



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:58 AM GMT

PDB ID : 2JIX
Title : Crystal structure of ABT-007 FAB fragment with the soluble domain of EPO receptor
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Deposited on : 2007-07-02
Resolution : 3.20 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

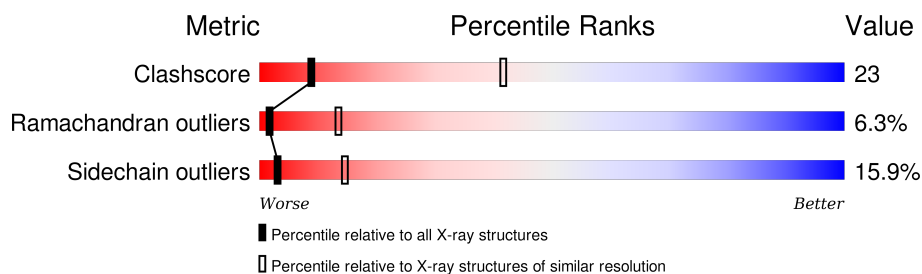
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)



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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	
1	G	214	
1	L	214	
2	B	225	
2	C	225	
2	E	225	
3	D	217	

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Mol	Chain	Length	Quality of chain
3	F	217	 56% 36% 7%
3	H	217	 47% 42% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14781 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 ABT-007 FAB FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1642	1023	281	333	5			
1	G	214	Total	C	N	O	S	0	0	0
			1642	1023	281	333	5			
1	L	214	Total	C	N	O	S	0	0	0
			1642	1023	281	333	5			

- Molecule 2 is a protein called ERYTHROPOIETIN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	1
			1680	1065	297	311	7			
2	C	215	Total	C	N	O	S	0	0	1
			1665	1056	295	307	7			
2	E	217	Total	C	N	O	S	0	0	1
			1680	1065	297	311	7			

- Molecule 3 is a protein called ABT-007 FAB FRAGMENT.

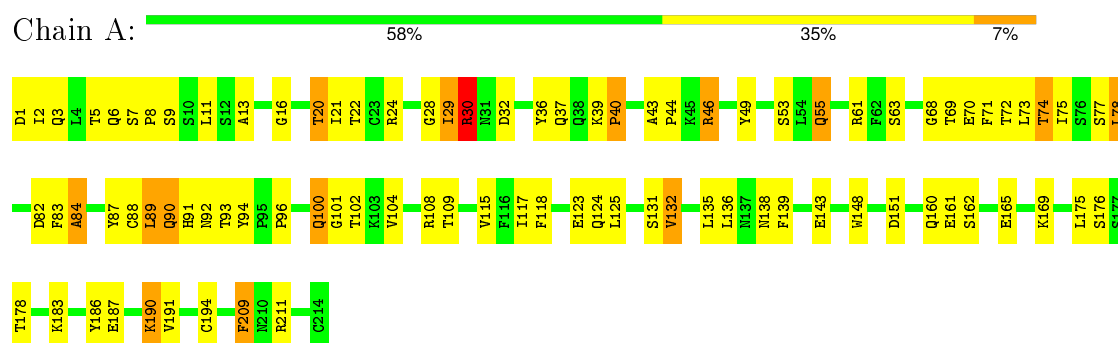
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	217	Total	C	N	O	S	0	0	1
			1607	1015	268	320	4			
3	F	217	Total	C	N	O	S	0	0	1
			1607	1015	268	320	4			
3	H	217	Total	C	N	O	S	0	0	0
			1616	1021	269	322	4			

3 Residue-property plots

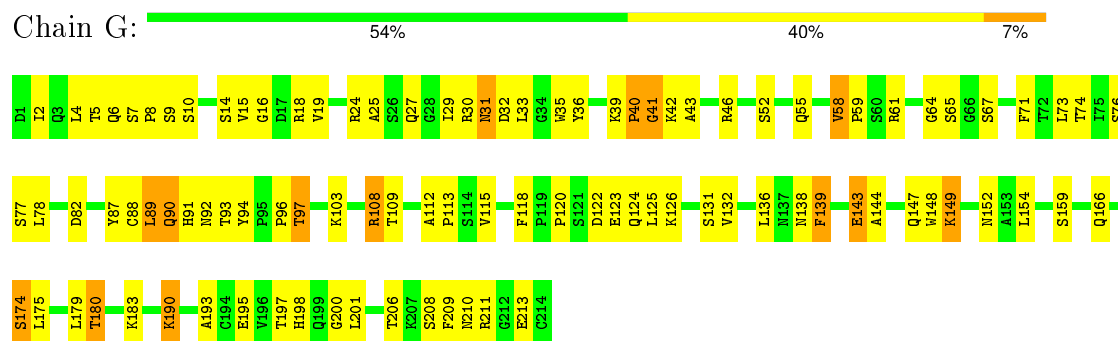
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

