Full wwPDB X-ray Structure Validation Report (i)

Apr 3, 2016 – 08:56 AM EDT

PDB ID	:	5ENQ
Title	:	MBX3132 bound structure of bacterial efflux pump.
Authors	:	Sjuts, H.; Ornik, A.R.; Pos, K.M.
Deposited on	:	2015-11-09
Resolution	:	1.80 Å(reported)

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

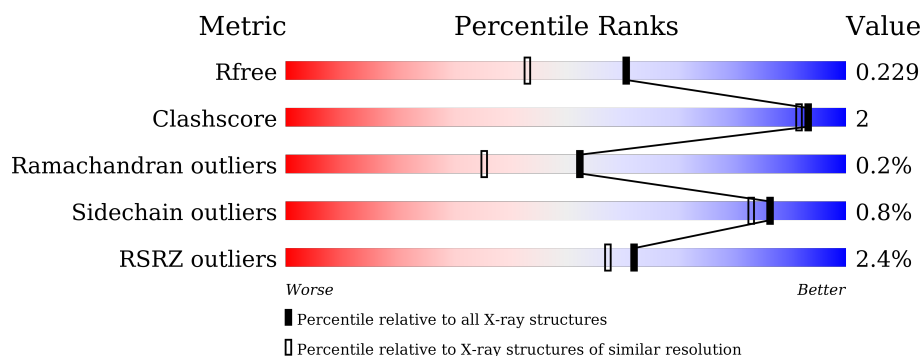|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 1.80 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	Percentile Ranks	Value
Rfree		0.229
Clashscore		2
Ramachandran outliers		0.2%
Sidechain outliers		0.8%
RSRZ outliers		2.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	609	3% / 89% / 6% / 5%
1	B	609	% / 89% / 6% / 5%
1	C	609	% / 90% / 5% / 5%
2	D	169	3% / 89% / 7% / •
2	E	169	4% / 89% / • / 8%
2	F	169	2% / 92% / • / •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18265 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 Multidrug efflux pump subunit AcrB,Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	1	0
			4424	2777	750	875	22			
1	B	578	Total	C	N	O	S	0	0	0
			4405	2766	746	871	22			
1	C	578	Total	C	N	O	S	0	1	0
			4404	2766	745	871	22			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	GLY	-	linker	UNP P31224
A	553	GLY	-	linker	UNP P31224
A	554	SER	-	linker	UNP P31224
A	555	GLY	-	linker	UNP P31224
A	556	GLY	-	linker	UNP P31224
A	557	SER	-	linker	UNP P31224
A	558	GLY	-	linker	UNP P31224
A	559	GLY	-	linker	UNP P31224
A	560	SER	-	linker	UNP P31224
B	552	GLY	-	linker	UNP P31224
B	553	GLY	-	linker	UNP P31224
B	554	SER	-	linker	UNP P31224
B	555	GLY	-	linker	UNP P31224
B	556	GLY	-	linker	UNP P31224
B	557	SER	-	linker	UNP P31224
B	558	GLY	-	linker	UNP P31224
B	559	GLY	-	linker	UNP P31224
B	560	SER	-	linker	UNP P31224
C	552	GLY	-	linker	UNP P31224
C	553	GLY	-	linker	UNP P31224
C	554	SER	-	linker	UNP P31224
C	555	GLY	-	linker	UNP P31224

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	556	GLY	-	linker	UNP P31224
C	557	SER	-	linker	UNP P31224
C	558	GLY	-	linker	UNP P31224
C	559	GLY	-	linker	UNP P31224
C	560	SER	-	linker	UNP P31224

- Molecule 2 is a protein called DARPin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	162	Total	C	N	O	S	0	0	0
			1237	777	224	235	1			
2	E	155	Total	C	N	O	S	0	0	0
			1168	736	204	227	1			
2	F	162	Total	C	N	O	S	0	0	0
			1237	777	224	235	1			

