



Full wwPDB EM Validation Report ⓘ

Oct 26, 2025 – 12:20 AM JST

PDB ID : 9K07 / pdb_00009k07
EMDB ID : EMD-61941
Title : Cryo-EM structure of the DSO-5a-bound human BRS3-Gq complex
Authors : Li, J.; Li, C.; Zhou, Q.; Han, W.; Fang, M.; Xu, Y.; Mai, Y.; Cui, J.; Xu, H.;
Zhang, Y.; Yin, W.; Wang, M.
Deposited on : 2024-10-15
Resolution : 2.83 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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

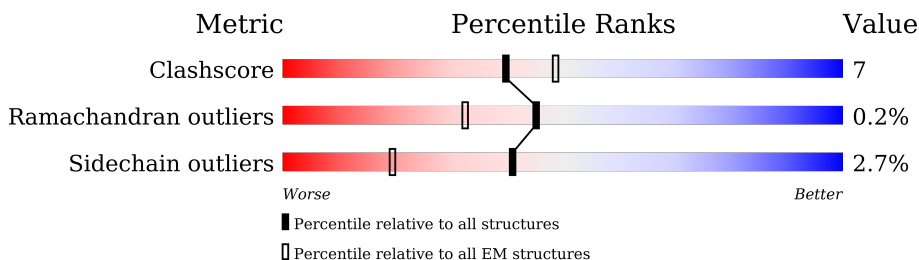
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	R	612	
2	A	246	
3	E	267	
4	B	345	
5	G	70	
6	N	140	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9618 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 Bombesin receptor subtype-3, Oplophorus-luciferin 2-monooxygenase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	273	Total	C	N	O	S	0	0
			2165	1445	349	361	10		

There are 85 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-15	MET	-	initiating methionine	UNP P32247
R	-14	LYS	-	expression tag	UNP P32247
R	-13	THR	-	expression tag	UNP P32247
R	-12	ILE	-	expression tag	UNP P32247
R	-11	ILE	-	expression tag	UNP P32247
R	-10	ALA	-	expression tag	UNP P32247
R	-9	LEU	-	expression tag	UNP P32247
R	-8	SER	-	expression tag	UNP P32247
R	-7	TYR	-	expression tag	UNP P32247
R	-6	ILE	-	expression tag	UNP P32247
R	-5	PHE	-	expression tag	UNP P32247
R	-4	CYS	-	expression tag	UNP P32247
R	-3	LEU	-	expression tag	UNP P32247
R	-2	VAL	-	expression tag	UNP P32247
R	-1	PHE	-	expression tag	UNP P32247
R	0	ALA	-	expression tag	UNP P32247
R	400	GLY	-	linker	UNP P32247
R	401	SER	-	linker	UNP P32247
R	402	SER	-	linker	UNP P32247
R	403	GLY	-	linker	UNP P32247
R	404	GLY	-	linker	UNP P32247
R	405	GLY	-	linker	UNP P32247
R	406	GLY	-	linker	UNP P32247
R	407	SER	-	linker	UNP P32247
R	408	GLY	-	linker	UNP P32247
R	409	GLY	-	linker	UNP P32247
R	410	GLY	-	linker	UNP P32247

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Chain	Residue	Modelled	Actual	Comment	Reference
R	411	GLY	-	linker	UNP P32247
R	412	SER	-	linker	UNP P32247
R	413	SER	-	linker	UNP P32247
R	414	GLY	-	linker	UNP P32247
R	415	VAL	-	linker	UNP P32247
R	419	GLU	ALA	conflict	UNP Q9GV45
R	426	GLU	GLN	conflict	UNP Q9GV45
R	430	ALA	GLY	conflict	UNP Q9GV45
R	433	LEU	GLN	conflict	UNP Q9GV45
R	442	VAL	LEU	conflict	UNP Q9GV45
R	446	LEU	PHE	conflict	UNP Q9GV45
R	448	ASN	ALA	conflict	UNP Q9GV45
R	450	ALA	GLY	conflict	UNP Q9GV45
R	458	ARG	LYS	conflict	UNP Q9GV45
R	459	ILE	VAL	conflict	UNP Q9GV45
R	461	ARG	LEU	conflict	UNP Q9GV45
R	466	ALA	GLY	conflict	UNP Q9GV45
R	469	ILE	ALA	conflict	UNP Q9GV45
R	482	ALA	GLY	conflict	UNP Q9GV45
R	483	ASP	PHE	conflict	UNP Q9GV45
R	486	ALA	GLY	conflict	UNP Q9GV45
R	487	GLN	LEU	conflict	UNP Q9GV45
R	490	GLU	MET	conflict	UNP Q9GV45
R	491	VAL	ILE	conflict	UNP Q9GV45
R	505	VAL	ILE	conflict	UNP Q9GV45
R	508	PRO	HIS	conflict	UNP Q9GV45
R	522	LEU	ILE	conflict	UNP Q9GV45
R	523	ASN	ASP	conflict	UNP Q9GV45
R	530	GLU	PRO	conflict	UNP Q9GV45
R	539	LYS	GLN	conflict	UNP Q9GV45
R	553	ILE	TYR	conflict	UNP Q9GV45
R	559	THR	ASN	conflict	UNP Q9GV45
R	564	MET	LEU	conflict	UNP Q9GV45
R	572	SER	-	expression tag	UNP Q9GV45
R	573	GLY	-	expression tag	UNP Q9GV45
R	574	GLY	-	expression tag	UNP Q9GV45
R	575	SER	-	expression tag	UNP Q9GV45
R	576	GLU	-	expression tag	UNP Q9GV45
R	577	ASN	-	expression tag	UNP Q9GV45
R	578	LEU	-	expression tag	UNP Q9GV45
R	579	TYR	-	expression tag	UNP Q9GV45
R	580	PHE	-	expression tag	UNP Q9GV45

