Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:47 PM GMT

PDB ID	:	3UXM
Title	:	Structure Guided Development of Novel Thymidine Mimetics targeting Pseudomonas aeruginosa Thymidylate Kinase: from Hit to Lead Generation
Authors	:	Choi, J.Y.; Plummer, M.S.; Starr, J.; Desbonnet, C.R.; Soutter, H.H.; Chang, J.; Miller, J.R.; Dillman, K.; Miller, A.A.; Roush, W.R.
Deposited on	:	2011-12-05
Resolution	:	1.95 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 (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 1.95 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		0.238
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		3.7%
RSRZ outliers		0.5%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
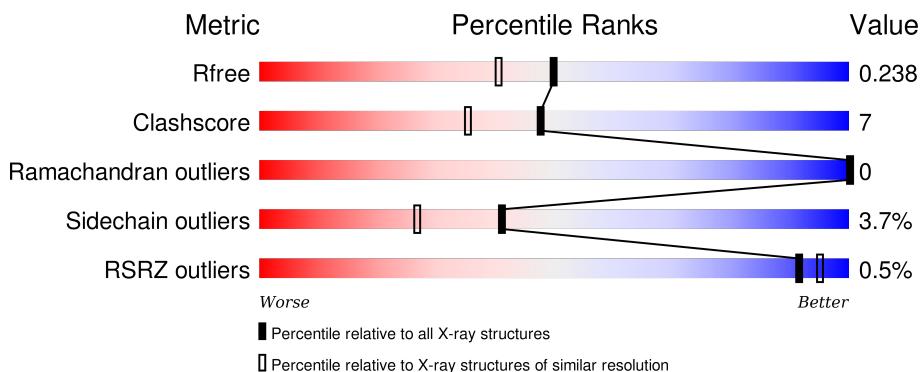
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	211	81% .... 12% · 7%
1	B	211	81% .... 14% · ·
1	C	211	% 81% .... 12% · 5%
1	D	211	84% .... 11% · ·
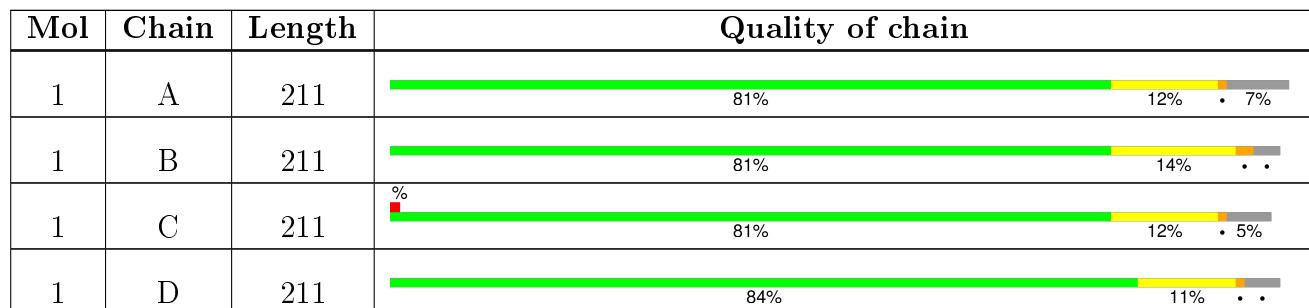
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6691 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 Thymidylate kinase.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	1	0
