



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:34 am GMT

PDB ID : 4NSO
Title : Crystal structure of the effector-immunity protein complex
Authors : Dong, C.
Deposited on : 2013-11-28
Resolution : 2.40 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

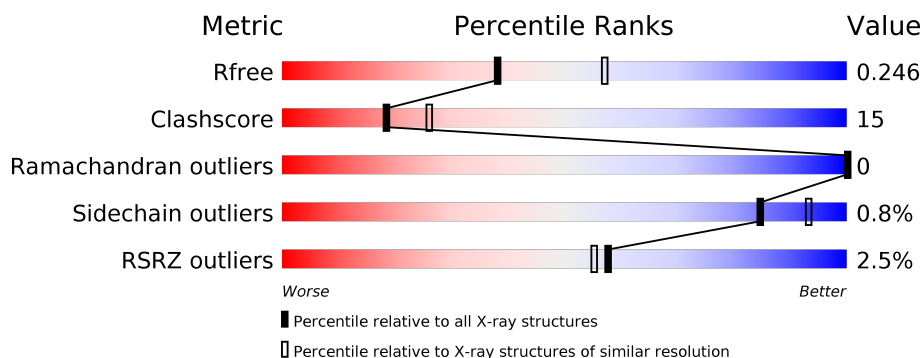
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	301	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>11%</div> <div>35%</div> </div> </div>
2	B	108	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>13%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2450 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 Effector protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	Se	0	0	0
			1591	1014	277	296	1	3			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	717	MSE	-	EXPRESSION TAG	UNP Q9KN42
A	718	ALA	-	EXPRESSION TAG	UNP Q9KN42
A	719	SER	-	EXPRESSION TAG	UNP Q9KN42
A	720	MSE	-	EXPRESSION TAG	UNP Q9KN42
A	721	THR	-	EXPRESSION TAG	UNP Q9KN42
A	722	GLY	-	EXPRESSION TAG	UNP Q9KN42
A	723	GLY	-	EXPRESSION TAG	UNP Q9KN42
A	724	GLN	-	EXPRESSION TAG	UNP Q9KN42
A	725	GLN	-	EXPRESSION TAG	UNP Q9KN42
A	726	MSE	-	EXPRESSION TAG	UNP Q9KN42
A	727	GLY	-	EXPRESSION TAG	UNP Q9KN42
A	728	ARG	-	EXPRESSION TAG	UNP Q9KN42
A	729	GLY	-	EXPRESSION TAG	UNP Q9KN42
A	730	SER	-	EXPRESSION TAG	UNP Q9KN42
A	1010	LEU	-	EXPRESSION TAG	UNP Q9KN42
A	1011	GLU	-	EXPRESSION TAG	UNP Q9KN42
A	1012	HIS	-	EXPRESSION TAG	UNP Q9KN42
A	1013	HIS	-	EXPRESSION TAG	UNP Q9KN42
A	1014	HIS	-	EXPRESSION TAG	UNP Q9KN42
A	1015	HIS	-	EXPRESSION TAG	UNP Q9KN42
A	1016	HIS	-	EXPRESSION TAG	UNP Q9KN42
A	1017	HIS	-	EXPRESSION TAG	UNP Q9KN42

- Molecule 2 is a protein called Immunity protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	B	94	Total	C	N	O	S	Se	0	0	0
			752	471	127	148	3	3			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	MSE	-	EXPRESSION TAG	UNP Q9KN41
B	25	GLY	-	EXPRESSION TAG	UNP Q9KN41
B	123	LEU	-	EXPRESSION TAG	UNP Q9KN41
B	124	LEU	-	EXPRESSION TAG	UNP Q9KN41
B	125	GLU	-	EXPRESSION TAG	UNP Q9KN41
B	126	HIS	-	EXPRESSION TAG	UNP Q9KN41
B	127	HIS	-	EXPRESSION TAG	UNP Q9KN41
B	128	HIS	-	EXPRESSION TAG	UNP Q9KN41
B	129	HIS	-	EXPRESSION TAG	UNP Q9KN41
B	130	HIS	-	EXPRESSION TAG	UNP Q9KN41
B	131	HIS	-	EXPRESSION TAG	UNP Q9KN41

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total	O	0	0
			67	67		
3	B	40	Total	O	0	0
			40	40		

