wwPDB X-ray Structure Validation Summary Report (i)

Mar 8, 2026 – 06:01 PM UTC

PDB ID	:	12E8 / pdb_000012e8
Title	:	2E8 FAB FRAGMENT
Authors	:	Rupp, B.; Trakhanov, S.
Deposited on	:	1998-03-14
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:

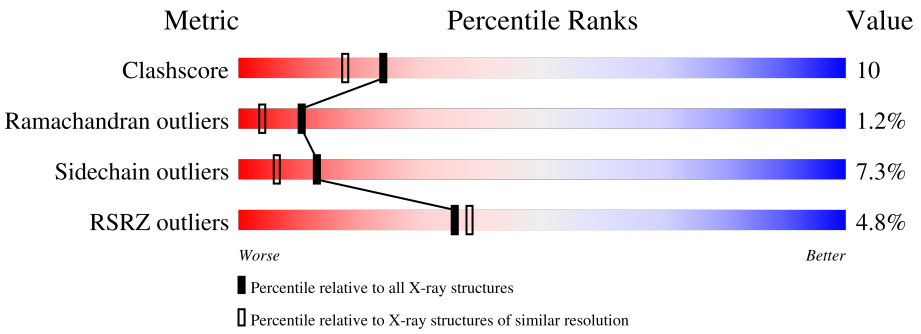
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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	L	214	2%, 76%, 22%, •
1	M	214	2%, 79%, 19%, •
2	H	221	5%, 71%, 26%, •
2	P	221	9%, 72%, 23%, 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7429 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 IGG1-KAPPA 2E8 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	214	1649	1020	277	342	10	0	0	0
1	M	214	1649	1020	277	342	10	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	21	ILE	VAL	conflict	GB 10121892
L	32	ALA	ASN	conflict	GB 10121892
L	46	LEU	ALA	conflict	GB 10121892
L	47	MET	LEU	conflict	GB 10121892
L	53	ASN	TYR	conflict	GB 10121892
L	56	THR	SER	conflict	GB 10121892
L	78	MET	VAL	conflict	GB 10121892
L	85	ASP	GLU	conflict	GB 10121892
L	92	SER	ASN	conflict	GB 10121892
L	163	ALA	TRP	conflict	GB 10121892
M	21	ILE	VAL	conflict	GB 10121892
M	32	ALA	ASN	conflict	GB 10121892
M	46	LEU	ALA	conflict	GB 10121892
M	47	MET	LEU	conflict	GB 10121892
M	53	ASN	TYR	conflict	GB 10121892
M	56	THR	SER	conflict	GB 10121892
M	78	MET	VAL	conflict	GB 10121892
M	85	ASP	GLU	conflict	GB 10121892
M	92	SER	ASN	conflict	GB 10121892
M	163	ALA	TRP	conflict	GB 10121892

- Molecule 2 is a protein called IGG1-KAPPA 2E8 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	221	1682	1064	276	336	6	40	0	0
2	P	221	1682	1064	276	336	6	40	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	3	GLN	LYS	conflict	PIR S49220
H	5	GLN	LEU	conflict	PIR S49220
H	6	GLN	GLU	conflict	PIR S49220
H	11	VAL	LEU	conflict	PIR S49220
H	13	ARG	LYS	conflict	PIR S49220
H	32	TYR	THR	conflict	PIR S49220
H	34	ILE	MET	conflict	PIR S49220
H	43	LYS	GLN	conflict	PIR S49220
H	50	TRP	ARG	conflict	PIR S49220
H	53	GLU	ALA	conflict	PIR S49220
H	54	ILE	ASN	conflict	PIR S49220
H	56	ASP	GLU	conflict	PIR S49220
H	57	THR	ILE	conflict	PIR S49220
H	58	GLU	LYS	conflict	PIR S49220
H	60	VAL	ASP	conflict	PIR S49220
H	66	LYS	THR	conflict	PIR S49220
H	69	MET	ILE	conflict	PIR S49220
H	75	SER	THR	conflict	PIR S49220
H	?	-	VAL	deletion	PIR S49220
H	93	ASN	ARG	conflict	PIR S49220
H	94	ALA	ARG	conflict	PIR S49220
H	96	HIS	-	insertion	PIR S49220
H	97	ASP	-	insertion	PIR S49220
H	99	ASP	GLY	conflict	PIR S49220
H	100	ARG	SER	conflict	PIR S49220
H	100A	GLY	SER	conflict	PIR S49220
H	100B	ARG	GLN	conflict	PIR S49220
H	100C	PHE	GLU	conflict	PIR S49220
H	108	LEU	THR	conflict	PIR S49220
H	109	VAL	LEU	conflict	PIR S49220
H	113	ALA	SER	conflict	PIR S49220
P	3	GLN	LYS	conflict	PIR S49220
P	5	GLN	LEU	conflict	PIR S49220
P	6	GLN	GLU	conflict	PIR S49220
P	11	VAL	LEU	conflict	PIR S49220

