Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 04:39 PM EDT

PDB ID	:	4IT5
Title	:	Chaperone HscB from Vibrio cholerae
Authors	:	Osipiuk, J.; Gu, M.; Papazisi, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2013-01-17
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

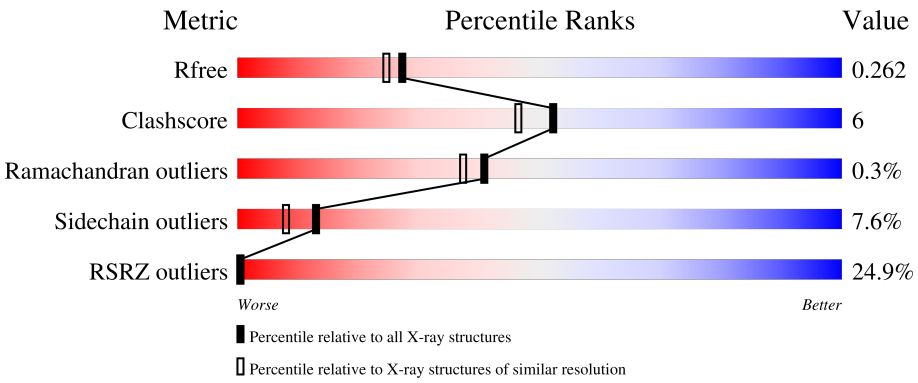
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	174	20% 82% 11% • 6%
1	B	174	24% 75% 20% • •
1	C	174	17% 78% 14% • 6%
1	D	174	31% 74% 22% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5469 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 Co-chaperone protein HscB homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	164	1326	838	228	252	1	7	0	0	0
1	B	169	1365	861	235	262	1	6	0	0	0
1	C	163	1317	833	226	250	1	7	0	0	0
1	D	169	1365	861	235	262	1	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q9KTX9
A	-1	ASN	-	EXPRESSION TAG	UNP Q9KTX9
A	0	ALA	-	EXPRESSION TAG	UNP Q9KTX9
B	-2	SER	-	EXPRESSION TAG	UNP Q9KTX9
B	-1	ASN	-	EXPRESSION TAG	UNP Q9KTX9
B	0	ALA	-	EXPRESSION TAG	UNP Q9KTX9
C	-2	SER	-	EXPRESSION TAG	UNP Q9KTX9
C	-1	ASN	-	EXPRESSION TAG	UNP Q9KTX9
C	0	ALA	-	EXPRESSION TAG	UNP Q9KTX9
D	-2	SER	-	EXPRESSION TAG	UNP Q9KTX9
D	-1	ASN	-	EXPRESSION TAG	UNP Q9KTX9
D	0	ALA	-	EXPRESSION TAG	UNP Q9KTX9

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	C	1	1	1	0	0
			Total	Ca		
2	D	2	2	2	0	0

- Molecule 3 is water.

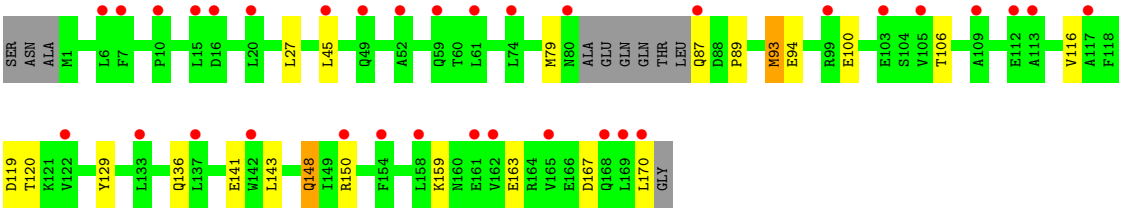
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	26	26	26	0	0
			Total	O		
3	B	15	15	15	0	0
			Total	O		
3	C	36	36	36	0	0
			Total	O		
3	D	14	14	14	0	0

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.

