



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 09:09 PM UTC

PDB ID : 5XUA / pdb_00005xua
Title : The ligand-free dimer of chemoreceptor MCP2201 ligand binding domain
Authors : Hong, Y.; Li, D.F.; Wang, D.C.
Deposited on : 2017-06-23
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

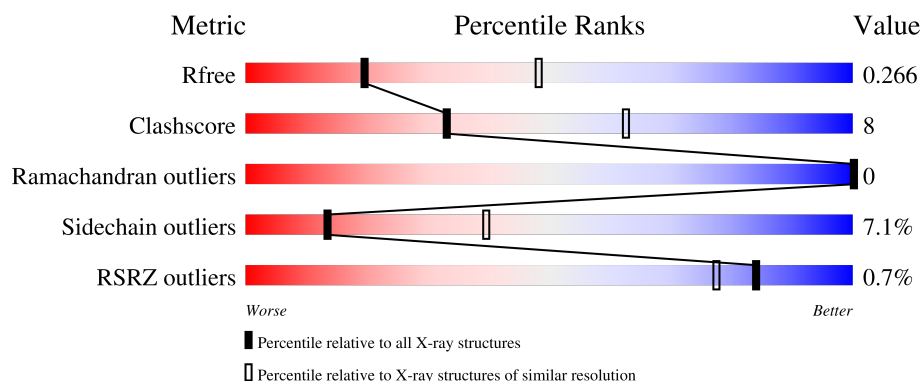
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	154	
1	B	154	
1	C	154	
1	D	154	
1	E	154	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	154	% 69%18%•12%
1	G	154	71%16%•10%
1	H	154	64%22%•12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8363 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Methyl-accepting chemotaxis sensory transducer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1082	675	185	218	4			
1	B	137	Total	C	N	O	S	0	0	0
			1040	649	179	208	4			
1	C	138	Total	C	N	O	S	0	0	0
			1047	654	180	209	4			
1	D	137	Total	C	N	O	S	0	0	0
			1040	649	179	208	4			
1	E	137	Total	C	N	O	S	0	0	0
			1040	649	179	208	4			
1	F	136	Total	C	N	O	S	0	0	0
			1032	644	178	207	3			
1	G	139	Total	C	N	O	S	0	0	0
			1056	659	181	212	4			
1	H	135	Total	C	N	O	S	0	0	0
			1026	641	177	204	4			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	expression tag	UNP D0IVL9
A	51	HIS	-	expression tag	UNP D0IVL9
A	52	HIS	-	expression tag	UNP D0IVL9
A	53	HIS	-	expression tag	UNP D0IVL9
A	54	HIS	-	expression tag	UNP D0IVL9
A	55	HIS	-	expression tag	UNP D0IVL9
A	56	HIS	-	expression tag	UNP D0IVL9
B	50	MET	-	expression tag	UNP D0IVL9
B	51	HIS	-	expression tag	UNP D0IVL9
B	52	HIS	-	expression tag	UNP D0IVL9
B	53	HIS	-	expression tag	UNP D0IVL9
B	54	HIS	-	expression tag	UNP D0IVL9
B	55	HIS	-	expression tag	UNP D0IVL9

Continued on next page...

Continued from previous page...

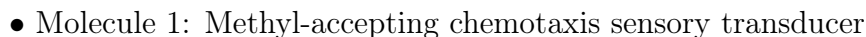
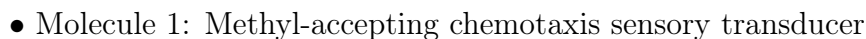
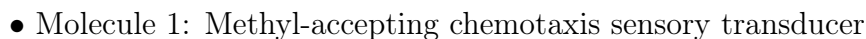
Chain	Residue	Modelled	Actual	Comment	Reference
B	56	HIS	-	expression tag	UNP D0IVL9
C	50	MET	-	expression tag	UNP D0IVL9
C	51	HIS	-	expression tag	UNP D0IVL9
C	52	HIS	-	expression tag	UNP D0IVL9
C	53	HIS	-	expression tag	UNP D0IVL9
C	54	HIS	-	expression tag	UNP D0IVL9
C	55	HIS	-	expression tag	UNP D0IVL9
C	56	HIS	-	expression tag	UNP D0IVL9
D	50	MET	-	expression tag	UNP D0IVL9
D	51	HIS	-	expression tag	UNP D0IVL9
D	52	HIS	-	expression tag	UNP D0IVL9
D	53	HIS	-	expression tag	UNP D0IVL9
D	54	HIS	-	expression tag	UNP D0IVL9
D	55	HIS	-	expression tag	UNP D0IVL9
D	56	HIS	-	expression tag	UNP D0IVL9
E	50	MET	-	expression tag	UNP D0IVL9
E	51	HIS	-	expression tag	UNP D0IVL9
E	52	HIS	-	expression tag	UNP D0IVL9
E	53	HIS	-	expression tag	UNP D0IVL9
E	54	HIS	-	expression tag	UNP D0IVL9
E	55	HIS	-	expression tag	UNP D0IVL9
E	56	HIS	-	expression tag	UNP D0IVL9
F	50	MET	-	expression tag	UNP D0IVL9
F	51	HIS	-	expression tag	UNP D0IVL9
F	52	HIS	-	expression tag	UNP D0IVL9
F	53	HIS	-	expression tag	UNP D0IVL9
F	54	HIS	-	expression tag	UNP D0IVL9
F	55	HIS	-	expression tag	UNP D0IVL9
F	56	HIS	-	expression tag	UNP D0IVL9
G	50	MET	-	expression tag	UNP D0IVL9
G	51	HIS	-	expression tag	UNP D0IVL9
G	52	HIS	-	expression tag	UNP D0IVL9
G	53	HIS	-	expression tag	UNP D0IVL9
G	54	HIS	-	expression tag	UNP D0IVL9
G	55	HIS	-	expression tag	UNP D0IVL9
G	56	HIS	-	expression tag	UNP D0IVL9
H	50	MET	-	expression tag	UNP D0IVL9
H	51	HIS	-	expression tag	UNP D0IVL9
H	52	HIS	-	expression tag	UNP D0IVL9
H	53	HIS	-	expression tag	UNP D0IVL9
H	54	HIS	-	expression tag	UNP D0IVL9
H	55	HIS	-	expression tag	UNP D0IVL9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	56	HIS	-	expression tag	UNP D0IVL9

