Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 04:13 AM EDT

PDB ID	:	2DFU
Title	:	Crystal structure of the 2-hydroxyhepta-2,4-diene-1,7-dioate isomerase from Thermus Thermophilus HB8
Authors	:	Mizutani, H.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-03-03
Resolution	:	2.20 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:

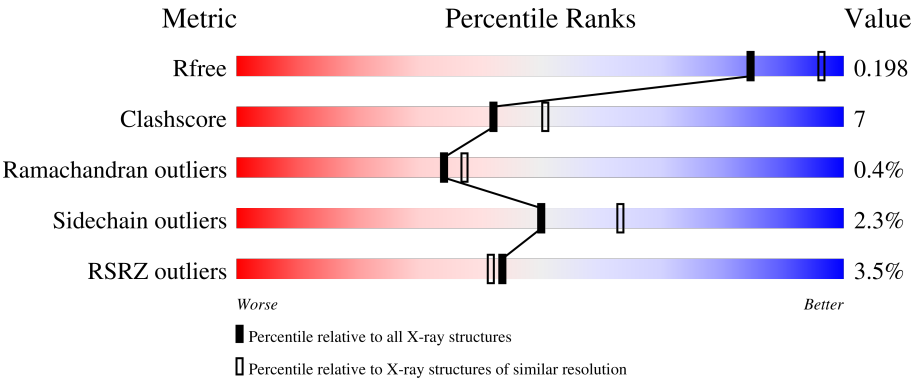
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	264	% 80% 13% • 5%
1	B	264	7% 80% 13% • 6%
1	C	264	3% 83% 11% 6%
1	D	264	2% 76% 17% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8438 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 probable 2-hydroxyhepta-2,4-diene-1,7-dioate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1967	1261	338	363	5			
1	B	249	Total	C	N	O	S	0	0	0
			1948	1249	333	361	5			
1	C	249	Total	C	N	O	S	0	0	0
			1948	1249	333	361	5			
1	D	247	Total	C	N	O	S	0	0	0
			1932	1238	330	359	5			

- Molecule 2 is water.

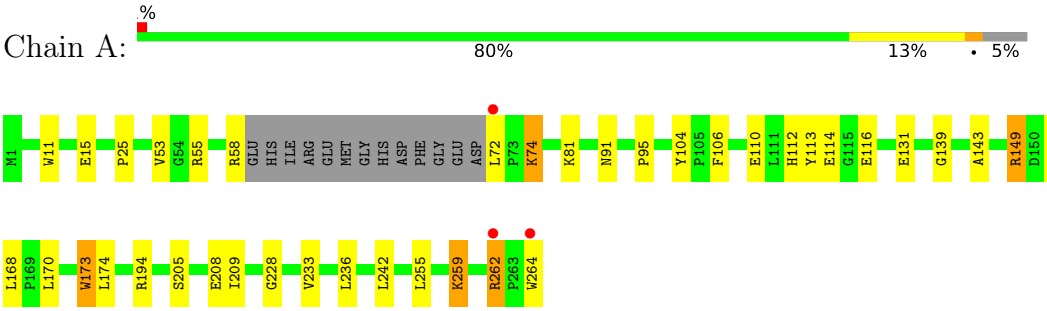
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	197	Total	O	0	0
			197	197		
2	B	136	Total	O	0	0
			136	136		
2	C	151	Total	O	0	0
			151	151		
2	D	159	Total	O	0	0
			159	159		

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.

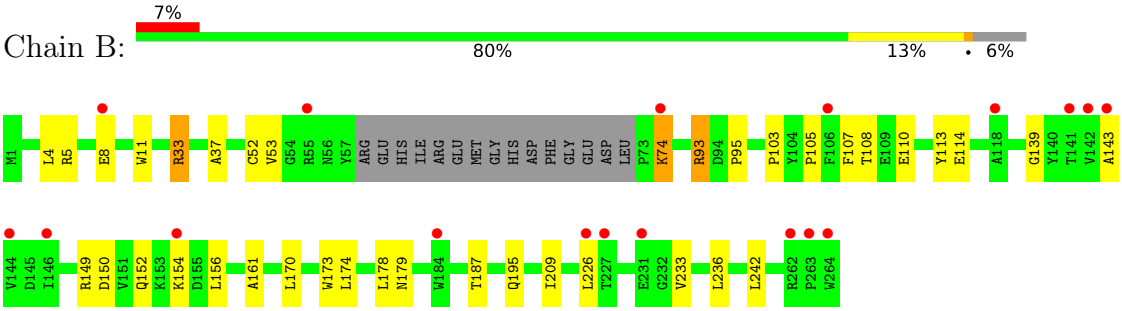
• Molecule 1: probable 2-hydroxyhepta-2,4-diene-1,7-dioate isomerase

