Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:06 PM GMT

PDB ID	:	4KKU
Title	:	Structure of BesA (Selenomethinone derivative - P212121)
Authors	:	Greene, N.P.; Hinchliffe, P.; Crow, A.; Ababou, A.; Hughes, C.; Koronakis, V.
Deposited on	:	2013-05-06
Resolution	:	2.35 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 (1)) were used in the production of this report:

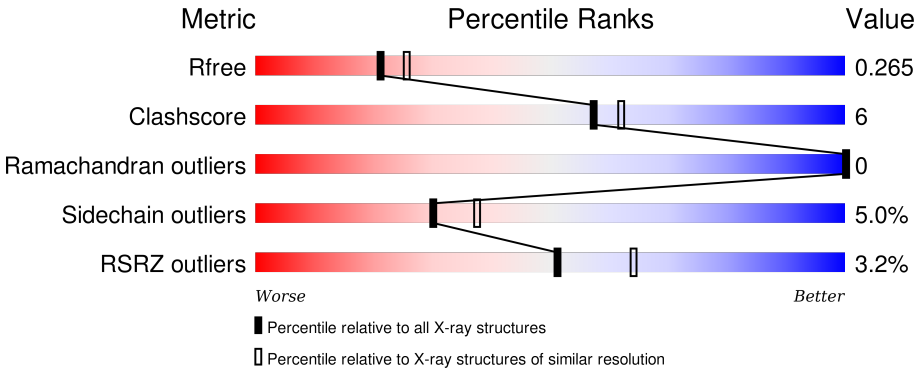
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	2% 78% 9% • 10%
1	B	296	2% 77% 11% • 10%
1	C	296	2% 79% 8% • 11%
1	D	296	6% 78% 9% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8454 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	266	Total	C	N	O	Se	0	3	0
			2075	1331	340	399	5			
1	B	267	Total	C	N	O	Se	0	3	0
			2084	1339	342	398	5			
1	C	264	Total	C	N	O	Se	0	1	0
			2043	1311	337	391	4			
1	D	266	Total	C	N	O	Se	0	3	0
			2074	1330	340	400	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	MSE	-	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	MSE	-	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	MSE	-	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	MSE	-	EXPRESSION TAG	UNP O51166

- Molecule 2 is water.

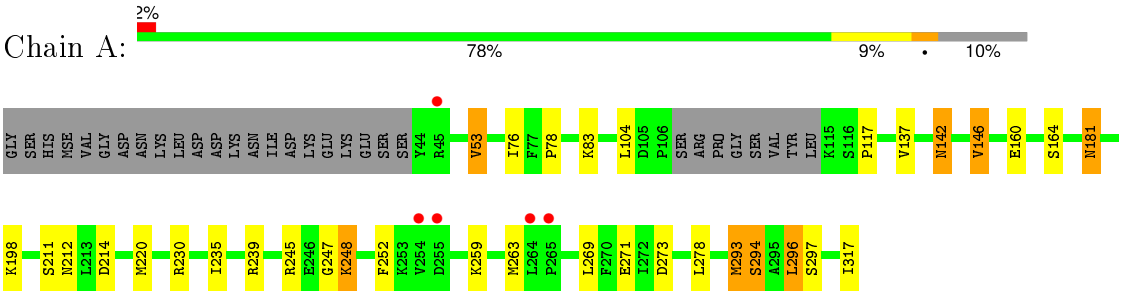
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	50	Total O 50 50	0	0
2	B	47	Total O 47 47	0	0
2	C	37	Total O 37 37	0	0
2	D	44	Total O 44 44	0	0

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.

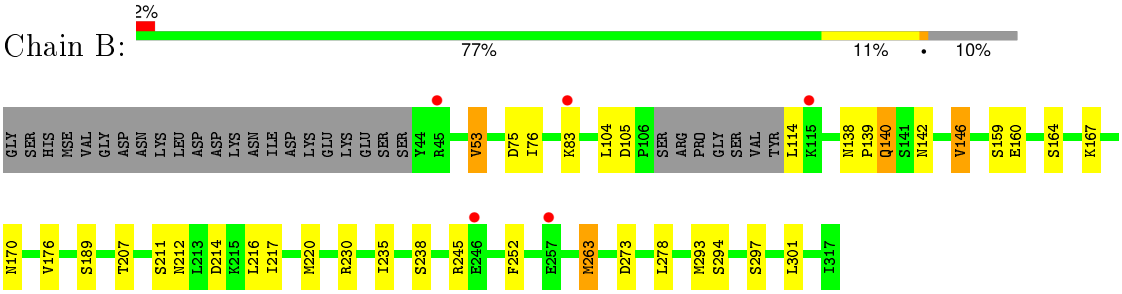
- Molecule 1: Membrane fusion protein

Chain A:



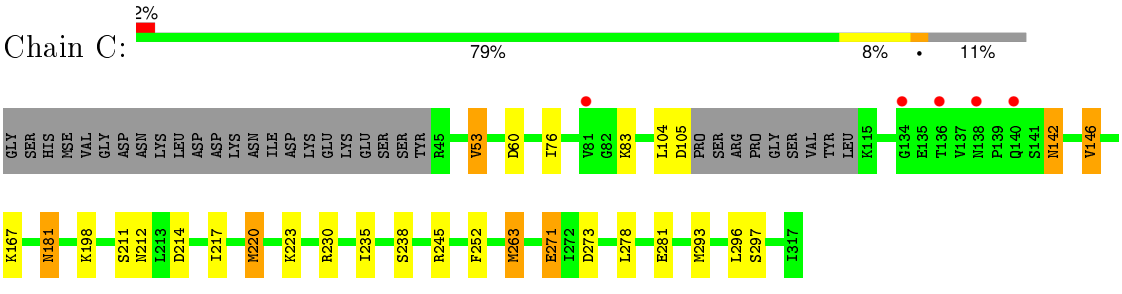
- Molecule 1: Membrane fusion protein

Chain B:



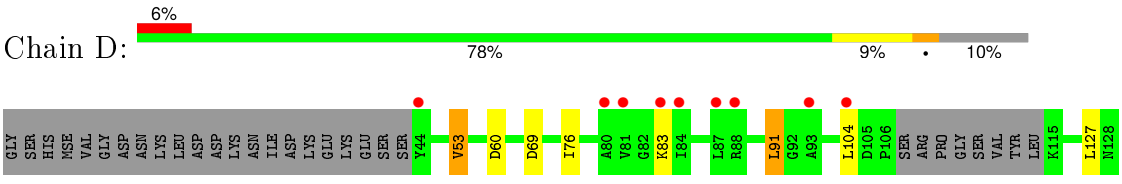
- Molecule 1: Membrane fusion protein

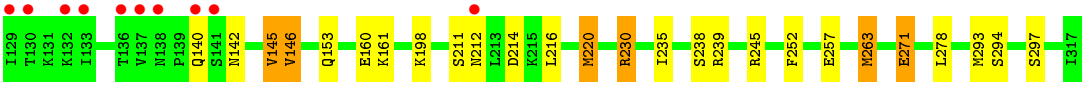
Chain C:



- Molecule 1: Membrane fusion protein

Chain D:




I129
T130
K131
K132
I133
T136
V137
N138
P139
Q140
S141
N142
V145
V146
Q153
E160
K161
K198
S211
N212
I213
D214
K215
I216
M220
R230
I235
S238
R239
R245
F252
E257
M263
E271
L278
M293
S294
S297
I317

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.74Å 152.13Å 155.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.74 – 2.35 77.75 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (77.74-2.35) 98.5 (77.75-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.236 , 0.264 0.240 , 0.265	Depositor DCC
R_{free} test set	3697 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 30.2	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	7 of 72538 reflections (0.010%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8454	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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 54.73 % 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 3.5035e-05.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	0.89	0/2094	0.93	3/2814 (0.1%)
1	B	0.92	0/2103	0.92	4/2825 (0.1%)
1	C	0.89	2/2060 (0.1%)	0.94	6/2766 (0.2%)
1	D	0.84	1/2093 (0.0%)	0.98	8/2813 (0.3%)
All	All	0.88	3/8350 (0.0%)	0.94	21/11218 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	271	GLU	CD-OE1	7.57	1.33	1.25
1	C	281	GLU	CG-CD	7.45	1.63	1.51
1	D	271	GLU	CD-OE1	6.02	1.32	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	220	MSE	CA-CB-CG	13.70	136.59	113.30
1	D	220	MSE	CG-SE-CE	-9.66	77.64	98.90
1	D	220	MSE	N-CA-CB	-9.15	94.13	110.60
1	A	146	VAL	CB-CA-C	-7.55	97.05	111.40
1	B	146	VAL	CB-CA-C	-7.46	97.23	111.40
1	C	146	VAL	CB-CA-C	-7.04	98.02	111.40
1	D	91	LEU	CA-CB-CG	6.83	131.01	115.30
1	C	230	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	D	146	VAL	CB-CA-C	-6.58	98.91	111.40
1	D	230	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	C	281	GLU	OE1-CD-OE2	-6.01	116.09	123.30
1	A	230	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	263	MSE	CG-SE-CE	5.95	111.99	98.90
1	D	263	MSE	CG-SE-CE	5.75	111.55	98.90
1	B	140	GLN	CA-CB-CG	5.69	125.91	113.40
1	A	230	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	60	ASP	CB-CG-OD1	5.56	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	263	MSE	CG-SE-CE	5.40	110.78	98.90
1	D	60	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	230	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	230	ARG	NE-CZ-NH2	-5.01	117.79	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	2075	0	2199	34	0
1	B	2084	0	2219	30	0
1	C	2043	0	2180	23	0
1	D	2074	0	2197	25	0
2	A	50	0	0	7	0
2	B	47	0	0	4	0
2	C	37	0	0	5	0
2	D	44	0	0	5	0
All	All	8454	0	8795	102	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 6.

