Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2021 – 11:02 am BST

PDB ID	:	6YEV
Title	:	Crystal structure of MsrA C206 and Trx C35S complex from Escherichia coli
Authors	:	Napolitano, S.; Zyla, D.; Glockshuber, R.
Deposited on	:	2020-03-25
Resolution	:	2.94 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 following versions of software and data (see references ⓘ) were used in the production of this report:

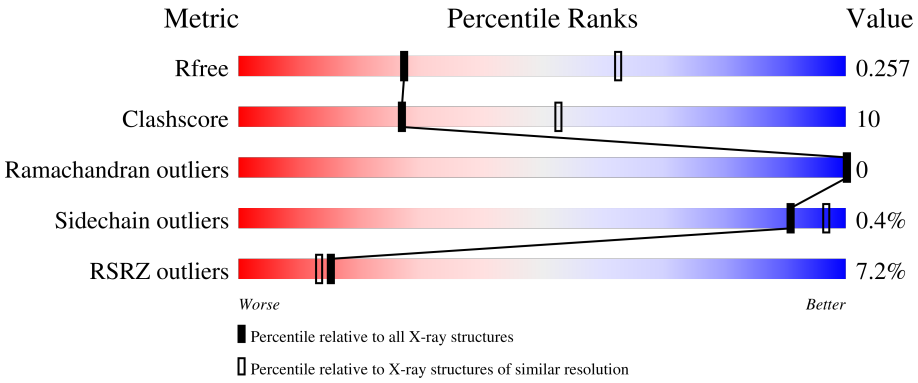
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	E	109	7% 65% 29% 6%
1	F	109	16% 80% 19%
1	G	109	28% 52% 43%
2	A	212	% 83% 15%
2	B	212	2% 83% 14%

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Mol	Chain	Length	Quality of chain
2	C	212	2% 82% 16%
2	D	212	7% 78% 17% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8822 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 Thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	103	Total	C	N	O	S	0	0	0
			787	508	126	151	2			
1	F	108	Total	C	N	O	S	0	0	0
			822	528	132	160	2			
1	G	106	Total	C	N	O	S	0	0	0
			798	512	129	155	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	35	SER	CYS	engineered mutation	UNP P0AA25
F	35	SER	CYS	engineered mutation	UNP P0AA25
G	35	SER	CYS	engineered mutation	UNP P0AA25

- Molecule 2 is a protein called Peptide methionine sulfoxide reductase MsrA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	209	Total	C	N	O	S	0	0	0
			1613	1019	277	310	7			
2	B	207	Total	C	N	O	S	0	0	0
			1596	1007	275	307	7			
2	C	208	Total	C	N	O	S	0	1	0
			1616	1019	281	309	7			
2	D	201	Total	C	N	O	S	0	0	0
			1552	979	269	297	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ALA	CYS	engineered mutation	UNP P0A744
A	86	ALA	CYS	engineered mutation	UNP P0A744
A	198	ALA	CYS	engineered mutation	UNP P0A744

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Chain	Residue	Modelled	Actual	Comment	Reference
B	51	ALA	CYS	engineered mutation	UNP P0A744
B	86	ALA	CYS	engineered mutation	UNP P0A744
B	198	ALA	CYS	engineered mutation	UNP P0A744
C	51	ALA	CYS	engineered mutation	UNP P0A744
C	86	ALA	CYS	engineered mutation	UNP P0A744
C	198	ALA	CYS	engineered mutation	UNP P0A744
D	51	ALA	CYS	engineered mutation	UNP P0A744
D	86	ALA	CYS	engineered mutation	UNP P0A744
D	198	ALA	CYS	engineered mutation	UNP P0A744

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0

- Molecule 4 is water.

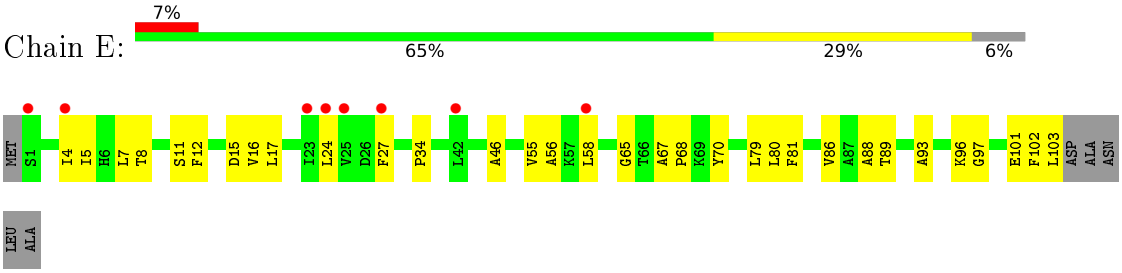
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	9	Total O 9 9	0	0
4	C	7	Total O 7 7	0	0
4	D	5	Total O 5 5	0	0

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.