			1548	973	284	288	3			
1	B	204	Total	C	N	O	S	0	1	0
			1583	993	292	295	3			
1	C	200	Total	C	N	O	S	0	0	0
			1545	974	280	288	3			
1	D	203	Total	C	N	O	S	0	0	0
			1566	984	287	292	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	GLY	-	EXPRESSION TAG	UNP Q9HZN8
A	212	SER	-	EXPRESSION TAG	UNP Q9HZN8
B	211	GLY	-	EXPRESSION TAG	UNP Q9HZN8
B	212	SER	-	EXPRESSION TAG	UNP Q9HZN8
C	211	GLY	-	EXPRESSION TAG	UNP Q9HZN8
C	212	SER	-	EXPRESSION TAG	UNP Q9HZN8
D	211	GLY	-	EXPRESSION TAG	UNP Q9HZN8
D	212	SER	-	EXPRESSION TAG	UNP Q9HZN8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 5'-DEOXY-5'-FLUOROTHYMIDINE (three-letter code: 0DN) (formula: $C_{10}H_{13}FN_2O_4$).
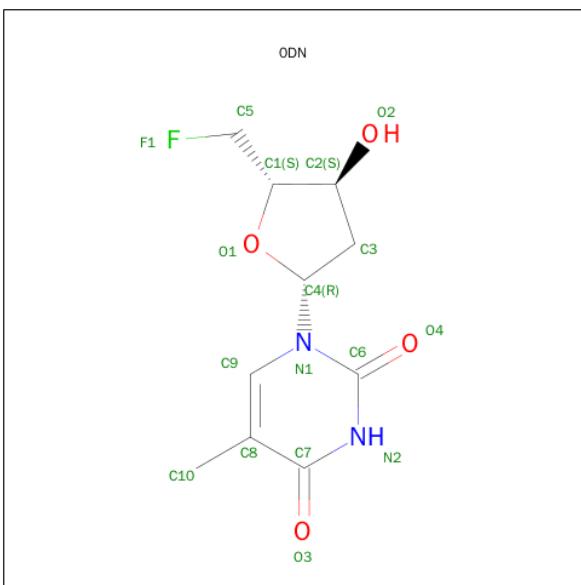
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			17	10	1	2	4		
3	B	1	Total	C	F	N	O	0	0
			17	10	1	2	4		
3	C	1	Total	C	F	N	O	0	0
			17	10	1	2	4		
3	D	1	Total	C	F	N	O	0	0
			17	10	1	2	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	102	Total	O	0	0
			102	102		
4	C	94	Total	O	0	0
			94	94		
4	D	87	Total	O	0	0
			87	87		

