Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 04:48 AM EDT

PDB ID	:	3E9N / pdb_00003e9n
Title	:	Crystal structure of a putative short-chain dehydrogenase/reductase from Corynebacterium glutamicum
Authors	:	Bonanno, J.B.; Gilmore, M.; Bain, K.T.; Hu, S.; Romero, R.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-08-22
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:

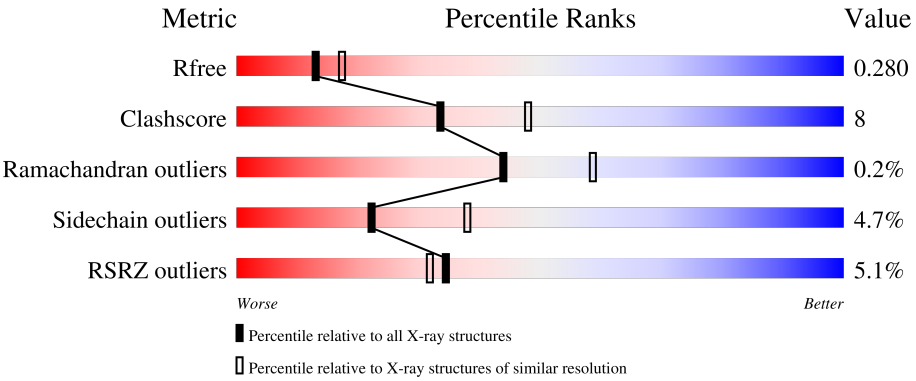
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (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	245	2% 59% 18% 23%
1	B	245	% 61% 12% • 26%
1	C	245	4% 60% 12% • 26%
1	D	245	4% 54% 18% • 27%
1	E	245	6% 61% 12% • 26%

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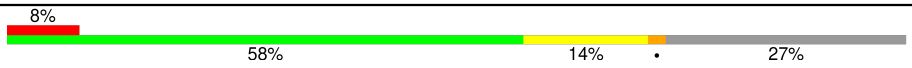
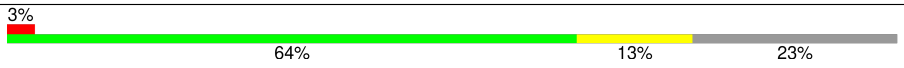
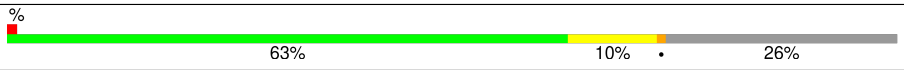
Mol	Chain	Length	Quality of chain
1	F	245	
1	G	245	
1	H	245	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10879 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 SHORT-CHAIN DEHYDROGENASE/REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	1	0
			1397	881	248	265	3			
1	B	181	Total	C	N	O	S	0	1	0
			1339	845	239	252	3			
1	C	181	Total	C	N	O	S	0	1	0
			1334	838	236	257	3			
1	D	180	Total	C	N	O	S	0	1	0
			1315	829	235	248	3			
1	E	182	Total	C	N	O	S	0	1	0
			1331	837	237	254	3			
1	F	180	Total	C	N	O	S	0	1	0
			1319	831	234	251	3			
1	G	189	Total	C	N	O	S	0	1	0
			1386	876	247	260	3			
1	H	181	Total	C	N	O	S	0	1	0
			1331	838	237	253	3			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q8NMW9
A	0	SER	-	expression tag	UNP Q8NMW9
A	1	LEU	-	expression tag	UNP Q8NMW9
A	236	GLU	-	expression tag	UNP Q8NMW9
A	237	GLY	-	expression tag	UNP Q8NMW9
A	238	HIS	-	expression tag	UNP Q8NMW9
A	239	HIS	-	expression tag	UNP Q8NMW9
A	240	HIS	-	expression tag	UNP Q8NMW9
A	241	HIS	-	expression tag	UNP Q8NMW9
A	242	HIS	-	expression tag	UNP Q8NMW9
A	243	HIS	-	expression tag	UNP Q8NMW9
B	-1	MET	-	expression tag	UNP Q8NMW9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP Q8NMW9
B	1	LEU	-	expression tag	UNP Q8NMW9
B	236	GLU	-	expression tag	UNP Q8NMW9
B	237	GLY	-	expression tag	UNP Q8NMW9
B	238	HIS	-	expression tag	UNP Q8NMW9
B	239	HIS	-	expression tag	UNP Q8NMW9
B	240	HIS	-	expression tag	UNP Q8NMW9
B	241	HIS	-	expression tag	UNP Q8NMW9
B	242	HIS	-	expression tag	UNP Q8NMW9
B	243	HIS	-	expression tag	UNP Q8NMW9
C	-1	MET	-	expression tag	UNP Q8NMW9
C	0	SER	-	expression tag	UNP Q8NMW9
C	1	LEU	-	expression tag	UNP Q8NMW9
C	236	GLU	-	expression tag	UNP Q8NMW9
C	237	GLY	-	expression tag	UNP Q8NMW9
C	238	HIS	-	expression tag	UNP Q8NMW9
C	239	HIS	-	expression tag	UNP Q8NMW9
C	240	HIS	-	expression tag	UNP Q8NMW9
C	241	HIS	-	expression tag	UNP Q8NMW9
C	242	HIS	-	expression tag	UNP Q8NMW9
C	243	HIS	-	expression tag	UNP Q8NMW9
D	-1	MET	-	expression tag	UNP Q8NMW9
D	0	SER	-	expression tag	UNP Q8NMW9
D	1	LEU	-	expression tag	UNP Q8NMW9
D	236	GLU	-	expression tag	UNP Q8NMW9
D	237	GLY	-	expression tag	UNP Q8NMW9
D	238	HIS	-	expression tag	UNP Q8NMW9
D	239	HIS	-	expression tag	UNP Q8NMW9
D	240	HIS	-	expression tag	UNP Q8NMW9
D	241	HIS	-	expression tag	UNP Q8NMW9
D	242	HIS	-	expression tag	UNP Q8NMW9
D	243	HIS	-	expression tag	UNP Q8NMW9
E	-1	MET	-	expression tag	UNP Q8NMW9
E	0	SER	-	expression tag	UNP Q8NMW9
E	1	LEU	-	expression tag	UNP Q8NMW9
E	236	GLU	-	expression tag	UNP Q8NMW9
E	237	GLY	-	expression tag	UNP Q8NMW9
E	238	HIS	-	expression tag	UNP Q8NMW9
E	239	HIS	-	expression tag	UNP Q8NMW9
E	240	HIS	-	expression tag	UNP Q8NMW9
E	241	HIS	-	expression tag	UNP Q8NMW9
E	242	HIS	-	expression tag	UNP Q8NMW9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	243	HIS	-	expression tag	UNP Q8NMW9
F	-1	MET	-	expression tag	UNP Q8NMW9
F	0	SER	-	expression tag	UNP Q8NMW9
F	1	LEU	-	expression tag	UNP Q8NMW9
F	236	GLU	-	expression tag	UNP Q8NMW9
F	237	GLY	-	expression tag	UNP Q8NMW9
F	238	HIS	-	expression tag	UNP Q8NMW9
F	239	HIS	-	expression tag	UNP Q8NMW9
F	240	HIS	-	expression tag	UNP Q8NMW9
F	241	HIS	-	expression tag	UNP Q8NMW9
F	242	HIS	-	expression tag	UNP Q8NMW9
F	243	HIS	-	expression tag	UNP Q8NMW9
G	-1	MET	-	expression tag	UNP Q8NMW9
G	0	SER	-	expression tag	UNP Q8NMW9
G	1	LEU	-	expression tag	UNP Q8NMW9
G	236	GLU	-	expression tag	UNP Q8NMW9
G	237	GLY	-	expression tag	UNP Q8NMW9
G	238	HIS	-	expression tag	UNP Q8NMW9
G	239	HIS	-	expression tag	UNP Q8NMW9
G	240	HIS	-	expression tag	UNP Q8NMW9
G	241	HIS	-	expression tag	UNP Q8NMW9
G	242	HIS	-	expression tag	UNP Q8NMW9
G	243	HIS	-	expression tag	UNP Q8NMW9
H	-1	MET	-	expression tag	UNP Q8NMW9
H	0	SER	-	expression tag	UNP Q8NMW9
H	1	LEU	-	expression tag	UNP Q8NMW9
H	236	GLU	-	expression tag	UNP Q8NMW9
H	237	GLY	-	expression tag	UNP Q8NMW9
H	238	HIS	-	expression tag	UNP Q8NMW9
H	239	HIS	-	expression tag	UNP Q8NMW9
H	240	HIS	-	expression tag	UNP Q8NMW9
H	241	HIS	-	expression tag	UNP Q8NMW9
H	242	HIS	-	expression tag	UNP Q8NMW9
H	243	HIS	-	expression tag	UNP Q8NMW9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	32	Total O 32 32	0	0
2	B	24	Total O 24 24	0	0