- Molecule 3 is {N}-[4-[2-[[5-cyano-8-[(2 {S},6 {R})-2,6-dimethylmorpholin-4-yl]-3,3-dimethyl-1,4-dihydropyrano[3,4-c]pyridin-6-yl]sulfanyl]ethyl]phenyl]ethanamide (three-letter code: 5QE) (formula: $C_{27}H_{34}N_4O_3S$).
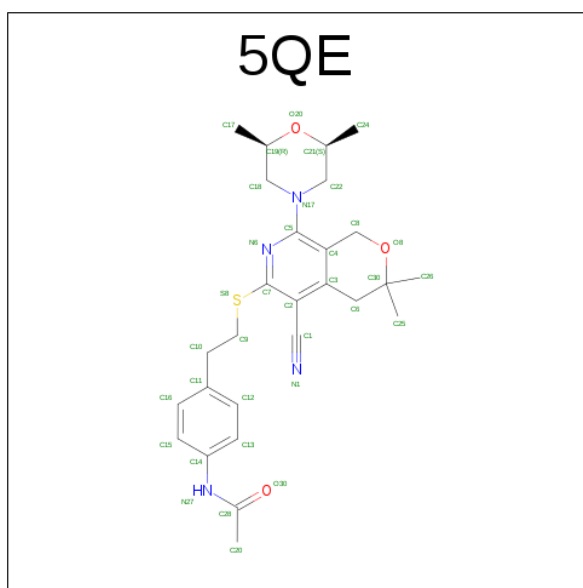
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			35	27	4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	386	Total 386	O 386	0	0
4	B	389	Total 389	O 389	0	0
4	C	402	Total 402	O 402	0	0
4	D	69	Total 69	O 69	0	0
4	E	52	Total 52	O 52	0	0
4	F	57	Total 57	O 57	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.
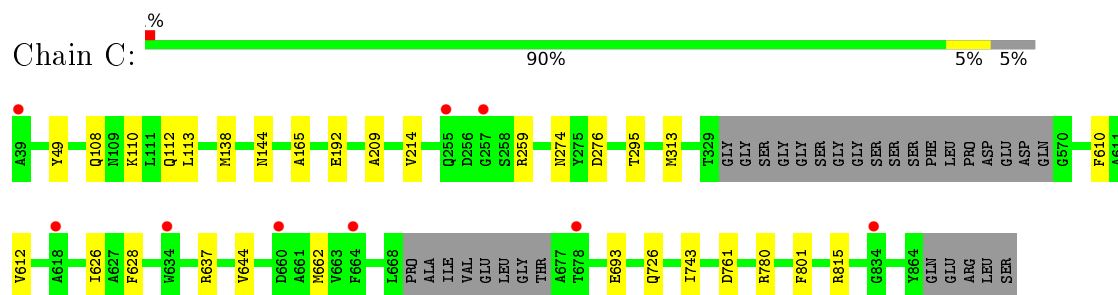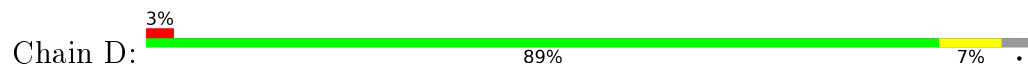
• Molecule 1: Multidrug efflux pump subunit AcrB,Multidrug efflux pump subunit AcrB
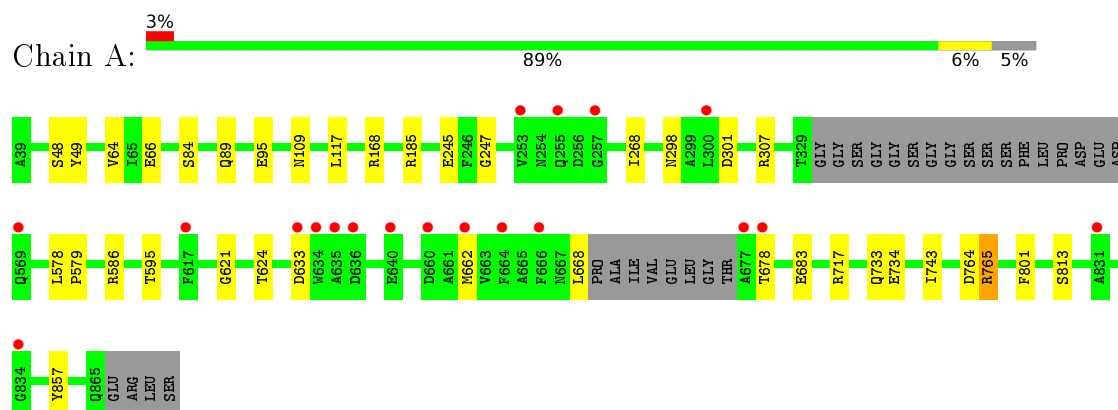
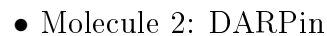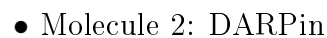• Molecule 1: Multidrug efflux pump subunit AcrB,Multidrug efflux pump subunit AcrB
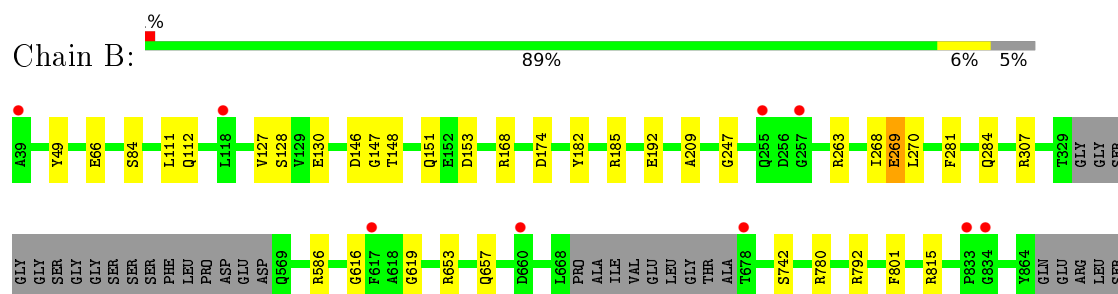
• Molecule 1: Multidrug efflux pump subunit AcrB,Multidrug efflux pump subunit AcrB

