Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 04:55 PM EDT

PDB ID	:	7L4S
Title	:	Crystal structure of the OxyR regulatory domain of Shewanella oneidensis MR-1, reduced form
Authors	:	Tao, Y.J.; Gao, H.
Deposited on	:	2020-12-21
Resolution	:	2.40 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 ⓘ 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 ⓘ) were used in the production of this report:

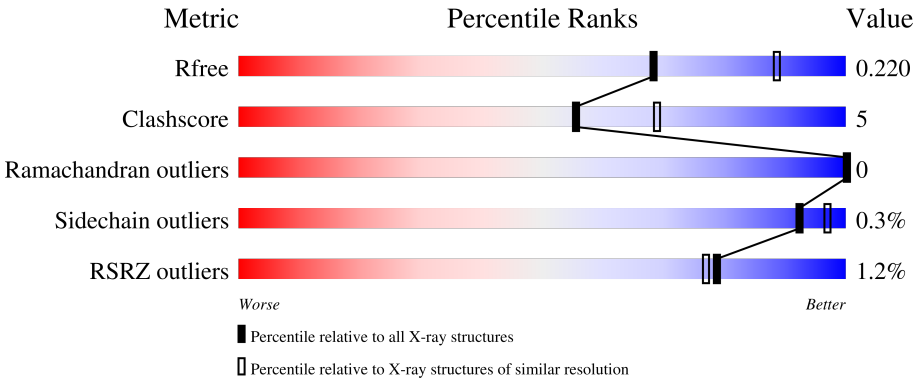
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	304	62% 6% 32%
1	B	304	56% 9% 35%
1	C	304	59% 7% 33%
1	D	304	55% 10% 35%
1	E	304	58% 8% 35%

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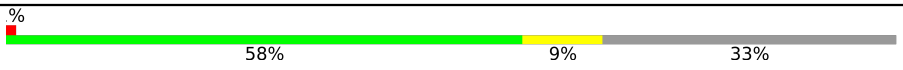
Mol	Chain	Length	Quality of chain
1	F	304	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9621 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 Transcriptional regulator of oxidative stress OxyR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1589	1018	264	297	10			
1	B	199	Total	C	N	O	S	0	0	0
			1532	982	253	287	10			
1	C	203	Total	C	N	O	S	0	0	0
			1560	1000	257	293	10			
1	D	197	Total	C	N	O	S	0	0	0
			1512	969	250	283	10			
1	E	198	Total	C	N	O	S	0	0	0
			1520	972	253	285	10			
1	F	204	Total	C	N	O	S	0	0	0
			1571	1006	259	296	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	SER	CYS	engineered mutation	UNP Q8EHA1
B	203	SER	CYS	engineered mutation	UNP Q8EHA1
C	203	SER	CYS	engineered mutation	UNP Q8EHA1
D	203	SER	CYS	engineered mutation	UNP Q8EHA1
E	203	SER	CYS	engineered mutation	UNP Q8EHA1
F	203	SER	CYS	engineered mutation	UNP Q8EHA1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	60	Total	O	0	0
			60	60		
2	B	60	Total	O	0	0
			60	60		
2	C	65	Total	O	0	0
			65	65		

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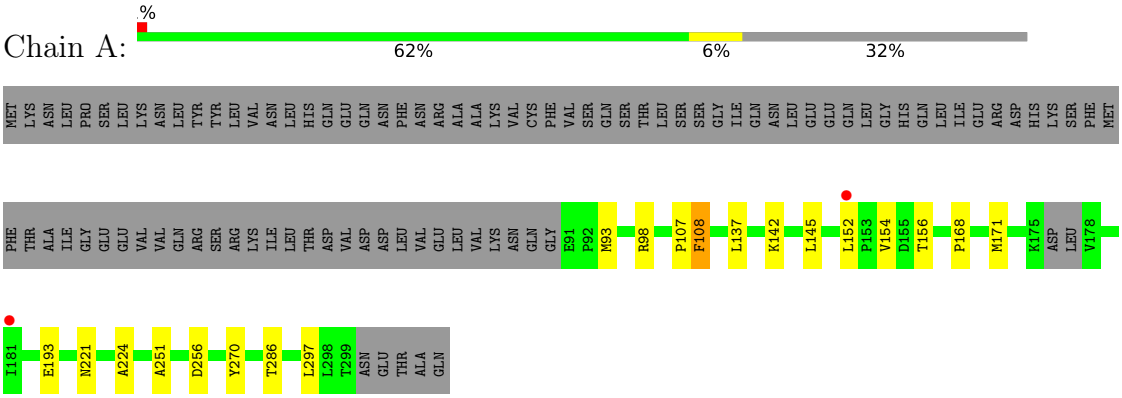
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	41	Total O 41 41	0	0
2	E	57	Total O 57 57	0	0
2	F	54	Total O 54 54	0	0

