Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:07 PM GMT

PDB ID	:	4KKT
Title	:	Crystal Structure of BesA (P21 form)
Authors	:	Greene, N.P.; Hinchliffe, P.; Crow, A.; Ababou, A.; Hughes, C.; Koronakis, V.
Deposited on	:	2013-05-06
Resolution	:	2.53 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:

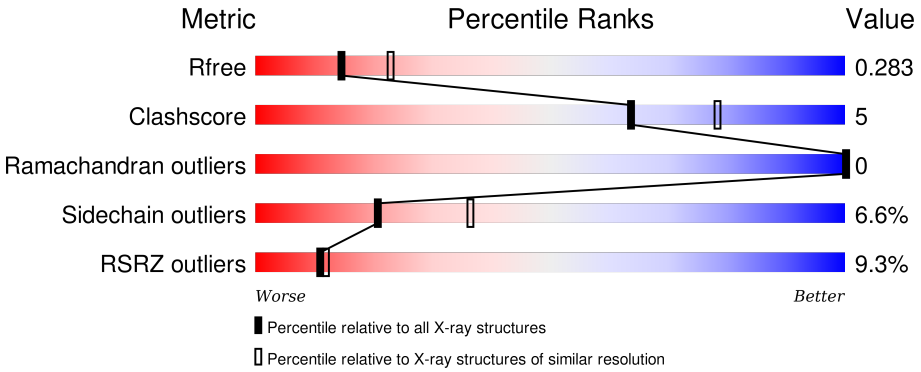
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 2.53 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}	91344	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	296	7% 77% 10% • 10%
1	B	296	6% 77% 11% • 11%
1	C	296	7% 77% 10% • 11%
1	D	296	13% 76% 11% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8267 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 Membrane fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	1	0
			2048	1314	337	393	4			
1	B	262	Total	C	N	O	S	0	3	0
			2043	1311	335	393	4			
1	C	262	Total	C	N	O	S	0	0	0
			2019	1296	332	387	4			
1	D	263	Total	C	N	O	S	0	2	0
			2046	1313	335	394	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	EXPRESSION TAG	UNP O51166
A	23	SER	-	EXPRESSION TAG	UNP O51166
A	24	HIS	-	EXPRESSION TAG	UNP O51166
A	25	MET	-	EXPRESSION TAG	UNP O51166
B	22	GLY	-	EXPRESSION TAG	UNP O51166
B	23	SER	-	EXPRESSION TAG	UNP O51166
B	24	HIS	-	EXPRESSION TAG	UNP O51166
B	25	MET	-	EXPRESSION TAG	UNP O51166
C	22	GLY	-	EXPRESSION TAG	UNP O51166
C	23	SER	-	EXPRESSION TAG	UNP O51166
C	24	HIS	-	EXPRESSION TAG	UNP O51166
C	25	MET	-	EXPRESSION TAG	UNP O51166
D	22	GLY	-	EXPRESSION TAG	UNP O51166
D	23	SER	-	EXPRESSION TAG	UNP O51166
D	24	HIS	-	EXPRESSION TAG	UNP O51166
D	25	MET	-	EXPRESSION TAG	UNP O51166

- Molecule 2 is water.

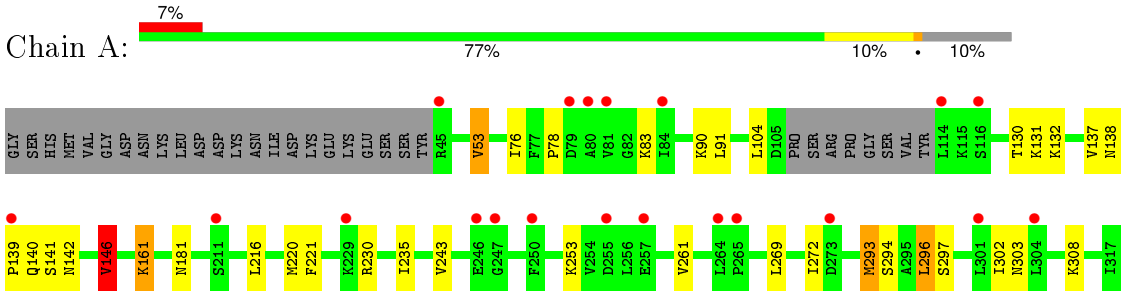
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	30	Total O 30 30	0	0
2	C	23	Total O 23 23	0	0
2	D	29	Total O 29 29	0	0

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.

