WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2018 – 06:21 AM EST

PDB ID	:	1M7Q
Title	:	Crystal structure of p38 MAP kinase in complex with a dihydroquinazolinone inhibitor
Authors	:	Stelmach, J.E.; Liu, L.; Patel, S.B.; Pivnichny, J.V.; Scapin, G.; Singh, S.; Hop, C.E.C.A.; Wang, Z.; Cameron, P.M.; Nichols, E.A.; O'Keefe, S.J.; O'Neill, E.A.; Schmatz, D.M.; Schwartz, C.D.; Thompson, C.M.; Zaller, D.M.; Doherty, J.B.
Deposited on	:	2002-07-22
Resolution	:	2.40 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
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)	:	rb-20030736
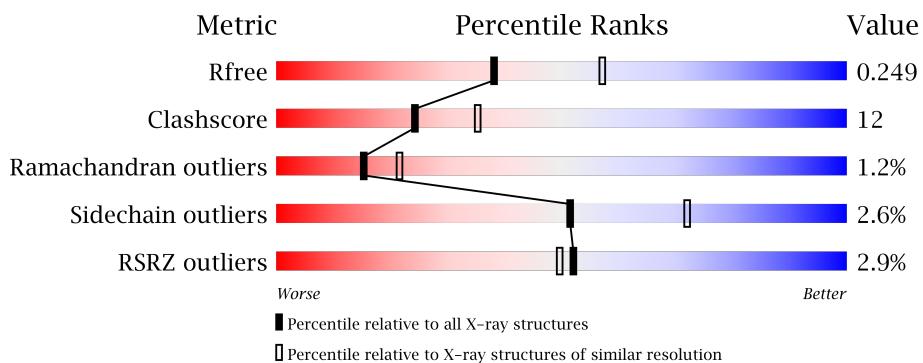
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	366	3% / 70% / 23% / • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2952 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.
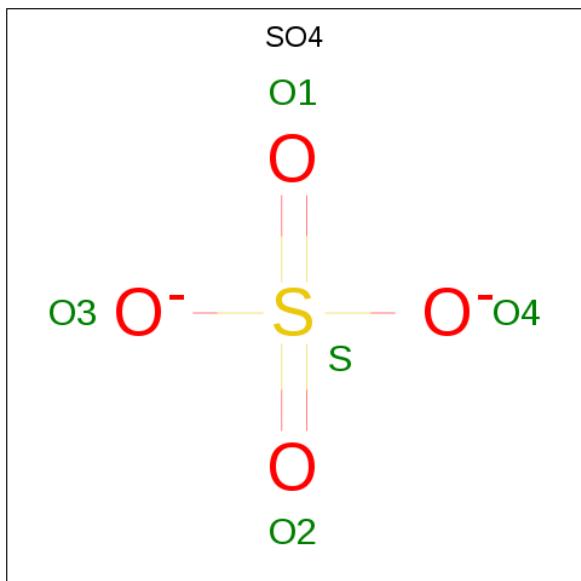
- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total 2800	C 1792	N 476	O 519	S 13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:
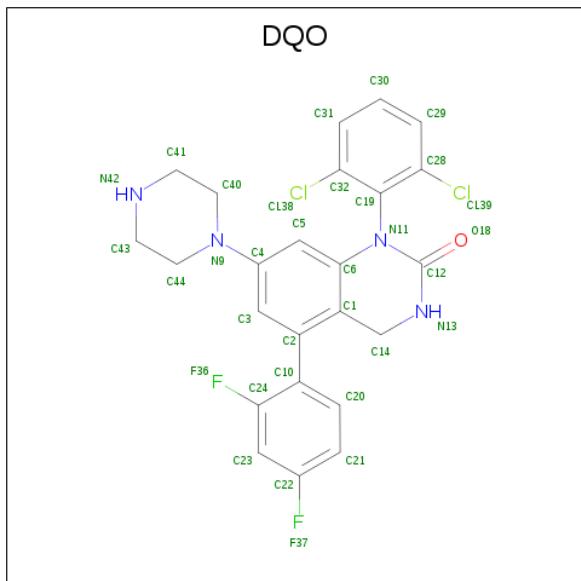
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	INSERTION	UNP Q16539
A	-4	SER	-	INSERTION	UNP Q16539
A	-3	HIS	-	INSERTION	UNP Q16539
A	-2	MET	-	INSERTION	UNP Q16539
A	-1	LEU	-	INSERTION	UNP Q16539
A	0	GLU	-	INSERTION	UNP Q16539