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.

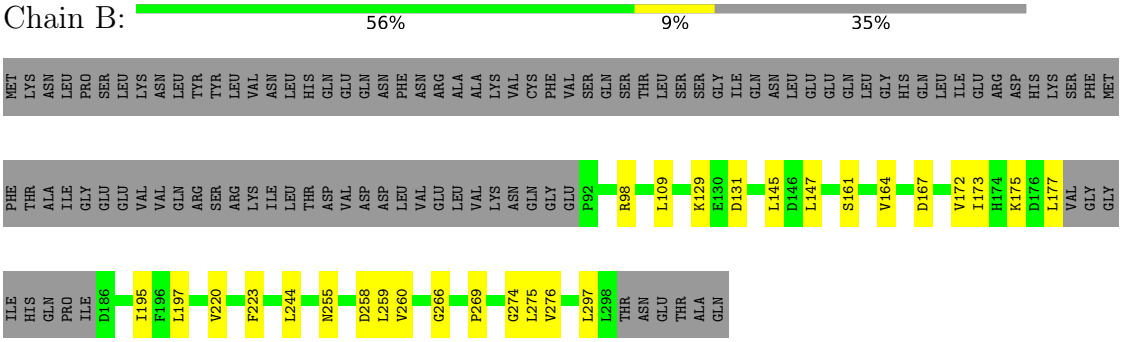
• Molecule 1: Transcriptional regulator of oxidative stress OxyR

Chain A:



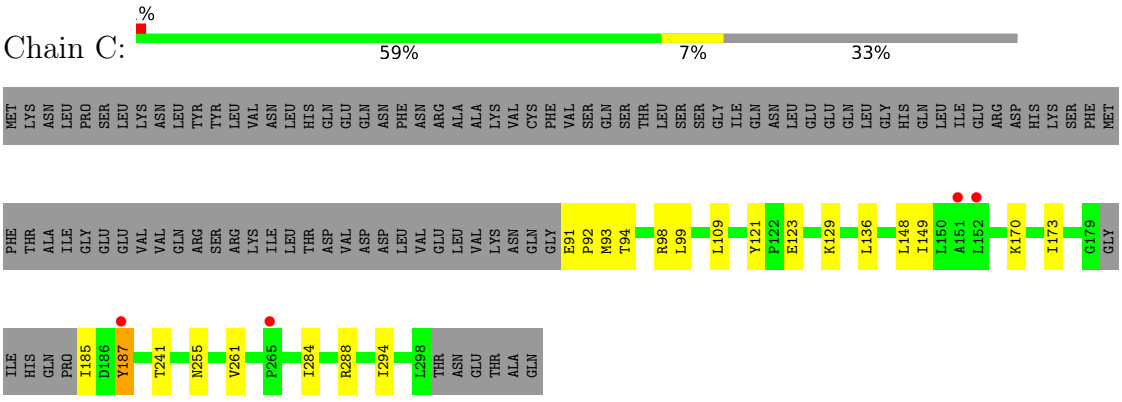
• Molecule 1: Transcriptional regulator of oxidative stress OxyR

Chain B:



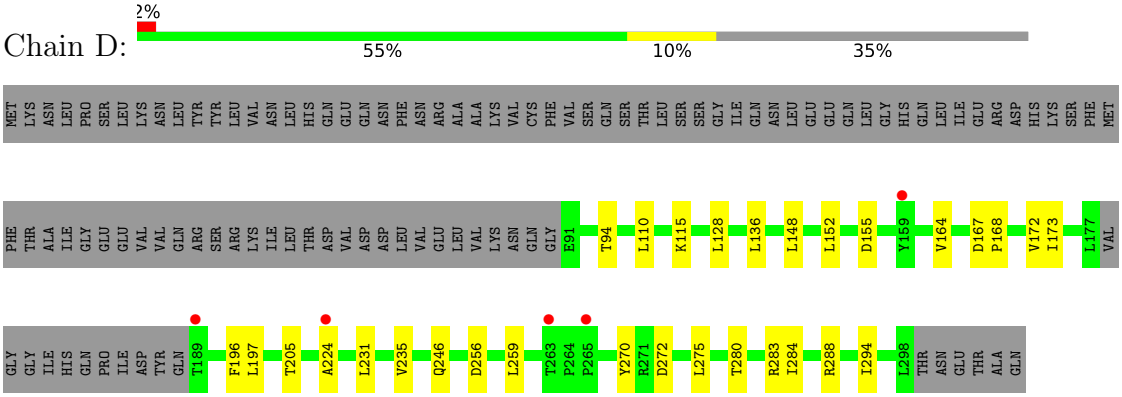
• Molecule 1: Transcriptional regulator of oxidative stress OxyR

Chain C:



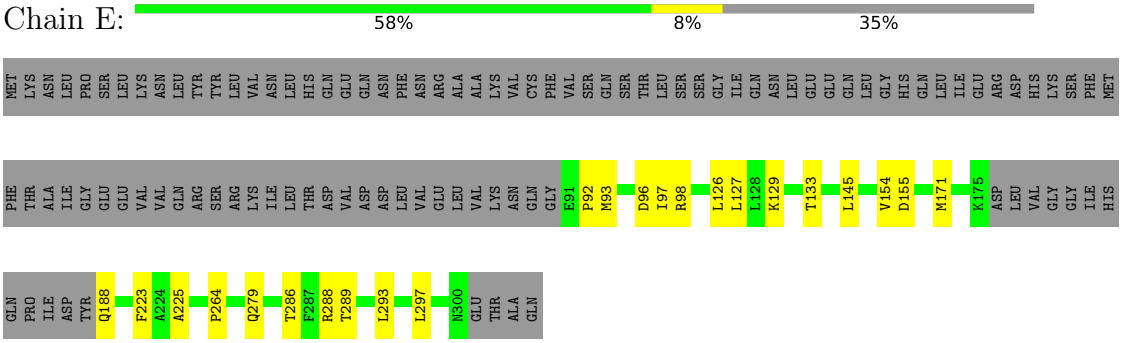
• Molecule 1: Transcriptional regulator of oxidative stress OxyR

Chain D:



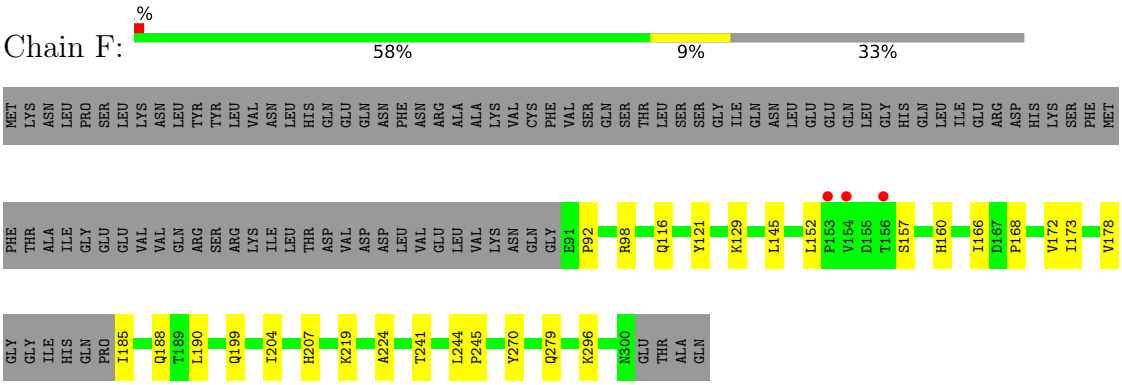
• Molecule 1: Transcriptional regulator of oxidative stress OxyR