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Chain	Residue	Modelled	Actual	Comment	Reference
R	581	GLN	-	expression tag	UNP Q9GV45
R	582	GLY	-	expression tag	UNP Q9GV45
R	583	GLY	-	expression tag	UNP Q9GV45
R	584	SER	-	expression tag	UNP Q9GV45
R	585	ALA	-	expression tag	UNP Q9GV45
R	586	GLY	-	expression tag	UNP Q9GV45
R	587	SER	-	expression tag	UNP Q9GV45
R	588	ALA	-	expression tag	UNP Q9GV45
R	589	HIS	-	expression tag	UNP Q9GV45
R	590	HIS	-	expression tag	UNP Q9GV45
R	591	HIS	-	expression tag	UNP Q9GV45
R	592	HIS	-	expression tag	UNP Q9GV45
R	593	HIS	-	expression tag	UNP Q9GV45
R	594	HIS	-	expression tag	UNP Q9GV45
R	595	HIS	-	expression tag	UNP Q9GV45
R	596	HIS	-	expression tag	UNP Q9GV45

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	212	Total	C	N	O	S	0	0
			1655	1053	292	303	7		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	CYS	conflict	UNP P04899
A	31	ARG	ALA	conflict	UNP P04899
A	33	THR	GLU	conflict	UNP P04899
A	34	LEU	VAL	conflict	UNP P04899
A	35	ARG	LYS	conflict	UNP P04899
A	42	ASP	GLY	conflict	UNP P63092
A	43	ASN	GLU	conflict	UNP P63092
A	58	GLY	-	linker	UNP P63092
A	59	GLY	-	linker	UNP P63092
A	60	SER	-	linker	UNP P63092
A	61	GLY	-	linker	UNP P63092
A	62	GLY	-	linker	UNP P63092
A	63	SER	-	linker	UNP P63092
A	64	GLY	-	linker	UNP P63092
A	65	GLY	-	linker	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
A	111	ASP	ALA	conflict	UNP P63092
A	114	ASP	SER	conflict	UNP P63092
A	124	ASP	LEU	conflict	UNP P63092
A	195	LYS	ASP	conflict	UNP P63092
A	198	VAL	LEU	conflict	UNP P63092
A	199	ASP	ARG	conflict	UNP P63092
A	210	ILE	TYR	conflict	UNP P63092
A	224	ALA	ILE	conflict	UNP P63092
A	227	ILE	VAL	conflict	UNP P63092
A	232	LYS	ARG	conflict	UNP P63092
A	236	LEU	GLN	conflict	UNP P63092
A	237	GLN	ARG	conflict	UNP P63092
A	239	ASN	HIS	conflict	UNP P63092
A	242	GLU	GLN	conflict	UNP P63092
A	244	ASN	GLU	conflict	UNP P63092
A	246	VAL	LEU	conflict	UNP P63092

- Molecule 3 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	231	Total	C	N	O	S	0	0
			1776	1128	294	344	10		

- 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 P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311