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: Thymidylate kinase
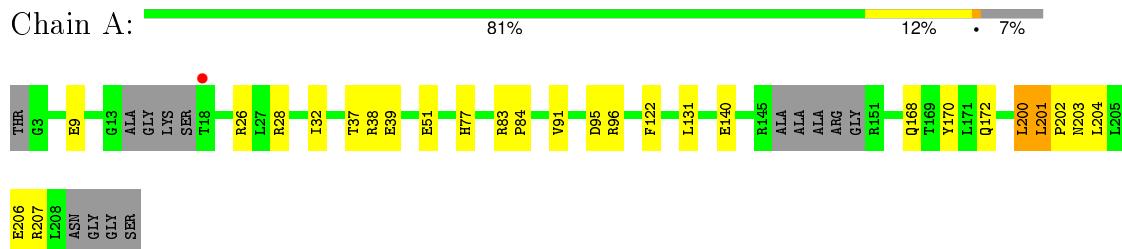
- Molecule 1: Thymidylate kinase
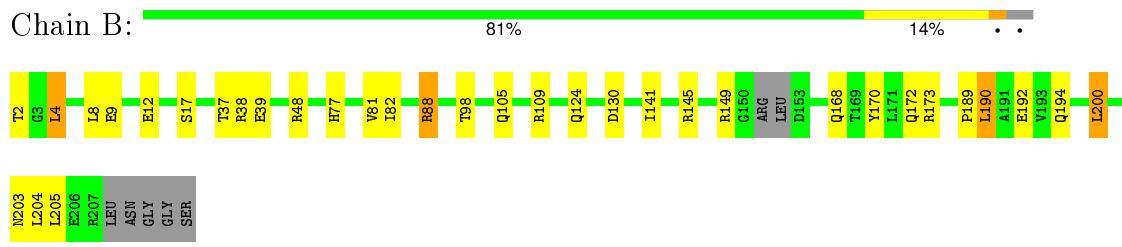
- Molecule 1: Thymidylate kinase
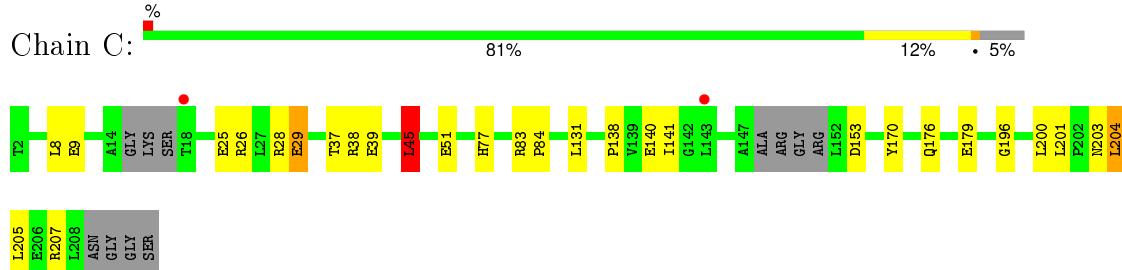
- Molecule 1: Thymidylate kinase
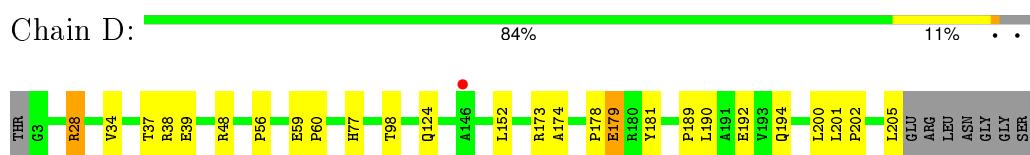
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	73.88Å 41.54Å 117.89Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	24.60 – 1.95 24.63 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.1 (24.60-1.95) 97.1 (24.63-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.236 0.179 , 0.238	Depositor DCC
R_{free} test set	2620 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 31.9	EDS
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 51330 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6691	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.53% 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, 0.375 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: 0DN, MG

