



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 08:07 AM UTC

PDB ID : 2E3D / pdb_00002e3d
Title : Crystal structure of E. coli glucose-1-phosphate uridylyltransferase
Authors : Thoden, J.B.; Holden, H.M.
Deposited on : 2006-11-22
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

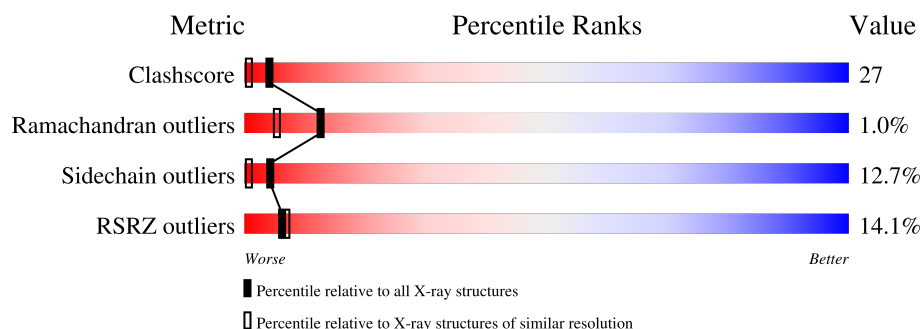
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	302	11% 46% 38% 10% • 5%
1	B	302	12% 45% 34% 12% • 7%
1	C	302	13% 47% 37% 9% • 5%
1	D	302	18% 43% 35% 12% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9442 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 UTP--glucose-1-phosphate uridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	2	0
			2199	1400	363	420	16			
1	B	281	Total	C	N	O	S	0	3	0
			2166	1376	361	413	16			
1	C	288	Total	C	N	O	S	0	0	0
			2195	1396	362	422	15			
1	D	278	Total	C	N	O	S	0	0	0
			2096	1331	346	404	15			

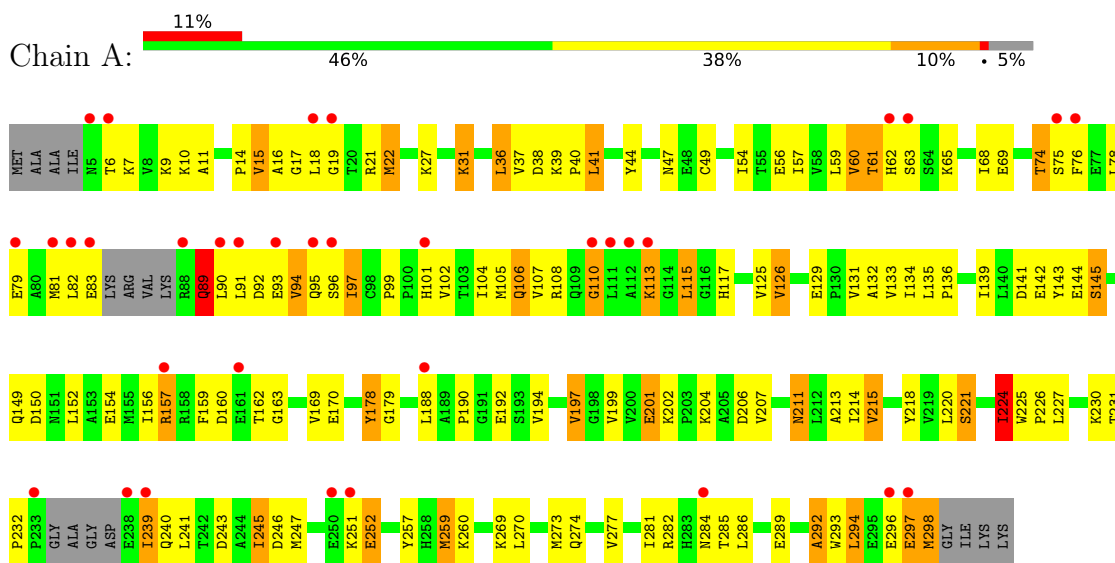
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	249	Total	O	0	0
			249	249		
2	B	194	Total	O	0	0
			194	194		
2	C	187	Total	O	0	0
			187	187		
2	D	156	Total	O	0	0
			156	156		

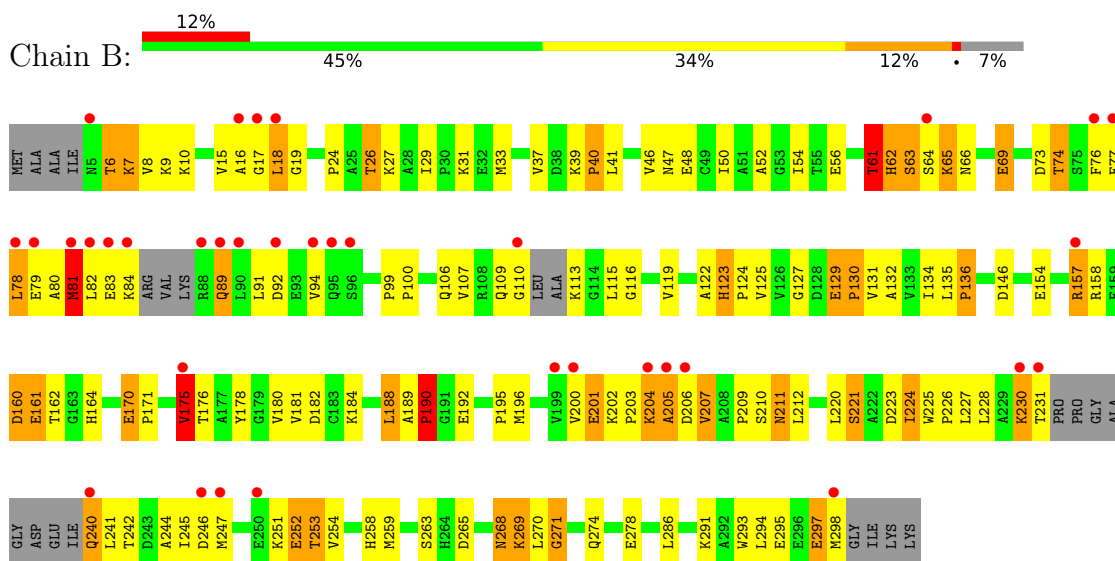
3 Residue-property plots [i](#)

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.

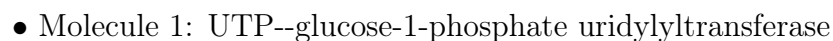
- Molecule 1: UTP--glucose-1-phosphate uridylyltransferase



- Molecule 1: UTP--glucose-1-phosphate uridylyltransferase



- Molecule 1: UTP--glucose-1-phosphate uridylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.90Å 109.30Å 100.50Å 90.00° 93.80° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 30.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-1.95) 98.7 (30.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 1.91Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.198 , 0.243 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 125.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9442	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.06	3/2250 (0.1%)	1.81	60/3058 (2.0%)
1	B	0.99	1/2219 (0.0%)	1.80	47/3011 (1.6%)
1	C	1.11	7/2235 (0.3%)	1.91	66/3038 (2.2%)
