



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:12 PM GMT

PDB ID : 1SM3
Title : CRYSTAL STRUCTURE OF THE TUMOR SPECIFIC ANTIBODY SM3
COMPLEX WITH ITS PEPTIDE EPITOPE
Authors : Dokurno, P.; Bates, P.A.; Band, H.A.; Stewart, L.M.D.; Lally, J.M.; Burchell,
J.M.; Taylor-Papadimitriou, J.; Sternberg, M.J.E.; Snary, D.; Freemont, P.S.
Deposited on : 1997-12-23
Resolution : 1.95 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
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

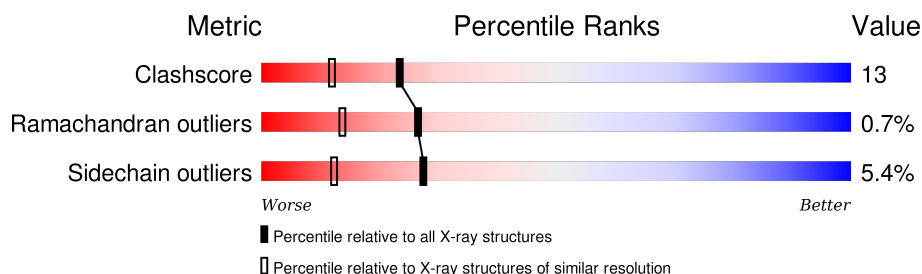
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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	L	215	
2	H	218	
3	P	13	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3564 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 SM3 ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total	C	N	O	S	0	0	0
			1581	991	266	318	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	108	SER	GLN	CONFLICT	UNP P01723
L	109	GLU	PRO	CONFLICT	UNP P01723

- Molecule 2 is a protein called SM3 ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	211	Total	C	N	O	S	0	0	0
			1580	1006	266	300	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	3	GLN	LYS	CONFLICT	UNP P01801
H	5	GLN	GLU	CONFLICT	UNP P01801
H	20	LEU	VAL	CONFLICT	UNP P01801
H	28	THR	ALA	CONFLICT	UNP P01801
H	31	ASN	TYR	CONFLICT	UNP P01801
H	43	LYS	ARG	CONFLICT	UNP P01801
H	48	VAL	ILE	CONFLICT	UNP P01801
H	52A	LEU	PHE	CONFLICT	UNP P01801
H	56	ALA	-	INSERTION	UNP P01801
H	94	GLY	ARG	CONFLICT	UNP P01801
H	95	VAL	GLU	CONFLICT	UNP P01801
H	?	-	ILE	DELETION	UNP P01801
H	?	-	TYR	DELETION	UNP P01801
H	?	-	TYR	DELETION	UNP P01801

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Chain	Residue	Modelled	Actual	Comment	Reference
H	97	GLN	PRO	CONFLICT	UNP P01801
H	108	THR	LEU	CONFLICT	UNP P01801
H	113	SER	ALA	CONFLICT	UNP P01801
H	120	THR	SER	CONFLICT	UNP P01801
H	129	ASN	ALA	CONFLICT	UNP P01801
H	131	ALA	GLN	CONFLICT	UNP P01801
H	132	SER	THR	CONFLICT	UNP P01801
H	133	GLN	ASN	CONFLICT	UNP P01801
H	160	ALA	SER	CONFLICT	UNP P01801
H	208	ALA	LYS	CONFLICT	UNP P01801

- Molecule 3 is a protein called PEPTIDE EPITOPE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	0	0	0
			62	38	12	12			

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	4	Total	Cd	0	0
			4	4		
4	L	4	Total	Cd	0	0
			4	4		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Cl	0	0
			2	2		

- Molecule 6 is water.