- Molecule 1: Effector protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.63Å 78.66Å 47.86Å 90.00° 101.52° 90.00°	Depositor
Resolution (Å)	38.16 – 2.40 40.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.8 (38.16-2.40) 96.4 (40.50-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.215 , 0.259 0.207 , 0.246	Depositor DCC
R_{free} test set	1846 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2450	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.96% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/1626	0.51	0/2186
2	B	0.49	0/758	0.56	0/1014
All	All	0.45	0/2384	0.53	0/3200

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	960	GLU	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	A	1591	0	1558	60	5
2	B	752	0	746	10	5
3	A	67	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	40	0	0	3	0
All	All	2450	0	2304	69	5

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 15.

All (69) 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:929:ARG:CG	1:A:1011:GLU:OE1	1.74	1.35
1:A:929:ARG:CB	1:A:1011:GLU:OE1	1.73	1.33
1:A:1008:GLU:O	1:A:1011:GLU:CG	1.74	1.32
1:A:1008:GLU:HG2	1:A:1011:GLU:OE2	1.21	1.32
1:A:929:ARG:HG2	1:A:1011:GLU:CB	1.57	1.31
1:A:1008:GLU:CG	1:A:1011:GLU:OE2	1.86	1.22
1:A:1008:GLU:O	1:A:1011:GLU:HG2	0.94	1.10
1:A:929:ARG:HG2	1:A:1011:GLU:OE1	1.41	1.09
1:A:929:ARG:HB3	1:A:1011:GLU:OE1	1.52	1.09
1:A:929:ARG:CG	1:A:1011:GLU:CB	2.36	1.04
1:A:929:ARG:HG2	1:A:1011:GLU:HB2	1.37	1.03
1:A:907:LYS:NZ	3:A:1151:HOH:O	1.92	1.01
1:A:929:ARG:CG	1:A:1011:GLU:HB2	1.90	1.01
1:A:853:MSE:HE1	1:A:863:TYR:CD2	1.97	0.99
1:A:929:ARG:CD	1:A:1011:GLU:HB2	1.93	0.97
1:A:975:LYS:NZ	3:A:1161:HOH:O	1.79	0.96
1:A:929:ARG:HG2	1:A:1011:GLU:HB3	1.48	0.92
1:A:1008:GLU:C	1:A:1011:GLU:HG2	1.89	0.90
1:A:929:ARG:HG2	1:A:1011:GLU:CD	1.91	0.90
1:A:1011:GLU:O	1:A:1012:HIS:HB2	1.71	0.88
1:A:929:ARG:HG2	1:A:1011:GLU:CG	2.03	0.88
1:A:1008:GLU:CD	1:A:1011:GLU:OE2	2.16	0.83
2:B:124:LEU:HD12	2:B:124:LEU:C	2.01	0.81
2:B:124:LEU:CD1	2:B:124:LEU:C	2.50	0.80
1:A:1011:GLU:O	1:A:1012:HIS:CB	2.33	0.77
1:A:929:ARG:CG	1:A:1011:GLU:HB3	2.10	0.75
1:A:929:ARG:CD	1:A:1011:GLU:CB	2.64	0.74
1:A:929:ARG:HD3	1:A:1011:GLU:HB2	1.70	0.71
1:A:865:GLN:NE2	3:A:1143:HOH:O	2.28	0.67
1:A:1008:GLU:O	1:A:1011:GLU:CD	2.33	0.66
1:A:929:ARG:HB2	1:A:1011:GLU:OE1	1.90	0.65
1:A:1011:GLU:CD	3:A:1113:HOH:O	2.39	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:ARG:HD2	1:A:930:ALA:H	1.68	0.59
2:B:74:GLN:NE2	3:B:231:HOH:O	2.20	0.57
1:A:929:ARG:NE	1:A:1011:GLU:CB	2.68	0.56
1:A:1011:GLU:HG3	1:A:1012:HIS:N	2.21	0.56
1:A:817:TRP:CD1	1:A:930:ALA:HB1	2.41	0.56
2:B:69:ASP:OD2	2:B:69:ASP:N	2.37	0.56
1:A:1008:GLU:OE2	1:A:1011:GLU:OE2	2.25	0.55
1:A:1008:GLU:HG2	1:A:1011:GLU:CD	2.17	0.54
1:A:1008:GLU:HA	1:A:1011:GLU:CD	2.28	0.53
2:B:69:ASP:OD1	2:B:73:LYS:HE3	2.08	0.52
1:A:894:TYR:HB3	1:A:897:GLU:HB2	1.92	0.50
1:A:986:SER:OG	1:A:989:TRP:HD1	1.94	0.49
2:B:83:MSE:SE	2:B:97:MSE:HE2	2.61	0.49
1:A:853:MSE:SE	1:A:863:TYR:HB2	2.63	0.49
1:A:1008:GLU:O	1:A:1011:GLU:OE2	2.32	0.47
1:A:1011:GLU:O	1:A:1012:HIS:CG	2.67	0.47
2:B:109:ASP:OD1	3:B:230:HOH:O	2.20	0.47
1:A:853:MSE:SE	1:A:863:TYR:CB	3.13	0.47
2:B:54:ARG:O	3:B:234:HOH:O	2.20	0.47
1:A:954:LEU:HG	1:A:962:MSE:HE1	1.96	0.46
1:A:842:ASP:OD2	2:B:71:TYR:OH	2.31	0.45
1:A:925:PHE:C	1:A:927:HIS:HA	2.35	0.45
1:A:960:GLU:O	1:A:961:SER:HB3	2.16	0.45
1:A:987:PRO:HA	1:A:990:TRP:CE2	2.51	0.45
1:A:911:TYR:OH	1:A:933:HIS:ND1	2.33	0.45
1:A:1011:GLU:CG	1:A:1012:HIS:N	2.79	0.45
2:B:124:LEU:C	2:B:124:LEU:HD13	2.37	0.43
1:A:926:GLU:N	1:A:927:HIS:HA	2.34	0.42
1:A:1011:GLU:O	1:A:1012:HIS:CD2	2.73	0.42
1:A:1011:GLU:HG3	1:A:1012:HIS:H	1.83	0.41
1:A:967:ILE:O	1:A:971:VAL:HG13	2.21	0.41
1:A:929:ARG:HE	1:A:1011:GLU:HB3	1.86	0.41
1:A:935:LEU:HD11	1:A:971:VAL:CG2	2.51	0.41
1:A:927:HIS:HB2	1:A:933:HIS:NE2	2.37	0.40
1:A:853:MSE:HE1	1:A:863:TYR:CG	2.51	0.40
1:A:1011:GLU:CG	1:A:1012:HIS:H	2.34	0.40
1:A:826:TYR:CD1	1:A:996:ARG:HD2	2.57	0.40

