



wwPDB X-ray Structure Validation Summary Report

Feb 15, 2017 – 03:31 am GMT

PDB ID : 2BYS
Title : CRYSTAL STRUCTURE OF ACHBP FROM APLYSIA CALIFORNICA IN COMPLEX WITH LOBELINE
Authors : Hansen, S.B.; Sulzenbacher, G.; Huxford, T.; Marchot, P.; Taylor, P.; Bourne, Y.
Deposited on : 2005-08-04
Resolution : 2.05 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

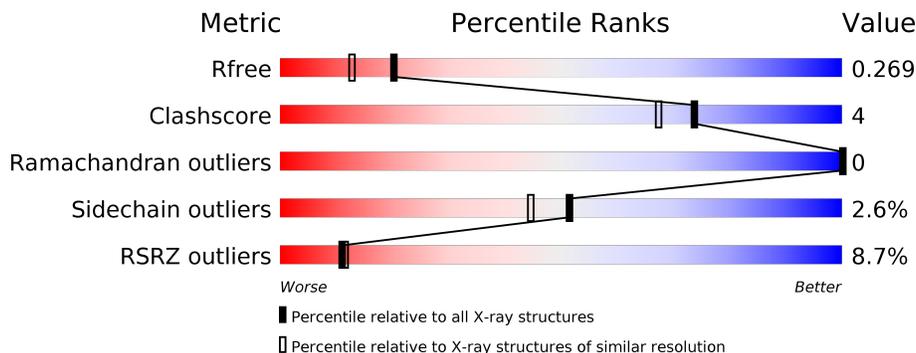
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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))
R_{free}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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.

Mol	Chain	Length	Quality of chain
1	A	227	 7% 78% 12% • 10%
1	B	227	 5% 82% 8% 9%
1	C	227	 5% 79% 10% • 11%
1	D	227	 8% 82% 8% 10%
1	E	227	 12% 82% 8% 9%
1	F	227	 6% 83% 7% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	227	
1	H	227	
1	I	227	
1	J	227	

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
2	LOB	D	301	-	-	-	X

2 Entry composition [i](#)

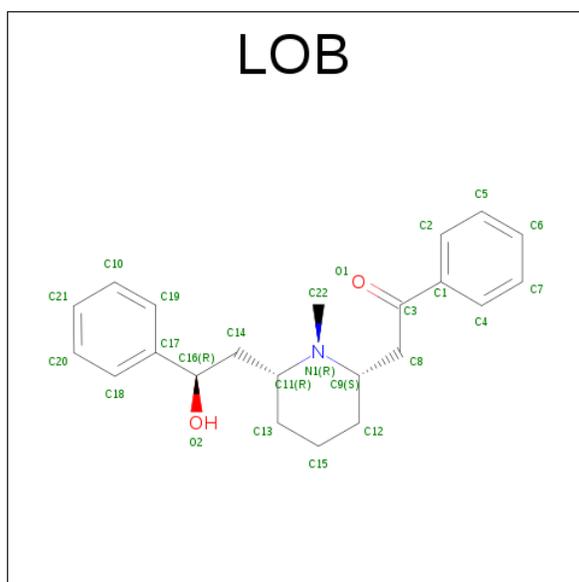
There are 3 unique types of molecules in this entry. The entry contains 18491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	205	Total 1670	C 1054	N 278	O 330	S 8	0	10	0
1	B	206	Total 1682	C 1063	N 282	O 329	S 8	0	7	0
1	C	203	Total 1656	C 1047	N 274	O 327	S 8	0	7	0
1	D	205	Total 1689	C 1068	N 279	O 334	S 8	0	10	0
1	E	206	Total 1666	C 1054	N 277	O 327	S 8	0	3	0
1	F	204	Total 1653	C 1044	N 273	O 328	S 8	0	8	0
1	G	203	Total 1664	C 1054	N 276	O 326	S 8	0	8	0
1	H	204	Total 1663	C 1051	N 278	O 326	S 8	0	6	0
1	I	206	Total 1681	C 1062	N 282	O 329	S 8	0	6	0
1	J	204	Total 1658	C 1047	N 278	O 325	S 8	0	4	0