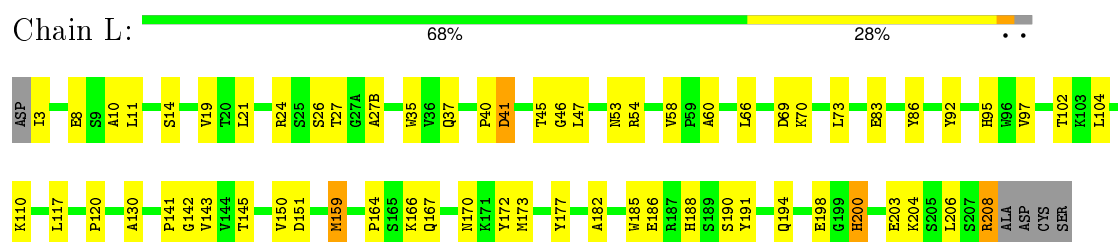
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	162	Total	O	0	0
			162	162		
6	L	156	Total	O	0	0
			156	156		
6	P	13	Total	O	0	0
			13	13		

3 Residue-property plots

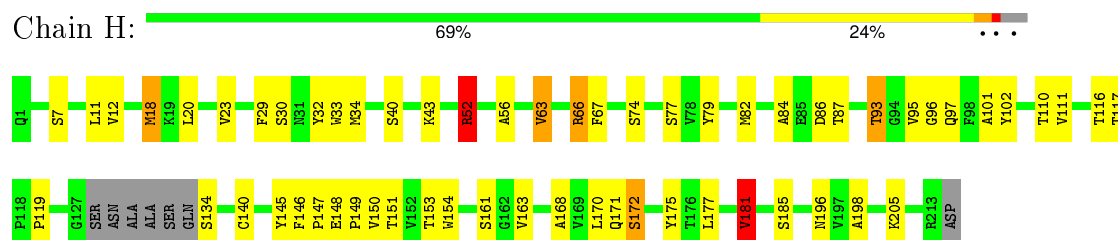
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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: SM3 ANTIBODY



• Molecule 2: SM3 ANTIBODY



• Molecule 3: PEPTIDE EPITOPE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.20 Å 83.73 Å 67.24 Å 90.00° 93.30° 90.00°	Depositor
Resolution (Å)	8.00 – 1.95	Depositor
% Data completeness (in resolution range)	85.6 (8.00-1.95)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.213 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3564	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CD

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	0.87	0/1618	0.80	0/2212
2	H	0.90	1/1622 (0.1%)	0.91	6/2219 (0.3%)
3	P	0.92	0/64	0.99	0/89
All	All	0.89	1/3304 (0.0%)	0.86	6/4520 (0.1%)

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	L	0	1
2	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	74	SER	CA-CB	6.19	1.62	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	H	52	ARG	NE-CZ-NH1	6.91	123.76	120.30
2	H	66	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	H	181	VAL	CB-CA-C	-6.88	98.33	111.40
2	H	66	ARG	NE-CZ-NH2	-6.70	116.95	120.30
2	H	147	PRO	CA-N-CD	-5.70	103.52	111.50
2	H	149	PRO	CA-N-CD	-5.22	104.20	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	79	TYR	Sidechain
1	L	86	TYR	Sidechain

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	L	1581	0	1524	52	0
2	H	1580	0	1529	33	0
3	P	62	0	56	2	0
4	H	4	0	0	0	0
4	L	4	0	0	0	0
5	H	2	0	0	0	0
6	H	162	0	0	1	0
6	L	156	0	0	7	0
6	P	13	0	0	0	0
All	All	3564	0	3109	84	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 13.