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	0.76	0/1571	0.81	1/2126 (0.0%)
1	B	0.72	0/1607	0.81	1/2176 (0.0%)
1	C	0.78	1/1568 (0.1%)	0.82	2/2125 (0.1%)
1	D	0.74	0/1591	0.80	1/2156 (0.0%)
All	All	0.75	1/6337 (0.0%)	0.81	5/8583 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	29	GLU	CB-CG	-5.91	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	28	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	28	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	C	45	LEU	CA-CB-CG	5.58	128.14	115.30
1	C	28	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	200	LEU	CA-CB-CG	5.13	127.11	115.30

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	1548	0	1549	25	0
1	B	1583	0	1591	30	0
1	C	1545	0	1546	25	0
1	D	1566	0	1575	16	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0
3	A	17	0	13	0	0
3	B	17	0	13	0	0
3	C	17	0	13	0	0
3	D	17	0	13	0	0
4	A	94	0	0	2	1
4	B	102	0	0	3	1
4	C	94	0	0	3	0
4	D	87	0	0	0	0
All	All	6691	0	6313	94	1

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 7.

All (94) 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:B:189:PRO:HG2	1:B:192:GLU:HG3	1.26	1.18
1:B:77:HIS:CE1	1:B:81[B]:VAL:HG21	1.98	0.97
1:A:203:ASN:HD21	1:A:207:ARG:HE	1.22	0.87
1:A:203:ASN:ND2	1:A:207:ARG:HE	1.78	0.82
1:B:77:HIS:O	1:B:81[B]:VAL:HG22	1.82	0.79
1:B:77:HIS:ND1	1:B:81[B]:VAL:HG21	1.96	0.79
1:C:203:ASN:HD21	1:C:207:ARG:HH21	1.34	0.76
1:C:200:LEU:CD1	4:C:346:HOH:O	2.34	0.74
1:C:39:GLU:OE2	1:C:77:HIS:HD2	1.71	0.74
1:D:37:THR:OG1	1:D:77:HIS:HE1	1.71	0.73
1:A:200:LEU:C	1:A:200:LEU:HD23	2.10	0.70
1:A:140:GLU:CB	4:A:276:HOH:O	2.41	0.68
1:D:179:GLU:CD	1:D:179:GLU:H	1.94	0.68
1:C:140:GLU:HB2	4:C:286:HOH:O	1.92	0.68
1:B:39:GLU:OE2	1:B:77:HIS:HD2	1.75	0.68
1:B:12:GLU:HB3	1:B:149:ARG:NH1	2.09	0.68
1:D:178:PRO:HD2	1:D:179:GLU:OE2	1.94	0.67
1:A:203:ASN:HD21	1:A:207:ARG:NE	1.91	0.67
1:D:28:ARG:NH2	1:D:34:VAL:O	2.28	0.67
1:B:81[B]:VAL:HG23	1:B:82:ILE:N	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:OE2	1:A:77:HIS:HD2	1.76	0.66
1:D:37:THR:OG1	1:D:77:HIS:CE1	2.48	0.65
1:D:39:GLU:OE2	1:D:77:HIS:HD2	1.78	0.65
1:B:203:ASN:HB2	4:B:377:HOH:O	1.95	0.65
1:B:81[B]:VAL:HG23	1:B:82:ILE:HG13	1.79	0.64
1:C:131:LEU:HD22	1:C:204:LEU:HD22	1.77	0.64
1:A:131:LEU:CD2	1:A:204:LEU:HD11	2.28	0.64
1:B:77:HIS:ND1	1:B:81[B]:VAL:CG2	2.60	0.64
1:B:37:THR:OG1	1:B:77:HIS:HE1	1.81	0.63
1:B:168:GLN:O	1:B:172:GLN:HG3	1.99	0.62
1:A:26:ARG:HB3	1:A:201:LEU:HD21	1.80	0.62
1:B:37:THR:OG1	1:B:77:HIS:CE1	2.54	0.60
1:A:200:LEU:C	1:A:200:LEU:CD2	2.71	0.59
1:B:190:LEU:O	1:B:194:GLN:HG3	2.03	0.58
1:B:189:PRO:CG	1:B:192:GLU:HG3	2.18	0.57