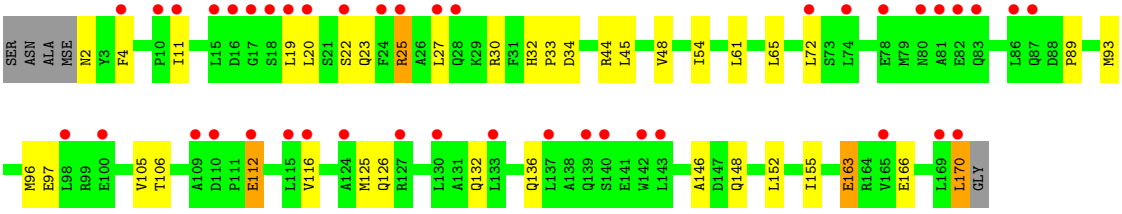
• Molecule 1: Co-chaperone protein HscB homolog

Chain A:



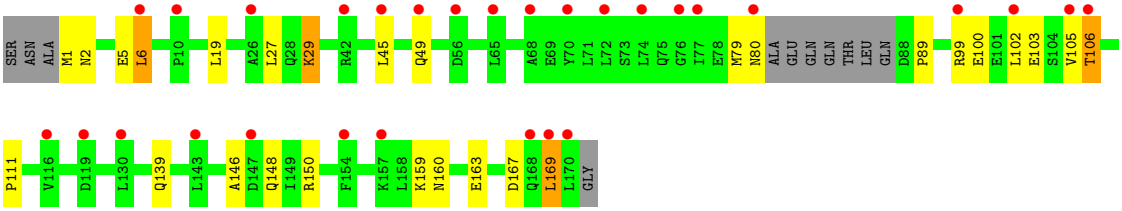
• Molecule 1: Co-chaperone protein HscB homolog

Chain B:



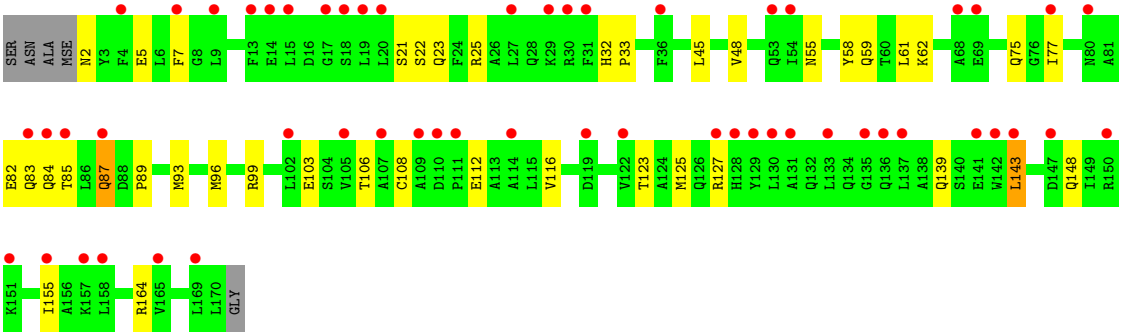
• Molecule 1: Co-chaperone protein HscB homolog

Chain C:



• Molecule 1: Co-chaperone protein HscB homolog

Chain D:


SER ASN ALA MSE N2 Y3 F4 E5 L6 F7 G8 L9 F13 E14 L15 D16 G17 S18 L19 L20 S21 S22 Q23 F24 R25 A26 L27 Q28 K29 R30 F31 H32 P33 F36 L45 V48 Q53 I54 N55 Y58 Q59 T60 L61 K62 A68 E69 Q75 G76 I77 N80 A81
E82 Q83 Q84 T85 L86 Q87 D88 P89 M93 M96 R99 L102 E103 S104 V105 T106 A107 C108 A109 D110 P111 E112 A113 A114 L115 V116 D119 V122 T123 A124 M125 Q126 R127 H128 Y129 L130 A131 Q132 L133 Q134 G135 Q136 L137 A138 Q139 S140 E141 W142 L143 D147 Q148 I149 R150
K151 I155 A156 K157 L158 R164 V165 L169 L170 GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.43Å 100.71Å 70.35Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	48.56 – 2.15 48.56 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.56-2.15) 96.9 (48.56-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.220 , 0.259 0.222 , 0.262	Depositor DCC
R_{free} test set	2099 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.439 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5469	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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: CA

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	0.26	0/1340	0.40	0/1794
1	B	0.25	0/1380	0.40	0/1851
1	C	0.26	0/1331	0.41	0/1782
1	D	0.25	0/1380	0.42	0/1851
All	All	0.26	0/5431	0.41	0/7278

There are no bond length outliers.

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	1326	0	1317	14	0
1	B	1365	0	1351	22	0
1	C	1317	0	1309	12	0
1	D	1365	0	1351	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	26	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	4	0
3	C	36	0	0	1	0
3	D	14	0	0	0	0
All	All	5469	0	5328	59	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 6.