1	D	1.00	4/2131 (0.2%)	1.81	45/2893 (1.6%)
All	All	1.04	15/8835 (0.2%)	1.83	218/12000 (1.8%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	273	MET	SD-CE	-18.23	1.33	1.79
1	C	22	MET	SD-CE	11.11	2.07	1.79
1	D	33	MET	SD-CE	8.16	2.00	1.79
1	B	33	MET	SD-CE	8.08	1.99	1.79
1	C	258	HIS	CA-CB	6.31	1.61	1.53
1	C	219	VAL	CA-CB	-6.15	1.45	1.54
1	A	259	MET	SD-CE	6.07	1.94	1.79
1	A	133	VAL	CA-CB	-5.95	1.47	1.54
1	A	224	ILE	CA-CB	5.73	1.61	1.54
1	C	264	HIS	CA-CB	5.71	1.62	1.53
1	D	74	THR	CA-CB	-5.60	1.45	1.53
1	C	277	VAL	CA-CB	-5.44	1.48	1.54
1	D	189	ALA	CA-CB	-5.33	1.47	1.54
1	D	12	VAL	CA-CB	5.17	1.60	1.54
1	C	71	HIS	CA-CB	5.10	1.61	1.53

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	GLY	N-CA-C	-14.12	93.32	112.81
1	A	61	THR	N-CA-C	10.72	126.37	109.65
1	B	83	GLU	N-CA-C	-10.29	98.84	111.40
1	C	204	LYS	N-CA-C	-9.86	94.51	109.60
1	B	175	VAL	N-CA-C	9.68	123.19	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	ALA	N-CA-C	-9.65	100.07	112.23
1	B	61	THR	N-CA-C	9.23	124.54	109.96
1	A	201	GLU	N-CA-C	9.19	123.21	108.41
1	A	252	GLU	N-CA-CB	-8.97	97.65	111.46
1	B	74	THR	CB-CA-C	8.86	124.15	109.53
1	A	162	THR	N-CA-C	8.67	121.87	111.82
1	C	89	GLN	N-CA-C	8.66	121.50	111.11
1	C	178	TYR	N-CA-C	8.56	120.93	108.86
1	B	66	ASN	N-CA-C	8.45	122.57	111.75
1	C	136	PRO	N-CA-C	8.31	124.25	113.86
1	D	7	LYS	N-CA-C	8.30	121.26	111.71
1	B	211	ASN	N-CA-C	-8.30	101.62	112.41
1	D	81	MET	N-CA-C	8.29	121.51	111.40
1	D	136	PRO	N-CA-C	8.23	124.64	114.35
1	A	135	LEU	CA-C-O	8.12	125.71	119.46
1	A	204	LYS	N-CA-C	-8.08	97.44	110.20
1	D	178	TYR	N-CA-C	8.00	122.13	109.65
1	D	90	LEU	N-CA-C	7.89	120.58	111.11
1	C	61	THR	N-CA-C	7.89	122.43	109.96
1	A	179	GLY	N-CA-C	-7.81	97.36	110.95
1	C	182	ASP	CA-C-N	-7.72	111.66	123.17
1	C	182	ASP	C-N-CA	-7.72	111.66	123.17
1	B	134	ILE	N-CA-CB	-7.67	101.39	111.82
1	A	19	GLY	N-CA-C	7.58	131.14	113.18
1	D	220	LEU	N-CA-C	7.53	121.72	109.59
1	D	95	GLN	N-CA-C	-7.44	103.11	111.14
1	B	65	LYS	N-CA-C	7.33	121.94	112.92
1	C	11	ALA	CA-C-N	-7.29	114.16	123.19
1	C	11	ALA	C-N-CA	-7.29	114.16	123.19
1	C	7	LYS	N-CA-C	-7.26	104.45	113.38
1	A	292	ALA	N-CA-C	-7.22	103.10	110.97
