



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID : 2BMK
Title : FAB FRAGMENT OF PLP-DEPENDENT CATALYTIC ANTIBODY 15A9
IN COMPLEX WITH PHOSPHOPYRIDOXYL-D-ALANINE
Authors : Golinelli-Pimpaneau, B.; Christen, P.
Deposited on : 2005-03-14
Resolution : 2.30 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

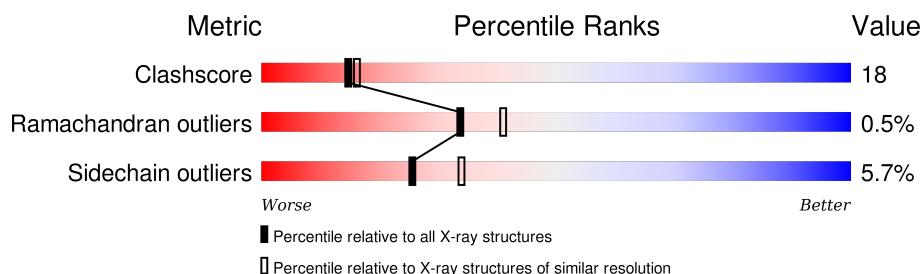
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	213	
1	L	213	
2	B	226	
2	H	226	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	B	1215	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6967 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 FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1610	1003	264	334	9			
1	L	213	Total	C	N	O	S	0	0	0
			1629	1016	271	333	9			

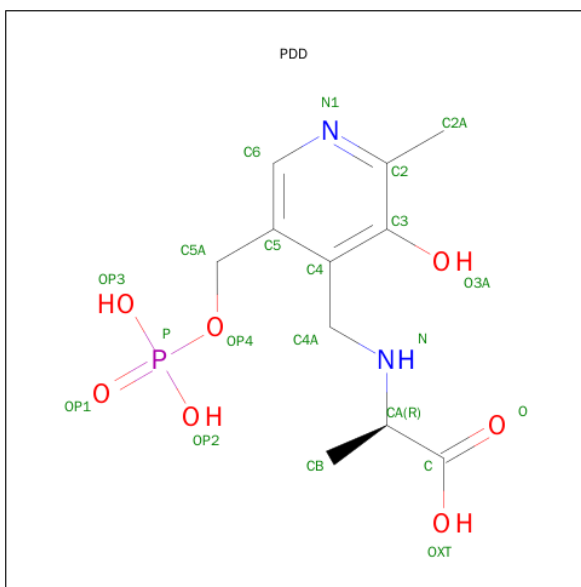
- Molecule 2 is a protein called FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	224	Total	C	N	O	S	0	0	1
			1658	1053	276	322	7			
2	H	222	Total	C	N	O	S	0	0	1
			1668	1059	282	320	7			

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	3	Total	I	0	0
			3	3		
3	B	3	Total	I	0	0
			3	3		

- Molecule 4 is N-(5'-PHOSPHOPYRIDOXYL)-D-ALANINE (three-letter code: PDD) (formula: C₁₁H₁₇N₂O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
4	L	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 5 is water.

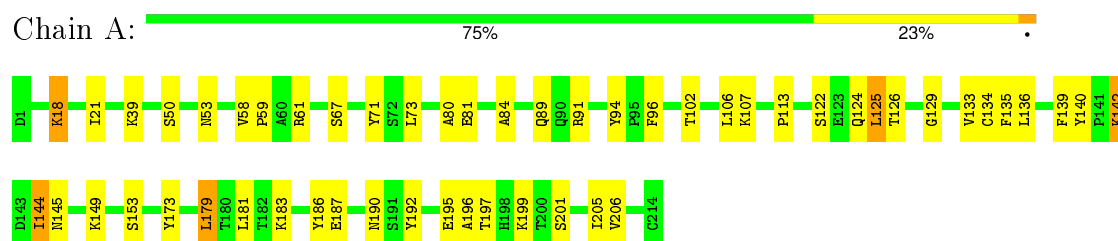
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O	0	0
			81	81		
5	B	82	Total	O	0	0
			82	82		
5	H	94	Total	O	0	0
			94	94		
5	L	97	Total	O	0	0
			97	97		