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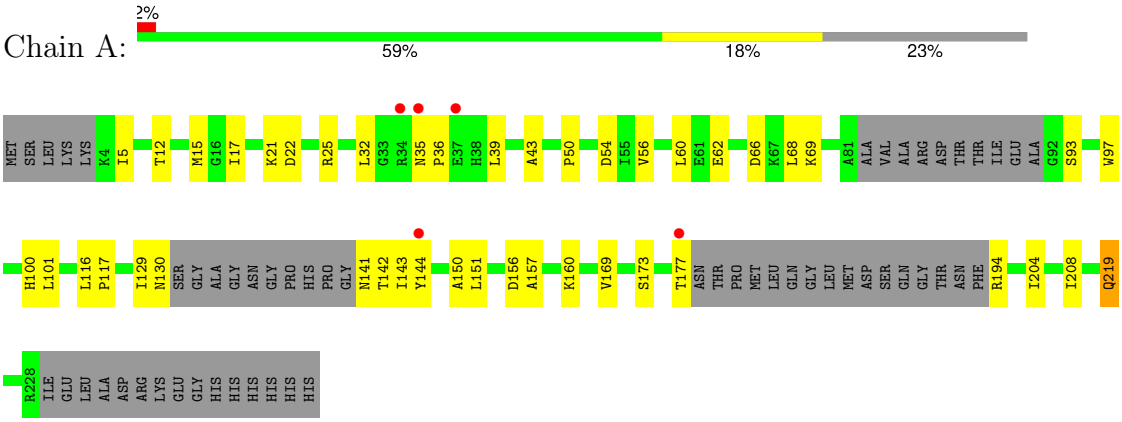
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	7	Total O 7 7	0	0
2	D	9	Total O 9 9	0	0
2	E	11	Total O 11 11	0	0
2	F	6	Total O 6 6	0	0
2	G	18	Total O 18 18	0	0
2	H	20	Total O 20 20	0	0

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.