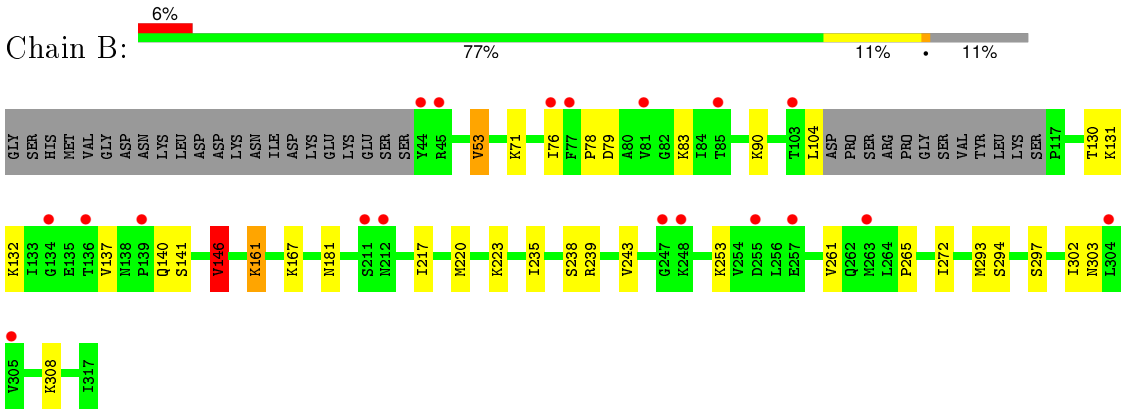
- Molecule 1: Membrane fusion protein

Chain A:



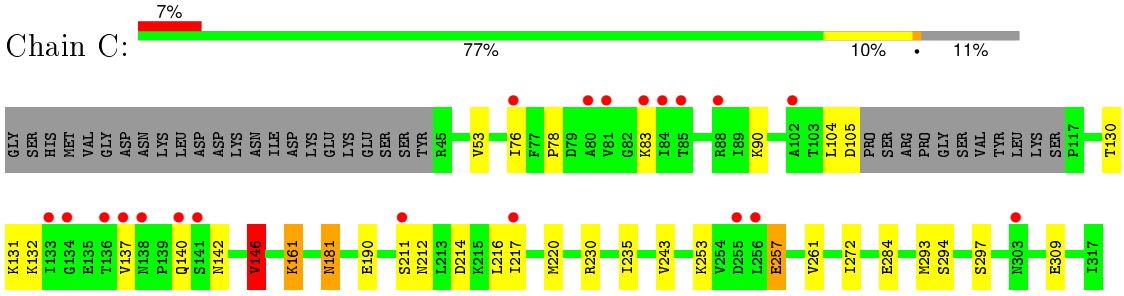
- Molecule 1: Membrane fusion protein

Chain B:



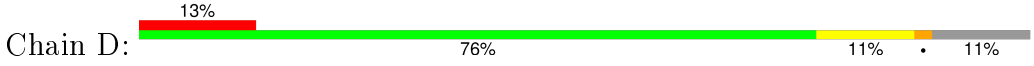
- Molecule 1: Membrane fusion protein

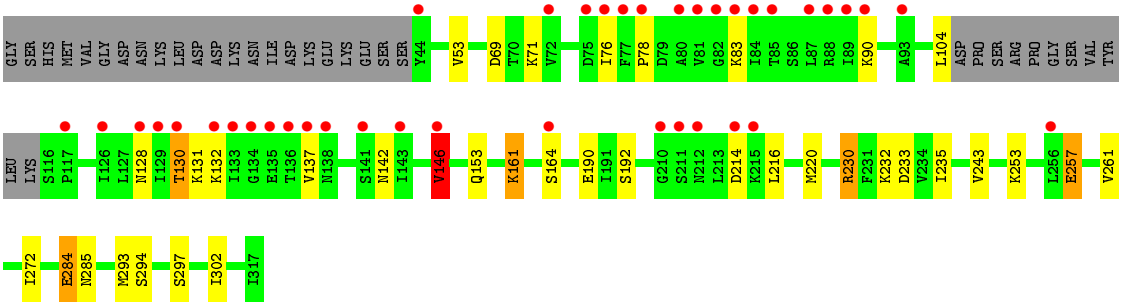
Chain C:



- Molecule 1: Membrane fusion protein

Chain D:




GLY SER HIS MET VAL GLY ASP ASN LYS LEU ASP ASP LYS ASN ILE ASP LYS GLU LYS GLU SER SER Y44 V53 D69 T70 K71 V72 D75 I76 F77 P78 D79 A80 V81 G82 K83 I84 T85 S86 L87 R88 I89 K90 A93 L104 ASP PRO SER ARG PRO GLY SER VAL TYR
LEU LYS S116 P117 I126 L127 N128 I129 T130 K131 K132 I133 G134 E135 T136 V137 N138 S141 N142 I143 V149 Q153 K161 S164 E190 I191 S192 G210 S211 N212 L213 D214 K215 L216 M220 R230 F231 K232 D233 V234 I235 V243 K253 L256 E257 V261
I272 E284 N285 M293 S294 S297 I302 I317

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.20Å 73.74Å 152.23Å 90.00° 98.06° 90.00°	Depositor
Resolution (Å)	73.27 – 2.53 73.17 – 2.53	Depositor EDS
% Data completeness (in resolution range)	95.2 (73.27-2.53) 95.2 (73.17-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.52 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.257 , 0.285 0.261 , 0.283	Depositor DCC
R_{free} test set	2928 reflections (5.63%)	DCC
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	4 of 54835 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8267	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.47 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.1511e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.75	0/2069	0.86	4/2786 (0.1%)
1	B	0.76	0/2065	0.84	1/2781 (0.0%)
1	C	0.72	0/2040	0.83	2/2747 (0.1%)
1	D	0.71	0/2068	0.82	2/2786 (0.1%)
All	All	0.73	0/8242	0.84	9/11100 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	MET	CG-SD-CE	6.64	110.83	100.20
1	B	146	VAL	CB-CA-C	-6.57	98.92	111.40
1	A	230	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	146	VAL	CB-CA-C	-6.08	99.85	111.40
1	C	146	VAL	CB-CA-C	-6.01	99.97	111.40
1	A	230	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	C	230	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	146	VAL	CB-CA-C	-5.77	100.44	111.40
1	D	230	ARG	NE-CZ-NH2	-5.40	117.60	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2048	0	2183	25	0
1	B	2043	0	2167	22	0
1	C	2019	0	2151	23	0
1	D	2046	0	2168	23	0
2	A	29	0	0	2	0
2	B	30	0	0	5	0
2	C	23	0	0	1	0
2	D	29	0	0	9	0
All	All	8267	0	8669	87	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 5.

