Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 06:12 AM EDT

PDB ID	:	2HTB
Title	:	Crystal Structure of a putative mutarotase (YeaD) from Salmonella typhimurium in monoclinic form
Authors	:	Chittori, S.; Simanshu, D.K.; Savithri, H.S.; Murthy, M.R.N.
Deposited on	:	2006-07-25
Resolution	:	2.50 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:

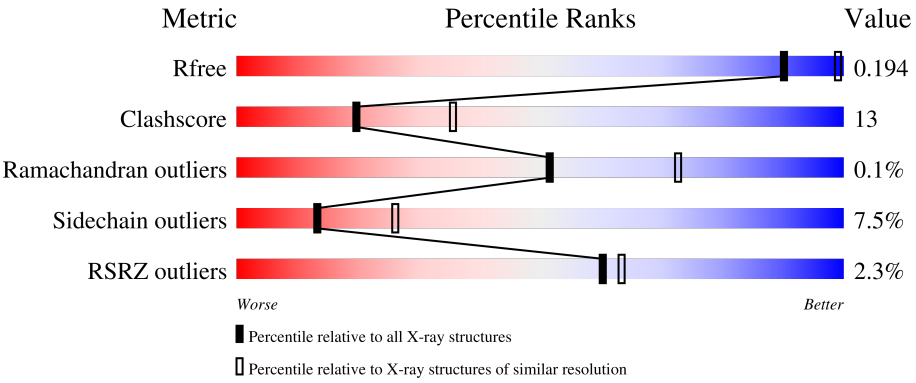
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	309	2% 66% 23% 6%
1	B	309	3% 69% 23%
1	C	309	2% 68% 22% 6% 5%
1	D	309	3% 71% 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9434 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 related to aldose 1-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2286	1458	395	424	9			
1	B	296	Total	C	N	O	S	0	0	0
			2256	1438	387	422	9			
1	C	295	Total	C	N	O	S	0	0	0
			2287	1457	397	424	9			
1	D	296	Total	C	N	O	S	0	0	0
			2283	1455	396	423	9			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	cloning artifact	UNP Q8ZPV9
A	-13	ARG	-	cloning artifact	UNP Q8ZPV9
A	-12	GLY	-	cloning artifact	UNP Q8ZPV9
A	-11	SER	-	cloning artifact	UNP Q8ZPV9
A	-10	HIS	-	expression tag	UNP Q8ZPV9
A	-9	HIS	-	expression tag	UNP Q8ZPV9
A	-8	HIS	-	expression tag	UNP Q8ZPV9
A	-7	HIS	-	expression tag	UNP Q8ZPV9
A	-6	HIS	-	expression tag	UNP Q8ZPV9
A	-5	HIS	-	expression tag	UNP Q8ZPV9
A	-4	GLY	-	cloning artifact	UNP Q8ZPV9
A	-3	MET	-	cloning artifact	UNP Q8ZPV9
A	-2	ALA	-	cloning artifact	UNP Q8ZPV9
A	-1	SER	-	cloning artifact	UNP Q8ZPV9
A	0	HIS	-	cloning artifact	UNP Q8ZPV9
B	-14	MET	-	cloning artifact	UNP Q8ZPV9
B	-13	ARG	-	cloning artifact	UNP Q8ZPV9
B	-12	GLY	-	cloning artifact	UNP Q8ZPV9
B	-11	SER	-	cloning artifact	UNP Q8ZPV9
B	-10	HIS	-	expression tag	UNP Q8ZPV9
B	-9	HIS	-	expression tag	UNP Q8ZPV9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP Q8ZPV9
B	-7	HIS	-	expression tag	UNP Q8ZPV9
B	-6	HIS	-	expression tag	UNP Q8ZPV9
B	-5	HIS	-	expression tag	UNP Q8ZPV9
B	-4	GLY	-	cloning artifact	UNP Q8ZPV9
B	-3	MET	-	cloning artifact	UNP Q8ZPV9
B	-2	ALA	-	cloning artifact	UNP Q8ZPV9
B	-1	SER	-	cloning artifact	UNP Q8ZPV9
B	0	HIS	-	cloning artifact	UNP Q8ZPV9
C	-14	MET	-	cloning artifact	UNP Q8ZPV9
C	-13	ARG	-	cloning artifact	UNP Q8ZPV9
C	-12	GLY	-	cloning artifact	UNP Q8ZPV9
C	-11	SER	-	cloning artifact	UNP Q8ZPV9
C	-10	HIS	-	expression tag	UNP Q8ZPV9
C	-9	HIS	-	expression tag	UNP Q8ZPV9
C	-8	HIS	-	expression tag	UNP Q8ZPV9
C	-7	HIS	-	expression tag	UNP Q8ZPV9
C	-6	HIS	-	expression tag	UNP Q8ZPV9
C	-5	HIS	-	expression tag	UNP Q8ZPV9
C	-4	GLY	-	cloning artifact	UNP Q8ZPV9
C	-3	MET	-	cloning artifact	UNP Q8ZPV9
C	-2	ALA	-	cloning artifact	UNP Q8ZPV9
C	-1	SER	-	cloning artifact	UNP Q8ZPV9
C	0	HIS	-	cloning artifact	UNP Q8ZPV9
D	-14	MET	-	cloning artifact	UNP Q8ZPV9
D	-13	ARG	-	cloning artifact	UNP Q8ZPV9
D	-12	GLY	-	cloning artifact	UNP Q8ZPV9
D	-11	SER	-	cloning artifact	UNP Q8ZPV9
D	-10	HIS	-	expression tag	UNP Q8ZPV9
D	-9	HIS	-	expression tag	UNP Q8ZPV9
D	-8	HIS	-	expression tag	UNP Q8ZPV9
D	-7	HIS	-	expression tag	UNP Q8ZPV9
D	-6	HIS	-	expression tag	UNP Q8ZPV9
D	-5	HIS	-	expression tag	UNP Q8ZPV9
D	-4	GLY	-	cloning artifact	UNP Q8ZPV9
D	-3	MET	-	cloning artifact	UNP Q8ZPV9
D	-2	ALA	-	cloning artifact	UNP Q8ZPV9
D	-1	SER	-	cloning artifact	UNP Q8ZPV9
D	0	HIS	-	cloning artifact	UNP Q8ZPV9