3 Residue-property plots

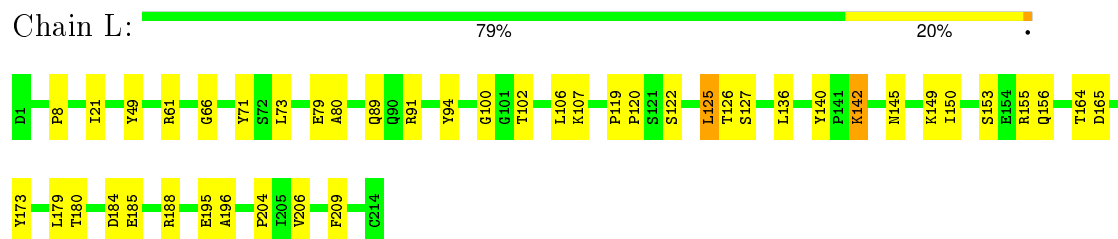
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

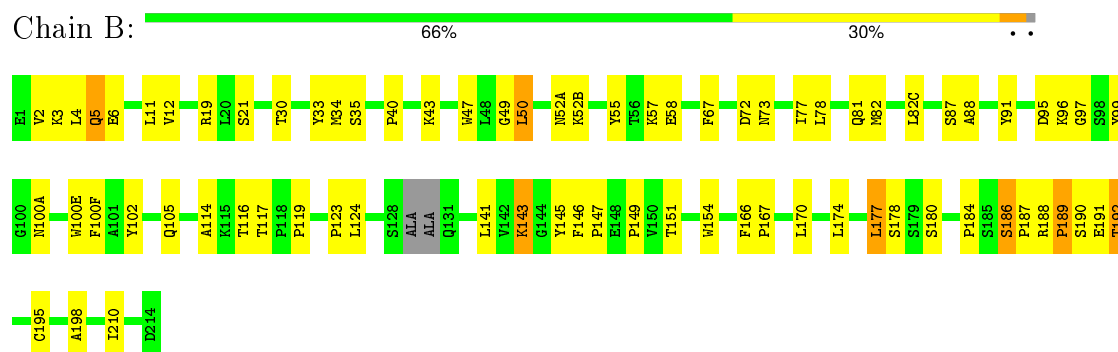
• Molecule 1: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, LIGHT CHAIN



• Molecule 1: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, LIGHT CHAIN



• Molecule 2: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, HEAVY CHAIN



• Molecule 2: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, HEAVY CHAIN



E1	E2	R3	L4	Q5	E6	S21	C22	A23	Y33	W36	Q39	P40	K43	L44	L45	E46	W47	L48	G49	L50	L51	R52	G54	Y55	T56	R57	E58	I69	D72	W73	S74	Q75	I77	L78	Y79	L80	Q81	W82	L82C	R83	A84	E85	A88	Y93	D95	R96
Y99	Y100B	E100C	F100F	Q105	T108	V111	K115	T116	T117	P118	P119	S120	V121	Y122	P123	L124	S128	ALA	ALA	GLN	THR	W133	S134	M135	V136	T137	L138	L141	V142	K143	G144	Y145	F146	P147	E148	P149	W154	L159	H164	T165	F166	P167	A168	V169	L170	Y175
T176	L177	S178	S179	T182	W183	P184	S185	S186	P187	R188	P189	S190	E191	T192	V193	T194	H199	S202	V206	D207	K208	R209	I210	V211	P212	R213	D214																			

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	63.15Å 81.15Å 79.33Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30	Depositor
% Data completeness (in resolution range)	90.2 (40.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6967	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/1649	0.62	0/2247
1	L	0.39	0/1668	0.65	0/2267
2	B	0.38	0/1703	0.66	0/2333
2	H	0.39	0/1713	0.68	1/2341 (0.0%)
All	All	0.38	0/6733	0.65	1/9188 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	50	LEU	CA-CB-CG	5.42	127.77	115.30

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	A	1610	0	1499	40	0
1	L	1629	0	1547	38	0
2	B	1658	0	1571	82	0
2	H	1668	0	1611	91	0
3	B	3	0	0	3	0
3	H	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	21	0	13	0	0
4	L	21	0	13	1	0
5	A	81	0	0	3	0
5	B	82	0	0	6	0
5	H	94	0	0	3	0
5	L	97	0	0	4	0
All	All	6967	0	6254	229	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 18.

