Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:02 am BST

PDB ID	:	1A4S
Title	:	BETAINE ALDEHYDE DEHYDROGENASE FROM COD LIVER
Authors	:	Johansson, K.; El Ahmad, M.; Hjelmqvist, L.; Ramaswamy, S.; Jornvall, H.; Eklund, H.
Deposited on	:	1998-02-03
Resolution	:	2.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

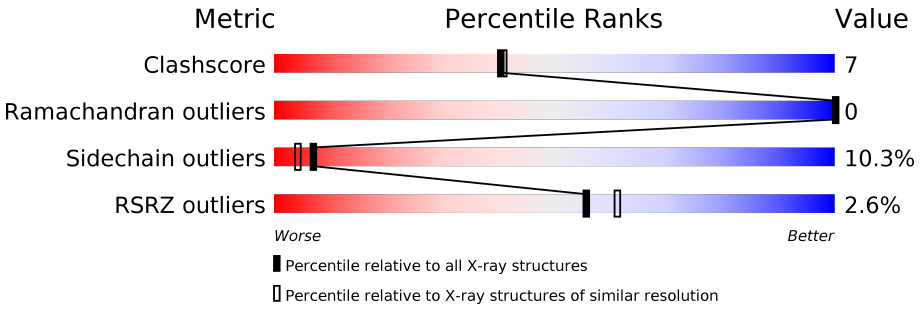
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	503	6% 75% 20%
1	B	503	% 76% 18% 5%
1	C	503	% 77% 18%
1	D	503	2% 77% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15925 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 BETAINE ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			3808	2408	651	719	30			
1	B	503	Total	C	N	O	S	0	0	0
			3808	2408	651	719	30			
1	C	503	Total	C	N	O	S	0	0	0
			3808	2408	651	719	30			
1	D	503	Total	C	N	O	S	0	0	0
			3808	2408	651	719	30			

- Molecule 2 is water.

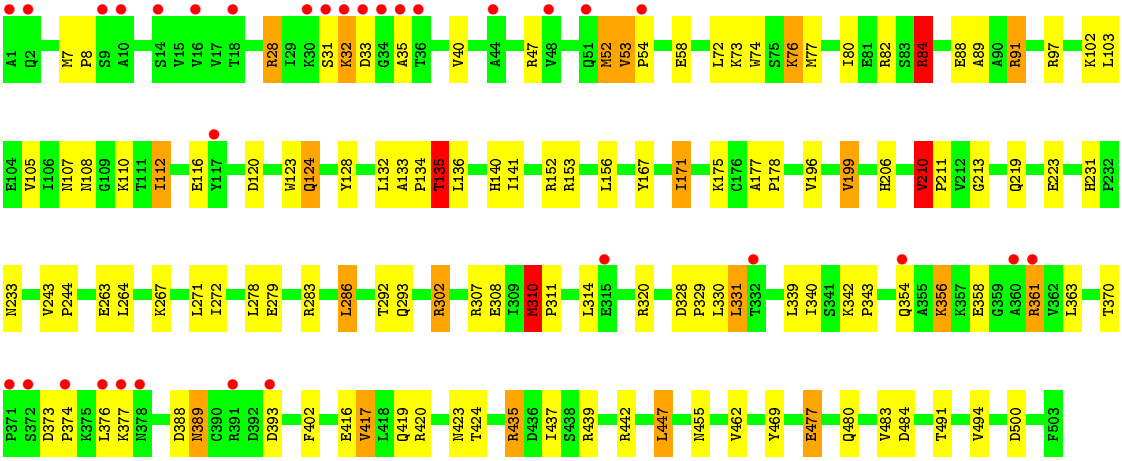
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		
2	B	211	Total	O	0	0
			211	211		
2	C	170	Total	O	0	0
			170	170		
2	D	198	Total	O	0	0
			198	198		

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 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.

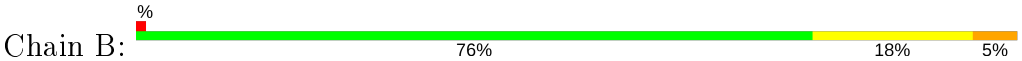
- Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE

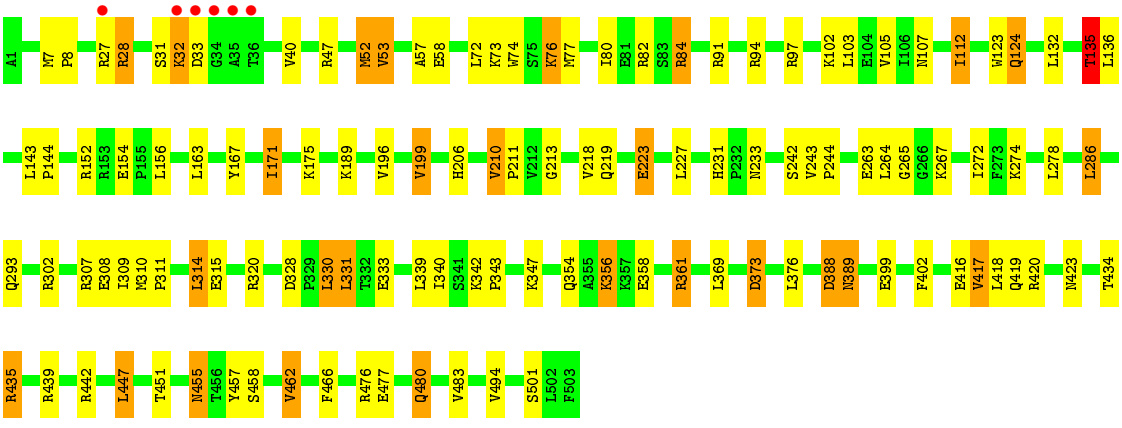
Chain A:



- Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE

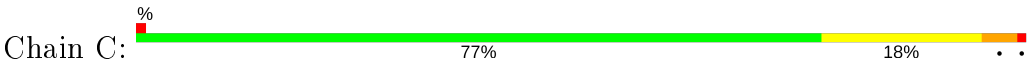
Chain B:

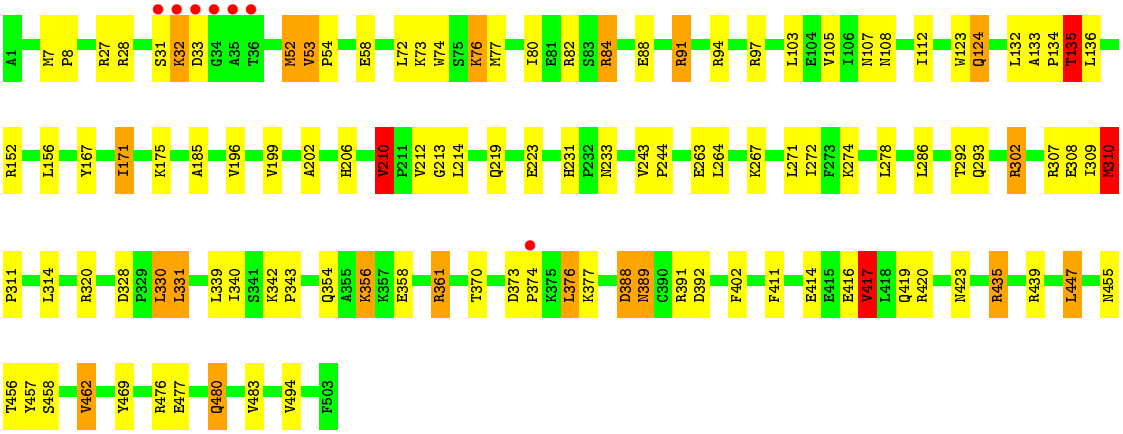




- Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE

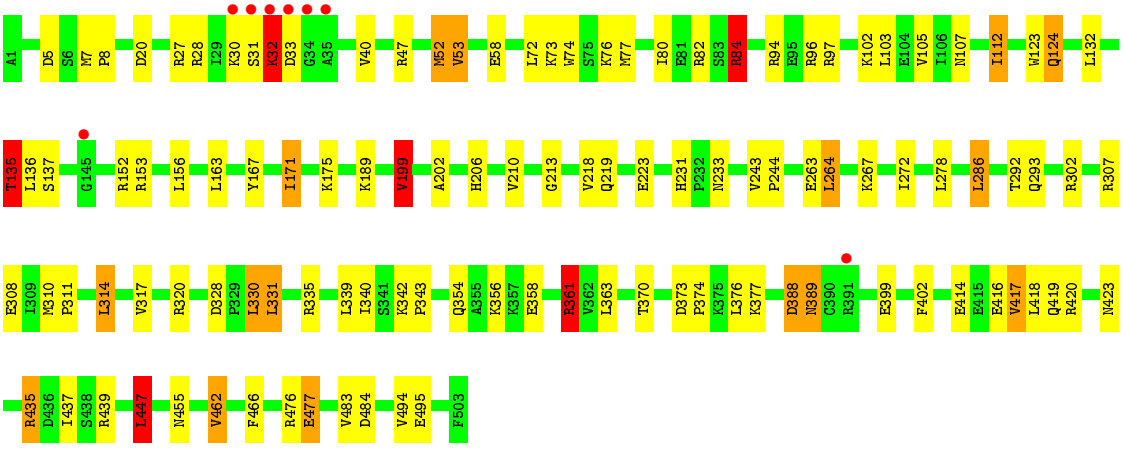
Chain C:





• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.17Å 86.22Å 88.33Å 105.20° 115.13° 100.02°	Depositor
Resolution (Å)	8.00 – 2.10 20.11 – 2.10	Depositor EDS
% Data completeness (in resolution range)	75.2 (8.00-2.10) 75.3 (20.11-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.63 (at 2.09Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.223 , 0.253 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.8	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	0.92	EDS
Total number of atoms	15925	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.61	0/3882	1.36	38/5265 (0.7%)
1	B	0.61	0/3882	1.59	39/5265 (0.7%)
1	C	0.57	0/3882	1.38	39/5265 (0.7%)
1	D	0.58	0/3882	1.35	38/5265 (0.7%)
All	All	0.59	0/15528	1.42	154/21060 (0.7%)

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	A	0	6
1	B	0	5
1	C	0	4
1	D	0	4
All	All	0	19

There are no bond length outliers.

