Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:27 AM GMT

PDB ID	:	2AHU
Title	:	Crystal structure of Acyl-CoA transferase (YdiF) apoenzyme from Escherichia coli O157:H7.
Authors	:	Rangarajan, E.S.; Li, Y.; Ajamian, E.; Iannuzzi, P.; Kernaghan, S.D.; Fraser, M.E.; Cygler, M.; Matte, A.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2005-07-28
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

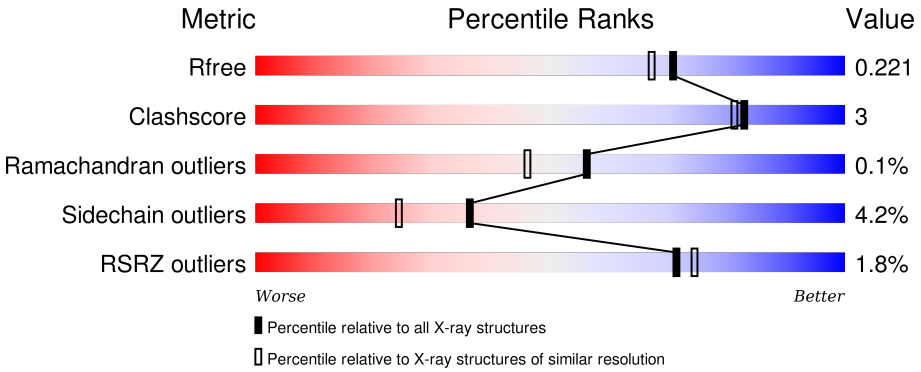
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	531	2% 85% 12%
1	B	531	2% 83% 13%
1	C	531	2% 84% 12%
1	D	531	% 83% 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16967 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 putative enzyme ydiF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	Se	0	0	0
			3924	2497	669	742	6	10			
1	B	515	Total	C	N	O	S	Se	0	0	0
			3924	2497	669	742	6	10			
1	C	515	Total	C	N	O	S	Se	0	0	0
			3924	2497	669	742	6	10			
1	D	515	Total	C	N	O	S	Se	0	0	0
			3924	2497	669	742	6	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
A	204	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
A	223	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
A	224	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
A	229	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
A	299	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
A	359	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
A	397	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
A	499	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
A	512	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
A	522	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
B	204	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
B	223	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
B	224	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
B	229	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
B	299	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
B	359	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
B	397	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
B	499	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
B	512	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	522	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
C	204	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
C	223	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
C	224	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
C	229	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
C	299	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
C	359	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
C	397	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
C	499	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
C	512	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
C	522	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
D	204	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
D	223	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
D	224	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
D	229	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
D	299	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
D	359	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
D	397	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
D	499	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
D	512	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6
D	522	MSE	MET	MODIFIED RESIDUE	UNP Q8X5X6

- Molecule 2 is water.

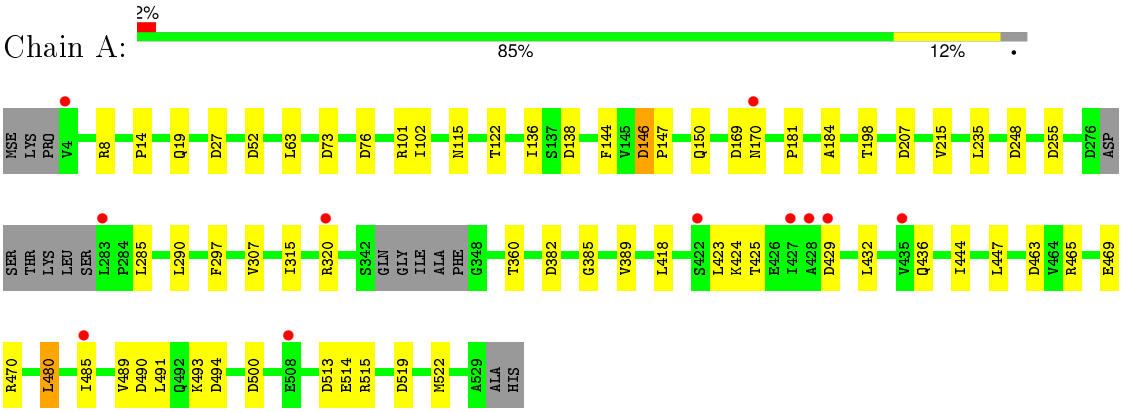
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	291	Total O 291 291	0	0
2	B	285	Total O 285 285	0	0
2	C	362	Total O 362 362	0	0
2	D	333	Total O 333 333	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

