HD3	1.76	0.68
2:C:53:MET:HE3	2:C:332:VAL:HG22	1.75	0.68
1:A:93:TRP:CZ3	1:A:100:CYS:SG	2.87	0.68
1:A:36:LEU:HG	1:A:37:GLU:N	2.09	0.67
4:G:58:GLU:N	4:G:58:GLU:OE1	2.28	0.67
1:A:34:LEU:O	1:A:37:GLU:HB2	1.96	0.66
1:A:182:ILE:O	1:A:183:CYS:SG	2.53	0.65
3:B:27:ASP:OD1	3:B:28:ALA:N	2.29	0.65
3:B:130:GLU:OE1	3:B:130:GLU:N	2.30	0.65
3:B:245:SER:OG	3:B:247:ASP:OD1	2.15	0.65
1:A:33:VAL:O	1:A:37:GLU:HG2	1.99	0.63
3:B:271:CYS:HB2	3:B:290:ASP:HB2	1.80	0.63
1:A:93:TRP:N	1:A:93:TRP:CD1	2.64	0.62
2:C:252:SER:O	2:C:256:ASN:ND2	2.32	0.62
1:A:227:LYS:O	1:A:231:THR:HG23	1.99	0.62
4:G:56:ALA:O	4:G:62:ARG:NH1	2.32	0.61
1:A:83:VAL:O	1:A:87:TYR:CD1	2.53	0.61
1:A:274:LEU:HA	1:A:277:PHE:CE2	2.35	0.61
1:A:184:HIS:CE1	1:A:258:LEU:CG	2.84	0.60
4:G:8:SER:OG	4:G:9:ILE:N	2.30	0.60
3:B:74:SER:OG	3:B:76:ASP:OD1	2.17	0.59
1:A:229:ALA:HA	2:C:353:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:O	1:A:158:LEU:HG	2.04	0.58
5:S:22:CYS:HB3	5:S:79:LEU:HB3	1.84	0.58
3:B:9:GLN:HG2	3:B:10:GLU:OE2	2.04	0.58
3:B:22:ARG:O	3:B:259:GLN:NE2	2.37	0.57
1:A:93:TRP:CE3	1:A:100:CYS:SG	2.98	0.57
1:A:277:PHE:HA	1:A:280:LEU:HD12	1.86	0.57
1:A:26:ILE:HA	1:A:29:VAL:HG22	1.87	0.56
5:S:40:ALA:HB3	5:S:43:LYS:HB2	1.87	0.56
1:A:27:ALA:HA	1:A:87:TYR:HD2	1.71	0.56
3:B:16:ASN:OD1	3:B:19:ARG:NH2	2.35	0.56
3:B:320:VAL:HG22	3:B:327:VAL:HG22	1.87	0.55
1:A:93:TRP:N	1:A:93:TRP:HD1	2.03	0.55
1:A:197:PHE:CD2	1:A:248:VAL:HG21	2.41	0.55
1:A:53:CYS:SG	1:A:54:PHE:N	2.80	0.55
3:B:331:SER:OG	3:B:333:ASP:OD1	2.18	0.55
1:A:60:LYS:H	1:A:63:ARG:HB2	1.72	0.55
5:S:142:GLN:NE2	5:S:229:CYS:SG	2.67	0.54
1:A:266:CYS:HA	1:A:269:TYR:HB2	1.88	0.54
2:C:325:CYS:N	2:C:328:ASP:OD2	2.41	0.54
1:A:129:VAL:HG22	2:C:348:LEU:HD21	1.89	0.54
3:B:58:ILE:O	3:B:316:SER:OG	2.25	0.53
3:B:286:LEU:HG	3:B:296:VAL:HG12	1.90	0.53
1:A:251:ARG:HD2	1:A:254:ILE:HD11	1.91	0.53
1:A:271:SER:HA	1:A:274:LEU:HD21	1.91	0.52
2:C:274:PHE:O	2:C:278:ILE:HG22	2.09	0.52
1:A:93:TRP:HZ3	1:A:100:CYS:SG	2.31	0.52
1:A:250:VAL:CG2	1:A:279:THR:HG21	2.34	0.52
3:B:180:PHE:HE1	3:B:216:GLY:HA2	1.75	0.52
2:C:276:GLU:OE2	2:C:279:LYS:HD3	2.10	0.51
1:A:31:PRO:HA	1:A:87:TYR:OH	2.09	0.51
2:C:251:ASP:OD1	2:C:255:ASN:ND2	2.44	0.51
1:A:86:TYR:CD1	1:A:93:TRP:HB3	2.46	0.51
1:A:74:PHE:O	1:A:78:ILE:HG23	2.10	0.50
1:A:45:ASN:ND2	1:A:74:PHE:HD1	2.09	0.50
2:C:48:THR:O	2:C:52:GLN:HG2	2.12	0.50
1:A:38:PHE:HZ	1:A:81:PRO:HA	1.77	0.49
1:A:276:PHE:O	1:A:280:LEU:HD12	2.12	0.49
1:A:177:CYS:SG	1:A:177:CYS:O	2.70	0.49