1	D	17	GLY	N-CA-C	-7.21	102.87	112.82
1	C	238	GLU	N-CA-C	7.09	120.94	110.30
1	B	63	SER	N-CA-C	7.08	118.99	111.28
1	B	52	ALA	CA-C-N	-7.01	111.50	122.51
1	B	52	ALA	C-N-CA	-7.01	111.50	122.51
1	D	69	GLU	CA-CB-CG	-6.84	100.42	114.10
1	B	81	MET	CA-C-N	6.80	129.39	120.28
1	B	81	MET	C-N-CA	6.80	129.39	120.28
1	B	130	PRO	CA-C-N	-6.76	113.65	122.51
1	B	130	PRO	C-N-CA	-6.76	113.65	122.51
1	C	137	ASP	CA-C-N	-6.76	114.28	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	ASP	C-N-CA	-6.76	114.28	123.14
1	A	144	GLU	N-CA-C	6.74	121.67	113.17
1	C	182	ASP	CB-CA-C	-6.71	99.85	110.79
1	A	240	GLN	N-CA-C	6.69	119.83	109.07
1	D	192	GLU	CB-CA-C	-6.68	97.69	109.71
1	C	126	VAL	N-CA-C	6.66	116.79	110.53
1	C	225	TRP	N-CA-C	6.64	121.78	112.75
1	C	21	ARG	N-CA-C	-6.63	105.05	113.01
1	D	179	GLY	N-CA-C	-6.54	100.71	110.71
1	B	135	LEU	CA-C-N	6.53	126.16	119.56
1	B	135	LEU	C-N-CA	6.53	126.16	119.56
1	D	61	THR	N-CA-C	6.51	119.81	109.65
1	B	62[A]	HIS	N-CA-CB	-6.43	101.21	111.62
1	B	62[B]	HIS	N-CA-CB	-6.43	101.21	111.62
1	A	94	VAL	N-CA-C	6.38	117.90	110.62
1	D	19	GLY	N-CA-C	6.37	128.29	113.18
1	A	286	LEU	N-CA-C	6.37	122.00	113.72
1	C	252	GLU	N-CA-C	6.36	116.84	107.88
1	D	224	ILE	CB-CA-C	-6.34	102.00	112.26
1	C	219	VAL	N-CA-C	-6.33	96.60	107.24
1	A	150	ASP	CB-CA-C	-6.32	98.45	111.22
1	B	129	GLU	O-C-N	6.29	126.25	121.65
1	A	113	LYS	N-CA-C	6.27	121.79	112.94
1	A	141	ASP	N-CA-C	6.27	119.30	109.96
1	D	242	THR	N-CA-C	-6.26	104.38	111.07
1	C	97	ILE	N-CA-C	6.24	119.78	111.17
1	D	20	THR	N-CA-C	6.22	124.05	110.80
1	A	178	TYR	N-CA-C	6.22	117.63	108.86
1	C	49	CYS	CA-C-O	6.20	127.12	120.55
1	A	142	GLU	N-CA-C	6.20	119.01	111.82
1	A	145	SER	N-CA-C	-6.18	99.75	108.96
1	A	224	ILE	CB-CG1-CD1	-6.18	100.83	113.80
1	C	45	VAL	N-CA-C	6.18	116.92	110.62
1	A	59	LEU	CA-C-N	-6.17	114.72	123.11
1	A	59	LEU	C-N-CA	-6.17	114.72	123.11
1	C	19	GLY	N-CA-C	6.17	127.80	113.18
1	A	246	ASP	CB-CA-C	6.16	122.49	110.67
1	D	252	GLU	N-CA-C	6.12	117.19	108.74
1	C	273	MET	CG-SD-CE	-6.12	87.45	100.90
1	C	63	SER	N-CA-C	6.10	117.93	111.28
1	C	134	ILE	CB-CA-C	-6.10	102.11	110.77
1	B	8	VAL	CB-CA-C	-6.10	105.73	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	293	TRP	N-CA-C	-6.09	104.76	111.82