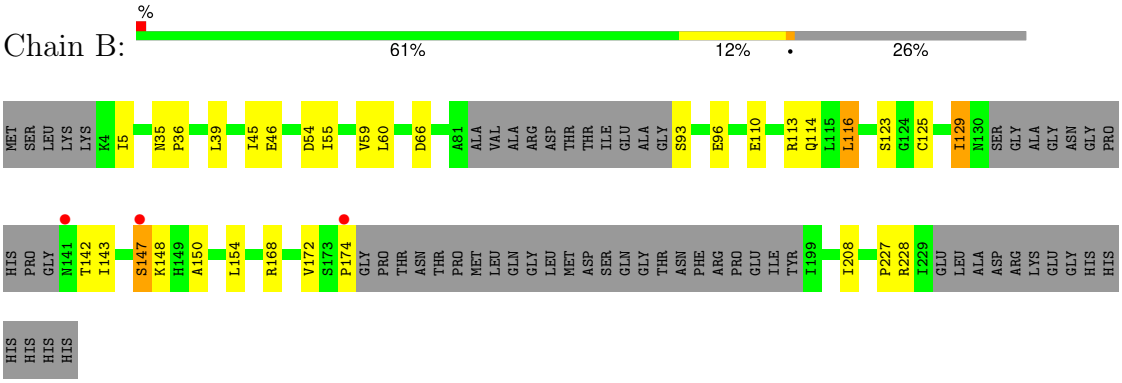
• Molecule 1: PUTATIVE SHORT-CHAIN DEHYDROGENASE/REDUCTASE

Chain A:



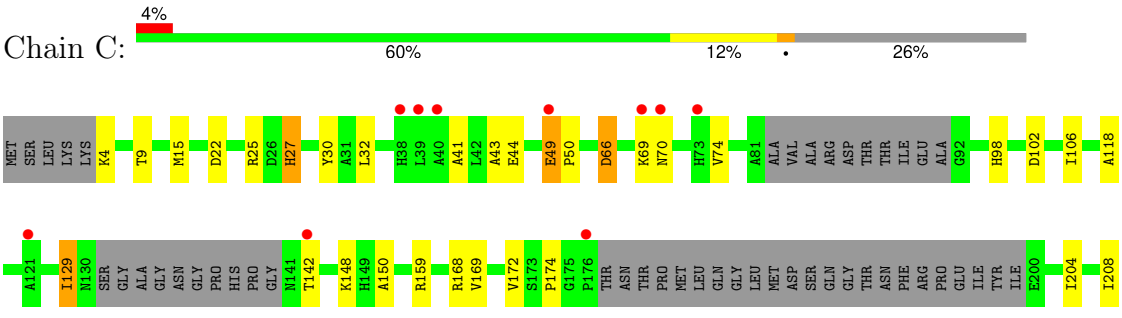
• Molecule 1: PUTATIVE SHORT-CHAIN DEHYDROGENASE/REDUCTASE

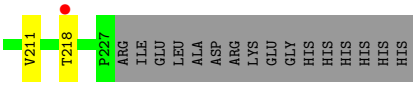
Chain B:



• Molecule 1: PUTATIVE SHORT-CHAIN DEHYDROGENASE/REDUCTASE

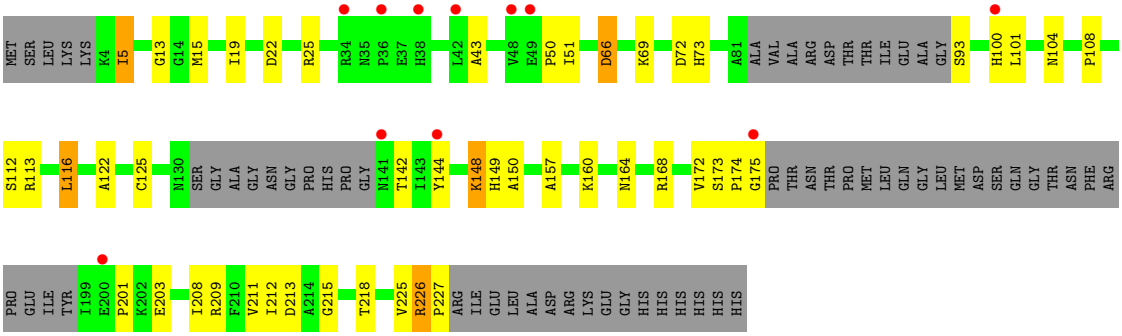
Chain C:





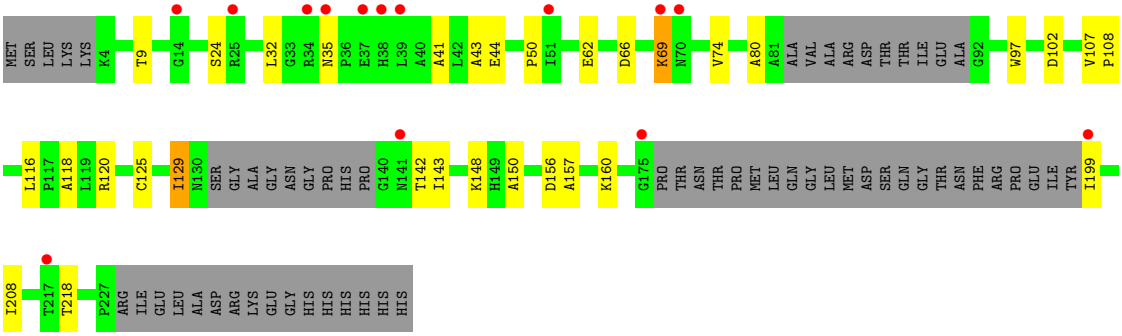
• Molecule 1: PUTATIVE SHORT-CHAIN DEHYDROGENASE/REDUCTASE

