



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5L36 / pdb_00005l36
Title : Crystal Structure of a human FasL mutant in complex with human DcR3
Authors : Liu, W.; Bonanno, J.B.; Almo, S.C.
Deposited on : 2016-08-03
Resolution : 3.10 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
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

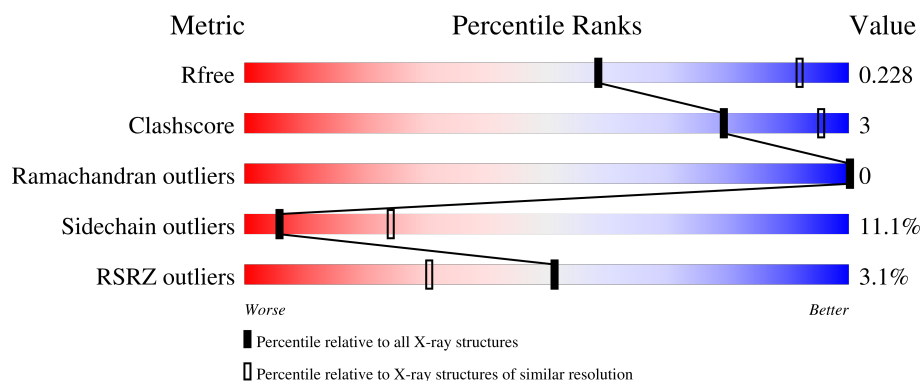
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	B	174	4% 75% 13% 12%
2	A	153	% 68% 21% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2277 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 Tumor necrosis factor receptor superfamily member 6B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	153	Total	C	N	O	S	0	0	0
			1167	706	224	219	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	196	THR	-	expression tag	UNP O95407
B	197	GLY	-	expression tag	UNP O95407
B	198	HIS	-	expression tag	UNP O95407
B	199	HIS	-	expression tag	UNP O95407
B	200	HIS	-	expression tag	UNP O95407
B	201	HIS	-	expression tag	UNP O95407
B	202	HIS	-	expression tag	UNP O95407
B	203	HIS	-	expression tag	UNP O95407

- Molecule 2 is a protein called Tumor necrosis factor ligand superfamily member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	138	Total	C	N	O	S	0	0	0
			1106	713	184	200	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	MET	-	initiating methionine	UNP P48023
A	164	HIS	ASP	conflict	UNP P48023
A	165	GLU	THR	conflict	UNP P48023
A	166	LEU	TYR	conflict	UNP P48023
A	168	LEU	ILE	conflict	UNP P48023
A	169	ALA	VAL	conflict	UNP P48023

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0

- Molecule 4 is water.

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

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	127.27Å 127.27Å 206.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 3.10 50.01 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.01-3.10) 98.9 (50.01-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.178 , 0.223 0.184 , 0.228	Depositor DCC
R_{free} test set	570 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2277	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: NA

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	B	1.12	0/1204	1.18	4/1642 (0.2%)
2	A	1.18	2/1131 (0.2%)	1.21	3/1521 (0.2%)
All	All	1.15	2/2335 (0.1%)	1.19	7/3163 (0.2%)

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
2	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	183	ILE	CA-C	-5.22	1.47	1.52
2	A	264	LEU	N-CA	-5.07	1.40	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	SER	N-CA-C	7.34	114.83	108.22
2	A	262	SER	N-CA-C	6.83	120.09	111.69
2	A	248	VAL	CB-CA-C	-5.99	102.53	110.98
2	A	260	ASN	N-CA-CB	-5.58	102.91	111.56
1	B	158	PHE	N-CA-C	5.49	117.14	108.96
1	B	146	GLN	N-CA-C	5.34	117.19	109.07
1	B	105	CYS	N-CA-C	-5.30	102.01	109.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	260	ASN	Peptide

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	B	1167	0	1052	4	0
2	A	1106	0	1101	8	1
3	B	1	0	0	0	0
4	A	3	0	0	0	0
All	All	2277	0	2153	12	1

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 3.

All (12) 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:129:HIS:CD2	1:B:142:GLY:HA3	2.31	0.66
2:A:184:ASN:C	2:A:184:ASN:HD22	2.06	0.62
2:A:149:LEU:HB3	2:A:162:TRP:HB3	1.94	0.49
1:B:154:PRO:O	1:B:157:THR:OG1	2.28	0.49
2:A:146:VAL:HG12	2:A:172:SER:HB3	1.97	0.47
1:B:140:ALA:HB3	1:B:149:GLN:HG3	1.99	0.45
1:B:153:CYS:HB2	1:B:187:SER:HB2	1.98	0.44
2:A:278:LEU:C	2:A:278:LEU:HD12	2.42	0.44
2:A:184:ASN:C	2:A:184:ASN:ND2	2.76	0.43
2:A:194:LYS:HA	2:A:243:SER:O	2.20	0.41
2:A:176:TYR:HA	2:A:180:GLY:O	2.20	0.41
2:A:185:GLU:O	2:A:186:THR:C	2.61	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:279:TYR:OH	2:A:279:TYR:OH[2_555]	2.02	0.18

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	B	149/174 (86%)	138 (93%)	11 (7%)	0	100	100
2	A	134/153 (88%)	128 (96%)	6 (4%)	0	100	100
All	All	283/327 (86%)	266 (94%)	17 (6%)	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	B	130/146 (89%)	119 (92%)	11 (8%)	10	35
2	A	122/136 (90%)	105 (86%)	17 (14%)	3	15
All	All	252/282 (89%)	224 (89%)	28 (11%)	6	24

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	33	THR
1	B	45	GLU
1	B	94	LEU

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Mol	Chain	Res	Type
1	B	97	GLU
1	B	103	ARG
1	B	145	SER
1	B	148	THR
1	B	161	SER
1	B	188	SER
1	B	192	LEU
1	B	193	CYS
2	A	152	LYS
2	A	156	ARG
2	A	157	SER
2	A	184	ASN
2	A	195	VAL
2	A	200	GLN
2	A	205	LEU
2	A	206	PRO
2	A	213	MET
2	A	216	SER
2	A	228	LYS
2	A	234	THR
2	A	237	GLN
2	A	242	SER
2	A	253	SER
2	A	261	VAL
2	A	268	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	169	GLN
2	A	184	ASN
2	A	268	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 1 ligands modelled in this entry, 1 is 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 [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	B	153/174 (87%)	0.11	7 (4%) 37 20	35, 61, 120, 146	0
2	A	138/153 (90%)	-0.46	2 (1%) 73 53	26, 45, 75, 124	0
All	All	291/327 (88%)	-0.16	9 (3%) 51 30	26, 50, 109, 146	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	CYS	5.9
1	B	192	LEU	3.7
2	A	155	SER	3.1
1	B	43	THR	2.6
2	A	143	LEU	2.6
1	B	184	PRO	2.6
1	B	41	ALA	2.3
1	B	64	ARG	2.1
1	B	44	GLY	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
3	NA	B	301	1/1	0.98	0.16	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.