



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 09:52 PM BST

PDB ID : 4E7I
Title : PFV intasome freeze-trapped prior to 3'-processing, Mn-bound form (UI-Mn)
Authors : Hare, S.; Cherepanov, P.
Deposited on : 2012-03-17
Resolution : 2.53 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

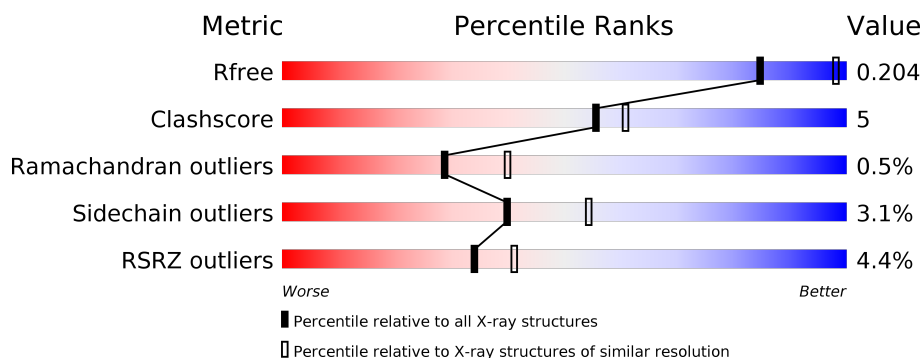
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 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 $\leq 5\%$. 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	395	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>7%</div> </div> </div>
1	B	395	<div> <div>3%</div> <div> <div></div> <div>40%</div> <div>7%</div> <div>53%</div> </div> </div>
2	C	19	<div> <div>21%</div> <div>63%</div> <div>16%</div> </div>
3	D	19	<div> <div>47%</div> <div>47%</div> <div>5%</div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5483 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 Pro-Pol polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2922	1873	515	530	4			
1	B	184	Total	C	N	O	S	0	0	0
			1423	922	233	267	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P14350
A	-1	PRO	-	EXPRESSION TAG	UNP P14350
A	0	GLY	-	EXPRESSION TAG	UNP P14350
A	217	SER	GLY	VARIANT	UNP P14350
A	218	GLY	SER	VARIANT	UNP P14350
B	-2	GLY	-	EXPRESSION TAG	UNP P14350
B	-1	PRO	-	EXPRESSION TAG	UNP P14350
B	0	GLY	-	EXPRESSION TAG	UNP P14350
B	217	SER	GLY	VARIANT	UNP P14350
B	218	GLY	SER	VARIANT	UNP P14350

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*TP*TP*GP*TP*CP*AP*TP*GP*GP*AP*AP*TP*TP*TP*CP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	19	Total	C	N	O	P	0	0	0
			387	187	68	114	18			

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*GP*CP*GP*AP*AP*AP*TP*TP*CP*CP*AP*TP*GP*AP*CP*AP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	19	Total	C	N	O	P	0	0	0
			386	186	72	110	18			

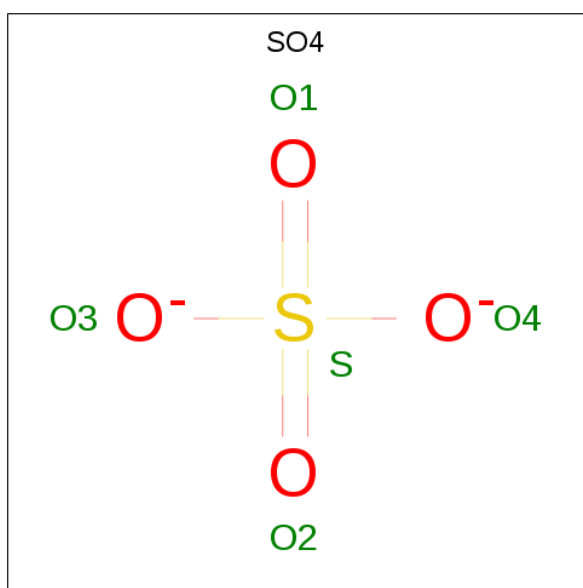
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	A	2	Total	Mn	0	0
			2	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



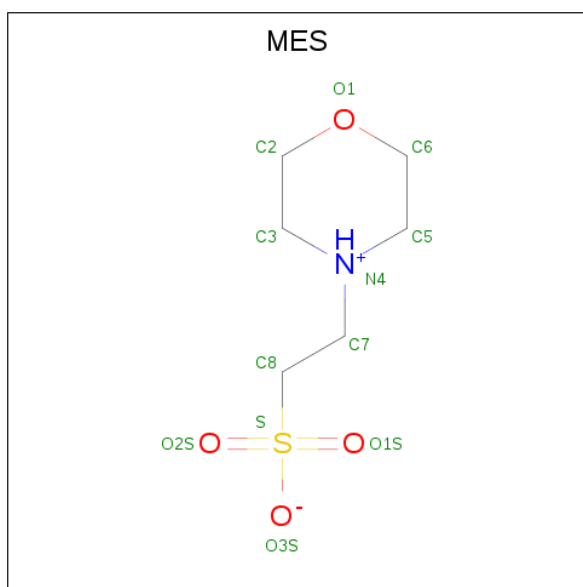
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