All (59) 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:A:170:LEU:HD11	1:B:163:GLU:HG3	1.62	0.80
1:B:163:GLU:OE2	3:B:315:HOH:O	2.00	0.77
1:C:1:MSE:HE3	1:C:6:LEU:HD12	1.72	0.71
1:A:136:GLN:HB2	1:A:141:GLU:HB2	1.73	0.69
1:B:45:LEU:HD22	1:D:89:PRO:HB2	1.77	0.67
1:A:159:LYS:NZ	1:A:163:GLU:OE2	2.28	0.67
1:B:89:PRO:HB2	1:D:45:LEU:HD22	1.76	0.65
1:D:125:MSE:HE2	1:D:155:ILE:HD11	1.82	0.62
1:B:166:GLU:HG2	1:B:170:LEU:HD23	1.82	0.61
1:B:125:MSE:HE2	1:B:155:ILE:HD11	1.83	0.59
1:A:163:GLU:OE1	3:B:315:HOH:O	2.16	0.58
1:D:21:SER:O	1:D:25:ARG:HG3	2.06	0.55
1:A:45:LEU:HD22	1:C:89:PRO:HB2	1.87	0.55
1:D:55:ASN:O	1:D:59:GLN:HG2	2.06	0.55
1:A:129:TYR:HD1	1:A:148:GLN:HE21	1.54	0.54
1:A:79:MSE:HE3	1:A:150:ARG:HH12	1.73	0.54
1:B:33:PRO:HG2	1:D:96:MSE:SE	2.57	0.54
1:A:167:ASP:OD2	3:A:421:HOH:O	2.18	0.54
1:A:119:ASP:OD2	3:A:423:HOH:O	2.19	0.53
1:B:65:LEU:HD11	1:B:152:LEU:HB3	1.91	0.53
1:C:167:ASP:OD2	3:C:314:HOH:O	2.19	0.53
1:C:159:LYS:NZ	1:C:163:GLU:OE2	2.42	0.52
1:D:7:PHE:O	1:D:23:GLN:HG3	2.11	0.50
1:A:116:VAL:O	1:A:120:THR:HG23	2.11	0.50
1:B:27:LEU:HB3	1:B:54:ILE:HD13	1.93	0.50
1:A:79:MSE:HE2	1:A:150:ARG:HH22	1.77	0.49
1:B:126:GLN:HB2	1:B:155:ILE:HG21	1.95	0.48
1:D:112:GLU:O	1:D:116:VAL:HG23	2.13	0.48
1:D:82:GLU:O	1:D:85:THR:HG22	2.13	0.48
1:C:2:ASN:ND2	1:C:5:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:THR:O	1:C:106:THR:OG1	2.26	0.47
1:D:2:ASN:HB3	1:D:5:GLU:HG3	1.97	0.47
1:B:22:SER:HA	1:B:25:ARG:HD2	1.96	0.46
1:B:132:GLN:O	1:B:136:GLN:HG2	2.16	0.46
1:B:2:ASN:OD1	1:B:4:PHE:N	2.48	0.46
1:A:93:MSE:HE2	1:A:93:MSE:HB2	1.81	0.45
1:C:102:LEU:O	1:C:105:VAL:HG22	2.16	0.45
1:A:89:PRO:HB2	1:C:45:LEU:HD22	1.98	0.45
1:B:163:GLU:HG2	3:B:306:HOH:O	2.16	0.45
1:A:79:MSE:HB3	1:A:150:ARG:HH12	1.81	0.44
1:B:93:MSE:HG2	1:D:48:VAL:HG21	1.98	0.44
1:C:99:ARG:NH2	1:C:103:GLU:OE1	2.51	0.44
1:C:146:ALA:O	1:C:150:ARG:HG2	2.17	0.44
1:B:48:VAL:HG21	1:D:93:MSE:HG3	1.99	0.43
1:D:123:THR:HG22	1:D:127:ARG:HD3	1.99	0.43
1:C:111:PRO:HB2	1:C:169:LEU:HD21	2.00	0.43
1:D:84:GLN:O	1:D:87:GLN:HB3	2.19	0.43
1:B:32:HIS:CE1	1:B:34:ASP:HB2	2.54	0.43
1:B:112:GLU:O	1:B:116:VAL:HG23	2.19	0.42
1:D:75:GLN:HB2	1:D:77:ILE:HG13	2.00	0.42
1:B:166:GLU:OE1	3:B:315:HOH:O	2.22	0.41
1:D:58:TYR:OH	1:D:62:LYS:NZ	2.52	0.41
1:B:72:LEU:HD21	1:B:146:ALA:HB2	2.02	0.41
1:D:82:GLU:HG2	1:D:83:GLN:N	2.36	0.41
1:C:29:LYS:NZ	1:C:29:LYS:HB2	2.36	0.41
1:D:99:ARG:O	1:D:103:GLU:HG2	2.21	0.41
1:B:96:MSE:SE	1:D:33:PRO:HG2	2.71	0.40
1:D:143:LEU:HD23	1:D:143:LEU:HA	1.94	0.40
1:B:44:ARG:O	1:B:48:VAL:HG23	2.22	0.40