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	320	ARG	NE-CZ-NH2	49.09	144.84	120.30
1	B	320	ARG	NH1-CZ-NH2	-33.48	82.58	119.40
1	B	320	ARG	NE-CZ-NH1	24.50	132.55	120.30
1	A	320	ARG	NE-CZ-NH1	18.64	129.62	120.30
1	D	320	ARG	NE-CZ-NH2	18.44	129.52	120.30
1	C	320	ARG	NE-CZ-NH2	16.11	128.35	120.30
1	C	91	ARG	NE-CZ-NH2	-15.84	112.38	120.30
1	C	320	ARG	NE-CZ-NH1	15.65	128.12	120.30
1	D	435	ARG	NE-CZ-NH2	-15.24	112.68	120.30
1	C	82	ARG	CD-NE-CZ	14.55	143.97	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	320	ARG	NH1-CZ-NH2	-14.45	103.51	119.40
1	D	320	ARG	NH1-CZ-NH2	-14.37	103.59	119.40
1	C	84	ARG	NE-CZ-NH2	14.24	127.42	120.30
1	B	420	ARG	NE-CZ-NH2	-14.21	113.19	120.30
1	C	439	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	D	420	ARG	NE-CZ-NH2	-13.82	113.39	120.30
1	A	455	ASN	OD1-CG-ND2	-13.73	90.31	121.90
1	D	320	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	B	435	ARG	NE-CZ-NH1	13.07	126.84	120.30
1	A	82	ARG	CD-NE-CZ	12.63	141.28	123.60
1	D	82	ARG	CD-NE-CZ	12.45	141.03	123.60
1	D	82	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	A	320	ARG	NH1-CZ-NH2	-12.12	106.07	119.40
1	A	82	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	B	435	ARG	NE-CZ-NH2	-11.67	114.47	120.30
1	D	152	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	C	435	ARG	NE-CZ-NH2	-10.69	114.96	120.30
1	B	82	ARG	CD-NE-CZ	10.62	138.47	123.60
1	C	152	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	B	82	ARG	NE-CZ-NH2	-10.23	115.19	120.30
1	C	435	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	A	91	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	C	94	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	B	84	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	D	476	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	A	455	ASN	CB-CG-ND2	8.60	137.34	116.70
1	A	435	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	A	439	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	C	82	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	28	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	C	28	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	A	417	VAL	CB-CA-C	-8.22	95.78	111.40
1	D	97	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	A	97	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	320	ARG	NE-CZ-NH2	8.01	124.31	120.30
1	C	152	ARG	CD-NE-CZ	7.72	134.41	123.60
1	D	153	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	C	469	TYR	CB-CG-CD1	7.50	125.50	121.00
1	A	120	ASP	CB-CG-OD1	7.49	125.04	118.30
1	C	417	VAL	CB-CA-C	-7.44	97.26	111.40
1	B	439	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	C	91	ARG	CD-NE-CZ	7.39	133.95	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	82	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	D	361	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	D	455	ASN	OD1-CG-ND2	-7.24	105.25	121.90
1	D	94	ARG	CD-NE-CZ	7.16	133.62	123.60
1	A	47	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	388	ASP	CB-CG-OD2	7.12	124.71	118.30
1	D	417	VAL	CB-CA-C	-7.05	98.00	111.40
1	B	417	VAL	CB-CA-C	-6.97	98.15	111.40
1	B	28	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	C	97	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	82	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	B	154	GLU	OE1-CD-OE2	-6.80	115.14	123.30
1	B	152	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	373	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	417	VAL	N-CA-CB	6.69	126.21	111.50
1	A	484	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	152	ARG	CD-NE-CZ	6.64	132.90	123.60
1	A	420	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	47	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	D	135	THR	N-CA-CB	-6.45	98.05	110.30
1	D	435	ARG	NH1-CZ-NH2	6.45	126.49	119.40
1	C	414	GLU	OE1-CD-OE2	-6.44	115.58	123.30
1	D	439	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	135	THR	N-CA-CB	-6.41	98.11	110.30
1	D	388	ASP	CB-CG-OD2	6.37	124.03	118.30
1	C	356	LYS	CA-CB-CG	6.36	127.39	113.40
