Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:01 PM GMT

PDB ID	:	1IBU
Title	:	STRUCTURE OF THE D53,54N MUTANT OF HISTIDINE DECARBOXY-LASE AT 25 C
Authors	:	Worley, S.; Schelp, E.; Monzingo, A.F.; Ernst, S.; Robertus, J.D.
Deposited on	:	2001-03-29
Resolution	:	3.10 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:

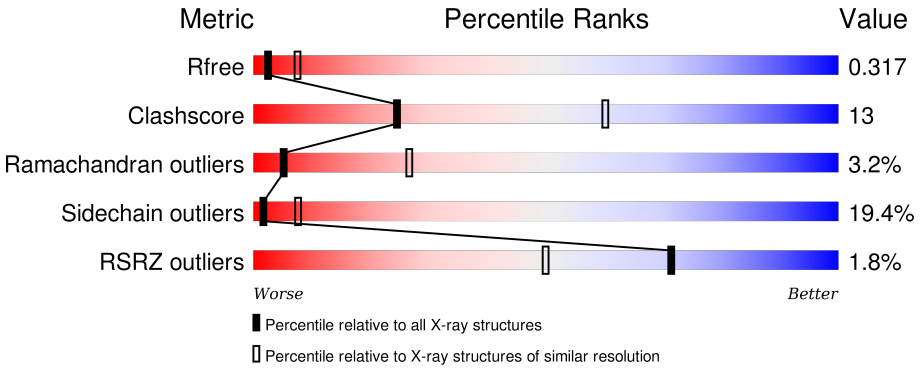
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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.



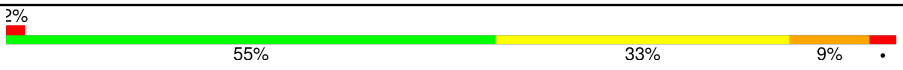
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	81	56% 17% 7% 20%
1	C	81	58% 19% 6% 17%
1	E	81	60% 16% 10% 14%
2	B	229	59% 31% 9%
2	D	229	4% 57% 31% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	229	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6856 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 HISTIDINE DECARBOXYLASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	65	Total	C	N	O	S	0	0	0
			493	307	87	97	2			
1	C	67	Total	C	N	O	S	0	0	0
			506	314	89	101	2			
1	E	70	Total	C	N	O	S	0	0	0
			529	328	95	104	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ASN	ASP	ENGINEERED	UNP P00862
A	54	ASN	ASP	ENGINEERED	UNP P00862
C	53	ASN	ASP	ENGINEERED	UNP P00862
C	54	ASN	ASP	ENGINEERED	UNP P00862
E	53	ASN	ASP	ENGINEERED	UNP P00862
E	54	ASN	ASP	ENGINEERED	UNP P00862

- Molecule 2 is a protein called HISTIDINE DECARBOXYLASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1776	1127	286	352	11			
2	D	229	Total	C	N	O	S	0	0	0
			1776	1127	286	352	11			
2	F	229	Total	C	N	O	S	0	0	0
			1776	1127	286	352	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	PYR	SER	MODIFIED RESIDUE	UNP P00862
D	82	PYR	SER	MODIFIED RESIDUE	UNP P00862

Continued on next page...

Continued from previous page...

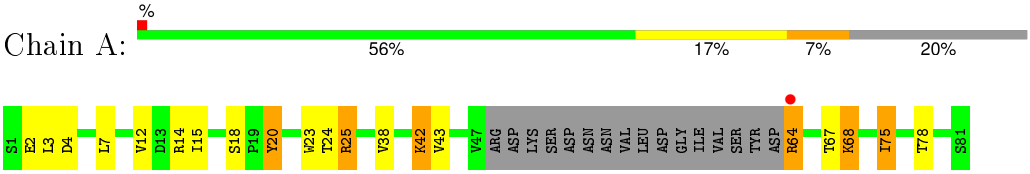
Chain	Residue	Modelled	Actual	Comment	Reference
F	82	PYR	SER	MODIFIED RESIDUE	UNP P00862

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.

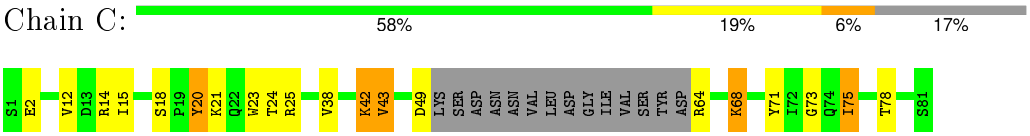
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain A:



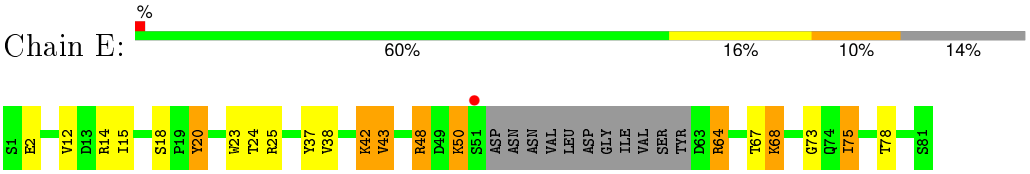
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain C:



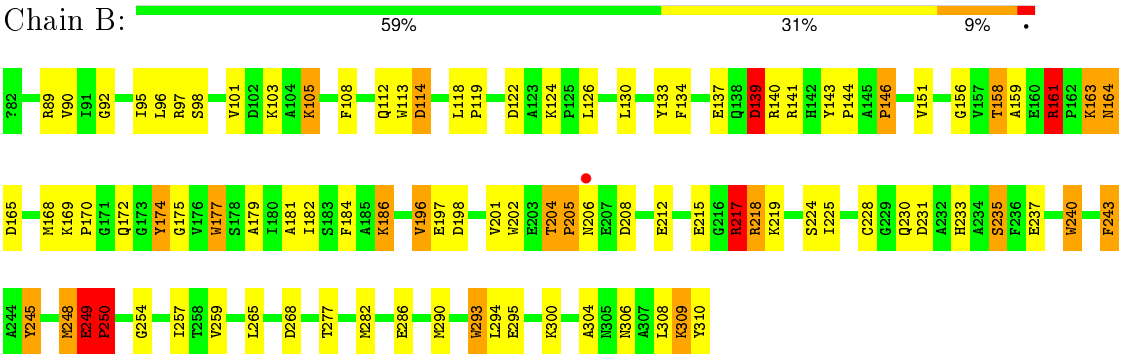
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain E:



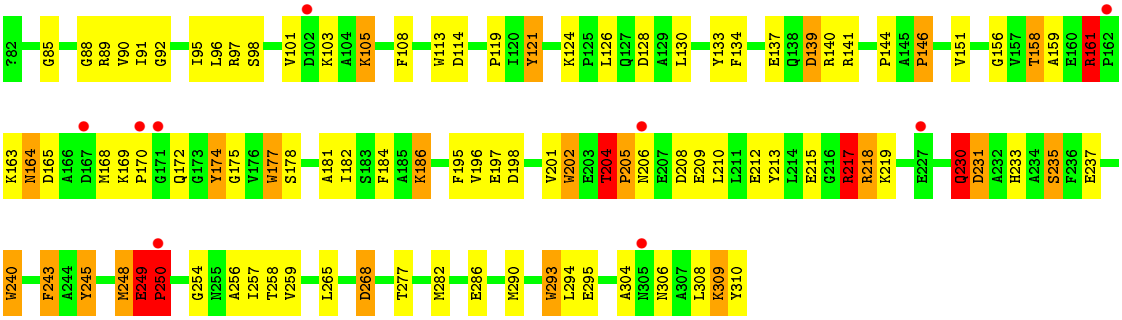
- Molecule 2: HISTIDINE DECARBOXYLASE ALPHA CHAIN

Chain B:



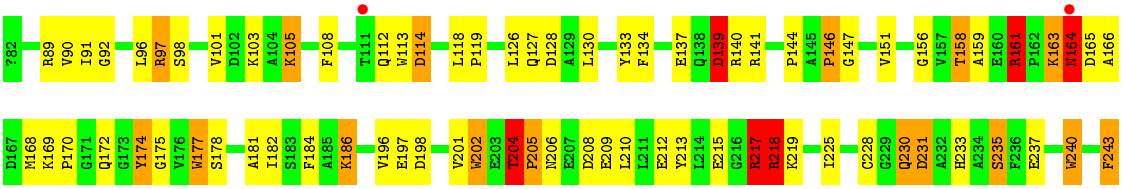
- Molecule 2: HISTIDINE DECARBOXYLASE ALPHA CHAIN

Chain D:



- Molecule 2: HISTIDINE DECARBOXYLASE ALPHA CHAIN

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	98.28Å 119.04Å 203.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 9.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.10) 81.8 (9.98-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 3.10Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.270 , 0.330 0.255 , 0.317	Depositor DCC
R_{free} test set	845 reflections (4.84%)	DCC
Wilson B-factor (Å^2)	82.7	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 89.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 17467 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6856	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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

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

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	0.91	0/499	2.31	9/670 (1.3%)
1	C	0.93	2/512 (0.4%)	1.67	8/688 (1.2%)
1	E	1.00	1/535 (0.2%)	1.87	14/719 (1.9%)
2	B	0.96	0/1816	1.69	32/2463 (1.3%)
2	D	0.95	0/1816	1.85	31/2463 (1.3%)
2	F	0.94	0/1816	1.72	38/2463 (1.5%)
All	All	0.95	3/6994 (0.0%)	1.80	132/9466 (1.4%)

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
2	B	0	1
2	D	0	1
2	F	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	23	TRP	NE1-CE2	-5.36	1.30	1.37
1	C	23	TRP	CG-CD2	-5.23	1.34	1.43
1	E	48	ARG	NE-CZ	5.03	1.39	1.33