• Molecule 2: DARPin

• Molecule 2: DARPin

Chain E:

• Molecule 2: DARPin

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.73Å 145.52Å 173.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 49.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.80) 99.8 (49.51-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.182 , 0.223 0.191 , 0.229	Depositor DCC
R_{free} test set	12426 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 251469 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18265	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5QE

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	0.98	4/4502 (0.1%)	0.97	8/6100 (0.1%)
1	B	0.93	3/4480 (0.1%)	0.96	10/6070 (0.2%)
1	C	0.95	1/4482 (0.0%)	0.91	8/6073 (0.1%)
2	D	0.86	1/1262 (0.1%)	0.90	1/1716 (0.1%)
2	E	0.81	0/1187	0.89	2/1614 (0.1%)
2	F	0.88	1/1262 (0.1%)	0.89	2/1716 (0.1%)
All	All	0.93	10/17175 (0.1%)	0.94	31/23289 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	SER	CB-OG	11.27	1.56	1.42
2	F	57	TRP	CB-CG	6.20	1.61	1.50
1	B	742	SER	CB-OG	-5.87	1.34	1.42
1	B	128	SER	CB-OG	-5.46	1.35	1.42
1	C	693	GLU	CD-OE1	5.45	1.31	1.25
1	B	66	GLU	CD-OE1	5.36	1.31	1.25
1	A	48	SER	CB-OG	-5.36	1.35	1.42
1	A	66	GLU	CD-OE1	5.21	1.31	1.25
2	D	57	TRP	CB-CG	5.11	1.59	1.50
1	A	813	SER	CB-OG	5.09	1.48	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	765	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	C	780	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	A	765	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	C	815	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	C	815	ARG	NE-CZ-NH2	-7.58	116.51	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	780	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	C	637	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	792	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	B	168	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	B	586	ARG	NE-CZ-NH1	-6.43	117.08	120.30
2	F	105	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	815	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	168	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	307	ARG	NE-CZ-NH1	6.09	123.34	120.30
2	E	77	ASP	CB-CG-OD1	6.06	123.76	118.30
1	A	185	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	717	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	780	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	263	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	780	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	138	MET	CA-CB-CG	5.64	122.89	113.30
2	D	138	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	662	MET	CG-SD-CE	5.50	109.00	100.20
1	A	307	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	761	ASP	CB-CG-OD1	5.25	123.02	118.30
2	F	77	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	586	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	E	138	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	653	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	185	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	245	GLU	OE1-CD-OE2	-5.03	117.26	123.30