1	A	84	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	C	91	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	D	84	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	C	94	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	97	ARG	CD-NE-CZ	6.16	132.22	123.60
1	A	152	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	442	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	152	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	B	94	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	135	THR	N-CA-CB	-6.02	98.87	110.30
1	B	223	GLU	OE1-CD-OE2	-5.98	116.12	123.30
1	B	27	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	C	392	ASP	CB-CG-OD1	5.93	123.64	118.30
1	D	447	LEU	CA-CB-CG	5.89	128.86	115.30
1	B	307	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	420	ARG	CD-NE-CZ	5.81	131.74	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	302	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	307	ARG	CD-NE-CZ	5.75	131.65	123.60
1	D	484	ASP	CB-CG-OD2	5.75	123.47	118.30
1	C	417	VAL	N-CA-CB	5.73	124.11	111.50
1	C	307	ARG	CD-NE-CZ	5.71	131.59	123.60
1	A	47	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	356	LYS	CA-CB-CG	5.67	125.88	113.40
1	C	439	ARG	CD-NE-CZ	5.66	131.52	123.60
1	B	47	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	286	LEU	CA-CB-CG	5.58	128.12	115.30
1	C	388	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	B	439	ARG	CD-NE-CZ	5.54	131.35	123.60
1	D	414	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	B	462	VAL	CB-CA-C	-5.47	101.01	111.40
1	B	210	VAL	N-CA-CB	-5.45	99.52	111.50
1	B	455	ASN	OD1-CG-ND2	-5.44	109.38	121.90
1	C	302	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	442	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	C	185	ALA	N-CA-CB	5.40	117.66	110.10
1	D	96	ARG	CD-NE-CZ	5.38	131.13	123.60
1	A	307	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	455	ASN	CB-CG-OD1	5.37	132.34	121.60
1	C	447	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	135	THR	N-CA-CB	-5.36	100.12	110.30
1	B	333	GLU	CG-CD-OE1	5.36	129.01	118.30
1	B	28	ARG	NH1-CZ-NH2	-5.35	113.52	119.40
1	D	420	ARG	NH1-CZ-NH2	5.33	125.26	119.40
1	A	356	LYS	CA-CB-CG	5.33	125.12	113.40
1	B	47	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	462	VAL	CB-CA-C	-5.32	101.29	111.40
1	C	310	MET	CG-SD-CE	-5.32	91.69	100.20
1	A	153	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	477	GLU	CG-CD-OE2	5.30	128.91	118.30
1	B	112	ILE	N-CA-CB	5.29	122.96	110.80
1	C	455	ASN	OD1-CG-ND2	-5.25	109.83	121.90
1	A	469	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	D	335	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	476	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	D	388	ASP	CB-CG-OD1	-5.21	113.62	118.30
1	B	417	VAL	N-CA-CB	5.18	122.90	111.50
1	C	84	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	D	439	ARG	CD-NE-CZ	5.18	130.85	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	447	LEU	CA-CB-CG	5.16	127.18	115.30
1	A	477	GLU	CG-CD-OE2	5.16	128.62	118.30
1	A	310	MET	CG-SD-CE	-5.13	91.99	100.20
1	A	393	ASP	CB-CG-OD1	5.13	122.92	118.30
1	D	307	ARG	CD-NE-CZ	5.13	130.78	123.60
1	C	271	LEU	CA-CB-CG	5.11	127.05	115.30
1	D	5	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	210	VAL	CA-CB-CG1	5.09	118.53	110.90
1	D	112	ILE	N-CA-CB	5.09	122.50	110.80
1	B	152	ARG	CD-NE-CZ	5.08	130.71	123.60
1	D	286	LEU	CA-CB-CG	5.06	126.93	115.30
1	D	417	VAL	N-CA-CB	5.06	122.63	111.50
1	D	462	VAL	CB-CA-C	-5.06	101.79	111.40
1	B	388	ASP	CB-CA-C	-5.05	100.30	110.40
1	B	91	ARG	CD-NE-CZ	5.03	130.65	123.60
1	B	286	LEU	CA-CB-CG	5.02	126.85	115.30
1	A	210	VAL	N-CA-CB	-5.02	100.46	111.50
1	D	476	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	TYR	Mainchain
1	A	308	GLU	Mainchain
1	A	370	THR	Mainchain
1	A	424	THR	Mainchain
1	A	480	GLN	Mainchain
1	A	89	ALA	Mainchain
1	B	242	SER	Mainchain
1	B	265	GLY	Mainchain
1	B	308	GLU	Mainchain
1	B	40	VAL	Mainchain
1	B	480	GLN	Mainchain
1	C	308	GLU	Mainchain
1	C	370	THR	Mainchain
1	C	391	ARG	Mainchain
1	C	480	GLN	Mainchain
1	D	199	VAL	Mainchain
1	D	308	GLU	Mainchain
1	D	32	LYS	Mainchain
1	D	370	THR	Mainchain