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	ARG	NE-CZ-NH2	-30.27	105.17	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	217	ARG	NE-CZ-NH2	-25.93	107.34	120.30
2	D	217	ARG	NE-CZ-NH1	25.60	133.10	120.30
1	A	25	ARG	NE-CZ-NH1	23.62	132.11	120.30
1	A	25	ARG	CD-NE-CZ	17.99	148.79	123.60
2	D	217	ARG	CD-NE-CZ	17.67	148.34	123.60
1	E	25	ARG	NE-CZ-NH1	-15.07	112.77	120.30
2	B	217	ARG	NE-CZ-NH1	-14.43	113.08	120.30
1	C	25	ARG	NE-CZ-NH1	-12.61	114.00	120.30
1	E	25	ARG	NE-CZ-NH2	10.37	125.48	120.30
2	B	141	ARG	NE-CZ-NH1	-10.12	115.24	120.30
2	B	250	PRO	CA-N-CD	-9.46	98.25	111.50
2	F	250	PRO	N-CA-C	9.46	136.69	112.10
2	B	250	PRO	N-CA-C	9.43	136.61	112.10
2	F	250	PRO	CA-N-CD	-9.35	98.41	111.50
2	D	250	PRO	CA-N-CD	-9.15	98.69	111.50
2	D	250	PRO	N-CA-C	9.12	135.82	112.10
2	F	245	TYR	CB-CG-CD1	-8.91	115.65	121.00
2	F	177	TRP	CD1-CG-CD2	8.88	113.41	106.30
2	B	245	TYR	CB-CG-CD1	-8.85	115.69	121.00
2	F	217	ARG	NE-CZ-NH1	-8.83	115.89	120.30
2	F	293	TRP	CD1-CG-CD2	8.77	113.31	106.30
2	D	177	TRP	CD1-CG-CD2	8.57	113.15	106.30
2	F	113	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	A	20	TYR	CB-CG-CD2	-8.47	115.92	121.00
2	F	202	TRP	CE2-CD2-CG	-8.38	100.59	107.30
2	D	141	ARG	NE-CZ-NH1	-8.27	116.17	120.30
2	B	217	ARG	NE-CZ-NH2	8.27	124.43	120.30
2	F	217	ARG	CD-NE-CZ	8.27	135.17	123.60
1	E	23	TRP	CD1-CG-CD2	8.24	112.89	106.30
2	B	177	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	A	23	TRP	CE2-CD2-CG	-8.06	100.85	107.30
2	F	177	TRP	CE2-CD2-CG	-8.06	100.85	107.30
2	F	202	TRP	CD1-CG-CD2	8.03	112.73	106.30
2	D	293	TRP	CD1-CG-CD2	8.03	112.72	106.30
2	F	113	TRP	CE2-CD2-CG	-8.03	100.88	107.30
2	D	202	TRP	CE2-CD2-CG	-8.00	100.90	107.30
2	D	113	TRP	CD1-CG-CD2	7.89	112.61	106.30
2	D	202	TRP	CD1-CG-CD2	7.86	112.59	106.30
2	D	293	TRP	CE2-CD2-CG	-7.75	101.10	107.30
2	D	177	TRP	CE2-CD2-CG	-7.71	101.13	107.30
2	B	202	TRP	CE2-CD2-CG	-7.71	101.14	107.30
2	F	217	ARG	NE-CZ-NH2	7.68	124.14	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	TRP	CD1-CG-CD2	7.62	112.40	106.30
2	F	174	TYR	CB-CG-CD1	-7.54	116.48	121.00
2	B	245	TYR	CB-CG-CD2	7.53	125.52	121.00
2	B	293	TRP	CE2-CD2-CG	-7.53	101.28	107.30
2	B	202	TRP	CD1-CG-CD2	7.53	112.32	106.30
2	F	245	TYR	CB-CG-CD2	7.52	125.51	121.00
2	B	217	ARG	CD-NE-CZ	7.41	133.97	123.60
1	E	23	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	C	25	ARG	NE-CZ-NH2	7.38	123.99	120.30
2	D	113	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	E	50	LYS	N-CA-C	7.31	130.73	111.00
2	F	293	TRP	CE2-CD2-CG	-7.20	101.54	107.30
2	B	177	TRP	CE2-CD2-CG	-7.19	101.55	107.30
2	F	97	ARG	NE-CZ-NH1	-7.13	116.73	120.30
2	D	240	TRP	CE2-CD2-CG	-7.11	101.61	107.30
2	F	240	TRP	CD1-CG-CD2	7.07	111.96	106.30
1	C	23	TRP	CD1-CG-CD2	7.07	111.95	106.30
2	F	213	TYR	CB-CG-CD2	-6.97	116.82	121.00
2	B	113	TRP	CD1-CG-CD2	6.96	111.87	106.30