1	A	252	GLU	CB-CG-CD	-6.07	102.29	112.60
1	D	131	VAL	N-CA-C	5.99	117.31	108.45
1	B	160	ASP	N-CA-C	-5.99	104.67	111.07
1	A	41	LEU	CB-CA-C	-5.98	100.51	110.68
1	C	165	SER	CA-C-O	-5.97	115.23	121.55
1	C	181	VAL	N-CA-C	5.96	117.74	109.45
1	A	17	GLY	CA-C-N	5.95	130.33	122.30
1	A	17	GLY	C-N-CA	5.95	130.33	122.30
1	B	136	PRO	N-CA-C	5.94	121.28	113.86
1	C	224	ILE	CB-CA-C	-5.93	98.31	111.77
1	A	159	PHE	N-CA-C	-5.93	104.90	111.36
1	B	134	ILE	CB-CA-C	-5.90	102.45	110.42
1	B	40	PRO	CA-C-N	-5.87	112.34	120.38
1	B	40	PRO	C-N-CA	-5.87	112.34	120.38
1	C	22	MET	CG-SD-CE	5.85	113.77	100.90
1	A	60	VAL	N-CA-C	-5.84	98.73	107.37
1	A	297	GLU	N-CA-C	5.84	120.25	113.18
1	C	41	LEU	CB-CA-C	-5.82	100.78	110.68
1	C	256	ALA	N-CA-C	-5.81	100.24	109.76
1	C	20	THR	N-CA-C	5.80	123.15	110.80
1	C	36	LEU	N-CA-C	-5.80	96.33	107.57
1	C	131	VAL	N-CA-CB	-5.78	100.15	112.00
1	D	80	ALA	N-CA-C	-5.77	105.08	111.71
1	C	212	LEU	N-CA-C	5.76	117.69	108.41
1	B	269	LYS	N-CA-C	5.76	118.02	111.11
1	A	14	PRO	CB-CA-C	-5.74	106.17	111.40
1	C	217	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	A	68	ILE	N-CA-C	-5.72	104.94	110.72
1	B	246	ASP	N-CA-C	5.71	119.35	112.38
1	C	54	ILE	CB-CA-C	-5.71	103.73	111.15
1	C	194	VAL	N-CA-CB	-5.71	103.22	111.21
1	A	145	SER	CB-CA-C	-5.70	98.14	111.09
1	C	196	MET	N-CA-C	-5.70	99.72	109.24
1	D	107	VAL	CB-CA-C	-5.70	102.13	110.62
1	C	276	PHE	CA-C-O	5.70	126.80	120.82
1	C	172	VAL	N-CA-C	5.70	116.08	108.11
1	A	36	LEU	N-CA-C	-5.67	95.96	107.41
1	A	211	ASN	N-CA-C	-5.66	105.05	112.41
1	D	244	ALA	N-CA-C	-5.65	105.20	111.36
1	B	157	ARG	N-CA-C	-5.64	105.04	111.07
1	C	225	TRP	CA-C-N	5.63	125.16	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	TRP	C-N-CA	5.63	125.16	119.19
1	B	127	GLY	N-CA-C	-5.62	103.74	112.45
1	A	245	ILE	CA-C-N	-5.60	111.79	120.31
1	A	245	ILE	C-N-CA	-5.60	111.79	120.31
1	C	197	VAL	N-CA-CB	-5.60	105.04	112.26
1	A	277	VAL	CB-CA-C	-5.60	104.58	112.14
1	B	254	VAL	N-CA-C	-5.60	100.17	108.45
1	D	100	PRO	CA-C-N	-5.59	112.25	122.38
1	D	100	PRO	C-N-CA	-5.59	112.25	122.38
1	A	285	THR	N-CA-C	5.59	119.27	112.23