All (87) 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:D:69:ASP:OD2	2:D:403:HOH:O	1.69	1.08
1:A:78:PRO:HG3	1:A:137:VAL:HG11	1.56	0.88
1:D:190:GLU:OE2	2:D:409:HOH:O	2.01	0.78
1:A:78:PRO:HG3	1:A:137:VAL:CG1	2.12	0.78
1:D:230:ARG:HG3	2:D:428:HOH:O	1.83	0.77
1:C:257:GLU:HA	1:C:257:GLU:OE2	1.85	0.75
1:A:293:MET:HA	1:A:296:LEU:HD22	1.70	0.73
1:A:78:PRO:CG	1:A:137:VAL:CG1	2.69	0.70
1:D:232:LYS:O	1:D:233[B]:ASP:OD1	2.10	0.69
1:A:303:ASN:HA	2:A:425:HOH:O	1.93	0.67
1:D:233[B]:ASP:CG	1:D:233[B]:ASP:O	2.36	0.63
1:A:137:VAL:HG13	1:A:141[B]:SER:HB3	1.80	0.63
1:B:303:ASN:HA	2:B:425:HOH:O	1.97	0.63
1:A:137:VAL:HG13	1:A:141[A]:SER:HB2	1.81	0.62
1:C:53:VAL:CG1	1:C:235:ILE:HD12	2.33	0.59
1:A:131:LYS:HE3	1:A:137:VAL:HG22	1.85	0.58
1:C:211:SER:O	1:C:212:ASN:HB3	2.02	0.58
1:D:53:VAL:CG1	1:D:235:ILE:HD12	2.35	0.57
1:B:53:VAL:CG1	1:B:235:ILE:HD12	2.35	0.56
1:B:79[B]:ASP:OD1	1:B:79[B]:ASP:O	2.23	0.56
1:B:217:ILE:HD12	1:B:220:MET:HE1	1.87	0.56
1:B:272:ILE:HD12	1:C:161:LYS:HB3	1.88	0.56
1:A:53:VAL:CG1	1:A:235:ILE:HD12	2.36	0.56
1:D:153:GLN:NE2	2:D:403:HOH:O	2.38	0.56
1:A:272:ILE:HD12	1:D:161:LYS:HB3	1.88	0.55
1:A:161:LYS:HB3	1:D:272:ILE:HD12	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:LYS:O	1:D:104:LEU:HA	2.07	0.55
2:A:405:HOH:O	1:D:161:LYS:HD3	2.08	0.54
1:B:83:LYS:O	1:B:104:LEU:HA	2.08	0.54
1:A:91:LEU:HD12	1:B:181:ASN:HB3	1.90	0.53
1:A:76:ILE:HD11	1:A:146:VAL:HG22	1.89	0.53
1:C:220:MET:CE	2:D:412:HOH:O	2.58	0.52
1:B:76:ILE:HD11	1:B:146:VAL:HG22	1.91	0.52
1:C:76:ILE:HD11	1:C:146:VAL:HG22	1.93	0.51
1:D:76:ILE:HD11	1:D:146:VAL:HG22	1.91	0.50
1:D:192:SER:HA	2:D:409:HOH:O	2.11	0.50
1:A:78:PRO:HG2	1:A:137:VAL:CG1	2.42	0.49
1:B:161:LYS:HB3	1:C:272:ILE:HD12	1.94	0.49
1:A:137:VAL:CG1	1:A:138:ASN:N	2.76	0.49
1:C:83:LYS:O	1:C:104:LEU:HA	2.12	0.49
1:A:221:PHE:CE2	1:B:223:LYS:HD2	2.47	0.48
2:B:405:HOH:O	1:C:161:LYS:HD3	2.14	0.48
1:B:141[A]:SER:OG	2:B:410:HOH:O	1.99	0.48
1:A:83:LYS:O	1:A:104:LEU:HA	2.13	0.48
1:C:217:ILE:HD12	1:C:220:MET:HE1	1.96	0.48
1:A:78:PRO:HB3	1:A:104:LEU:HD11	1.98	0.46
1:B:78:PRO:HG3	1:B:137:VAL:HG21	1.97	0.46
1:C:211:SER:O	1:C:212:ASN:CB	2.64	0.46
1:C:190:GLU:HA	2:C:412:HOH:O	2.15	0.46
1:B:131:LYS:HE3	1:B:137:VAL:HG12	1.98	0.45
1:D:164:SER:HB2	2:D:406:HOH:O	2.15	0.45
1:D:253:LYS:O	1:D:261:VAL:HA	2.17	0.45
1:B:217:ILE:HD12	1:B:220:MET:CE	2.47	0.45
1:D:257[B]:GLU:H	1:D:257[B]:GLU:HG2	1.44	0.44
1:B:239:ARG:NH2	2:B:420:HOH:O	2.50	0.44
1:B:302:ILE:HD12	1:B:302:ILE:C	2.38	0.44
1:A:78:PRO:CG	1:A:137:VAL:HG12	2.45	0.44
1:C:257:GLU:OE2	1:C:257:GLU:CA	2.62	0.44
1:D:128:ASN:OD1	1:D:130:THR:HG23	2.17	0.44
1:A:302:ILE:C	1:A:302:ILE:HD12	2.38	0.44
1:C:78:PRO:HG3	1:C:137:VAL:HG21	1.99	0.44
1:D:131:LYS:HE3	1:D:137:VAL:HG12	2.00	0.43
1:C:217:ILE:HB	1:C:220:MET:HE3	1.99	0.43
1:C:78:PRO:HB3	1:C:104:LEU:HD11	2.00	0.43
1:B:217:ILE:HB	1:B:220:MET:HE3	2.01	0.43
1:C:220:MET:HE2	2:D:412:HOH:O	2.18	0.43
1:B:78:PRO:HG3	1:B:137:VAL:CG2	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LYS:HE3	1:C:137:VAL:HG12	2.01	0.43
1:C:253:LYS:O	1:C:261:VAL:HA	2.19	0.43
1:B:78:PRO:HB3	1:B:104:LEU:HD11	2.00	0.42
1:C:220:MET:HE1	2:D:412:HOH:O	2.19	0.42
1:A:253:LYS:O	1:A:261:VAL:HA	2.19	0.42
1:B:253:LYS:O	1:B:261:VAL:HA	2.19	0.42
1:A:78:PRO:CG	1:A:137:VAL:HG11	2.34	0.42
1:D:78:PRO:HB3	1:D:104:LEU:HD11	2.01	0.42
1:D:216:LEU:HA	1:D:216:LEU:HD12	1.89	0.42
1:D:78:PRO:HG3	1:D:137:VAL:HG21	2.00	0.42
1:B:265:PRO:O	2:B:424:HOH:O	2.22	0.42
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.86	0.41
1:D:284:GLU:O	1:D:285:ASN:HB2	2.20	0.41
1:C:78:PRO:HG3	1:C:137:VAL:CG2	2.50	0.41
1:B:308:LYS:HB3	1:B:308:LYS:HE3	1.88	0.41
1:C:181:ASN:H	1:C:181:ASN:HD22	1.69	0.41
1:A:308:LYS:HB3	1:A:308:LYS:HE3	1.89	0.41
1:C:216:LEU:HA	1:C:216:LEU:HD12	1.90	0.41
1:A:138:ASN:HB2	1:A:139:PRO:HD2	2.03	0.41
1:D:302:ILE:C	1:D:302:ILE:HD12	2.41	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	A	262/296 (88%)	256 (98%)	6 (2%)	0	100	100
1	B	261/296 (88%)	258 (99%)	3 (1%)	0	100	100
1	C	258/296 (87%)	253 (98%)	5 (2%)	0	100	100
1	D	261/296 (88%)	256 (98%)	5 (2%)	0	100	100
All	All	1042/1184 (88%)	1023 (98%)	19 (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	235/262 (90%)	220 (94%)	15 (6%)	22	38
1	B	234/262 (89%)	219 (94%)	15 (6%)	22	38
1	C	231/262 (88%)	214 (93%)	17 (7%)	17	30
1	D	234/262 (89%)	218 (93%)	16 (7%)	20	35
All	All	934/1048 (89%)	871 (93%)	63 (7%)	21	36