All (84) 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:L:3:ILE:HD13	1:L:27:THR:HG23	1.56	0.86
2:H:20:LEU:HG	2:H:82:MET:HE2	1.62	0.82
1:L:3:ILE:HD12	1:L:26:SER:OG	1.87	0.74
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.71	0.73
1:L:3:ILE:HG23	1:L:97:VAL:HG21	1.72	0.71
2:H:198:ALA:HB2	2:H:205:LYS:HD3	1.74	0.69
1:L:3:ILE:CG2	1:L:97:VAL:HG21	2.23	0.68
1:L:188:HIS:HB2	1:L:191:TYR:OH	1.96	0.66
1:L:24:ARG:HB3	1:L:70:LYS:HD3	1.78	0.65
1:L:3:ILE:HG12	1:L:92:TYR:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:27(B):ALA:HA	1:L:69:ASP:HB3	1.79	0.64
1:L:3:ILE:HG21	6:L:281:HOH:O	1.98	0.64
2:H:40:SER:OG	2:H:43:LYS:HB2	2.00	0.62
1:L:194:GLN:HG2	1:L:203:GLU:HG3	1.82	0.62
1:L:186:GLU:HG2	6:L:358:HOH:O	2.02	0.60
2:H:134:SER:N	2:H:185:SER:HG	1.98	0.60
1:L:3:ILE:HD13	1:L:27:THR:CG2	2.28	0.60
2:H:18:MET:HG3	2:H:82:MET:HE3	1.84	0.59
1:L:188:HIS:HB2	1:L:191:TYR:CZ	2.39	0.57
1:L:159:MET:H	1:L:159:MET:HE2	1.69	0.56
2:H:20:LEU:HG	2:H:82:MET:CE	2.35	0.55
2:H:66:ARG:HD3	6:H:284:HOH:O	2.06	0.55
1:L:3:ILE:CD1	1:L:27:THR:HG23	2.33	0.53
1:L:24:ARG:HB3	1:L:70:LYS:CD	2.38	0.53
1:L:95:HIS:CD2	6:L:293:HOH:O	2.63	0.52
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.42	0.52
2:H:153:THR:OG1	2:H:196:ASN:HB2	2.10	0.52
2:H:116:THR:HA	2:H:146:PHE:O	2.11	0.51
2:H:23:VAL:HG12	2:H:77:SER:OG	2.11	0.51
2:H:29:PHE:CE1	2:H:34:MET:HG3	2.45	0.51
1:L:47:LEU:HA	1:L:58:VAL:HG21	1.95	0.49
1:L:164:PRO:HA	1:L:173:MET:O	2.14	0.48
2:H:84:ALA:HA	2:H:111:VAL:HB	1.95	0.48
1:L:198:GLU:O	1:L:200:HIS:CD2	2.66	0.48
1:L:117:LEU:HD23	1:L:206:LEU:HG	1.96	0.47
2:H:33:TRP:CD2	3:P:5:ASP:HB2	2.50	0.47
1:L:24:ARG:HB3	1:L:70:LYS:HG2	1.97	0.46
2:H:148:GLU:HG3	2:H:175:TYR:CE2	2.50	0.46
2:H:170:LEU:HD13	2:H:175:TYR:CE1	2.49	0.46
1:L:182:ALA:O	1:L:186:GLU:HG3	2.15	0.46
1:L:186:GLU:O	1:L:208:ARG:NH1	2.49	0.46
2:H:146:PHE:CD1	2:H:146:PHE:C	2.89	0.46
2:H:163:VAL:HG22	2:H:181:VAL:HG13	1.98	0.45
1:L:54:ARG:CZ	1:L:60:ALA:HA	2.46	0.45
2:H:32:TYR:OH	3:P:10:PRO:HD3	2.16	0.45
1:L:166:LYS:HG2	1:L:170:ASN:HA	1.98	0.45
2:H:96:GLY:HA2	2:H:97:GLN:NE2	2.32	0.45
1:L:203:GLU:O	1:L:204:LYS:HD3	2.16	0.45
1:L:186:GLU:HB2	6:L:255:HOH:O	2.16	0.45
2:H:153:THR:HG1	2:H:196:ASN:HB2	1.83	0.44
1:L:120:PRO:HG3	1:L:130:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:151:THR:OG1	2:H:198:ALA:HB3	2.18	0.43
1:L:150:VAL:HG22	1:L:191:TYR:CD1	2.54	0.43
1:L:37:GLN:HB2	1:L:47:LEU:HD11	2.01	0.43
1:L:185:TRP:CZ2	1:L:208:ARG:HG3	2.53	0.43
1:L:10:ALA:O	1:L:11:LEU:HD23	2.19	0.43
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.00	0.43
1:L:159:MET:HA	1:L:177:TYR:O	2.19	0.43
1:L:143:VAL:HG13	6:L:355:HOH:O	2.18	0.43
1:L:151:ASP:HA	1:L:190:SER:HB3	2.00	0.42
1:L:110:LYS:HG2	1:L:141:PRO:HD3	2.00	0.42
1:L:14:SER:HB3	6:L:294:HOH:O	2.19	0.42
1:L:46:GLY:HA3	2:H:101:ALA:HA	2.00	0.42
2:H:52:ARG:HG2	2:H:56:ALA:O	2.20	0.42
1:L:21:LEU:HD12	1:L:21:LEU:N	2.35	0.42
2:H:87:THR:HG23	2:H:110:THR:HA	2.00	0.42
2:H:93:THR:HA	2:H:102:TYR:O	2.19	0.42
2:H:18:MET:HG3	2:H:82:MET:CE	2.48	0.42
1:L:203:GLU:HG2	1:L:204:LYS:N	2.34	0.42
2:H:154:TRP:CD2	2:H:181:VAL:HG22	2.54	0.42
1:L:35:TRP:CD2	1:L:73:LEU:HB2	2.56	0.41
1:L:204:LYS:HD3	1:L:204:LYS:HA	1.83	0.41
2:H:171:GLN:O	2:H:172:SER:CB	2.67	0.41
1:L:54:ARG:HG3	1:L:58:VAL:HB	2.03	0.41
1:L:8:GLU:O	1:L:102:THR:HA	2.20	0.41
1:L:200:HIS:CD2	1:L:200:HIS:N	2.88	0.41
1:L:40:PRO:O	1:L:41:ASP:CB	2.68	0.41
2:H:168:ALA:HA	2:H:177:LEU:HB3	2.02	0.41
1:L:159:MET:H	1:L:159:MET:CE	2.34	0.40
1:L:167:GLN:HG2	1:L:173:MET:CE	2.51	0.40
1:L:45:THR:HG22	6:L:351:HOH:O	2.21	0.40
2:H:117:THR:N	2:H:146:PHE:O	2.48	0.40
1:L:142:GLY:HA3	1:L:172:TYR:CD1	2.56	0.40
1:L:83:GLU:HG3	1:L:104:LEU:O	2.21	0.40