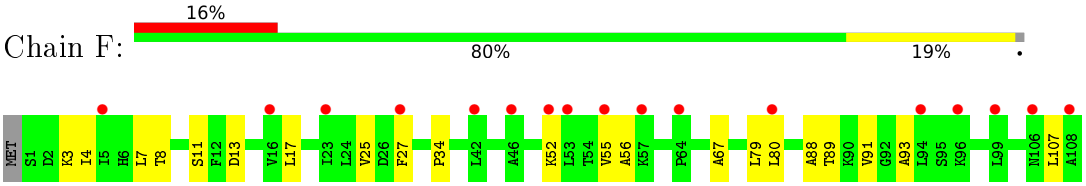
- Molecule 1: Thioredoxin 1

Chain E:



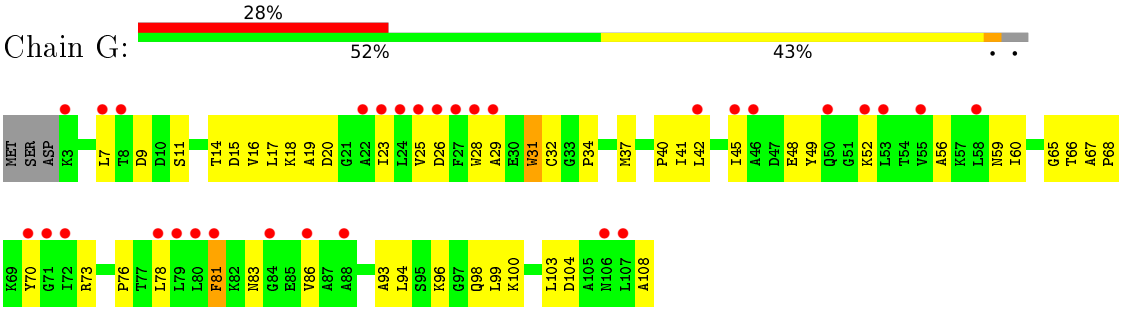
- Molecule 1: Thioredoxin 1

Chain F:



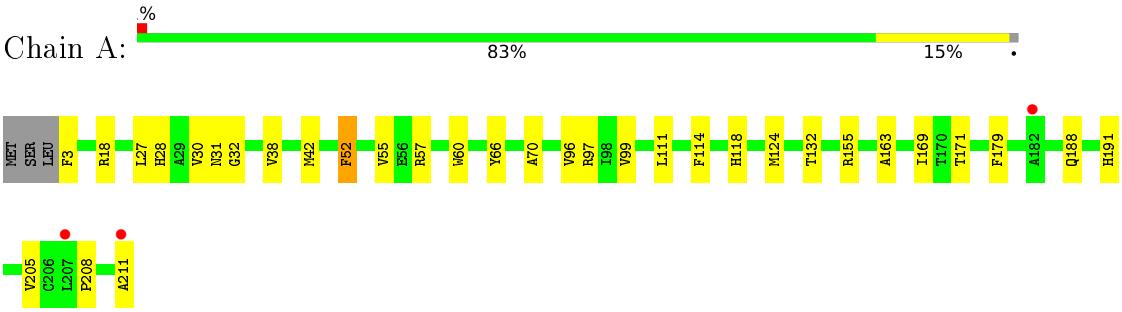
- Molecule 1: Thioredoxin 1

Chain G:



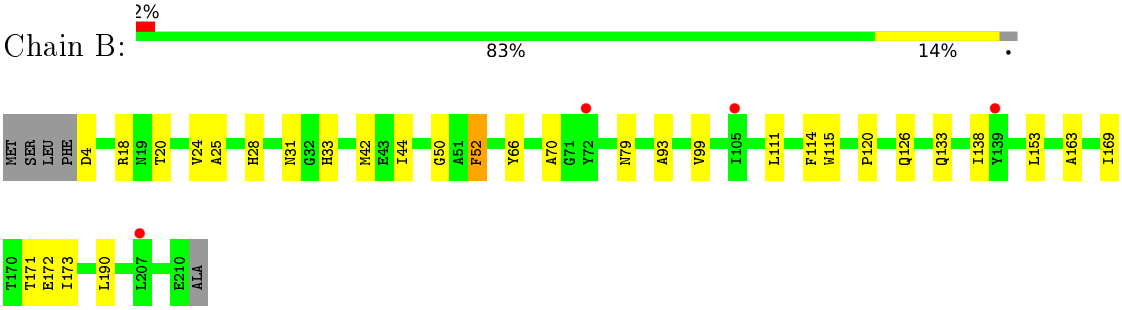
- Molecule 2: Peptide methionine sulfoxide reductase MsrA

Chain A:



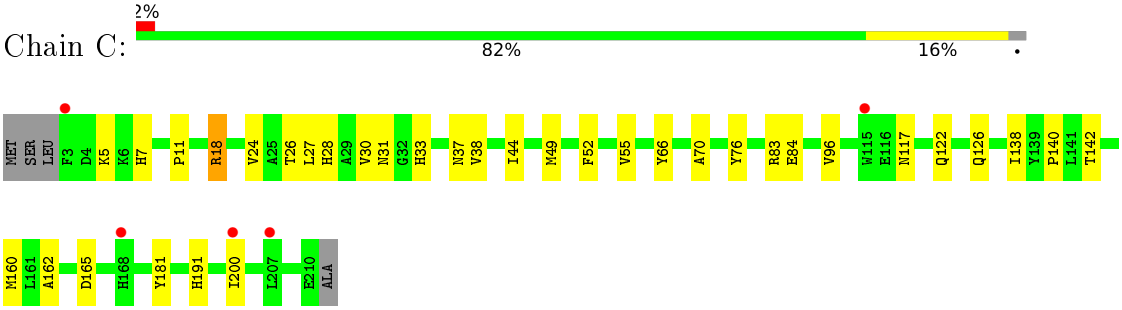
• Molecule 2: Peptide methionine sulfoxide reductase MsrA

Chain B:



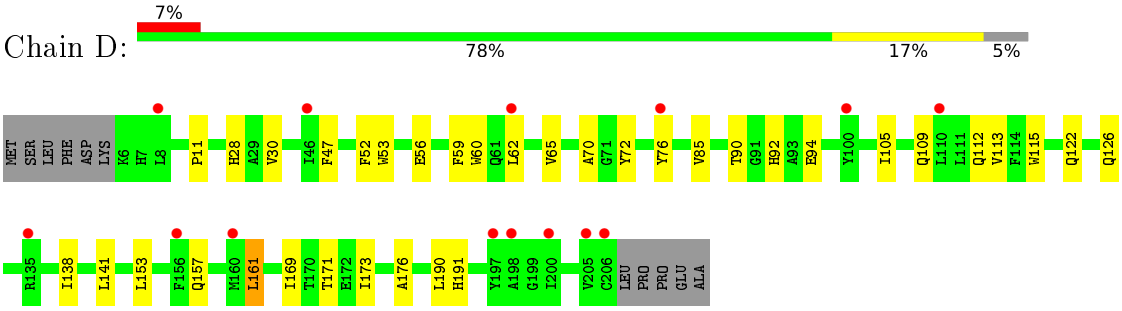
• Molecule 2: Peptide methionine sulfoxide reductase MsrA

Chain C:



• Molecule 2: Peptide methionine sulfoxide reductase MsrA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.91Å 139.91Å 218.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.71 – 2.94 49.71 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.71-2.94) 99.9 (49.71-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.17rc5_3630	Depositor
R, R_{free}	0.229 , 0.258 0.229 , 0.257	Depositor DCC
R_{free} test set	2656 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	87.4	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 75.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.158 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8822	wwPDB-VP
Average B, all atoms (Å^2)	97.0	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.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	E	0.36	0/802	0.62	0/1087
1	F	0.32	0/837	0.62	0/1134
1	G	0.31	0/812	0.63	0/1102
2	A	0.41	0/1663	0.64	0/2274
2	B	0.41	0/1645	0.66	0/2251
2	C	0.46	0/1665	0.67	0/2276
2	D	0.39	0/1599	0.64	1/2186 (0.0%)
All	All	0.39	0/9023	0.65	1/12310 (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	E	0	1
1	G	0	3
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	161	LEU	CB-CG-CD2	5.19	119.83	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	101	GLU	Peptide
1	G	31	TRP	Peptide
1	G	67	ALA	Peptide
1	G	81	PHE	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	E	787	0	801	26	0
1	F	822	0	832	12	0
1	G	798	0	802	36	0
2	A	1613	0	1495	21	0
2	B	1596	0	1480	23	0
2	C	1616	0	1506	26	0
2	D	1552	0	1445	33	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	13	0	0	1	0
4	B	9	0	0	0	0
4	C	7	0	0	0	0
4	D	5	0	0	0	0
All	All	8822	0	8361	174	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 10.

