wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2024 – 09:43 PM EDT

PDB ID	:	1XED
Title	:	Crystal Structure of a Ligand-Binding Domain of the Human Polymeric Ig Receptor, pIgR
Authors	:	Hamburger, A.E.; West Jr., A.P.; Bjorkman, P.J.
Deposited on	:	2004-09-10
Resolution	:	1.90 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 (i) 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 (1)) were used in the production of this report:

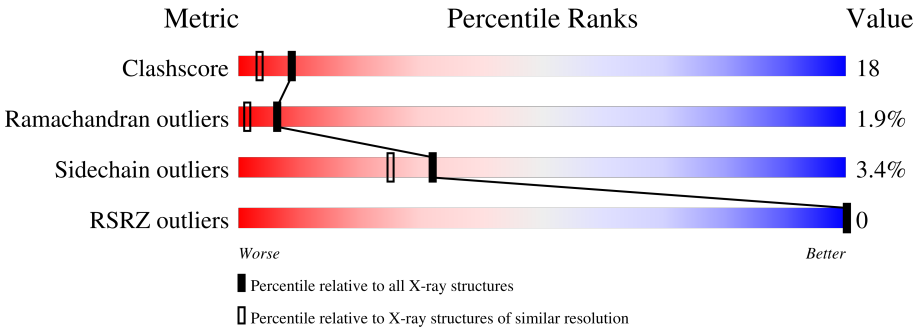
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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 <=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	117	65% 29% • 5%
1	B	117	61% 27% 5% 7%
1	C	117	50% 35% • 10%
1	D	117	52% 36% • 10%
1	E	117	67% 27% • 5%
1	F	117	61% 32% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5148 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 Polymeric-immunoglobulin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			865	539	155	167	4			
1	B	109	Total	C	N	O	S	0	0	0
			848	530	151	163	4			
1	C	105	Total	C	N	O	S	0	0	0
			803	503	138	158	4			
1	D	105	Total	C	N	O	S	0	0	0
			804	503	138	159	4			
1	E	111	Total	C	N	O	S	0	0	0
			832	518	144	166	4			
1	F	111	Total	C	N	O	S	0	0	0
			836	520	144	168	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	-	expression tag	UNP P01833
A	111	GLU	-	expression tag	UNP P01833
A	112	HIS	-	expression tag	UNP P01833
A	113	HIS	-	expression tag	UNP P01833
A	114	HIS	-	expression tag	UNP P01833
A	115	HIS	-	expression tag	UNP P01833
A	116	HIS	-	expression tag	UNP P01833
A	117	HIS	-	expression tag	UNP P01833
B	110	LEU	-	expression tag	UNP P01833
B	111	GLU	-	expression tag	UNP P01833
B	112	HIS	-	expression tag	UNP P01833
B	113	HIS	-	expression tag	UNP P01833
B	114	HIS	-	expression tag	UNP P01833
B	115	HIS	-	expression tag	UNP P01833
B	116	HIS	-	expression tag	UNP P01833
B	117	HIS	-	expression tag	UNP P01833
C	110	LEU	-	expression tag	UNP P01833