1	E	23	TRP	CG-CD2-CE3	6.90	140.11	133.90
2	F	141	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	C	23	TRP	CE2-CD2-CG	-6.89	101.78	107.30
1	E	20	TYR	CB-CG-CD2	-6.89	116.87	121.00
2	B	113	TRP	CE2-CD2-CG	-6.83	101.84	107.30
2	B	293	TRP	CD1-CG-CD2	6.82	111.75	106.30
2	D	174	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	E	25	ARG	CD-NE-CZ	6.75	133.06	123.60
2	D	240	TRP	CD1-CG-CD2	6.61	111.59	106.30
2	F	202	TRP	CB-CG-CD1	-6.49	118.56	127.00
2	D	245	TYR	CB-CG-CD2	6.47	124.88	121.00
2	B	205	PRO	CA-N-CD	-6.46	102.46	111.50
1	C	20	TYR	CB-CG-CD2	-6.45	117.13	121.00
2	D	202	TRP	CB-CG-CD1	-6.43	118.64	127.00
2	B	174	TYR	CB-CG-CD1	-6.35	117.19	121.00
2	F	240	TRP	CE2-CD2-CG	-6.31	102.25	107.30
2	F	202	TRP	CG-CD2-CE3	6.26	139.53	133.90
2	F	113	TRP	CB-CG-CD1	-6.23	118.91	127.00
2	F	218	ARG	NE-CZ-NH1	-6.21	117.19	120.30
2	D	245	TYR	CB-CG-CD1	-6.17	117.30	121.00
1	A	23	TRP	CG-CD2-CE3	6.17	139.45	133.90
1	C	25	ARG	CD-NE-CZ	6.16	132.23	123.60
2	F	205	PRO	CA-N-CD	-6.13	102.92	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	202	TRP	CG-CD2-CE3	6.10	139.39	133.90
2	B	240	TRP	CD1-CG-CD2	6.10	111.18	106.30
2	B	202	TRP	CB-CG-CD1	-5.99	119.21	127.00
1	C	23	TRP	CG-CD2-CE3	5.99	139.29	133.90
2	D	202	TRP	CG-CD2-CE3	5.91	139.22	133.90
2	D	205	PRO	CA-N-CD	-5.91	103.22	111.50
2	B	139	ASP	CB-CG-OD1	5.81	123.53	118.30
2	B	141	ARG	NE-CZ-NH2	5.81	123.20	120.30
2	B	204	THR	CA-C-N	5.77	133.25	117.10
1	E	48	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	64	ARG	NE-CZ-NH2	5.74	123.17	120.30
2	F	243	PHE	CB-CA-C	-5.74	98.93	110.40
2	F	139	ASP	CB-CG-OD1	5.67	123.40	118.30
2	B	240	TRP	CE2-CD2-CG	-5.64	102.79	107.30
1	E	23	TRP	CB-CG-CD1	-5.64	119.66	127.00
2	F	293	TRP	CB-CG-CD1	-5.64	119.66	127.00
2	F	293	TRP	CG-CD1-NE1	-5.56	104.54	110.10
2	B	143	TYR	CB-CG-CD2	-5.55	117.67	121.00
2	B	113	TRP	CB-CG-CD1	-5.55	119.79	127.00
1	E	37	TYR	CB-CG-CD2	-5.53	117.68	121.00
2	F	128	ASP	CB-CG-OD2	5.53	123.28	118.30
2	B	243	PHE	CB-CA-C	-5.52	99.36	110.40
1	E	23	TRP	CG-CD1-NE1	-5.51	104.59	110.10
2	D	204	THR	CA-C-N	5.50	132.51	117.10
2	F	177	TRP	CB-CG-CD1	-5.49	119.87	127.00
1	E	48	ARG	CG-CD-NE	5.47	123.29	111.80
2	D	113	TRP	CB-CG-CD1	-5.46	119.90	127.00
2	B	177	TRP	CG-CD2-CE3	5.43	138.79	133.90
2	F	293	TRP	CG-CD2-CE3	5.39	138.75	133.90
2	F	113	TRP	CG-CD2-CE3	5.36	138.72	133.90
2	D	243	PHE	CB-CA-C	-5.35	99.70	110.40
1	C	23	TRP	CB-CG-CD1	-5.34	120.05	127.00
2	F	230	GLN	CA-CB-CG	5.33	125.12	113.40
2	F	204	THR	CA-C-N	5.31	131.96	117.10
2	D	139	ASP	CB-CG-OD1	5.30	123.07	118.30
2	F	177	TRP	CG-CD1-NE1	-5.26	104.84	110.10
2	F	262	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	E	50	LYS	CA-C-N	-5.17	105.83	117.20
2	D	293	TRP	CG-CD2-CE3	5.16	138.55	133.90
2	B	177	TRP	CG-CD1-NE1	-5.16	104.94	110.10
2	D	213	TYR	CB-CG-CD2	-5.13	117.92	121.00
