



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 11:15 AM JST

PDB ID : 8KFY
EMDB ID : EMD-37208
Title : Gi bound CCR8 complex with nonpeptide agonist ZK 756326
Authors : Jiang, S.; Lin, X.; Wu, L.J.; Xu, F.
Deposited on : 2023-08-16
Resolution : 3.06 Å(reported)

This is a wwPDB EM Validation Summary 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	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.39

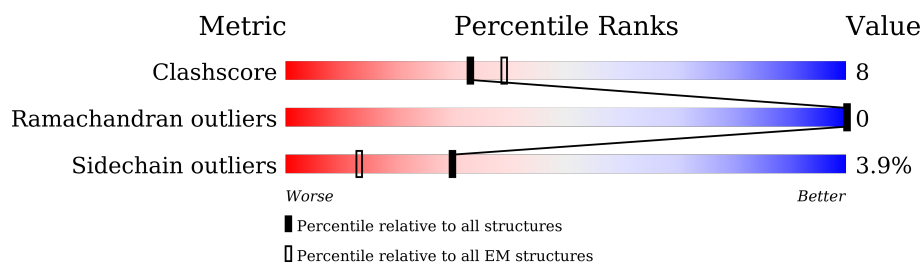
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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	A	354	
2	B	366	
3	C	71	
4	R	575	
5	S	297	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8992 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1812	1151	301	346	14		

There are 3 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	326	SER	ALA	conflict	UNP P63096

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

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

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	341	GLY	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	354	SER	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	VAL	-	expression tag	UNP P62873
B	357	SER	-	expression tag	UNP P62873
B	358	GLY	-	expression tag	UNP P62873
B	359	TRP	-	expression tag	UNP P62873
B	360	ARG	-	expression tag	UNP P62873
B	361	LEU	-	expression tag	UNP P62873
B	362	PHE	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	LYS	-	expression tag	UNP P62873
B	365	ILE	-	expression tag	UNP P62873
B	366	SER	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

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

- Molecule 4 is a protein called C-C chemokine receptor type 8,Fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	288	Total	C	N	O	S	0	0
			2342	1578	364	382	18		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-26	MET	-	initiating methionine	UNP P51685
R	-25	LYS	-	expression tag	UNP P51685
R	-24	THR	-	expression tag	UNP P51685
R	-23	ILE	-	expression tag	UNP P51685
R	-22	ILE	-	expression tag	UNP P51685
R	-21	ALA	-	expression tag	UNP P51685
R	-20	LEU	-	expression tag	UNP P51685
R	-19	SER	-	expression tag	UNP P51685
R	-18	TYR	-	expression tag	UNP P51685
R	-17	ILE	-	expression tag	UNP P51685
R	-16	PHE	-	expression tag	UNP P51685
R	-15	CYS	-	expression tag	UNP P51685

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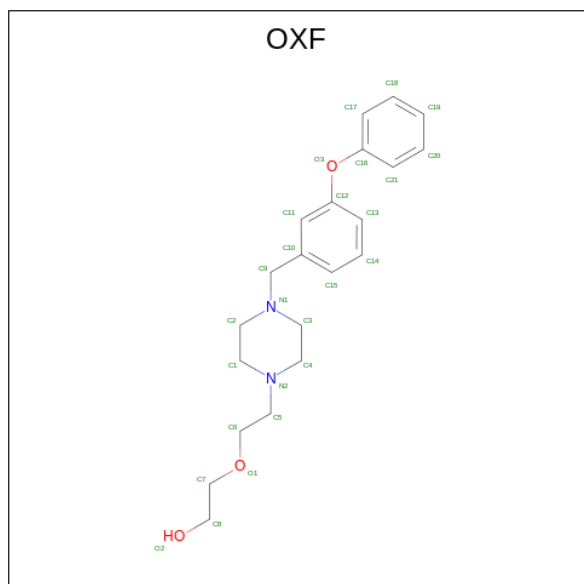
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Chain	Residue	Modelled	Actual	Comment	Reference
R	-14	LEU	-	expression tag	UNP P51685
R	-13	VAL	-	expression tag	UNP P51685
R	-12	PHE	-	expression tag	UNP P51685
R	-11	ALA	-	expression tag	UNP P51685
R	-10	ASP	-	expression tag	UNP P51685
R	-9	TYR	-	expression tag	UNP P51685
R	-8	LYS	-	expression tag	UNP P51685
R	-7	ASP	-	expression tag	UNP P51685
R	-6	ASP	-	expression tag	UNP P51685
R	-5	ASP	-	expression tag	UNP P51685
R	-4	ASP	-	expression tag	UNP P51685
R	-3	ALA	-	expression tag	UNP P51685
R	-2	GLY	-	expression tag	UNP P51685
R	-1	ARG	-	expression tag	UNP P51685
R	0	ALA	-	expression tag	UNP P51685

- Molecule 5 is a protein called scFv16.