All (229) 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:61:ARG:CZ	1:L:79:GLU:HG3	2.00	0.91
2:H:186:SER:HB2	2:H:187:PRO:HD3	1.58	0.85
2:H:191:GLU:O	2:H:192:THR:HB	1.78	0.84
1:L:142:LYS:HD3	1:L:173:TYR:CE1	2.14	0.83
1:L:195:GLU:HG3	1:L:204:PRO:HB3	1.63	0.81
2:B:19:ARG:HD2	2:H:75:GLN:OE1	1.81	0.81
2:B:191:GLU:O	2:B:192:THR:HB	1.82	0.80
2:H:184:PRO:O	2:H:187:PRO:HD2	1.85	0.76
1:L:61:ARG:NE	1:L:79:GLU:HG3	2.02	0.74
1:A:89:GLN:NE2	1:A:91:ARG:HE	1.86	0.73
1:L:100:GLY:HA3	5:L:2052:HOH:O	1.87	0.72
2:B:50:LEU:HD23	2:B:50:LEU:C	2.10	0.72
2:H:184:PRO:HG2	2:H:187:PRO:HG2	1.71	0.71
1:A:94:TYR:CD2	2:B:58:GLU:HG2	2.27	0.70
2:B:184:PRO:HG2	2:B:187:PRO:HG2	1.73	0.70
2:B:184:PRO:HG2	2:B:187:PRO:CD	2.22	0.70
2:B:124:LEU:HD11	2:B:141:LEU:HB2	1.74	0.70
2:H:40:PRO:HG2	2:H:43:LYS:CB	2.24	0.68
1:L:142:LYS:HD3	1:L:173:TYR:CD1	2.29	0.68
1:L:21:ILE:HD12	1:L:102:THR:HG21	1.75	0.68
2:B:184:PRO:O	2:B:187:PRO:HD2	1.95	0.67
1:L:120:PRO:HB2	1:L:125:LEU:HD21	1.78	0.65
1:A:125:LEU:HG	1:A:183:LYS:HZ3	1.61	0.65
2:B:186:SER:CB	2:B:187:PRO:HD3	2.27	0.65
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.79	0.64
2:B:105:GLN:H	2:B:105:GLN:CD	2.00	0.64
2:B:184:PRO:HG2	2:B:187:PRO:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:TYR:HB2	2:B:95:ASP:HB3	1.80	0.63
2:B:184:PRO:HG2	2:B:187:PRO:CG	2.29	0.63
2:B:33:TYR:CB	2:B:95:ASP:HB3	2.29	0.62
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.33	0.62
1:A:106:LEU:HD13	1:A:107:LYS:O	1.99	0.62
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.35	0.62
2:B:97:GLY:HA3	3:B:1215:IOD:I	2.69	0.62
2:B:143:LYS:NZ	2:B:143:LYS:HB2	2.15	0.62
2:H:83:ARG:HG3	2:H:85:GLU:HG2	1.81	0.62
1:A:80:ALA:HA	1:A:106:LEU:HG	1.82	0.61
2:B:81:GLN:NE2	2:H:75:GLN:HE22	1.98	0.61
1:A:149:LYS:HA	1:A:153:SER:O	2.01	0.61
2:H:177:LEU:HD12	2:H:177:LEU:C	2.21	0.61
2:H:23:ALA:HA	2:H:77:ILE:HD13	1.83	0.60
2:H:100(C):GLU:HB3	1:L:49:TYR:CZ	2.36	0.60
1:A:124:GLN:HG2	1:A:129:GLY:O	2.01	0.60
2:B:177:LEU:C	2:B:177:LEU:HD12	2.21	0.60
2:H:40:PRO:HG2	2:H:43:LYS:HB2	1.84	0.60
1:L:122:SER:O	1:L:126:THR:HG23	2.02	0.60
1:A:21:ILE:HD12	1:A:102:THR:HG21	1.83	0.60
2:H:33:TYR:HB2	2:H:95:ASP:HB3	1.84	0.59
2:H:100(B):TYR:HB2	5:H:2058:HOH:O	2.03	0.58
2:H:108:THR:CG2	2:H:149:PRO:HD3	2.33	0.58
2:B:143:LYS:HB2	2:B:143:LYS:HZ3	1.69	0.58
2:B:6:GLU:H	2:B:105:GLN:HE22	1.51	0.58
2:B:100(A):ASN:ND2	5:B:2048:HOH:O	2.36	0.57
1:A:18:LYS:HB2	1:A:18:LYS:NZ	2.19	0.56
1:A:67:SER:HA	1:A:71:TYR:CZ	2.39	0.56
2:H:99:TYR:HB2	3:H:1216:IOD:I	2.75	0.56
2:B:154:TRP:CZ3	2:B:195:CYS:HB3	2.39	0.56
2:H:123:PRO:O	2:H:124:LEU:HD12	2.05	0.56
2:B:5:GLN:HA	2:B:105:GLN:HE22	1.70	0.56
1:A:122:SER:O	1:A:126:THR:HG23	2.06	0.56