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	90	LYS
1	A	130	THR
1	A	132	LYS
1	A	140	GLN
1	A	142	ASN
1	A	146	VAL
1	A	161	LYS
1	A	181	ASN
1	A	243	VAL
1	A	269	LEU
1	A	293	MET
1	A	294	SER
1	A	296	LEU
1	A	297	SER
1	B	53	VAL
1	B	71	LYS
1	B	90	LYS
1	B	130	THR
1	B	132	LYS
1	B	140	GLN
1	B	146	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	161	LYS
1	B	167	LYS
1	B	238[A]	SER
1	B	238[B]	SER
1	B	243	VAL
1	B	293	MET
1	B	294	SER
1	B	297	SER
1	C	90	LYS
1	C	105	ASP
1	C	130	THR
1	C	132	LYS
1	C	140	GLN
1	C	142	ASN
1	C	146	VAL
1	C	161	LYS
1	C	181	ASN
1	C	214	ASP
1	C	243	VAL
1	C	257	GLU
1	C	284	GLU
1	C	293	MET
1	C	294	SER
1	C	297	SER
1	C	309	GLU
1	D	71	LYS
1	D	90	LYS
1	D	130	THR
1	D	132	LYS
1	D	142	ASN
1	D	146	VAL
1	D	161	LYS
1	D	214	ASP
1	D	220	MET
1	D	243	VAL
1	D	257[A]	GLU
1	D	257[B]	GLU
1	D	284	GLU
1	D	293	MET
1	D	294	SER
1	D	297	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	B	96	GLN
1	B	165	ASN
1	B	170	ASN
1	C	153	GLN
1	C	165	ASN
1	C	181	ASN
1	C	274	ASN
1	D	153	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

There are no ligands in this entry.