1:C:204:LEU:N	1:C:204:LEU:HD23	2.20	0.56
1:A:203:ASN:HD21	1:A:207:ARG:HH21	1.55	0.55
1:A:202:PRO:HG3	1:C:51:GLU:HG2	1.88	0.55
1:C:200:LEU:HD13	4:C:346:HOH:O	2.04	0.54
1:B:141:ILE:O	1:B:145:ARG:HG3	2.08	0.54
1:A:140:GLU:HB3	4:A:276:HOH:O	2.06	0.54
1:B:105:GLN:O	1:B:109:ARG:HB2	2.08	0.54
1:C:8:LEU:N	1:C:8:LEU:HD12	2.22	0.53
1:A:37:THR:OG1	1:A:77:HIS:HE1	1.91	0.52
1:C:201:LEU:O	1:C:205:LEU:HG	2.09	0.52
1:B:4:LEU:HD22	1:B:130:ASP:CG	2.30	0.52
1:C:25:GLU:O	1:C:29:GLU:HG3	2.12	0.50
1:C:203:ASN:HD21	1:C:207:ARG:NH2	2.06	0.50
1:B:81[B]:VAL:CG2	1:B:82:ILE:N	2.76	0.49
1:C:203:ASN:ND2	1:C:207:ARG:HE	2.10	0.49
1:C:45:LEU:HB2	1:D:59:GLU:OE1	2.13	0.49
1:A:37:THR:OG1	1:A:77:HIS:CE1	2.66	0.48
1:D:174:ALA:HA	1:D:181:TYR:CD2	2.48	0.48
1:B:4:LEU:HD22	1:B:130:ASP:OD1	2.14	0.48
1:A:203:ASN:HD21	1:A:207:ARG:NH2	2.12	0.48
1:D:189:PRO:HD2	1:D:192:GLU:HG3	1.95	0.47
1:B:88:ARG:NH2	4:B:260:HOH:O	2.47	0.47
1:B:8:LEU:N	1:B:8:LEU:HD12	2.30	0.47
1:C:39:GLU:OE2	1:C:77:HIS:CD2	2.61	0.46
1:B:9:GLU:HB3	1:B:170:TYR:CE1	2.51	0.46
1:C:131:LEU:CD2	1:C:204:LEU:HD22	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ARG:HB2	1:C:84:PRO:HD3	1.98	0.45
1:C:9:GLU:HB3	1:C:170:TYR:CE1	2.51	0.45
1:B:203:ASN:CB	4:B:377:HOH:O	2.61	0.45
1:A:95:ASP:OD1	1:A:96:ARG:HG3	2.16	0.45
1:C:37:THR:OG1	1:C:77:HIS:HE1	1.99	0.44
1:A:9:GLU:HB3	1:A:170:TYR:CE1	2.53	0.44
1:D:201:LEU:O	1:D:205:LEU:HG	2.19	0.43
1:B:12:GLU:HB3	1:B:149:ARG:HH12	1.81	0.43
1:C:203:ASN:ND2	1:C:207:ARG:HH21	2.10	0.43
1:B:48:ARG:HA	1:B:48:ARG:NE	2.34	0.43
1:D:190:LEU:O	1:D:194:GLN:HG3	2.18	0.42
1:A:203:ASN:HD21	1:A:207:ARG:CZ	2.32	0.42
1:C:196:GLY:O	1:C:200:LEU:HD13	2.19	0.42
1:A:200:LEU:O	1:A:200:LEU:HD23	2.19	0.42
1:B:204:LEU:HA	1:B:204:LEU:HD23	1.89	0.42
1:A:168:GLN:O	1:A:172:GLN:HG3	2.19	0.42
1:A:122:PHE:C	1:A:122:PHE:CD1	2.92	0.42
1:C:26:ARG:HB3	1:C:201:LEU:HD11	2.02	0.42
1:C:153:ASP:C	1:C:153:ASP:OD1	2.59	0.41
1:B:168:GLN:O	1:B:172:GLN:CG	2.68	0.41
1:D:201:LEU:N	1:D:202:PRO:CD	2.82	0.41
1:C:138:PRO:HD2	1:C:141:ILE:HD12	2.01	0.41
1:D:59:GLU:HA	1:D:60:PRO:HD3	1.89	0.41
1:B:98:THR:OG1	1:B:124:GLN:NE2	2.52	0.41
1:A:204:LEU:C	1:A:206:GLU:N	2.73	0.41
1:A:32:ILE:HG21	1:A:91:VAL:HG23	2.02	0.41
1:B:39:GLU:OE2	1:B:77:HIS:CD2	2.66	0.40
1:C:37:THR:OG1	1:C:77:HIS:CE1	2.74	0.40
1:D:98:THR:OG1	1:D:124:GLN:NE2	2.55	0.40
1:A:83:ARG:HB2	1:A:84:PRO:HD3	2.04	0.40
1:D:174:ALA:HA	1:D:181:TYR:CG	2.56	0.40
1:A:122:PHE:CD1	1:A:122:PHE:O	2.75	0.40
1:D:56:PRO:HD3	1:D:152:LEU:HG	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:282:HOH:O	4:B:279:HOH:O[2_565]	2.06	0.14