2:H:188:ARG:HA	2:H:190:SER:H	1.69	0.56
1:A:50:SER:HB2	1:A:53:ASN:HD22	1.71	0.56
1:L:150:ILE:HD12	1:L:155:ARG:HE	1.70	0.55
2:B:188:ARG:HA	2:B:190:SER:H	1.71	0.55
2:B:177:LEU:HD12	2:B:178:SER:N	2.22	0.55
2:H:184:PRO:HG2	2:H:187:PRO:CG	2.35	0.55
1:A:195:GLU:HA	1:A:206:VAL:HG12	1.87	0.55
1:A:107:LYS:HA	1:A:140:TYR:OH	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:89:GLN:NE2	1:L:91:ARG:HE	2.05	0.54
1:L:80:ALA:HA	1:L:106:LEU:HD22	1.89	0.54
1:A:205:ILE:N	1:A:205:ILE:HD12	2.23	0.54
2:H:199:HIS:ND1	2:H:202:SER:HB2	2.22	0.54
1:A:201:SER:HB3	1:A:205:ILE:HD11	1.90	0.54
1:L:188:ARG:NH2	5:L:2086:HOH:O	2.40	0.54
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.90	0.54
2:H:83:ARG:HE	2:H:85:GLU:CD	2.11	0.53
1:A:179:LEU:HD22	1:A:181:LEU:HG	1.91	0.53
1:A:183:LYS:O	1:A:187:GLU:HG3	2.07	0.53
2:B:186:SER:HB3	2:B:187:PRO:HD3	1.90	0.53
2:H:50:LEU:HD23	2:H:50:LEU:C	2.29	0.53
1:A:67:SER:HB3	5:A:2039:HOH:O	2.08	0.53
2:H:137:THR:O	2:H:138:LEU:HD23	2.09	0.53
2:B:33:TYR:CZ	2:B:96:LYS:HD3	2.44	0.53
1:A:142:LYS:HG2	1:A:173:TYR:CE2	2.44	0.52
2:H:170:LEU:HB2	2:H:175:TYR:CE1	2.44	0.52
1:L:66:GLY:HA3	1:L:71:TYR:HA	1.92	0.52
1:A:142:LYS:HD3	1:A:173:TYR:CD1	2.44	0.52
1:L:195:GLU:CG	1:L:204:PRO:HB3	2.37	0.52
2:H:33:TYR:CB	2:H:95:ASP:HB3	2.40	0.52
2:H:121:VAL:HG21	2:H:206:VAL:CG2	2.40	0.51
2:B:6:GLU:H	2:B:105:GLN:NE2	2.08	0.51
2:H:211:VAL:HG13	2:H:212:PRO:HD2	1.92	0.51
1:A:61:ARG:NH2	1:A:81:GLU:HG3	2.26	0.51
2:H:93:VAL:HG11	2:H:100(F):PHE:CD2	2.46	0.51
2:B:188:ARG:HA	2:B:190:SER:N	2.26	0.51
2:H:33:TYR:CZ	2:H:96:LYS:HD3	2.46	0.50
2:B:40:PRO:HG2	2:B:43:LYS:CB	2.41	0.50
2:H:52:ARG:O	2:H:55:TYR:HA	2.11	0.50
1:L:142:LYS:HD3	1:L:173:TYR:CZ	2.45	0.50
2:H:154:TRP:CZ3	2:H:210:ILE:HD11	2.46	0.50
2:B:77:ILE:HD13	5:B:2035:HOH:O	2.10	0.50
1:A:89:GLN:HE22	1:A:91:ARG:HH21	1.59	0.50
2:B:50:LEU:C	2:B:50:LEU:CD2	2.79	0.50
2:H:118:PRO:HB3	2:H:202:SER:OG	2.11	0.50
2:B:151:THR:CG2	2:B:198:ALA:HB3	2.42	0.49
2:H:184:PRO:HG2	2:H:187:PRO:CD	2.43	0.49
2:B:170:LEU:HD12	2:B:174:LEU:O	2.13	0.49
2:H:47:TRP:HZ2	2:H:50:LEU:HD13	1.78	0.49
1:A:136:LEU:HD21	1:A:196:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:PRO:C	2:B:124:LEU:HD12	2.33	0.49
2:B:188:ARG:HG2	2:B:189:PRO:HA	1.95	0.49
1:L:184:ASP:HA	5:L:2084:HOH:O	2.13	0.49
2:H:57:LYS:HD2	2:H:57:LYS:N	2.28	0.49
1:A:73:LEU:HD23	1:A:73:LEU:C	2.33	0.49
2:B:5:GLN:NE2	5:B:2004:HOH:O	2.37	0.49
2:B:191:GLU:O	2:B:192:THR:CB	2.55	0.48
2:B:154:TRP:CZ3	2:B:210:ILE:HD11	2.48	0.48
2:B:188:ARG:C	2:B:188:ARG:HD3	2.34	0.48
2:B:19:ARG:HH12	2:H:72:ASP:HB3	1.77	0.48
2:H:188:ARG:HH22	2:H:212:PRO:HA	1.78	0.48
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.48	0.48