Chain E:



• Molecule 1: Transcriptional regulator of oxidative stress OxyR

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	84.00Å 84.00Å 185.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.00 – 2.40 42.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.00-2.40) 97.9 (42.00-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.174 , 0.222 0.175 , 0.220	Depositor DCC
R_{free} test set	2828 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 23.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.117 for -h,-k,l 0.435 for h,-h-k,-l 0.118 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9621	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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

5.1 Standard geometry

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	0.32	0/1618	0.58	0/2200
1	B	0.31	0/1559	0.57	0/2118
1	C	0.35	0/1587	0.59	1/2157 (0.0%)
1	D	0.30	0/1538	0.56	0/2090
1	E	0.29	0/1546	0.55	1/2101 (0.0%)
1	F	0.31	0/1598	0.55	0/2173
All	All	0.31	0/9446	0.57	2/12839 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	187	TYR	CA-CB-CG	5.36	123.59	113.40
1	E	293	LEU	CB-CG-CD2	5.16	119.77	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1589	0	1641	17	0
1	B	1532	0	1585	18	0
1	C	1560	0	1613	15	0
1	D	1512	0	1569	19	0
1	E	1520	0	1575	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1571	0	1623	20	0
2	A	60	0	0	2	0
2	B	60	0	0	0	0
2	C	65	0	0	4	0
2	D	41	0	0	1	0
2	E	57	0	0	4	0
2	F	54	0	0	3	0
All	All	9621	0	9606	97	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 (97) 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:F:173:ILE:HD13	1:F:241:THR:HG22	1.76	0.68
1:D:197:LEU:HD23	1:D:205:THR:HG23	1.80	0.64
1:D:280:THR:HG22	1:F:166:ILE:HD13	1.82	0.61
1:E:188:GLN:N	2:E:406:HOH:O	2.34	0.60
1:E:92:PRO:O	1:E:286:THR:OG1	2.20	0.59
1:C:185:ILE:N	2:C:406:HOH:O	2.36	0.58
1:A:193:GLU:O	1:A:221:ASN:ND2	2.29	0.57
1:C:98:ARG:NH2	2:C:408:HOH:O	2.38	0.56
1:F:116:GLN:OE1	1:F:296:LYS:NZ	2.37	0.56
1:B:129:LYS:HD3	1:B:145:LEU:HD11	1.89	0.55
1:D:110:LEU:HD21	1:D:128:LEU:HD22	1.89	0.55
1:D:136:LEU:HB3	1:D:148:LEU:HD22	1.90	0.54
1:A:107:PRO:HB2	1:A:108:PHE:CE1	2.43	0.54
1:D:275:LEU:HD21	1:D:294:ILE:HD12	1.88	0.53
1:B:255:ASN:ND2	1:D:256:ASP:OD2	2.41	0.53
1:A:256:ASP:OD2	1:C:255:ASN:ND2	2.42	0.53
1:D:167:ASP:N	1:D:167:ASP:OD1	2.42	0.52
1:B:167:ASP:OD2	1:B:167:ASP:N	2.41	0.52
1:C:91:GLU:N	2:C:411:HOH:O	2.43	0.52
1:B:266:GLY:HA2	1:B:269:PRO:HG3	1.92	0.51
1:B:164:VAL:HG22	1:B:274:GLY:HA2	1.93	0.51