1:A:285:MET:O	1:A:289:LEU:HB2	2.13	0.48
1:A:91:SER:O	1:A:175:ASN:CB	2.62	0.48
1:A:243:CYS:SG	1:A:286:ASN:HB3	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:138:ILE:HD12	5:S:138:ILE:H	1.78	0.48
3:B:274:THR:OG1	3:B:315:VAL:O	2.25	0.48
1:A:188:TRP:O	1:A:189:HIS:C	2.57	0.48
3:B:262:MET:HB2	3:B:262:MET:HE2	1.73	0.48
1:A:45:ASN:OD1	1:A:46:GLY:N	2.47	0.47
1:A:229:ALA:O	1:A:233:ILE:HG22	2.14	0.47
1:A:246:PRO:O	1:A:250:VAL:HG23	2.14	0.47
1:A:30:LEU:N	1:A:31:PRO:CD	2.77	0.47
3:B:225:HIS:CE1	3:B:251:ARG:HD2	2.50	0.47
1:A:284:TYR:O	1:A:288:MET:HG2	2.15	0.47
1:A:195:LEU:C	1:A:197:PHE:H	2.22	0.47
3:B:172:GLU:OE1	3:B:172:GLU:N	2.46	0.46
1:A:68:ASN:OD1	1:A:148:SER:HB2	2.15	0.46
1:A:107:PHE:O	1:A:110:ASN:N	2.48	0.46
1:A:192:MET:HE2	1:A:192:MET:HB2	1.59	0.46
3:B:195:ASP:OD1	3:B:195:ASP:N	2.41	0.46
1:A:184:HIS:CG	1:A:258:LEU:HD21	2.51	0.46
1:A:198:PHE:O	1:A:199:LEU:C	2.58	0.46
1:A:38:PHE:HZ	1:A:81:PRO:CA	2.29	0.46
1:A:80:LEU:N	1:A:81:PRO:HD2	2.31	0.46
1:A:138:LYS:HB2	1:A:138:LYS:HE2	1.70	0.46
1:A:289:LEU:O	1:A:290:ASP:C	2.59	0.45
3:B:161:SER:OG	3:B:163:ASP:OD1	2.32	0.45
1:A:107:PHE:O	1:A:108:ALA:C	2.59	0.45
1:A:197:PHE:O	1:A:197:PHE:CG	2.69	0.45
1:A:212:ILE:HD12	1:A:230:ILE:HG23	1.98	0.45
2:C:33:GLU:HG2	2:C:195:HIS:HB3	1.98	0.45
5:S:152:GLY:N	5:S:219:LEU:O	2.40	0.45
3:B:48:ARG:HA	3:B:48:ARG:HD3	1.75	0.45
1:A:112:GLN:HE21	1:A:192:MET:CG	2.30	0.45
1:A:250:VAL:O	1:A:254:ILE:HG12	2.17	0.45
3:B:308:LEU:HD12	3:B:339:TRP:CD2	2.53	0.45
1:A:50:TRP:O	1:A:55:HIS:ND1	2.48	0.44
1:A:124:ASP:O	1:A:128:ARG:HG3	2.17	0.44
3:B:165:THR:HG22	3:B:181:THR:HG22	1.98	0.44
3:B:256:ARG:HB3	4:G:28:ILE:HG12	1.99	0.44
1:A:31:PRO:CD	1:A:87:TYR:HE2	2.29	0.44
3:B:264:TYR:HE2	3:B:285:LEU:HD13	1.81	0.44
1:A:100:CYS:C	1:A:104:LEU:HD22	2.37	0.44
1:A:281:SER:O	1:A:284:TYR:CE2	2.70	0.44
1:A:285:MET:O	1:A:289:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:54:HIS:NE2	3:B:72:SER:OG	2.37	0.44
2:C:299:ALA:C	2:C:301:ALA:H	2.25	0.44
3:B:128:THR:OG1	3:B:132:ASN:O	2.36	0.44
1:A:184:HIS:CE1	1:A:258:LEU:CD2	3.01	0.44
1:A:31:PRO:CB	1:A:32:PRO:HD3	2.47	0.44
1:A:18:CYS:SG	1:A:182:ILE:O	2.76	0.43
1:A:133:HIS:HE1	2:C:343:ILE:HD12	1.83	0.43
1:A:181:SER:O	1:A:182:ILE:C	2.60	0.43
1:A:197:PHE:CG	1:A:248:VAL:HG21	2.53	0.43
3:B:10:GLU:O	3:B:13:GLN:HG3	2.19	0.43
3:B:168:LEU:HD23	3:B:177:THR:HB	2.00	0.43
1:A:282:PHE:O	1:A:283:THR:C	2.60	0.43
1:A:108:ALA:C	1:A:159:THR:HG21	2.43	0.43
1:A:38:PHE:CZ	1:A:80:LEU:HB3	2.54	0.43