1:L:120:PRO:HB2	1:L:125:LEU:CD2	2.42	0.48
2:H:199:HIS:ND1	2:H:202:SER:CB	2.77	0.48
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.95	0.48
2:B:100(A):ASN:ND2	5:B:2050:HOH:O	2.41	0.48
2:B:114:ALA:HB3	2:B:146:PHE:CE2	2.49	0.48
2:H:115:LYS:HG2	2:H:116:THR:N	2.28	0.47
2:H:40:PRO:HG2	2:H:43:LYS:HB3	1.97	0.47
1:A:106:LEU:HD13	1:A:106:LEU:C	2.35	0.47
2:H:168:ALA:HA	2:H:177:LEU:HB3	1.97	0.47
2:H:188:ARG:HG2	2:H:189:PRO:HA	1.97	0.47
2:B:30:THR:O	2:B:52(A):ASN:HB2	2.14	0.47
2:B:151:THR:HG23	5:B:2068:HOH:O	2.13	0.47
2:B:19:ARG:NH2	2:H:72:ASP:HB2	2.30	0.47
2:B:97:GLY:CA	3:B:1215:IOD:I	3.32	0.47
2:H:58:GLU:HG2	1:L:94:TYR:CE2	2.48	0.47
1:A:89:GLN:HE22	1:A:91:ARG:HE	1.61	0.47
2:H:188:ARG:C	2:H:188:ARG:HD3	2.34	0.47
2:B:6:GLU:N	2:B:105:GLN:HE22	2.12	0.47
2:H:57:LYS:NZ	2:H:69:ILE:O	2.48	0.47
2:B:19:ARG:NH1	2:H:72:ASP:CB	2.79	0.46
1:L:106:LEU:HG	1:L:107:LYS:N	2.30	0.46
1:L:73:LEU:HD23	1:L:73:LEU:C	2.36	0.46
1:L:80:ALA:CB	1:L:106:LEU:HD22	2.45	0.46
2:H:100(C):GLU:HA	1:L:49:TYR:CD1	2.51	0.46
2:B:99:TYR:HB2	3:B:1215:IOD:I	2.86	0.46
1:L:145:ASN:O	1:L:196:ALA:HA	2.16	0.46
1:A:135:PHE:CE2	2:B:180:SER:HB3	2.51	0.46
1:A:94:TYR:CE2	2:B:58:GLU:HG2	2.51	0.46
1:A:186:TYR:HA	1:A:192:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:MET:HB3	2:B:82(C):LEU:HD21	1.98	0.46
2:B:2:VAL:HB	2:B:102:TYR:CE1	2.51	0.46
2:B:19:ARG:HH12	2:H:72:ASP:CB	2.29	0.45
2:B:19:ARG:HH22	2:H:72:ASP:HB2	1.81	0.45
2:B:81:GLN:NE2	2:H:75:GLN:NE2	2.64	0.45
2:H:164:HIS:O	2:H:179:SER:HA	2.17	0.45
2:H:108:THR:HG21	2:H:149:PRO:HD3	1.97	0.45
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.98	0.45
1:A:197:THR:HG23	5:A:2081:HOH:O	2.16	0.45
1:L:195:GLU:HA	1:L:206:VAL:HG12	1.98	0.45
2:H:100(C):GLU:HA	1:L:49:TYR:CE1	2.52	0.45
2:H:187:PRO:O	2:H:191:GLU:N	2.46	0.45
2:B:6:GLU:OE2	2:B:91:TYR:HA	2.17	0.45
2:H:100(C):GLU:CB	1:L:49:TYR:CZ	2.99	0.44
2:B:12:VAL:HG11	2:B:82(C):LEU:HD13	2.00	0.44
2:H:184:PRO:C	2:H:187:PRO:HD2	2.38	0.44
2:B:19:ARG:NH2	2:H:79:TYR:HE2	2.15	0.44
2:B:6:GLU:HA	2:B:21:SER:O	2.17	0.44
2:H:115:LYS:HD2	2:H:116:THR:O	2.17	0.44
2:H:95:ASP:OD1	4:L:1215:PDD:N1	2.50	0.44
1:L:150:ILE:HD12	1:L:155:ARG:HH21	1.83	0.44
2:B:188:ARG:HD3	2:B:189:PRO:N	2.33	0.44
2:H:208:LYS:HA	2:H:208:LYS:HD2	1.90	0.44
2:H:21:SER:HG	2:H:79:TYR:HE1	1.63	0.44
1:A:91:ARG:HA	1:A:96:PHE:CD2	2.53	0.44
2:H:188:ARG:HA	2:H:190:SER:N	2.33	0.44
1:A:142:LYS:HG2	1:A:173:TYR:CD2	2.53	0.44
2:H:23:ALA:HA	2:H:77:ILE:CD1	2.49	0.43
1:L:195:GLU:HG3	1:L:204:PRO:CB	2.41	0.43
2:B:81:GLN:HE21	2:H:75:GLN:NE2	2.17	0.43
1:L:107:LYS:HA	1:L:140:TYR:OH	2.19	0.43
2:H:194:THR:HG23	2:H:208:LYS:C	2.39	0.43
2:H:54:GLY:HA2	5:H:2034:HOH:O	2.17	0.43