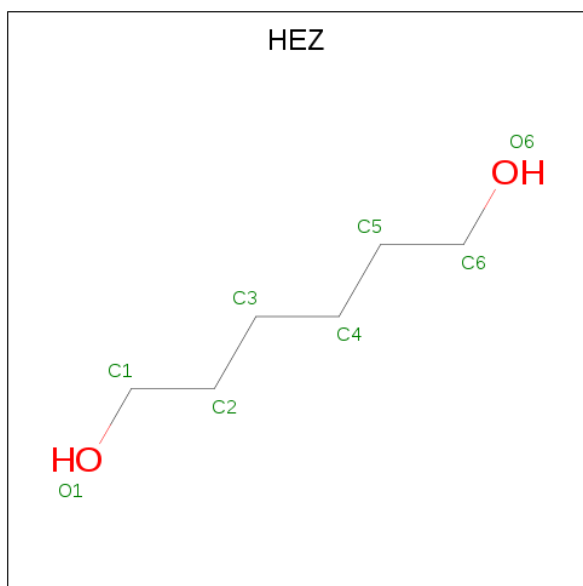
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 9 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	160	Total 160	O 160	0	0
10	B	50	Total 50	O 50	0	0
10	C	35	Total 35	O 35	0	0
10	D	22	Total 22	O 22	0	0



- Molecule 3: DNA (5'-D(*TP*GP*CP*GP*AP*AP*AP*TP*TP*CP*CP*AP*TP*GP*AP*CP*AP*AP*T)-3')

Chain D: 47% 47% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	160.15Å 160.15Å 124.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.84 – 2.53 38.84 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.84-2.53) 99.8 (38.84-2.53)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.183 , 0.211 0.177 , 0.204	Depositor DCC
R_{free} test set	2746 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5483	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL, ZN, MN, HEZ, SO4, MES

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	0.50	0/3001	0.65	0/4096
1	B	0.51	0/1463	0.62	0/2003
2	C	0.98	0/433	1.94	17/667 (2.5%)
3	D	1.00	0/433	1.98	12/666 (1.8%)
All	All	0.61	0/5330	1.01	29/7432 (0.4%)

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	7	DA	O4'-C1'-N9	-13.30	98.69	108.00
3	D	17	DA	O4'-C1'-N9	12.64	116.84	108.00
3	D	12	DA	O4'-C1'-N9	-10.30	100.79	108.00
2	C	15	DT	O4'-C1'-N1	-9.86	101.10	108.00
3	D	13	DT	O4'-C1'-N1	-9.10	101.63	108.00

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	2922	0	2952	26	0
1	B	1423	0	1384	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	387	0	218	6	0
3	D	386	0	216	2	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	15	0	0	0	0
6	B	5	0	0	1	0
7	A	30	0	40	4	0
7	B	6	0	8	2	0
7	C	6	0	8	0	0
7	D	12	0	16	0	0
8	A	12	0	13	4	0
9	B	8	0	14	1	0
10	A	160	0	0	4	1
10	B	50	0	0	0	0
10	C	35	0	0	0	0
10	D	22	0	0	1	0
All	All	5483	0	4869	51	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 5.

The worst 5 of 51 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)
2:C:1:DA:H4'	2:C:2:DT:H5'	1.43	1.01
7:A:408:GOL:HO1	7:A:408:GOL:HO3	0.92	0.89
1:A:137:GLN:H	7:A:406:GOL:H2	1.46	0.81
1:B:250:GLN:HE22	9:B:403:HEZ:H22	1.52	0.74
1:B:219:LYS:HE2	1:B:261:LEU:HD12	1.71	0.72

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)
10:A:528:HOH:O	10:A:632:HOH:O[8_554]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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	366/395 (93%)	356 (97%)	10 (3%)	0	100	100
1	B	182/395 (46%)	168 (92%)	11 (6%)	3 (2%)	9	12
All	All	548/790 (69%)	524 (96%)	21 (4%)	3 (0%)	29	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	216	SER
1	B	260	VAL
1	B	298	ILE

5.3.2 Protein sidechains

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	327/354 (92%)	318 (97%)	9 (3%)	43	58
1	B	154/354 (44%)	148 (96%)	6 (4%)	32	44
All	All	481/708 (68%)	466 (97%)	15 (3%)	40	54

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	SER
1	A	332	SER
1	B	282	ASP

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Mol	Chain	Res	Type
1	A	306	SER
1	B	274	SER