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0

- Molecule 3 is 1-(2,6-DICHLOROPHENYL)-5-(2,4-DIFLUOROPHENYL)-7-PIPERAZ IN-1-YL-3,4-DIHYDROQUINAZOLIN-2(1H)-ONE (three-letter code: DQO) (formula: $C_{24}H_{20}Cl_2F_2N_4O$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 33	C 24	Cl 2	F 2	N 4	O 1	0	0
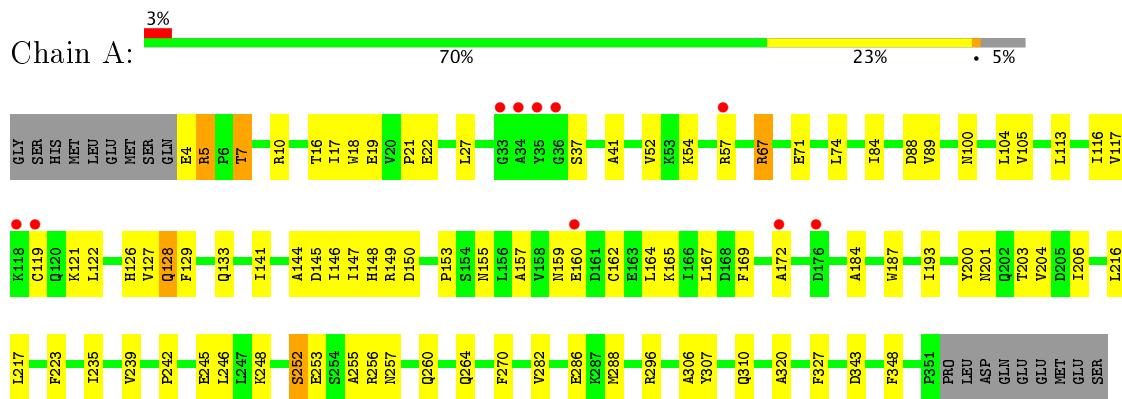
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total 114	O 114	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 the various outlier classes 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: Mitogen-activated protein kinase 14

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	45.52Å 87.16Å 124.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40	Depositor
	38.39 – 2.41	EDS
% Data completeness	91.4 (25.00-2.40)	Depositor
(in resolution range)	93.0 (38.39-2.41)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.22 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.254	Depositor
	0.211 , 0.249	DCC
R_{free} test set	897 reflections (5.13%)	DCC
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.9	EDS
L-test for twinning[2]	$<|L|> = 0.46$, $<L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2952	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ 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: DQO, SO4

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	0.57	0/2865	0.67	0/3892

There are no bond length outliers.

There are no bond angle outliers.

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	2800	0	2777	69	0
2	A	5	0	0	0	0
3	A	33	0	20	2	0
4	A	114	0	0	5	0
All	All	2952	0	2797	70	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 12.