1	D	34	LEU	CA-C-N	-5.58	114.23	120.14
1	D	34	LEU	C-N-CA	-5.58	114.23	120.14
1	B	254	VAL	CB-CA-C	-5.58	101.06	110.71
1	D	19	GLY	CA-C-N	5.58	132.19	121.54
1	D	19	GLY	C-N-CA	5.58	132.19	121.54
1	A	297	GLU	CB-CA-C	5.57	121.03	109.95
1	A	215	VAL	CB-CA-C	-5.55	104.95	111.94
1	D	219	VAL	N-CA-CB	5.52	118.83	112.15
1	B	116	GLY	N-CA-C	-5.52	105.98	113.37
1	A	163	GLY	N-CA-C	-5.51	108.03	115.36
1	D	284	ASN	N-CA-C	5.51	118.05	111.71
1	A	144	GLU	CA-C-O	-5.50	112.91	119.35
1	B	271	GLY	N-CA-C	-5.48	105.76	112.77
1	C	226	PRO	CB-CA-C	-5.46	104.13	112.11
1	B	48	GLU	N-CA-C	-5.44	105.43	111.36
1	A	49	CYS	N-CA-C	-5.42	105.45	111.36
1	A	131	VAL	N-CA-CB	-5.42	102.33	112.36
1	D	36	LEU	N-CA-C	-5.42	96.95	107.62
1	A	134	ILE	N-CA-CB	-5.41	104.47	111.82
1	D	176	THR	N-CA-C	-5.40	105.47	111.36
1	D	230	LYS	CB-CA-C	-5.40	99.20	109.95
1	D	60	VAL	N-CA-C	-5.39	99.47	107.51
1	C	245	ILE	CB-CA-C	5.39	119.65	112.22
1	A	89	GLN	N-CA-C	-5.38	105.50	111.36
1	A	246	ASP	N-CA-CB	5.38	118.61	110.28
1	C	125	VAL	CB-CA-C	-5.37	105.18	111.94
1	A	19	GLY	CA-C-N	5.37	131.79	121.54
1	A	19	GLY	C-N-CA	5.37	131.79	121.54
1	C	53	GLY	CA-C-N	-5.37	114.26	121.66
1	C	53	GLY	C-N-CA	-5.37	114.26	121.66
1	B	129	GLU	CA-C-N	5.35	125.29	119.78
1	B	129	GLU	C-N-CA	5.35	125.29	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	79	GLU	N-CA-C	-5.34	105.63	111.82
1	B	123	HIS	CA-C-O	5.32	123.44	118.44
1	B	170	GLU	O-C-N	5.32	125.57	121.85
1	B	26	THR	CB-CA-C	-5.31	102.83	111.06
1	C	180	VAL	N-CA-C	5.30	115.94	108.36
1	A	230	LYS	N-CA-C	5.29	118.57	110.20
1	A	102	VAL	CA-C-O	-5.29	114.87	120.48
1	C	12	VAL	CA-C-O	-5.28	114.88	120.48
1	C	171	PRO	N-CA-C	5.28	119.15	110.55
1	C	269	LYS	CG-CD-CE	-5.27	99.18	111.30
1	C	134	ILE	N-CA-C	5.26	115.43	107.75
1	B	161	GLU	N-CA-C	5.22	116.97	111.28
1	B	204	LYS	N-CA-C	-5.22	100.67	108.96
1	A	15	VAL	CB-CA-C	-5.20	102.76	111.29
1	D	130	PRO	N-CA-C	-5.20	103.11	111.38
1	B	113	LYS	N-CA-C	5.20	125.55	111.00
1	A	197	VAL	N-CA-CB	-5.18	105.39	112.28
1	C	56	GLU	CB-CA-C	5.16	118.40	110.14
1	D	279	TYR	CA-C-N	-5.16	114.32	120.00
1	D	279	TYR	C-N-CA	-5.16	114.32	120.00
1	A	206	ASP	N-CA-C	5.15	119.19	113.01