All (174) 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:D:52:PHE:HD1	2:D:94:GLU:HB3	1.39	0.86
1:G:34:PRO:HB3	1:G:93:ALA:HB2	1.57	0.84
1:F:52:LYS:HE3	1:F:107:LEU:HD22	1.61	0.80
2:D:53:TRP:HB3	2:D:190:LEU:HD11	1.63	0.78
1:G:52:LYS:HD2	1:G:108:ALA:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3:PHE:N	4:A:401:HOH:O	2.20	0.74
1:G:11:SER:OG	1:G:15:ASP:OD2	2.05	0.74
2:C:52:PHE:HA	2:C:55:VAL:HG22	1.69	0.74
2:D:157:GLN:HE21	2:D:161:LEU:HG	1.55	0.72
1:G:29:ALA:HB1	1:G:31:TRP:HD1	1.55	0.71
2:C:52:PHE:CE2	2:C:70:ALA:HB1	2.26	0.70
1:G:20:ASP:HB2	1:G:83:ASN:HD21	1.57	0.69
2:B:52:PHE:H	2:B:52:PHE:HD1	1.41	0.68
1:E:88:ALA:HB2	1:E:102:PHE:HE2	1.59	0.68
1:E:88:ALA:HB2	1:E:102:PHE:CE2	2.30	0.67
2:C:162:ALA:HB2	1:G:73:ARG:HB2	1.78	0.66
1:G:7:LEU:HD22	1:G:56:ALA:HB1	1.77	0.66
1:F:4:ILE:HG23	1:F:55:VAL:HG23	1.79	0.65
1:E:34:PRO:HB3	1:E:93:ALA:HB2	1.79	0.64
2:C:38:VAL:HG21	2:C:44:ILE:HD11	1.79	0.64
2:C:18:ARG:HH22	2:C:84:GLU:CD	2.02	0.62
2:C:49:MET:HB2	2:C:55:VAL:HG11	1.81	0.62
1:G:70:TYR:HE2	1:G:86:VAL:HG11	1.65	0.61
1:E:7:LEU:HD11	1:E:56:ALA:HB1	1.84	0.60
2:D:52:PHE:CD1	2:D:94:GLU:HB3	2.29	0.60
2:D:62:LEU:O	2:D:65:VAL:HG12	2.03	0.59
1:F:79:LEU:HD22	1:F:89:THR:HG22	1.85	0.58
2:D:62:LEU:HD23	2:D:105:ILE:HD11	1.85	0.58
1:E:81:PHE:CE1	1:E:86:VAL:HG22	2.39	0.57
1:G:20:ASP:N	1:G:83:ASN:OD1	2.37	0.57
2:B:52:PHE:CE2	2:B:70:ALA:HB1	2.40	0.57
2:C:52:PHE:CD2	2:C:70:ALA:HB1	2.40	0.57
2:B:52:PHE:CD2	2:B:70:ALA:HB1	2.40	0.56
2:A:52:PHE:CE2	2:A:70:ALA:HB1	2.40	0.56
1:G:81:PHE:CE1	1:G:86:VAL:HG12	2.41	0.56
1:G:19:ALA:HB3	1:G:23:ILE:HD11	1.88	0.56
2:C:24:VAL:HG11	2:C:181:TYR:CD2	2.41	0.55
1:E:16:VAL:HG13	1:E:17:LEU:HD12	1.88	0.55
1:G:104:ASP:HA	1:G:108:ALA:OXT	2.07	0.55
1:E:103:LEU:H	1:E:103:LEU:HD23	1.71	0.55
2:A:97:ARG:HB2	2:A:179:PHE:CZ	2.42	0.55
2:B:33:HIS:HB3	2:B:66:TYR:CZ	2.42	0.55
2:C:52:PHE:H	2:C:52:PHE:HD1	1.54	0.55
2:B:20:THR:HG22	2:C:142:THR:HG22	1.89	0.55
2:C:83[A]:ARG:HG3	2:C:83[A]:ARG:HH11	1.70	0.54
1:G:20:ASP:HB2	1:G:83:ASN:ND2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:ILE:HG22	2:D:171:THR:H	1.72	0.54
2:D:62:LEU:HD21	2:D:113:VAL:HG21	1.89	0.53
2:D:59:PHE:HA	2:D:62:LEU:HD13	1.89	0.53
2:B:44:ILE:HD13	2:B:99:VAL:HG22	1.91	0.53
2:A:124:MET:SD	2:A:132:THR:HG22	2.49	0.52
2:A:42:MET:CE	2:A:66:TYR:HB2	2.39	0.52
2:D:30:VAL:HG22	2:D:191:HIS:CG	2.44	0.52
2:A:169:ILE:HG22	2:A:171:THR:H	1.74	0.52
2:C:55:VAL:HG23	2:C:96:VAL:HG21	1.91	0.51
2:C:11:PRO:HG3	2:C:76:TYR:CE1	2.46	0.51
2:D:47:PHE:HE1	2:D:138:ILE:HG23	1.75	0.51
1:E:80:LEU:HB3	1:E:88:ALA:HB3	1.93	0.50
1:G:26:ASP:HB3	1:G:78:LEU:HD23	1.94	0.50
2:D:28:HIS:CE1	2:D:30:VAL:HB	2.46	0.50
2:B:18:ARG:HG2	2:B:20:THR:H	1.76	0.50
2:A:155:ARG:HD2	2:A:211:ALA:HB3	1.93	0.50
2:D:138:ILE:HB	2:D:173:ILE:HG12	1.94	0.50
1:G:25:VAL:HA	1:G:56:ALA:O	2.12	0.49