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Chain	Residue	Modelled	Actual	Comment	Reference
C	111	GLU	-	expression tag	UNP P01833
C	112	HIS	-	expression tag	UNP P01833
C	113	HIS	-	expression tag	UNP P01833
C	114	HIS	-	expression tag	UNP P01833
C	115	HIS	-	expression tag	UNP P01833
C	116	HIS	-	expression tag	UNP P01833
C	117	HIS	-	expression tag	UNP P01833
D	110	LEU	-	expression tag	UNP P01833
D	111	GLU	-	expression tag	UNP P01833
D	112	HIS	-	expression tag	UNP P01833
D	113	HIS	-	expression tag	UNP P01833
D	114	HIS	-	expression tag	UNP P01833
D	115	HIS	-	expression tag	UNP P01833
D	116	HIS	-	expression tag	UNP P01833
D	117	HIS	-	expression tag	UNP P01833
E	110	LEU	-	expression tag	UNP P01833
E	111	GLU	-	expression tag	UNP P01833
E	112	HIS	-	expression tag	UNP P01833
E	113	HIS	-	expression tag	UNP P01833
E	114	HIS	-	expression tag	UNP P01833
E	115	HIS	-	expression tag	UNP P01833
E	116	HIS	-	expression tag	UNP P01833
E	117	HIS	-	expression tag	UNP P01833
F	110	LEU	-	expression tag	UNP P01833
F	111	GLU	-	expression tag	UNP P01833
F	112	HIS	-	expression tag	UNP P01833
F	113	HIS	-	expression tag	UNP P01833
F	114	HIS	-	expression tag	UNP P01833
F	115	HIS	-	expression tag	UNP P01833
F	116	HIS	-	expression tag	UNP P01833
F	117	HIS	-	expression tag	UNP P01833

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is water.

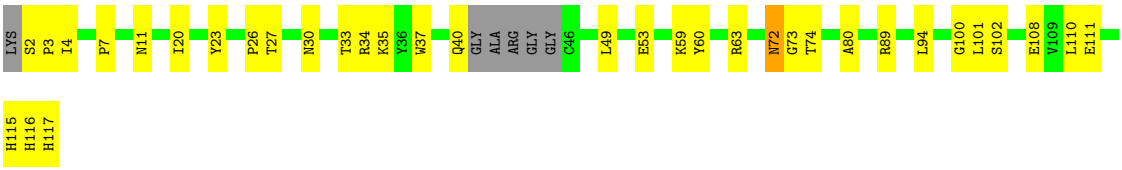
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	B	29	Total O 29 29	0	0
3	C	22	Total O 22 22	0	0
3	D	14	Total O 14 14	0	0
3	E	35	Total O 35 35	0	0
3	F	31	Total O 31 31	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

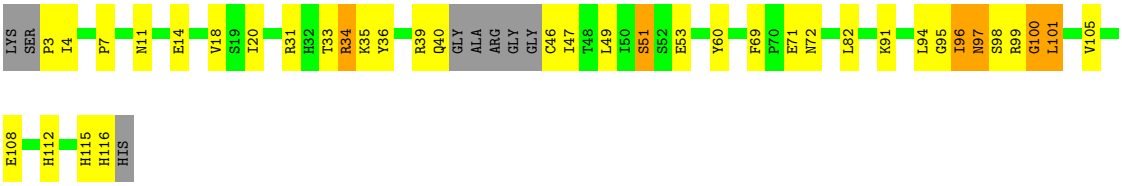
• Molecule 1: Polymeric-immunoglobulin receptor

Chain A:



• Molecule 1: Polymeric-immunoglobulin receptor

Chain B:

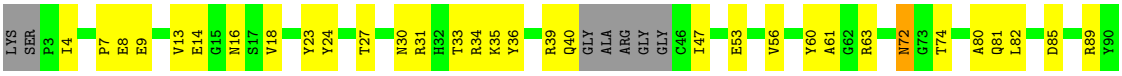


• Molecule 1: Polymeric-immunoglobulin receptor

Chain C:

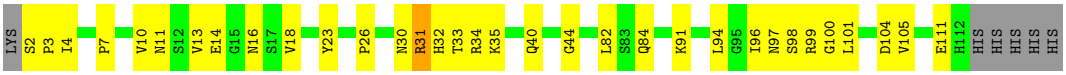
• Molecule 1: Polymeric-immunoglobulin receptor

Chain D:



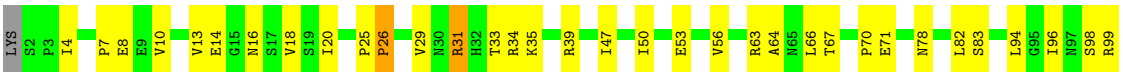
• Molecule 1: Polymeric-immunoglobulin receptor