- Molecule 2 is water.

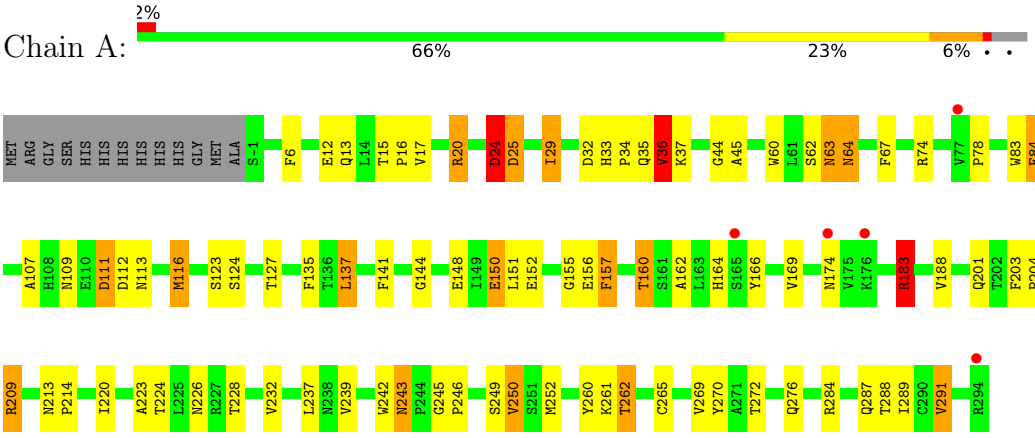
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	98	Total O 98 98	0	0
2	B	45	Total O 45 45	0	0
2	C	75	Total O 75 75	0	0
2	D	104	Total O 104 104	0	0

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.

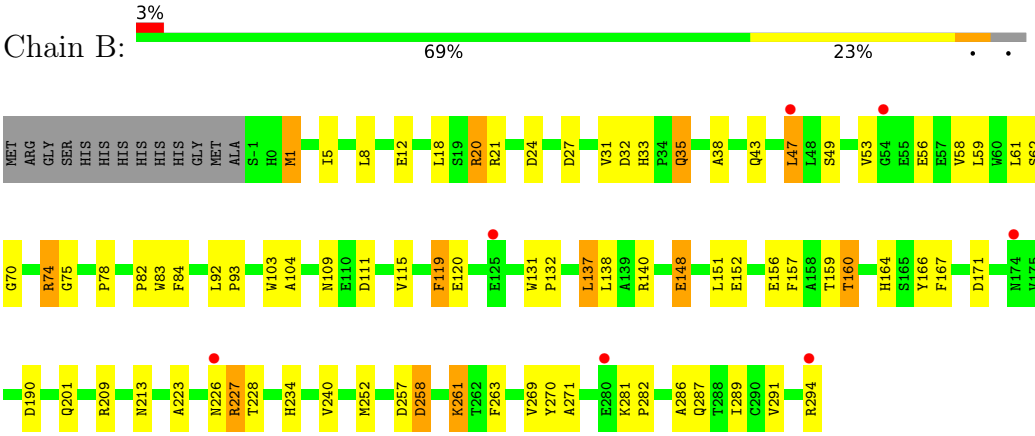
• Molecule 1: Putative enzyme related to aldose 1-epimerase

Chain A:



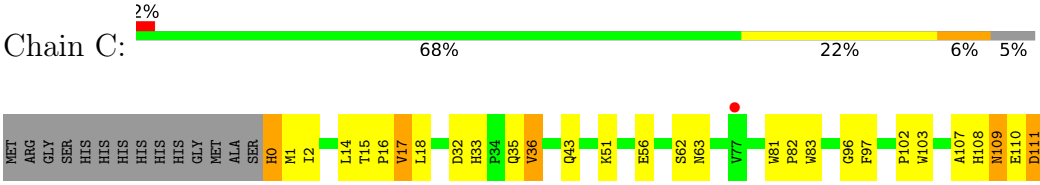
• Molecule 1: Putative enzyme related to aldose 1-epimerase