2:D:157:GLN:NE2	2:D:161:LEU:HG	2.24	0.49
2:D:56:GLU:HG2	2:D:60:TRP:CE3	2.48	0.49
2:B:120:PRO:HB2	2:B:169:ILE:HG23	1.94	0.49
2:A:55:VAL:HG12	2:A:96:VAL:HG11	1.95	0.48
1:G:29:ALA:C	1:G:31:TRP:H	2.17	0.48
1:E:17:LEU:HD11	1:E:70:TYR:OH	2.14	0.48
2:C:18:ARG:NH2	2:C:84:GLU:OE1	2.43	0.48
1:G:32:CYS:SG	1:G:34:PRO:HD2	2.53	0.48
1:G:94:LEU:HD22	1:G:98:GLN:HB3	1.95	0.48
1:G:70:TYR:CE2	1:G:86:VAL:HG11	2.48	0.48
1:F:34:PRO:HB3	1:F:93:ALA:HB2	1.96	0.48
2:C:28:HIS:HB3	2:C:31:ASN:OD1	2.14	0.48
1:E:8:THR:H	1:E:11:SER:HB3	1.77	0.47
2:D:115:TRP:HH2	2:D:153:LEU:HD23	1.79	0.47
2:D:141:LEU:HD23	2:D:176:ALA:HB3	1.97	0.47
2:B:18:ARG:CZ	2:B:18:ARG:HB2	2.44	0.47
2:D:53:TRP:HB3	2:D:190:LEU:CD1	2.39	0.47
1:G:14:THR:HA	1:G:18:LYS:NZ	2.29	0.47
2:A:28:HIS:HB3	2:A:31:ASN:OD1	2.14	0.47
2:C:117:ASN:HB3	2:C:200:ILE:HD12	1.97	0.47
2:D:90:THR:HB	2:D:92:HIS:HD2	1.79	0.47
2:D:52:PHE:CD2	2:D:70:ALA:HB1	2.50	0.46
1:G:16:VAL:HG13	1:G:17:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:PHE:CZ	1:E:16:VAL:HG11	2.50	0.46
1:F:27:PHE:HE2	1:F:67:ALA:HA	1.81	0.46
2:A:155:ARG:NH1	2:A:208:PRO:O	2.48	0.46
2:D:56:GLU:HG2	2:D:60:TRP:HE3	1.81	0.46
2:D:72:TYR:CD1	2:D:85:VAL:HG11	2.50	0.46
1:E:7:LEU:HB2	1:E:58:LEU:HD13	1.98	0.46
1:E:79:LEU:HD22	1:E:89:THR:HG22	1.97	0.45
2:B:28:HIS:HB3	2:B:31:ASN:OD1	2.16	0.45
2:D:30:VAL:HG22	2:D:191:HIS:CD2	2.50	0.45
2:D:52:PHE:CE2	2:D:70:ALA:HB1	2.52	0.45
1:G:65:GLY:O	1:G:68:PRO:HD2	2.16	0.45
2:D:90:THR:HB	2:D:92:HIS:CD2	2.52	0.45
2:D:115:TRP:CH2	2:D:153:LEU:HD23	2.51	0.45
2:C:26:THR:HG22	2:C:27:LEU:HD12	1.98	0.45
1:G:9:ASP:O	1:G:66:THR:HG21	2.15	0.45
1:E:4:ILE:HG12	1:E:55:VAL:CG2	2.47	0.45
1:E:11:SER:OG	1:E:15:ASP:OD2	2.35	0.45
2:D:109:GLN:HA	2:D:112:GLN:HG2	1.99	0.45
2:A:28:HIS:CD2	2:A:188:GLN:HE21	2.34	0.44
1:F:25:VAL:HA	1:F:56:ALA:O	2.17	0.44
1:G:42:LEU:HA	1:G:45:ILE:HG13	1.99	0.44
2:C:28:HIS:CE1	2:C:30:VAL:HB	2.52	0.44
2:D:122:GLN:OE1	2:D:126:GLN:HA	2.17	0.44
2:A:30:VAL:HG22	2:A:191:HIS:CG	2.53	0.44
1:G:28:TRP:O	1:G:60:ILE:HG13	2.18	0.44
2:B:115:TRP:HH2	2:B:153:LEU:HD12	1.83	0.44
1:G:28:TRP:HB2	1:G:59:ASN:HA	2.00	0.44
2:B:4:ASP:OD2	2:B:172:GLU:HB2	2.17	0.44
2:B:114:PHE:CE2	2:B:138:ILE:HD11	2.53	0.44
2:D:47:PHE:CE1	2:D:138:ILE:HG23	2.52	0.44
1:G:37:MET:O	1:G:40:PRO:HD2	2.17	0.44
1:E:46:ALA:HB2	1:E:55:VAL:HG22	2.00	0.43
1:E:67:ALA:HB3	1:E:68:PRO:HD3	2.00	0.43
2:C:122:GLN:OE1	2:C:126:GLN:HA	2.19	0.43
1:E:65:GLY:O	1:E:68:PRO:HD2	2.18	0.43
1:E:5:ILE:HG22	1:E:7:LEU:HD12	2.00	0.43
1:F:7:LEU:CD1	1:F:56:ALA:HB1	2.47	0.43
2:B:138:ILE:HB	2:B:173:ILE:HG12	2.01	0.43
1:G:16:VAL:HG23	1:G:23:ILE:HG21	2.00	0.43
2:A:52:PHE:H	2:A:52:PHE:HD1	1.65	0.43
2:A:163:ALA:HB2	2:A:205:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:28:HIS:CD2	2:A:188:GLN:NE2	2.86	0.43
2:D:109:GLN:O	2:D:112:GLN:HG2	2.19	0.43