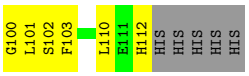
Chain E:



• Molecule 1: Polymeric-immunoglobulin receptor

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.00Å 157.19Å 53.86Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 99.4 (20.00-1.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.244 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.355 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5148	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 8.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG

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	0.36	0/887	0.63	0/1203
1	B	0.37	0/869	0.65	0/1179
1	C	0.38	0/820	0.64	0/1114
1	D	0.38	0/821	0.62	0/1115
1	E	0.41	0/850	0.66	0/1156
1	F	0.38	0/854	0.65	0/1161
All	All	0.38	0/5101	0.64	0/6928

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	865	0	804	27	0
1	B	848	0	793	34	0
1	C	803	0	751	36	0
1	D	804	0	754	37	0
1	E	832	0	775	23	0
1	F	836	0	779	29	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	27	0	0	1	0
3	B	29	0	0	0	0
3	C	22	0	0	1	0
3	D	14	0	0	0	0
3	E	35	0	0	0	0
3	F	31	0	0	0	0
All	All	5148	0	4656	177	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 18.

The worst 5 of 177 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:34:ARG:HG3	1:A:53:GLU:HG2	1.44	0.98
1:D:4:ILE:HD11	1:D:94:LEU:HG	1.51	0.92
1:E:4:ILE:HD11	1:E:101:LEU:HG	1.58	0.86
1:F:18:VAL:HG13	1:F:82:LEU:HD11	1.59	0.83
1:D:91:LYS:HE2	1:D:104:ASP:OD1	1.84	0.78

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	107/117 (92%)	100 (94%)	6 (6%)	1 (1%)	14 7
1	B	105/117 (90%)	98 (93%)	3 (3%)	4 (4%)	2 0
1	C	101/117 (86%)	92 (91%)	8 (8%)	1 (1%)	13 5
1	D	101/117 (86%)	91 (90%)	10 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	109/117 (93%)	100 (92%)	7 (6%)	2 (2%)	7 2
1	F	109/117 (93%)	98 (90%)	7 (6%)	4 (4%)	2 0
All	All	632/702 (90%)	579 (92%)	41 (6%)	12 (2%)	6 1

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	LEU
1	F	63	ARG
1	B	97	ASN
1	B	99	ARG
1	E	99	ARG

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	97/101 (96%)	96 (99%)	1 (1%)	73 74
1	B	95/101 (94%)	91 (96%)	4 (4%)	25 18
1	C	89/101 (88%)	81 (91%)	8 (9%)	8 3
1	D	90/101 (89%)	87 (97%)	3 (3%)	33 26
1	E	91/101 (90%)	89 (98%)	2 (2%)	47 43
1	F	92/101 (91%)	91 (99%)	1 (1%)	70 71
All	All	554/606 (91%)	535 (97%)	19 (3%)	32 25

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	85	ASP
1	E	34	ARG
1	F	31	ARG
1	E	31	ARG
1	C	63	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	72	ASN
1	F	84	GLN
1	D	40	GLN
1	F	32	HIS
1	D	30	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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 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, 95^{th} 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	111/117 (94%)	-1.22	0	100	100	19, 29, 44, 56	0
1	B	109/117 (93%)	-1.19	0	100	100	19, 30, 47, 61	0
1	C	105/117 (89%)	-1.19	0	100	100	19, 31, 53, 69	0
1	D	105/117 (89%)	-1.12	0	100	100	20, 34, 64, 72	0
1	E	111/117 (94%)	-1.24	0	100	100	19, 28, 44, 52	0
1	F	111/117 (94%)	-1.20	0	100	100	20, 29, 48, 58	0
All	All	652/702 (92%)	-1.19	0	100	100	19, 31, 52, 72	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
2	MG	A	200	1/1	1.00	0.02	18,18,18,18	0
2	MG	B	201	1/1	1.00	0.01	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.