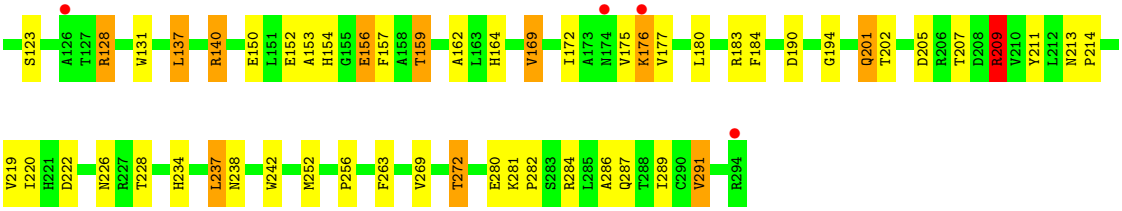
Chain B:



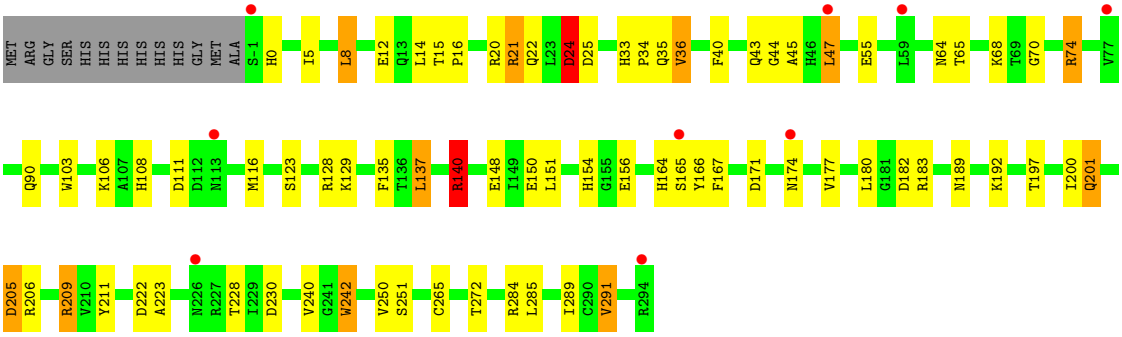
• Molecule 1: Putative enzyme related to aldose 1-epimerase

Chain C:





• Molecule 1: Putative enzyme related to aldose 1-epimerase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	219.55Å 47.60Å 138.09Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	27.80 – 2.50 25.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (27.80-2.50) 99.1 (25.60-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.240 0.186 , 0.194	Depositor DCC
R_{free} test set	2526 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9434	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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	1.36	13/2347 (0.6%)	1.20	16/3204 (0.5%)
1	B	1.23	3/2317 (0.1%)	1.16	14/3172 (0.4%)
1	C	1.32	4/2348 (0.2%)	1.23	12/3206 (0.4%)
1	D	1.31	6/2345 (0.3%)	1.19	18/3206 (0.6%)
All	All	1.31	26/9357 (0.3%)	1.20	60/12788 (0.5%)

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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	GLU	CB-CG	7.58	1.66	1.52
1	A	67	PHE	CE1-CZ	6.66	1.50	1.37
1	A	166	TYR	CE1-CZ	6.26	1.46	1.38
1	A	111	ASP	CB-CG	-5.86	1.39	1.51
1	A	107	ALA	CA-CB	5.51	1.64	1.52
1	D	148	GLU	CB-CG	5.45	1.62	1.52
1	C	56	GLU	CG-CD	5.44	1.60	1.51
1	D	140	ARG	CG-CD	5.37	1.65	1.51
1	D	242	TRP	CE3-CZ3	5.33	1.47	1.38
1	B	119	PHE	CE1-CZ	5.33	1.47	1.37
1	C	280	GLU	CG-CD	5.24	1.59	1.51
1	D	148	GLU	CG-CD	5.23	1.59	1.51
1	A	270	TYR	CD1-CE1	5.22	1.47	1.39
1	A	150	GLU	CG-CD	5.19	1.59	1.51
1	A	116	MET	CB-CG	5.18	1.68	1.51
1	B	148	GLU	CG-CD	5.16	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	223	ALA	CA-CB	5.16	1.63	1.52
1	A	261	LYS	CD-CE	5.12	1.64	1.51
1	C	176	LYS	CE-NZ	5.09	1.61	1.49
1	D	166	TYR	CD2-CE2	-5.07	1.31	1.39
1	A	84	PHE	CD1-CE1	5.04	1.49	1.39
1	A	157	PHE	CE1-CZ	5.03	1.47	1.37
1	D	156	GLU	CD-OE1	5.02	1.31	1.25
1	C	156	GLU	CG-CD	5.01	1.59	1.51
1	A	250	VAL	CB-CG1	5.01	1.63	1.52
1	A	156	GLU	CD-OE2	5.00	1.31	1.25