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Chain	Residue	Modelled	Actual	Comment	Reference
P	13	ARG	LYS	conflict	PIR S49220
P	32	TYR	THR	conflict	PIR S49220
P	34	ILE	MET	conflict	PIR S49220
P	43	LYS	GLN	conflict	PIR S49220
P	50	TRP	ARG	conflict	PIR S49220
P	53	GLU	ALA	conflict	PIR S49220
P	54	ILE	ASN	conflict	PIR S49220
P	56	ASP	GLU	conflict	PIR S49220
P	57	THR	ILE	conflict	PIR S49220
P	58	GLU	LYS	conflict	PIR S49220
P	60	VAL	ASP	conflict	PIR S49220
P	66	LYS	THR	conflict	PIR S49220
P	69	MET	ILE	conflict	PIR S49220
P	75	SER	THR	conflict	PIR S49220
P	?	-	VAL	deletion	PIR S49220
P	93	ASN	ARG	conflict	PIR S49220
P	94	ALA	ARG	conflict	PIR S49220
P	96	HIS	-	insertion	PIR S49220
P	97	ASP	-	insertion	PIR S49220
P	99	ASP	GLY	conflict	PIR S49220
P	100	ARG	SER	conflict	PIR S49220
P	100A	GLY	SER	conflict	PIR S49220
P	100B	ARG	GLN	conflict	PIR S49220
P	100C	PHE	GLU	conflict	PIR S49220
P	108	LEU	THR	conflict	PIR S49220
P	109	VAL	LEU	conflict	PIR S49220
P	113	ALA	SER	conflict	PIR S49220

- Molecule 3 is water.

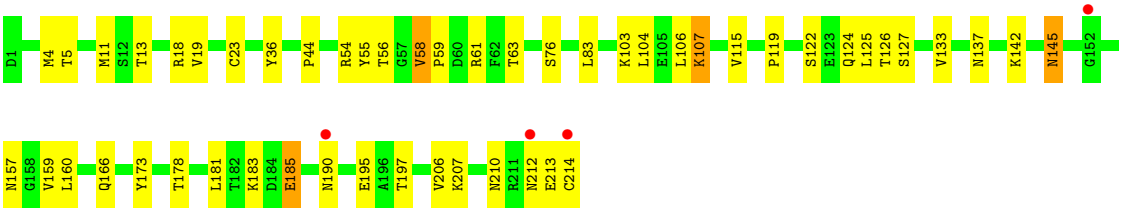
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	L	202	202	202	0	0
			Total	O		
3	H	194	194	194	0	0
			Total	O		
3	M	191	191	191	0	0
			Total	O		
3	P	180	180	180	0	0

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.

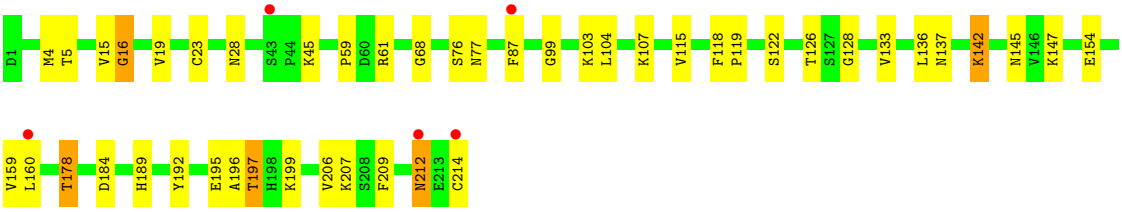
• Molecule 1: IGG1-KAPPA 2E8 FAB (LIGHT CHAIN)

Chain L:



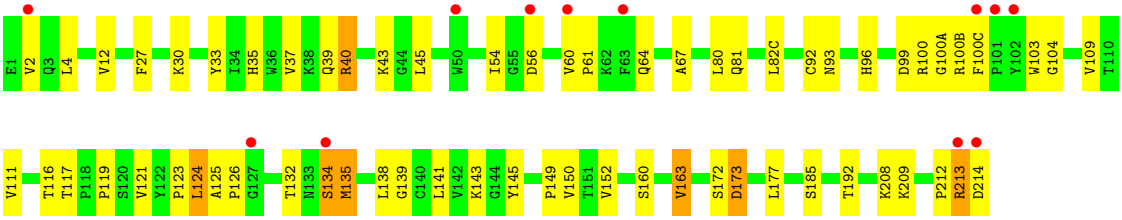
• Molecule 1: IGG1-KAPPA 2E8 FAB (LIGHT CHAIN)

Chain M:



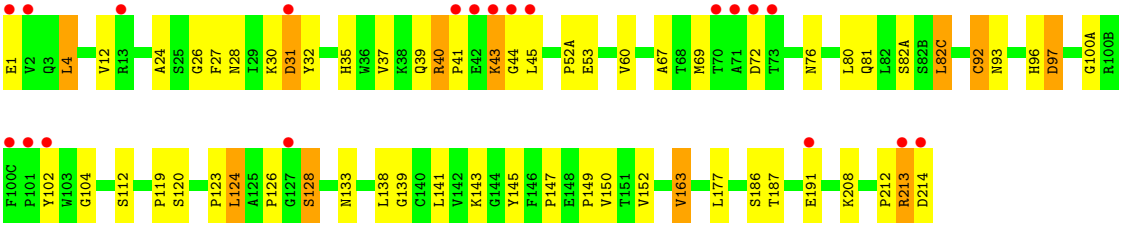
• Molecule 2: IGG1-KAPPA 2E8 FAB (HEAVY CHAIN)

Chain H:



• Molecule 2: IGG1-KAPPA 2E8 FAB (HEAVY CHAIN)

Chain P:


E1
V2
Q3
L4
V12
R13
A24
S25
G26
F27
N28
I29
K30
D31
Y32
H35
W36
V37
K38
Q39
R40
P41
E42
K43
G44
L45
P52A
E53
V60
A67
T68
M69
T70
A71
D72
T73
N76
L80
Q81
L82
S82A
S82B
L82C
C92
N93
H96
D97
G100A
R100B

F100C
P101
Y102
W103
G104
S112
P119
S120
P123
L124
A125
P126
G127
S128
N133
L138
G139
C140
L141
V142
K143
G144
Y145
F146
P147
E148
P149
V150
T151
V152
V163
L177
S186
T187
E191
K208
P212
R213
D214

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.56Å 65.57Å 103.22Å 90.00° 97.04° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.4 (20.00-1.90) 84.3 (20.00-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	0.55 (at 1.84Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.221 , 0.271 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	10.9	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7429	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.38% 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 (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	L	0.63	0/1682	0.98	4/2278 (0.2%)
1	M	0.65	0/1682	0.99	6/2278 (0.3%)
2	H	0.63	0/1728	1.02	9/2366 (0.4%)
2	P	0.62	0/1728	1.04	8/2366 (0.3%)
All	All	0.63	0/6820	1.01	27/9288 (0.3%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	60	VAL	N-CA-C	-9.50	100.46	108.63
1	M	137	ASN	N-CA-C	6.71	120.97	110.17
2	P	92	CYS	N-CA-C	-6.70	99.30	109.95
2	H	92	CYS	N-CA-C	-6.25	100.02	109.95
1	L	137	ASN	N-CA-C	6.18	120.12	110.17

There are no chirality outliers.

There are no planarity outliers.

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	L	1649	0	1578	27	0
1	M	1649	0	1578	25	0
2	H	1682	0	1625	35	0
2	P	1682	0	1625	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	194	0	0	10	0
3	L	202	0	0	9	0
3	M	191	0	0	6	0
3	P	180	0	0	22	0
All	All	7429	0	6406	130	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 10.

The worst 5 of 130 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:P:32:TYR:HA	3:P:378:HOH:O	1.66	0.93
1:L:63:THR:HG23	3:L:398:HOH:O	1.76	0.84
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.58	0.83
2:P:39:GLN:HB2	2:P:45:LEU:HD23	1.60	0.83
2:P:92:CYS:SG	3:P:376:HOH:O	2.38	0.80

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	L	212/214 (99%)	208 (98%)	4 (2%)	0	100 100
1	M	212/214 (99%)	208 (98%)	4 (2%)	0	100 100
2	H	219/221 (99%)	209 (95%)	3 (1%)	7 (3%)	3 0
2	P	219/221 (99%)	207 (94%)	9 (4%)	3 (1%)	9 3
All	All	862/870 (99%)	832 (96%)	20 (2%)	10 (1%)	10 4

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	132	THR
2	H	213	ARG
2	P	128	SER
2	P	213	ARG
2	H	100(A)	GLY

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	L	189/189 (100%)	174 (92%)	15 (8%)	11 5
1	M	189/189 (100%)	174 (92%)	15 (8%)	11 5
2	H	189/189 (100%)	178 (94%)	11 (6%)	18 10
2	P	189/189 (100%)	175 (93%)	14 (7%)	13 6
All	All	756/756 (100%)	701 (93%)	55 (7%)	13 6

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	59	PRO
1	M	160	LEU
2	P	163	VAL
2	P	133	ASN
1	M	103	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	53	ASN
1	M	212	ASN
2	P	96	HIS
2	P	39	GLN
2	H	64	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 oligosaccharides 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	L	214/214 (100%)	0.18	4 (1%)	66	70	4, 13, 31, 59	0
1	M	214/214 (100%)	0.15	5 (2%)	61	65	4, 12, 26, 62	0
2	H	215/221 (97%)	0.34	12 (5%)	30	32	5, 12, 30, 49	0
2	P	215/221 (97%)	0.54	20 (9%)	14	15	5, 15, 36, 51	0
All	All	858/870 (98%)	0.30	41 (4%)	35	38	4, 13, 32, 62	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	214	CYS	6.1
2	H	102	TYR	5.6
2	P	214	ASP	5.1
1	M	43	SER	5.1
1	M	87	PHE	4.5

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.