All (5) 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)
1:A:921:LYS:NZ	2:B:124:LEU:CD2[2_656]	0.51	1.69
1:A:921:LYS:NZ	2:B:124:LEU:CG[2_656]	1.10	1.10
1:A:921:LYS:CE	2:B:124:LEU:CD2[2_656]	1.71	0.49
1:A:921:LYS:NZ	2:B:124:LEU:CD1[2_656]	2.07	0.13
1:A:921:LYS:NZ	2:B:124:LEU:CB[2_656]	2.10	0.10

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	195/301 (65%)	185 (95%)	10 (5%)	0	100	100
2	B	92/108 (85%)	90 (98%)	2 (2%)	0	100	100
All	All	287/409 (70%)	275 (96%)	12 (4%)	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	171/246 (70%)	170 (99%)	1 (1%)	89	95
2	B	86/95 (90%)	85 (99%)	1 (1%)	75	88
All	All	257/341 (75%)	255 (99%)	2 (1%)	85	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	898	PHE
2	B	124	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	910	HIS
1	A	1012	HIS

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](#)

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 [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	194/301 (64%)	-0.23	6 (3%)	49 47	31, 50, 97, 140	0
2	B	91/108 (84%)	-0.35	1 (1%)	80 79	27, 37, 82, 117	0
All	All	285/409 (69%)	-0.27	7 (2%)	58 55	27, 46, 96, 140	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	926	GLU	3.5
1	A	924	LEU	2.8
1	A	961	SER	2.7
1	A	929	ARG	2.4
1	A	919	ARG	2.3
1	A	927	HIS	2.2
2	B	60	LYS	2.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.