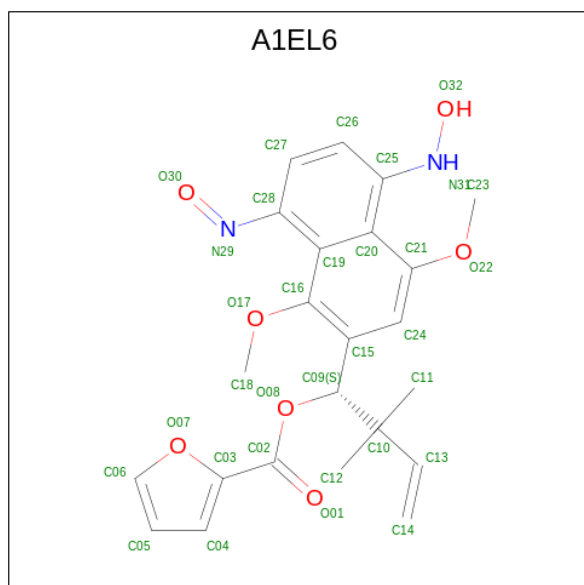
- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

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		

- Molecule 7 is [(1 {S})-1-[1,4-dimethoxy-8-nitroso-5-(oxidanylamino)naphthalen-2-yl]-2,2-dimethyl-but-3-enyl] furan-2-carboxylate (CCD ID: A1EL6) (formula: C₂₃H₂₄N₂O₇) (labeled as "Ligand of Interest" by depositor).

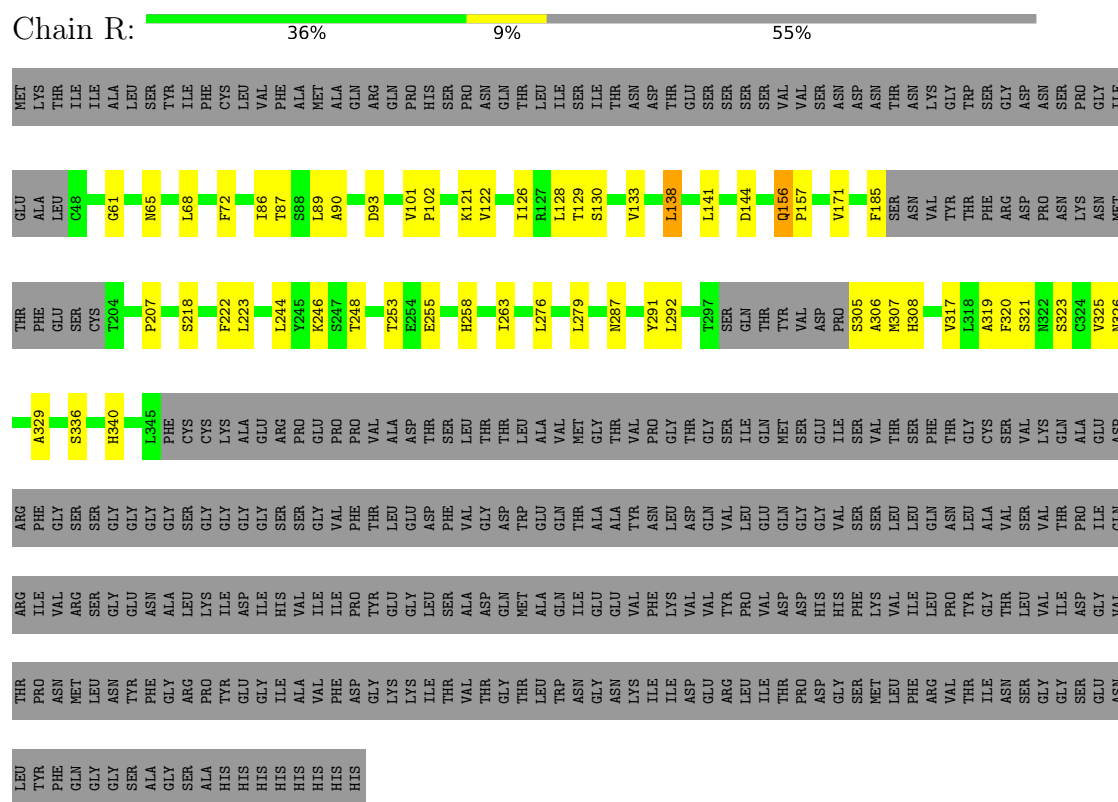


Mol	Chain	Residues	Atoms				AltConf
7	R	1	Total	C	N	O	0
			32	23	2	7	

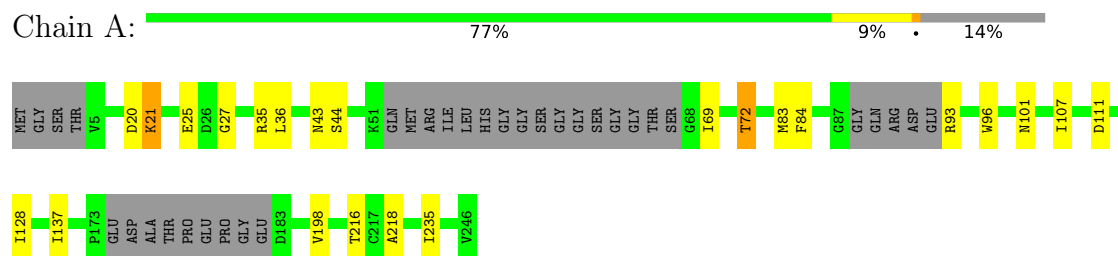
3 Residue-property plots

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: Bombesin receptor subtype-3,Oplophorus-luciferin 2-monooxygenase catalytic subunit