Chain A:



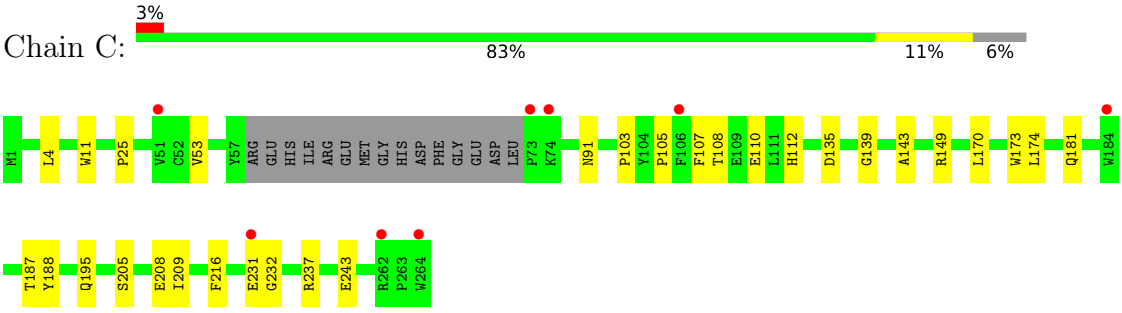
• Molecule 1: probable 2-hydroxyhepta-2,4-diene-1,7-dioate isomerase

Chain B:



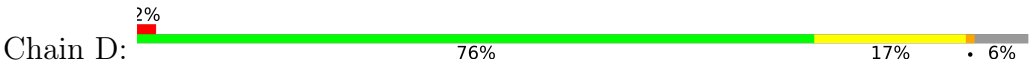
• Molecule 1: probable 2-hydroxyhepta-2,4-diene-1,7-dioate isomerase

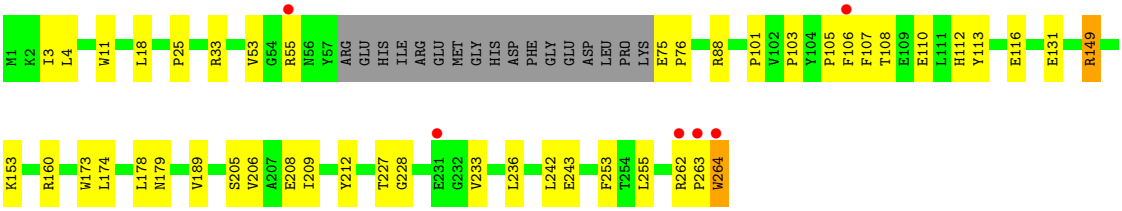
Chain C:



• Molecule 1: probable 2-hydroxyhepta-2,4-diene-1,7-dioate isomerase

Chain D:




M1
K2
I3
L4
W11
L18
P25
R33
V53
G54
R55
N56
Y57
ARG
GLU
HIS
ILE
ARG
GLU
MET
GLY
HIS
ASP
PHE
GLY
GLU
ASP
LEU
PRO
LYS
E75
P76
R88
P101
V102
P103
Y104
P105
F106
F107
T108
E109
E110
L111
H112
Y113
E116
E131
R149

K153
R160
W173
L174
L178
N179
V189
S205
V206
A207
E208
I209
Y212
T227
G228
E231
G232
V233
L236
L242
E243
F253
T254
L255
R262
P263
W264

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.34Å 73.41Å 122.63Å 90.00° 111.78° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.20) 100.0 (29.60-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.224 0.199 , 0.198	Depositor DCC
R_{free} test set	3942 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8438	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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	0.48	2/2020 (0.1%)	0.70	0/2757
1	B	0.31	0/2001	0.62	0/2731
1	C	0.33	0/2001	0.62	0/2731
1	D	0.46	2/1984 (0.1%)	0.68	0/2709
All	All	0.40	4/8006 (0.0%)	0.66	0/10928

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	264	TRP	NE1-CE2	8.72	1.48	1.37
1	A	173	TRP	NE1-CE2	8.64	1.48	1.37
1	D	173	TRP	NE1-CE2	8.49	1.48	1.37
1	A	264	TRP	NE1-CE2	8.31	1.48	1.37

There are no bond angle outliers.