- Molecule 2 is LOBELINE (three-letter code: LOB) (formula: $C_{22}H_{27}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	22	1	2		
2	B	1	Total	C	N	O	0	0
			25	22	1	2		
2	C	1	Total	C	N	O	0	0
			25	22	1	2		
2	D	1	Total	C	N	O	0	0
			25	22	1	2		
2	E	1	Total	C	N	O	0	0
			25	22	1	2		
2	F	1	Total	C	N	O	0	0
			25	22	1	2		
2	G	1	Total	C	N	O	0	0
			25	22	1	2		
2	H	1	Total	C	N	O	0	0
			25	22	1	2		
2	I	1	Total	C	N	O	0	0
			25	22	1	2		
2	J	1	Total	C	N	O	0	0
			25	22	1	2		

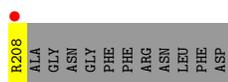
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total	O	0	0
			164	164		
3	B	186	Total	O	0	0
			186	186		

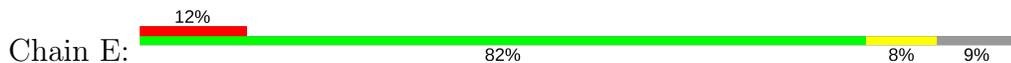
Continued on next page...

Continued from previous page...

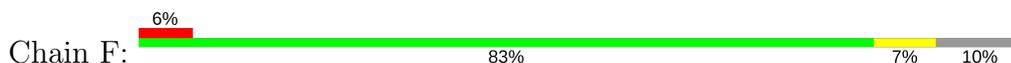
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	150	Total 150	O 150	0	0
3	D	181	Total 181	O 181	0	0
3	E	170	Total 170	O 170	0	0
3	F	158	Total 158	O 158	0	0
3	G	158	Total 158	O 158	0	0
3	H	104	Total 104	O 104	0	0
3	I	133	Total 133	O 133	0	0
3	J	155	Total 155	O 155	0	0



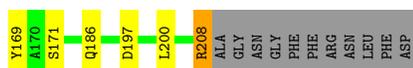
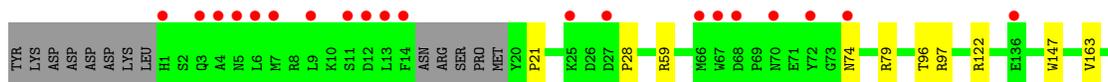
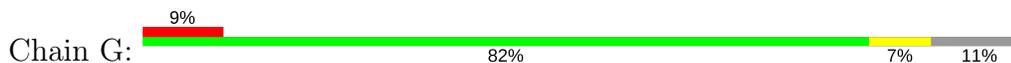
- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN



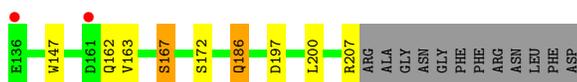
- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN



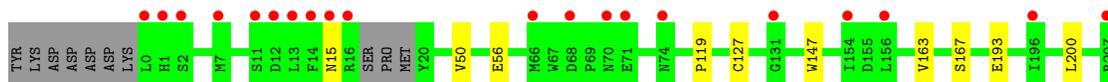
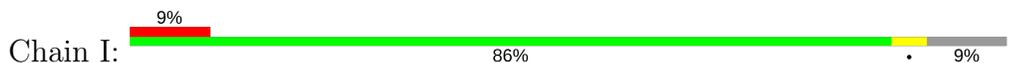
- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN



- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

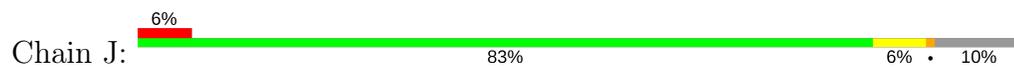


- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN





● Molecule 1: ACETYLCHOLINE-BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.76Å 85.73Å 117.32Å 89.95° 97.33° 106.64°	Depositor
Resolution (Å)	47.73 – 2.05 34.55 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.5 (47.73-2.05) 76.3 (34.55-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.97Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.258 0.230 , 0.269	Depositor DCC
R_{free} test set	4134 reflections (3.12%)	DCC
Wilson B-factor (Å ²)	21.7	Xtrriage
Anisotropy	0.817	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18491	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.41	0/1727	0.64	0/2351
1	B	0.43	0/1736	0.61	0/2363
1	C	0.39	0/1712	0.59	0/2332
1	D	0.39	0/1756	0.60	0/2392
1	E	0.39	0/1714	0.58	0/2333
1	F	0.39	0/1703	0.59	0/2320
1	G	0.37	0/1724	0.56	0/2348
1	H	0.35	0/1716	0.57	0/2335
1	I	0.37	0/1735	0.57	0/2363
1	J	0.37	0/1708	0.61	0/2325
All	All	0.39	0/17231	0.59	0/23462