2	D	293	TRP	CB-CG-CD1	-5.12	120.35	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	113	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	A	4	ASP	CB-CG-OD1	5.09	122.88	118.30
2	B	196	VAL	N-CA-C	-5.09	97.27	111.00
2	D	230	GLN	CA-CB-CG	5.08	124.59	113.40
2	B	177	TRP	CB-CG-CD1	-5.07	120.42	127.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	161	ARG	Peptide
2	D	161	ARG	Peptide
2	F	161	ARG	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	493	0	491	14	0
1	C	506	0	497	18	0
1	E	529	0	521	21	0
2	B	1776	0	1706	46	0
2	D	1776	0	1706	56	0
2	F	1776	0	1706	57	0
All	All	6856	0	6627	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:218:ARG:HG2	2:F:243:PHE:HZ	1.44	0.82
2:D:218:ARG:HG2	2:D:243:PHE:HZ	1.46	0.81
2:B:218:ARG:HG2	2:B:243:PHE:HZ	1.46	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:ARG:NE	2:D:249:GLU:HA	2.00	0.77
2:F:249:GLU:HB2	2:F:250:PRO:HD2	1.66	0.77
2:B:161:ARG:NE	2:B:249:GLU:HA	2.02	0.75
2:D:249:GLU:HB2	2:D:250:PRO:HD2	1.68	0.75
2:D:175:GLY:HA2	2:D:248:MET:SD	2.27	0.74
2:B:249:GLU:HB2	2:B:250:PRO:HD2	1.70	0.74
2:F:161:ARG:HG3	2:F:174:TYR:HA	1.70	0.73
2:D:161:ARG:HG3	2:D:174:TYR:HA	1.71	0.73
2:F:175:GLY:HA2	2:F:248:MET:SD	2.31	0.70
2:F:161:ARG:NE	2:F:249:GLU:HA	2.05	0.70
1:E:38:VAL:HG11	2:F:265:LEU:HD21	1.77	0.67
2:B:161:ARG:HG3	2:B:174:TYR:HA	1.78	0.65
2:D:156:GLY:HA2	2:D:257:ILE:HG22	1.81	0.63
2:F:156:GLY:HA2	2:F:257:ILE:HG22	1.79	0.63
2:D:231:ASP:HB3	1:E:67:THR:HG21	1.82	0.62
2:B:156:GLY:HA2	2:B:257:ILE:HG22	1.83	0.60
2:B:175:GLY:HA2	2:B:248:MET:SD	2.43	0.59
1:E:42:LYS:HB3	2:F:259:VAL:HG13	1.86	0.58
2:D:161:ARG:HE	2:D:249:GLU:HA	1.68	0.58
1:A:67:THR:HG21	2:F:231:ASP:HB3	1.86	0.57
1:C:38:VAL:HG11	2:D:265:LEU:HD21	1.86	0.57
1:E:75:ILE:HD11	2:F:144:PRO:HB2	1.87	0.56
2:F:218:ARG:HG2	2:F:243:PHE:CZ	2.33	0.56
1:C:14:ARG:HB2	2:D:89:ARG:NH1	2.21	0.56
1:C:42:LYS:HB3	2:D:259:VAL:HG13	1.88	0.55
2:D:218:ARG:HG2	2:D:243:PHE:CZ	2.34	0.55
1:C:75:ILE:HD11	2:D:144:PRO:HB2	1.89	0.55
1:A:14:ARG:HB2	2:B:89:ARG:NH1	2.21	0.55
1:A:38:VAL:HG11	2:B:265:LEU:HD21	1.88	0.54
1:A:42:LYS:HB3	2:B:259:VAL:HG13	1.89	0.54
2:D:92:GLY:O	2:D:97:ARG:HA	2.08	0.54
2:B:218:ARG:HG2	2:B:243:PHE:CZ	2.36	0.54
1:A:75:ILE:HD11	2:B:144:PRO:HB2	1.90	0.53
2:B:92:GLY:O	2:B:97:ARG:HA	2.09	0.53
1:E:48:ARG:HB3	2:F:253:ILE:HG23	1.91	0.53
2:D:101:VAL:HG13	2:D:240:TRP:CH2	2.44	0.53
2:B:177:TRP:HH2	2:B:217:ARG:HH11	1.58	0.52
2:F:92:GLY:O	2:F:97:ARG:HA	2.08	0.52
2:F:161:ARG:HE	2:F:249:GLU:HA	1.72	0.52
2:F:182:ILE:HG23	2:F:240:TRP:HB2	1.92	0.52
1:E:68:LYS:HZ2	1:E:68:LYS:HB2	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:PHE:CZ	2:B:219:LYS:HG2	2.46	0.51
2:B:161:ARG:HE	2:B:249:GLU:HA	1.74	0.51
2:D:85:GLY:HA3	2:F:147:GLY:HA3	1.92	0.51
2:F:309:LYS:NZ	2:F:310:TYR:HA	2.25	0.51
2:F:103:LYS:O	2:F:105:LYS:NZ	2.44	0.51
1:C:12:VAL:HG22	1:E:20:TYR:CE1	2.47	0.50