1	A	126	VAL	CB-CA-C	-5.15	105.34	112.24
1	D	256	ALA	CA-C-N	-5.15	115.73	122.99
1	D	256	ALA	C-N-CA	-5.15	115.73	122.99
1	C	274	GLN	CA-CB-CG	-5.14	103.83	114.10
1	C	10	LYS	N-CA-C	5.13	117.85	109.59
1	D	134	ILE	N-CA-C	5.11	115.22	107.75
1	D	155	MET	N-CA-C	-5.11	106.30	112.54
1	A	104	ILE	CB-CA-C	-5.11	103.98	110.98
1	D	13	ILE	CB-CA-C	-5.11	106.23	111.08
1	C	62	HIS	N-CA-CB	-5.10	102.68	111.55
1	C	163	GLY	N-CA-C	-5.09	108.68	115.40
1	B	286	LEU	N-CA-C	5.09	119.44	112.88
1	D	13	ILE	N-CA-C	5.08	113.18	108.15
1	B	253	THR	N-CA-C	-5.08	102.96	110.48
1	A	224	ILE	N-CA-C	-5.08	105.44	112.50
1	A	144	GLU	O-C-N	5.07	128.68	122.34
1	C	138	VAL	N-CA-C	-5.07	101.02	108.11
1	A	143	TYR	N-CA-C	-5.06	106.62	112.89
1	B	190	PRO	CB-CA-C	-5.05	105.14	111.56
1	C	160	ASP	CB-CA-C	-5.05	100.97	110.67
1	D	159	PHE	CA-C-N	5.05	127.56	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	159	PHE	C-N-CA	5.05	127.56	120.28
1	C	82	LEU	N-CA-C	-5.04	107.68	113.88
1	C	179	GLY	N-CA-C	-5.01	101.31	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2199	0	2224	125	0
1	B	2166	0	2187	149	0
1	C	2195	0	2215	104	0
1	D	2096	0	2076	133	0
2	A	249	0	0	21	0
2	B	194	0	0	12	0
2	C	187	0	0	7	0
2	D	156	0	0	6	0
All	All	9442	0	8702	477	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 27.

All (477) 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:22:MET:SD	1:C:22:MET:CE	2.07	1.42
1:D:117:HIS:HB2	1:D:239:ILE:HD13	1.17	1.11
1:B:295:GLU:HG2	1:D:298:MET:HE1	1.12	1.11
1:C:21:ARG:H	1:C:21:ARG:HD3	1.24	1.01
1:D:117:HIS:HB2	1:D:239:ILE:CD1	1.90	1.00
1:A:149:GLN:O	1:A:157:ARG:NH2	1.94	1.00
1:B:295:GLU:CG	1:D:298:MET:HE1	1.94	0.97
1:A:273:MET:HE1	1:C:286:LEU:CD1	1.96	0.95
1:A:273:MET:HE1	1:C:286:LEU:HD12	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:O	2:A:495:HOH:O	1.85	0.94
1:B:188:LEU:CD2	1:B:192:GLU:HB2	1.97	0.94
1:D:7:LYS:CD	1:D:130:PRO:HG3	1.98	0.93
1:D:285:THR:HG22	1:D:286:LEU:HG	1.51	0.92
1:B:298:MET:HE2	1:D:294:LEU:HB3	1.50	0.91
1:B:298:MET:HE3	1:D:295:GLU:HG3	1.54	0.89
1:B:295:GLU:HG2	1:D:298:MET:CE	2.02	0.89
1:A:16:ALA:HB2	1:A:61:THR:HA	1.56	0.88
1:A:298:MET:HE2	1:C:294:LEU:HB3	1.55	0.88