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	209	ARG	NE-CZ-NH1	14.34	127.47	120.30
1	C	209	ARG	NE-CZ-NH2	-12.45	114.08	120.30
1	C	140	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	A	74	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	C	140	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	C	183	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	D	205	ASP	CB-CG-OD2	8.25	125.73	118.30
1	A	209	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	D	21	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	A	209	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	C	36	VAL	CB-CA-C	-7.73	96.72	111.40
1	B	20	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	74	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	74	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	36	VAL	CB-CA-C	-7.63	96.90	111.40
1	D	182	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	27	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	111	ASP	CB-CG-OD1	-7.32	111.71	118.30
1	A	20	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	D	230	ASP	CB-CG-OD1	7.21	124.79	118.30
1	B	74	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	B	27	ASP	CB-CG-OD1	7.13	124.72	118.30
1	D	36	VAL	CB-CA-C	-7.05	98.00	111.40
1	D	21	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	24	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	B	32	ASP	CB-CG-OD1	6.63	124.27	118.30
1	D	230	ASP	CB-CG-OD2	-6.61	112.36	118.30
1	A	291	VAL	CB-CA-C	-6.57	98.92	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	20	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	C	291	VAL	CB-CA-C	-6.38	99.28	111.40
1	B	171	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	25	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	209	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	D	74	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	D	183	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	D	201	GLN	CB-CA-C	-5.91	98.59	110.40
1	A	205	ASP	CB-CG-OD2	5.85	123.56	118.30
1	B	32	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	C	14	LEU	CB-CG-CD2	-5.78	101.17	111.00
1	B	227	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	64	ASN	CB-CA-C	-5.72	98.95	110.40
1	D	47	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	112	ASP	CB-CG-OD1	5.70	123.42	118.30
1	B	257	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	24	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	111	ASP	CB-CA-C	-5.53	99.35	110.40
1	C	140	ARG	CD-NE-CZ	5.52	131.32	123.60
1	C	205	ASP	CB-CG-OD2	5.48	123.23	118.30
1	D	171	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	183	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	140	ARG	CG-CD-NE	-5.39	100.49	111.80
1	B	64	ASN	CB-CA-C	-5.32	99.75	110.40
1	C	190	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	222	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	190	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	291	VAL	CB-CA-C	-5.16	101.60	111.40
1	A	183	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	24	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	D	284	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	29	ILE	CG1-CB-CG2	-5.01	100.37	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	0	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	2286	0	2209	71	0
1	B	2256	0	2150	59	0
1	C	2287	0	2221	66	0
1	D	2283	0	2205	43	0
2	A	98	0	0	3	0
2	B	45	0	0	1	0
2	C	75	0	0	7	0
2	D	104	0	0	1	0
All	All	9434	0	8785	228	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 13.

