wwPDB X-ray Structure Validation Summary Report (i)

Dec 13, 2023 – 10:40 pm GMT

PDB ID	:	4D6O
Title	:	THE CRYSTAL STRUCTURE OF I-DMOI IN COMPLEX WITH ITS TARGET DNA AT 1H INCUBATION IN 5MM MG (STATE 2)
Authors	:	Molina, R.; Stella, S.; Redondo, P.; Gomez, H.; Marcaida, M.J.; Orozco, M.; Prieto, J.; Montoya, G.
Deposited on	:	2014-11-13
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

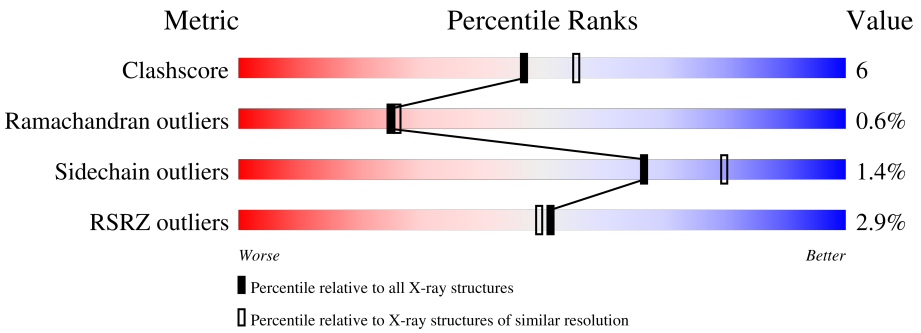
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	199	4%, 76%, 15%, •, 9%
1	D	199	2%, 79%, 17%, •
1	G	199	4%, 72%, 16%, •, 12%
2	B	25	84%, 12%, •
2	H	25	88%, 12%
3	C	25	84%, 16%

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Mol	Chain	Length	Quality of chain
3	I	25	4% 96%
4	E	25	64% 36%
5	F	25	4% 72% 28%

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
7	ACT	D	1198	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7979 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 HOMING ENDONUCLEASE I-DMOI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	182	1523	984	279	257	3	0	5	0
1	D	191	1621	1050	293	275	3	0	8	0
1	G	176	1509	975	278	253	3	0	7	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP P21505
A	189	ALA	-	expression tag	UNP P21505
A	190	ALA	-	expression tag	UNP P21505
A	191	ALA	-	expression tag	UNP P21505
A	192	LEU	-	expression tag	UNP P21505
A	193	GLU	-	expression tag	UNP P21505
A	194	HIS	-	expression tag	UNP P21505
A	195	HIS	-	expression tag	UNP P21505
A	196	HIS	-	expression tag	UNP P21505
A	197	HIS	-	expression tag	UNP P21505
A	198	HIS	-	expression tag	UNP P21505
A	199	HIS	-	expression tag	UNP P21505
D	1	ALA	-	expression tag	UNP P21505
D	189	ALA	-	expression tag	UNP P21505
D	190	ALA	-	expression tag	UNP P21505
D	191	ALA	-	expression tag	UNP P21505
D	192	LEU	-	expression tag	UNP P21505
D	193	GLU	-	expression tag	UNP P21505
D	194	HIS	-	expression tag	UNP P21505
D	195	HIS	-	expression tag	UNP P21505
D	196	HIS	-	expression tag	UNP P21505
D	197	HIS	-	expression tag	UNP P21505
D	198	HIS	-	expression tag	UNP P21505

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Chain	Residue	Modelled	Actual	Comment	Reference
D	199	HIS	-	expression tag	UNP P21505
G	1	ALA	-	expression tag	UNP P21505
G	189	ALA	-	expression tag	UNP P21505
G	190	ALA	-	expression tag	UNP P21505
G	191	ALA	-	expression tag	UNP P21505
G	192	LEU	-	expression tag	UNP P21505
G	193	GLU	-	expression tag	UNP P21505
G	194	HIS	-	expression tag	UNP P21505
G	195	HIS	-	expression tag	UNP P21505
G	196	HIS	-	expression tag	UNP P21505
G	197	HIS	-	expression tag	UNP P21505
G	198	HIS	-	expression tag	UNP P21505
G	199	HIS	-	expression tag	UNP P21505

- Molecule 2 is a DNA chain called 25MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	25	511	242	94	151	24	0	0	0
2	H	25	511	242	94	151	24	0	0	0

- Molecule 3 is a DNA chain called 25MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	25	508	240	99	145	24	0	0	0
3	I	25	508	240	99	145	24	0	0	0

- Molecule 4 is a DNA chain called 25MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	E	25	510	242	94	150	24	0	0	0