1:D:168:PRO:HA	1:D:270:TYR:HA	1.91	0.51
1:F:190:LEU:O	1:F:219:LYS:NZ	2.42	0.51
1:B:129:LYS:HE2	1:B:131:ASP:HB2	1.93	0.50
1:D:172:VAL:HG23	1:D:235:VAL:HG11	1.92	0.50
1:D:152:LEU:HB2	1:D:272:ASP:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:PHE:CD2	1:E:225:ALA:HB2	2.48	0.49
1:B:172:VAL:HG11	1:B:244:LEU:HD12	1.94	0.49
1:E:98:ARG:HB3	1:E:145:LEU:HD23	1.94	0.49
1:F:129:LYS:HD3	1:F:145:LEU:HD11	1.94	0.49
1:B:109:LEU:HD11	1:B:297:LEU:HB3	1.95	0.48
1:A:93:MET:SD	1:A:286:THR:HA	2.54	0.48
1:C:173:ILE:HD13	1:C:241:THR:HG22	1.95	0.48
1:A:171:MET:N	2:A:401:HOH:O	2.32	0.48
1:E:289:THR:HG23	1:F:92:PRO:HG2	1.96	0.47
1:D:164:VAL:HG11	1:D:275:LEU:HD23	1.97	0.47
1:C:99:LEU:HD11	1:C:149:ILE:HG13	1.95	0.47
1:D:224:ALA:O	2:D:401:HOH:O	2.20	0.47
1:E:288:ARG:NH1	2:E:410:HOH:O	2.39	0.46
1:F:188:GLN:NE2	2:F:411:HOH:O	2.46	0.46
1:E:93:MET:HB2	1:F:121:TYR:HE1	1.81	0.46
1:A:193:GLU:HB3	1:A:221:ASN:HA	1.98	0.46
1:A:193:GLU:N	2:A:413:HOH:O	2.47	0.46
1:B:195:ILE:HB	1:B:220:VAL:HA	1.98	0.46
1:C:109:LEU:HD21	1:C:294:ILE:HG23	1.98	0.45
1:E:133:THR:HG21	1:E:154:VAL:HG21	1.97	0.45
1:A:152:LEU:O	1:A:154:VAL:N	2.48	0.45
1:A:98:ARG:HB3	1:A:145:LEU:HD23	1.98	0.45
1:B:98:ARG:NE	1:E:155:ASP:OD1	2.49	0.45
1:F:204:ILE:HD11	1:F:245:PRO:HD3	1.99	0.45
1:B:172:VAL:HA	1:B:260:VAL:O	2.16	0.45
1:F:168:PRO:HA	1:F:270:TYR:HA	1.98	0.45
1:B:147:LEU:HD11	1:B:275:LEU:HB3	1.98	0.44
1:B:173:ILE:HD11	1:B:177:LEU:HD22	1.98	0.44
1:C:170:LYS:HB3	1:C:261:VAL:HG13	1.99	0.44
1:E:96:ASP:HB3	1:E:127:LEU:HD11	2.00	0.44
1:A:224:ALA:HB3	1:C:129:LYS:HG3	2.00	0.44
1:F:173:ILE:HG23	1:F:178:VAL:HG22	2.00	0.44
1:A:107:PRO:HB2	1:A:108:PHE:CD1	2.53	0.44
1:F:157:SER:N	2:F:415:HOH:O	2.50	0.44
1:A:168:PRO:HA	1:A:270:TYR:HA	1.99	0.44
1:B:175:LYS:HG2	1:B:258:ASP:HB3	2.00	0.44
1:C:284:ILE:HD11	1:C:288:ARG:HH21	1.83	0.44
1:D:173:ILE:O	1:D:259:LEU:HA	2.18	0.43
1:C:136:LEU:HB3	1:C:148:LEU:HD22	1.99	0.43
1:F:185:ILE:N	2:F:416:HOH:O	2.51	0.43
1:A:137:LEU:HD21	1:A:156:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:HG2	1:F:160:HIS:CD2	2.54	0.43
1:C:93:MET:HB3	1:C:121:TYR:HB3	2.01	0.43
1:D:94:THR:O	1:D:283:ARG:NH1	2.45	0.43
1:F:199:GLN:HG2	1:F:224:ALA:HB1	1.99	0.43
1:D:196:PHE:HB3	1:D:231:LEU:HD22	2.00	0.42
1:B:173:ILE:O	1:B:259:LEU:HA	2.19	0.42
1:C:91:GLU:HA	1:C:92:PRO:HD2	1.90	0.42
1:E:97:ILE:HG23	1:E:126:LEU:HD23	2.01	0.42
1:F:296:LYS:HE3	1:F:296:LYS:HB3	1.84	0.42
1:E:129:LYS:NZ	2:E:409:HOH:O	2.36	0.42
1:A:108:PHE:HD2	1:A:251:ALA:HB3	1.85	0.42
1:D:284:ILE:HD11	1:D:288:ARG:HE	1.84	0.42