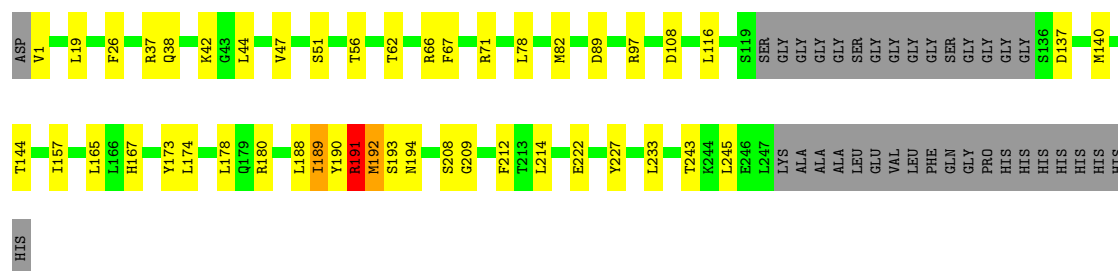


- Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-2,Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



- Molecule 3: scFv16

Chain E:  69% 16% 13%



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

Chain B:  75% 22%



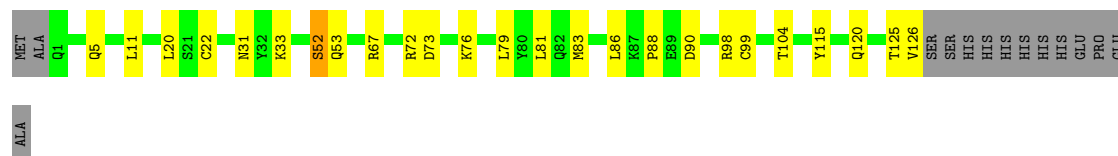
- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:  69% 11% 20%



- Molecule 6: Nanobody-35

Chain N:  72% 17% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	311433	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 10	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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

Bond lengths and bond angles in the following residue types are not validated in this section: A1EL6