2:D:108:PHE:CZ	2:D:219:LYS:HG2	2.46	0.50
1:A:68:LYS:HB2	1:A:68:LYS:HZ2	1.76	0.50
2:D:309:LYS:NZ	2:D:310:TYR:HA	2.27	0.50
2:D:103:LYS:O	2:D:105:LYS:NZ	2.45	0.49
2:B:103:LYS:O	2:B:105:LYS:NZ	2.45	0.49
2:F:108:PHE:CZ	2:F:219:LYS:HG2	2.47	0.49
2:F:178:SER:OG	2:F:256:ALA:HB1	2.13	0.49
2:D:133:TYR:HD1	2:D:293:TRP:CH2	2.31	0.49
2:B:182:ILE:HG23	2:B:240:TRP:HB2	1.94	0.49
1:A:15:ILE:HA	2:B:282:MET:HG3	1.95	0.48
1:C:15:ILE:HA	2:D:282:MET:HG3	1.94	0.48
1:A:75:ILE:CD1	2:B:144:PRO:HB2	2.43	0.48
1:E:75:ILE:CD1	2:F:144:PRO:HB2	2.44	0.48
2:D:182:ILE:HG23	2:D:240:TRP:HB2	1.95	0.48
2:D:186:LYS:NZ	2:D:235:SER:OG	2.47	0.48
2:B:309:LYS:NZ	2:B:310:TYR:HA	2.29	0.48
2:F:91:ILE:HD12	2:F:130:LEU:HD13	1.95	0.48
2:B:101:VAL:HG13	2:B:240:TRP:CH2	2.49	0.47
2:F:177:TRP:HH2	2:F:217:ARG:HH11	1.61	0.47
2:B:137:GLU:O	2:B:140:ARG:NH1	2.47	0.47
1:E:78:THR:HB	2:F:151:VAL:HA	1.97	0.47
2:F:225:ILE:O	2:F:228:CYS:HB3	2.14	0.47
2:B:90:VAL:HG21	2:B:184:PHE:HE1	1.80	0.47
1:E:15:ILE:HA	2:F:282:MET:HG3	1.96	0.47
1:A:78:THR:HB	2:B:151:VAL:HA	1.97	0.46
2:F:156:GLY:CA	2:F:257:ILE:HG22	2.45	0.46
1:E:73:GLY:O	1:E:75:ILE:HD13	2.15	0.46
2:F:202:TRP:CD1	2:F:210:LEU:HD13	2.50	0.46
2:F:101:VAL:HG13	2:F:240:TRP:CH2	2.50	0.46
2:D:177:TRP:HH2	2:D:217:ARG:NH1	2.13	0.46
1:C:75:ILE:CD1	2:D:144:PRO:HB2	2.45	0.46
1:E:14:ARG:HB2	2:F:89:ARG:NH1	2.31	0.46
1:C:68:LYS:HB2	1:C:68:LYS:HZ2	1.81	0.46
2:D:290:MET:O	2:D:294:LEU:HD12	2.16	0.46
1:C:78:THR:HB	2:D:151:VAL:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:VAL:HG21	2:D:184:PHE:HE1	1.81	0.46
2:B:95:ILE:HD12	2:B:96:LEU:HD13	1.98	0.45
2:D:181:ALA:N	2:D:196:VAL:O	2.49	0.45
2:D:96:LEU:O	2:D:290:MET:HB2	2.16	0.45
1:C:68:LYS:N	1:C:68:LYS:HZ2	2.15	0.45
2:B:290:MET:O	2:B:294:LEU:HD12	2.17	0.45
2:B:96:LEU:O	2:B:290:MET:HB2	2.18	0.44
2:B:139:ASP:OD2	2:B:300:LYS:NZ	2.51	0.44
2:B:89:ARG:HH21	2:B:286:GLU:CD	2.21	0.44
2:B:177:TRP:HH2	2:B:217:ARG:NH1	2.16	0.44
2:D:202:TRP:CD1	2:D:210:LEU:HD13	2.53	0.44
2:F:139:ASP:OD2	2:F:300:LYS:NZ	2.51	0.44
2:B:118:LEU:HA	2:B:119:PRO:HD2	1.88	0.44
1:C:21:LYS:HZ3	2:D:268:ASP:CG	2.21	0.44
2:F:174:TYR:O	2:F:248:MET:SD	2.76	0.43
2:B:156:GLY:CA	2:B:257:ILE:HG22	2.47	0.43
2:F:89:ARG:HH21	2:F:286:GLU:CD	2.22	0.43
2:D:249:GLU:HB2	2:D:250:PRO:CD	2.44	0.43
1:C:43:VAL:HA	2:D:257:ILE:O	2.18	0.43
2:F:159:ALA:HB1	2:F:172:GLN:HA	2.00	0.43
2:B:186:LYS:NZ	2:B:235:SER:OG	2.50	0.43
2:B:159:ALA:HB1	2:B:172:GLN:HA	2.00	0.43
2:B:163:LYS:NZ	2:B:250:PRO:O	2.50	0.43
2:B:130:LEU:HD11	2:B:134:PHE:CE1	2.54	0.43
2:D:137:GLU:O	2:D:140:ARG:NH1	2.50	0.43
2:B:133:TYR:HD1	2:B:293:TRP:CH2	2.36	0.43
2:D:158:THR:HA	2:D:254:GLY:O	2.18	0.43
2:D:156:GLY:CA	2:D:257:ILE:HG22	2.45	0.43
1:C:73:GLY:O	1:C:75:ILE:HD13	2.18	0.43
1:A:68:LYS:N	1:A:68:LYS:HZ2	2.17	0.43
2:F:186:LYS:NZ	2:F:235:SER:OG	2.52	0.43
2:F:249:GLU:HB2	2:F:250:PRO:CD	2.43	0.43
