



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2017 – 11:00 AM EDT

PDB ID : 5L7H
Title : MCR IN COMPLEX WITH ligand
Authors : Xue, Y.; Aagaard, A.; Backstrom, S.; Edman, K.
Deposited on : unknown
Resolution : 1.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

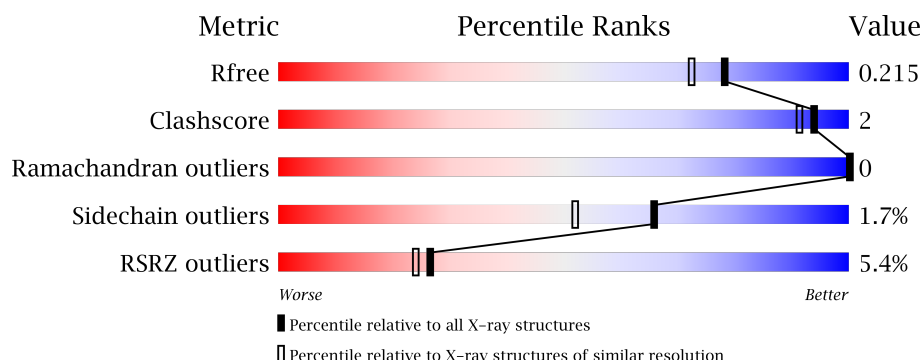
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	100719	2964 (1.86-1.82)
Clashscore	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)
RSRZ outliers	101464	2973 (1.86-1.82)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	305	<div> <div>5%</div> <div>78%</div> <div>18%</div> </div>
2	B	10	<div> <div>100%</div> </div>

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
4	NHE	A	1102	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2414 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 Mineralocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	6	0
			2091	1355	340	382	14			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	713	MET	-	initiating methionine	UNP P08235
A	714	HIS	-	expression tag	UNP P08235
A	715	ASN	-	expression tag	UNP P08235
A	716	HIS	-	expression tag	UNP P08235
A	717	ASN	-	expression tag	UNP P08235
A	718	HIS	-	expression tag	UNP P08235
A	719	ASN	-	expression tag	UNP P08235
A	720	HIS	-	expression tag	UNP P08235
A	721	ASN	-	expression tag	UNP P08235
A	722	HIS	-	expression tag	UNP P08235
A	723	ASN	-	expression tag	UNP P08235
A	724	HIS	-	expression tag	UNP P08235
A	725	ASN	-	expression tag	UNP P08235
A	726	GLY	-	expression tag	UNP P08235
A	727	GLY	-	expression tag	UNP P08235
A	728	GLU	-	expression tag	UNP P08235
A	729	ASN	-	expression tag	UNP P08235
A	730	LEU	-	expression tag	UNP P08235
A	731	TYR	-	expression tag	UNP P08235
A	732	PHE	-	expression tag	UNP P08235
A	733	GLN	-	expression tag	UNP P08235
A	734	GLY	-	expression tag	UNP P08235
A	808	SER	CYS	conflict	UNP P08235
A	810	LEU	SER	conflict	UNP P08235
A	910	SER	CYS	conflict	UNP P08235
A	985	GLY	-	expression tag	UNP P08235
A	986	GLY	-	expression tag	UNP P08235