2:H:6:GLU:H	2:H:105:GLN:HE22	1.66	0.43
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	2.01	0.43
2:H:100(B):TYR:HD1	2:H:100(C):GLU:N	2.17	0.42
1:A:113:PRO:HB3	1:A:139:PHE:HB3	2.00	0.42
2:H:6:GLU:HA	2:H:21:SER:O	2.19	0.42
2:H:58:GLU:HG2	1:L:94:TYR:CD2	2.53	0.42
2:B:143:LYS:NZ	2:B:143:LYS:CB	2.82	0.42
2:B:34:MET:HB3	2:B:78:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HG13	1:A:145:ASN:N	2.33	0.42
2:H:138:LEU:HD11	2:H:188:ARG:HD2	2.01	0.42
1:L:136:LEU:HD21	1:L:196:ALA:HB2	2.01	0.42
2:H:72:ASP:C	2:H:72:ASP:OD2	2.59	0.42
1:A:106:LEU:HD11	5:A:2056:HOH:O	2.19	0.42
2:H:119:PRO:CB	2:H:145:TYR:HB3	2.48	0.41
2:B:146:PHE:HA	2:B:147:PRO:HA	1.79	0.41
2:H:166:PHE:CD2	1:L:164:THR:HG23	2.55	0.41
1:L:100:GLY:CA	5:L:2052:HOH:O	2.60	0.41
1:L:149:LYS:HA	1:L:153:SER:O	2.21	0.41
2:B:151:THR:HG22	2:B:198:ALA:HB3	2.03	0.41
2:B:19:ARG:NH1	2:H:79:TYR:OH	2.53	0.41
2:B:50:LEU:HD23	2:B:50:LEU:O	2.20	0.41
2:B:100(E):TRP:HB2	5:B:2049:HOH:O	2.20	0.41
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.85	0.41
2:B:67:PHE:HA	2:B:81:GLN:O	2.20	0.41
2:H:50:LEU:C	2:H:50:LEU:CD2	2.88	0.41
2:H:168:ALA:HB2	2:H:177:LEU:HD23	2.03	0.41
1:A:18:LYS:HB2	1:A:18:LYS:HZ3	1.86	0.41
2:H:39:GLN:C	2:H:88:ALA:HB1	2.41	0.41
1:L:119:PRO:HB3	1:L:209:PHE:CZ	2.56	0.41
2:H:135:MET:CE	2:H:182:THR:HG22	2.51	0.41
2:H:3:LYS:HA	5:H:2002:HOH:O	2.21	0.41
2:H:83:ARG:C	2:H:111:VAL:HG11	2.41	0.41
2:B:87:SER:O	2:B:88:ALA:HB2	2.21	0.41
2:B:5:GLN:HB3	2:B:5:GLN:HE21	1.47	0.41
2:B:11:LEU:HB2	2:B:147:PRO:HG3	2.03	0.41
1:A:133:VAL:HG12	1:A:134:CYS:N	2.36	0.41
2:B:116:THR:HG22	2:B:117:THR:N	2.35	0.41
2:B:67:PHE:CD1	2:B:67:PHE:N	2.88	0.41
2:B:99:TYR:HB2	2:B:100(A):ASN:HD22	1.86	0.41
2:H:55:TYR:CZ	2:H:73:ASN:ND2	2.88	0.41
1:A:39:LYS:HG2	1:A:84:ALA:HB2	2.03	0.41
2:B:55:TYR:CZ	2:B:73:ASN:ND2	2.89	0.41
2:H:57:LYS:CD	2:H:57:LYS:N	2.85	0.40
2:B:166:PHE:HA	2:B:167:PRO:HD3	1.96	0.40
1:L:8:PRO:O	1:L:102:THR:HG23	2.20	0.40
2:B:72:ASP:OD1	2:H:73:ASN:HB2	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	A	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
1	L	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
2	B	220/226 (97%)	202 (92%)	16 (7%)	2 (1%)	21	24
2	H	218/226 (96%)	205 (94%)	11 (5%)	2 (1%)	21	24
All	All	860/878 (98%)	817 (95%)	39 (4%)	4 (0%)	34	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	192	THR
2	H	192	THR
2	H	189	PRO
2	B	189	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	178/185 (96%)	171 (96%)	7 (4%)	39	53
1	L	182/185 (98%)	174 (96%)	8 (4%)	35	46
2	B	178/192 (93%)	166 (93%)	12 (7%)	20	26
2	H	182/192 (95%)	168 (92%)	14 (8%)	16	20
All	All	720/754 (96%)	679 (94%)	41 (6%)	25	34