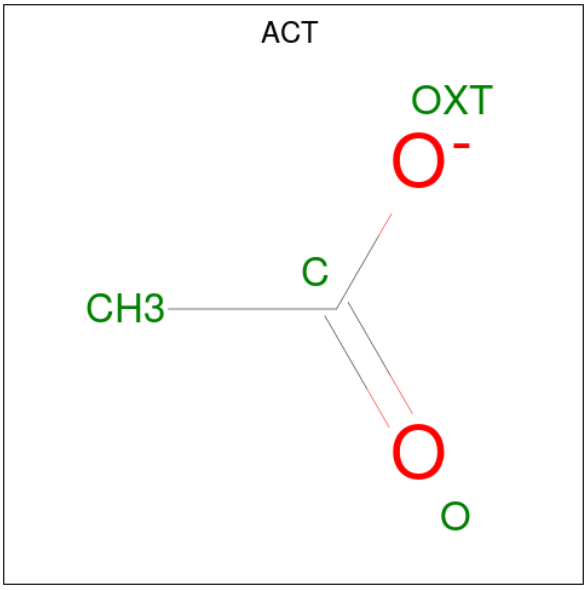
- Molecule 5 is a DNA chain called 25MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	F	25	509	241	98	146	24	0	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Mg 2 2	0	0
6	D	2	Total Mg 2 2	0	0
6	G	2	Total Mg 2 2	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	57	Total O 57 57	0	0
8	B	21	Total O 21 21	0	0
8	C	7	Total O 7 7	0	0
8	D	80	Total O 80 80	0	0
8	E	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	F	10	10	10	0	0
			Total	O		
8	G	55	55	55	0	0
			Total	O		
8	H	11	11	11	0	0
			Total	O		
8	I	10	10	10	0	0

3 Residue-property plots (i)

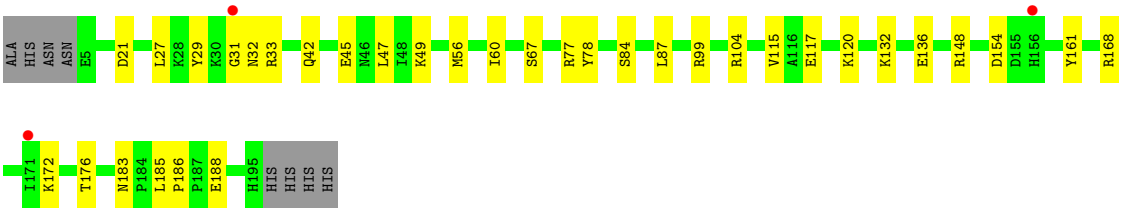
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HOMING ENDONUCLEASE I-DMOI

Chain A:

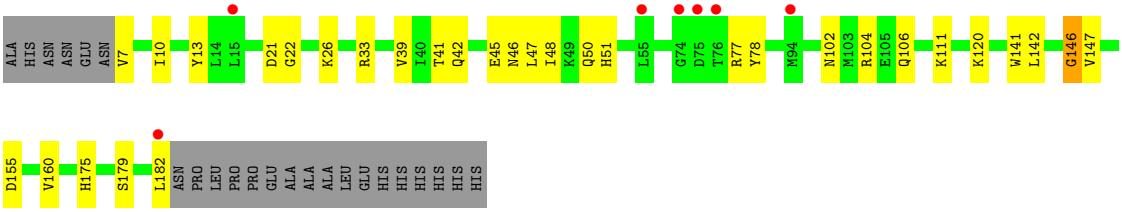
• Molecule 1: HOMING ENDONUCLEASE I-DMOI

Chain D:



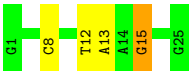
• Molecule 1: HOMING ENDONUCLEASE I-DMOI

Chain G:



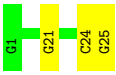
• Molecule 2: 25MER

Chain B:



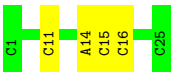
- Molecule 2: 25MER

Chain H:



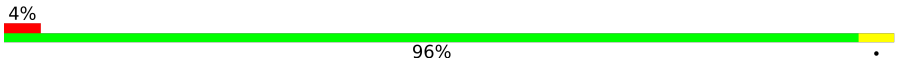
- Molecule 3: 25MER

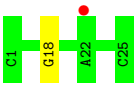
Chain C:



- Molecule 3: 25MER

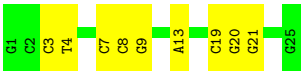
Chain I:





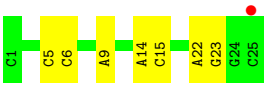
- Molecule 4: 25MER

Chain E:



- Molecule 5: 25MER

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.89Å 70.67Å 107.14Å 90.00° 119.80° 90.00°	Depositor
Resolution (Å)	46.49 – 2.20 46.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.49-2.20) 99.5 (46.49-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.186 , 0.220 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h-l,k,h 0.020 for l,k,-h-l 0.015 for h,-k,-h-l 0.014 for -h-l,-k,l 0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7979	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, 0.333 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: ACT, 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	0.45	0/1566	0.63	1/2107 (0.0%)
1	D	0.42	0/1677	0.57	2/2257 (0.1%)
1	G	0.45	0/1552	0.60	0/2084
2	B	1.02	2/572 (0.3%)	1.03	0/882
2	H	0.87	0/572	1.00	0/882
3	C	0.88	1/570 (0.2%)	0.92	0/877
3	I	0.93	0/570	0.97	0/877
4	E	0.81	0/571	1.05	0/880
5	F	0.89	0/571	1.01	1/879 (0.1%)
All	All	0.67	3/8221 (0.0%)	0.80	4/11725 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	15	DC	P-O5'	5.61	1.65	1.59
2	B	15	DG	N1-C2	-5.55	1.33	1.37
2	B	15	DG	N7-C5	5.12	1.42	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	27	LEU	CA-CB-CG	6.07	129.25	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	LEU	CA-CB-CG	5.56	128.08	115.30
5	F	9	DA	O4'-C1'-N9	5.33	111.73	108.00
1	D	77	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	HIS	Sidechain

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	1523	0	1596	23	0
1	D	1621	0	1712	28	0
1	G	1509	0	1588	21	0
2	B	511	0	282	8	0
2	H	511	0	282	2	0
3	C	508	0	279	3	0
3	I	508	0	279	1	0
4	E	510	0	282	7	0
5	F	509	0	280	3	0
6	A	2	0	0	0	0
6	D	2	0	0	0	0
6	G	2	0	0	0	0
7	D	4	0	3	2	0
8	A	57	0	0	5	1
8	B	21	0	0	1	0
8	C	7	0	0	3	0
8	D	80	0	0	9	0
8	E	8	0	0	1	0
8	F	10	0	0	0	1
8	G	55	0	0	5	0
8	H	11	0	0	0	0
8	I	10	0	0	1	0
All	All	7979	0	6583	88	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 6.

The worst 5 of 88 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:G:21:ASP:OD1	8:G:2005:HOH:O	1.91	0.89
3:I:18:DG:OP1	8:I:2007:HOH:O	1.89	0.88
3:C:11:DC:OP1	8:C:2005:HOH:O	1.92	0.87
1:G:120:LYS:HG2	8:G:2033:HOH:O	1.81	0.80
2:B:12:DT:O2	8:B:2008:HOH:O	2.04	0.73

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)
8:A:2056:HOH:O	8:F:2007:HOH:O[2_645]	1.88	0.32

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	185/199 (93%)	177 (96%)	7 (4%)	1 (0%)	29	31
1	D	197/199 (99%)	193 (98%)	4 (2%)	0	100	100
1	G	181/199 (91%)	174 (96%)	5 (3%)	2 (1%)	14	12
All	All	563/597 (94%)	544 (97%)	16 (3%)	3 (0%)	25	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	PRO
1	G	147	VAL

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Mol	Chain	Res	Type
1	G	146	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	166/178 (93%)	163 (98%)	3 (2%)	59	72
1	D	179/178 (101%)	174 (97%)	5 (3%)	43	56
1	G	165/178 (93%)	165 (100%)	0	100	100
All	All	510/534 (96%)	502 (98%)	8 (2%)	67	76

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	185	LEU
1	D	183	ASN
1	D	136[A]	GLU
1	D	32	ASN
1	D	136[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
7	ACT	D	1198	-	3,3,3	0.69	0	3,3,3	1.60	1 (33%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1198	ACT	OXT-C-CH3	2.06	123.68	115.18

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
7	D	1198	ACT	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	182/199 (91%)	0.37	8 (4%)	34	32	32, 45, 72, 98	0
1	D	191/199 (95%)	0.23	3 (1%)	72	70	30, 44, 64, 77	0
1	G	176/199 (88%)	0.57	7 (3%)	38	36	30, 42, 64, 120	0
2	B	25/25 (100%)	-0.20	0	100	100	40, 50, 62, 67	0
2	H	25/25 (100%)	0.13	0	100	100	39, 54, 60, 63	0
3	C	25/25 (100%)	0.07	0	100	100	38, 53, 71, 74	0
3	I	25/25 (100%)	0.40	1 (4%)	38	36	38, 49, 78, 85	0
4	E	25/25 (100%)	0.12	0	100	100	37, 55, 72, 77	0
5	F	25/25 (100%)	0.24	1 (4%)	38	36	39, 52, 87, 89	0
All	All	699/747 (93%)	0.33	20 (2%)	51	49	30, 46, 71, 120	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	HIS	6.0
1	A	75	ASP	4.3
1	A	184	PRO	4.0
1	D	31	GLY	3.8
1	G	182	LEU	3.7

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
6	MG	A	1187	1/1	0.74	0.10	42,42,42,42	0
6	MG	G	1184	1/1	0.87	0.08	39,39,39,39	0
7	ACT	D	1198	4/4	0.89	0.23	45,49,49,60	0
6	MG	D	1197	1/1	0.95	0.11	36,36,36,36	0
6	MG	D	1196	1/1	0.98	0.22	25,25,25,25	0
6	MG	A	1186	1/1	0.99	0.17	29,29,29,29	0
6	MG	G	1183	1/1	0.99	0.17	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.