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	1967	0	1965	33	0
1	B	1948	0	1942	25	0
1	C	1948	0	1942	19	0
1	D	1932	0	1921	32	0
2	A	197	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	136	0	0	0	0
2	C	151	0	0	1	0
2	D	159	0	0	1	0
All	All	8438	0	7770	108	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 7.

All (108) 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:139:GLY:HA3	1:A:174:LEU:HD13	1.59	0.82
1:D:3:ILE:HB	1:D:174:LEU:CD1	2.19	0.72
1:D:3:ILE:HB	1:D:174:LEU:HD11	1.72	0.72
1:B:187:THR:HB	1:B:195:GLN:HB2	1.76	0.68
1:B:105:PRO:HB2	1:B:108:THR:HG22	1.77	0.67
1:D:189:VAL:HG22	1:D:242:LEU:HD23	1.74	0.67
1:A:53:VAL:HG21	1:A:209:ILE:HD13	1.76	0.67
1:A:112:HIS:ND1	1:A:149:ARG:HG3	2.11	0.66
1:D:106:PHE:CZ	1:D:262:ARG:HG2	2.36	0.61
1:D:18:LEU:HD11	1:D:33:ARG:HD2	1.83	0.60
1:D:116:GLU:HG2	1:D:228:GLY:O	2.03	0.59
1:B:143:ALA:HB2	1:B:170:LEU:HD12	1.86	0.58
1:B:53:VAL:HG21	1:B:209:ILE:HD13	1.85	0.58
1:A:110:GLU:HG3	1:A:112:HIS:HE1	1.69	0.58
1:C:110:GLU:HG3	1:C:112:HIS:HE1	1.69	0.57
1:B:52:CYS:SG	1:B:226:LEU:HD22	2.45	0.57
1:B:74:LYS:HB2	1:B:74:LYS:NZ	2.20	0.57
1:C:11:TRP:CE2	1:C:25:PRO:HG3	2.39	0.57
1:B:113:TYR:HB3	1:B:236:LEU:HD11	1.88	0.56
1:B:37:ALA:HB2	1:B:93:ARG:HG2	1.87	0.56
1:D:205:SER:OG	1:D:208:GLU:HG3	2.05	0.56
1:A:262:ARG:HG3	1:A:262:ARG:HH11	1.70	0.56
1:A:58:ARG:NH2	2:A:424:HOH:O	2.30	0.55
1:C:110:GLU:HG3	1:C:112:HIS:CE1	2.41	0.55
1:D:75:GLU:O	1:D:75:GLU:HG3	2.06	0.55
1:A:11:TRP:CE2	1:A:25:PRO:HG3	2.42	0.54
1:D:113:TYR:HB3	1:D:236:LEU:HD11	1.90	0.54
1:A:236:LEU:HD21	1:A:242:LEU:HD21	1.89	0.54
1:B:33:ARG:O	1:B:33:ARG:HD3	2.08	0.53
1:A:110:GLU:HG3	1:A:112:HIS:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLU:OE1	1:B:150:ASP:HB3	2.09	0.53
1:A:205:SER:OG	1:A:208:GLU:HG3	2.08	0.53
1:D:149:ARG:HD2	1:D:153:LYS:HE3	1.91	0.53
1:C:4:LEU:HD23	1:C:4:LEU:N	2.24	0.52
1:B:105:PRO:HB3	1:B:107:PHE:CE2	2.44	0.52
1:A:255:LEU:HD12	1:A:255:LEU:C	2.30	0.52
1:C:187:THR:HB	1:C:195:GLN:HB2	1.92	0.52
1:A:104:TYR:HB3	1:A:259:LYS:HA	1.90	0.52
1:D:101:PRO:O	1:D:103:PRO:HD3	2.10	0.52
1:A:151:VAL:HG12	1:A:154:LYS:HE2	1.92	0.51
1:C:205:SER:OG	1:C:208:GLU:HG3	2.10	0.51
1:A:74:LYS:HB2	1:A:74:LYS:NZ	2.26	0.51
1:B:139:GLY:HA3	1:B:174:LEU:HD13	1.91	0.51
1:A:55:ARG:NH2	1:A:72:LEU:HD23	2.26	0.50
1:A:114:GLU:HG2	1:A:233:VAL:HG22	1.93	0.50
1:A:262:ARG:HH11	1:A:262:ARG:CG	2.24	0.50
1:D:110:GLU:HG3	1:D:112:HIS:HE1	1.77	0.50
1:A:151:VAL:HA	1:A:154:LYS:HG2	1.93	0.49
1:C:11:TRP:CZ2	1:C:25:PRO:HG3	2.47	0.49
1:D:105:PRO:HB2	1:D:108:THR:HG22	1.94	0.49
1:D:18:LEU:CD1	1:D:33:ARG:HD2	2.42	0.49
1:A:116:GLU:HG2	1:A:228:GLY:O	2.13	0.49
1:C:139:GLY:HA3	1:C:174:LEU:HD13	1.95	0.48
1:A:143:ALA:HB2	1:A:170:LEU:HD12	1.95	0.48