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	0.16	0/2219	0.36	1/3019 (0.0%)
2	A	0.16	0/1683	0.27	0/2274
3	E	0.34	2/1820 (0.1%)	0.48	3/2468 (0.1%)
4	B	0.17	0/2647	0.29	0/3589
5	G	0.11	0/435	0.21	0/587
6	N	0.15	0/981	0.27	0/1329
All	All	0.20	2/9785 (0.0%)	0.34	4/13266 (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
3	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	193	SER	CA-CB	-6.16	1.45	1.54
3	E	189	ILE	C-O	-5.35	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	121	LYS	N-CA-C	-7.09	104.49	113.43
3	E	194	ASN	CB-CA-C	6.73	120.80	109.84
3	E	191	ARG	CB-CA-C	5.67	121.70	110.42
3	E	190	TYR	CA-CB-CG	5.31	123.46	113.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	191	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	R	2165	0	2258	33	0
2	A	1655	0	1591	14	0
3	E	1776	0	1716	25	0
4	B	2600	0	2505	51	0
5	G	429	0	441	7	0
6	N	961	0	928	12	0
7	R	32	0	0	1	0
All	All	9618	0	9439	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)
1:R:255:GLU:HB3	2:A:198:VAL:HG11	1.61	0.82
4:B:294:CYS:HB2	4:B:308:LEU:HB2	1.67	0.77
4:B:160:SER:HB3	4:B:190:LEU:HD23	1.69	0.75
4:B:271:CYS:HB2	4:B:290:ASP:HB2	1.68	0.74
2:A:101:ASN:OD1	4:B:57:LYS:NZ	2.23	0.71
3:E:180:ARG:NH1	3:E:222:GLU:O	2.27	0.68
1:R:317:VAL:O	1:R:321:SER:OG	2.11	0.67
4:B:250:CYS:HB2	4:B:264:TYR:HB2	1.80	0.64
2:A:21:LYS:O	2:A:25:GLU:HG2	1.98	0.63
1:R:336:SER:O	1:R:340:HIS:ND1	2.30	0.63
2:A:72:THR:HG23	2:A:83:MET:HB3	1.80	0.63
4:B:274:THR:OG1	4:B:315:VAL:O	2.13	0.62
1:R:248:THR:HG23	1:R:263:ILE:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:290:ASP:OD1	4:B:314:ARG:NE	2.31	0.60
3:E:19:LEU:HG	3:E:82:MET:HE2	1.83	0.60
4:B:8:ARG:HH12	6:N:120:GLN:HB3	1.67	0.59
1:R:89:LEU:HD21	1:R:326:ASN:HB3	1.82	0.59
4:B:256:ARG:HB3	5:G:28:ILE:HG12	1.85	0.58
6:N:73:ASP:OD2	6:N:76:LYS:NZ	2.35	0.58
6:N:52:SER:O	6:N:72:ARG:NH1	2.36	0.58
6:N:11:LEU:HD13	6:N:125:THR:HG23	1.86	0.58
4:B:51:LEU:HB2	4:B:336:LEU:HB2	1.86	0.58
1:R:68:LEU:HD21	1:R:86:ILE:HG22	1.85	0.57
1:R:287:ASN:HB2	1:R:319:ALA:HB2	1.86	0.57
6:N:83:MET:HB3	6:N:86:LEU:HD21	1.84	0.57
3:E:97:ARG:NE	3:E:108:ASP:OD2	2.36	0.57
2:A:96:TRP:HB2	4:B:117:LEU:HD21	1.86	0.57
1:R:61:GLY:O	1:R:65:ASN:ND2	2.36	0.57
4:B:33:ILE:HG22	5:G:38:MET:HE2	1.87	0.57
2:A:27:GLY:HA3	4:B:55:LEU:HD13	1.86	0.56
1:R:72:PHE:CG	1:R:87:THR:HG21	2.40	0.56
2:A:44:SER:HA	2:A:111:ASP:HB2	1.87	0.56
1:R:93:ASP:OD1	1:R:323:SER:HB3	2.06	0.56
3:E:66:ARG:NH2	3:E:89:ASP:OD2	2.29	0.56
4:B:58:ILE:O	4:B:316:SER:OG	2.18	0.56
4:B:30:LEU:HD23	4:B:262:MET:HB2	1.88	0.55
3:E:51:SER:O	3:E:71:ARG:NH1	2.40	0.54
4:B:276:VAL:HG13	4:B:285:LEU:HD11	1.88	0.54
1:R:307:MET:SD	1:R:308:HIS:N	2.82	0.53
4:B:79:LEU:HB2	4:B:93:ILE:HB	1.90	0.53
4:B:101:MET:HE1	4:B:145:TYR:CD1	2.43	0.53
1:R:72:PHE:CD1	1:R:87:THR:HG21	2.44	0.53
1:R:222:PHE:HB2	1:R:292:LEU:HD21	1.91	0.53
3:E:157:ILE:HB	3:E:214:LEU:HB3	1.91	0.52
1:R:156:GLN:H	1:R:157:PRO:HD2	1.74	0.52
2:A:20:ASP:OD1	4:B:89:LYS:NZ	2.42	0.52
1:R:133:VAL:HG23	1:R:171:VAL:HG12	1.93	0.51
2:A:35:ARG:HB3	2:A:84:PHE:HE2	1.76	0.50
3:E:38:GLN:HB2	3:E:44:LEU:HD23	1.93	0.50
6:N:22:CYS:HB3	6:N:79:LEU:HB3	1.93	0.50
6:N:67:ARG:NH1	6:N:90:ASP:OD2	2.32	0.50
6:N:20:LEU:HD12	6:N:81:LEU:HD23	1.94	0.50
2:A:93:ARG:HG3	2:A:96:TRP:CZ2	2.47	0.49
1:R:86:ILE:HD13	1:R:141:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:178:LEU:HD13	3:E:227:TYR:CE2	2.48	0.49
3:E:174:LEU:HD22	3:E:212:PHE:CG	2.48	0.49
1:R:317:VAL:HA	1:R:320:PHE:CZ	2.47	0.49
4:B:331:SER:OG	4:B:332:TRP:N	2.45	0.49
4:B:215:GLU:HB3	4:B:217:MET:SD	2.53	0.48
