Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2018 – 10:50 PM EST

PDB ID	:	4KQV
Title	:	Topoisomerase iv atp binding domain of francisella tularensis in complex with a small molecule inhibitor
Authors	:	Bensen, D.C.; Akers-Rodriguez, S.; Lam, T.; Tari, L.W.
Deposited on	:	2013-05-15
Resolution	:	2.38 Å(reported)

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

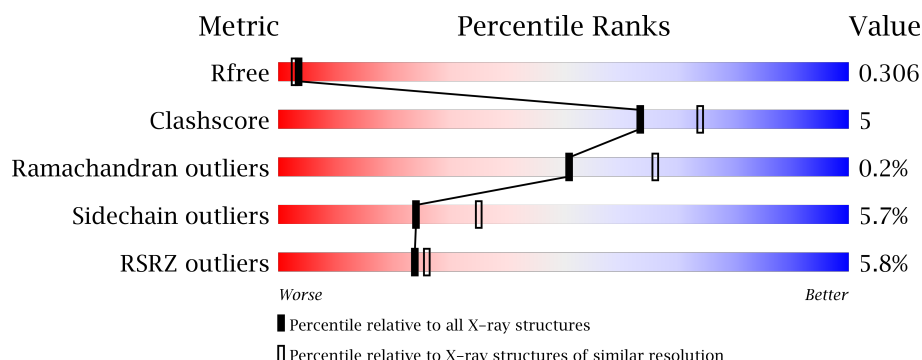|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.38 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		0.306
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		5.7%
RSRZ outliers		5.8%

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}	100719	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

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	390	3% 80% 9% · 9%
1	B	390	5% 42% 7% · 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DOO	B	403	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4586 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 Topoisomerase IV, subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total 2826	C 1805	N 476	O 537	S 8	0	3	0
1	B	196	Total 1559	C 996	N 263	O 294	S 6	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	PRO	LEU	VARIANT	UNP Q2A1P5
A	383	LEU	-	EXPRESSION TAG	UNP Q2A1P5
A	384	GLU	-	EXPRESSION TAG	UNP Q2A1P5
A	385	HIS	-	EXPRESSION TAG	UNP Q2A1P5
A	386	HIS	-	EXPRESSION TAG	UNP Q2A1P5
A	387	HIS	-	EXPRESSION TAG	UNP Q2A1P5
A	388	HIS	-	EXPRESSION TAG	UNP Q2A1P5
A	389	HIS	-	EXPRESSION TAG	UNP Q2A1P5
A	390	HIS	-	EXPRESSION TAG	UNP Q2A1P5
B	258	PRO	LEU	VARIANT	UNP Q2A1P5
B	383	LEU	-	EXPRESSION TAG	UNP Q2A1P5
B	384	GLU	-	EXPRESSION TAG	UNP Q2A1P5
B	385	HIS	-	EXPRESSION TAG	UNP Q2A1P5
B	386	HIS	-	EXPRESSION TAG	UNP Q2A1P5
B	387	HIS	-	EXPRESSION TAG	UNP Q2A1P5
B	388	HIS	-	EXPRESSION TAG	UNP Q2A1P5
B	389	HIS	-	EXPRESSION TAG	UNP Q2A1P5
B	390	HIS	-	EXPRESSION TAG	UNP Q2A1P5

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	I 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	I	0	0
			6	6		

- Molecule 3 is 6-fluoro-4-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-N-methyl-2-[(2-methylpyrimidin-5-yl)oxy]-9H-pyrimido[4,5-b]indol-8-amine (three-letter code: DOO) (formula: $C_{22}H_{23}FN_8O$).
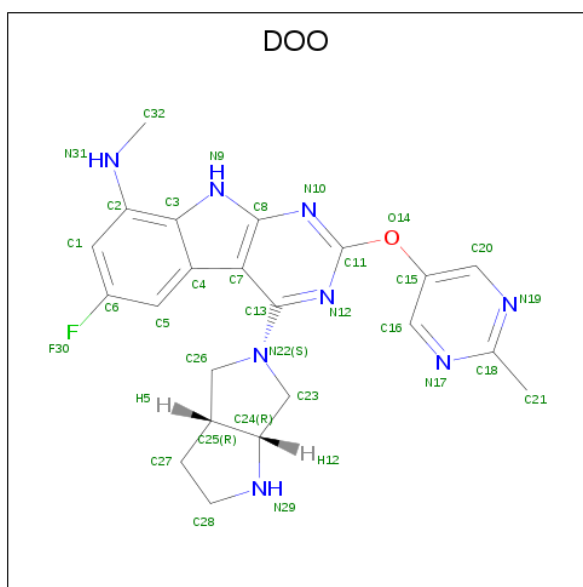
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			32	22	1	8	1		
3	B	1	Total	C	F	N	O	0	0
			32	22	1	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	107	Total	O	0	0
			107	107		
4	B	22	Total	O	0	0
			22	22		