Chain D:



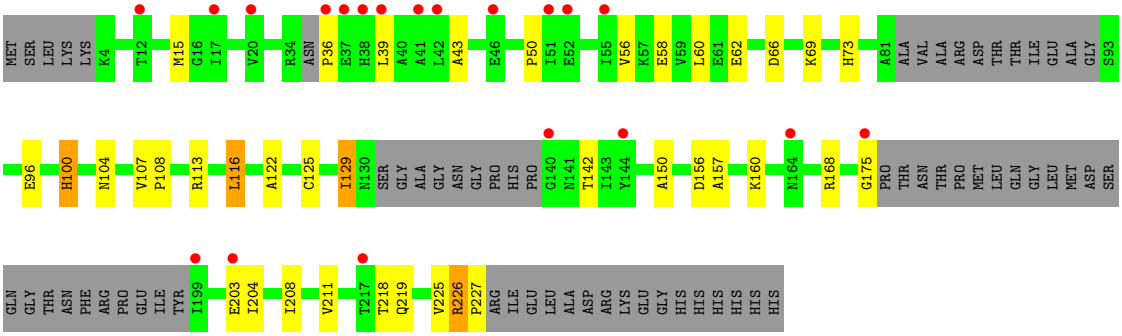
• Molecule 1: PUTATIVE SHORT-CHAIN DEHYDROGENASE/REDUCTASE

Chain E:



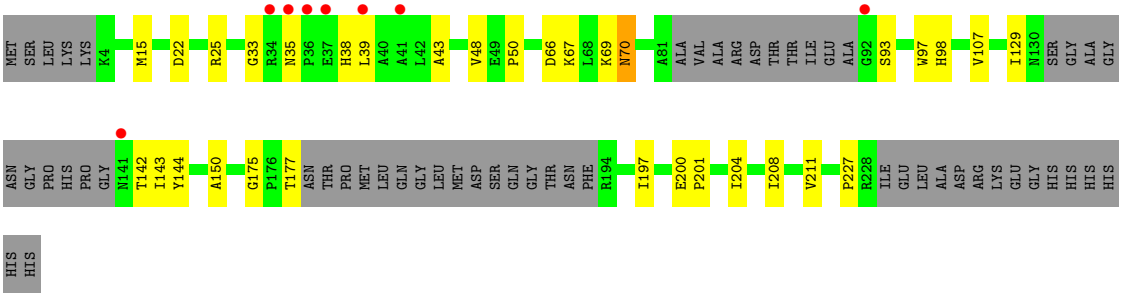
• Molecule 1: PUTATIVE SHORT-CHAIN DEHYDROGENASE/REDUCTASE

Chain F:



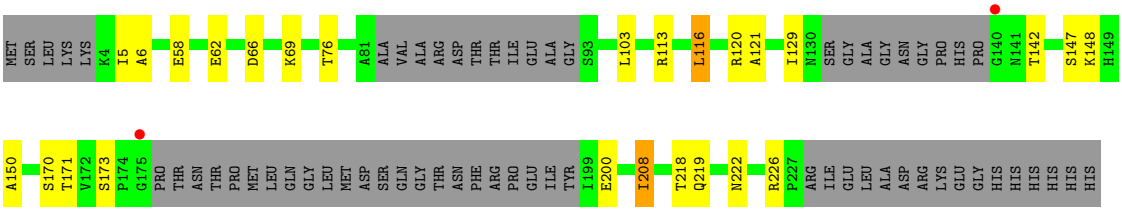
• Molecule 1: PUTATIVE SHORT-CHAIN DEHYDROGENASE/REDUCTASE

Chain G:



• Molecule 1: PUTATIVE SHORT-CHAIN DEHYDROGENASE/REDUCTASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	238.11Å 62.26Å 127.30Å 90.00° 99.19° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.40) 99.7 (20.00-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.276 0.232 , 0.280	Depositor DCC
R_{free} test set	3613 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10879	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9874e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	1.08	0/1420	1.12	4/1935 (0.2%)
1	B	1.04	1/1359 (0.1%)	1.14	2/1850 (0.1%)
1	C	0.88	0/1355	1.09	2/1846 (0.1%)
1	D	0.91	0/1335	1.06	2/1820 (0.1%)
1	E	0.94	0/1351	1.09	4/1840 (0.2%)
1	F	0.92	1/1338 (0.1%)	1.03	2/1820 (0.1%)
1	G	1.07	1/1409 (0.1%)	1.17	2/1921 (0.1%)
1	H	1.06	0/1351	1.14	2/1839 (0.1%)
All	All	0.99	3/10918 (0.0%)	1.11	20/14871 (0.1%)