3:B:248:ALA:HB1	3:B:269:ILE:HG22	2.01	0.43
1:A:66:LEU:HD22	1:A:295:TYR:CE1	2.54	0.43
3:B:220:GLN:NE2	3:B:258:ASP:OD1	2.50	0.43
1:A:85:ASP:O	1:A:89:ARG:HG2	2.19	0.43
3:B:217:MET:HE3	3:B:219:ARG:HH21	1.82	0.43
3:B:290:ASP:HA	3:B:314:ARG:HG2	2.00	0.43
2:C:254:CYS:SG	2:C:317:LYS:NZ	2.73	0.43
1:A:257:LEU:HA	1:A:260:THR:OG1	2.19	0.43
2:C:315:ASP:OD1	2:C:315:ASP:N	2.46	0.42
3:B:340:ASN:O	3:B:340:ASN:ND2	2.46	0.42
1:A:205:LEU:HD12	1:A:205:LEU:HA	1.91	0.42
1:A:284:TYR:CD2	1:A:284:TYR:N	2.60	0.42
1:A:161:HIS:HD2	1:A:189:HIS:CG	2.37	0.42
1:A:36:LEU:O	1:A:37:GLU:C	2.63	0.42
2:C:8:GLU:OE2	5:S:175:TYR:OH	2.36	0.42
2:C:224:CYS:SG	2:C:269:ASN:ND2	2.92	0.42
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.79	0.42
1:A:225:LYS:NZ	2:C:349:LYS:HB2	2.35	0.42
2:C:210:LYS:HD3	2:C:210:LYS:HA	1.78	0.42
2:C:276:GLU:OE2	2:C:276:GLU:HA	2.20	0.42
1:A:108:ALA:HB1	1:A:159:THR:HG22	2.01	0.41
1:A:112:GLN:HE21	1:A:192:MET:HG3	1.84	0.41
1:A:288:MET:O	1:A:291:PRO:HG2	2.20	0.41
3:B:99:TRP:HB3	3:B:117:LEU:HD12	2.02	0.41
1:A:90:ARG:HD3	1:A:90:ARG:HA	1.65	0.41
1:A:284:TYR:O	1:A:285:MET:C	2.63	0.41
2:C:268:LEU:HD12	2:C:323:PHE:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:HB3	1:A:92:ASP:OD2	2.20	0.41
1:A:94:LYS:HB2	1:A:95:PHE:H	1.55	0.41
1:A:109:MET:HE2	1:A:109:MET:HB3	1.64	0.41
2:C:233:VAL:HA	2:C:241:ASN:HB3	2.02	0.41
1:A:289:LEU:HA	1:A:289:LEU:HD12	1.81	0.41
2:C:48:THR:HA	2:C:51:LYS:HG2	2.02	0.41
2:C:313:ARG:CZ	2:C:313:ARG:HB2	2.50	0.41
2:C:325:CYS:SG	2:C:326:SER:N	2.91	0.41
3:B:76:ASP:OD1	3:B:76:ASP:N	2.53	0.41
5:S:165:LEU:HD23	5:S:233:LEU:HD12	2.03	0.41
1:A:115:ILE:HD11	1:A:244:PHE:CE1	2.56	0.41
5:S:64:VAL:HA	5:S:67:ARG:HH21	1.86	0.41
5:S:82:GLN:OE1	5:S:83:MET:N	2.54	0.41
3:B:34:THR:O	3:B:301:LYS:NZ	2.53	0.41
5:S:219:LEU:HD12	5:S:220:GLU:N	2.36	0.40
1:A:31:PRO:HD3	1:A:87:TYR:HE2	1.87	0.40
1:A:184:HIS:CE1	1:A:258:LEU:HD21	2.56	0.40
1:A:45:ASN:OD1	1:A:45:ASN:C	2.64	0.40
5:S:222:GLU:H	5:S:222:GLU:HG3	1.48	0.40
1:A:245:LEU:O	1:A:249:VAL:HG23	2.20	0.40
1:A:104:LEU:O	1:A:107:PHE:HB2	2.21	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	283/387 (73%)	241 (85%)	41 (14%)	1 (0%)	30	60
2	C	209/351 (60%)	204 (98%)	5 (2%)	0	100	100
3	B	335/337 (99%)	329 (98%)	6 (2%)	0	100	100
4	G	54/56 (96%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	229/247 (93%)	218 (95%)	11 (5%)	0	100	100
All	All	1110/1378 (81%)	1044 (94%)	65 (6%)	1 (0%)	49	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	TRP