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 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: Topoisomerase IV, subunit B
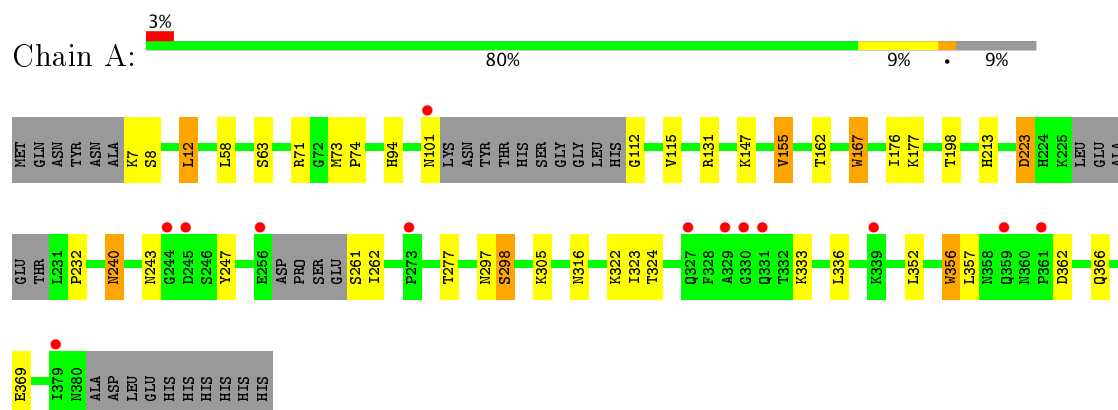
- Molecule 1: Topoisomerase IV, subunit B
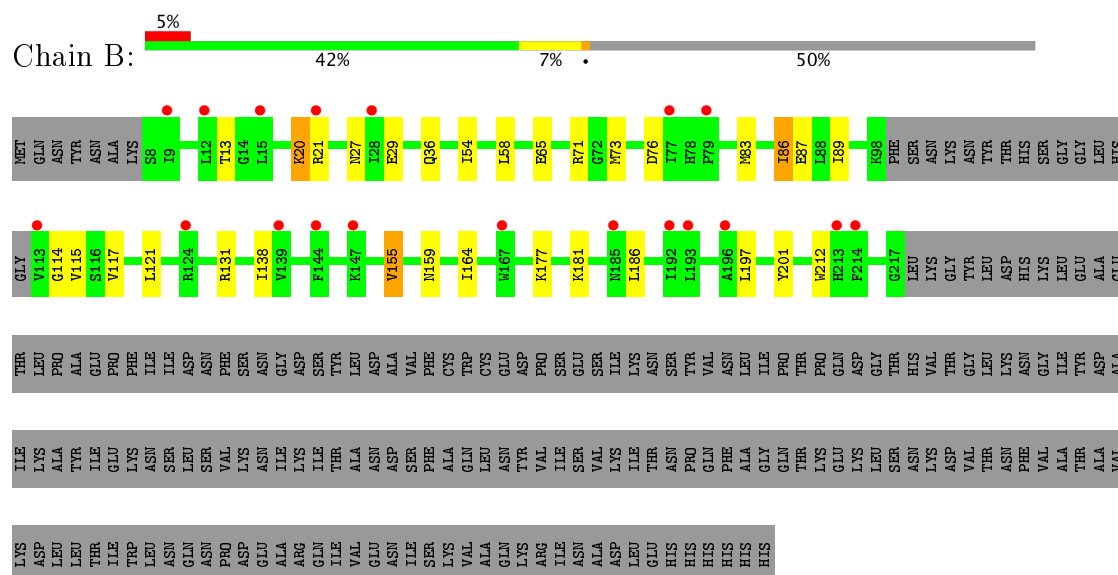
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.20Å 163.16Å 72.28Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	66.06 – 2.38 44.18 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.1 (66.06-2.38) 98.1 (44.18-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.99 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.255 , 0.299 0.261 , 0.306	Depositor DCC
R_{free} test set	2007 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.6	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4586	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, DOO

