Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:42 PM GMT

PDB ID	:	1YEG
Title	:	STRUCTURE OF IGG2A FAB FRAGMENT (D2.3) COMPLEXED WITH REACTION PRODUCT
Authors	:	Gigant, B.; Knossow, M.
Deposited on	:	1997-05-29
Resolution	:	2.00 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

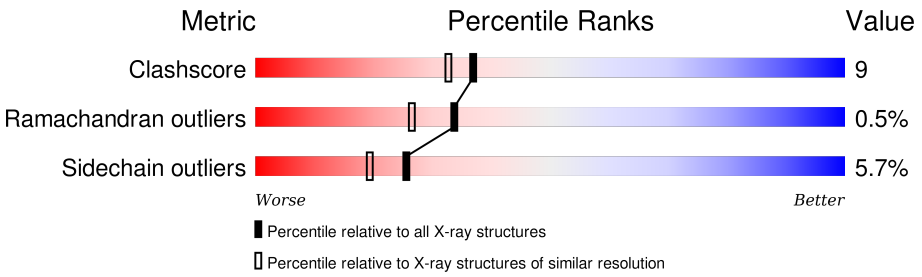
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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 <=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	219	82% 16% •
2	H	222	77% 19% •

2 Entry composition (i)

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 IGG2A FAB FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	219	1686	1054	286	339	7	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	ILE	VAL	CONFLICT	PIR S16112
L	7	SER	THR	CONFLICT	PIR S16112
L	10	THR	SER	CONFLICT	PIR S16112
L	12	SER	PRO	CONFLICT	PIR S16112
L	14	THR	SER	CONFLICT	PIR S16112
L	15	ILE	LEU	CONFLICT	PIR S16112
L	17	GLN	ASP	CONFLICT	PIR S16112
L	18	PRO	GLN	CONFLICT	PIR S16112
L	24	LYS	ARG	CONFLICT	PIR S16112
L	27B	LEU	VAL	CONFLICT	PIR S16112
L	27D	TYR	HIS	CONFLICT	PIR S16112
L	30	LYS	ASN	CONFLICT	PIR S16112
L	34	ASN	TYR	CONFLICT	PIR S16112
L	36	LEU	TYR	CONFLICT	PIR S16112
L	39	ARG	LYS	CONFLICT	PIR S16112
L	46	ARG	PRO	CONFLICT	PIR S16112
L	49	HIS	TYR	CONFLICT	PIR S16112
L	50	LEU	ARG	CONFLICT	PIR S16112
L	53	LYS	ASN	CONFLICT	PIR S16112
L	54	LEU	ARG	CONFLICT	PIR S16112
L	55	ASP	PHE	CONFLICT	PIR S16112
L	62	ILE	PHE	CONFLICT	PIR S16112
L	63	THR	SER	CONFLICT	PIR S16112
L	81	ALA	GLU	CONFLICT	PIR S16112
L	87	TYR	PHE	CONFLICT	PIR S16112
L	89	VAL	PHE	CONFLICT	PIR S16112
L	94	PHE	VAL	CONFLICT	PIR S16112

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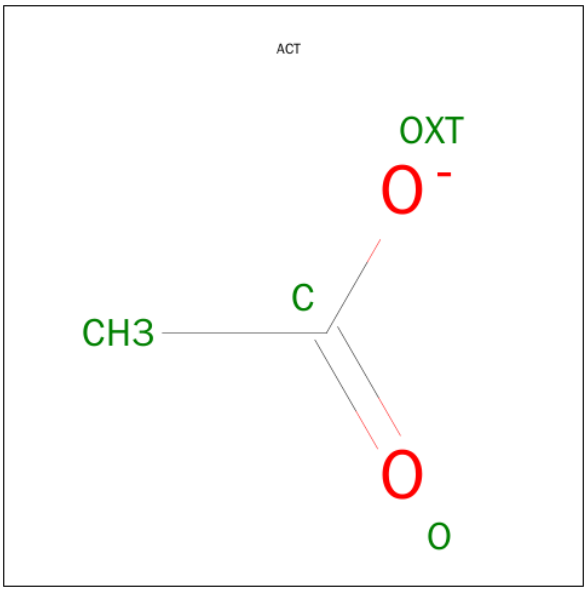
Chain	Residue	Modelled	Actual	Comment	Reference
L	103	LYS	ARG	CONFLICT	PIR S16112
L	107	LEU	LYS	CONFLICT	PIR S16112
L	109	GLY	ALA	CONFLICT	PIR S16112

- Molecule 2 is a protein called IGG2A FAB FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	222	1702	1084	275	335	8	0	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