1:E:7:LEU:CD1	1:E:56:ALA:HB1	2.48	0.43
1:F:91:VAL:HB	2:B:163:ALA:HA	2.01	0.43
2:D:11:PRO:HG3	2:D:76:TYR:CZ	2.54	0.43
1:G:99:LEU:O	1:G:103:LEU:HD13	2.18	0.43
1:E:24:LEU:HB3	1:E:55:VAL:HG12	2.01	0.42
2:B:42:MET:SD	2:B:66:TYR:HB2	2.59	0.42
1:F:13:ASP:OD1	1:F:17:LEU:HD12	2.19	0.42
2:A:114:PHE:CZ	2:A:118:HIS:HE1	2.37	0.42
2:C:83[A]:ARG:HG3	2:C:83[A]:ARG:NH1	2.34	0.42
2:A:66:TYR:N	2:A:99:VAL:O	2.50	0.42
1:G:15:ASP:O	1:G:19:ALA:HB2	2.20	0.42
1:E:16:VAL:HG22	1:E:81:PHE:CD2	2.54	0.42
2:B:190:LEU:HA	2:B:190:LEU:HD23	1.75	0.42
2:A:57:ARG:HA	2:A:60:TRP:CE3	2.54	0.42
2:B:18:ARG:O	2:B:79:ASN:HB2	2.19	0.42
2:B:111:LEU:O	2:B:114:PHE:HB3	2.20	0.42
1:G:41:ILE:HD12	1:G:96:LYS:HB2	2.02	0.42
1:F:80:LEU:HB3	1:F:88:ALA:HB3	2.02	0.42
1:G:45:ILE:HA	1:G:48:GLU:HB3	2.02	0.42
2:C:5:LYS:O	2:C:7:HIS:N	2.52	0.42
1:G:17:LEU:HD13	1:G:83:ASN:O	2.20	0.42
2:A:27:LEU:HD22	2:A:32:GLY:O	2.19	0.41
2:C:30:VAL:HG22	2:C:191:HIS:CG	2.53	0.41
2:C:33:HIS:HB3	2:C:66:TYR:CZ	2.55	0.41
2:C:138:ILE:O	2:C:140:PRO:HD3	2.20	0.41
2:D:59:PHE:O	2:D:65:VAL:HG11	2.20	0.41
1:E:27:PHE:HE2	1:E:79:LEU:HD12	1.85	0.41
1:F:8:THR:H	1:F:11:SER:HB3	1.86	0.41
2:C:37:ASN:OD1	2:C:38:VAL:N	2.53	0.41
2:D:62:LEU:HD23	2:D:105:ILE:CD1	2.51	0.41
2:B:50:GLY:HA3	2:B:126:GLN:HG2	2.02	0.41
2:B:93:ALA:HA	2:B:133:GLN:HA	2.03	0.41
1:E:4:ILE:HG12	1:E:55:VAL:HG23	2.02	0.41
2:B:169:ILE:HG22	2:B:171:THR:H	1.86	0.41
1:G:34:PRO:HB2	1:G:76:PRO:HD3	2.03	0.41
1:E:96:LYS:HG3	1:E:97:GLY:H	1.86	0.40
2:A:38:VAL:O	2:A:38:VAL:HG23	2.21	0.40
2:A:111:LEU:HD23	2:A:111:LEU:HA	1.93	0.40
1:G:48:GLU:HG2	1:G:49:TYR:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:LYS:O	1:G:104:ASP:N	2.44	0.40
2:B:24:VAL:HG12	2:B:25:ALA:O	2.21	0.40
1:E:96:LYS:HG3	1:E:97:GLY:N	2.36	0.40
1:F:3:LYS:HD2	1:F:3:LYS:HA	1.93	0.40
2:C:160:MET:HE3	2:C:165:ASP:OD2	2.20	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	E	101/109 (93%)	92 (91%)	9 (9%)	0	100	100
1	F	106/109 (97%)	100 (94%)	6 (6%)	0	100	100
1	G	104/109 (95%)	89 (86%)	15 (14%)	0	100	100
2	A	207/212 (98%)	199 (96%)	8 (4%)	0	100	100
2	B	205/212 (97%)	196 (96%)	9 (4%)	0	100	100
2	C	207/212 (98%)	199 (96%)	8 (4%)	0	100	100
2	D	199/212 (94%)	190 (96%)	9 (4%)	0	100	100
All	All	1129/1175 (96%)	1065 (94%)	64 (6%)	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	E	84/88 (96%)	84 (100%)	0	100 100
1	F	87/88 (99%)	87 (100%)	0	100 100
1	G	83/88 (94%)	83 (100%)	0	100 100
2	A	162/166 (98%)	160 (99%)	2 (1%)	71 89
2	B	161/166 (97%)	160 (99%)	1 (1%)	86 95
2	C	163/166 (98%)	162 (99%)	1 (1%)	86 95
2	D	156/166 (94%)	156 (100%)	0	100 100
All	All	896/928 (97%)	892 (100%)	4 (0%)	91 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	18	ARG
2	A	52	PHE
2	B	52	PHE
2	C	18	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	188	GLN
2	D	157	GLN
2	D	191	HIS