All (102) 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:230:ARG:HG3	2:D:420:HOH:O	1.49	1.11
1:D:245:ARG:NH2	1:D:263:MSE:HE1	1.91	0.86
1:A:142:ASN:ND2	2:A:412:HOH:O	2.09	0.84
1:B:245:ARG:NH2	1:B:263:MSE:HE1	1.93	0.83
1:D:69:ASP:OD2	2:D:441:HOH:O	1.99	0.80
1:C:142:ASN:ND2	2:C:416:HOH:O	2.14	0.80
1:C:252:PHE:HZ	1:C:263:MSE:HE2	1.48	0.77
1:C:252:PHE:HZ	1:C:263:MSE:CE	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220[A]:MSE:HE1	1:B:220[A]:MSE:CE	2.15	0.75
1:A:293:MSE:HA	1:A:296:LEU:HD22	1.70	0.74
1:B:252:PHE:HZ	1:B:263:MSE:HE2	1.54	0.73
1:C:252:PHE:CZ	1:C:263:MSE:CE	2.71	0.73
1:D:252:PHE:HZ	1:D:263:MSE:HE2	1.53	0.72
1:C:252:PHE:CZ	1:C:263:MSE:HE2	2.26	0.71
1:D:252:PHE:HZ	1:D:263:MSE:CE	2.04	0.69
1:D:252:PHE:CZ	1:D:263:MSE:CE	2.75	0.69
1:B:273:ASP:OD2	2:B:447:HOH:O	2.11	0.69
1:B:252:PHE:HZ	1:B:263:MSE:CE	2.06	0.68
1:D:252:PHE:CZ	1:D:263:MSE:HE2	2.28	0.68
1:B:252:PHE:CZ	1:B:263:MSE:HE2	2.28	0.68
1:B:301:LEU:HG	2:B:439:HOH:O	1.94	0.68
1:A:78:PRO:HG3	1:A:137:VAL:HG11	1.74	0.67
1:D:239:ARG:NH2	2:D:437:HOH:O	2.14	0.67
1:A:220[A]:MSE:CE	1:B:220[A]:MSE:CE	2.71	0.67
1:A:245:ARG:NH2	1:A:296:LEU:O	2.28	0.66
1:B:252:PHE:CZ	1:B:263:MSE:CE	2.78	0.66
1:C:223:LYS:HE3	2:C:419:HOH:O	1.95	0.66
1:A:220[A]:MSE:HE1	1:B:220[A]:MSE:HE2	1.77	0.66
1:A:273:ASP:OD2	2:A:406:HOH:O	2.15	0.65
1:A:252:PHE:HZ	1:A:263:MSE:HE2	1.61	0.65
1:A:252:PHE:HZ	1:A:263:MSE:CE	2.10	0.64
1:A:252:PHE:CZ	1:A:263:MSE:CE	2.81	0.64
1:C:245:ARG:NH1	2:C:430:HOH:O	2.31	0.64
1:A:294:SER:OG	2:A:434:HOH:O	2.12	0.64
1:A:220[A]:MSE:HE1	1:B:176:VAL:HB	1.80	0.63
1:C:245:ARG:NH2	1:C:296:LEU:O	2.32	0.62
1:A:220[A]:MSE:CE	1:B:220[A]:MSE:HE1	2.29	0.62
1:A:252:PHE:CZ	1:A:263:MSE:HE2	2.34	0.62
1:D:127:LEU:HB2	1:D:145:VAL:HG22	1.81	0.62
1:D:153:GLN:NE2	2:D:441:HOH:O	2.32	0.62
1:A:220[A]:MSE:HE1	1:B:220[A]:MSE:HE1	1.82	0.60
1:D:127:LEU:HB2	1:D:145:VAL:CG2	2.32	0.60
1:A:78:PRO:CG	1:A:137:VAL:CG1	2.80	0.60
1:C:252:PHE:CZ	1:C:263:MSE:HE3	2.36	0.59
1:D:245:ARG:NH2	1:D:263:MSE:CE	2.64	0.57
1:A:78:PRO:HG2	1:A:137:VAL:CG1	2.34	0.57
1:B:245:ARG:NH2	1:B:263:MSE:CE	2.67	0.57
2:A:407:HOH:O	1:D:161:LYS:HD3	2.04	0.56
1:B:76:ILE:HD11	1:B:146:VAL:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HD11	1:A:146:VAL:HG22	1.88	0.56
1:A:160:GLU:OE2	1:D:271:GLU:OE1	2.25	0.55
1:D:252:PHE:CZ	1:D:263:MSE:HE3	2.41	0.55
1:D:76:ILE:HD11	1:D:146:VAL:HG22	1.87	0.55
1:B:212:ASN:N	2:B:429:HOH:O	2.39	0.53
1:C:181:ASN:H	1:C:181:ASN:HD22	1.57	0.53
1:D:220:MSE:HE1	2:D:405:HOH:O	2.08	0.52