All (228) 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:C:201:GLN:HG3	1:C:211:TYR:OH	1.54	1.06
1:B:84:PHE:H	1:B:160:THR:HG23	1.26	0.98
1:A:183:ARG:HH11	1:A:183:ARG:HG2	1.29	0.96
1:A:127:THR:HG22	2:A:299:HOH:O	1.67	0.93
1:D:140:ARG:HG2	1:D:140:ARG:HH11	1.36	0.88
1:B:84:PHE:H	1:B:160:THR:CG2	1.87	0.87
1:A:89:GLN:HE21	1:C:107:ALA:HA	1.40	0.85
1:C:111:ASP:HB3	1:C:113:ASN:H	1.42	0.85
1:B:201:GLN:HE22	1:B:209:ARG:HH11	1.22	0.84
1:D:140:ARG:HH11	1:D:140:ARG:CG	1.89	0.84
1:A:89:GLN:NE2	1:C:107:ALA:HA	1.95	0.81
1:B:33:HIS:HD2	1:B:35:GLN:H	1.28	0.80
1:A:111:ASP:HB3	1:A:113:ASN:H	1.47	0.80
1:D:33:HIS:HD2	1:D:35:GLN:H	1.29	0.79
1:A:36:VAL:HG22	1:A:144:GLY:HA2	1.66	0.78
1:A:89:GLN:NE2	1:C:108:HIS:H	1.82	0.77
1:B:33:HIS:CD2	1:B:35:GLN:H	2.02	0.77
1:D:33:HIS:CD2	1:D:35:GLN:H	2.04	0.76
1:B:84:PHE:N	1:B:160:THR:HG23	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:TRP:HA	1:B:160:THR:HG22	1.69	0.75
1:A:89:GLN:HE21	1:C:107:ALA:CA	1.99	0.74
1:A:36:VAL:CG2	1:A:144:GLY:HA2	2.18	0.73
1:B:18:LEU:HD21	1:B:115:VAL:HG11	1.69	0.73
1:A:60:TRP:CD1	1:A:262:THR:HG22	2.24	0.72
1:A:84:PHE:H	1:A:160:THR:CG2	2.03	0.71
1:A:174:ASN:ND2	1:A:224:THR:OG1	2.23	0.71
1:A:84:PHE:H	1:A:160:THR:HG22	1.54	0.71
1:A:183:ARG:HG2	1:A:183:ARG:NH1	2.06	0.71
1:D:164:HIS:O	1:D:164:HIS:CD2	2.44	0.70
1:A:103:TRP:CH2	1:A:137:LEU:HD13	2.27	0.69
1:A:209:ARG:HD2	2:A:321:HOH:O	1.93	0.69
1:C:103:TRP:CH2	1:C:137:LEU:HD13	2.28	0.69
1:C:164:HIS:O	1:C:164:HIS:CD2	2.46	0.69
1:A:60:TRP:NE1	1:A:262:THR:HG22	2.09	0.68
1:D:103:TRP:CH2	1:D:137:LEU:HD13	2.27	0.68
1:D:164:HIS:O	1:D:164:HIS:HD2	1.76	0.68
1:A:83:TRP:HA	1:A:160:THR:HG22	1.75	0.68
1:A:89:GLN:HE22	1:C:108:HIS:H	1.42	0.68
1:B:201:GLN:HE22	1:B:209:ARG:NH1	1.92	0.67
1:B:137:LEU:HD22	1:B:151:LEU:HD22	1.77	0.66
1:A:33:HIS:HD2	1:A:35:GLN:H	1.44	0.66
1:D:108:HIS:HA	1:D:116:MET:O	1.97	0.65
1:C:207:THR:O	1:C:242:TRP:HA	1.97	0.65
1:C:164:HIS:O	1:C:164:HIS:HD2	1.78	0.64
1:D:140:ARG:HG2	1:D:140:ARG:NH1	2.12	0.64
1:A:33:HIS:CD2	1:A:35:GLN:H	2.16	0.64
1:B:33:HIS:HE1	1:B:111:ASP:O	1.81	0.64
1:C:109:ASN:HD22	1:C:110:GLU:H	1.44	0.64
1:C:1:MET:H	1:C:63:ASN:ND2	1.97	0.62
1:C:238:ASN:HD21	1:C:272:THR:HB	1.65	0.62
1:D:201:GLN:CG	1:D:211:TYR:OH	2.48	0.61
1:D:201:GLN:OE1	1:D:209:ARG:NH1	2.32	0.61
1:C:159:THR:HG21	2:C:309:HOH:O	1.99	0.61
1:D:5:ILE:HA	1:D:8:LEU:HD22	1.81	0.61
1:C:33:HIS:HD2	1:C:35:GLN:H	1.49	0.60
1:D:14:LEU:HD12	1:D:14:LEU:N	2.17	0.60
1:C:33:HIS:CD2	1:C:35:GLN:H	2.20	0.59
1:D:140:ARG:HD2	1:D:150:GLU:HB2	1.84	0.59
1:D:123:SER:HB3	1:D:135:PHE:CD2	2.36	0.59
1:A:124:SER:H	1:A:127:THR:HB	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ASN:ND2	1:C:110:GLU:H	2.00	0.59
1:C:17:VAL:HG22	1:C:32:ASP:O	2.03	0.59
1:B:83:TRP:CA	1:B:160:THR:HG22	2.32	0.58
1:A:84:PHE:N	1:A:160:THR:HG22	2.18	0.58
1:B:140:ARG:HH21	1:B:152:GLU:CD	2.07	0.58
1:C:33:HIS:HE1	1:C:111:ASP:O	1.86	0.58
1:D:33:HIS:HE1	1:D:111:ASP:O	1.85	0.58
1:C:201:GLN:NE2	1:C:202:THR:O	2.36	0.58
1:C:234:HIS:HB2	1:C:286:ALA:HB3	1.86	0.57
1:D:201:GLN:HG3	1:D:211:TYR:OH	2.04	0.57
1:D:103:TRP:HH2	1:D:137:LEU:HD13	1.68	0.57
1:B:1:MET:HB3	1:B:61:LEU:HD23	1.86	0.57
1:B:5:ILE:O	1:B:8:LEU:HB2	2.03	0.57
1:B:92:LEU:HB3	1:B:93:PRO:HD2	1.86	0.57
1:B:47:LEU:HD13	1:B:59:LEU:HD11	1.87	0.57
1:B:47:LEU:HD13	1:B:59:LEU:CD1	2.35	0.57
1:C:0:HIS:H2	1:C:2:ILE:H	1.53	0.56
1:A:12:GLU:OE2	1:B:20:ARG:HD2	2.05	0.56
1:A:89:GLN:NE2	1:C:108:HIS:N	2.54	0.55
1:C:169:VAL:HG11	1:C:175:VAL:HG21	1.89	0.55