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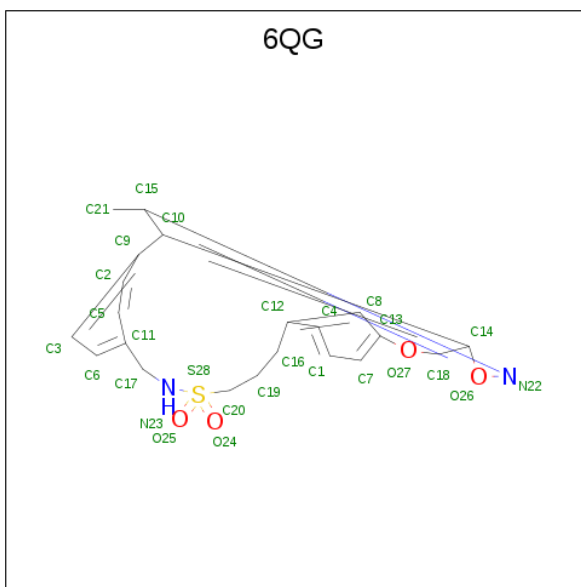
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Chain	Residue	Modelled	Actual	Comment	Reference
A	987	SER	-	expression tag	UNP P08235
A	988	LEU	-	expression tag	UNP P08235
A	989	VAL	-	expression tag	UNP P08235
A	990	PRO	-	expression tag	UNP P08235
A	991	ARG	-	expression tag	UNP P08235
A	992	GLY	-	expression tag	UNP P08235
A	993	SER	-	expression tag	UNP P08235
A	994	GLY	-	expression tag	UNP P08235
A	995	GLY	-	expression tag	UNP P08235
A	996	GLY	-	expression tag	UNP P08235
A	997	SER	-	expression tag	UNP P08235
A	998	GLY	-	expression tag	UNP P08235
A	999	GLY	-	expression tag	UNP P08235
A	1000	SER	-	expression tag	UNP P08235
A	1001	GLY	-	expression tag	UNP P08235
A	1002	GLY	-	expression tag	UNP P08235
A	1003	PRO	-	expression tag	UNP P08235
A	1004	GLN	-	expression tag	UNP P08235
A	1005	ALA	-	expression tag	UNP P08235
A	1006	GLN	-	expression tag	UNP P08235
A	1007	GLN	-	expression tag	UNP P08235
A	1008	LYS	-	expression tag	UNP P08235
A	1009	SER	-	expression tag	UNP P08235
A	1010	LEU	-	expression tag	UNP P08235
A	1011	LEU	-	expression tag	UNP P08235
A	1012	GLN	-	expression tag	UNP P08235
A	1013	GLN	-	expression tag	UNP P08235
A	1014	LEU	-	expression tag	UNP P08235
A	1015	LEU	-	expression tag	UNP P08235
A	1016	THR	-	expression tag	UNP P08235
A	1017	GLU	-	expression tag	UNP P08235

- Molecule 2 is a protein called NCOA1 peptide.

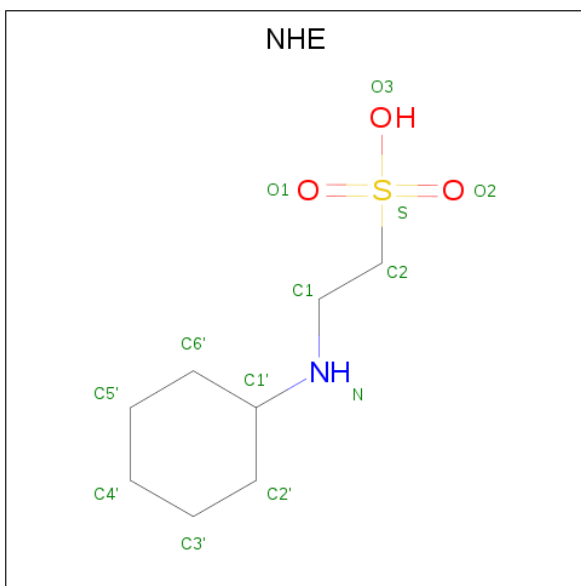
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	1	0
			90	58	14	18			

- Molecule 3 is 3-methyl-5,8-dioxa-17lambda-thia-4,18-diazatetracyclo[18.2.2.1,.0]pentaco sa-1(22),2(6),3,9,11,13(25),20,23-octaene-17,17-dione (three-letter code: 6QG) (formula: C₂₁H₂₂N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	21	2	4	1		

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $\text{C}_8\text{H}_{17}\text{NO}_3\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	188	Total 188	O 188	0	0
5	B	4	Total 4	O 4	0	0

i

- Molecule 1: Mineralocorticoid receptor



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.67Å 77.89Å 78.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.27 – 1.84 39.31 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.27-1.84) 99.9 (39.31-1.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.84Å)	Xtriage
Refinement program	BUSTER 2.11.6 PACIOREK	Depositor
R, R_{free}	0.194 , 0.224 0.181 , 0.215	Depositor DCC
R_{free} test set	1343 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2414	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NHE, 6QG

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	0.51	0/2140	0.56	0/2887
2	B	0.42	0/89	0.50	0/117
All	All	0.51	0/2229	0.56	0/3004

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 ⓘ

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	2091	0	2089	6	0
2	B	90	0	100	0	0
3	A	28	0	0	0	0
4	A	13	0	16	1	0
5	A	188	0	0	1	0
5	B	4	0	0	0	0
All	All	2414	0	2205	7	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 2.