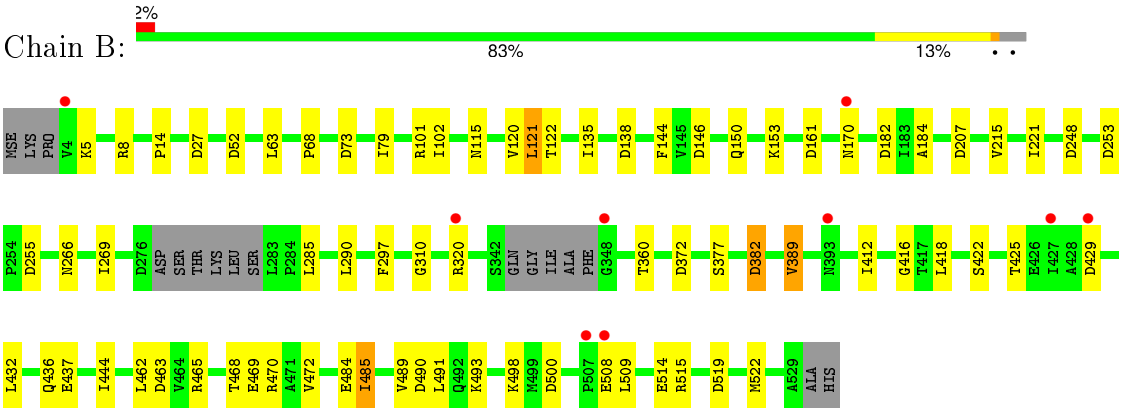
- Molecule 1: putative enzyme ydiF

Chain A:



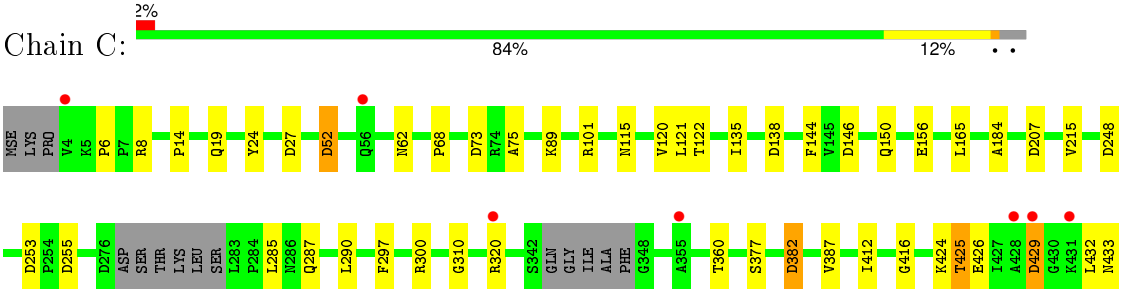
- Molecule 1: putative enzyme ydiF

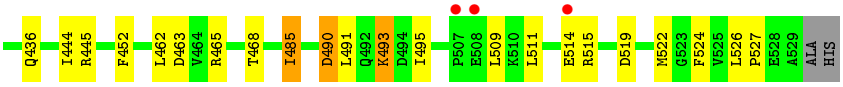
Chain B:



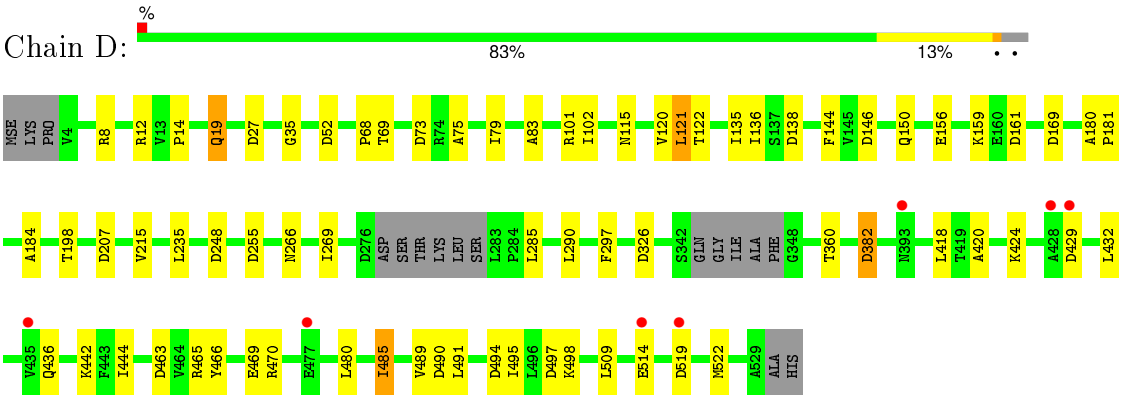
- Molecule 1: putative enzyme ydiF

Chain C:





- Molecule 1: putative enzyme ydiF



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.13Å 133.31Å 105.84Å 90.00° 100.57° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 40.86 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-1.90) 94.3 (40.86-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.220 0.188 , 0.221	Depositor DCC
R_{free} test set	15015 reflections (10.09%)	DCC
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 163804 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16967	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.40	0/3980	0.77	15/5372 (0.3%)
1	B	0.40	0/3980	0.75	16/5372 (0.3%)
1	C	0.42	0/3980	0.77	14/5372 (0.3%)
1	D	0.42	0/3980	0.75	16/5372 (0.3%)
All	All	0.41	0/15920	0.76	61/21488 (0.3%)

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	ASP	CB-CG-OD2	7.38	124.95	118.30
1	C	138	ASP	CB-CG-OD2	7.37	124.93	118.30
1	D	463	ASP	CB-CG-OD2	7.25	124.82	118.30
1	D	27	ASP	CB-CG-OD2	7.16	124.75	118.30
1	C	27	ASP	CB-CG-OD2	6.91	124.52	118.30
1	B	73	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	463	ASP	CB-CG-OD2	6.65	124.29	118.30
1	B	146	ASP	CB-CG-OD2	6.63	124.27	118.30
1	C	463	ASP	CB-CG-OD2	6.62	124.25	118.30
1	B	519	ASP	CB-CG-OD2	6.61	124.24	118.30
1	C	207	ASP	CB-CG-OD2	6.60	124.24	118.30
1	C	146	ASP	CB-CG-OD2	6.59	124.23	118.30
1	D	382	ASP	CB-CG-OD2	6.42	124.08	118.30
1	D	138	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	146	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	248	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	207	ASP	CB-CG-OD2	6.38	124.04	118.30
1	D	519	ASP	CB-CG-OD2	6.38	124.04	118.30
1	C	429	ASP	CB-CG-OD2	6.34	124.01	118.30
1	C	382	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	382	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	207	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	73	ASP	CB-CG-OD2	6.29	123.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	27	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	248	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	519	ASP	CB-CG-OD2	6.18	123.86	118.30
1	D	146	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	382	ASP	CB-CG-OD2	6.10	123.79	118.30
1	D	429	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	429	ASP	CB-CG-OD2	6.07	123.77	118.30
1	B	429	ASP	CB-CG-OD2	5.97	123.68	118.30
1	B	463	ASP	CB-CG-OD2	5.88	123.59	118.30
1	C	52	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	73	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	519	ASP	CB-CG-OD2	5.85	123.56	118.30
1	D	248	ASP	CB-CG-OD2	5.73	123.46	118.30
1	D	207	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	248	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	52	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	138	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	490	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	27	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	490	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	490	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	255	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	76	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	169	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	255	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	253	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	253	ASP	CB-CG-OD2	5.21	122.98	118.30
1	D	255	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	161	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	372	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	255	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	513	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	169	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	490	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	497	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	182	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	326	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	73	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3924	0	3981	20	0
1	B	3924	0	3981	25	0
1	C	3924	0	3981	26	0
1	D	3924	0	3981	27	0
2	A	291	0	0	0	0
2	B	285	0	0	0	0
2	C	362	0	0	0	0
2	D	333	0	0	0	0
All	All	16967	0	15924	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 3.