All (70) 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:27:LEU:HD23	1:A:41:ALA:HB2	1.45	0.99
1:A:10:ARG:HH22	1:A:17:ILE:HD13	1.46	0.81
1:A:193:ILE:HG22	1:A:200:TYR:HB3	1.64	0.79
1:A:157:ALA:HB2	3:A:501:DQO:CL39	2.30	0.68
1:A:84:ILE:HG23	1:A:84:ILE:O	1.97	0.65
1:A:242:PRO:HB3	1:A:246:LEU:HD23	1.79	0.63
1:A:10:ARG:NH2	1:A:17:ILE:HD13	2.14	0.60
1:A:10:ARG:NH2	1:A:17:ILE:HG21	2.15	0.60
1:A:16:THR:HG23	1:A:18:TRP:HE1	1.67	0.59
1:A:150:ASP:O	1:A:155:ASN:ND2	2.36	0.59
1:A:67:ARG:NH2	1:A:71:GLU:OE1	2.36	0.59
1:A:89:VAL:HG23	1:A:104:LEU:HD23	1.85	0.59
1:A:256:ARG:O	1:A:260:GLN:HG3	2.03	0.58
1:A:18:TRP:HZ2	1:A:37:SER:HB2	1.71	0.56
1:A:16:THR:HG23	1:A:18:TRP:NE1	2.21	0.56
1:A:201:ASN:O	1:A:204:VAL:HG22	2.07	0.55
1:A:282:VAL:O	1:A:286:GLU:HG3	2.06	0.55
1:A:200:TYR:CD1	1:A:200:TYR:C	2.80	0.55
1:A:27:LEU:CD2	1:A:41:ALA:HB2	2.30	0.54
1:A:147:ILE:HG22	1:A:149:ARG:HG3	1.90	0.54
1:A:67:ARG:HD2	1:A:172:ALA:HB2	1.90	0.54
1:A:144:ALA:HB2	1:A:320:ALA:HB3	1.89	0.53
1:A:203:THR:HB	1:A:296:ARG:HD2	1.91	0.53
1:A:88:ASP:HA	1:A:348:PHE:CE2	2.44	0.52
1:A:252:SER:HB2	1:A:255:ALA:HB3	1.91	0.52
1:A:113:LEU:HB3	1:A:153:PRO:HB3	1.93	0.51
1:A:253:GLU:HG2	1:A:253:GLU:O	2.10	0.51
1:A:200:TYR:HB2	1:A:204:VAL:HG11	1.93	0.50
1:A:245:GLU:HA	1:A:248:LYS:HE2	1.93	0.50
1:A:206:ILE:CG2	1:A:288:MET:HG2	2.42	0.49
1:A:57:ARG:HG3	1:A:57:ARG:HH11	1.78	0.49
1:A:223:PHE:CE1	1:A:235:ILE:HA	2.48	0.49
1:A:253:GLU:O	1:A:257:ASN:HB2	2.13	0.48
1:A:343:ASP:HB2	4:A:692:HOH:O	2.15	0.47
1:A:148:HIS:O	1:A:149:ARG:HB2	2.13	0.47
1:A:193:ILE:HG22	1:A:200:TYR:CB	2.40	0.47
1:A:184:ALA:HA	1:A:187:TRP:CE3	2.50	0.47
1:A:122:LEU:HA	1:A:126:HIS:ND1	2.30	0.46
1:A:116:ILE:HG22	1:A:117:VAL:N	2.31	0.46
1:A:127:VAL:HG21	1:A:217:LEU:HD23	1.98	0.46
1:A:7:THR:O	1:A:22:GLU:HG3	2.15	0.46
1:A:141:ILE:HG22	1:A:146:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:HG22	1:A:105:VAL:HG22	1.98	0.45
1:A:16:THR:CG2	1:A:18:TRP:HE1	2.28	0.45
1:A:310:GLN:HB3	4:A:627:HOH:O	2.15	0.45
1:A:122:LEU:CD1	1:A:216:LEU:HD22	2.46	0.45
1:A:167:LEU:HD12	1:A:167:LEU:N	2.32	0.45
1:A:84:ILE:CG2	1:A:84:ILE:O	2.63	0.45
1:A:193:ILE:CG2	1:A:200:TYR:HB3	2.42	0.45
1:A:128:GLN:HG3	1:A:307:TYR:CZ	2.52	0.45
1:A:206:ILE:HG23	1:A:288:MET:HG2	1.98	0.44
1:A:16:THR:HG23	1:A:18:TRP:CD1	2.53	0.44
1:A:10:ARG:HG2	1:A:19:GLU:HG3	2.00	0.43
1:A:327:PHE:HD1	4:A:705:HOH:O	2.01	0.43
1:A:159:ASN:O	1:A:162:CYS:N	2.44	0.43
1:A:5:ARG:CG	1:A:5:ARG:HH11	2.32	0.43
1:A:164:LEU:HD23	1:A:165:LYS:N	2.34	0.42
1:A:200:TYR:O	1:A:200:TYR:CD1	2.72	0.42
1:A:270:PHE:HB3	1:A:282:VAL:HG13	2.01	0.42
1:A:129:PHE:CE2	1:A:133:GLN:NE2	2.86	0.42
1:A:235:ILE:O	1:A:239:VAL:HG22	2.20	0.41
1:A:121:LYS:HD2	1:A:121:LYS:HA	1.74	0.41
1:A:21:PRO:HG2	4:A:671:HOH:O	2.20	0.41
1:A:16:THR:OG1	1:A:54:LYS:HE2	2.21	0.41
1:A:116:ILE:HD12	1:A:116:ILE:N	2.35	0.41
1:A:74:LEU:HD13	1:A:169:PHE:HB3	2.01	0.41
3:A:501:DQO:H412	4:A:696:HOH:O	2.20	0.41
1:A:200:TYR:HB2	1:A:204:VAL:CG1	2.50	0.41
1:A:147:ILE:HB	1:A:149:ARG:NH1	2.36	0.40
1:A:193:ILE:CG2	1:A:200:TYR:CB	2.99	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	346/366 (94%)	326 (94%)	16 (5%)	4 (1%)	15 21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	SER
1	A	306	ALA
1	A	100	ASN
1	A	160	GLU