1:C:116:MET:HB2	2:C:364:HOH:O	2.06	0.55
1:D:55:GLU:HB3	2:D:373:HOH:O	2.05	0.55
1:C:209:ARG:HD2	2:C:302:HOH:O	2.06	0.55
1:A:60:TRP:HE1	1:A:262:THR:HG22	1.71	0.55
1:A:276:GLN:HE22	1:C:154:HIS:HE1	1.54	0.54
1:B:103:TRP:CH2	1:B:137:LEU:HD13	2.42	0.54
1:C:109:ASN:HD22	1:C:110:GLU:N	2.04	0.54
1:A:174:ASN:HB3	1:A:223:ALA:HB3	1.89	0.54
1:A:6:PHE:CE1	1:A:37:LYS:HB3	2.43	0.53
1:D:209:ARG:O	1:D:240:VAL:HA	2.08	0.53
1:B:226:ASN:HD21	1:B:294:ARG:CB	2.22	0.53
1:B:201:GLN:NE2	1:B:209:ARG:HH11	2.01	0.52
1:B:226:ASN:O	1:B:294:ARG:N	2.36	0.52
1:C:1:MET:H	1:C:63:ASN:HD22	1.55	0.52
1:A:207:THR:CG2	1:A:209:ARG:HD3	2.38	0.52
1:A:246:PRO:O	1:A:250:VAL:HG23	2.09	0.52
1:B:82:PRO:HB2	1:B:159:THR:HG22	1.91	0.52
1:B:137:LEU:CD2	1:B:151:LEU:HD22	2.40	0.52
1:B:234:HIS:HB2	1:B:286:ALA:HB3	1.92	0.52
1:A:152:GLU:OE2	1:A:284:ARG:NH1	2.44	0.51
1:D:33:HIS:HD2	1:D:35:GLN:N	2.03	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:HIS:CD2	1:D:34:PRO:HD2	2.45	0.51
1:A:116:MET:HA	1:A:141:PHE:O	2.10	0.51
1:D:135:PHE:HA	1:D:154:HIS:O	2.11	0.51
1:C:43:GLN:HA	1:C:102:PRO:HA	1.93	0.51
1:A:78:PRO:HD2	1:A:164:HIS:O	2.12	0.50
1:C:15:THR:HB	1:C:16:PRO:CD	2.41	0.50
1:A:287:GLN:HE21	1:A:289:ILE:HD11	1.77	0.50
1:C:201:GLN:CG	1:C:211:TYR:OH	2.44	0.50
1:B:74:ARG:CZ	1:B:252:MET:CE	2.90	0.50
1:C:172:ILE:HD13	1:C:263:PHE:O	2.12	0.50
1:D:20:ARG:HG2	1:D:21:ARG:N	2.27	0.50
1:A:15:THR:HB	1:A:16:PRO:HD2	1.94	0.49
1:A:33:HIS:HE1	1:A:111:ASP:O	1.95	0.49
1:B:226:ASN:ND2	1:B:294:ARG:CB	2.75	0.49
1:A:89:GLN:HE21	1:C:107:ALA:CB	2.25	0.49
1:C:184:PHE:CZ	1:C:194:GLY:HA3	2.48	0.49
1:C:222:ASP:C	1:C:222:ASP:OD1	2.51	0.49
1:C:140:ARG:NH2	1:C:152:GLU:OE2	2.46	0.49
1:B:78:PRO:HD2	1:B:164:HIS:HB3	1.94	0.49
1:A:243:ASN:ND2	1:A:245:GLY:H	2.11	0.49
1:B:74:ARG:NH2	1:B:252:MET:HE3	2.29	0.48
1:D:15:THR:HB	1:D:16:PRO:HD2	1.95	0.48
1:A:232:VAL:HB	1:A:288:THR:HB	1.95	0.48
1:C:238:ASN:ND2	1:C:272:THR:HB	2.29	0.48
1:C:162:ALA:HB2	1:C:269:VAL:HG22	1.96	0.48
1:B:83:TRP:HA	1:B:160:THR:O	2.14	0.48
1:C:51:LYS:HE2	2:C:339:HOH:O	2.13	0.48
1:B:281:LYS:HA	1:B:282:PRO:HD2	1.54	0.47
1:B:56:GLU:HB3	1:B:227:ARG:NH1	2.29	0.47
1:D:44:GLY:O	1:D:45:ALA:C	2.51	0.47
1:B:58:VAL:HG21	1:B:291:VAL:HG21	1.96	0.47
1:B:177:VAL:HG12	1:B:180:LEU:HD11	1.95	0.47
1:D:167:PHE:HE2	1:D:289:ILE:HD13	1.80	0.47
1:B:269:VAL:CG1	1:B:270:TYR:N	2.78	0.47
1:A:203:PHE:N	1:A:204:PRO:CD	2.78	0.47
1:B:38:ALA:HA	1:B:49:SER:O	2.15	0.47
1:B:109:ASN:HA	2:B:297:HOH:O	2.14	0.47
1:C:169:VAL:CG1	1:C:175:VAL:HG21	2.45	0.47
1:C:281:LYS:HA	1:C:282:PRO:HD2	1.79	0.47
1:B:43:GLN:HE22	1:B:70:GLY:H	1.63	0.46
1:C:201:GLN:OE1	1:C:209:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:TRP:CH2	1:A:62:SER:HB2	2.50	0.46
1:A:214:PRO:HG3	1:A:239:VAL:HG23	1.97	0.46
1:A:24:ASP:HB3	1:A:25:ASP:H	1.15	0.46
1:C:180:LEU:CD1	1:C:201:GLN:HB2	2.45	0.46
1:B:258:ASP:O	1:B:261:LYS:HG3	2.16	0.46
1:B:269:VAL:HG12	1:B:270:TYR:N	2.30	0.46
1:D:65:THR:HB	1:D:74:ARG:HB3	1.97	0.46
1:B:62:SER:HB3	1:B:65:THR:HB	1.97	0.46
1:B:287:GLN:HE21	1:B:289:ILE:HD11	1.81	0.45
1:C:15:THR:HB	1:C:16:PRO:HD2	1.98	0.45
1:B:131:TRP:HA	1:B:132:PRO:HD3	1.64	0.45
1:A:20:ARG:HD2	1:B:12:GLU:OE2	2.17	0.45
1:D:177:VAL:O	1:D:200:ILE:HA	2.17	0.45
1:A:141:PHE:HA	1:A:148:GLU:O	2.17	0.44
1:D:174:ASN:HB3	1:D:223:ALA:HB3	1.99	0.44
1:D:242:TRP:HE3	1:D:265:CYS:HG	1.64	0.44
1:D:189:ASN:O	1:D:192:LYS:HG3	2.17	0.44
1:A:33:HIS:CD2	1:A:34:PRO:HD2	2.53	0.44
1:C:82:PRO:HD3	1:C:97:PHE:CE1	2.52	0.44