1:B:252:PHE:CZ	1:B:263:MSE:HE3	2.45	0.52
1:A:78:PRO:HG3	1:A:137:VAL:CG1	2.38	0.52
1:C:76:ILE:HD11	1:C:146:VAL:HG22	1.91	0.52
1:A:252:PHE:CZ	1:A:263:MSE:HE3	2.45	0.50
1:B:217:ILE:HD12	1:B:220[B]:MSE:HE3	1.93	0.50
1:A:117:PRO:HD2	2:A:410:HOH:O	2.11	0.50
1:C:53:VAL:HG13	1:C:235:ILE:HD12	1.94	0.49
1:A:181:ASN:H	1:A:181:ASN:HD22	1.59	0.49
1:C:217:ILE:O	1:C:220:MSE:HB2	2.13	0.49
1:D:53:VAL:HG13	1:D:235:ILE:HD12	1.94	0.48
1:A:78:PRO:HG2	1:A:137:VAL:HG13	1.95	0.47
1:D:278:LEU:HD12	1:D:278:LEU:C	2.35	0.46
1:C:223:LYS:CE	2:C:419:HOH:O	2.56	0.46
1:A:245:ARG:HE	1:A:263:MSE:HE1	1.80	0.46
1:B:142:ASN:OD1	2:B:416:HOH:O	2.20	0.45
1:D:83:LYS:O	1:D:104:LEU:HA	2.17	0.44
1:A:53:VAL:HG13	1:A:235:ILE:HD12	1.99	0.44
1:D:216:LEU:HD12	1:D:216:LEU:HA	1.88	0.44
1:B:138:ASN:HB2	1:B:139:PRO:CD	2.48	0.44
1:A:278:LEU:C	1:A:278:LEU:HD12	2.37	0.44
1:A:239:ARG:NH2	2:A:433:HOH:O	2.50	0.44
1:A:247:GLY:O	1:A:248:LYS:HD2	2.18	0.43
1:B:167:LYS:H	1:B:170:ASN:ND2	2.16	0.43
1:B:53:VAL:HG13	1:B:235:ILE:HD12	1.99	0.43
1:B:278:LEU:C	1:B:278:LEU:HD12	2.39	0.43
1:C:252:PHE:CE1	1:C:263:MSE:HE3	2.53	0.43
1:A:83:LYS:O	1:A:104:LEU:HA	2.18	0.43
1:D:252:PHE:CE1	1:D:263:MSE:HE3	2.54	0.43
1:C:83:LYS:O	1:C:104:LEU:HA	2.19	0.43
1:C:278:LEU:C	1:C:278:LEU:HD12	2.40	0.42
2:A:407:HOH:O	1:D:161:LYS:CD	2.65	0.42
1:B:211:SER:O	1:B:212:ASN:CB	2.68	0.42
1:C:167[B]:LYS:HE3	1:C:167[B]:LYS:HB2	1.84	0.42
1:A:271:GLU:OE2	1:D:160:GLU:OE2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ASP:OD2	2:C:435:HOH:O	2.22	0.42
1:B:160:GLU:OE2	1:C:271:GLU:OE1	2.38	0.41
1:C:181:ASN:N	1:C:181:ASN:HD22	2.18	0.41
1:B:75:ASP:CG	1:B:142:ASN:ND2	2.74	0.41
1:B:189[B]:SER:HB3	1:B:207:THR:HG1	1.84	0.41
1:D:211:SER:O	1:D:212:ASN:CB	2.69	0.41
1:B:83:LYS:O	1:B:104:LEU:HA	2.19	0.41
1:A:211:SER:O	1:A:212:ASN:CB	2.67	0.41
1:A:220[A]:MSE:HE2	1:B:220[A]:MSE:CE	2.50	0.41
1:C:211:SER:O	1:C:212:ASN:CB	2.68	0.41
1:C:245:ARG:HE	1:C:263:MSE:HE1	1.86	0.40
1:B:216:LEU:HA	1:B:216:LEU:HD12	1.86	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	265/296 (90%)	256 (97%)	9 (3%)	0	100	100
1	B	266/296 (90%)	257 (97%)	9 (3%)	0	100	100
1	C	261/296 (88%)	254 (97%)	7 (3%)	0	100	100
1	D	265/296 (90%)	257 (97%)	8 (3%)	0	100	100
All	All	1057/1184 (89%)	1024 (97%)	33 (3%)	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	238/257 (93%)	223 (94%)	15 (6%)	22	25
1	B	239/257 (93%)	228 (95%)	11 (5%)	33	42
1	C	234/257 (91%)	224 (96%)	10 (4%)	35	45
1	D	238/257 (93%)	226 (95%)	12 (5%)	30	37
All	All	949/1028 (92%)	901 (95%)	48 (5%)	30	36