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	202/349 (58%)	176 (87%)	26 (13%)	4	18
2	C	182/304 (60%)	181 (100%)	1 (0%)	81	83
3	B	276/280 (99%)	276 (100%)	0	100	100
4	G	35/46 (76%)	34 (97%)	1 (3%)	37	64
5	S	190/200 (95%)	188 (99%)	2 (1%)	65	77
All	All	885/1179 (75%)	855 (97%)	30 (3%)	33	61

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	80	LEU
1	A	81	PRO
1	A	83	VAL
1	A	89	ARG
1	A	90	ARG
1	A	92	ASP
1	A	93	TRP
1	A	94	LYS
1	A	102	LEU
1	A	104	LEU

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Mol	Chain	Res	Type
1	A	106	MET
1	A	109	MET
1	A	110	ASN
1	A	111	ARG
1	A	184	HIS
1	A	192	MET
1	A	193	PHE
1	A	195	LEU
1	A	199	LEU
1	A	201	LEU
1	A	223	HIS
1	A	274	LEU
1	A	284	TYR
1	A	286	ASN
1	A	289	LEU
2	C	294	ASN
4	G	63	GLU
5	S	192	MET
5	S	235	TYR

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

Mol	Chain	Res	Type
1	A	112	GLN
1	A	161	HIS
1	A	189	HIS
2	C	195	HIS
2	C	244	HIS
2	C	255	ASN
2	C	306	GLN
2	C	331	ASN
3	B	44	GLN
3	B	91	HIS
5	S	171	ASN

5.3.3 RNA ⓘ

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	P9X	A	401	-	16,17,17	5.31	8 (50%)	16,25,25	2.48	8 (50%)