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	160/174 (92%)	157 (98%)	3 (2%)	0	100	100
1	B	167/174 (96%)	163 (98%)	3 (2%)	1 (1%)	25	18
1	C	159/174 (91%)	153 (96%)	5 (3%)	1 (1%)	25	18
1	D	167/174 (96%)	163 (98%)	4 (2%)	0	100	100
All	All	653/696 (94%)	636 (97%)	15 (2%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	169	LEU
1	B	19	LEU

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	140/140 (100%)	132 (94%)	8 (6%)	20	16
1	B	144/140 (103%)	131 (91%)	13 (9%)	9	5
1	C	139/140 (99%)	127 (91%)	12 (9%)	10	6
1	D	144/140 (103%)	134 (93%)	10 (7%)	15	10
All	All	567/560 (101%)	524 (92%)	43 (8%)	13	8

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	87	GLN
1	A	93	MSE
1	A	94	GLU
1	A	100	GLU
1	A	106	THR
1	A	143	LEU
1	A	148	GLN
1	B	11	ILE

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Mol	Chain	Res	Type
1	B	20	LEU
1	B	23	GLN
1	B	25	ARG
1	B	30	ARG
1	B	61	LEU
1	B	97	GLU
1	B	105	VAL
1	B	106	THR
1	B	112	GLU
1	B	148	GLN
1	B	163	GLU
1	B	170	LEU
1	C	6	LEU
1	C	19	LEU
1	C	27	LEU
1	C	29	LYS
1	C	49	GLN
1	C	79	MSE
1	C	80	ASN
1	C	100	GLU
1	C	106	THR
1	C	139	GLN
1	C	148	GLN
1	C	160	ASN
1	D	22	SER
1	D	32	HIS
1	D	61	LEU
1	D	87	GLN
1	D	106	THR
1	D	108	CYS
1	D	139	GLN
1	D	143	LEU
1	D	148	GLN
1	D	164	ARG