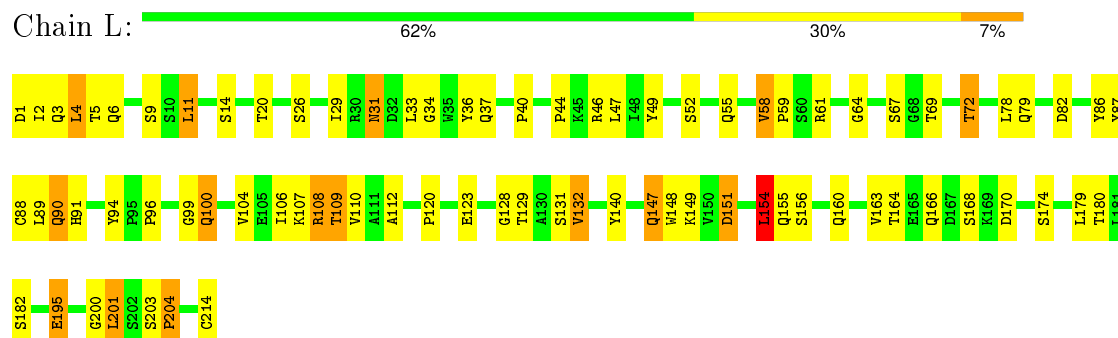
• Molecule 1: ABT-007 FAB FRAGMENT



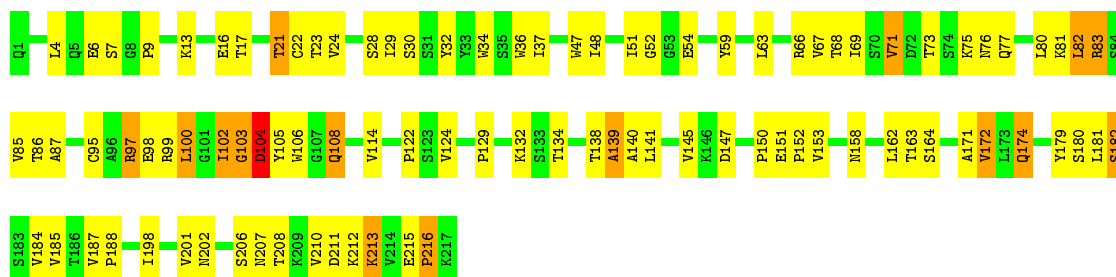
• Molecule 1: ABT-007 FAB FRAGMENT



• Molecule 1: ABT-007 FAB FRAGMENT

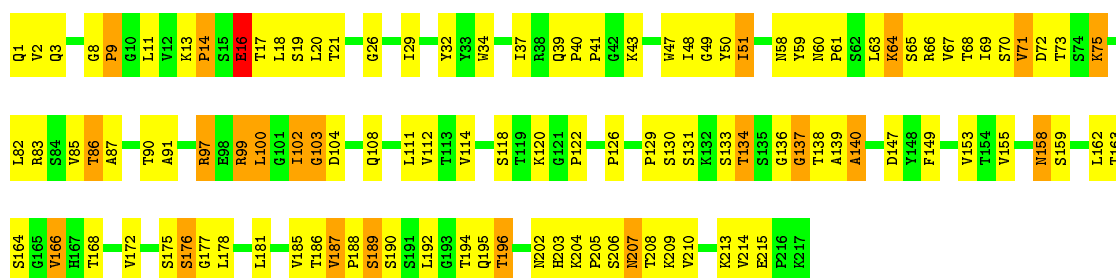


Chain F:  56% 36% 7%



• Molecule 3: ABT-007 FAB FRAGMENT

Chain H:  47% 42% 10%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.95Å 156.17Å 164.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.23 – 3.20	Depositor
% Data completeness (in resolution range)	97.3 (113.23-3.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.257 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14781	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