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	P9X	A	401	-	-	5/10/25/25	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	401	P9X	C1-C2	-15.19	1.40	1.54
6	A	401	P9X	C3-C4	9.74	1.51	1.35
6	A	401	P9X	O1-C4	7.78	1.52	1.36
6	A	401	P9X	C1-C6	-5.19	1.44	1.53
6	A	401	P9X	C3-C2	-3.97	1.37	1.44
6	A	401	P9X	C8-C9	-2.37	1.31	1.38
6	A	401	P9X	C8-C7	-2.13	1.34	1.38
6	A	401	P9X	O2-C5	-2.08	1.24	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	401	P9X	C3-C4-C5	-4.54	123.45	132.57
6	A	401	P9X	O-C2-C3	-4.32	120.03	128.86
6	A	401	P9X	C-C1-C2	4.29	116.28	110.13
6	A	401	P9X	C10-C11-C6	-3.14	117.46	120.76
6	A	401	P9X	C7-C6-C1	-2.65	116.31	120.62
6	A	401	P9X	C7-C6-C11	2.64	121.91	117.97
6	A	401	P9X	C-C1-C6	-2.32	106.85	113.74
6	A	401	P9X	O1-C1-C2	2.07	106.42	104.89

There are no chirality outliers.

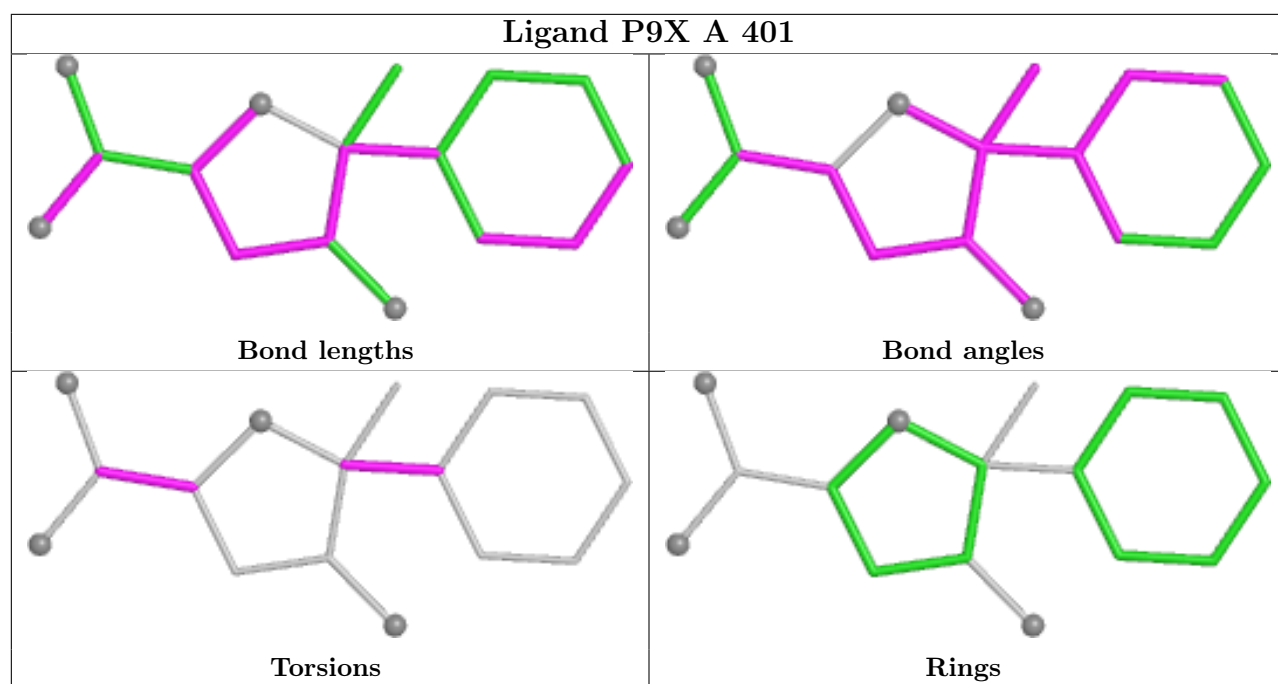
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	P9X	C-C1-C6-C11
6	A	401	P9X	C-C1-C6-C7
6	A	401	P9X	C3-C4-C5-O2
6	A	401	P9X	C2-C1-C6-C11
6	A	401	P9X	C2-C1-C6-C7

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.



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.