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	190	CYS	Peptide

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	1670	0	1613	19	0
1	B	1682	0	1629	10	0
1	C	1656	0	1600	16	0
1	D	1689	0	1635	11	0
1	E	1666	0	1612	13	0
1	F	1653	0	1590	15	0
1	G	1664	0	1614	13	0
1	H	1663	0	1609	13	0
1	I	1681	0	1629	5	0
1	J	1658	0	1604	10	0
2	A	25	0	27	2	0
2	B	25	0	27	1	0
2	C	25	0	27	4	0
2	D	25	0	27	1	0
2	E	25	0	27	5	0
2	F	25	0	27	3	0
2	G	25	0	27	3	0
2	H	25	0	27	2	0
2	I	25	0	27	2	0
2	J	25	0	27	4	0
3	A	164	0	0	1	0
3	B	186	0	0	1	0
3	C	150	0	0	1	0
3	D	181	0	0	0	0
3	E	170	0	0	1	0
3	F	158	0	0	2	0
3	G	158	0	0	0	0
3	H	104	0	0	1	0
3	I	133	0	0	0	0
3	J	155	0	0	2	0
All	All	18491	0	16405	128	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 4.

The worst 5 of 128 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:A:38[B]:GLN:HA	1:A:38[B]:GLN:HE21	1.32	0.94
1:F:38[B]:GLN:HE22	1:F:167:SER:HB2	1.34	0.92
1:F:105[B]:GLN:HA	1:F:105[B]:GLN:HE21	1.40	0.86
1:A:38[B]:GLN:CA	1:A:38[B]:GLN:HE21	1.89	0.85
1:J:147:TRP:O	2:J:301:LOB:H8C1	1.81	0.81

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	A	207/227 (91%)	201 (97%)	6 (3%)	0	100	100
1	B	207/227 (91%)	200 (97%)	7 (3%)	0	100	100
1	C	205/227 (90%)	202 (98%)	3 (2%)	0	100	100
1	D	210/227 (92%)	209 (100%)	1 (0%)	0	100	100
1	E	205/227 (90%)	199 (97%)	6 (3%)	0	100	100
1	F	204/227 (90%)	200 (98%)	4 (2%)	0	100	100
1	G	206/227 (91%)	203 (98%)	3 (2%)	0	100	100
1	H	204/227 (90%)	200 (98%)	4 (2%)	0	100	100
1	I	207/227 (91%)	203 (98%)	4 (2%)	0	100	100
1	J	204/227 (90%)	201 (98%)	3 (2%)	0	100	100
All	All	2059/2270 (91%)	2018 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	192/205 (94%)	180 (94%)	12 (6%)	21	11
1	B	192/205 (94%)	186 (97%)	6 (3%)	45	38
1	C	190/205 (93%)	179 (94%)	11 (6%)	23	13
1	D	195/205 (95%)	193 (99%)	2 (1%)	80	79
1	E	190/205 (93%)	188 (99%)	2 (1%)	78	77
1	F	189/205 (92%)	186 (98%)	3 (2%)	68	65
1	G	191/205 (93%)	185 (97%)	6 (3%)	45	38
1	H	190/205 (93%)	178 (94%)	12 (6%)	21	11
1	I	192/205 (94%)	190 (99%)	2 (1%)	80	79
1	J	189/205 (92%)	184 (97%)	5 (3%)	51	44
All	All	1910/2050 (93%)	1849 (97%)	61 (3%)	51	36

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	186[B]	GLN
1	F	74[A]	ASN
1	J	8	ARG
1	C	208	ARG
1	D	208	ARG

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

Mol	Chain	Res	Type
1	F	186	GLN
1	G	3	GLN
1	I	70	ASN
1	E	186	GLN
1	G	74	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](#)

10 ligands are modelled in this entry.