1:F:160:HIS:HB2	1:F:279:GLN:OE1	2.19	0.42
1:E:279:GLN:HE21	1:E:279:GLN:HB3	1.64	0.41
1:F:98:ARG:HB3	1:F:145:LEU:HD23	2.02	0.41
1:D:115:LYS:HD2	1:D:115:LYS:HA	1.79	0.41
1:D:167:ASP:HB2	1:D:246:GLN:HB3	2.01	0.41
1:C:170:LYS:NZ	2:C:415:HOH:O	2.52	0.41
1:B:195:ILE:HG22	1:B:197:LEU:HG	2.03	0.41
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.90	0.41
1:F:172:VAL:HG11	1:F:244:LEU:HD12	2.03	0.41
1:D:155:ASP:N	1:D:155:ASP:OD1	2.54	0.41
1:E:98:ARG:NH2	2:E:414:HOH:O	2.54	0.41
1:F:152:LEU:HB3	1:F:207:HIS:CE1	2.56	0.41
1:A:108:PHE:CD1	1:A:108:PHE:N	2.89	0.41
1:E:297:LEU:HD23	1:E:297:LEU:HA	1.94	0.40
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.95	0.40
1:C:94:THR:HG23	1:C:123:GLU:HB3	2.02	0.40
1:E:171:MET:HG3	1:E:264:PRO:HB3	2.02	0.40
1:B:161:SER:HB3	1:B:276:VAL:HG22	2.03	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	203/304 (67%)	192 (95%)	11 (5%)	0	100	100
1	B	195/304 (64%)	192 (98%)	3 (2%)	0	100	100
1	C	199/304 (66%)	191 (96%)	8 (4%)	0	100	100
1	D	193/304 (64%)	184 (95%)	9 (5%)	0	100	100
1	E	194/304 (64%)	186 (96%)	8 (4%)	0	100	100
1	F	200/304 (66%)	190 (95%)	10 (5%)	0	100	100
All	All	1184/1824 (65%)	1135 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	180/269 (67%)	179 (99%)	1 (1%)	86	94
1	B	174/269 (65%)	173 (99%)	1 (1%)	86	94
1	C	177/269 (66%)	176 (99%)	1 (1%)	86	94
1	D	172/269 (64%)	172 (100%)	0	100	100
1	E	173/269 (64%)	173 (100%)	0	100	100
1	F	179/269 (66%)	179 (100%)	0	100	100
All	All	1055/1614 (65%)	1052 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	PHE
1	B	223	PHE
1	C	187	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	C	199	GLN
1	C	213	GLN
1	E	279	GLN
1	F	188	GLN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	207/304 (68%)	-0.51	2 (0%) 82 80	14, 23, 34, 50	0
1	B	199/304 (65%)	-0.35	0 100 100	16, 31, 43, 68	0
1	C	203/304 (66%)	-0.45	4 (1%) 65 63	13, 25, 43, 58	0
1	D	197/304 (64%)	-0.07	5 (2%) 57 55	28, 41, 59, 85	0
1	E	198/304 (65%)	-0.40	0 100 100	14, 24, 39, 53	0
1	F	204/304 (67%)	-0.41	3 (1%) 73 72	15, 26, 40, 63	0
All	All	1208/1824 (66%)	-0.36	14 (1%) 79 77	13, 28, 50, 85	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	189	THR	4.3
1	F	154	VAL	4.1
1	C	187	TYR	3.6
1	D	265	PRO	2.9
1	C	151	ALA	2.6
1	D	159	TYR	2.6
1	C	152	LEU	2.5
1	F	156	THR	2.5
1	F	153	PRO	2.3
1	D	224	ALA	2.3
1	A	152	LEU	2.3
1	C	265	PRO	2.2
1	A	181	ILE	2.2
1	D	263	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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.