1:D:255:LEU:HD23	1:D:255:LEU:N	2.29	0.48
1:A:55:ARG:CZ	1:A:72:LEU:HD23	2.43	0.48
1:A:106:PHE:HA	1:A:259:LYS:HE3	1.94	0.48
1:C:105:PRO:HB2	1:C:108:THR:HG22	1.97	0.47
1:D:18:LEU:HD11	1:D:33:ARG:CD	2.45	0.47
1:B:113:TYR:O	1:B:233:VAL:HG13	2.15	0.46
1:B:4:LEU:HD23	1:B:4:LEU:N	2.30	0.46
1:D:206:VAL:HG22	1:D:227:THR:HG21	1.97	0.46
1:D:263:PRO:HB2	1:D:264:TRP:CE3	2.51	0.46
1:C:53:VAL:HG21	1:C:209:ILE:HD13	1.98	0.46
1:D:131:GLU:H	1:D:131:GLU:CD	2.18	0.46
1:D:243:GLU:HG3	1:D:253:PHE:CE1	2.51	0.46
1:B:4:LEU:HD23	1:B:4:LEU:H	1.81	0.46
1:D:105:PRO:HB3	1:D:107:PHE:CE2	2.51	0.46
1:C:143:ALA:HB2	1:C:170:LEU:HD12	1.98	0.45
1:A:255:LEU:HD12	1:A:255:LEU:O	2.15	0.45
1:A:11:TRP:CZ2	1:A:25:PRO:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:HD12	1:B:242:LEU:N	2.32	0.45
1:B:103:PRO:O	1:B:105:PRO:HD3	2.17	0.45
1:A:91:ASN:HB2	2:A:275:HOH:O	2.16	0.44
1:A:81:LYS:HE2	1:A:168:LEU:HD13	1.99	0.44
1:D:189:VAL:HG22	1:D:242:LEU:CD2	2.45	0.44
1:A:106:PHE:HZ	1:A:262:ARG:NH1	2.16	0.44
1:A:262:ARG:CG	1:A:262:ARG:NH1	2.80	0.44
1:D:110:GLU:HG3	1:D:112:HIS:CE1	2.52	0.44
1:A:113:TYR:HD2	1:A:236:LEU:HG	1.82	0.44
1:B:8:GLU:H	1:B:8:GLU:CD	2.20	0.44
1:D:11:TRP:CE2	1:D:25:PRO:HG3	2.53	0.43
1:B:5:ARG:HG3	1:B:11:TRP:CZ3	2.53	0.43
1:C:91:ASN:HB2	2:C:296:HOH:O	2.18	0.43
1:D:178:LEU:HG	1:D:179:ASN:N	2.33	0.43
1:A:194:ARG:NE	2:A:296:HOH:O	2.23	0.43
1:D:18:LEU:C	1:D:18:LEU:HD23	2.39	0.43
1:D:76:PRO:HD2	1:D:212:TYR:CD2	2.54	0.43
1:B:74:LYS:HB2	1:B:74:LYS:HZ2	1.82	0.42
1:C:4:LEU:HD23	1:C:4:LEU:H	1.84	0.42
1:D:53:VAL:HG21	1:D:209:ILE:HD13	2.00	0.42
1:B:178:LEU:HG	1:B:179:ASN:N	2.34	0.42
1:A:15:GLU:OE1	1:A:15:GLU:HA	2.19	0.42
1:A:112:HIS:CE1	1:A:149:ARG:HG3	2.54	0.42
1:C:188:TYR:HB2	1:C:243:GLU:HB3	2.02	0.42
1:D:264:TRP:CD1	1:D:264:TRP:C	2.93	0.42
1:A:131:GLU:H	1:A:131:GLU:CD	2.24	0.41
1:B:150:ASP:OD1	1:B:150:ASP:N	2.53	0.41
1:D:11:TRP:CZ2	1:D:25:PRO:HG3	2.55	0.41
1:D:88:ARG:NH1	2:D:265:HOH:O	2.53	0.41
1:B:114:GLU:HG2	1:B:233:VAL:HG22	2.01	0.41
1:B:174:LEU:C	1:B:174:LEU:HD12	2.41	0.41
1:C:195:GLN:HG2	1:C:232:GLY:HA3	2.02	0.41
1:C:103:PRO:O	1:C:105:PRO:HD3	2.20	0.41
1:C:105:PRO:HB3	1:C:107:PHE:CE2	2.56	0.41
1:C:181:GLN:NE2	1:C:181:GLN:HA	2.36	0.40
1:B:152:GLN:HB2	1:B:161:ALA:HB1	2.03	0.40
1:C:216:PHE:CE2	1:D:160:ARG:HB3	2.56	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	247/264 (94%)	231 (94%)	15 (6%)	1 (0%)	34 37
1	B	245/264 (93%)	230 (94%)	14 (6%)	1 (0%)	34 37
1	C	245/264 (93%)	234 (96%)	11 (4%)	0	100 100
1	D	243/264 (92%)	231 (95%)	10 (4%)	2 (1%)	19 19
All	All	980/1056 (93%)	926 (94%)	50 (5%)	4 (0%)	34 37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	55	ARG
1	A	95	PRO
1	B	95	PRO
1	D	233	VAL