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	0.60	3/1677 (0.2%)	3.73	17/2275 (0.7%)
1	G	0.66	3/1677 (0.2%)	3.74	16/2275 (0.7%)
1	L	0.53	0/1677	0.67	0/2275
2	B	0.70	0/1726	0.82	1/2356 (0.0%)
2	C	0.83	2/1710 (0.1%)	0.80	3/2333 (0.1%)
2	E	0.70	0/1726	0.76	0/2356
3	D	0.56	0/1646	0.73	2/2249 (0.1%)
3	F	0.50	0/1646	0.66	0/2249
3	H	0.54	0/1655	0.70	0/2258
All	All	0.63	8/15140 (0.1%)	1.87	39/20626 (0.2%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	67	CYS	CB-SG	16.80	2.10	1.82
1	A	209	PHE	CD1-CE1	5.63	1.50	1.39
1	G	139	PHE	CD1-CE1	5.43	1.50	1.39
1	A	139	PHE	CD1-CE1	5.25	1.49	1.39
1	G	209	PHE	CD2-CE2	5.18	1.49	1.39

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	PHE	CZ-CE2-CD2	-58.96	49.35	120.10
1	A	139	PHE	CZ-CE2-CD2	-58.49	49.91	120.10
1	G	209	PHE	CD1-CE1-CZ	-58.43	49.99	120.10
1	G	139	PHE	CZ-CE2-CD2	-58.35	50.08	120.10
1	G	139	PHE	CD1-CE1-CZ	-58.12	50.36	120.10

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	1642	0	1599	78	0
1	G	1642	0	1599	72	0
1	L	1642	0	1599	56	0
2	B	1680	0	1633	89	0
2	C	1665	0	1624	100	0
2	E	1680	0	1633	65	0
3	D	1607	0	1592	84	0
3	F	1607	0	1592	102	0
3	H	1616	0	1605	79	0
All	All	14781	0	14476	685	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 23.

The worst 5 of 685 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)
2:C:67:CYS:SG	2:C:67:CYS:CB	2.10	1.38
2:E:201:ALA:O	2:E:205:PHE:HD1	1.32	1.11
3:H:102:ILE:HG22	3:H:103:GLY:H	1.06	1.11
3:F:102:ILE:HG13	3:F:106:TRP:HE1	0.99	1.10
2:B:87:THR:HA	2:B:90:THR:OG1	1.55	1.07

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	212/214 (99%)	176 (83%)	30 (14%)	6 (3%)	6	37
1	G	212/214 (99%)	178 (84%)	27 (13%)	7 (3%)	5	32
1	L	212/214 (99%)	188 (89%)	17 (8%)	7 (3%)	5	32
2	B	215/225 (96%)	172 (80%)	28 (13%)	15 (7%)	1	10
2	C	213/225 (95%)	163 (76%)	33 (16%)	17 (8%)	1	7
2	E	215/225 (96%)	169 (79%)	30 (14%)	16 (7%)	1	9
3	D	215/217 (99%)	163 (76%)	31 (14%)	21 (10%)	1	4
3	F	215/217 (99%)	164 (76%)	37 (17%)	14 (6%)	1	13
3	H	215/217 (99%)	161 (75%)	36 (17%)	18 (8%)	1	6
All	All	1924/1968 (98%)	1534 (80%)	269 (14%)	121 (6%)	2	13

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	123	GLU
2	B	116	ASN
2	B	168	SER
2	C	23	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	187/187 (100%)	163 (87%)	24 (13%)	5	25
1	G	187/187 (100%)	163 (87%)	24 (13%)	5	25
1	L	187/187 (100%)	159 (85%)	28 (15%)	3	17
2	B	178/186 (96%)	143 (80%)	35 (20%)	1	8
2	C	176/186 (95%)	141 (80%)	35 (20%)	1	8
2	E	178/186 (96%)	150 (84%)	28 (16%)	3	15
3	D	184/185 (100%)	149 (81%)	35 (19%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	184/185 (100%)	168 (91%)	16 (9%)	13	45
3	H	185/185 (100%)	148 (80%)	37 (20%)	1	8
All	All	1646/1674 (98%)	1384 (84%)	262 (16%)	3	14

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	144	LEU
2	E	159	ASP
1	L	46	ARG
3	D	172	VAL
2	E	37	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	108	GLN
2	E	170	GLN
1	L	160	GLN
3	D	158	ASN
3	F	5	GLN

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.