1:B:18:LEU:CD2	1:B:31:VAL:HG22	2.48	0.44
1:B:33:HIS:HD2	1:B:35:GLN:N	2.04	0.44
1:C:162:ALA:CB	1:C:269:VAL:HG22	2.47	0.44
1:C:287:GLN:HE21	1:C:289:ILE:HD11	1.82	0.44
1:B:160:THR:OG1	1:B:271:ALA:HA	2.17	0.44
1:A:84:PHE:HB3	1:A:160:THR:HG23	1.99	0.44
1:A:13:GLN:NE2	1:A:15:THR:O	2.50	0.44
1:C:180:LEU:HD12	1:C:201:GLN:HB2	2.00	0.44
1:C:153:ALA:O	1:C:282:PRO:CB	2.66	0.44
1:A:17:VAL:O	1:A:17:VAL:CG1	2.66	0.43
1:A:17:VAL:HG22	1:A:32:ASP:O	2.18	0.43
1:A:252:MET:O	2:A:306:HOH:O	2.21	0.43
1:C:201:GLN:HG3	1:C:211:TYR:HH	1.75	0.43
1:A:36:VAL:HG21	1:A:144:GLY:HA2	1.96	0.43
1:C:177:VAL:HA	1:C:219:VAL:O	2.19	0.43
1:B:140:ARG:NH2	1:B:152:GLU:OE1	2.51	0.43
1:D:12:GLU:OE2	1:D:20:ARG:NH1	2.52	0.43
1:A:188:VAL:O	1:A:188:VAL:HG12	2.19	0.43
1:A:242:TRP:HE3	1:A:265:CYS:HG	1.66	0.43
1:B:8:LEU:O	1:B:21:ARG:HD3	2.19	0.43
1:B:35:GLN:HE21	1:B:35:GLN:HA	1.82	0.43
1:D:205:ASP:O	1:D:206:ARG:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:THR:HG23	1:A:209:ARG:HD3	2.00	0.42
1:D:33:HIS:CG	1:D:34:PRO:HD2	2.54	0.42
1:C:83:TRP:CE2	1:C:96:GLY:HA2	2.54	0.42
1:C:111:ASP:HB3	1:C:113:ASN:N	2.22	0.42
1:B:209:ARG:O	1:B:240:VAL:HA	2.19	0.42
1:C:62:SER:OG	1:C:256:PRO:HD3	2.19	0.42
1:D:180:LEU:HD13	1:D:211:TYR:CZ	2.55	0.42
1:A:64:ASN:HD22	1:A:64:ASN:HA	1.49	0.42
1:B:83:TRP:CB	1:B:160:THR:HG22	2.49	0.42
1:C:213:ASN:HA	1:C:214:PRO:HD2	1.65	0.42
1:A:103:TRP:CD1	1:A:103:TRP:N	2.84	0.42
1:D:165:SER:O	1:D:265:CYS:HA	2.19	0.42
1:B:84:PHE:N	1:B:160:THR:CG2	2.68	0.42
1:C:33:HIS:HD2	1:C:35:GLN:N	2.15	0.42
1:D:285:LEU:HD12	1:D:285:LEU:HA	1.88	0.42
1:A:44:GLY:O	1:A:45:ALA:C	2.58	0.42
1:A:155:GLY:HA3	1:A:157:PHE:CE2	2.55	0.42
1:B:75:GLY:HA2	1:B:166:TYR:CD1	2.54	0.42
1:C:128:ARG:HA	1:C:131:TRP:O	2.20	0.42
1:A:6:PHE:CZ	1:A:37:LYS:HB3	2.55	0.41
1:C:284:ARG:HD3	2:C:356:HOH:O	2.20	0.41
1:A:63:ASN:OD1	1:A:63:ASN:N	2.53	0.41
1:C:237:LEU:CD1	1:C:272:THR:HG22	2.50	0.41
1:A:249:SER:HB2	1:A:260:TYR:HB3	2.03	0.41
1:A:162:ALA:CB	1:A:269:VAL:HG22	2.50	0.41
1:D:14:LEU:HD12	1:D:14:LEU:H	1.85	0.41
1:D:15:THR:HB	1:D:16:PRO:CD	2.49	0.41
1:B:104:ALA:O	1:B:119:PHE:HA	2.20	0.41
1:B:120:GLU:HB2	1:B:138:LEU:CD2	2.50	0.41
1:D:43:GLN:NE2	1:D:70:GLY:H	2.18	0.41
1:A:17:VAL:HG11	1:A:33:HIS:HB2	2.03	0.41
1:A:201:GLN:HE22	1:A:209:ARG:HH21	1.67	0.41
1:C:150:GLU:HG2	2:C:333:HOH:O	2.20	0.41
1:C:81:TRP:CG	1:C:82:PRO:HA	2.56	0.41
1:C:220:ILE:O	1:C:228:THR:HA	2.21	0.41
1:A:123:SER:HB3	1:A:135:PHE:CD1	2.56	0.40
1:A:272:THR:O	1:C:284:ARG:NH2	2.47	0.40
1:D:40:PHE:CD1	1:D:40:PHE:N	2.89	0.40
1:A:83:TRP:CA	1:A:160:THR:HG22	2.46	0.40
1:A:84:PHE:N	1:A:160:THR:CG2	2.78	0.40
1:B:83:TRP:HA	1:B:160:THR:CG2	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ASP:HB3	1:D:25:ASP:H	1.55	0.40
1:A:220:ILE:O	1:A:228:THR:HA	2.22	0.40
1:B:167:PHE:O	1:B:263:PHE:HA	2.21	0.40
1:C:252:MET:O	2:C:358:HOH:O	2.22	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	294/309 (95%)	279 (95%)	15 (5%)	0	100 100
1	B	294/309 (95%)	278 (95%)	15 (5%)	1 (0%)	41 61
1	C	293/309 (95%)	278 (95%)	15 (5%)	0	100 100
1	D	294/309 (95%)	278 (95%)	16 (5%)	0	100 100
All	All	1175/1236 (95%)	1113 (95%)	61 (5%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	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	241/261 (92%)	222 (92%)	19 (8%)	12	24
1	B	236/261 (90%)	223 (94%)	13 (6%)	21	41
1	C	244/261 (94%)	224 (92%)	20 (8%)	11	22
1	D	243/261 (93%)	223 (92%)	20 (8%)	11	22
All	All	964/1044 (92%)	892 (92%)	72 (8%)	13	26