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	142	ASN
1	A	164	SER
1	A	181	ASN
1	A	198	LYS
1	A	214[A]	ASP
1	A	214[B]	ASP
1	A	248	LYS
1	A	259	LYS
1	A	269	LEU
1	A	293	MSE
1	A	294	SER
1	A	296	LEU
1	A	297	SER
1	A	317	ILE
1	B	53	VAL
1	B	105	ASP
1	B	114	LEU
1	B	140	GLN
1	B	159	SER
1	B	164	SER
1	B	214	ASP
1	B	238	SER
1	B	293	MSE
1	B	294	SER
1	B	297	SER
1	C	53	VAL
1	C	105	ASP

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Mol	Chain	Res	Type
1	C	142	ASN
1	C	181	ASN
1	C	198	LYS
1	C	214	ASP
1	C	220	MSE
1	C	238	SER
1	C	293	MSE
1	C	297	SER
1	D	53	VAL
1	D	91	LEU
1	D	140	GLN
1	D	142	ASN
1	D	145	VAL
1	D	198	LYS
1	D	214	ASP
1	D	238	SER
1	D	257	GLU
1	D	293	MSE
1	D	294	SER
1	D	297	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	B	96	GLN
1	B	170	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	262/296 (88%)	0.31	5 (1%)	70	81	18, 35, 72, 115	0
1	B	263/296 (88%)	0.27	5 (1%)	70	81	17, 33, 68, 98	0
1	C	260/296 (87%)	0.30	5 (1%)	70	81	19, 37, 96, 112	0
1	D	262/296 (88%)	0.46	19 (7%)	18	27	21, 40, 107, 130	0
All	All	1047/1184 (88%)	0.34	34 (3%)	51	64	17, 36, 90, 130	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	133	ILE	6.5
1	D	84	ILE	4.7
1	D	137	VAL	3.8
1	C	136	THR	3.5
1	D	129	ILE	3.5
1	D	130	THR	3.4
1	D	140	GLN	3.3
1	D	83	LYS	3.3
1	D	81	VAL	3.3
1	B	45	ARG	3.1
1	D	104	LEU	3.0
1	D	132	LYS	3.0
1	D	88	ARG	2.9
1	C	81	VAL	2.8
1	B	257	GLU	2.8
1	D	44	TYR	2.8
1	D	212	ASN	2.8
1	D	93	ALA	2.7
1	D	141	SER	2.7
1	A	264	LEU	2.6
1	A	255	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	80	ALA	2.5
1	C	134	GLY	2.4
1	A	45	ARG	2.4
1	B	246	GLU	2.4
1	A	265	PRO	2.3
1	B	115	LYS	2.3
1	D	136	THR	2.2
1	C	138	ASN	2.2
1	B	83	LYS	2.1
1	C	140	GLN	2.1
1	A	254	VAL	2.1
1	D	87	LEU	2.1
1	D	138	ASN	2.0

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.