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	4424	0	4362	21	0
1	B	4405	0	4343	16	0
1	C	4404	0	4345	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1237	0	1201	7	0
2	E	1168	0	1151	2	0
2	F	1237	0	1201	4	0
3	C	35	0	0	1	0
4	A	386	0	0	8	0
4	B	389	0	0	8	0
4	C	402	0	0	5	0
4	D	69	0	0	4	0
4	E	52	0	0	0	0
4	F	57	0	0	0	0
All	All	18265	0	16603	65	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 2.

All (65) 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:64:VAL:HG23	4:A:1004:HOH:O	1.56	1.05
1:A:678:THR:O	4:A:901:HOH:O	1.89	0.90
1:A:95:GLU:HG3	4:A:1221:HOH:O	1.85	0.77
2:D:150:PHE:CE2	2:D:154:ILE:HD11	2.21	0.75
1:B:84:SER:HB3	4:B:1138:HOH:O	1.86	0.74
2:D:5:HIS:N	4:D:201:HOH:O	2.21	0.74
1:C:626:ILE:HD13	1:C:628:PHE:CE2	2.23	0.73
1:B:192:GLU:HG3	4:B:1237:HOH:O	1.89	0.72
1:A:109[A]:ASN:OD1	1:C:108:GLN:HG3	1.89	0.70
1:B:148:THR:HG21	4:B:985:HOH:O	1.92	0.68
1:C:726:GLN:OE1	4:C:1001:HOH:O	2.10	0.68
1:A:668:LEU:HD12	4:A:1240:HOH:O	1.94	0.67
1:B:209:ALA:HB1	1:C:743:ILE:HG21	1.78	0.65
1:A:743:ILE:HD11	4:A:1063:HOH:O	1.95	0.65
1:C:144:ASN:O	4:C:1002:HOH:O	2.15	0.64
1:C:644:VAL:HG23	4:C:1250:HOH:O	1.99	0.63
1:B:84:SER:CB	4:B:1138:HOH:O	2.45	0.60
2:F:34:MET:SD	2:F:40:VAL:HG12	2.41	0.60
1:A:678:THR:O	1:A:678:THR:CG2	2.50	0.59
2:F:34:MET:CE	2:F:40:VAL:HG12	2.33	0.58
1:C:612:VAL:HB	1:C:626:ILE:HD12	1.86	0.58
1:A:298:ASN:HD22	1:A:301:ASP:H	1.52	0.57
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:THR:HG21	4:A:1243:HOH:O	2.06	0.55
1:C:612:VAL:HB	1:C:626:ILE:CD1	2.37	0.54
1:A:678:THR:O	1:A:678:THR:HG22	2.07	0.54
3:C:901:5QE:C8	3:C:901:5QE:C18	2.86	0.54
1:A:89:GLN:NE2	4:A:909:HOH:O	2.42	0.51
1:A:764:ASP:OD1	1:A:765:ARG:HD3	2.11	0.51
1:B:247:GLY:HA2	1:B:268:ILE:HD13	1.93	0.50
1:B:657:GLN:HB2	4:B:966:HOH:O	2.10	0.50
1:C:274:ASN:ND2	1:C:276:ASP:OD2	2.38	0.50
1:B:269:GLU:HG3	1:B:270:LEU:O	2.12	0.50
2:E:69:ASN:HD22	2:E:69:ASN:N	2.10	0.50
1:A:621:GLY:O	1:A:624:THR:HG22	2.12	0.50
1:C:108:GLN:NE2	1:C:112:GLN:HG3	2.28	0.49
2:D:150:PHE:HE2	2:D:154:ILE:HD11	1.75	0.49
1:B:153:ASP:OD1	1:B:182:TYR:OH	2.30	0.49
1:C:214:VAL:HB	4:C:1313:HOH:O	2.13	0.48
2:D:5:HIS:CA	4:D:201:HOH:O	2.59	0.48
4:A:908:HOH:O	1:C:214:VAL:HG13	2.12	0.48
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.95	0.47
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.45	0.46
1:B:616:GLY:O	1:B:619:GLY:N	2.48	0.45