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	29	ILE
1	A	36	VAL
1	A	63	ASN
1	A	64	ASN
1	A	89	GLN
1	A	109	ASN
1	A	137	LEU
1	A	150	GLU
1	A	151	LEU
1	A	160	THR
1	A	169	VAL
1	A	183	ARG
1	A	213	ASN
1	A	226	ASN
1	A	237	LEU
1	A	243	ASN
1	A	262	THR
1	A	291	VAL
1	B	1	MET
1	B	35	GLN
1	B	47	LEU
1	B	64	ASN
1	B	137	LEU
1	B	148	GLU
1	B	156	GLU
1	B	157	PHE
1	B	160	THR
1	B	213	ASN
1	B	228	THR
1	B	258	ASP
1	B	261	LYS
1	C	17	VAL

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Mol	Chain	Res	Type
1	C	18	LEU
1	C	36	VAL
1	C	109	ASN
1	C	111	ASP
1	C	116	MET
1	C	123	SER
1	C	128	ARG
1	C	137	LEU
1	C	156	GLU
1	C	157	PHE
1	C	159	THR
1	C	169	VAL
1	C	176	LYS
1	C	201	GLN
1	C	209	ARG
1	C	226	ASN
1	C	237	LEU
1	C	272	THR
1	C	291	VAL
1	D	0	HIS
1	D	8	LEU
1	D	22	GLN
1	D	24	ASP
1	D	36	VAL
1	D	47	LEU
1	D	68	LYS
1	D	90	GLN
1	D	106	LYS
1	D	128	ARG
1	D	129	LYS
1	D	137	LEU
1	D	140	ARG
1	D	151	LEU
1	D	197	THR
1	D	228	THR
1	D	250	VAL
1	D	251	SER
1	D	272	THR
1	D	291	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	35	GLN
1	A	64	ASN
1	A	89	GLN
1	A	109	ASN
1	A	113	ASN
1	A	122	GLN
1	A	174	ASN
1	A	201	GLN
1	A	243	ASN
1	A	276	GLN
1	A	287	GLN
1	B	33	HIS
1	B	35	GLN
1	B	43	GLN
1	B	64	ASN
1	B	201	GLN
1	B	226	ASN
1	B	287	GLN
1	C	3	ASN
1	C	22	GLN
1	C	33	HIS
1	C	35	GLN
1	C	63	ASN
1	C	109	ASN
1	C	164	HIS
1	C	287	GLN
1	D	33	HIS
1	D	43	GLN
1	D	90	GLN
1	D	108	HIS
1	D	122	GLN
1	D	164	HIS
1	D	213	ASN
1	D	287	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	296/309 (95%)	-0.18	5 (1%)	70	72	20, 31, 45, 70	11 (3%)
1	B	296/309 (95%)	-0.09	8 (2%)	54	58	24, 36, 53, 60	12 (4%)
1	C	295/309 (95%)	-0.11	5 (1%)	70	72	22, 32, 46, 65	11 (3%)
1	D	296/309 (95%)	-0.23	9 (3%)	50	53	20, 29, 41, 59	11 (3%)
All	All	1183/1236 (95%)	-0.15	27 (2%)	60	63	20, 32, 47, 70	45 (3%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-1	SER	7.5
1	D	174	ASN	5.3
1	C	174	ASN	5.1
1	A	174	ASN	4.3
1	B	174	ASN	4.3
1	B	294	ARG	4.2
1	C	294	ARG	3.6
1	A	294	ARG	3.2
1	A	176	LYS	3.2
1	B	125	GLU	3.1
1	B	47	LEU	3.1
1	C	77	VAL	3.1
1	A	77	VAL	2.8
1	C	176	LYS	2.8
1	D	47	LEU	2.8
1	D	294	ARG	2.6
1	B	226	ASN	2.6
1	B	54	GLY	2.5
1	D	165	SER	2.5
1	D	113	ASN	2.5
1	D	77	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	165	SER	2.4
1	D	59	LEU	2.3
1	C	126	ALA	2.2
1	B	176	LYS	2.2
1	B	280	GLU	2.1
1	D	226	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.