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$
2	LOB	A	301	-	27,27,27	0.79	0	33,36,36	2.09	5 (15%)
2	LOB	B	301	-	27,27,27	0.81	1 (3%)	33,36,36	2.22	10 (30%)
2	LOB	C	301	-	27,27,27	0.78	0	33,36,36	2.05	6 (18%)
2	LOB	D	301	-	27,27,27	0.75	0	33,36,36	2.27	8 (24%)
2	LOB	E	301	-	27,27,27	0.68	0	33,36,36	2.09	8 (24%)
2	LOB	F	301	-	27,27,27	0.74	1 (3%)	33,36,36	2.05	7 (21%)
2	LOB	G	301	-	27,27,27	0.69	0	33,36,36	2.20	6 (18%)
2	LOB	H	301	-	27,27,27	0.76	0	33,36,36	2.09	7 (21%)
2	LOB	I	301	-	27,27,27	0.66	0	33,36,36	2.16	5 (15%)
2	LOB	J	301	-	27,27,27	0.66	0	33,36,36	2.06	6 (18%)

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
2	LOB	A	301	-	-	0/16/30/30	0/3/3/3
2	LOB	B	301	-	-	0/16/30/30	0/3/3/3
2	LOB	C	301	-	-	0/16/30/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LOB	D	301	-	-	0/16/30/30	0/3/3/3
2	LOB	E	301	-	-	0/16/30/30	0/3/3/3
2	LOB	F	301	-	-	0/16/30/30	0/3/3/3
2	LOB	G	301	-	-	0/16/30/30	0/3/3/3
2	LOB	H	301	-	-	0/16/30/30	0/3/3/3
2	LOB	I	301	-	-	0/16/30/30	0/3/3/3
2	LOB	J	301	-	-	0/16/30/30	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	LOB	C11-N1	2.12	1.50	1.47
2	B	301	LOB	C11-N1	2.60	1.50	1.47

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	LOB	C8-C9-N1	-4.80	105.74	114.59
2	H	301	LOB	C8-C9-N1	-4.73	105.86	114.59
2	G	301	LOB	C8-C9-N1	-4.53	106.23	114.59
2	C	301	LOB	C8-C9-N1	-4.46	106.36	114.59
2	J	301	LOB	C8-C9-N1	-4.23	106.79	114.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	LOB	2	0
2	B	301	LOB	1	0
2	C	301	LOB	4	0
2	D	301	LOB	1	0
2	E	301	LOB	5	0
2	F	301	LOB	3	0
2	G	301	LOB	3	0
2	H	301	LOB	2	0
2	I	301	LOB	2	0
2	J	301	LOB	4	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](#)

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	A	205/227 (90%)	0.44	16 (7%) 14 15	20, 34, 72, 88	4 (1%)
1	B	206/227 (90%)	0.28	12 (5%) 24 26	20, 34, 77, 92	2 (0%)
1	C	203/227 (89%)	0.27	12 (5%) 23 25	22, 37, 65, 74	1 (0%)
1	D	205/227 (90%)	0.39	18 (8%) 11 11	21, 32, 70, 89	1 (0%)
1	E	206/227 (90%)	0.53	27 (13%) 4 3	22, 34, 72, 94	0
1	F	204/227 (89%)	0.24	14 (6%) 18 19	24, 35, 73, 82	4 (1%)
1	G	203/227 (89%)	0.39	20 (9%) 8 9	24, 36, 83, 100	1 (0%)
1	H	204/227 (89%)	0.57	24 (11%) 5 5	27, 43, 78, 89	1 (0%)
1	I	206/227 (90%)	0.53	21 (10%) 7 8	26, 36, 71, 87	1 (0%)
1	J	204/227 (89%)	0.42	14 (6%) 18 19	25, 35, 65, 72	0
All	All	2046/2270 (90%)	0.41	178 (8%) 11 11	20, 36, 73, 100	15 (0%)

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	HIS	7.4
1	A	17	SER	7.2
1	I	11	SER	6.9
1	G	1	HIS	6.6
1	G	74	ASN	6.4

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	LOB	D	301	25/25	0.88	0.21	2.03	25,29,33,33	0
2	LOB	H	301	25/25	0.90	0.21	1.79	32,33,34,34	0
2	LOB	B	301	25/25	0.93	0.16	1.78	25,31,35,35	0
2	LOB	C	301	25/25	0.88	0.16	1.61	27,28,31,31	0
2	LOB	G	301	25/25	0.92	0.15	1.20	32,34,37,37	0
2	LOB	F	301	25/25	0.89	0.14	0.51	32,34,37,37	0
2	LOB	I	301	25/25	0.89	0.16	0.42	27,31,35,35	0
2	LOB	J	301	25/25	0.92	0.13	0.11	27,29,31,31	0
2	LOB	A	301	25/25	0.89	0.12	-0.10	30,32,36,36	0
2	LOB	E	301	25/25	0.92	0.12	-0.12	28,30,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.