wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 03:24 PM EDT

PDB ID	:	3C8H
Title	:	Crystal structure of the enterobactin esterase FES from Shigella flexneri in the presence of 2,3-Di-hydroxy-N-benzoyl-serine
Authors	:	Kim, Y.; Maltseva, N.; Abergel, R.; Holzle, D.; Raymond, K.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-02-12
Resolution	:	2.48 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:

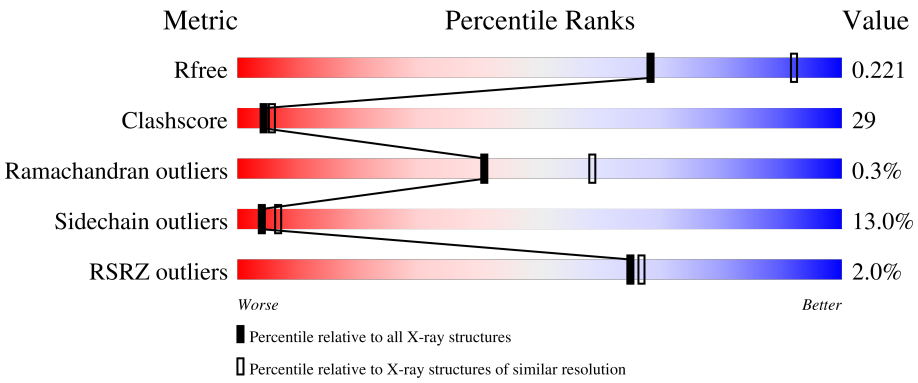
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	403	.% 53% 36% 5% 5%
1	B	403	3% 51% 35% 8% 5%
1	C	403	.% 43% 42% 9% 5%
1	D	403	2% 49% 39% 7% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12711 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 Enterochelin esterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	383	3091	1988	543	548	5	7	0	0	0
1	B	383	3090	1987	542	549	5	7	0	0	0
1	C	383	3091	1988	543	548	5	7	0	0	0
1	D	383	3106	1996	544	554	5	7	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q83SB9
A	-1	ASN	-	expression tag	UNP Q83SB9
A	0	ALA	-	expression tag	UNP Q83SB9
B	-2	SER	-	expression tag	UNP Q83SB9
B	-1	ASN	-	expression tag	UNP Q83SB9
B	0	ALA	-	expression tag	UNP Q83SB9
C	-2	SER	-	expression tag	UNP Q83SB9
C	-1	ASN	-	expression tag	UNP Q83SB9
C	0	ALA	-	expression tag	UNP Q83SB9
D	-2	SER	-	expression tag	UNP Q83SB9
D	-1	ASN	-	expression tag	UNP Q83SB9
D	0	ALA	-	expression tag	UNP Q83SB9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	80	80	80	0	0
2	B	85	85	85	0	0

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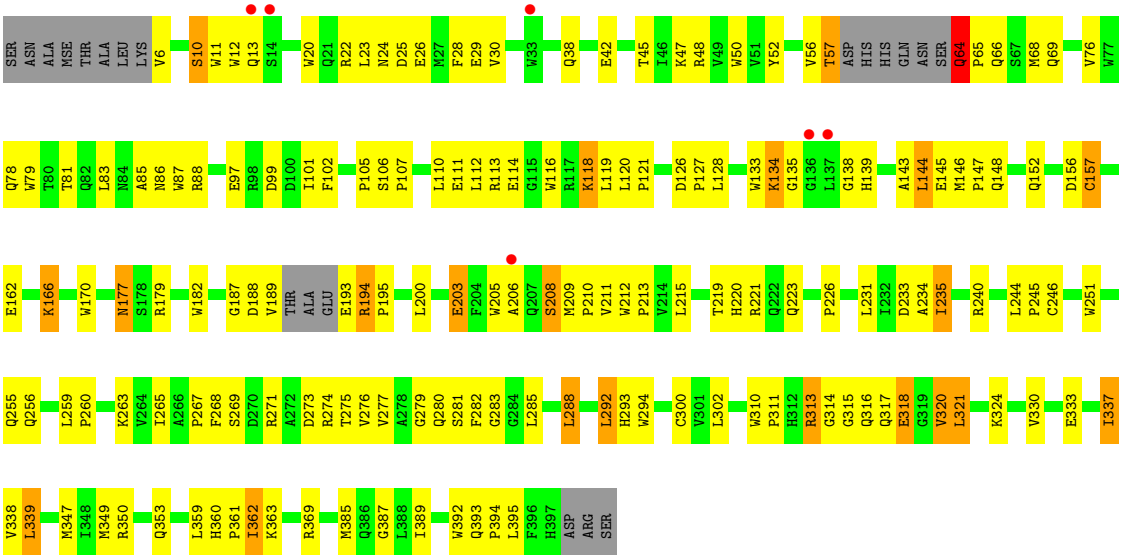
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	C	90	90	90	0	0
			Total	O		
2	D	78	78	78	0	0