1:C:43:VAL:HG12	2:D:258:THR:HA	2.01	0.43
2:F:90:VAL:HG21	2:F:184:PHE:HE1	1.83	0.43
1:E:68:LYS:HZ2	1:E:68:LYS:N	2.17	0.43
2:D:175:GLY:CA	2:D:248:MET:SD	3.03	0.43
2:F:161:ARG:CZ	2:F:174:TYR:HD1	2.32	0.42
1:A:20:TYR:CD1	1:E:12:VAL:HG22	2.54	0.42
1:A:12:VAL:HG22	1:C:20:TYR:CE1	2.54	0.42
2:D:119:PRO:HB2	2:D:121:TYR:CE1	2.54	0.42
2:D:174:TYR:O	2:D:248:MET:SD	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:309:LYS:HZ2	2:D:310:TYR:HA	1.84	0.42
2:D:159:ALA:HB1	2:D:172:GLN:HA	2.01	0.42
2:B:122:ASP:OD2	2:B:124:LYS:HB2	2.19	0.42
2:F:181:ALA:N	2:F:196:VAL:O	2.52	0.42
2:B:158:THR:HA	2:B:254:GLY:O	2.19	0.42
2:D:88:GLY:O	2:D:89:ARG:HG3	2.19	0.42
2:F:130:LEU:HD11	2:F:134:PHE:CE1	2.54	0.42
2:F:137:GLU:O	2:F:140:ARG:NH1	2.52	0.42
2:F:204:THR:HG21	2:F:209:GLU:HB2	2.02	0.42
2:D:89:ARG:HH21	2:D:286:GLU:CD	2.22	0.42
1:E:42:LYS:HB3	2:F:259:VAL:CG1	2.48	0.42
2:F:289:THR:CB	2:F:291:PRO:HD2	2.50	0.42
2:F:118:LEU:HA	2:F:119:PRO:HD2	1.95	0.42
2:D:95:ILE:HD12	2:D:96:LEU:HD13	2.02	0.42
2:B:181:ALA:N	2:B:196:VAL:O	2.53	0.42
2:D:161:ARG:CZ	2:D:174:TYR:HD1	2.33	0.41
2:F:177:TRP:HH2	2:F:217:ARG:NH1	2.18	0.41
2:B:179:ALA:HB2	2:B:243:PHE:CD1	2.55	0.41
2:D:91:ILE:HD12	2:D:130:LEU:HD13	2.02	0.41
1:E:43:VAL:HA	2:F:257:ILE:O	2.20	0.41
1:A:42:LYS:HB3	2:B:259:VAL:CG1	2.51	0.41
2:D:230:GLN:OE1	1:E:64:ARG:NH1	2.53	0.41
2:F:133:TYR:HD1	2:F:293:TRP:CH2	2.38	0.41
1:E:48:ARG:HB3	2:F:253:ILE:CG2	2.50	0.41
2:F:163:LYS:NZ	2:F:250:PRO:O	2.53	0.41
2:F:127:GLN:HB3	2:F:310:TYR:OH	2.20	0.41
1:E:64:ARG:HD2	1:E:64:ARG:HH11	1.68	0.41
2:B:112:GLN:HB2	2:B:114:ASP:OD2	2.20	0.41
1:C:12:VAL:HG22	1:E:20:TYR:CD1	2.56	0.41
2:D:204:THR:HG21	2:D:209:GLU:HB2	2.02	0.41
2:F:158:THR:HA	2:F:254:GLY:O	2.21	0.41
1:C:71:TYR:CZ	1:C:73:GLY:HA3	2.56	0.41
2:D:97:ARG:HH21	2:D:97:ARG:HD3	1.75	0.41
2:B:225:ILE:O	2:B:228:CYS:HB3	2.21	0.41
2:F:274:SER:HB3	2:F:277:THR:OG1	2.21	0.41
1:C:42:LYS:HB3	2:D:259:VAL:CG1	2.49	0.41
2:D:181:ALA:O	2:D:195:PHE:HA	2.21	0.41
2:D:130:LEU:HD11	2:D:134:PHE:CE1	2.55	0.41
2:F:164:ASN:O	2:F:166:ALA:N	2.54	0.41
2:F:112:GLN:HB2	2:F:114:ASP:OD2	2.21	0.41
2:F:96:LEU:O	2:F:290:MET:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:PHE:CE1	2:B:219:LYS:HE3	2.57	0.40
1:A:3:LEU:O	1:A:7:LEU:HB2	2.21	0.40
2:F:284:ILE:HG21	2:F:284:ILE:HD13	1.91	0.40
1:E:68:LYS:HZ2	1:E:68:LYS:CB	2.33	0.40
2:D:124:LYS:HG3	2:D:128:ASP:OD1	2.22	0.40
2:B:161:ARG:HH11	2:B:161:ARG:HD3	1.74	0.40
2:D:178:SER:OG	2:D:256:ALA:HB1	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	61/81 (75%)	51 (84%)	10 (16%)	0	100 100
1	C	63/81 (78%)	52 (82%)	11 (18%)	0	100 100
1	E	66/81 (82%)	55 (83%)	10 (15%)	1 (2%)	13 46
2	B	226/229 (99%)	194 (86%)	23 (10%)	9 (4%)	4 21
2	D	226/229 (99%)	194 (86%)	23 (10%)	9 (4%)	4 21
2	F	226/229 (99%)	194 (86%)	23 (10%)	9 (4%)	4 21
All	All	868/930 (93%)	740 (85%)	100 (12%)	28 (3%)	5 26