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	125	LEU
1	A	142	LYS
1	A	144	ILE
1	A	179	LEU
1	A	190	ASN
1	A	199	LYS
2	B	3	LYS
2	B	4	LEU
2	B	5	GLN
2	B	35	SER
2	B	50	LEU
2	B	52(B)	LYS
2	B	57	LYS
2	B	100(F)	PHE
2	B	143	LYS
2	B	149	PRO
2	B	177	LEU
2	B	186	SER
2	H	5	GLN
2	H	50	LEU
2	H	57	LYS
2	H	100(B)	TYR
2	H	100(C)	GLU
2	H	100(F)	PHE
2	H	115	LYS
2	H	134	SER
2	H	141	LEU
2	H	143	LYS
2	H	147	PRO
2	H	149	PRO
2	H	159	LEU
2	H	177	LEU
1	L	125	LEU
1	L	127	SER
1	L	142	LYS
1	L	156	GLN
1	L	165	ASP
1	L	179	LEU
1	L	180	THR
1	L	185	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	89	GLN
1	A	137	ASN
1	A	212	ASN
2	B	81	GLN
2	B	100(A)	ASN
2	B	105	GLN
2	B	164	HIS
2	H	5	GLN
2	H	81	GLN
2	H	82(A)	ASN
2	H	164	HIS
1	L	31	ASN
1	L	89	GLN
1	L	137	ASN
1	L	190	ASN
1	L	212	ASN