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	3808	0	3826	61	0
1	B	3808	0	3826	58	0
1	C	3808	0	3826	54	0
1	D	3808	0	3826	54	0
2	A	114	0	0	3	0
2	B	211	0	0	10	0
2	C	170	0	0	5	0
2	D	198	0	0	4	0
All	All	15925	0	15304	220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (220) 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:B:206:HIS:HE1	1:B:213:GLY:H	1.21	0.85
1:D:206:HIS:HE1	1:D:213:GLY:H	1.21	0.84
1:B:315:GLU:HG3	2:B:665:HOH:O	1.79	0.81
1:D:231:HIS:HD2	1:D:233:ASN:H	1.29	0.80
1:A:206:HIS:HE1	1:A:213:GLY:H	1.28	0.79
1:A:58:GLU:HB3	2:A:596:HOH:O	1.82	0.77
1:C:231:HIS:HD2	1:C:233:ASN:H	1.34	0.76
1:A:243:VAL:HB	1:A:244:PRO:HD3	1.66	0.76
1:C:206:HIS:HE1	1:C:213:GLY:H	1.31	0.75
1:B:231:HIS:HD2	1:B:233:ASN:H	1.34	0.74
1:B:243:VAL:HB	1:B:244:PRO:HD3	1.69	0.74
1:C:243:VAL:HB	1:C:244:PRO:HD3	1.69	0.73
1:B:171:ILE:HD11	1:B:175:LYS:HE2	1.70	0.73
1:C:293:GLN:HB3	1:C:339:LEU:HD22	1.71	0.73
1:A:32:LYS:O	1:A:33:ASP:HB3	1.89	0.72
1:D:171:ILE:HD11	1:D:175:LYS:HE2	1.69	0.72
1:A:171:ILE:HD11	1:A:175:LYS:HE2	1.70	0.72
1:D:243:VAL:HB	1:D:244:PRO:HD3	1.73	0.71
1:A:231:HIS:HD2	1:A:233:ASN:H	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:LYS:HB3	1:D:343:PRO:HD3	1.72	0.69
1:B:293:GLN:HB3	1:B:339:LEU:HD22	1.75	0.68
1:D:293:GLN:HB3	1:D:339:LEU:HD22	1.76	0.68
1:B:263:GLU:HB3	2:B:517:HOH:O	1.92	0.68
1:C:231:HIS:CD2	1:C:233:ASN:H	2.13	0.67
1:C:27:ARG:NH2	2:C:535:HOH:O	2.26	0.67
1:C:171:ILE:HD11	1:C:175:LYS:HE2	1.75	0.67
1:B:32:LYS:O	1:B:33:ASP:HB3	1.95	0.67
1:B:52:MET:CE	1:B:219:GLN:HB3	2.25	0.67
1:A:342:LYS:HB3	1:A:343:PRO:HD3	1.77	0.66
1:B:74:TRP:HA	1:B:77:MET:HE3	1.76	0.66
1:A:293:GLN:HB3	1:A:339:LEU:HD22	1.78	0.65
1:B:231:HIS:CD2	1:B:233:ASN:H	2.15	0.65
1:C:263:GLU:HB3	2:C:554:HOH:O	1.95	0.65
1:A:132:LEU:O	1:A:135:THR:HB	1.97	0.65
1:D:74:TRP:HA	1:D:77:MET:HE3	1.79	0.65
1:B:206:HIS:CE1	1:B:213:GLY:H	2.11	0.64
1:D:231:HIS:CD2	1:D:233:ASN:H	2.12	0.64
1:C:342:LYS:HB3	1:C:343:PRO:HD3	1.79	0.64
1:A:73:LYS:HG3	1:A:77:MET:CE	2.29	0.63
1:B:73:LYS:HG3	1:B:77:MET:CE	2.27	0.63
1:D:263:GLU:HB3	2:D:591:HOH:O	1.99	0.63
1:A:283:ARG:HB3	1:B:501:SER:HB2	1.81	0.63
1:D:52:MET:HE3	1:D:219:GLN:HB3	1.79	0.63
1:D:361:ARG:HB3	1:D:388:ASP:HB3	1.81	0.62
1:A:74:TRP:HA	1:A:77:MET:HE3	1.82	0.62
1:B:342:LYS:HB3	1:B:343:PRO:HD3	1.81	0.62
1:C:73:LYS:HG3	1:C:77:MET:CE	2.31	0.60
1:C:132:LEU:O	1:C:135:THR:HB	2.01	0.60
1:D:73:LYS:HG3	1:D:77:MET:CE	2.31	0.60
1:C:52:MET:CE	1:C:219:GLN:HB3	2.32	0.60
1:D:52:MET:CE	1:D:219:GLN:HB3	2.31	0.60
1:A:231:HIS:CD2	1:A:233:ASN:H	2.19	0.60
1:C:52:MET:HE3	1:C:219:GLN:HB3	1.83	0.59
1:C:74:TRP:HA	1:C:77:MET:HE3	1.83	0.59
1:C:373:ASP:HB3	1:C:376:LEU:HD22	1.83	0.58
1:A:373:ASP:HB3	1:A:376:LEU:HD22	1.85	0.58
1:C:32:LYS:O	1:C:33:ASP:HB3	2.03	0.58
1:D:373:ASP:HB3	1:D:376:LEU:HD22	1.85	0.58
1:B:52:MET:HE1	1:B:219:GLN:HB3	1.85	0.57
1:D:132:LEU:O	1:D:135:THR:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ARG:NH2	2:B:696:HOH:O	2.37	0.57
1:C:167:TYR:O	1:C:171:ILE:HG22	2.04	0.57
1:B:361:ARG:HB3	1:B:388:ASP:HB3	1.85	0.57
1:B:58:GLU:CD	1:B:58:GLU:H	2.08	0.57
1:D:206:HIS:CE1	1:D:213:GLY:H	2.12	0.57
1:D:31:SER:HB3	1:D:53:VAL:HG11	1.87	0.57
1:B:52:MET:HE1	1:B:219:GLN:CB	2.35	0.57
1:C:58:GLU:H	1:C:58:GLU:CD	2.08	0.56
1:B:52:MET:HE3	1:B:219:GLN:HB3	1.87	0.56
1:B:31:SER:HB3	1:B:53:VAL:HG11	1.87	0.56
1:C:416:GLU:O	1:C:419:GLN:HG3	2.06	0.55
1:D:310:MET:HE1	1:D:314:LEU:HD13	1.89	0.55