1:B:146:ASP:HB2	1:B:148:THR:HG22	1.98	0.45
2:D:30:VAL:O	2:D:34:MET:HG2	2.16	0.45
4:B:901:HOH:O	1:C:113:LEU:HG	2.16	0.44
2:D:5:HIS:HA	4:D:201:HOH:O	2.18	0.44
1:B:112:GLN:OE1	4:B:901:HOH:O	2.21	0.43
2:E:34:MET:HE1	2:E:69:ASN:HB2	2.00	0.43
1:C:165:ALA:HB3	1:C:313:MET:CE	2.48	0.42
1:B:148:THR:OG1	1:B:148:THR:O	2.37	0.42
1:A:734:GLU:OE2	1:C:259:ARG:NH1	2.51	0.42
1:B:281:PHE:O	1:B:284:GLN:HG2	2.20	0.42
2:F:30:VAL:O	2:F:34:MET:HG2	2.20	0.42
1:A:743:ILE:HD13	1:C:209:ALA:HB1	2.02	0.41
4:B:908:HOH:O	1:C:110:LYS:NZ	2.53	0.41
1:A:733:GLN:OE1	1:A:743:ILE:HD11	2.21	0.41
2:D:98:VAL:HG23	4:D:203:HOH:O	2.20	0.41
1:A:298:ASN:ND2	1:A:301:ASP:H	2.18	0.41
1:A:683:GLU:O	1:A:857:TYR:HA	2.21	0.41
1:B:130:GLU:OE1	1:B:174:ASP:OD1	2.39	0.41
2:F:34:MET:HE1	2:F:40:VAL:HG12	2.01	0.41
1:A:117:LEU:HD22	1:A:117:LEU:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLU:HG3	4:C:1338:HOH:O	2.22	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	575/609 (94%)	558 (97%)	17 (3%)	0	100	100
1	B	572/609 (94%)	558 (98%)	13 (2%)	1 (0%)	52	35
1	C	573/609 (94%)	556 (97%)	17 (3%)	0	100	100
2	D	160/169 (95%)	157 (98%)	1 (1%)	2 (1%)	15	4
2	E	153/169 (90%)	151 (99%)	2 (1%)	0	100	100
2	F	160/169 (95%)	156 (98%)	3 (2%)	1 (1%)	30	14
All	All	2193/2334 (94%)	2136 (97%)	53 (2%)	4 (0%)	52	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	13	ASP
2	F	9	HIS
2	D	11	GLY
1	B	147	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	A	472/492 (96%)	468 (99%)	4 (1%)	86	83
1	B	470/492 (96%)	466 (99%)	4 (1%)	84	80
1	C	470/492 (96%)	466 (99%)	4 (1%)	84	80
2	D	126/132 (96%)	124 (98%)	2 (2%)	70	59
2	E	119/132 (90%)	118 (99%)	1 (1%)	86	83
2	F	126/132 (96%)	126 (100%)	0	100	100
All	All	1783/1872 (95%)	1768 (99%)	15 (1%)	86	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TYR
1	A	633	ASP
1	A	662	MET
1	A	801	PHE
1	B	49	TYR
1	B	151	GLN
1	B	269	GLU
1	B	801	PHE
1	C	49	TYR
1	C	295	THR
1	C	610	PHE
1	C	801	PHE
2	D	27	ASP
2	D	68	LYS
2	E	23	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
1	A	687	GLN
1	B	70	ASN
1	B	112	GLN
1	B	569	GLN
1	C	58	GLN
1	C	108	GLN
1	C	284	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	726	GLN
2	D	5	HIS
2	E	69	ASN
2	E	112	ASN
2	F	5	HIS

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)

1 ligand is 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	#$|Z| > 2$
3	5QE	C	901	-	36,38,38	2.23	8 (22%)	36,55,55	2.03	13 (36%)

