



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:47 PM UTC

PDB ID : 6V02 / pdb_00006v02
Title : N-terminal 5 domains of CI-MPR
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Deposited on : 2019-11-18
Resolution : 2.46 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

<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)	:	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

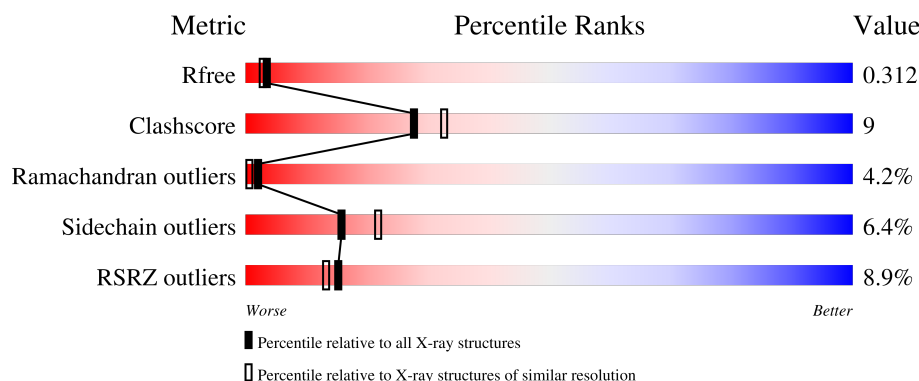
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	731	7% 57% 18% • 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4570 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 Cation-independent mannose-6-phosphate receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	0	0
			4482	2819	756	872	35			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP P11717
A	4	SER	-	expression tag	UNP P11717
A	5	THR	-	expression tag	UNP P11717
A	6	GLN	-	expression tag	UNP P11717
A	7	ALA	-	expression tag	UNP P11717
A	729	ALA	-	expression tag	UNP P11717
A	730	LEU	-	expression tag	UNP P11717
A	731	VAL	-	expression tag	UNP P11717
A	732	PRO	-	expression tag	UNP P11717
A	733	ARG	-	expression tag	UNP P11717

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.78Å 66.22Å 124.53Å 90.00° 100.53° 90.00°	Depositor
Resolution (Å)	35.91 – 2.46 35.91 – 2.46	Depositor EDS
% Data completeness (in resolution range)	66.0 (35.91-2.46) 66.1 (35.91-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.240 , 0.308 0.248 , 0.312	Depositor DCC
R_{free} test set	996 reflections (3.36%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4570	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: NAG

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	0/4574	0.84	3/6191 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	CYS	N-CA-C	5.55	119.88	113.38
1	A	89	HIS	N-CA-C	5.15	119.65	112.90
1	A	684	ARG	N-CA-C	-5.03	105.26	111.40

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	4482	0	4292	79	0
2	A	14	0	13	0	0
3	A	74	0	0	0	0
All	All	4570	0	4305	79	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 9.

