



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:06 am GMT

PDB ID : 5AO6
Title : Endo180 D1-4, trigonal form
Authors : Paracuellos, P.; Briggs, D.C.; Carafoli, F.; Loncar, T.; Hohenester, E.
Deposited on : 2015-09-09
Resolution : 3.36 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

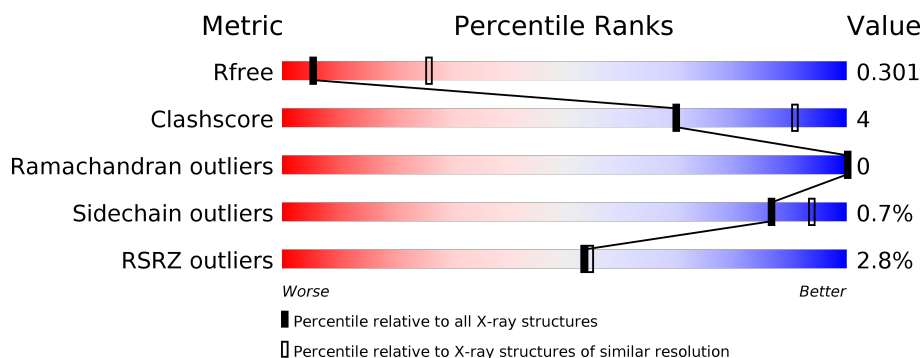
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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	1156 (3.42-3.30)
Clashscore	112137	1231 (3.42-3.30)
Ramachandran outliers	110173	1212 (3.42-3.30)
Sidechain outliers	110143	1211 (3.42-3.30)
RSRZ outliers	101464	1165 (3.42-3.30)

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	491	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>12%</div> </div> </div>
1	B	491	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>11%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12948 atoms, of which 6115 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 C-TYPE MANNOSE RECEPTOR 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	430	Total	C	H	N	O	S	0	0	0
			6361	2127	2990	574	644	26			
1	B	436	Total	C	H	N	O	S	0	0	0
			6587	2176	3125	601	659	26			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	-	EXPRESSION TAG	UNP Q9UBG0
A	32	PRO	-	EXPRESSION TAG	UNP Q9UBG0
A	33	LEU	-	EXPRESSION TAG	UNP Q9UBG0
A	34	ALA	-	EXPRESSION TAG	UNP Q9UBG0
A	512	GLY	-	EXPRESSION TAG	UNP Q9UBG0
A	513	ALA	-	EXPRESSION TAG	UNP Q9UBG0
A	514	ALA	-	EXPRESSION TAG	UNP Q9UBG0
A	515	ALA	-	EXPRESSION TAG	UNP Q9UBG0
A	516	HIS	-	EXPRESSION TAG	UNP Q9UBG0
A	517	HIS	-	EXPRESSION TAG	UNP Q9UBG0
A	518	HIS	-	EXPRESSION TAG	UNP Q9UBG0
A	519	HIS	-	EXPRESSION TAG	UNP Q9UBG0
A	520	HIS	-	EXPRESSION TAG	UNP Q9UBG0
A	521	HIS	-	EXPRESSION TAG	UNP Q9UBG0
B	31	ALA	-	EXPRESSION TAG	UNP Q9UBG0
B	32	PRO	-	EXPRESSION TAG	UNP Q9UBG0
B	33	LEU	-	EXPRESSION TAG	UNP Q9UBG0
B	34	ALA	-	EXPRESSION TAG	UNP Q9UBG0
B	512	GLY	-	EXPRESSION TAG	UNP Q9UBG0
B	513	ALA	-	EXPRESSION TAG	UNP Q9UBG0
B	514	ALA	-	EXPRESSION TAG	UNP Q9UBG0
B	515	ALA	-	EXPRESSION TAG	UNP Q9UBG0
B	516	HIS	-	EXPRESSION TAG	UNP Q9UBG0
B	517	HIS	-	EXPRESSION TAG	UNP Q9UBG0
B	518	HIS	-	EXPRESSION TAG	UNP Q9UBG0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	519	HIS	-	EXPRESSION TAG	UNP Q9UBG0
B	520	HIS	-	EXPRESSION TAG	UNP Q9UBG0
B	521	HIS	-	EXPRESSION TAG	UNP Q9UBG0

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.00Å 87.00Å 321.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.21 – 3.36 68.21 – 3.36	Depositor EDS
% Data completeness (in resolution range)	99.1 (68.21-3.36) 99.0 (68.21-3.36)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.220 , 0.306 0.238 , 0.301	Depositor DCC
R_{free} test set	1064 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12948	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.62% 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

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	0.30	0/3470	0.48	0/4727
1	B	0.30	0/3561	0.50	0/4840
All	All	0.30	0/7031	0.49	0/9567

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	3371	2990	3048	37	1
1	B	3462	3125	3171	18	0
All	All	6833	6115	6219	55	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 4.