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

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, 95^{th} 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	265/296 (89%)	0.79	20 (7%) 17 19	15, 30, 57, 97	0
1	B	262/296 (88%)	0.83	19 (7%) 18 20	13, 29, 60, 77	0
1	C	262/296 (88%)	0.73	20 (7%) 17 18	16, 32, 83, 101	0
1	D	263/296 (88%)	1.01	39 (14%) 3 3	15, 33, 99, 134	0
All	All	1052/1184 (88%)	0.84	98 (9%) 11 12	13, 31, 77, 134	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	THR	6.3
1	D	81	VAL	5.8
1	D	133	ILE	5.8
1	D	132	LYS	5.8
1	D	212	ASN	5.6
1	D	83	LYS	5.5
1	D	141	SER	5.1
1	D	137	VAL	4.9
1	A	247	GLY	4.9
1	A	80	ALA	4.6
1	D	84	ILE	4.5
1	D	129	ILE	4.5
1	C	136	THR	4.2
1	A	257	GLU	4.1
1	A	45	ARG	4.1
1	D	80	ALA	4.1
1	C	134	GLY	3.8
1	C	138	ASN	3.8
1	D	138	ASN	3.8
1	D	130	THR	3.7
1	A	304	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	81	VAL	3.6
1	D	117	PRO	3.6
1	D	134	GLY	3.6
1	A	211	SER	3.6
1	B	247	GLY	3.5
1	A	114	LEU	3.5
1	D	214	ASP	3.4
1	D	211	SER	3.4
1	C	85	THR	3.3
1	A	255	ASP	3.3
1	D	76	ILE	3.3
1	B	212	ASN	3.2
1	B	45	ARG	3.2
1	A	229	LYS	3.1
1	D	128	ASN	3.1
1	C	84	ILE	3.0
1	B	255	ASP	3.0
1	B	85	THR	3.0
1	B	44	TYR	3.0
1	D	126	ILE	2.9
1	D	210	GLY	2.9
1	D	215	LYS	2.8
1	D	93	ALA	2.8
1	A	246	GLU	2.8
1	D	87	LEU	2.8
1	D	143	ILE	2.8
1	C	256	LEU	2.8
1	B	305	VAL	2.8
1	D	85	THR	2.7
1	C	80	ALA	2.7
1	D	78	PRO	2.7
1	D	75	ASP	2.7
1	A	81	VAL	2.7
1	D	88	ARG	2.7
1	D	89	ILE	2.6
1	B	134	GLY	2.6
1	C	137	VAL	2.6
1	D	164	SER	2.6
1	C	83	LYS	2.6
1	D	90	LYS	2.6
1	C	133	ILE	2.6
1	B	136	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	211	SER	2.5
1	D	135	GLU	2.5
1	B	103	THR	2.4
1	D	256	LEU	2.4
1	C	140	GLN	2.4
1	B	81	VAL	2.4
1	C	217	ILE	2.4
1	A	84	ILE	2.4
1	B	248	LYS	2.3
1	D	44	TYR	2.3
1	A	264	LEU	2.3
1	B	304	LEU	2.3
1	A	79	ASP	2.3
1	B	76	ILE	2.3
1	C	141	SER	2.3
1	A	139	PRO	2.3
1	A	250	PHE	2.3
1	C	211	SER	2.2
1	C	88	ARG	2.2
1	A	265	PRO	2.2
1	C	102	ALA	2.2
1	B	77	PHE	2.2
1	A	301	LEU	2.2
1	B	139	PRO	2.2
1	B	257	GLU	2.2
1	A	273	ASP	2.2
1	C	303	ASN	2.2
1	D	72	VAL	2.2
1	A	116	SER	2.1
1	D	146	VAL	2.1
1	B	263	MET	2.1
1	D	77	PHE	2.1
1	D	82	GLY	2.1
1	C	76	ILE	2.1
1	C	255	ASP	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.