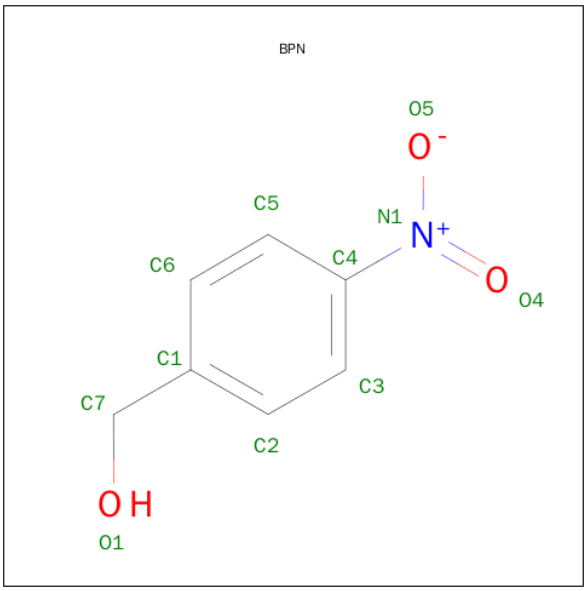


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	H	1	4	2	2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	L	7	7	7	0	0

- Molecule 5 is PARANITROBENZYL ALCOHOL (three-letter code: BPN) (formula: $C_7H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	L	1	11	7	1	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	H	66	66	66	0	0
			Total	O		
6	L	88	88	88	0	0

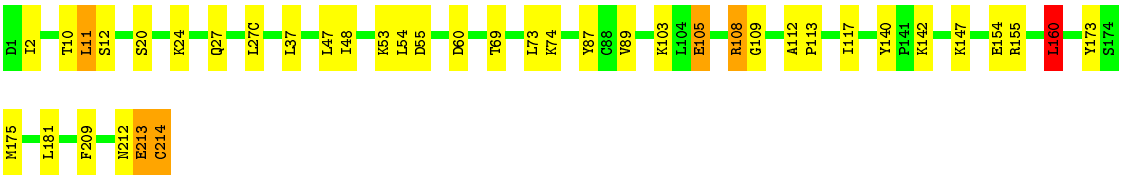
3 Residue-property plots (i)

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.

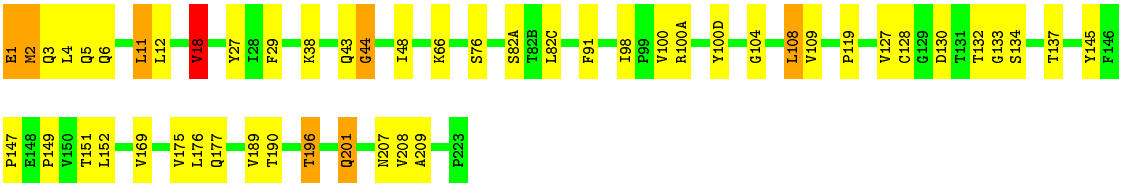
- Molecule 1: IGG2A FAB FRAGMENT

Chain L:



- Molecule 2: IGG2A FAB FRAGMENT

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	78.55Å 78.55Å 159.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.6 (7.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.199 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3564	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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: ZN, BPN, ACT

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	0.44	0/1722	0.75	2/2337 (0.1%)
2	H	0.47	0/1748	0.76	1/2385 (0.0%)
All	All	0.46	0/3470	0.76	3/4722 (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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	11	LEU	CA-CB-CG	5.96	129.01	115.30
2	H	18	VAL	CB-CA-C	-5.68	100.61	111.40
1	L	160	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	140	TYR	Sidechain

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	1686	0	1651	26	0
2	H	1702	0	1666	44	0
3	H	4	0	3	0	0
4	L	7	0	0	0	0
5	L	11	0	7	2	0
6	H	66	0	0	2	0
6	L	88	0	0	0	0
All	All	3564	0	3327	63	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 9.