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 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	157/174 (90%)	1.35	34 (21%)	0	0	32, 52, 80, 97	0
1	B	163/174 (93%)	1.58	42 (25%)	0	0	37, 66, 105, 113	0
1	C	156/174 (89%)	1.30	29 (18%)	1	1	32, 52, 75, 94	0
1	D	163/174 (93%)	1.64	54 (33%)	0	0	37, 65, 100, 119	0
All	All	639/696 (91%)	1.47	159 (24%)	0	0	32, 58, 95, 119	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	PHE	8.2
1	D	15	LEU	7.0
1	D	13	PHE	6.4
1	B	82	GLU	6.2
1	B	170	LEU	5.7
1	B	109	ALA	5.6
1	D	9	LEU	5.2
1	D	111	PRO	5.1
1	C	77	ILE	5.1
1	A	169	LEU	4.9
1	D	7	PHE	4.8
1	B	15	LEU	4.6
1	D	142	TRP	4.5
1	B	83	GLN	4.4
1	D	77	ILE	4.4
1	D	137	LEU	4.1
1	A	45	LEU	3.9
1	B	22	SER	3.8
1	C	168	GLN	3.8
1	B	25	ARG	3.8
1	C	170	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	16	ASP	3.7
1	D	169	LEU	3.6
1	B	139	GLN	3.6
1	D	109	ALA	3.6
1	A	74	LEU	3.6
1	A	80	ASN	3.5
1	B	72	LEU	3.5
1	A	105	VAL	3.5
1	B	110	ASP	3.5
1	D	80	ASN	3.4
1	D	110	ASP	3.4
1	D	141	GLU	3.4
1	D	135	GLY	3.4
1	C	70	TYR	3.3
1	A	109	ALA	3.3
1	C	80	ASN	3.3
1	B	20	LEU	3.3
1	D	83	GLN	3.3
1	B	18	SER	3.3
1	B	133	LEU	3.3
1	B	165	VAL	3.2
1	A	142	TRP	3.2
1	D	127	ARG	3.2
1	A	112	GLU	3.1
1	B	137	LEU	3.1
1	A	6	LEU	3.1
1	B	80	ASN	3.1
1	D	29	LYS	3.0
1	D	31	PHE	3.0
1	B	86	LEU	3.0
1	B	112	GLU	3.0
1	C	102	LEU	3.0
1	D	19	LEU	3.0
1	D	30	ARG	2.9
1	B	142	TRP	2.9
1	D	165	VAL	2.8
1	B	78	GLU	2.8
1	B	130	LEU	2.8
1	A	7	PHE	2.8
1	B	81	ALA	2.8
1	C	130	LEU	2.8
1	C	116	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	154	PHE	2.7
1	B	127	ARG	2.7
1	D	158	LEU	2.7
1	A	122	VAL	2.7
1	B	169	LEU	2.7
1	A	117	ALA	2.7
1	A	168	GLN	2.7
1	B	27	LEU	2.7
1	D	102	LEU	2.7
1	A	87	GLN	2.6
1	C	169	LEU	2.6
1	D	87	GLN	2.6
1	B	74	LEU	2.6
1	C	105	VAL	2.6
1	C	6	LEU	2.6
1	C	157	LYS	2.6
1	D	136	GLN	2.6
1	C	68	ALA	2.5
1	D	151	LYS	2.5
1	A	133	LEU	2.5
1	A	52	ALA	2.5
1	B	11	ILE	2.5
1	A	61	LEU	2.5
1	C	65	LEU	2.5
1	D	4	PHE	2.5
1	A	99	ARG	2.4
1	D	84	GLN	2.4
1	D	54	ILE	2.4
1	B	24	PHE	2.4
1	D	85	THR	2.4
1	A	15	LEU	2.4
1	A	20	LEU	2.4
1	D	129	TYR	2.4
1	B	143	LEU	2.4
1	B	17	GLY	2.4
1	D	119	ASP	2.4
1	D	143	LEU	2.4
1	B	115	LEU	2.4
1	D	17	GLY	2.4
1	A	165	VAL	2.3
1	D	105	VAL	2.3
1	C	76	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	161	GLU	2.3
1	B	87	GLN	2.3
1	C	72	LEU	2.3
1	C	42	ARG	2.3
1	D	128	HIS	2.3
1	C	143	LEU	2.3
1	C	56	ASP	2.3
1	C	26	ALA	2.3
1	C	74	LEU	2.3
1	D	114	ALA	2.3
1	A	16	ASP	2.3
1	D	147	ASP	2.3
1	D	53	GLN	2.3
1	C	119	ASP	2.2
1	B	19	LEU	2.2
1	C	45	LEU	2.2
1	D	107	ALA	2.2
1	D	130	LEU	2.2
1	C	154	PHE	2.2
1	D	122	VAL	2.2
1	A	10	PRO	2.2
1	C	10	PRO	2.2
1	D	150	ARG	2.2
1	D	36	PHE	2.2
1	A	59	GLN	2.2
1	A	162	VAL	2.2
1	B	124	ALA	2.2
1	A	158	LEU	2.1
1	C	147	ASP	2.1
1	C	99	ARG	2.1
1	D	69	GLU	2.1
1	B	98	LEU	2.1
1	D	27	LEU	2.1
1	D	133	LEU	2.1
1	A	113	ALA	2.1
1	B	10	PRO	2.1
1	A	150	ARG	2.1
1	A	103	GLU	2.1
1	B	116	VAL	2.1
1	C	49	GLN	2.1
1	D	155	ILE	2.1
1	D	18	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	157	LYS	2.1
1	A	49	GLN	2.0
1	A	137	LEU	2.0
1	A	170	LEU	2.0
1	D	20	LEU	2.0
1	D	68	ALA	2.0
1	C	106	THR	2.0
1	D	14	GLU	2.0
1	B	140	SER	2.0
1	B	100	GLU	2.0
1	D	131	ALA	2.0
1	B	28	GLN	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 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
2	CA	B	201	1/1	0.68	0.13	60,60,60,60	0
2	CA	D	201	1/1	0.88	0.09	61,61,61,61	0
2	CA	D	202	1/1	0.92	0.12	55,55,55,55	0
2	CA	A	301	1/1	0.95	0.06	62,62,62,62	0
2	CA	C	201	1/1	0.97	0.10	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.