6:N:88:PRO:HA	6:N:126:VAL:HG21	1.95	0.48
3:E:37:ARG:HG3	3:E:47:VAL:HG21	1.94	0.48
4:B:262:MET:HG2	4:B:264:TYR:CE1	2.48	0.48
4:B:27:ASP:H	5:G:30:VAL:HG12	1.78	0.48
4:B:247:ASP:OD1	4:B:247:ASP:N	2.45	0.48
4:B:147:SER:OG	4:B:187:VAL:O	2.21	0.48
4:B:220:GLN:NE2	4:B:258:ASP:OD1	2.43	0.48
3:E:192:MET:HE2	3:E:192:MET:HB3	1.58	0.48
4:B:294:CYS:SG	4:B:315:VAL:HG11	2.55	0.47
3:E:1:VAL:HG12	3:E:26:PHE:HB3	1.96	0.47
4:B:192:LEU:HD23	4:B:199:PHE:HB3	1.95	0.47
4:B:212:ASP:OD2	4:B:219:ARG:NH1	2.48	0.47
2:A:216:THR:HG22	2:A:218:ALA:H	1.79	0.47
3:E:178:LEU:HB2	3:E:188:LEU:HD11	1.97	0.47
1:R:279:LEU:HD13	1:R:325:VAL:HG21	1.96	0.47
1:R:68:LEU:HD22	1:R:90:ALA:HB2	1.95	0.46
3:E:227:TYR:CE2	3:E:245:LEU:HD13	2.51	0.46
1:R:305:SER:O	1:R:307:MET:N	2.49	0.45
2:A:36:LEU:HD13	2:A:107:ILE:HD11	1.97	0.45
1:R:101:VAL:N	1:R:102:PRO:HD2	2.32	0.45
4:B:155:ASN:HD21	4:B:172:GLU:HB2	1.82	0.45
1:R:126:ILE:HA	1:R:129:THR:HG22	2.00	0.44
4:B:292:PHE:N	4:B:292:PHE:CD1	2.86	0.44
5:G:28:ILE:HD12	5:G:32:LYS:HB3	2.00	0.44
3:E:71:ARG:HB3	3:E:78:LEU:HD12	2.00	0.44
4:B:61:MET:HE2	4:B:61:MET:HB2	1.82	0.44
4:B:145:TYR:O	4:B:162:GLY:N	2.46	0.44
1:R:218:SER:HA	1:R:291:TYR:HE2	1.83	0.43
3:E:140:MET:HE3	3:E:140:MET:HB3	1.85	0.43
1:R:305:SER:OG	1:R:306:ALA:N	2.51	0.43
3:E:51:SER:HB2	3:E:56:THR:HB	1.99	0.43
3:E:208:SER:OG	3:E:209:GLY:N	2.51	0.43
1:R:122:VAL:O	1:R:126:ILE:HG12	2.17	0.43
1:R:276:LEU:HD21	1:R:329:ALA:HB2	2.01	0.43
4:B:165:THR:HG22	4:B:181:THR:HG22	2.01	0.43
1:R:185:PHE:HD2	1:R:207:PRO:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:67:PHE:CE1	3:E:82:MET:HB3	2.53	0.43
1:R:287:ASN:ND2	7:R:601:A1EL6:O07	2.51	0.42
4:B:333:ASP:OD1	4:B:333:ASP:N	2.52	0.42
4:B:9:GLN:O	4:B:12:GLU:HG3	2.19	0.42
4:B:150:ARG:HD3	4:B:150:ARG:HA	1.84	0.42
6:N:53:GLN:OE1	6:N:53:GLN:N	2.52	0.42
1:R:138:LEU:HD11	1:R:326:ASN:ND2	2.35	0.42
3:E:165:LEU:HA	3:E:233:LEU:HD22	2.01	0.42
4:B:279:SER:HB2	4:B:284:LEU:HB2	2.01	0.42
3:E:167:HIS:HB2	3:E:173:TYR:HE2	1.85	0.42
3:E:82:MET:HE1	3:E:116:LEU:HD22	2.00	0.42
4:B:59:TYR:CD1	4:B:101:MET:HB3	2.55	0.42
1:R:144:ASP:OD1	1:R:144:ASP:C	2.63	0.41
4:B:48:ARG:HE	4:B:340:ASN:HB3	1.85	0.41
4:B:323:ASP:OD1	4:B:323:ASP:N	2.52	0.41
4:B:236:PRO:HB2	5:G:40:TYR:CE2	2.56	0.41
1:R:244:LEU:HD23	1:R:244:LEU:HA	1.90	0.41
4:B:123:ILE:O	4:B:136:SER:N	2.39	0.41
4:B:258:ASP:HB3	5:G:27:ARG:HD3	2.02	0.41
4:B:180:PHE:CE1	4:B:216:GLY:HA2	2.56	0.41
6:N:33:LYS:O	6:N:99:CYS:HB2	2.21	0.41
3:E:137:ASP:OD1	3:E:137:ASP:N	2.53	0.41
3:E:144:THR:O	3:E:243:THR:HG22	2.20	0.41
5:G:14:LYS:HE3	5:G:14:LYS:HB3	1.83	0.41
1:R:130:SER:HA	1:R:133:VAL:HG12	2.03	0.41
1:R:320:PHE:CD2	1:R:320:PHE:C	2.98	0.41
2:A:101:ASN:HA	2:A:137:ILE:HD11	2.02	0.40
4:B:214:ARG:NH1	4:B:214:ARG:HG3	2.36	0.40
4:B:251:ARG:NH1	4:B:260:GLU:OE2	2.43	0.40
4:B:312:ASP:OD2	4:B:312:ASP:C	2.64	0.40
4:B:134:ARG:HG2	4:B:134:ARG:HH11	1.87	0.40
2:A:43:ASN:OD1	2:A:43:ASN:C	2.65	0.40
4:B:161:SER:OG	4:B:162:GLY:N	2.55	0.40
4:B:245:SER:OG	4:B:246:ASP:N	2.54	0.40
3:E:42:LYS:HE2	3:E:42:LYS:HB2	1.94	0.40
6:N:98:ARG:O	6:N:115:TYR:OH	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	267/612 (44%)	247 (92%)	18 (7%)	2 (1%)	19	36
2	A	204/246 (83%)	201 (98%)	3 (2%)	0	100	100
3	E	227/267 (85%)	216 (95%)	11 (5%)	0	100	100
4	B	336/345 (97%)	327 (97%)	9 (3%)	0	100	100
5	G	54/70 (77%)	53 (98%)	1 (2%)	0	100	100
6	N	124/140 (89%)	120 (97%)	4 (3%)	0	100	100
All	All	1212/1680 (72%)	1164 (96%)	46 (4%)	2 (0%)	45	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	156	GLN
1	R	253	THR