All (63) 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:209:PHE:HB3	2:H:128:CYS:SG	2.16	0.86
2:H:127:VAL:HG13	2:H:128:CYS:SG	2.16	0.85
1:L:160:LEU:HD11	2:H:175:VAL:HB	1.63	0.79
2:H:12:LEU:HD23	2:H:109:VAL:HG13	1.67	0.77
1:L:213:GLU:O	1:L:214:CYS:HB2	1.85	0.76
2:H:18:VAL:HG22	2:H:82(C):LEU:HD11	1.72	0.72
2:H:44:GLY:HA3	6:H:610:HOH:O	1.91	0.70
2:H:169:VAL:HG12	2:H:189:VAL:HG23	1.75	0.68
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.77	0.68
1:L:2:ILE:HD12	1:L:27:GLN:HG3	1.80	0.64
1:L:48:ILE:HG12	1:L:54:LEU:HD12	1.85	0.59
1:L:147:LYS:HE3	1:L:154:GLU:OE2	2.04	0.57
2:H:2:MET:HE1	2:H:3:GLN:N	2.20	0.57
2:H:137:THR:HG22	2:H:190:THR:HG23	1.87	0.56
2:H:11:LEU:O	2:H:12:LEU:HD13	2.07	0.55
1:L:155:ARG:NH2	1:L:181:LEU:HD23	2.22	0.54
1:L:108:ARG:HD3	1:L:109:GLY:O	2.06	0.54
2:H:108:LEU:HD13	6:H:567:HOH:O	2.05	0.54
2:H:127:VAL:HG13	2:H:128:CYS:N	2.23	0.54
1:L:160:LEU:HD23	2:H:177:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:209:PHE:HB3	2:H:128:CYS:HG	1.74	0.53
2:H:2:MET:CE	2:H:4:LEU:HD12	2.39	0.53
2:H:151:THR:HB	2:H:209:ALA:HB3	1.90	0.52
2:H:2:MET:HE2	2:H:27:TYR:CD1	2.44	0.52
1:L:20:SER:HB3	1:L:74:LYS:HG2	1.91	0.52
1:L:209:PHE:CB	2:H:128:CYS:SG	2.96	0.51
1:L:54:LEU:HD21	1:L:60:ASP:HA	1.93	0.51
2:H:2:MET:HE3	2:H:27:TYR:HE1	1.75	0.51
2:H:12:LEU:CD2	2:H:109:VAL:HG13	2.38	0.50
1:L:10:THR:HG22	1:L:103:LYS:HB3	1.93	0.50
1:L:117:ILE:HG22	2:H:128:CYS:HB2	1.94	0.49
2:H:133:GLY:O	2:H:134:SER:HB3	2.13	0.49
1:L:24:LYS:HA	1:L:69:THR:O	2.13	0.48
1:L:53:LYS:N	1:L:53:LYS:HD2	2.27	0.48
1:L:2:ILE:CD1	1:L:27:GLN:HG3	2.42	0.48
2:H:12:LEU:HD22	2:H:12:LEU:N	2.28	0.48
2:H:2:MET:HE3	2:H:27:TYR:CE1	2.50	0.47
2:H:132:THR:HG22	2:H:133:GLY:H	1.80	0.47
2:H:2:MET:HE2	2:H:27:TYR:HD1	1.77	0.47
1:L:12:SER:HA	1:L:105:GLU:O	2.14	0.47
1:L:87:TYR:OH	2:H:43:GLN:HA	2.14	0.46
2:H:100:VAL:HG13	2:H:100(A):ARG:HG2	1.97	0.46
1:L:48:ILE:HD12	1:L:73:LEU:CD1	2.47	0.45
2:H:128:CYS:C	2:H:130:ASP:H	2.20	0.45
2:H:127:VAL:CG1	2:H:128:CYS:N	2.79	0.45
2:H:6:GLN:HE21	2:H:104:GLY:HA3	1.81	0.45
2:H:1:GLU:CD	2:H:1:GLU:N	2.70	0.45
1:L:89:VAL:HG22	5:L:551:BPN:H6	1.99	0.44
2:H:2:MET:CE	2:H:27:TYR:CE1	3.00	0.44
2:H:6:GLN:HE22	2:H:91:PHE:HA	1.83	0.44
2:H:151:THR:O	2:H:208:VAL:HA	2.18	0.44
2:H:29:PHE:CD2	2:H:76:SER:HA	2.54	0.43
1:L:112:ALA:HA	1:L:113:PRO:HD3	1.89	0.43
2:H:196:THR:O	2:H:201:GLN:HG3	2.19	0.43
1:L:147:LYS:HD2	1:L:147:LYS:HA	1.85	0.42
2:H:152:LEU:HA	2:H:207:ASN:O	2.19	0.42
2:H:38:LYS:HB2	2:H:48:ILE:HD11	2.02	0.41
2:H:132:THR:HG22	2:H:133:GLY:N	2.35	0.41
2:H:66:LYS:HE2	2:H:82(A):SER:O	2.20	0.41
1:L:89:VAL:CG2	5:L:551:BPN:H6	2.51	0.41
1:L:142:LYS:HB3	1:L:173:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100(D):TYR:CD1	2:H:100(D):TYR:N	2.89	0.41
2:H:98:ILE:HG22	2:H:100:VAL:HG12	2.02	0.40

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	217/219 (99%)	209 (96%)	7 (3%)	1 (0%)	34	26
2	H	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	34	26
All	All	437/441 (99%)	418 (96%)	17 (4%)	2 (0%)	34	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	212	ASN
2	H	44	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	195/195 (100%)	184 (94%)	11 (6%)	26	20
2	H	193/193 (100%)	182 (94%)	11 (6%)	25	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	388/388 (100%)	366 (94%)	22 (6%)	25 19

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	11	LEU
1	L	27(C)	LEU
1	L	37	LEU
1	L	47	LEU
1	L	55	ASP
1	L	105	GLU
1	L	108	ARG
1	L	160	LEU
1	L	175	MET
1	L	213	GLU
1	L	214	CYS
2	H	1	GLU
2	H	2	MET
2	H	5	GLN
2	H	11	LEU
2	H	18	VAL
2	H	108	LEU
2	H	147	PRO
2	H	149	PRO
2	H	176	LEU
2	H	196	THR
2	H	201	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	6	GLN
2	H	177	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)

Of 9 ligands modelled in this entry, 7 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	$\#\|Z\| > 2$
3	ACT	H	552	-	1,3,3	3.20	1 (100%)	0,3,3	0.00	-
5	BPN	L	551	-	9,11,11	0.41	0	12,14,14	0.84	0

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
3	ACT	H	552	-	-	0/0/0/0	0/0/0/0
5	BPN	L	551	-	-	0/6/6/6	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	552	ACT	CH3-C	3.20	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	551	BPN	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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