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.

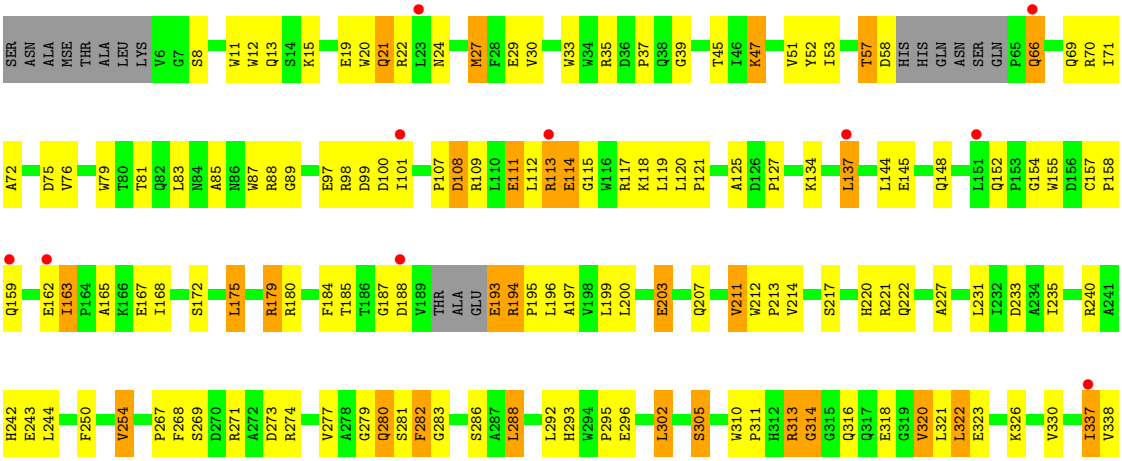
• Molecule 1: Enterochelin esterase

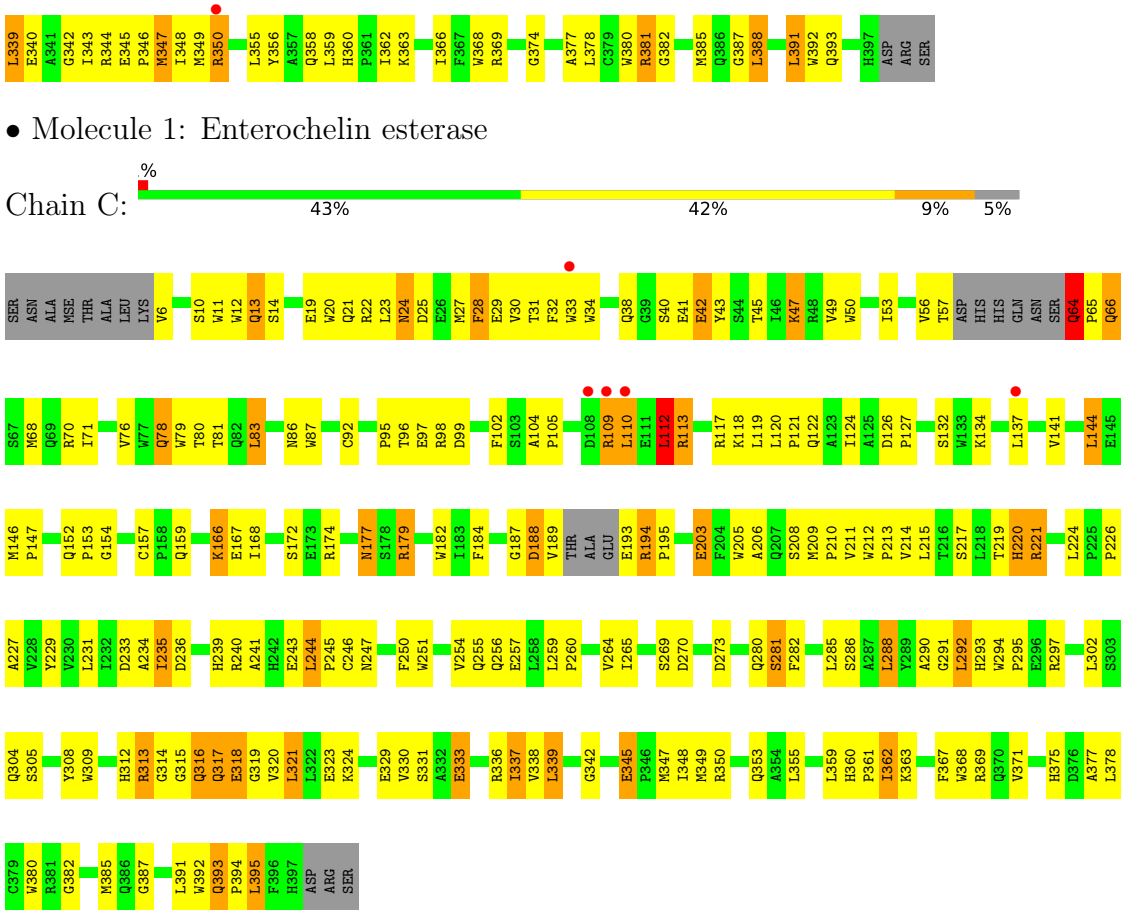