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	R	240/531 (45%)	235 (98%)	5 (2%)	48	72
2	A	169/213 (79%)	164 (97%)	5 (3%)	36	61
3	E	195/216 (90%)	191 (98%)	4 (2%)	48	72
4	B	281/287 (98%)	272 (97%)	9 (3%)	34	59
5	G	45/57 (79%)	44 (98%)	1 (2%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	N	104/116 (90%)	100 (96%)	4 (4%)	28 53
All	All	1034/1420 (73%)	1006 (97%)	28 (3%)	41 65

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	128	LEU
1	R	138	LEU
1	R	223	LEU
1	R	246	LYS
1	R	258	HIS
2	A	21	LYS
2	A	69	ILE
2	A	72	THR
2	A	128	ILE
2	A	235	ILE
3	E	62	THR
3	E	189	ILE
3	E	191	ARG
3	E	192	MET
4	B	27	ASP
4	B	46	ARG
4	B	118	ASP
4	B	175	GLN
4	B	176	GLN
4	B	215	GLU
4	B	275	SER
4	B	331	SER
4	B	336	LEU
5	G	47	GLU
6	N	5	GLN
6	N	31	ASN
6	N	52	SER
6	N	104	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	344	GLN
2	A	123	ASN
2	A	223	ASN

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Mol	Chain	Res	Type
2	A	244	ASN
3	E	2	GLN
3	E	81	GLN
4	B	175	GLN
6	N	82	GLN

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
7	A1EL6	R	601	-	27,34,34	1.73	3 (11%)	32,49,49	2.47	14 (43%)

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
7	A1EL6	R	601	-	-	14/25/29/29	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	601	A1EL6	C15-C09	6.53	1.59	1.51
7	R	601	A1EL6	C16-C15	3.73	1.40	1.37
7	R	601	A1EL6	C25-C20	2.49	1.46	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	601	A1EL6	O08-C02-C03	7.53	127.71	113.41
7	R	601	A1EL6	C16-C15-C09	6.05	128.42	119.73
7	R	601	A1EL6	O08-C02-O01	-4.00	117.00	123.53
7	R	601	A1EL6	C19-C28-N29	3.40	127.47	119.40
7	R	601	A1EL6	C15-C16-C19	2.99	125.38	122.73
7	R	601	A1EL6	C21-C24-C15	2.75	123.78	120.75
7	R	601	A1EL6	C26-C25-C20	-2.53	117.61	120.27
7	R	601	A1EL6	C11-C10-C09	2.45	111.95	108.62
7	R	601	A1EL6	O22-C21-C24	-2.40	119.06	123.34
7	R	601	A1EL6	C12-C10-C09	2.33	111.78	108.62
7	R	601	A1EL6	C04-C05-C06	-2.32	104.66	112.92
7	R	601	A1EL6	O30-N29-C28	2.32	122.36	114.95
7	R	601	A1EL6	C09-O08-C02	2.26	119.84	117.29
7	R	601	A1EL6	O17-C16-C19	-2.09	116.14	120.30