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

Of 4 ligands modelled in this entry, 4 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

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	E	103/109 (94%)	0.61	8 (7%) 13 11	70, 110, 147, 159	0
1	F	108/109 (99%)	0.83	17 (15%) 2 1	83, 109, 156, 164	0
1	G	106/109 (97%)	1.41	31 (29%) 0 0	101, 166, 216, 237	0
2	A	209/212 (98%)	0.50	3 (1%) 75 77	61, 73, 99, 191	0
2	B	207/212 (97%)	0.49	4 (1%) 66 67	58, 73, 121, 149	0
2	C	208/212 (98%)	0.61	5 (2%) 59 59	60, 74, 109, 170	0
2	D	201/212 (94%)	0.66	14 (6%) 16 14	70, 97, 156, 179	0
All	All	1142/1175 (97%)	0.67	82 (7%) 15 13	58, 86, 167, 237	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	86	VAL	9.5
1	G	23	ILE	6.5
2	D	206	CYS	6.1
1	G	80	LEU	5.7
2	D	205	VAL	5.5
1	G	106	ASN	5.4
2	D	200	ILE	5.1
1	G	84	GLY	4.8
1	G	22	ALA	4.8
2	A	211	ALA	4.7
1	G	46	ALA	4.7
1	G	88	ALA	4.5
1	G	42	LEU	4.4
1	G	81	PHE	4.4
2	C	207	LEU	4.3
1	G	55	VAL	4.2
1	G	8	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	53	LEU	4.2
1	F	52	LYS	3.9
1	G	27	PHE	3.8
1	G	45	ILE	3.7
1	G	50	GLN	3.7
1	G	70	TYR	3.6
1	E	42	LEU	3.6
1	G	28	TRP	3.5
1	E	1	SER	3.4
1	G	79	LEU	3.4
1	G	107	LEU	3.3
1	F	80	LEU	3.3
1	F	53	LEU	3.2
1	E	58	LEU	3.2
2	D	76	TYR	3.0
1	F	42	LEU	2.9
1	F	46	ALA	2.9
1	G	24	LEU	2.8
2	D	46	ILE	2.8
2	D	198	ALA	2.8
1	G	71	GLY	2.8
1	G	26	ASP	2.8
1	G	29	ALA	2.7
1	G	72	ILE	2.7
2	C	200	ILE	2.6
1	F	55	VAL	2.6
1	F	99	LEU	2.6
1	G	3	LYS	2.5
1	E	4	ILE	2.5
2	D	156	PHE	2.5
1	G	78	LEU	2.5
1	F	5	ILE	2.5
2	B	105	ILE	2.4
2	C	115	TRP	2.4
2	A	207	LEU	2.4
1	E	25	VAL	2.4
2	D	135	ARG	2.4
2	D	62	LEU	2.4
2	B	207	LEU	2.3
1	E	24	LEU	2.3
2	D	110	LEU	2.3
1	F	57	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	72	TYR	2.3
2	D	197	TYR	2.3
1	G	58	LEU	2.3
2	A	182	ALA	2.3
1	G	52	LYS	2.2
2	C	3	PHE	2.2
1	F	94	LEU	2.2
2	B	139	TYR	2.2
1	F	23	ILE	2.2
1	F	16	VAL	2.2
1	F	108	ALA	2.2
1	F	106	ASN	2.2
2	D	8	LEU	2.1
1	G	7	LEU	2.1
2	C	168	HIS	2.1
2	D	100	TYR	2.1
1	E	27	PHE	2.1
1	G	25	VAL	2.0
2	D	160	MET	2.0
1	F	96	LYS	2.0
1	E	23	ILE	2.0
1	F	27	PHE	2.0
1	F	64	PRO	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, 95^{th} 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	A	301	1/1	0.85	0.19	73,73,73,73	0
3	NA	C	301	1/1	0.86	0.24	71,71,71,71	0
3	NA	D	301	1/1	0.93	0.21	90,90,90,90	0
3	NA	B	301	1/1	0.96	0.21	81,81,81,81	0

6.5 Other polymers (i)

There are no such residues in this entry.