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:D:485:ILE:HD11	1:D:509:LEU:HD11	1.48	0.94
1:A:297:PHE:CZ	1:A:522:MSE:HE1	2.23	0.74
1:C:297:PHE:CZ	1:C:522:MSE:HE1	2.26	0.71
1:C:514:GLU:CD	1:C:514:GLU:H	1.95	0.69
1:C:8:ARG:HG2	1:C:14:PRO:HD3	1.76	0.68
1:D:297:PHE:CE1	1:D:522:MSE:HE1	2.29	0.68
1:C:184:ALA:HB2	1:C:215:VAL:HG21	1.76	0.66
1:B:297:PHE:HZ	1:B:522:MSE:HE1	1.59	0.66
1:C:120:VAL:HG13	1:C:135:ILE:HD11	1.79	0.65
1:B:297:PHE:CZ	1:B:522:MSE:HE1	2.35	0.62
1:A:144:PHE:HB2	1:A:150:GLN:HE21	1.64	0.61
1:B:515:ARG:HB2	1:B:522:MSE:HE3	1.82	0.61
1:D:8:ARG:HG2	1:D:14:PRO:HD3	1.82	0.61
1:D:297:PHE:CZ	1:D:522:MSE:HE1	2.36	0.61
1:D:120:VAL:HG13	1:D:135:ILE:HD11	1.82	0.61
1:D:144:PHE:HB2	1:D:150:GLN:HE21	1.67	0.60
1:A:297:PHE:CE1	1:A:522:MSE:HE1	2.37	0.60
1:D:184:ALA:HB2	1:D:215:VAL:HG21	1.83	0.59
1:D:266:ASN:HB3	1:D:269:ILE:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLU:H	1:A:514:GLU:CD	2.06	0.58
1:A:297:PHE:HZ	1:A:522:MSE:HE1	1.67	0.58
1:B:184:ALA:HB2	1:B:215:VAL:HG21	1.84	0.58
1:C:297:PHE:HZ	1:C:522:MSE:HE1	1.69	0.58
1:C:144:PHE:HB2	1:C:150:GLN:HE21	1.69	0.57
1:B:79:ILE:O	1:B:102:ILE:HD11	2.05	0.57
1:A:8:ARG:HG2	1:A:14:PRO:HD3	1.86	0.56
1:B:485:ILE:HG12	1:B:509:LEU:HD11	1.88	0.56
1:A:198:THR:HG23	1:A:235:LEU:HD13	1.88	0.56
1:C:122:THR:HG23	1:C:360:THR:HG23	1.87	0.56
1:A:184:ALA:HB2	1:A:215:VAL:HG21	1.87	0.56
1:B:144:PHE:HB2	1:B:150:GLN:HE21	1.70	0.55
1:B:5:LYS:HG2	1:B:221:ILE:HG12	1.88	0.55
1:C:62:ASN:HB3	1:C:89:LYS:HD2	1.89	0.55
1:C:297:PHE:CE1	1:C:522:MSE:HE1	2.41	0.55
1:B:122:THR:HG23	1:B:360:THR:HG23	1.89	0.54
1:B:472:VAL:HB	1:B:484:GLU:HB2	1.90	0.54
1:A:515:ARG:HB2	1:A:522:MSE:HE3	1.90	0.54
1:D:156:GLU:O	1:D:159:LYS:HE3	2.08	0.53
1:A:181:PRO:HB2	1:A:215:VAL:HG22	1.91	0.53
1:C:515:ARG:HB2	1:C:522:MSE:HE3	1.91	0.53
1:D:68:PRO:HA	1:D:121:LEU:HD13	1.90	0.52
1:C:424:LYS:HB2	1:C:436:GLN:HB3	1.91	0.52
1:B:444:ILE:HA	1:B:500:ASP:HB2	1.92	0.51
1:A:489:VAL:HG13	1:A:494:ASP:HB2	1.92	0.51
1:C:310:GLY:HA3	1:C:377:SER:OG	2.11	0.51
1:C:300:ARG:HD3	1:C:527:PRO:HB2	1.93	0.51
1:D:418:LEU:HD22	1:D:470:ARG:HD2	1.92	0.50
1:A:424:LYS:HB2	1:A:436:GLN:HB3	1.94	0.50
1:D:79:ILE:HD12	1:D:102:ILE:HD13	1.92	0.50
1:D:19:GLN:H	1:D:19:GLN:NE2	2.09	0.49
1:B:120:VAL:HG13	1:B:135:ILE:HD11	1.94	0.49
1:C:416:GLY:O	1:C:468:THR:HA	2.13	0.48
1:D:489:VAL:HG13	1:D:494:ASP:HB2	1.95	0.48
1:B:8:ARG:HG2	1:B:14:PRO:HD3	1.95	0.47
1:C:412:ILE:HD11	1:C:462:LEU:HD13	1.95	0.47