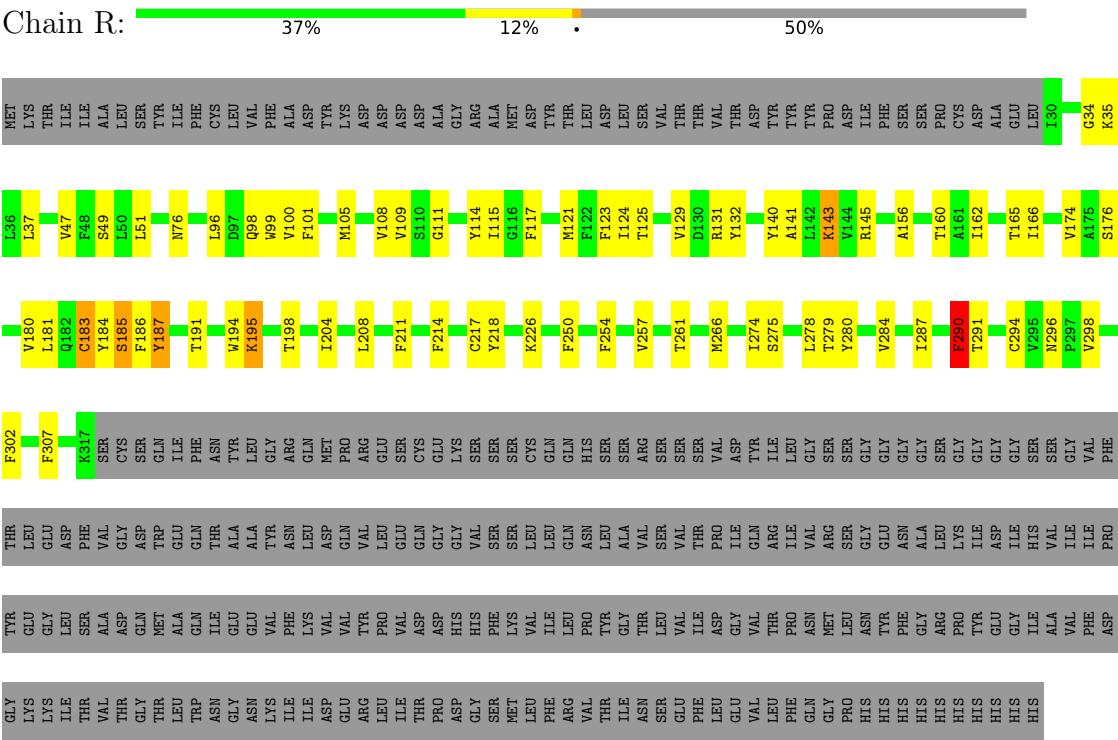
Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	232	Total	C	N	O	S	0	0
			1783	1131	295	347	10		

- Molecule 6 is 2-[2-[4-[(3-phenoxyphenyl)methyl]piperazin-1-yl]ethoxy]ethanol (three-letter code: OXF) (formula: C₂₁H₂₈N₂O₃) (labeled as "Ligand of Interest" by depositor).

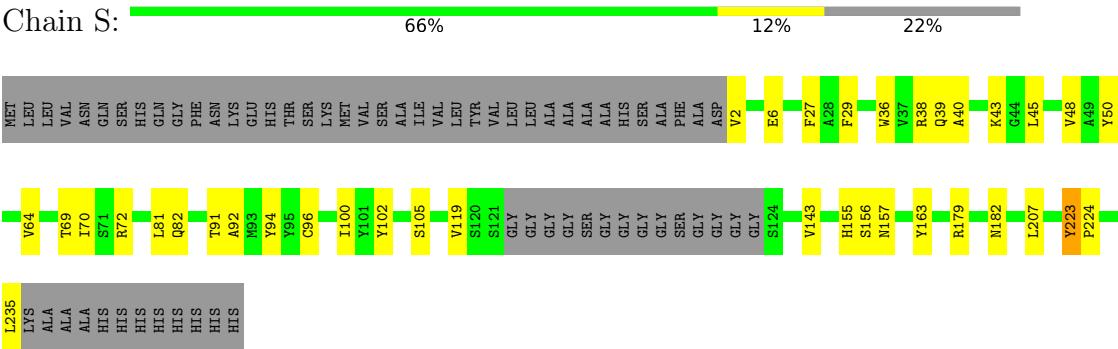


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	R	1	26	21	2	3	0

● Molecule 4: C-C chemokine receptor type 8,Fusion protein



● Molecule 5: scFv16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124576	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/1842	0.45	0/2472
2	B	0.28	0/2647	0.52	0/3589
3	C	0.27	0/435	0.44	0/587
4	R	0.28	0/2403	0.43	0/3265
5	S	0.29	0/1827	0.49	0/2477
All	All	0.28	0/9154	0.47	0/12390

