



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1MCR / pdb_00001mcr
Title : PRINCIPLES AND PITFALLS IN DESIGNING SITE DIRECTED PEPTIDE LIGANDS
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Deposited on : 1993-02-25
Resolution : 2.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

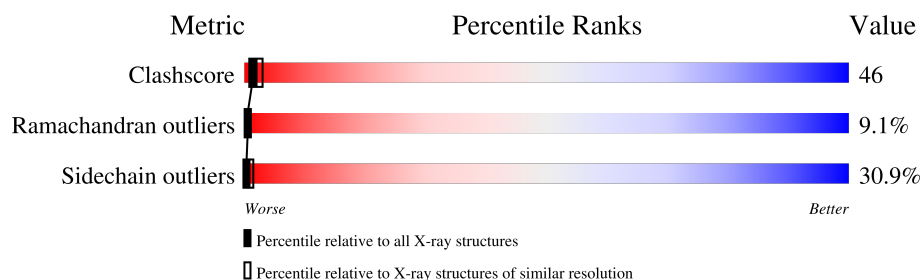
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	216	
1	B	216	
2	P	3	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3231 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 IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1605	1000	266	334	5			
1	B	216	Total	C	N	O	S	0	0	0
			1605	1000	266	334	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ILE	PHE	conflict	PIR S14675
A	23	THR	SER	conflict	PIR S14675
A	29	VAL	ILE	conflict	PIR S14675
A	31	GLY	ASN	conflict	PIR S14675
A	39	GLN	ARG	conflict	PIR S14675
A	42	ALA	PRO	conflict	PIR S14675
A	48	VAL	LEU	conflict	PIR S14675
A	49	ILE	MET	conflict	PIR S14675
A	54	ASN	THR	conflict	PIR S14675
A	62	ASP	ASN	conflict	PIR S14675
A	94	GLU	ALA	conflict	PIR S14675
A	97	ASP	ASN	conflict	PIR S14675
A	98	ASN	SER	conflict	PIR S14675
A	99	PHE	LEU	conflict	PIR S14675
A	100	VAL	ILE	conflict	PIR S14675
A	103	THR	GLY	conflict	PIR S14675
A	106	LYS	ARG	conflict	PIR S14675
A	107	VAL	LEU	conflict	PIR S14675
A	116	ASN	ALA	conflict	PIR S14675
A	118	THR	SER	conflict	PIR S14675
A	156	GLY	SER	conflict	PIR S14675
A	167	LYS	THR	conflict	PIR S14675
B	20	ILE	PHE	conflict	PIR S14675
B	23	THR	SER	conflict	PIR S14675

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	VAL	ILE	conflict	PIR S14675
B	31	GLY	ASN	conflict	PIR S14675
B	39	GLN	ARG	conflict	PIR S14675
B	42	ALA	PRO	conflict	PIR S14675
B	48	VAL	LEU	conflict	PIR S14675
B	49	ILE	MET	conflict	PIR S14675
B	54	ASN	THR	conflict	PIR S14675
B	62	ASP	ASN	conflict	PIR S14675
B	94	GLU	ALA	conflict	PIR S14675
B	97	ASP	ASN	conflict	PIR S14675
B	98	ASN	SER	conflict	PIR S14675
B	99	PHE	LEU	conflict	PIR S14675
B	100	VAL	ILE	conflict	PIR S14675
B	103	THR	GLY	conflict	PIR S14675
B	106	LYS	ARG	conflict	PIR S14675
B	107	VAL	LEU	conflict	PIR S14675
B	116	ASN	ALA	conflict	PIR S14675
B	118	THR	SER	conflict	PIR S14675
B	156	GLY	SER	conflict	PIR S14675
B	167	LYS	THR	conflict	PIR S14675

- Molecule 2 is a protein called PEPTIDE N-ACETYL-L-HIS-D-PRO-OH.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	3	Total	C	N	O	0	0	0
			21	13	4	4			



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.30 Å 72.30 Å 185.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.204 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3231	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.19	5/1644 (0.3%)	1.99	58/2241 (2.6%)
1	B	1.17	3/1644 (0.2%)	1.91	38/2241 (1.7%)
2	P	0.57	0/11	1.22	0/14
All	All	1.18	8/3299 (0.2%)	1.95	96/4496 (2.1%)

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	1
1	B	0	1
All	All	0	2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	THR	CA-CB	5.78	1.61	1.53
1	B	159	VAL	N-CA	5.67	1.52	1.46
1	B	85	GLU	N-CA	5.55	1.53	1.46
1	A	141	SER	N-CA	5.33	1.53	1.46
1	B	26	SER	C-O	5.29	1.30	1.24

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ASN	CA-CB-CG	11.57	124.17	112.60
1	B	143	PHE	CA-CB-CG	10.25	124.05	113.80
1	A	8	PRO	N-CA-C	9.60	125.72	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	PHE	CA-CB-CG	9.08	122.88	113.80
1	A	162	GLY	N-CA-C	-8.59	103.08	114.25

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	ARG	Sidechain
1	B	116	ASN	Peptide

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	1605	0	1540	153	0
1	B	1605	0	1540	149	0
2	P	21	0	17	1	0
All	All	3231	0	3097	293	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 46.

The worst 5 of 293 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:B:153:LYS:HZ1	1:B:198:GLN:HB2	1.04	1.09
1:A:136:LEU:HD11	1:A:184:LEU:HD11	1.58	0.86
1:A:4:LEU:O	1:A:102:GLY:HA3	1.77	0.84
1:B:34:TYR:OH	2:P:1:HIS:HB2	1.77	0.84
1:A:65:SER:OG	1:A:76:THR:HB	1.79	0.83

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	214/216 (99%)	162 (76%)	31 (14%)	21 (10%)	0	0
1	B	214/216 (99%)	163 (76%)	33 (15%)	18 (8%)	0	1
2	P	1/3 (33%)	0	1 (100%)	0	100	100
All	All	429/435 (99%)	325 (76%)	65 (15%)	39 (9%)	0	0

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	16	GLN
1	A	29	VAL
1	A	33	ASN
1	A	47	LYS

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	181/181 (100%)	124 (68%)	57 (32%)	0	1
1	B	181/181 (100%)	126 (70%)	55 (30%)	0	1
2	P	1/1 (100%)	1 (100%)	0	100	100
All	All	363/363 (100%)	251 (69%)	112 (31%)	0	1

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	THR
1	B	213	THR
1	B	53	VAL
1	B	206	VAL
1	B	159	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	112	GLN
1	B	192	HIS
1	B	201	HIS
1	B	198	GLN
1	A	174	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.