All (79) 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:13:LEU:HB2	1:A:33:ILE:HD11	1.79	0.65
1:A:362:ARG:HB2	1:A:381:GLY:HA3	1.82	0.62
1:A:650:ASP:O	1:A:651:GLU:HB2	1.99	0.62
1:A:92:GLN:NE2	1:A:94:SER:OG	2.33	0.61
1:A:670:ILE:HB	1:A:694:PHE:HB2	1.81	0.61
1:A:590:GLU:HG3	1:A:591:ASN:H	1.70	0.57
1:A:252:VAL:HB	1:A:278:ILE:HD13	1.86	0.57
1:A:258:ARG:NH1	1:A:696:CYS:O	2.38	0.57
1:A:605:LEU:C	1:A:607:PRO:HD2	2.29	0.57
1:A:243:HIS:ND1	1:A:711:ASP:OD2	2.34	0.56
1:A:362:ARG:HB2	1:A:381:GLY:CA	2.34	0.56
1:A:328:LEU:HA	1:A:345:ALA:O	2.06	0.56
1:A:67:ARG:HD3	1:A:74:LEU:HD11	1.89	0.55
1:A:318:ILE:O	1:A:318:ILE:HG23	2.07	0.54
1:A:330:VAL:HG12	1:A:331:CYS:SG	2.47	0.54
1:A:8:ALA:HB1	1:A:10:PHE:CE2	2.42	0.54
1:A:711:ASP:HB3	1:A:713:SER:H	1.73	0.54
1:A:392:MET:HB2	1:A:420:THR:HG23	1.90	0.54
1:A:320:ASP:HA	1:A:325:LEU:HD12	1.89	0.53
1:A:590:GLU:CG	1:A:591:ASN:H	2.22	0.53
1:A:676:GLY:O	1:A:687:PRO:HB2	2.08	0.53
1:A:702:VAL:HG22	1:A:723:TYR:HE2	1.72	0.53
1:A:309:LEU:O	1:A:330:VAL:HG22	2.09	0.52
1:A:679:PRO:HA	1:A:686:THR:O	2.07	0.52
1:A:548:THR:C	1:A:549:LEU:HD23	2.34	0.52
1:A:551:CYS:HB3	1:A:581:ALA:HB3	1.91	0.52
1:A:109:VAL:HG23	1:A:118:PHE:HA	1.92	0.51
1:A:63:ASP:OD2	1:A:65:VAL:HG22	2.11	0.51
1:A:414:THR:HG21	1:A:424:THR:HG23	1.93	0.51
1:A:307:THR:N	1:A:308:PRO:CD	2.75	0.50
1:A:551:CYS:HB3	1:A:582:CYS:H	1.76	0.50
1:A:108:PHE:HA	1:A:118:PHE:CD1	2.47	0.49
1:A:447:LYS:HB3	1:A:583:VAL:HG12	1.94	0.49
1:A:606:SER:N	1:A:607:PRO:HD2	2.28	0.49
1:A:444:ASP:O	1:A:446:LYS:N	2.46	0.48
1:A:73:LEU:HD13	1:A:417:VAL:HG23	1.94	0.48
1:A:385:CYS:O	1:A:387:SER:O	2.31	0.48
1:A:152:ASN:N	1:A:153:PRO:CD	2.76	0.48
1:A:636:PRO:HB2	1:A:653:THR:HG21	1.96	0.47
1:A:55:THR:O	1:A:57:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ILE:HG22	1:A:694:PHE:CE1	2.50	0.47
1:A:709:GLU:HG2	1:A:709:GLU:O	2.16	0.46
1:A:652:LYS:O	1:A:654:TRP:CZ3	2.69	0.46
1:A:609:THR:HG23	1:A:630:GLY:H	1.81	0.46
1:A:27:VAL:HG13	1:A:52:ASP:N	2.30	0.46
1:A:244:SER:O	1:A:272:ARG:NH1	2.48	0.45
1:A:217:LEU:HD11	1:A:225:LEU:HB3	1.98	0.45
1:A:683:GLU:HA	1:A:683:GLU:OE1	2.16	0.45
1:A:147:ARG:O	1:A:148:LYS:HB3	2.16	0.45
1:A:128:LYS:HA	1:A:128:LYS:HE3	1.99	0.44
1:A:595:PHE:HA	1:A:602:SER:HB3	1.99	0.44
1:A:646:VAL:HG22	1:A:653:THR:HG22	1.98	0.44
1:A:196:GLY:O	1:A:212:GLN:HG2	2.17	0.44
1:A:29:TYR:HA	1:A:49:CYS:O	2.17	0.44
1:A:142:PHE:CE1	1:A:148:LYS:HB2	2.52	0.44
1:A:225:LEU:HB2	1:A:251:PHE:HB2	2.00	0.44
1:A:121:ARG:NH2	1:A:397:PHE:O	2.51	0.43
1:A:365:ASN:HB3	1:A:380:PHE:HB2	2.00	0.43
1:A:640:ASP:HB3	1:A:658:LEU:HD23	2.01	0.43
1:A:28:LEU:HD13	1:A:146:LEU:HD22	2.00	0.43
1:A:78:THR:CG2	1:A:91:VAL:O	2.67	0.43
1:A:354:THR:C	1:A:356:GLN:H	2.28	0.42
1:A:549:LEU:HD22	1:A:576:TRP:HB3	2.00	0.42
1:A:620:LYS:O	1:A:621:LYS:HB2	2.19	0.42
1:A:129:ASP:N	1:A:129:ASP:OD1	2.53	0.42
1:A:262:ILE:HB	1:A:263:PRO:HD2	2.01	0.42
1:A:579:ALA:HB1	1:A:598:GLN:O	2.20	0.42
1:A:629:CYS:HA	1:A:660:ASN:O	2.20	0.42
1:A:65:VAL:HG23	1:A:66:LEU:HG	2.01	0.41
1:A:685:HIS:O	1:A:686:THR:C	2.62	0.41
1:A:702:VAL:HG22	1:A:723:TYR:CE2	2.54	0.41
1:A:632:VAL:HG12	1:A:641:SER:O	2.21	0.41
1:A:184:ARG:O	1:A:185:ASP:HB2	2.20	0.41
1:A:51:HIS:O	1:A:52:ASP:HB3	2.21	0.40
1:A:78:THR:HG22	1:A:91:VAL:O	2.21	0.40
1:A:317:TYR:O	1:A:327:TYR:HA	2.21	0.40
1:A:345:ALA:HB2	1:A:362:ARG:O	2.21	0.40
1:A:589:GLY:HA3	1:A:593:THR:O	2.22	0.40
1:A:258:ARG:HH21	1:A:278:ILE:HD11	1.86	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 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	549/731 (75%)	457 (83%)	69 (13%)	23 (4%)	2 0