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	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	154	LEU	C-O	5.63	1.30	1.24
1	G	107	VAL	CA-C	5.43	1.58	1.52
1	F	226	ARG	N-CA	5.37	1.50	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	211	VAL	N-CA-C	6.91	117.05	110.42
1	H	200	GLU	CA-C-N	6.75	127.01	119.32
1	H	200	GLU	C-N-CA	6.75	127.01	119.32
1	G	211	VAL	N-CA-C	5.93	116.71	110.72
1	G	38	HIS	N-CA-C	-5.82	104.90	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	ILE	N-CA-C	5.63	116.06	108.17
1	E	62	GLU	N-CA-C	5.58	120.24	113.38
1	E	129	ILE	CB-CA-C	-5.45	104.33	111.25
1	E	35	ASN	CA-C-N	5.44	125.05	119.56
1	E	35	ASN	C-N-CA	5.44	125.05	119.56
1	B	55	ILE	N-CA-C	5.42	116.19	110.72
1	F	129	ILE	CB-CA-C	-5.13	103.95	110.98
1	B	129	ILE	CB-CA-C	-5.11	104.76	111.25
1	C	129	ILE	CB-CA-C	-5.10	104.77	111.25
1	D	211	VAL	N-CA-C	5.09	115.31	110.42
1	F	211	VAL	N-CA-C	5.08	115.80	110.62
1	A	54	ASP	N-CA-C	-5.04	98.37	107.75
1	D	13	GLY	N-CA-C	-5.03	104.76	112.85
1	A	62	GLU	N-CA-C	5.02	119.05	113.02
1	A	68	LEU	N-CA-C	-5.00	107.21	113.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	27	HIS	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	A	1397	0	1391	26	0
1	B	1339	0	1343	17	0
1	C	1334	0	1322	16	0
1	D	1315	0	1307	28	0
1	E	1331	0	1321	19	0
1	F	1319	0	1312	31	0
1	G	1386	0	1379	18	0
1	H	1331	0	1329	16	0
2	A	32	0	0	2	0
2	B	24	0	0	0	0
2	C	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	9	0	0	2	0
2	E	11	0	0	1	0
2	F	6	0	0	2	0
2	G	18	0	0	0	0
2	H	20	0	0	1	0
All	All	10879	0	10704	162	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 8.