1:B:310:MET:HE1	1:B:314:LEU:HD13	1.89	0.55
1:C:133:ALA:HB3	1:C:134:PRO:HD3	1.89	0.55
1:C:73:LYS:HE3	1:C:77:MET:HE1	1.88	0.54
1:A:361:ARG:HB3	1:A:388:ASP:HB3	1.90	0.54
1:B:167:TYR:O	1:B:171:ILE:HG22	2.08	0.54
1:A:58:GLU:H	1:A:58:GLU:CD	2.11	0.53
1:B:373:ASP:HB3	1:B:376:LEU:HD22	1.90	0.53
1:A:500:ASP:HB2	2:A:603:HOH:O	2.09	0.53
1:D:27:ARG:NH1	2:D:647:HOH:O	2.42	0.53
1:B:328:ASP:HB3	1:B:331:LEU:HD22	1.90	0.53
1:C:361:ARG:HB3	1:C:388:ASP:HB3	1.90	0.53
1:D:58:GLU:CD	1:D:58:GLU:H	2.11	0.53
1:C:374:PRO:HA	1:C:377:LYS:HE2	1.90	0.53
1:A:133:ALA:HB3	1:A:134:PRO:HD3	1.92	0.52
1:A:31:SER:HB3	1:A:53:VAL:HG11	1.91	0.52
1:B:123:TRP:CZ3	1:B:124:GLN:HG2	2.45	0.52
1:B:347:LYS:HD3	2:B:552:HOH:O	2.09	0.52
1:C:354:GLN:O	1:C:358:GLU:HG3	2.10	0.52
1:A:52:MET:HE1	1:A:219:GLN:HB2	1.92	0.52
1:A:206:HIS:CE1	1:A:213:GLY:H	2.19	0.51
1:A:374:PRO:HA	1:A:377:LYS:HE2	1.92	0.51
1:C:212:VAL:HG23	2:C:649:HOH:O	2.10	0.51
1:B:105:VAL:HG11	1:B:330:LEU:HD13	1.92	0.51
1:D:167:TYR:O	1:D:171:ILE:HG22	2.11	0.51
1:A:328:ASP:HB3	1:A:331:LEU:HD22	1.92	0.51
1:C:31:SER:HB3	1:C:53:VAL:HG11	1.92	0.50
1:B:132:LEU:O	1:B:135:THR:HB	2.12	0.50
1:D:52:MET:HE2	1:D:53:VAL:N	2.27	0.50
1:C:52:MET:HE1	1:C:219:GLN:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASP:OD2	1:A:35:ALA:HB2	2.12	0.50
1:A:123:TRP:CZ3	1:A:124:GLN:HG2	2.48	0.49
1:A:292:THR:HG22	1:A:292:THR:O	2.13	0.49
1:D:328:ASP:HB3	1:D:331:LEU:HD22	1.93	0.49
1:A:52:MET:HE1	1:A:219:GLN:CB	2.42	0.49
1:B:57:ALA:HA	1:B:227:LEU:HD22	1.95	0.49
1:B:361:ARG:NH1	2:B:696:HOH:O	2.46	0.49
1:D:52:MET:HE1	1:D:219:GLN:CB	2.43	0.49
1:A:52:MET:CE	1:A:219:GLN:HB3	2.42	0.48
1:A:52:MET:HE2	1:A:53:VAL:N	2.28	0.48
1:C:328:ASP:HB3	1:C:331:LEU:HD22	1.96	0.48
1:D:105:VAL:HG11	1:D:330:LEU:HD13	1.95	0.48
1:D:32:LYS:O	1:D:33:ASP:HB3	2.12	0.48
1:A:437:ILE:HA	1:D:437:ILE:HB	1.95	0.48
1:A:52:MET:HE3	1:A:219:GLN:HB3	1.95	0.47
1:C:105:VAL:HG11	1:C:330:LEU:HD13	1.95	0.47
1:B:52:MET:HE2	1:B:53:VAL:N	2.29	0.47
1:D:416:GLU:O	1:D:419:GLN:HG3	2.15	0.47
1:C:292:THR:HG22	1:C:292:THR:O	2.15	0.47
1:D:310:MET:HB3	1:D:311:PRO:HD3	1.95	0.47
1:B:361:ARG:CZ	2:B:696:HOH:O	2.63	0.47
1:C:53:VAL:HG22	2:C:591:HOH:O	2.14	0.47
1:C:310:MET:HB3	1:C:311:PRO:HD3	1.97	0.47
1:A:354:GLN:O	1:A:358:GLU:HG3	2.15	0.47
1:A:416:GLU:O	1:A:419:GLN:HG3	2.15	0.47
1:A:105:VAL:HG13	1:A:110:LYS:O	2.15	0.46
1:B:369:LEU:HD21	2:B:583:HOH:O	2.15	0.46
1:C:374:PRO:HA	1:C:377:LYS:HD3	1.98	0.46
1:B:274:LYS:HA	1:B:309:ILE:HD13	1.98	0.46
1:A:267:LYS:HD2	1:A:302:ARG:HG3	1.97	0.46
1:B:354:GLN:O	1:B:358:GLU:HG3	2.16	0.46
1:B:418:LEU:HD23	1:B:447:LEU:HD13	1.97	0.46
1:D:361:ARG:HB2	1:D:389:ASN:HB2	1.97	0.46
1:B:416:GLU:O	1:B:419:GLN:HG3	2.15	0.46
1:C:52:MET:HE1	1:C:219:GLN:HB2	1.97	0.46
1:D:123:TRP:CZ3	1:D:124:GLN:HG2	2.50	0.46
1:D:52:MET:HE1	1:D:219:GLN:HB2	1.98	0.46
1:D:374:PRO:HA	1:D:377:LYS:HE2	1.97	0.45
1:D:267:LYS:HD2	1:D:302:ARG:HG3	1.96	0.45
1:C:7:MET:N	1:C:8:PRO:CD	2.79	0.45
1:D:52:MET:CE	1:D:219:GLN:CB	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:GLN:O	1:D:358:GLU:HG3	2.17	0.45
1:A:167:TYR:O	1:A:171:ILE:HG22	2.17	0.45
1:A:437:ILE:HB	1:D:437:ILE:HA	1.98	0.45
1:C:52:MET:CE	1:C:219:GLN:CB	2.95	0.45
1:A:140:HIS:O	1:D:137:SER:HB2	2.16	0.45
1:A:112:ILE:HG13	1:A:329:PRO:O	2.17	0.45
1:A:53:VAL:HA	1:A:54:PRO:HD2	1.85	0.45
1:B:361:ARG:HB2	1:B:389:ASN:HB2	1.99	0.45
1:C:480:GLN:HG3	2:C:637:HOH:O	2.16	0.45
1:D:374:PRO:HA	1:D:377:LYS:HD3	2.00	0.45