1:D:297:PHE:HE1	1:D:522:MSE:HE1	1.77	0.47
1:D:35:GLY:O	1:D:69:THR:HB	2.14	0.47
1:D:382:ASP:HA	1:D:444:ILE:O	2.15	0.47
1:C:490:ASP:HB3	1:C:493:LYS:HG2	1.97	0.47
1:C:426:GLU:HG2	1:C:433:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:GLU:CD	1:B:514:GLU:H	2.18	0.47
1:B:382:ASP:HA	1:B:444:ILE:O	2.15	0.46
1:C:382:ASP:HA	1:C:444:ILE:O	2.16	0.46
1:D:122:THR:HG23	1:D:360:THR:HG23	1.97	0.46
1:A:444:ILE:HD11	1:A:447:LEU:HD23	1.97	0.46
1:A:418:LEU:HD22	1:A:470:ARG:HD2	1.97	0.45
1:B:310:GLY:HA3	1:B:377:SER:OG	2.17	0.45
1:A:136:ILE:HD11	1:D:136:ILE:HD11	1.97	0.45
1:C:68:PRO:HA	1:C:121:LEU:HD13	1.99	0.44
1:B:68:PRO:HA	1:B:121:LEU:HD13	2.00	0.44
1:C:6:PRO:HD3	1:C:24:TYR:CE1	2.53	0.44
1:D:424:LYS:HB2	1:D:436:GLN:HB3	2.00	0.44
1:A:307:VAL:HG21	1:A:315:ILE:CG2	2.47	0.44
1:D:83:ALA:HB2	1:D:102:ILE:HG13	2.01	0.43
1:C:387:VAL:HB	1:C:452:PHE:HB3	1.99	0.43
1:A:122:THR:HG23	1:A:360:THR:HG23	2.00	0.43
1:D:198:THR:HG23	1:D:235:LEU:HD13	2.00	0.43
1:C:485:ILE:HG23	1:C:495:ILE:CD1	2.48	0.43
1:C:19:GLN:NE2	1:C:19:GLN:H	2.15	0.43
1:B:416:GLY:O	1:B:468:THR:HA	2.19	0.43
1:A:385:GLY:HA2	1:A:480:LEU:HD21	2.00	0.43
1:B:412:ILE:HD11	1:B:462:LEU:HD13	2.01	0.43
1:D:485:ILE:HG23	1:D:495:ILE:CD1	2.48	0.42
1:D:466:TYR:CE1	1:D:480:LEU:HD21	2.54	0.42
1:B:437:GLU:HG2	1:B:498:LYS:HE2	2.00	0.42
1:B:266:ASN:HB3	1:B:269:ILE:HD12	2.02	0.42
1:D:514:GLU:H	1:D:514:GLU:CD	2.23	0.42
1:B:153:LYS:NZ	1:B:161:ASP:OD1	2.50	0.41
1:C:287:GLN:HE21	1:C:425:THR:HB	1.85	0.41
1:C:524:PHE:CE1	1:C:526:LEU:HD23	2.55	0.41
1:D:420:ALA:HB2	1:D:442:LYS:HD2	2.01	0.41
1:B:515:ARG:CB	1:B:522:MSE:HE3	2.50	0.41
1:B:418:LEU:HD22	1:B:470:ARG:HD2	2.02	0.41
1:D:180:ALA:HA	1:D:181:PRO:HD3	1.90	0.40
1:A:444:ILE:HA	1:A:500:ASP:HB2	2.04	0.40
1:A:146:ASP:HA	1:A:147:PRO:HD3	1.99	0.40
1:B:422:SER:HB3	1:B:436:GLN:OE1	2.21	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	509/531 (96%)	499 (98%)	10 (2%)	0	100	100
1	B	509/531 (96%)	495 (97%)	13 (3%)	1 (0%)	52	42
1	C	509/531 (96%)	497 (98%)	11 (2%)	1 (0%)	52	42
1	D	509/531 (96%)	497 (98%)	11 (2%)	1 (0%)	52	42
All	All	2036/2124 (96%)	1988 (98%)	45 (2%)	3 (0%)	56	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	75	ALA
1	C	75	ALA
1	B	389	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	418/420 (100%)	398 (95%)	20 (5%)	31	19
1	B	418/420 (100%)	400 (96%)	18 (4%)	35	23
1	C	418/420 (100%)	400 (96%)	18 (4%)	35	23
1	D	418/420 (100%)	404 (97%)	14 (3%)	45	34
All	All	1672/1680 (100%)	1602 (96%)	70 (4%)	36	24