All (162) 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:157:ALA:HA	1:A:160:LYS:HE2	1.45	0.96
1:G:43:ALA:HB2	1:G:50:PRO:HG2	1.46	0.94
1:F:43:ALA:HB2	1:F:50:PRO:HG3	1.49	0.92
1:A:157:ALA:HA	1:A:160:LYS:CE	2.00	0.91
1:G:70:ASN:HD22	1:G:70:ASN:H	1.12	0.90
1:B:96:GLU:HG2	1:B:143:ILE:HD13	1.54	0.90
1:F:66:ASP:HA	1:F:69:LYS:HD2	1.55	0.87
1:A:66:ASP:HA	1:A:69:LYS:HD2	1.58	0.85
1:A:43:ALA:HB2	1:A:50:PRO:HG3	1.61	0.82
1:F:157:ALA:HA	1:F:160:LYS:CE	2.11	0.80
1:H:129:ILE:HD11	1:H:208:ILE:HD11	1.61	0.79
1:E:157:ALA:HA	1:E:160:LYS:CE	2.13	0.78
1:E:156:ASP:O	1:E:160:LYS:HE2	1.82	0.77
1:G:43:ALA:HB2	1:G:50:PRO:CG	2.14	0.77
1:D:43:ALA:HB2	1:D:50:PRO:HG3	1.66	0.77
1:F:157:ALA:HA	1:F:160:LYS:HE3	1.66	0.77
1:D:5:ILE:HD13	1:D:73:HIS:CE1	2.22	0.74
1:D:125[A]:CYS:SG	1:D:168:ARG:NH2	2.62	0.72
1:F:175:GLY:C	2:F:244:HOH:O	2.31	0.72
1:D:66:ASP:HA	1:D:69:LYS:HD2	1.72	0.71
1:E:150:ALA:HB2	1:G:150:ALA:HB2	1.73	0.70
1:E:157:ALA:HA	1:E:160:LYS:HE3	1.72	0.70
1:A:141:ASN:HB3	1:A:144:TYR:CD2	2.26	0.69
1:D:73:HIS:HB2	1:D:122:ALA:HB2	1.73	0.69
1:G:66:ASP:HA	1:G:69:LYS:HD2	1.73	0.69
1:B:129:ILE:HD11	1:B:208:ILE:HD11	1.73	0.69
1:C:218:THR:OG1	1:D:203:GLU:HG3	1.93	0.68
1:F:218:THR:HG22	1:F:219:GLN:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:HIS:HB2	1:F:122:ALA:HB2	1.76	0.68
1:G:70:ASN:H	1:G:70:ASN:ND2	1.88	0.68
1:C:30:TYR:CZ	1:C:49:GLU:OE1	2.47	0.67
1:D:175:GLY:O	1:D:227:PRO:HD3	1.94	0.67
1:F:218:THR:CG2	1:F:219:GLN:N	2.58	0.66
1:B:125[A]:CYS:SG	1:B:168:ARG:NH1	2.70	0.64
1:F:125[A]:CYS:SG	1:F:168:ARG:NH2	2.71	0.63
1:E:43:ALA:HB2	1:E:50:PRO:HG3	1.80	0.62
1:D:72:ASP:OD1	1:D:73:HIS:HD2	1.85	0.58
1:D:19:ILE:HG12	1:D:208:ILE:HD13	1.85	0.58
1:C:129:ILE:HD11	1:C:208:ILE:HD11	1.85	0.58
1:H:66:ASP:HA	1:H:69:LYS:HD2	1.84	0.58
1:H:218:THR:HG22	1:H:219:GLN:N	2.18	0.58
1:A:194:ARG:N	2:A:269:HOH:O	2.36	0.58
1:A:101:LEU:HD12	1:C:106:ILE:HD11	1.86	0.57
1:B:125[A]:CYS:SG	1:B:168:ARG:CZ	2.93	0.57
1:B:143:ILE:O	1:B:147:SER:OG	2.22	0.57
1:D:5:ILE:CD1	1:D:73:HIS:CE1	2.88	0.57
1:B:150:ALA:HB2	1:D:150:ALA:HB2	1.87	0.57
1:G:97:TRP:CE2	1:G:143:ILE:HG12	2.40	0.56
1:B:35:ASN:O	1:B:39:LEU:HG	2.04	0.56
1:A:22:ASP:OD1	1:A:25:ARG:NH1	2.38	0.56
1:F:150:ALA:HB2	1:H:150:ALA:HB2	1.87	0.56
1:F:157:ALA:HA	1:F:160:LYS:HE2	1.87	0.56
1:F:175:GLY:O	1:F:227:PRO:HD3	2.06	0.56
1:E:157:ALA:HA	1:E:160:LYS:HE2	1.86	0.55
1:D:100:HIS:NE2	1:D:144:TYR:HE1	2.04	0.55
1:A:56:VAL:HG13	1:A:60:LEU:HD12	1.88	0.55
1:A:100:HIS:NE2	1:A:144:TYR:HE1	2.05	0.55
1:F:218:THR:CG2	1:F:219:GLN:H	2.18	0.54
1:D:113:ARG:O	1:D:116:LEU:HB2	2.07	0.54
1:E:41:ALA:O	1:E:44:GLU:HG3	2.08	0.54
1:C:41:ALA:O	1:C:44:GLU:HB2	2.07	0.53
1:H:219:GLN:HG2	2:H:247:HOH:O	2.08	0.53
1:A:22:ASP:O	1:A:25:ARG:HD3	2.08	0.52
1:G:22:ASP:OD1	1:G:25:ARG:NH1	2.43	0.52
1:A:116:LEU:HB3	1:A:117:PRO:HD3	1.92	0.51
1:C:15:MET:HE2	1:C:204:ILE:HG13	1.92	0.51
1:A:100:HIS:NE2	1:A:144:TYR:CE1	2.78	0.51
1:D:209:ARG:HD2	1:D:213:ASP:OD2	2.10	0.51
1:F:58:GLU:HA	1:F:62:GLU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:ASP:CA	1:F:69:LYS:HD2	2.35	0.50
1:C:74:VAL:HG23	1:C:118:ALA:HB1	1.93	0.50
1:E:129:ILE:HD11	1:E:208:ILE:HD11	1.94	0.50
1:G:70:ASN:HD22	1:G:70:ASN:N	1.93	0.50
1:H:113:ARG:HA	1:H:116:LEU:HD22	1.93	0.49
1:A:17:ILE:O	1:A:21:LYS:HG3	2.12	0.49
1:B:113:ARG:O	1:B:116:LEU:HB2	2.13	0.49
1:D:227:PRO:C	2:D:246:HOH:O	2.56	0.49
1:D:172:VAL:O	1:D:174:PRO:HD3	2.13	0.49
1:F:15:MET:HE2	1:F:204:ILE:HG13	1.95	0.49
1:F:36:PRO:HA	1:F:39:LEU:HB2	1.93	0.49
1:D:15:MET:HA	1:D:201:PRO:HB3	1.95	0.48
1:H:103:LEU:O	1:H:103:LEU:HG	2.13	0.48
1:E:66:ASP:HA	1:E:69:LYS:CD	2.42	0.48
1:C:9:THR:HG22	1:C:32:LEU:HD22	1.96	0.48
1:D:22:ASP:OD1	1:D:25:ARG:NH1	2.44	0.48
1:F:129:ILE:HD11	1:F:208:ILE:HD11	1.96	0.48
1:F:107:VAL:HB	1:F:108:PRO:HD3	1.95	0.48