Chain A:



• Molecule 1: Enterochelin esterase

Chain B:



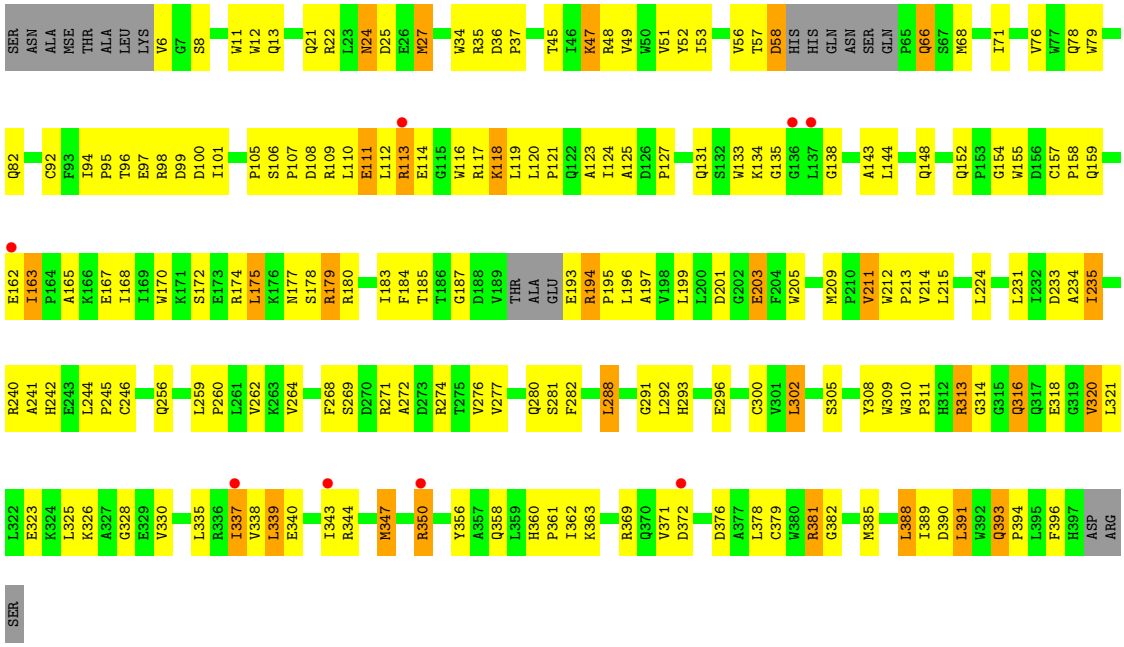


• Molecule 1: Enterochelin esterase

Chain C:

• Molecule 1: Enterochelin esterase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.51Å 48.78Å 156.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.23 – 2.48 47.23 – 2.48	Depositor EDS
% Data completeness (in resolution range)	94.2 (47.23-2.48) 94.2 (47.23-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.183 , 0.225 0.184 , 0.221	Depositor DCC
R_{free} test set	2889 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12711	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7823e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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)

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	0.49	1/3184 (0.0%)	0.57	1/4334 (0.0%)
1	B	0.46	0/3183	0.56	0/4332
1	C	0.48	0/3184	0.59	2/4334 (0.0%)
1	D	0.50	0/3198	0.59	0/4351
All	All	0.48	1/12749 (0.0%)	0.58	3/17351 (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	B	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	THR	C-O	7.07	1.36	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	GLN	N-CA-C	-5.89	95.10	111.00
1	C	64	GLN	N-CA-C	-5.36	96.53	111.00
1	C	112	LEU	CA-CB-CG	-5.16	103.42	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	314	GLY	Peptide
1	C	345	GLU	Peptide

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	3091	0	2996	173	1
1	B	3090	0	2993	179	0
1	C	3091	0	2996	207	1
1	D	3106	0	3004	196	0
2	A	80	0	0	14	0
2	B	85	0	0	9	0
2	C	90	0	0	7	0
2	D	78	0	0	8	0
All	All	12711	0	11989	710	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 29.

The worst 5 of 710 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:221:ARG:O	1:B:222:GLN:HG2	1.46	1.11
1:A:193:GLU:HB3	1:A:269:SER:HB2	1.35	1.08
1:B:152:GLN:OE1	1:B:381:ARG:HD2	1.53	1.06
1:D:337:ILE:HD11	1:D:339:LEU:HG	1.37	1.05
1:B:53:ILE:H	1:B:57:THR:HB	1.24	1.00

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)
1:A:157:CYS:SG	1:C:157:CYS:SG[2_645]	1.87	0.33

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	377/403 (94%)	358 (95%)	18 (5%)	1 (0%)	41	59
1	B	377/403 (94%)	361 (96%)	15 (4%)	1 (0%)	41	59
1	C	377/403 (94%)	358 (95%)	18 (5%)	1 (0%)	41	59
1	D	379/403 (94%)	355 (94%)	22 (6%)	2 (0%)	29	46
All	All	1510/1612 (94%)	1432 (95%)	73 (5%)	5 (0%)	41	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	235	ILE
1	A	235	ILE
1	D	235	ILE
1	B	235	ILE
1	D	105	PRO

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	324/333 (97%)	291 (90%)	33 (10%)	7	13
1	B	324/333 (97%)	277 (86%)	47 (14%)	3	5
1	C	324/333 (97%)	276 (85%)	48 (15%)	3	5
1	D	326/333 (98%)	286 (88%)	40 (12%)	4	8
All	All	1298/1332 (97%)	1130 (87%)	168 (13%)	4	7

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	313	ARG
1	D	168	ILE
1	C	320	VAL
1	D	24	ASN
1	D	277	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	255	GLN
1	D	256	GLN
1	C	38	GLN
1	D	242	HIS
1	D	66	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	376/403 (93%)	-0.12	6 (1%)	72	73	23, 58, 98, 118	5 (1%)
1	B	376/403 (93%)	-0.09	11 (2%)	51	54	27, 56, 94, 120	11 (2%)
1	C	376/403 (93%)	-0.33	5 (1%)	77	78	24, 49, 85, 119	5 (1%)
1	D	376/403 (93%)	-0.28	8 (2%)	63	65	17, 49, 93, 114	11 (2%)
All	All	1504/1612 (93%)	-0.21	30 (1%)	65	67	17, 53, 95, 120	32 (2%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	ILE	6.0
1	B	101	ILE	5.2
1	B	162	GLU	4.7
1	D	113	ARG	4.6
1	D	136	GLY	4.5

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.