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	52	ASP
1	A	63	LEU
1	A	101	ARG
1	A	102	ILE
1	A	115	ASN
1	A	170	ASN
1	A	285	LEU
1	A	290	LEU
1	A	320	ARG
1	A	389	VAL
1	A	423	LEU
1	A	425	THR
1	A	432	LEU
1	A	465	ARG
1	A	469	GLU
1	A	480	LEU
1	A	485	ILE
1	A	491	LEU
1	A	493	LYS
1	B	63	LEU
1	B	101	ARG
1	B	115	ASN
1	B	121	LEU
1	B	170	ASN
1	B	285	LEU
1	B	290	LEU
1	B	320	ARG
1	B	389	VAL
1	B	425	THR
1	B	432	LEU
1	B	465	ARG
1	B	469	GLU
1	B	485	ILE
1	B	489	VAL
1	B	491	LEU
1	B	493	LYS
1	B	508	GLU
1	C	52	ASP
1	C	101	ARG
1	C	115	ASN
1	C	156	GLU
1	C	165	LEU

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Mol	Chain	Res	Type
1	C	285	LEU
1	C	290	LEU
1	C	320	ARG
1	C	425	THR
1	C	429	ASP
1	C	432	LEU
1	C	445	ARG
1	C	465	ARG
1	C	485	ILE
1	C	491	LEU
1	C	493	LYS
1	C	509	LEU
1	C	511	LEU
1	D	12	ARG
1	D	19	GLN
1	D	52	ASP
1	D	101	ARG
1	D	115	ASN
1	D	121	LEU
1	D	285	LEU
1	D	290	LEU
1	D	432	LEU
1	D	465	ARG
1	D	469	GLU
1	D	485	ILE
1	D	491	LEU
1	D	498	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	150	GLN
1	A	287	GLN
1	A	350	ASN
1	B	150	GLN
1	B	287	GLN
1	B	350	ASN
1	C	19	GLN
1	C	150	GLN
1	C	287	GLN
1	C	350	ASN

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Mol	Chain	Res	Type
1	C	383	GLN
1	C	436	GLN
1	D	19	GLN
1	D	150	GLN
1	D	350	ASN

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 carbohydrates 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	505/531 (95%)	0.05	11 (2%) 65 68	16, 26, 41, 58	0
1	B	505/531 (95%)	-0.02	9 (1%) 71 74	16, 25, 45, 54	0
1	C	505/531 (95%)	-0.06	10 (1%) 68 71	17, 24, 36, 44	0
1	D	505/531 (95%)	-0.06	7 (1%) 78 80	15, 23, 41, 51	0
All	All	2020/2124 (95%)	-0.02	37 (1%) 71 74	15, 25, 41, 58	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	VAL	5.6
1	A	428	ALA	5.5
1	A	429	ASP	4.0
1	B	429	ASP	3.7
1	B	393	ASN	3.6
1	C	508	GLU	3.5
1	C	429	ASP	3.5
1	D	429	ASP	3.2
1	B	4	VAL	3.2
1	A	435	VAL	2.6
1	B	507	PRO	2.5
1	D	393	ASN	2.4
1	A	427	ILE	2.4
1	A	170	ASN	2.4
1	B	170	ASN	2.4
1	D	435	VAL	2.4
1	C	428	ALA	2.3
1	C	431	LYS	2.3
1	A	485	ILE	2.3
1	D	428	ALA	2.3
1	A	283	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	56	GLN	2.3
1	D	514	GLU	2.2
1	C	507	PRO	2.2
1	B	427	ILE	2.1
1	C	514	GLU	2.1
1	A	508	GLU	2.1
1	A	4	VAL	2.1
1	D	519	ASP	2.1
1	A	422	SER	2.1
1	A	320	ARG	2.1
1	C	320	ARG	2.1
1	B	348	GLY	2.1
1	C	355	ALA	2.0
1	B	320	ARG	2.0
1	B	508	GLU	2.0
1	D	477	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 carbohydrates 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.