1:A:374:PRO:HA	1:A:377:LYS:HD3	1.98	0.44
1:B:476:ARG:HH11	1:B:476:ARG:HD3	1.65	0.44
1:A:310:MET:HB3	1:A:311:PRO:HD3	1.98	0.44
1:B:457:TYR:O	1:B:458:SER:HB2	2.18	0.44
1:C:210:VAL:HG13	1:C:214:LEU:HB3	1.98	0.44
1:C:73:LYS:HG3	1:C:77:MET:HE1	1.98	0.44
1:B:310:MET:HB3	1:B:311:PRO:HD3	1.99	0.44
1:B:466:PHE:HA	2:B:525:HOH:O	2.18	0.44
1:D:243:VAL:HA	1:D:264:LEU:HG	2.00	0.44
1:D:28:ARG:NH2	1:D:199:VAL:HG22	2.32	0.44
1:D:418:LEU:HD23	1:D:447:LEU:HD13	1.99	0.44
1:A:141:ILE:HG12	1:D:137:SER:HB3	1.98	0.44
1:B:73:LYS:HG3	1:B:77:MET:HE2	1.98	0.44
1:A:84:ARG:HD3	1:A:84:ARG:HH11	1.61	0.44
1:C:202:ALA:O	1:C:206:HIS:HD2	2.01	0.44
1:A:177:ALA:N	1:A:178:PRO:HD2	2.33	0.43
1:C:53:VAL:HA	1:C:54:PRO:HD2	1.93	0.43
1:A:7:MET:N	1:A:8:PRO:CD	2.80	0.43
1:D:20:ASP:OD2	1:D:30:LYS:HG3	2.19	0.43
1:B:163:LEU:HD22	1:B:171:ILE:HD13	2.00	0.43
1:B:267:LYS:HD2	1:B:302:ARG:HG3	2.00	0.43
1:D:84:ARG:HH11	1:D:84:ARG:HD3	1.66	0.43
1:B:434:THR:H	1:B:455:ASN:HD21	1.67	0.43
1:A:361:ARG:HB2	1:A:389:ASN:HB2	2.01	0.43
1:B:480:GLN:HG3	2:B:655:HOH:O	2.17	0.43
1:B:28:ARG:NH2	1:B:199:VAL:HG22	2.34	0.43
1:B:76:LYS:HD2	1:B:76:LYS:HA	1.89	0.43
1:B:7:MET:N	1:B:8:PRO:CD	2.82	0.43
1:C:267:LYS:HD2	1:C:302:ARG:HG3	2.00	0.43
1:C:76:LYS:HA	1:C:76:LYS:HD2	1.89	0.43
1:A:112:ILE:O	1:A:116:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HG3	1:A:77:MET:HE2	2.00	0.42
1:B:77:MET:HE1	1:B:211:PRO:HG3	2.01	0.42
1:A:76:LYS:HD2	1:A:76:LYS:HA	1.91	0.42
1:C:274:LYS:HA	1:C:309:ILE:HD13	2.02	0.42
1:D:163:LEU:HD22	1:D:171:ILE:HD13	2.01	0.42
1:A:263:GLU:HB3	2:A:574:HOH:O	2.18	0.42
1:C:342:LYS:N	1:C:343:PRO:CD	2.82	0.42
1:B:189:LYS:HA	1:B:218:VAL:O	2.20	0.42
1:D:202:ALA:O	1:D:206:HIS:HD2	2.03	0.42
1:C:361:ARG:HB2	1:C:389:ASN:HB2	2.01	0.42
1:B:143:LEU:HB3	1:B:144:PRO:HD2	2.01	0.41
1:A:112:ILE:HG13	1:A:112:ILE:H	1.66	0.41
1:A:210:VAL:HA	1:A:211:PRO:HD3	1.99	0.41
1:A:28:ARG:NH2	1:A:199:VAL:HG22	2.34	0.41
1:A:491:THR:O	1:B:451:THR:HA	2.20	0.41
1:C:123:TRP:CZ3	1:C:124:GLN:HG2	2.55	0.41
1:C:411:PHE:CG	1:C:417:VAL:HG13	2.55	0.41
1:C:52:MET:HE2	1:C:53:VAL:N	2.35	0.41
1:D:189:LYS:HA	1:D:218:VAL:O	2.20	0.41
1:C:74:TRP:HA	1:C:77:MET:CE	2.49	0.41
1:A:73:LYS:HE3	1:A:77:MET:HE1	2.01	0.41
1:D:466:PHE:HA	2:D:589:HOH:O	2.20	0.41
1:D:292:THR:O	1:D:292:THR:HG22	2.20	0.41
1:B:361:ARG:HD3	2:B:667:HOH:O	2.20	0.41
1:B:52:MET:HE1	1:B:219:GLN:HB2	2.03	0.41
1:C:456:THR:HB	1:D:495:GLU:HB2	2.02	0.41
1:A:279:GLU:O	1:A:283:ARG:HG3	2.20	0.41
1:C:243:VAL:N	1:C:244:PRO:CD	2.83	0.41
1:D:30:LYS:HB2	2:D:648:HOH:O	2.21	0.41
1:A:88:GLU:OE1	1:A:91:ARG:NH2	2.53	0.41
1:A:177:ALA:HB3	1:A:178:PRO:HD3	2.04	0.40
1:C:457:TYR:O	1:C:458:SER:HB2	2.21	0.40
1:D:7:MET:N	1:D:8:PRO:CD	2.84	0.40
1:A:342:LYS:N	1:A:343:PRO:CD	2.84	0.40
1:A:363:LEU:HG	1:A:388:ASP:HB2	2.03	0.40
1:C:88:GLU:OE1	1:C:91:ARG:NH2	2.52	0.40
1:D:363:LEU:HG	1:D:388:ASP:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	501/503 (100%)	489 (98%)	12 (2%)	0	100	100
1	B	501/503 (100%)	487 (97%)	14 (3%)	0	100	100
1	C	501/503 (100%)	486 (97%)	15 (3%)	0	100	100
1	D	501/503 (100%)	485 (97%)	16 (3%)	0	100	100
All	All	2004/2012 (100%)	1947 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	410/410 (100%)	366 (89%)	44 (11%)	6	3
1	B	410/410 (100%)	369 (90%)	41 (10%)	7	5
1	C	410/410 (100%)	368 (90%)	42 (10%)	7	4
1	D	410/410 (100%)	368 (90%)	42 (10%)	7	4
All	All	1640/1640 (100%)	1471 (90%)	169 (10%)	7	4