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	5QE	C	901	-	-	0/15/39/39	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	5QE	C2-C1	-9.73	1.28	1.44
3	C	901	5QE	C7-S8	-4.49	1.70	1.76
3	C	901	5QE	C28-N27	-2.94	1.30	1.35
3	C	901	5QE	C6-C3	2.05	1.53	1.51
3	C	901	5QE	C5-N17	2.12	1.42	1.37
3	C	901	5QE	C14-N27	2.45	1.46	1.41
3	C	901	5QE	C16-C15	2.70	1.44	1.38
3	C	901	5QE	C7-N6	3.01	1.37	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	5QE	C2-C7-N6	-5.13	119.20	123.10
3	C	901	5QE	C14-N27-C28	-3.88	122.05	128.02
3	C	901	5QE	C15-C16-C11	-2.62	117.34	121.02
3	C	901	5QE	C15-C14-C13	-2.24	115.94	119.06
3	C	901	5QE	C25-C30-C26	-2.15	106.86	110.51
3	C	901	5QE	C7-C2-C1	-2.12	117.73	119.98
3	C	901	5QE	O30-C28-C20	-2.08	118.25	122.07
3	C	901	5QE	C3-C2-C1	2.29	122.57	119.67
3	C	901	5QE	C9-S8-C7	2.39	105.59	101.77
3	C	901	5QE	O20-C19-C17	2.97	112.84	106.69
3	C	901	5QE	C22-N17-C18	3.30	119.87	112.49
3	C	901	5QE	O20-C21-C24	3.71	114.37	106.69
3	C	901	5QE	C16-C15-C14	3.73	124.48	120.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	901	5QE	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 (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	580/609 (95%)	-0.00	19 (3%)	50	44	18, 32, 60, 93	0
1	B	578/609 (94%)	-0.21	9 (1%)	74	71	20, 31, 57, 87	0
1	C	578/609 (94%)	-0.09	9 (1%)	74	71	19, 31, 62, 90	0
2	D	162/169 (95%)	-0.12	5 (3%)	52	47	26, 38, 68, 114	0
2	E	155/169 (91%)	0.19	7 (4%)	37	31	27, 41, 72, 137	0
2	F	162/169 (95%)	-0.02	4 (2%)	61	56	26, 39, 68, 124	0
All	All	2215/2334 (94%)	-0.07	53 (2%)	62	57	18, 33, 63, 137	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	11	GLY	19.7
2	D	11	GLY	5.3
2	E	12	SER	5.1
1	A	677	ALA	4.6
1	C	255	GLN	4.2
2	E	31	ARG	4.2
1	B	255	GLN	3.9
2	F	10	HIS	3.8
2	E	28	ASP	3.7
1	A	678	THR	3.6
2	F	8	HIS	3.5
2	F	5	HIS	3.5
1	C	257	GLY	3.4
1	A	257	GLY	3.4
1	A	634	TRP	3.3
1	C	660	ASP	3.3
1	B	678	THR	3.3
1	A	255	GLN	3.2
1	B	660	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	634	TRP	3.0
2	D	12	SER	2.9
1	A	633	ASP	2.8
2	D	10	HIS	2.8
1	B	833	PRO	2.8
2	D	8	HIS	2.7
1	B	834	GLY	2.7
1	B	39	ALA	2.6
1	A	617	PHE	2.6
2	F	11	GLY	2.6
1	A	831	ALA	2.6
1	C	39	ALA	2.6
1	B	617	PHE	2.5
1	C	618	ALA	2.5
1	A	664	PHE	2.5
1	C	664	PHE	2.5
1	A	640	GLU	2.5
1	A	834	GLY	2.5
1	A	569	GLN	2.4
1	A	660	ASP	2.4
1	A	636	ASP	2.3
2	E	32	ILE	2.3
1	C	678	THR	2.3
1	A	253	VAL	2.3
2	D	35	ALA	2.3
1	A	662	MET	2.2
1	A	635	ALA	2.2
2	E	163	GLU	2.2
1	C	834	GLY	2.1
2	E	13	ASP	2.1
1	B	257	GLY	2.1
1	B	118	LEU	2.1
1	A	666	PHE	2.1
1	A	300	LEU	2.0

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

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
3	5QE	C	901	35/35	0.97	0.09	-0.13	21,29,36,40	0

6.5 Other polymers (i)

There are no such residues in this entry.