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	$\# Z > 2$
8	MES	A	412	-	12,12,12	1.80	3 (25%)	14,16,16	1.22	3 (21%)
7	GOL	D	102	-	5,5,5	0.31	0	5,5,5	0.70	0
6	SO4	A	405	-	4,4,4	0.16	0	6,6,6	0.31	0
7	GOL	A	408	-	5,5,5	0.40	0	5,5,5	0.84	0
7	GOL	A	407	-	5,5,5	0.39	0	5,5,5	0.69	0
7	GOL	D	101	-	5,5,5	0.41	0	5,5,5	0.41	0
7	GOL	A	409	-	5,5,5	0.49	0	5,5,5	0.92	0
7	GOL	A	411	-	5,5,5	0.36	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	404	-	5,5,5	0.47	0	5,5,5	0.45	0
6	SO4	B	402	-	4,4,4	0.21	0	6,6,6	0.29	0
7	GOL	A	406	-	5,5,5	0.32	0	5,5,5	0.76	0
9	HEZ	B	403	-	7,7,7	0.34	0	6,6,6	0.98	0
6	SO4	A	410	-	4,4,4	0.23	0	6,6,6	0.39	0
6	SO4	A	404	-	4,4,4	0.18	0	6,6,6	0.27	0
7	GOL	C	101	-	5,5,5	0.37	0	5,5,5	0.83	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
8	MES	A	412	-	-	0/6/14/14	0/1/1/1
7	GOL	A	411	-	-	2/4/4/4	-
7	GOL	A	407	-	-	0/4/4/4	-
7	GOL	D	101	-	-	4/4/4/4	-
7	GOL	A	409	-	-	4/4/4/4	-
7	GOL	D	102	-	-	0/4/4/4	-
7	GOL	B	404	-	-	2/4/4/4	-
7	GOL	A	406	-	-	2/4/4/4	-
9	HEZ	B	403	-	-	2/5/5/5	-
7	GOL	A	408	-	-	4/4/4/4	-
7	GOL	C	101	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	412	MES	C8-S	4.29	1.83	1.77
8	A	412	MES	O2S-S	2.96	1.53	1.45
8	A	412	MES	O1S-S	2.86	1.53	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	412	MES	O3S-S-C8	2.30	109.49	105.77
8	A	412	MES	O1S-S-C8	2.13	109.48	106.92
8	A	412	MES	O2S-S-C8	2.05	109.39	106.92

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	GOL	O1-C1-C2-C3
7	A	408	GOL	C1-C2-C3-O3
7	A	408	GOL	O2-C2-C3-O3
7	A	411	GOL	O1-C1-C2-C3
7	B	404	GOL	O1-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	412	MES	4	0
7	A	408	GOL	1	0
7	A	409	GOL	1	0
7	B	404	GOL	2	0
6	B	402	SO4	1	0
7	A	406	GOL	2	0
9	B	403	HEZ	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	368/395 (93%)	-0.03	14 (3%) 40 47	38, 51, 91, 126	0
1	B	184/395 (46%)	-0.09	12 (6%) 18 22	41, 58, 124, 141	0
2	C	19/19 (100%)	-0.33	0 100 100	42, 56, 84, 97	0
3	D	19/19 (100%)	-0.64	0 100 100	43, 51, 91, 96	0
All	All	590/828 (71%)	-0.08	26 (4%) 34 41	38, 53, 103, 141	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	LEU	7.3
1	B	280	ASN	4.6
1	B	260	VAL	4.1
1	B	294	LEU	3.7
1	A	15	LEU	3.6

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(\AA^2)	Q<0.9
7	GOL	A	407	6/6	0.84	0.26	71,76,93,95	0
7	GOL	A	408	6/6	0.85	0.24	56,64,78,89	0
9	HEZ	B	403	8/8	0.86	0.27	65,73,79,79	0
7	GOL	A	409	6/6	0.86	0.22	65,77,81,82	0
8	MES	A	412	12/12	0.88	0.28	48,74,89,96	12
7	GOL	D	101	6/6	0.88	0.24	59,76,78,80	0
7	GOL	D	102	6/6	0.90	0.22	67,70,85,92	0
6	SO4	A	410	5/5	0.90	0.22	64,66,74,82	5
7	GOL	A	411	6/6	0.91	0.37	76,78,82,91	0
7	GOL	A	406	6/6	0.92	0.13	66,73,81,91	0
7	GOL	B	404	6/6	0.92	0.35	64,72,76,90	0
6	SO4	A	405	5/5	0.92	0.21	57,68,72,80	5
6	SO4	B	402	5/5	0.96	0.20	78,78,90,97	0
7	GOL	C	101	6/6	0.97	0.14	49,52,60,70	0
6	SO4	A	404	5/5	0.99	0.17	66,71,88,106	0
5	MN	A	403	1/1	0.99	0.09	55,55,55,55	0
5	MN	B	401	1/1	1.00	0.13	58,58,58,58	0
5	MN	A	402	1/1	1.00	0.12	44,44,44,44	0
4	ZN	A	401	1/1	1.00	0.13	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.