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	601	A1EL6	C15-C09-C10-C11
7	R	601	A1EL6	O08-C09-C10-C11
7	R	601	A1EL6	C15-C09-C10-C12
7	R	601	A1EL6	O08-C09-C10-C12
7	R	601	A1EL6	C15-C09-C10-C13
7	R	601	A1EL6	O08-C09-C10-C13
7	R	601	A1EL6	C19-C28-N29-O30
7	R	601	A1EL6	C27-C28-N29-O30
7	R	601	A1EL6	C20-C21-O22-C23
7	R	601	A1EL6	C24-C21-O22-C23
7	R	601	A1EL6	C11-C10-C13-C14

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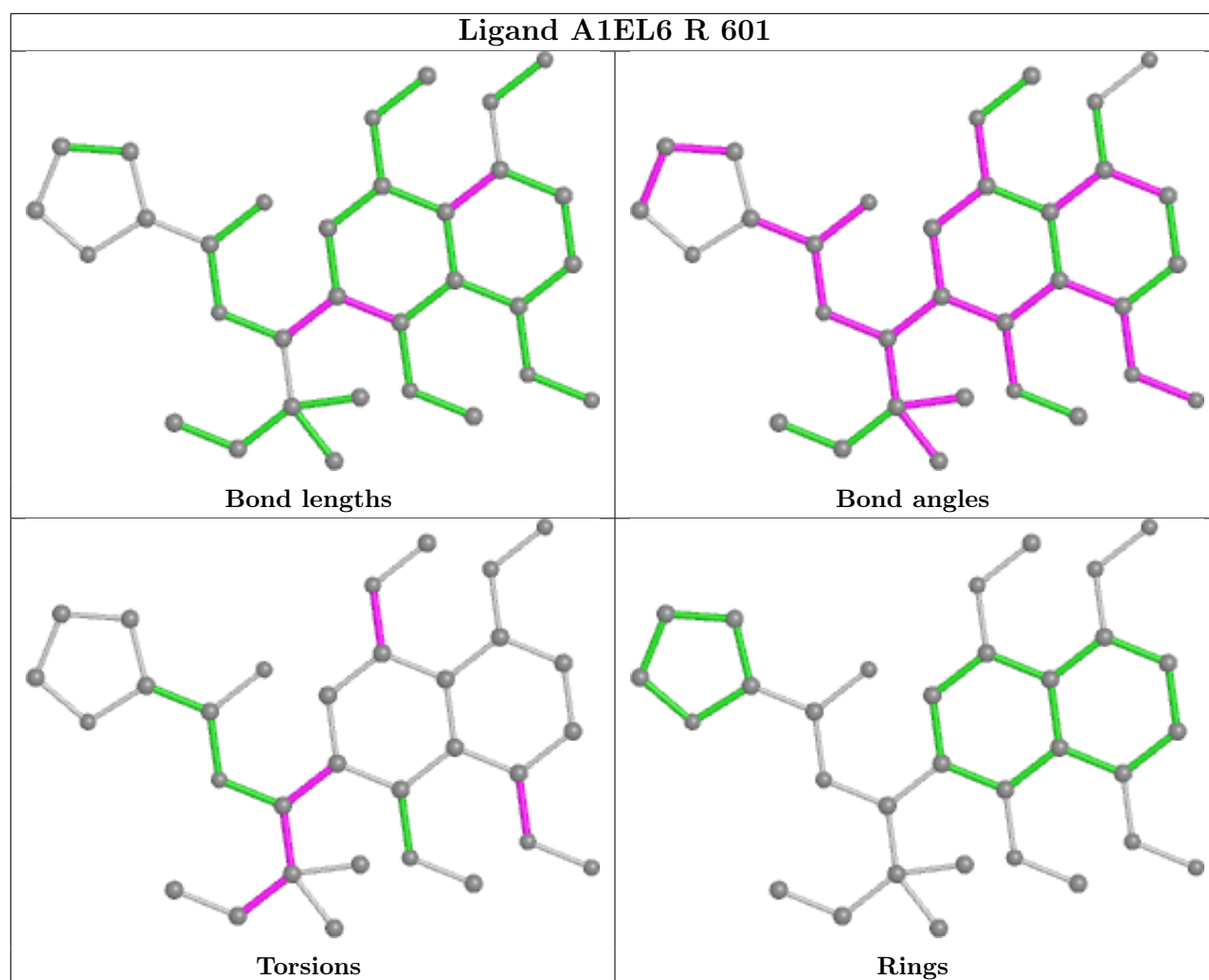
Mol	Chain	Res	Type	Atoms
7	R	601	A1EL6	C09-C10-C13-C14
7	R	601	A1EL6	O08-C09-C15-C16
7	R	601	A1EL6	C12-C10-C13-C14

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	601	A1EL6	1	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 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.