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	LYS
1	A	330	VAL
1	A	621	LYS
1	A	711	ASP
1	A	233	GLU
1	A	342	LYS
1	A	362	ARG
1	A	381	GLY
1	A	382	GLY
1	A	445	GLY
1	A	651	GLU
1	A	676	GLY
1	A	685	HIS
1	A	148	LYS
1	A	343	GLN
1	A	363	TYR
1	A	613	GLY
1	A	185	ASP
1	A	344	ALA
1	A	583	VAL
1	A	54	LYS
1	A	82	CYS
1	A	553	PRO

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	499/628 (80%)	467 (94%)	32 (6%)	16	22

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	28	LEU
1	A	52	ASP
1	A	63	ASP
1	A	70	THR
1	A	75	GLU
1	A	78	THR
1	A	88	ASN
1	A	121	ARG
1	A	128	LYS
1	A	129	ASP
1	A	130	ILE
1	A	157	LEU
1	A	225	LEU
1	A	262	ILE
1	A	342	LYS
1	A	363	TYR
1	A	365	ASN
1	A	387	SER
1	A	410	THR
1	A	417	VAL
1	A	427	THR
1	A	548	THR
1	A	549	LEU
1	A	550	VAL
1	A	592	CYS
1	A	602	SER
1	A	608	LEU
1	A	635	SER
1	A	651	GLU

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Mol	Chain	Res	Type
1	A	662	LYS
1	A	678	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	116	HIS
1	A	270	ASN
1	A	343	GLN
1	A	348	GLN
1	A	390	GLN
1	A	396	ASN
1	A	591	ASN
1	A	612	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](#)

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	$\# Z > 2$
2	NAG	A	801	1	14,14,15	0.40	0	17,19,21	0.82	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
2	NAG	A	801	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	573/731 (78%)	0.79	51 (8%) 15 13	36, 74, 112, 139	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	439	LEU	5.3
1	A	8	ALA	4.9
1	A	451	LEU	4.5
1	A	553	PRO	4.3
1	A	550	VAL	4.2
1	A	317	TYR	4.2
1	A	306	LEU	3.8
1	A	403	ALA	3.7
1	A	438	LEU	3.7
1	A	442	ALA	3.3
1	A	407	GLY	3.3
1	A	614	ALA	3.3
1	A	605	LEU	2.9
1	A	556	LEU	2.8
1	A	600	GLY	2.7
1	A	328	LEU	2.7
1	A	581	ALA	2.7
1	A	449	TYR	2.7
1	A	288	LEU	2.6
1	A	330	VAL	2.5
1	A	549	LEU	2.5
1	A	576	TRP	2.5
1	A	260	GLY	2.4
1	A	551	CYS	2.4
1	A	604	ASP	2.4
1	A	10	PHE	2.4
1	A	552	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	646	VAL	2.3
1	A	9	PRO	2.3
1	A	409	GLY	2.3
1	A	304	ILE	2.3
1	A	187	GLY	2.3
1	A	196	GLY	2.3
1	A	601	PHE	2.3
1	A	548	THR	2.2
1	A	235	GLY	2.2
1	A	583	VAL	2.2
1	A	318	ILE	2.2
1	A	638	GLN	2.1
1	A	440	CYS	2.1
1	A	232	GLU	2.1
1	A	453	ALA	2.1
1	A	616	LYS	2.1
1	A	40	VAL	2.1
1	A	429	TYR	2.1
1	A	50	MET	2.1
1	A	322	LYS	2.0
1	A	363	TYR	2.0
1	A	293	CYS	2.0
1	A	595	PHE	2.0
1	A	454	LEU	2.0

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](#)

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	801	14/15	0.69	0.13	84,92,96,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.