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](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PDD	B	1217	-	18,21,21	1.98	4 (22%)	23,30,30	1.52	5 (21%)
4	PDD	L	1215	-	18,21,21	1.99	4 (22%)	23,30,30	1.50	6 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PDD	B	1217	-	-	1/11/15/15	0/1/1/1
4	PDD	L	1215	-	-	1/11/15/15	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1217	PDD	CA-N	2.02	1.52	1.47
4	L	1215	PDD	CA-N	2.05	1.52	1.47
4	B	1217	PDD	C5-C4	3.47	1.45	1.40
4	B	1217	PDD	C3-C4	3.57	1.45	1.40
4	L	1215	PDD	C5-C4	3.60	1.45	1.40
4	L	1215	PDD	C3-C4	4.17	1.46	1.40
4	L	1215	PDD	C3-C2	4.88	1.44	1.40
4	B	1217	PDD	C3-C2	5.47	1.44	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1215	PDD	C3-C2-N1	-2.26	117.49	120.61
4	B	1217	PDD	C3-C2-N1	-2.25	117.50	120.61
4	B	1217	PDD	OP3-P-OP1	2.03	117.11	110.58
4	L	1215	PDD	OP3-P-OP1	2.13	117.42	110.58
4	L	1215	PDD	CB-CA-N	2.38	112.26	109.07
4	L	1215	PDD	C2A-C2-C3	2.40	123.94	121.04
4	B	1217	PDD	C2A-C2-C3	2.53	124.09	121.04
4	B	1217	PDD	C6-N1-C2	2.68	124.74	119.28
4	L	1215	PDD	C6-N1-C2	2.80	124.98	119.28
4	L	1215	PDD	C4A-C4-C5	3.50	122.83	119.71
4	B	1217	PDD	C4A-C4-C5	4.11	123.37	119.71

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1215	PDD	C-CA-N-C4A
4	B	1217	PDD	C-CA-N-C4A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1215	PDD	1	0

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.