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	306/325 (94%)	298 (97%)	8 (3%)	51 72

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	5	ARG
1	A	7	THR
1	A	67	ARG
1	A	119	CYS
1	A	128	GLN
1	A	145	ASP
1	A	264	GLN

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	14	ASN
1	A	60	GLN
1	A	64	HIS
1	A	100	ASN

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Mol	Chain	Res	Type
1	A	228	HIS
1	A	264	GLN
1	A	272	ASN
1	A	301	GLN
1	A	310	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)

2 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	#$|Z| > 2$
3	DQO	A	501	-	36,37,37	3.23	19 (52%)	42,54,54	3.11	13 (30%)
2	SO4	A	502	-	4,4,4	0.49	0	6,6,6	0.09	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	DQO	A	501	-	-	0/12/33/33	0/5/5/5
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	DQO	C19-N11	-9.34	1.20	1.44
3	A	501	DQO	C4-N9	-4.64	1.26	1.38
3	A	501	DQO	C32-CL38	2.08	1.78	1.73
3	A	501	DQO	C3-C2	2.29	1.43	1.39
3	A	501	DQO	C30-C31	2.31	1.43	1.38
3	A	501	DQO	C23-C24	2.38	1.41	1.37
3	A	501	DQO	C40-N9	2.54	1.50	1.46
3	A	501	DQO	C21-C20	2.58	1.43	1.38
3	A	501	DQO	C30-C29	2.73	1.44	1.38
3	A	501	DQO	C2-C1	2.74	1.45	1.41
3	A	501	DQO	C23-C22	2.76	1.42	1.37
3	A	501	DQO	C6-N11	3.13	1.48	1.41
3	A	501	DQO	C21-C22	3.24	1.43	1.37
3	A	501	DQO	C6-C1	3.42	1.45	1.40
3	A	501	DQO	C44-N9	3.74	1.52	1.46
3	A	501	DQO	C5-C6	3.93	1.46	1.39
3	A	501	DQO	C10-C24	5.36	1.45	1.39
3	A	501	DQO	C19-C28	5.41	1.47	1.39
3	A	501	DQO	C19-C32	8.30	1.51	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	DQO	C5-C4-N9	-8.91	111.40	121.34
3	A	501	DQO	C32-C19-N11	-8.47	115.31	121.19
3	A	501	DQO	C14-C1-C6	-4.09	117.49	120.25
3	A	501	DQO	C5-C6-C1	-2.57	117.44	121.15
3	A	501	DQO	F36-C24-C23	-2.28	114.32	118.63
3	A	501	DQO	C23-C24-C10	-2.02	121.51	124.07
3	A	501	DQO	C19-C32-CL38	2.08	123.19	120.13
3	A	501	DQO	O18-C12-N11	2.12	124.20	122.22
3	A	501	DQO	C20-C10-C24	2.40	118.43	115.87
3	A	501	DQO	F36-C24-C10	3.48	124.17	118.94
3	A	501	DQO	C44-N9-C40	4.17	120.40	111.57
3	A	501	DQO	C3-C4-N9	6.66	128.78	121.34
3	A	501	DQO	C28-C19-N11	10.32	128.35	121.19

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
3	A	501	DQO	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)

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	348/366 (95%)	-0.29	10 (2%)	52	50	25, 43, 70, 81	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	ALA	4.5
1	A	119	CYS	4.3
1	A	33	GLY	3.3
1	A	172	ALA	2.6
1	A	35	TYR	2.5
1	A	176	ASP	2.4
1	A	118	LYS	2.4
1	A	57	ARG	2.2
1	A	160	GLU	2.2
1	A	36	GLY	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)

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	DQO	A	501	33/33	0.85	0.18	0.30	47,53,65,67	0
2	SO4	A	502	5/5	0.96	0.11	-0.11	59,59,59,60	5

6.5 Other polymers (i)

There are no such residues in this entry.