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	0.51	2/2885 (0.1%)	0.60	0/3896
1	B	0.47	0/1588	0.58	0/2138
All	All	0.50	2/4473 (0.0%)	0.60	0/6034

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	TRP	CD2-CE2	5.27	1.47	1.41
1	A	356	TRP	CD2-CE2	5.09	1.47	1.41

There are no bond angle outliers.

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	2826	0	2865	24	0
1	B	1559	0	1595	16	0
2	A	6	0	0	0	0
2	B	2	0	0	1	0
3	A	32	0	23	7	0
3	B	32	0	23	3	0
4	A	107	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	22	0	0	0	0
All	All	4586	0	4506	44	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 (44) 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:73[B]:MET:SD	3:B:403:DOO:H4	2.07	0.93
1:A:73[A]:MET:SD	3:A:403:DOO:H4	2.20	0.82
1:B:86:ILE:HD12	1:B:138:ILE:HG21	1.70	0.73
1:A:261:SER:HB2	1:A:316:ASN:HD21	1.55	0.72
1:B:73[B]:MET:SD	3:B:403:DOO:C26	2.78	0.70
3:A:403:DOO:H2	3:A:403:DOO:C23	2.25	0.67
1:B:155:VAL:HG13	1:B:159:ASN:HB3	1.80	0.64
1:B:86:ILE:O	1:B:89:ILE:HG22	2.03	0.58
1:A:262:ILE:H	1:A:316:ASN:HD22	1.51	0.57
1:A:247:TYR:HB2	1:A:322:LYS:HB2	1.88	0.56
1:A:240:ASN:HD21	1:A:247:TYR:HD1	1.53	0.55
3:A:403:DOO:H2	3:A:403:DOO:H13	1.89	0.54
3:A:403:DOO:H2	3:A:403:DOO:H14	1.87	0.54
1:A:240:ASN:ND2	1:A:247:TYR:HD1	2.05	0.53
1:A:115:VAL:HG11	3:A:403:DOO:F30	2.00	0.52
1:B:20:LYS:HG3	1:B:21:ARG:HG3	1.92	0.51
1:B:83:MET:HG2	1:B:87:GLU:HB3	1.92	0.51
1:A:297:ASN:O	1:A:298:SER:HB3	2.11	0.51
1:A:73[B]:MET:HE2	1:A:162:THR:HG21	1.94	0.50
1:B:54:ILE:HG13	1:B:197:LEU:HD11	1.94	0.49
3:A:403:DOO:H14	3:A:403:DOO:C5	2.42	0.49
1:A:112:GLY:HA3	1:A:333:LYS:NZ	2.28	0.49
1:A:73[A]:MET:SD	3:A:403:DOO:C26	2.99	0.49
1:A:198:THR:HG23	1:A:213:HIS:HB2	1.94	0.48
1:B:36:GLN:HG3	1:B:186:LEU:HD21	1.96	0.47
1:A:223:ASP:OD1	1:A:223:ASP:N	2.45	0.47
1:A:362:ASP:O	1:A:366:GLN:HG3	2.15	0.47
1:B:164:ILE:HD12	3:B:403:DOO:C1	2.45	0.47
1:B:186:LEU:HD22	2:B:401:IOD:I	2.85	0.46
1:B:71:ARG:O	1:B:131:ARG:HG3	2.15	0.46
1:A:323:ILE:HD11	1:A:336:LEU:HD11	1.98	0.46
1:A:12:LEU:HD11	1:A:94:HIS:CE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:TYR:HB2	1:B:212:TRP:HZ3	1.80	0.45
1:A:232:PRO:HG3	1:A:356:TRP:CH2	2.52	0.45
1:A:262:ILE:H	1:A:316:ASN:ND2	2.14	0.44
1:B:27:ASN:OD1	1:B:29:GLU:HG2	2.17	0.44
1:B:65:GLU:HA	1:B:164:ILE:O	2.17	0.43
1:A:73[A]:MET:SD	1:A:74:PRO:HD2	2.59	0.43
1:A:63:SER:HB3	1:A:167:TRP:CD1	2.54	0.42
1:B:114:GLY:O	1:B:117:VAL:HB	2.18	0.42
1:A:155:VAL:HG22	4:A:569:HOH:O	2.18	0.42
1:A:71:ARG:O	1:A:131:ARG:HG2	2.20	0.42
1:A:297:ASN:O	1:A:298:SER:CB	2.68	0.42
1:A:262:ILE:N	1:A:316:ASN:HD22	2.17	0.41