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
4	R	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	R	290	PHE	Peptide

5.2 Too-close contacts [i](#)

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	1812	0	1798	38	0
2	B	2600	0	2505	42	0
3	C	429	0	441	8	0
4	R	2342	0	2443	45	0
5	S	1783	0	1717	24	0
6	R	26	0	0	0	0
All	All	8992	0	8904	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 146 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:33:GLU:HG3	1:A:195:HIS:HB2	1.64	0.79
4:R:111:GLY:O	4:R:115:ILE:HG13	1.93	0.69
1:A:23:LEU:HD22	2:B:78:LYS:HD3	1.75	0.68
1:A:335:VAL:O	1:A:339:VAL:HG23	1.94	0.67
1:A:271:LYS:HD2	1:A:323:PHE:HB3	1.78	0.66

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	221/354 (62%)	219 (99%)	2 (1%)	0	100	100
2	B	336/366 (92%)	326 (97%)	10 (3%)	0	100	100
3	C	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
4	R	286/575 (50%)	286 (100%)	0	0	100	100
5	S	228/297 (77%)	222 (97%)	6 (3%)	0	100	100
All	All	1125/1663 (68%)	1106 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	200/306 (65%)	192 (96%)	8 (4%)	27	55
2	B	281/298 (94%)	267 (95%)	14 (5%)	20	47
3	C	45/58 (78%)	43 (96%)	2 (4%)	24	51
4	R	265/514 (52%)	254 (96%)	11 (4%)	25	52
5	S	197/239 (82%)	193 (98%)	4 (2%)	50	71
All	All	988/1415 (70%)	949 (96%)	39 (4%)	30	55

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	R	187	TYR
5	S	50	TYR
4	R	195	LYS
4	R	266	MET
5	S	223	TYR

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

Mol	Chain	Res	Type
1	A	241	ASN
1	A	347	ASN
5	S	155	HIS

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	OXF	R	601	-	28,28,28	0.15	0	35,35,35	0.31	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	OXF	R	601	-	-	0/14/24/24	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

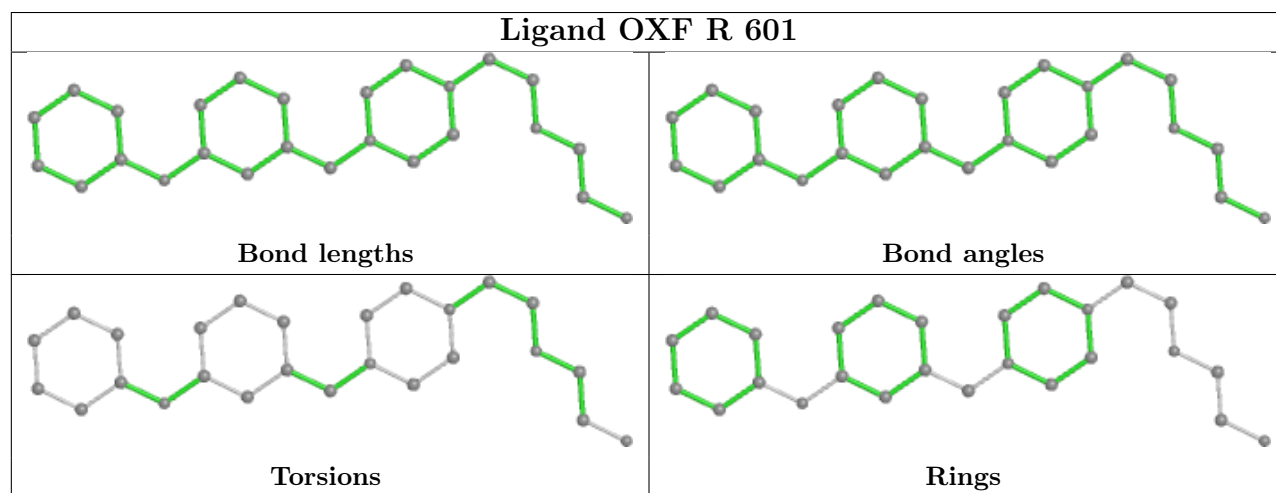
There are no torsion outliers.

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.