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	40	VAL

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Mol	Chain	Res	Type
1	A	52	MET
1	A	53	VAL
1	A	72	LEU
1	A	76	LYS
1	A	80	ILE
1	A	84	ARG
1	A	102	LYS
1	A	103	LEU
1	A	107	ASN
1	A	108	ASN
1	A	112	ILE
1	A	124	GLN
1	A	135	THR
1	A	136	LEU
1	A	156	LEU
1	A	171	ILE
1	A	196	VAL
1	A	199	VAL
1	A	210	VAL
1	A	223	GLU
1	A	264	LEU
1	A	271	LEU
1	A	272	ILE
1	A	278	LEU
1	A	286	LEU
1	A	310	MET
1	A	314	LEU
1	A	330	LEU
1	A	331	LEU
1	A	340	ILE
1	A	356	LYS
1	A	361	ARG
1	A	389	ASN
1	A	402	PHE
1	A	417	VAL
1	A	423	ASN
1	A	435	ARG
1	A	447	LEU
1	A	462	VAL
1	A	477	GLU
1	A	483	VAL
1	A	494	VAL

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Mol	Chain	Res	Type
1	B	32	LYS
1	B	52	MET
1	B	53	VAL
1	B	72	LEU
1	B	76	LYS
1	B	80	ILE
1	B	84	ARG
1	B	102	LYS
1	B	103	LEU
1	B	107	ASN
1	B	112	ILE
1	B	124	GLN
1	B	135	THR
1	B	136	LEU
1	B	156	LEU
1	B	171	ILE
1	B	196	VAL
1	B	199	VAL
1	B	210	VAL
1	B	223	GLU
1	B	264	LEU
1	B	272	ILE
1	B	278	LEU
1	B	286	LEU
1	B	314	LEU
1	B	330	LEU
1	B	331	LEU
1	B	340	ILE
1	B	356	LYS
1	B	361	ARG
1	B	389	ASN
1	B	399	GLU
1	B	402	PHE
1	B	417	VAL
1	B	423	ASN
1	B	435	ARG
1	B	447	LEU
1	B	462	VAL
1	B	477	GLU
1	B	483	VAL
1	B	494	VAL
1	C	32	LYS

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Mol	Chain	Res	Type
1	C	52	MET
1	C	53	VAL
1	C	72	LEU
1	C	76	LYS
1	C	80	ILE
1	C	84	ARG
1	C	103	LEU
1	C	107	ASN
1	C	108	ASN
1	C	112	ILE
1	C	124	GLN
1	C	135	THR
1	C	136	LEU
1	C	156	LEU
1	C	171	ILE
1	C	196	VAL
1	C	199	VAL
1	C	210	VAL
1	C	223	GLU
1	C	264	LEU
1	C	272	ILE
1	C	278	LEU
1	C	286	LEU
1	C	310	MET
1	C	314	LEU
1	C	330	LEU
1	C	331	LEU
1	C	340	ILE
1	C	356	LYS
1	C	361	ARG
1	C	376	LEU
1	C	389	ASN
1	C	402	PHE
1	C	417	VAL
1	C	423	ASN
1	C	435	ARG
1	C	447	LEU
1	C	462	VAL
1	C	477	GLU
1	C	483	VAL
1	C	494	VAL
1	D	32	LYS

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Mol	Chain	Res	Type
1	D	40	VAL
1	D	52	MET
1	D	53	VAL
1	D	72	LEU
1	D	76	LYS
1	D	80	ILE
1	D	84	ARG
1	D	102	LYS
1	D	103	LEU
1	D	107	ASN
1	D	112	ILE
1	D	124	GLN
1	D	135	THR
1	D	136	LEU
1	D	156	LEU
1	D	171	ILE
1	D	199	VAL
1	D	210	VAL
1	D	223	GLU
1	D	264	LEU
1	D	272	ILE
1	D	278	LEU
1	D	286	LEU
1	D	314	LEU
1	D	317	VAL
1	D	330	LEU
1	D	331	LEU
1	D	340	ILE
1	D	356	LYS
1	D	361	ARG
1	D	389	ASN
1	D	399	GLU
1	D	402	PHE
1	D	417	VAL
1	D	423	ASN
1	D	435	ARG
1	D	447	LEU
1	D	462	VAL
1	D	477	GLU
1	D	483	VAL
1	D	494	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	206	HIS
1	A	230	HIS
1	A	231	HIS
1	A	299	ASN
1	A	378	ASN
1	A	423	ASN
1	B	206	HIS
1	B	230	HIS
1	B	231	HIS
1	B	299	ASN
1	B	378	ASN
1	B	423	ASN
1	B	455	ASN
1	C	206	HIS
1	C	230	HIS
1	C	231	HIS
1	C	299	ASN
1	C	378	ASN
1	C	423	ASN
1	C	455	ASN
1	C	488	GLN
1	D	206	HIS
1	D	230	HIS
1	D	231	HIS
1	D	299	ASN
1	D	378	ASN
1	D	423	ASN
1	D	455	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	503/503 (100%)	0.11	32 (6%)	19	24	5, 15, 30, 107	0
1	B	503/503 (100%)	-0.20	6 (1%)	79	82	5, 15, 30, 107	0
1	C	503/503 (100%)	-0.25	7 (1%)	75	78	5, 15, 30, 107	0
1	D	503/503 (100%)	-0.26	8 (1%)	72	75	5, 15, 30, 107	0
All	All	2012/2012 (100%)	-0.15	53 (2%)	56	61	5, 15, 31, 107	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	34	GLY	15.7
1	C	33	ASP	11.2
1	B	34	GLY	11.1
1	C	34	GLY	10.4
1	B	33	ASP	10.3
1	D	33	ASP	9.6
1	D	31	SER	8.0
1	A	33	ASP	7.5
1	A	32	LYS	7.0
1	C	32	LYS	5.8
1	D	32	LYS	5.5
1	C	36	THR	5.4
1	A	34	GLY	5.3
1	B	35	ALA	5.2
1	A	35	ALA	5.1
1	A	374	PRO	5.0
1	B	32	LYS	4.7
1	C	35	ALA	4.7
1	A	36	THR	4.2
1	B	36	THR	3.8
1	D	35	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	372	SER	3.5
1	D	30	LYS	3.4
1	A	2	GLN	3.2
1	A	9	SER	3.1
1	A	361	ARG	3.0
1	A	371	PRO	2.8
1	A	31	SER	2.7
1	A	332	THR	2.7
1	A	378	ASN	2.7
1	A	391	ARG	2.6
1	A	51	GLN	2.6
1	A	30	LYS	2.5
1	A	14	SER	2.5
1	D	391	ARG	2.5
1	A	44	ALA	2.5
1	A	360	ALA	2.4
1	D	145	GLY	2.4
1	A	16	VAL	2.4
1	A	48	VAL	2.3
1	A	393	ASP	2.3
1	A	354	GLN	2.3
1	A	54	PRO	2.3
1	A	376	LEU	2.3
1	C	31	SER	2.3
1	A	18	THR	2.2
1	A	315	GLU	2.2
1	A	1	ALA	2.1
1	A	10	ALA	2.1
1	A	377	LYS	2.1
1	B	27	ARG	2.1
1	A	117	TYR	2.1
1	C	374	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.