All (55) 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:69:ASN:HB3	1:A:72:LEU:CD1	2.07	0.83
1:A:69:ASN:HB3	1:A:72:LEU:HD13	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:TYR:CE1	1:A:505:LYS:HB2	2.24	0.71
1:A:62:VAL:HG21	1:A:107:LEU:CD2	2.22	0.69
1:B:236:GLU:O	1:B:237:THR:OG1	2.12	0.67
1:A:419:SER:HB3	1:A:505:LYS:HE3	1.77	0.67
1:B:323:GLU:OE2	1:B:339:ARG:NH1	2.30	0.64
1:A:394:TYR:CD1	1:A:505:LYS:HB2	2.35	0.62
1:B:339:ARG:NH2	1:B:341:GLU:OE1	2.34	0.61
1:A:206:ARG:NH2	1:A:208:ASP:OD2	2.33	0.61
1:B:477:SER:O	1:B:479:GLU:N	2.35	0.60
1:B:166:ASP:OD1	1:B:167:LEU:N	2.35	0.59
1:A:286:ASN:N	1:A:287:GLY:HA3	2.17	0.58
1:B:286:ASN:N	1:B:287:GLY:HA3	2.18	0.58
1:A:306:SER:O	1:A:490:ARG:NH1	2.36	0.58
1:A:69:ASN:HB3	1:A:72:LEU:HD12	1.85	0.58
1:A:293:SER:HA	1:A:340:THR:HG21	1.86	0.57
1:B:383:GLU:HB3	1:B:384:PRO:HD2	1.86	0.57
1:A:444:LEU:HD23	1:A:482:VAL:HG21	1.88	0.56
1:A:110:TYR:HB3	1:A:114:ARG:HD3	1.88	0.55
1:B:163:SER:O	1:B:165:GLU:N	2.41	0.53
1:A:394:TYR:HE1	1:A:505:LYS:HB2	1.72	0.53
1:B:286:ASN:ND2	1:B:343:SER:O	2.43	0.52
1:A:383:GLU:HB3	1:A:384:PRO:HD2	1.91	0.50
1:A:107:LEU:HD12	1:A:133:LEU:HD22	1.94	0.49
1:A:242:ASP:HB2	1:A:284:TYR:CE2	2.48	0.48
1:B:40:GLU:N	1:B:41:PRO:CD	2.77	0.47
1:B:323:GLU:OE2	1:B:342:SER:OG	2.28	0.47
1:B:296:LEU:HG	1:B:356:PRO:HB2	1.96	0.47
1:A:339:ARG:NH2	1:A:341:GLU:OE1	2.47	0.47
1:A:416:ASP:OD1	1:A:417:LEU:N	2.43	0.46
1:A:51:LEU:HD22	1:A:64:VAL:HG11	1.98	0.45
1:A:313:ASP:OD2	1:A:315:SER:OG	2.34	0.45
1:A:419:SER:H	1:A:505:LYS:HD3	1.82	0.45
1:A:394:TYR:OH	1:A:425:GLU:OE2	2.23	0.45
1:A:218:ASP:OD1	1:A:221:LYS:N	2.51	0.44
1:A:40:GLU:N	1:A:41:PRO:CD	2.80	0.44
1:B:434:LYS:NZ	1:B:437:VAL:O	2.38	0.44
1:B:274:LEU:HD21	1:B:285:ILE:HD13	2.00	0.44
1:B:308:GLY:HA2	1:B:310:GLN:HG3	2.01	0.43
1:A:442:ILE:HD11	1:A:482:VAL:HG12	2.01	0.43
1:A:79:TRP:CZ2	1:A:123:CYS:HB3	2.54	0.43
1:A:464:THR:CG2	1:A:466:TRP:CD1	3.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASN:N	1:A:334:ASN:OD1	2.53	0.42
1:A:394:TYR:HE1	1:A:505:LYS:HD2	1.84	0.42
1:A:419:SER:HG	1:A:421:HIS:CE1	2.38	0.42
1:B:382:CYS:SG	1:B:388:PRO:HB3	2.60	0.42
1:B:441:TRP:CE3	1:B:483:THR:HG22	2.54	0.42
1:A:163:SER:O	1:A:165:GLU:N	2.51	0.42
1:B:340:THR:HG23	1:B:341:GLU:N	2.36	0.41
1:A:339:ARG:NH1	1:A:347:GLN:OE1	2.46	0.41
1:A:440:LEU:CD2	1:A:501:PRO:HB2	2.51	0.41
1:A:418:VAL:CG1	1:A:442:ILE:HG22	2.50	0.41
1:A:413:GLY:O	1:A:506:LYS:NZ	2.42	0.41
1:A:464:THR:HG23	1:A:466:TRP:CD1	2.55	0.40

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)
1:A:124:ARG:NH2	1:A:476:ASP:OD2[5_545]	2.17	0.03

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	422/491 (86%)	393 (93%)	29 (7%)	0	100	100
1	B	428/491 (87%)	402 (94%)	26 (6%)	0	100	100
All	All	850/982 (87%)	795 (94%)	55 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	357/424 (84%)	353 (99%)	4 (1%)	78	89
1	B	371/424 (88%)	370 (100%)	1 (0%)	94	98
All	All	728/848 (86%)	723 (99%)	5 (1%)	87	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	246	ASP
1	A	278	GLU
1	A	411	LEU
1	B	107	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	210	HIS
1	A	250	GLN
1	A	269	GLN
1	A	467	HIS

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 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

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	430/491 (87%)	0.47	14 (3%) 47 47	50, 76, 120, 222	0
1	B	436/491 (88%)	0.45	10 (2%) 61 61	39, 70, 104, 147	0
All	All	866/982 (88%)	0.46	24 (2%) 53 54	39, 72, 113, 222	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	VAL	3.9
1	A	46	ILE	3.2
1	B	136	ALA	3.1
1	A	52	GLN	2.8
1	A	68	CYS	2.6
1	B	87	ASN	2.5
1	B	76	ARG	2.5
1	A	77	TRP	2.4
1	B	60	GLY	2.4
1	A	199	HIS	2.3
1	B	77	TRP	2.3
1	B	376	ALA	2.3
1	B	48	SER	2.3
1	B	46	ILE	2.2
1	A	197	TRP	2.2
1	B	155	SER	2.2
1	A	381	GLU	2.2
1	A	380	VAL	2.2
1	A	58	GLN	2.2
1	A	94	LEU	2.1
1	B	65	THR	2.1
1	A	161	TYR	2.1
1	A	346	TRP	2.1
1	A	193	TYR	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 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.