1:H:173:SER:O	1:H:226:ARG:NH2	2.47	0.48
1:E:199:ILE:HG23	1:F:218:THR:OG1	2.14	0.48
1:F:225:VAL:C	1:F:226:ARG:HD2	2.38	0.47
1:D:157:ALA:HA	1:D:160:LYS:HE2	1.96	0.47
1:G:33:GLY:HA3	1:G:39:LEU:HD21	1.96	0.47
1:C:4:LYS:HB2	1:C:27:HIS:CD2	2.49	0.47
1:C:30:TYR:CE1	1:C:49:GLU:OE1	2.68	0.47
1:E:97:TRP:CE2	1:E:143:ILE:HG12	2.49	0.47
1:H:58:GLU:HA	1:H:62:GLU:HB2	1.96	0.47
1:A:150:ALA:HB2	1:C:150:ALA:HB2	1.97	0.47
1:F:225:VAL:O	1:F:226:ARG:HD2	2.14	0.47
1:F:156:ASP:O	1:F:160:LYS:HE2	2.14	0.46
1:E:102:ASP:OD2	1:G:98:HIS:HE1	1.98	0.46
1:C:98:HIS:O	1:C:102:ASP:HB2	2.15	0.46
1:E:9:THR:O	1:E:80:ALA:HB3	2.15	0.46
1:H:218:THR:CG2	1:H:219:GLN:N	2.78	0.46
1:A:129:ILE:HD11	1:A:208:ILE:HD11	1.98	0.46
1:A:156:ASP:O	1:A:160:LYS:HE2	2.16	0.46
1:D:108:PRO:O	1:D:112:SER:OG	2.30	0.45
1:G:144:TYR:CD1	1:G:144:TYR:N	2.81	0.45
1:B:110:GLU:HG3	1:B:114:GLN:NE2	2.30	0.45
1:C:43:ALA:HB2	1:C:50:PRO:HG3	1.97	0.45
1:A:97:TRP:CE2	1:A:143:ILE:HG12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ASN:HA	1:B:36:PRO:HD3	1.74	0.45
1:F:227:PRO:C	2:F:245:HOH:O	2.60	0.45
1:A:32:LEU:HD12	1:A:32:LEU:N	2.31	0.45
1:D:148:LYS:HG3	1:D:149:HIS:N	2.30	0.45
1:E:116:LEU:O	1:E:120:ARG:HG3	2.17	0.45
1:D:50:PRO:C	1:D:51:ILE:HG13	2.41	0.45
1:E:218:THR:OG1	1:F:203:GLU:HG3	2.16	0.45
1:D:72:ASP:OD1	1:D:73:HIS:CD2	2.68	0.44
1:G:48:VAL:O	1:G:50:PRO:HD3	2.18	0.44
1:B:59:VAL:HG12	1:B:60:LEU:HD23	1.98	0.44
1:D:101:LEU:HD23	1:D:101:LEU:HA	1.90	0.44
1:A:35:ASN:HA	1:A:36:PRO:HD3	1.67	0.44
1:B:172:VAL:O	1:B:174:PRO:HD3	2.17	0.44
1:C:159:ARG:HB2	1:C:169:VAL:HB	1.98	0.44
1:E:160:LYS:HE3	2:E:248:HOH:O	2.17	0.44
1:D:100:HIS:ND1	1:D:104:ASN:ND2	2.66	0.44
1:F:66:ASP:HA	1:F:69:LYS:CD	2.39	0.43
1:F:100:HIS:ND1	1:F:104:ASN:ND2	2.66	0.43
1:G:35:ASN:O	1:G:39:LEU:HG	2.18	0.43
1:C:22:ASP:OD1	1:C:25:ARG:NH1	2.51	0.43
1:H:120:ARG:O	1:H:121:ALA:C	2.60	0.43
1:B:227:PRO:O	1:B:228:ARG:C	2.61	0.43
1:A:160:LYS:HE3	2:A:261:HOH:O	2.18	0.43
1:B:45:ILE:O	1:B:46:GLU:C	2.62	0.43
1:H:113:ARG:O	1:H:116:LEU:HB2	2.19	0.43
1:F:56:VAL:HG13	1:F:60:LEU:HD12	2.02	0.42
1:G:175:GLY:O	1:G:227:PRO:HD3	2.20	0.42
1:E:32:LEU:HD12	1:E:32:LEU:N	2.35	0.42
1:D:113:ARG:HA	1:D:116:LEU:HD22	2.01	0.42
1:F:113:ARG:O	1:F:116:LEU:HB2	2.20	0.42
1:D:225:VAL:O	1:D:226:ARG:HD3	2.20	0.42
1:C:172:VAL:O	1:C:174:PRO:HD3	2.20	0.42
1:G:129:ILE:HD11	1:G:208:ILE:HD11	2.02	0.42
1:B:54:ASP:OD1	1:B:54:ASP:C	2.63	0.42
1:A:12:THR:HG21	1:A:39:LEU:HG	2.01	0.42
1:H:171:THR:O	1:H:222:ASN:HA	2.20	0.42
1:H:218:THR:HG22	1:H:219:GLN:H	1.84	0.42
1:A:169:VAL:H	1:A:219:GLN:HE22	1.66	0.41
1:G:200:GLU:HA	1:G:201:PRO:HD2	1.92	0.41
1:B:129:ILE:CD1	1:B:208:ILE:HD11	2.46	0.41
1:H:6:ALA:HA	1:H:76:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:MET:HE2	1:A:204:ILE:HG13	2.03	0.41
1:A:130:ASN:CG	1:A:151:LEU:HD23	2.46	0.41
1:F:218:THR:HG23	1:F:219:GLN:H	1.84	0.41
1:E:74:VAL:HG23	1:E:118:ALA:HB1	2.03	0.41
1:G:15:MET:HE2	1:G:204:ILE:HG13	2.03	0.41
1:F:66:ASP:OD1	1:F:69:LYS:NZ	2.48	0.41
1:D:144:TYR:CE2	2:D:245:HOH:O	2.71	0.40
1:H:218:THR:CG2	1:H:219:GLN:H	2.34	0.40
1:A:101:LEU:HA	1:A:101:LEU:HD23	1.83	0.40
1:E:107:VAL:HB	1:E:108:PRO:HD3	2.02	0.40
1:B:113:ARG:HA	1:B:116:LEU:HD22	2.04	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	182/245 (74%)	181 (100%)	1 (0%)	0	100	100
1	B	174/245 (71%)	172 (99%)	2 (1%)	0	100	100
1	C	174/245 (71%)	170 (98%)	3 (2%)	1 (1%)	22	33
1	D	173/245 (71%)	169 (98%)	3 (2%)	1 (1%)	22	33
1	E	175/245 (71%)	171 (98%)	4 (2%)	0	100	100
1	F	171/245 (70%)	165 (96%)	6 (4%)	0	100	100
1	G	182/245 (74%)	179 (98%)	2 (1%)	1 (0%)	25	38
1	H	174/245 (71%)	173 (99%)	1 (1%)	0	100	100
All	All	1405/1960 (72%)	1380 (98%)	22 (2%)	3 (0%)	44	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	67	LYS
1	C	66	ASP
1	D	215	GLY