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	350/390 (90%)	335 (96%)	14 (4%)	1 (0%)	44	59
1	B	193/390 (50%)	183 (95%)	10 (5%)	0	100	100
All	All	543/780 (70%)	518 (95%)	24 (4%)	1 (0%)	51	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	SER

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	317/344 (92%)	299 (94%)	18 (6%)	24	35
1	B	174/344 (51%)	164 (94%)	10 (6%)	24	35
All	All	491/688 (71%)	463 (94%)	28 (6%)	24	35

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	8	SER
1	A	12	LEU
1	A	58	LEU
1	A	101	ASN
1	A	147	LYS
1	A	155	VAL
1	A	176	ILE
1	A	177	LYS
1	A	223	ASP
1	A	240	ASN
1	A	243	ASN
1	A	277	THR
1	A	305	LYS
1	A	324	THR
1	A	352	LEU
1	A	357	LEU
1	A	369	GLU
1	B	13	THR
1	B	20	LYS
1	B	58	LEU
1	B	76	ASP
1	B	86	ILE
1	B	115	VAL
1	B	121	LEU
1	B	155	VAL
1	B	177	LYS

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Mol	Chain	Res	Type
1	B	181	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	137	HIS
1	A	224	HIS
1	A	240	ASN
1	A	243	ASN
1	A	316	ASN
1	A	343	ASN
1	A	358	ASN
1	A	370	ASN
1	B	36	GLN
1	B	134	ASN
1	B	137	HIS
1	B	154	ASN
1	B	185	ASN

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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	DOO	A	403	-	35,37,37	1.36	6 (17%)	35,55,55	1.93	15 (42%)
3	DOO	B	403	-	35,37,37	1.48	6 (17%)	35,55,55	2.30	13 (37%)