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	L	208/215 (97%)	197 (95%)	10 (5%)	1 (0%)	34	21
2	H	207/218 (95%)	200 (97%)	5 (2%)	2 (1%)	19	8
3	P	7/13 (54%)	6 (86%)	1 (14%)	0	100	100
All	All	422/446 (95%)	403 (96%)	16 (4%)	3 (1%)	26	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	41	ASP
2	H	172	SER
2	H	95	VAL

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	L	176/183 (96%)	169 (96%)	7 (4%)	38	23
2	H	172/185 (93%)	160 (93%)	12 (7%)	19	6
3	P	6/10 (60%)	6 (100%)	0	100	100
All	All	354/378 (94%)	335 (95%)	19 (5%)	27	12

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	19	VAL
1	L	53	ASN
1	L	66	LEU
1	L	145	THR
1	L	159	MET
1	L	200	HIS
1	L	208	ARG
2	H	7	SER
2	H	11	LEU
2	H	12	VAL
2	H	18	MET
2	H	30	SER
2	H	52	ARG
2	H	63	VAL
2	H	93	THR
2	H	140	CYS
2	H	150	VAL
2	H	161	SER
2	H	181	VAL

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

Mol	Chain	Res	Type
1	L	53	ASN
1	L	79	GLN
1	L	194	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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.