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	212/223 (95%)	207 (98%)	5 (2%)	49 62
1	B	210/223 (94%)	203 (97%)	7 (3%)	38 49
1	C	210/223 (94%)	205 (98%)	5 (2%)	49 62
1	D	208/223 (93%)	206 (99%)	2 (1%)	76 86
All	All	840/892 (94%)	821 (98%)	19 (2%)	50 63

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	A	149	ARG
1	A	173	TRP
1	A	259	LYS
1	A	262	ARG
1	B	33	ARG
1	B	74	LYS
1	B	93	ARG
1	B	149	ARG
1	B	154	LYS
1	B	156	LEU
1	B	173	TRP
1	C	135	ASP
1	C	149	ARG
1	C	173	TRP
1	C	231	GLU
1	C	237	ARG
1	D	4	LEU
1	D	149	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	C	112	HIS
1	D	28	ASN
1	D	112	HIS
1	D	127	HIS
1	D	201	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

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	251/264 (95%)	-0.24	3 (1%)	79	77	26, 35, 52, 73	0
1	B	249/264 (94%)	0.02	18 (7%)	15	14	28, 39, 63, 85	0
1	C	249/264 (94%)	-0.09	8 (3%)	47	45	26, 38, 57, 78	0
1	D	247/264 (93%)	-0.08	6 (2%)	59	56	25, 37, 61, 85	0
All	All	996/1056 (94%)	-0.10	35 (3%)	44	42	25, 37, 60, 85	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	LEU	5.3
1	D	264	TRP	5.2
1	B	231	GLU	4.9
1	C	264	TRP	4.8
1	D	263	PRO	4.5
1	B	262	ARG	4.3
1	B	74	LYS	4.0
1	A	264	TRP	4.0
1	D	55	ARG	3.7
1	B	106	PHE	3.7
1	C	262	ARG	3.5
1	C	74	LYS	3.5
1	C	106	PHE	3.4
1	B	264	TRP	3.3
1	B	226	LEU	3.2
1	C	231	GLU	3.1
1	D	262	ARG	3.1
1	A	262	ARG	2.9
1	C	184	TRP	2.9
1	B	142	VAL	2.8
1	B	55	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	51	VAL	2.5
1	D	231	GLU	2.5
1	D	106	PHE	2.4
1	B	144	VAL	2.4
1	B	263	PRO	2.3
1	B	141	THR	2.3
1	B	146	ILE	2.3
1	C	73	PRO	2.2
1	B	143	ALA	2.2
1	B	154	LYS	2.2
1	B	118	ALA	2.1
1	B	227	THR	2.1
1	B	184	TRP	2.1
1	B	8	GLU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.