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	DOO	A	403	-	-	0/10/28/28	0/6/6/6
3	DOO	B	403	-	-	0/10/28/28	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	DOO	C11-N10	2.11	1.36	1.33
3	B	403	DOO	C2-C3	2.21	1.48	1.43
3	A	403	DOO	C7-C8	2.22	1.48	1.43
3	B	403	DOO	C11-N12	2.28	1.36	1.33
3	A	403	DOO	C13-C7	2.75	1.48	1.43
3	A	403	DOO	C5-C6	2.85	1.40	1.36
3	A	403	DOO	C4-C3	2.86	1.47	1.42
3	B	403	DOO	C5-C6	2.88	1.40	1.36
3	B	403	DOO	C13-N12	3.00	1.36	1.32
3	B	403	DOO	C4-C3	3.22	1.48	1.42
3	A	403	DOO	C13-N12	3.28	1.37	1.32
3	B	403	DOO	C13-C7	3.65	1.50	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	403	DOO	C25-C26-N22	-4.66	97.33	103.30
3	B	403	DOO	N10-C11-N12	-4.00	122.21	127.80
3	A	403	DOO	C15-C20-N19	-3.37	118.76	122.72
3	B	403	DOO	C15-C16-N17	-3.22	118.93	122.72
3	B	403	DOO	N17-C18-N19	-3.01	120.45	125.58
3	A	403	DOO	C6-C5-C4	-3.00	117.50	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	DOO	N10-C11-N12	-2.96	123.67	127.80
3	B	403	DOO	C15-C20-N19	-2.94	119.26	122.72
3	A	403	DOO	N17-C18-N19	-2.87	120.69	125.58
3	A	403	DOO	C15-C16-N17	-2.45	119.84	122.72
3	A	403	DOO	C25-C26-N22	-2.11	100.59	103.30
3	A	403	DOO	C2-C1-C6	2.01	120.87	117.75
3	A	403	DOO	C21-C18-N17	2.01	119.33	117.06
3	B	403	DOO	C27-C25-C24	2.04	107.47	103.83
3	A	403	DOO	C27-C25-C24	2.07	107.52	103.83
3	A	403	DOO	C16-N17-C18	2.55	120.29	115.88
3	A	403	DOO	C21-C18-N19	2.58	119.97	117.06
3	B	403	DOO	C2-C1-C6	2.69	121.93	117.75
3	B	403	DOO	C21-C18-N17	2.81	120.24	117.06
3	A	403	DOO	C7-C13-N22	2.83	126.87	121.13
3	B	403	DOO	C16-N17-C18	2.84	120.78	115.88
3	A	403	DOO	C3-C2-N31	2.91	118.65	116.78
3	B	403	DOO	C20-N19-C18	2.94	120.97	115.88
3	A	403	DOO	C20-N19-C18	3.05	121.16	115.88
3	B	403	DOO	C7-C13-N22	3.61	128.44	121.13
3	A	403	DOO	C16-C15-C20	3.88	119.25	116.56
3	B	403	DOO	C16-C15-C20	4.40	119.61	116.56
3	B	403	DOO	C3-C2-N31	4.92	119.95	116.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	DOO	7	0
3	B	403	DOO	3	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(Å²)	Q<0.9
1	A	355/390 (91%)	0.14	13 (3%)	42	45	30, 50, 87, 117	0
1	B	196/390 (50%)	0.58	19 (9%)	8	9	45, 64, 90, 108	0
All	All	551/780 (70%)	0.30	32 (5%)	24	26	30, 57, 88, 117	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	GLN	6.2
1	A	245	ASP	4.8
1	A	339	LYS	4.4
1	B	214	PHE	4.4
1	A	329	ALA	3.9
1	B	12	LEU	3.5
1	A	359	GLN	3.5
1	B	196	ALA	3.1
1	B	213	HIS	3.0
1	A	101	ASN	3.0
1	A	330	GLY	3.0
1	A	379	ILE	2.9
1	A	327	GLN	2.8
1	B	144	PHE	2.8
1	B	193	LEU	2.8
1	B	15	LEU	2.7
1	B	28	ILE	2.7
1	A	361	PRO	2.6
1	B	185	ASN	2.6
1	B	9	ILE	2.6
1	B	167	TRP	2.5
1	B	192	ILE	2.5
1	A	273	PRO	2.4
1	B	113	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	139	VAL	2.3
1	B	21	ARG	2.3
1	B	77	ILE	2.3
1	A	256	GLU	2.2
1	B	124	ARG	2.2
1	B	147	LYS	2.1
1	A	244	GLY	2.1
1	B	79	PRO	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	DOO	B	403	32/32	0.92	0.21	3.14	47,62,71,73	0
3	DOO	A	403	32/32	0.95	0.14	0.36	34,37,47,47	0
2	IOD	A	402	1/1	0.99	0.07	-1.77	59,59,59,59	0
2	IOD	A	406	1/1	0.98	0.09	-2.02	107,107,107,107	0
2	IOD	A	404	1/1	0.95	0.07	-2.18	119,119,119,119	0
2	IOD	B	402	1/1	0.85	0.10	-	130,130,130,130	0
2	IOD	A	407	1/1	0.85	0.08	-	132,132,132,132	0
2	IOD	A	405	1/1	0.92	0.14	-	149,149,149,149	0
2	IOD	B	401	1/1	0.98	0.03	-	82,82,82,82	0
2	IOD	A	401	1/1	0.99	0.04	-	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.