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	192/211 (91%)	186 (97%)	6 (3%)	0	100	100
1	B	201/211 (95%)	194 (96%)	7 (4%)	0	100	100
1	C	194/211 (92%)	188 (97%)	6 (3%)	0	100	100
1	D	201/211 (95%)	196 (98%)	5 (2%)	0	100	100
All	All	788/844 (93%)	764 (97%)	24 (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	155/162 (96%)	151 (97%)	4 (3%)	54	43
1	B	157/162 (97%)	148 (94%)	9 (6%)	25	11
1	C	153/162 (94%)	148 (97%)	5 (3%)	45	32
1	D	155/162 (96%)	150 (97%)	5 (3%)	46	33
All	All	620/648 (96%)	597 (96%)	23 (4%)	41	27

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	51	GLU

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Mol	Chain	Res	Type
1	A	200	LEU
1	A	201	LEU
1	B	2	THR
1	B	4	LEU
1	B	17	SER
1	B	38	ARG
1	B	88	ARG
1	B	173	ARG
1	B	190	LEU
1	B	200	LEU
1	B	205	LEU
1	C	38	ARG
1	C	45	LEU
1	C	176	GLN
1	C	179	GLU
1	C	204	LEU
1	D	38	ARG
1	D	48	ARG
1	D	173	ARG
1	D	179	GLU
1	D	200	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	124	GLN
1	A	176	GLN
1	A	194	GLN
1	A	203	ASN
1	B	77	HIS
1	B	124	GLN
1	B	176	GLN
1	B	203	ASN
1	C	77	HIS
1	C	124	GLN
1	C	176	GLN
1	C	203	ASN
1	D	77	HIS
1	D	124	GLN
1	D	194	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)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	0DN	A	800	-	12,18,18	0.71	0	15,26,26	2.26	3 (20%)
3	0DN	B	801	-	12,18,18	0.64	0	15,26,26	1.90	2 (13%)
3	0DN	C	802	-	12,18,18	0.61	0	15,26,26	1.81	3 (20%)
3	0DN	D	803	-	12,18,18	0.72	0	15,26,26	2.51	2 (13%)

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	0DN	A	800	-	-	0/0/18/18	0/2/2/2
3	0DN	B	801	-	-	0/0/18/18	0/2/2/2
3	0DN	C	802	-	-	0/0/18/18	0/2/2/2
3	0DN	D	803	-	-	0/0/18/18	0/2/2/2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	803	0DN	C8-C7-N2	-5.87	118.60	125.14
3	A	800	0DN	C8-C7-N2	-4.92	119.66	125.14
3	B	801	0DN	C8-C7-N2	-4.34	120.30	125.14
3	C	802	0DN	C8-C7-N2	-4.15	120.52	125.14
3	C	802	0DN	C3-C4-N1	2.10	119.27	114.16
3	A	800	0DN	C10-C8-C7	2.12	122.79	120.05
3	C	802	0DN	C7-N2-C6	4.55	119.18	115.25
3	B	801	0DN	C7-N2-C6	5.19	119.74	115.25
3	A	800	0DN	C7-N2-C6	6.37	120.75	115.25
3	D	803	0DN	C7-N2-C6	7.06	121.35	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	197/211 (93%)	-0.29	1 (0%)	91	95	13, 22, 39, 47	0
1	B	204/211 (96%)	-0.34	0	100	100	13, 23, 41, 60	0
1	C	200/211 (94%)	-0.27	2 (1%)	84	89	14, 22, 40, 45	0
1	D	203/211 (96%)	-0.27	1 (0%)	91	95	14, 23, 39, 47	0
All	All	804/844 (95%)	-0.29	4 (0%)	91	95	13, 22, 40, 60	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	143	LEU	4.0
1	C	18	THR	2.4
1	A	18	THR	2.1
1	D	146	ALA	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)

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	0DN	B	801	17/17	0.96	0.09	0.38	15,17,21,21	0
3	0DN	C	802	17/17	0.97	0.09	-0.02	13,16,20,23	0
3	0DN	D	803	17/17	0.97	0.08	-0.62	15,18,21,23	0
3	0DN	A	800	17/17	0.98	0.07	-0.74	14,17,20,21	0
2	MG	C	213	1/1	0.95	0.07	-2.45	28,28,28,28	0
2	MG	C	214	1/1	0.72	0.10	-	38,38,38,38	0
2	MG	A	1	1/1	0.96	0.05	-	30,30,30,30	0
2	MG	A	213	1/1	0.90	0.10	-	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.