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	144/196 (74%)	139 (96%)	5 (4%)	31	51
1	B	138/196 (70%)	130 (94%)	8 (6%)	17	29
1	C	138/196 (70%)	131 (95%)	7 (5%)	20	35
1	D	134/196 (68%)	123 (92%)	11 (8%)	9	15
1	E	136/196 (69%)	130 (96%)	6 (4%)	24	41
1	F	135/196 (69%)	131 (97%)	4 (3%)	36	57
1	G	141/196 (72%)	136 (96%)	5 (4%)	31	51
1	H	137/196 (70%)	130 (95%)	7 (5%)	20	35
All	All	1103/1568 (70%)	1050 (95%)	53 (5%)	22	37

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	SER
1	A	142	THR
1	A	173	SER
1	A	177	THR
1	A	219	GLN
1	B	5	ILE
1	B	66	ASP
1	B	93	SER
1	B	116	LEU
1	B	123	SER
1	B	142	THR
1	B	147	SER
1	B	148	LYS

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Mol	Chain	Res	Type
1	C	49	GLU
1	C	66	ASP
1	C	69	LYS
1	C	70	ASN
1	C	142	THR
1	C	148	LYS
1	C	168	ARG
1	D	5	ILE
1	D	66	ASP
1	D	93	SER
1	D	116	LEU
1	D	142	THR
1	D	148	LYS
1	D	164	ASN
1	D	173	SER
1	D	212	ILE
1	D	218	THR
1	D	226	ARG
1	E	24	SER
1	E	69	LYS
1	E	125[A]	CYS
1	E	125[B]	CYS
1	E	142	THR
1	E	148	LYS
1	F	96	GLU
1	F	100	HIS
1	F	116	LEU
1	F	142	THR
1	G	70	ASN
1	G	93	SER
1	G	142	THR
1	G	177	THR
1	G	197	ILE
1	H	5	ILE
1	H	116	LEU
1	H	142	THR
1	H	147	SER
1	H	148	LYS
1	H	170	SER
1	H	208	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	219	GLN
1	B	73	HIS
1	B	98	HIS
1	B	164	ASN
1	C	164	ASN
1	D	27	HIS
1	D	38	HIS
1	D	70	ASN
1	D	73	HIS
1	D	98	HIS
1	D	104	ASN
1	E	70	ASN
1	E	98	HIS
1	E	164	ASN
1	F	98	HIS
1	F	104	ASN
1	F	164	ASN
1	G	70	ASN
1	G	98	HIS
1	G	164	ASN
1	H	164	ASN
1	H	222	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	189/245 (77%)	-0.04	5 (2%)	57	54	22, 38, 53, 61	1 (0%)
1	B	181/245 (73%)	0.23	3 (1%)	69	65	24, 42, 55, 60	1 (0%)
1	C	181/245 (73%)	0.52	11 (6%)	28	26	30, 49, 69, 83	1 (0%)
1	D	180/245 (73%)	0.60	11 (6%)	28	26	28, 48, 80, 85	1 (0%)
1	E	182/245 (74%)	0.48	14 (7%)	21	19	27, 47, 69, 79	1 (0%)
1	F	180/245 (73%)	0.70	20 (11%)	12	10	27, 50, 80, 104	1 (0%)
1	G	189/245 (77%)	0.16	8 (4%)	41	38	21, 39, 60, 74	1 (0%)
1	H	181/245 (73%)	-0.07	2 (1%)	77	75	24, 37, 51, 59	1 (0%)
All	All	1463/1960 (74%)	0.32	74 (5%)	34	32	21, 43, 66, 104	8 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	12	THR	5.3
1	G	34	ARG	5.2
1	F	144	TYR	5.2
1	C	70	ASN	4.9
1	E	175	GLY	4.5
1	D	48	VAL	4.2
1	E	70	ASN	4.0
1	F	175	GLY	4.0
1	F	36	PRO	4.0
1	F	37	GLU	4.0
1	F	39	LEU	3.9
1	F	38	HIS	3.9
1	H	175	GLY	3.8
1	A	144	TYR	3.6
1	G	35	ASN	3.5
1	D	175	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	217	THR	3.4
1	E	14	GLY	3.4
1	D	34	ARG	3.4
1	B	141	ASN	3.1
1	C	176	PRO	3.1
1	F	41	ALA	3.1
1	F	52	GLU	3.0
1	E	37	GLU	2.9
1	F	217	THR	2.9
1	D	144	TYR	2.9
1	C	49	GLU	2.9
1	F	199	ILE	2.8
1	G	36	PRO	2.8
1	B	147	SER	2.7
1	E	141	ASN	2.7
1	E	38	HIS	2.6
1	C	39	LEU	2.5
1	F	46	GLU	2.5
1	G	37	GLU	2.5
1	D	49	GLU	2.5
1	E	25	ARG	2.5
1	F	203	GLU	2.5
1	C	121	ALA	2.4
1	F	51	ILE	2.4
1	H	140	GLY	2.4
1	C	38	HIS	2.4
1	D	36	PRO	2.4
1	G	141	ASN	2.4
1	F	42	LEU	2.3
1	A	35	ASN	2.3
1	F	17	ILE	2.3
1	E	69	LYS	2.3
1	B	174	PRO	2.3
1	C	218	THR	2.3
1	F	55	ILE	2.3
1	F	140	GLY	2.2
1	C	142	THR	2.2
1	F	164	ASN	2.2
1	E	34	ARG	2.2
1	G	39	LEU	2.2
1	G	92	GLY	2.2
1	D	141	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	20	VAL	2.2
1	E	39	LEU	2.1
1	C	69	LYS	2.1
1	D	100	HIS	2.1
1	A	34	ARG	2.1
1	A	37	GLU	2.1
1	E	199	ILE	2.1
1	D	38	HIS	2.1
1	C	40	ALA	2.1
1	D	42	LEU	2.1
1	G	41	ALA	2.1
1	C	73	HIS	2.1
1	E	51	ILE	2.1
1	A	177	THR	2.0
1	D	200	GLU	2.0
1	E	35	ASN	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.