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	165	ASP
2	B	205	PRO
2	B	250	PRO
2	D	165	ASP
2	D	205	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	250	PRO
1	E	50	LYS
2	F	165	ASP
2	F	205	PRO
2	F	250	PRO
2	B	304	ALA
2	D	249	GLU
2	D	304	ALA
2	F	249	GLU
2	F	304	ALA
2	B	164	ASN
2	B	249	GLU
2	F	164	ASN
2	F	306	ASN
2	D	164	ASN
2	D	306	ASN
2	B	146	PRO
2	B	306	ASN
2	D	146	PRO
2	F	146	PRO
2	F	170	PRO
2	B	170	PRO
2	D	170	PRO

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	50/66 (76%)	41 (82%)	9 (18%)	2 10
1	C	51/66 (77%)	42 (82%)	9 (18%)	2 10
1	E	53/66 (80%)	45 (85%)	8 (15%)	3 15
2	B	188/188 (100%)	150 (80%)	38 (20%)	1 7
2	D	188/188 (100%)	150 (80%)	38 (20%)	1 7
2	F	188/188 (100%)	151 (80%)	37 (20%)	1 7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	718/762 (94%)	579 (81%)	139 (19%)	2 7

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	18	SER
1	A	24	THR
1	A	25	ARG
1	A	42	LYS
1	A	43	VAL
1	A	64	ARG
1	A	68	LYS
1	A	75	ILE
2	B	98	SER
2	B	105	LYS
2	B	114	ASP
2	B	126	LEU
2	B	139	ASP
2	B	146	PRO
2	B	158	THR
2	B	161	ARG
2	B	163	LYS
2	B	164	ASN
2	B	168	MET
2	B	169	LYS
2	B	186	LYS
2	B	197	GLU
2	B	198	ASP
2	B	201	VAL
2	B	204	THR
2	B	206	ASN
2	B	208	ASP
2	B	212	GLU
2	B	215	GLU
2	B	217	ARG
2	B	218	ARG
2	B	224	SER
2	B	230	GLN
2	B	231	ASP
2	B	233	HIS
2	B	235	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	237	GLU
2	B	245	TYR
2	B	248	MET
2	B	249	GLU
2	B	250	PRO
2	B	268	ASP
2	B	277	THR
2	B	295	GLU
2	B	308	LEU
2	B	309	LYS
1	C	2	GLU
1	C	18	SER
1	C	24	THR
1	C	42	LYS
1	C	43	VAL
1	C	49	ASP
1	C	64	ARG
1	C	68	LYS
1	C	75	ILE
2	D	98	SER
2	D	105	LYS
2	D	114	ASP
2	D	121	TYR
2	D	126	LEU
2	D	139	ASP
2	D	146	PRO
2	D	158	THR
2	D	161	ARG
2	D	163	LYS
2	D	164	ASN
2	D	168	MET
2	D	169	LYS
2	D	186	LYS
2	D	197	GLU
2	D	198	ASP
2	D	201	VAL
2	D	204	THR
2	D	206	ASN
2	D	208	ASP
2	D	212	GLU
2	D	215	GLU
2	D	217	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	218	ARG
2	D	230	GLN
2	D	231	ASP
2	D	233	HIS
2	D	235	SER
2	D	237	GLU
2	D	245	TYR
2	D	248	MET
2	D	249	GLU
2	D	250	PRO
2	D	268	ASP
2	D	277	THR
2	D	295	GLU
2	D	308	LEU
2	D	309	LYS
1	E	2	GLU
1	E	18	SER
1	E	24	THR
1	E	42	LYS
1	E	43	VAL
1	E	64	ARG
1	E	68	LYS
1	E	75	ILE
2	F	98	SER
2	F	105	LYS
2	F	114	ASP
2	F	126	LEU
2	F	139	ASP
2	F	146	PRO
2	F	158	THR
2	F	161	ARG
2	F	163	LYS
2	F	164	ASN
2	F	168	MET
2	F	169	LYS
2	F	186	LYS
2	F	197	GLU
2	F	198	ASP
2	F	201	VAL
2	F	204	THR
2	F	206	ASN
2	F	208	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	212	GLU
2	F	215	GLU
2	F	217	ARG
2	F	218	ARG
2	F	230	GLN
2	F	231	ASP
2	F	233	HIS
2	F	235	SER
2	F	237	GLU
2	F	245	TYR
2	F	248	MET
2	F	249	GLU
2	F	250	PRO
2	F	268	ASP
2	F	277	THR
2	F	295	GLU
2	F	308	LEU
2	F	309	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
2	B	87	GLN
1	C	69	ASN
2	D	87	GLN
2	F	87	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 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	65/81 (80%)	-0.66	1 (1%) 76 58	27, 44, 78, 93	0
1	C	67/81 (82%)	-0.57	0 100 100	27, 44, 91, 100	0
1	E	70/81 (86%)	-0.41	1 (1%) 78 60	26, 45, 94, 100	0
2	B	228/229 (99%)	-0.30	1 (0%) 93 85	24, 59, 94, 100	0
2	D	228/229 (99%)	-0.03	9 (3%) 43 21	22, 61, 94, 100	0
2	F	228/229 (99%)	-0.17	4 (1%) 71 50	24, 61, 93, 100	0
All	All	886/930 (95%)	-0.25	16 (1%) 71 50	22, 58, 94, 100	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	111	THR	3.6
1	E	51	SER	3.6
2	D	171	GLY	3.5
2	D	167	ASP	3.3
2	F	305	ASN	2.8
2	F	164	ASN	2.7
2	D	170	PRO	2.5
2	B	206	ASN	2.4
2	D	206	ASN	2.4
1	A	64	ARG	2.3
2	D	305	ASN	2.3
2	F	251	GLY	2.1
2	D	162	PRO	2.1
2	D	250	PRO	2.1
2	D	102	ASP	2.1
2	D	227	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.