- Molecule 1: Methyl-accepting chemotaxis sensory transducer



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.78Å 105.03Å 91.07Å 90.00° 90.95° 90.00°	Depositor
Resolution (Å)	53.20 – 2.80 53.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (53.20-2.80) 94.8 (53.20-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.222 , 0.266 0.224 , 0.266	Depositor DCC
R_{free} test set	1520 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8363	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.18	0/1091	0.46	0/1476
1	B	0.15	0/1049	0.42	0/1419
1	C	0.16	0/1056	0.44	0/1429
1	D	0.15	0/1049	0.40	0/1419
1	E	0.17	0/1049	0.41	0/1419
1	F	0.17	0/1041	0.44	0/1409
1	G	0.19	0/1065	0.41	0/1441
1	H	0.18	0/1035	0.45	0/1400
All	All	0.17	0/8435	0.43	0/11412

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 [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	1082	0	1117	24	0
1	B	1040	0	1077	15	0
1	C	1047	0	1086	18	0
1	D	1040	0	1077	15	0
1	E	1040	0	1077	18	0
1	F	1032	0	1068	14	0
1	G	1056	0	1092	19	0
1	H	1026	0	1066	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8363	0	8660	133	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 133 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:132:MET:SD	1:A:135:ARG:NH2	2.49	0.86
1:C:105:THR:HG21	1:H:150:ALA:HB1	1.66	0.78
1:B:61:PRO:HB2	1:B:187:LEU:HD13	1.72	0.72
1:E:78:ALA:O	1:E:82:THR:OG1	2.13	0.67
1:D:88:SER:O	1:D:149:LYS:NZ	2.28	0.67

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 X-ray entries followed by that with respect to entries of similar resolution.

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	140/154 (91%)	137 (98%)	3 (2%)	0	100	100
1	B	135/154 (88%)	129 (96%)	6 (4%)	0	100	100
1	C	136/154 (88%)	135 (99%)	1 (1%)	0	100	100
1	D	135/154 (88%)	129 (96%)	6 (4%)	0	100	100
1	E	135/154 (88%)	131 (97%)	4 (3%)	0	100	100
1	F	134/154 (87%)	130 (97%)	4 (3%)	0	100	100
1	G	137/154 (89%)	133 (97%)	4 (3%)	0	100	100
1	H	133/154 (86%)	128 (96%)	5 (4%)	0	100	100
All	All	1085/1232 (88%)	1052 (97%)	33 (3%)	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 X-ray entries followed by that with respect to entries of similar resolution.

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	117/129 (91%)	106 (91%)	11 (9%)	8	27
1	B	112/129 (87%)	106 (95%)	6 (5%)	20	51
1	C	113/129 (88%)	107 (95%)	6 (5%)	20	52
1	D	112/129 (87%)	102 (91%)	10 (9%)	9	29
1	E	112/129 (87%)	103 (92%)	9 (8%)	11	34
1	F	111/129 (86%)	103 (93%)	8 (7%)	13	39
1	G	114/129 (88%)	106 (93%)	8 (7%)	14	40
1	H	111/129 (86%)	105 (95%)	6 (5%)	20	51
All	All	902/1032 (87%)	838 (93%)	64 (7%)	13	39

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	195	GLU
1	H	67	LEU
1	D	73	SER
1	D	58	MET
1	H	82	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	133	GLN
1	F	163	ASN
1	H	121	GLN
1	H	110	ASN
1	C	163	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](#)

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	142/154 (92%)	-0.15	0 100 100	35, 58, 94, 121	0
1	B	137/154 (88%)	-0.17	1 (0%) 84 77	36, 54, 97, 116	0
1	C	138/154 (89%)	-0.22	1 (0%) 84 77	41, 56, 91, 102	0
1	D	137/154 (88%)	0.09	5 (3%) 46 37	41, 63, 108, 129	0
1	E	137/154 (88%)	-0.00	0 100 100	48, 72, 108, 119	0
1	F	136/154 (88%)	-0.09	1 (0%) 84 77	41, 61, 102, 133	0
1	G	139/154 (90%)	-0.19	0 100 100	44, 63, 95, 124	0
1	H	135/154 (87%)	-0.07	0 100 100	44, 67, 115, 126	0
All	All	1101/1232 (89%)	-0.10	8 (0%) 84 77	35, 62, 103, 133	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	ALA	3.3
1	D	153	MET	3.1
1	D	101	ALA	2.7
1	D	94	VAL	2.7
1	B	192	ALA	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.