All (7) 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:919:GLN:H	1:A:919:GLN:HE21	1.52	0.56
1:A:852:MET:HE3	1:A:934:LEU:HD21	1.86	0.56
1:A:749:ILE:HD11	1:A:828:TYR:HE1	1.71	0.55
1:A:916:GLN:HB2	1:A:919:GLN:HE22	1.79	0.48
1:A:920:ARG:HA	1:A:923:GLN:HE21	1.80	0.46
1:A:852:MET:HE3	1:A:934:LEU:CD2	2.47	0.44
4:A:1102:NHE:HC'1	5:A:1306:HOH:O	2.19	0.43

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 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	249/305 (82%)	247 (99%)	2 (1%)	0	100	100
2	B	9/10 (90%)	9 (100%)	0	0	100	100
All	All	258/315 (82%)	256 (99%)	2 (1%)	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 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	236/272 (87%)	232 (98%)	4 (2%)	66	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	11/10 (110%)	11 (100%)	0	100	100
All	All	247/282 (88%)	243 (98%)	4 (2%)	66	55

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	758	LYS
1	A	919	GLN
1	A	949	SER
1	A	950	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	792	ASN
1	A	823	ASN
1	A	850	GLN
1	A	919	GLN
1	A	923	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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
3	6QG	A	1101	-	25,31,31	1.29	2 (8%)	35,44,44	1.64	5 (14%)
4	NHE	A	1102	-	13,13,13	2.65	2 (15%)	15,17,17	2.23	3 (20%)

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
3	6QG	A	1101	-	-	0/20/22/22	0/0/4/4
4	NHE	A	1102	-	-	0/7/15/15	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	NHE	C2-S	-6.57	1.67	1.77
3	A	1101	6QG	C10-C9	-2.46	1.45	1.50
3	A	1101	6QG	S28-N23	4.63	1.73	1.60
4	A	1102	NHE	O2-S	6.59	1.64	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	6QG	C18-O27-C13	-4.27	106.97	117.61
3	A	1101	6QG	C16-C12-C8	-4.04	113.93	120.56
3	A	1101	6QG	O25-S28-C20	-2.24	104.09	107.96
3	A	1101	6QG	C16-C12-C4	2.17	126.65	121.24
4	A	1102	NHE	C4'-C3'-C2'	2.22	116.02	111.42
4	A	1102	NHE	O3-S-C2	4.29	111.33	106.06
3	A	1101	6QG	O27-C18-C14	4.99	117.07	107.96
4	A	1102	NHE	O1-S-C2	5.79	111.76	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1102	NHE	1	0

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	249/305 (81%)	0.22	14 (5%) 25 23	15, 26, 61, 102	0
2	B	10/10 (100%)	-0.01	0 100 100	28, 35, 54, 63	0
All	All	259/315 (82%)	0.21	14 (5%) 26 24	15, 26, 61, 102	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	952	LEU	7.7
1	A	951	ALA	7.1
1	A	911	PRO	7.0
1	A	915	GLY	6.9
1	A	950	HIS	5.8
1	A	914	SER	5.7
1	A	984	LYS	4.5
1	A	916	GLN	3.3
1	A	912	ASN	3.3
1	A	910	SER	2.6
1	A	731	TYR	2.6
1	A	846	TYR	2.4
1	A	732	PHE	2.4
1	A	884	ASP	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NHE	A	1102	13/13	0.84	0.23	2.69	38,51,54,55	0
3	6QG	A	1101	28/28	0.95	0.11	0.18	19,29,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.