1:D:241:LEU:HG	1:D:245:ILE:HD12	1.55	0.87
1:A:269:LYS:HB3	1:A:273:MET:CE	2.04	0.87
1:A:239:ILE:HD12	1:A:239:ILE:H	1.39	0.85
1:C:21:ARG:HD3	1:C:21:ARG:N	1.90	0.85
1:B:62[B]:HIS:CE1	1:B:64:SER:H	1.94	0.85
1:A:269:LYS:C	1:A:273:MET:HE3	2.02	0.85
1:B:298:MET:CE	1:D:295:GLU:HG3	2.07	0.83
1:A:79:GLU:HG2	1:A:91:LEU:HD11	1.60	0.83
1:B:80:ALA:HB1	1:B:84:LYS:HE3	1.59	0.82
1:B:16:ALA:CB	1:B:31:LYS:HD3	2.10	0.82
1:B:176:THR:O	1:B:202:LYS:HB3	1.78	0.81
1:A:22:MET:HE3	1:A:269:LYS:HG3	1.63	0.81
1:A:227:LEU:HD22	1:A:247:MET:HE2	1.63	0.81
1:A:83:GLU:HG2	1:A:91:LEU:CD2	2.10	0.80
1:B:200:VAL:HG11	1:B:209:PRO:CD	2.12	0.80
1:B:206:ASP:OD1	1:B:207:VAL:HG22	1.82	0.79
1:B:223:ASP:O	1:B:226:PRO:HD2	1.82	0.79
1:D:7:LYS:HD3	1:D:130:PRO:HG3	1.65	0.79
1:A:115:LEU:HD21	1:A:241:LEU:HD23	1.64	0.78
1:A:201:GLU:HG2	1:A:202:LYS:HG3	1.64	0.78
1:C:226:PRO:O	1:C:230:LYS:HG2	1.84	0.78
1:A:61:THR:HG21	1:A:106:GLN:OE1	1.84	0.78
1:D:247:MET:O	1:D:251:LYS:HD3	1.83	0.77
1:B:76:PHE:CD1	1:C:77:GLU:HG3	2.20	0.77
1:A:78:LEU:HG	1:A:82:LEU:HD11	1.65	0.77
1:D:162:THR:HG23	1:D:164:HIS:H	1.50	0.77
1:C:230:LYS:O	1:C:232:PRO:HD3	1.83	0.77
1:D:7:LYS:HD2	1:D:130:PRO:HG3	1.65	0.76
1:B:136:PRO:HG2	2:B:395:HOH:O	1.84	0.76
1:D:158:ARG:O	1:D:162:THR:HG22	1.84	0.76
1:D:159:PHE:O	1:D:163:GLY:N	2.19	0.76
1:C:31:LYS:HB2	2:C:419:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:LEU:O	1:D:119:VAL:HG23	1.87	0.75
1:C:123:HIS:HB3	1:C:124:PRO:HD3	1.68	0.74
1:B:39:LYS:HE3	2:B:316:HOH:O	1.85	0.74
1:B:200:VAL:HG11	1:B:209:PRO:HD3	1.68	0.74
1:B:294:LEU:HB3	1:D:298:MET:HE2	1.68	0.74
1:C:79:GLU:O	1:C:83:GLU:HG3	1.88	0.74
1:B:80:ALA:C	1:B:84:LYS:HE3	2.13	0.73
1:B:298:MET:CE	1:D:294:LEU:HB3	2.16	0.73
1:A:296:GLU:HB2	1:A:297:GLU:OE1	1.90	0.72
1:B:80:ALA:HB1	1:B:84:LYS:CE	2.19	0.72
1:A:243:ASP:O	1:A:247:MET:HG3	1.89	0.71
1:A:115:LEU:HD21	1:A:241:LEU:CD2	2.21	0.71
1:C:112:ALA:HB1	1:C:117:HIS:CG	2.26	0.70
1:B:80:ALA:CA	1:B:84:LYS:HE3	2.21	0.70
1:C:200:VAL:HG12	1:C:203:PRO:HG3	1.71	0.70
1:B:76:PHE:CE1	1:C:81:MET:HE2	2.26	0.70
1:D:117:HIS:CB	1:D:239:ILE:HD13	2.10	0.70
1:A:22:MET:HE3	1:A:269:LYS:CG	2.21	0.70
1:A:61:THR:HG21	1:A:106:GLN:CD	2.18	0.69
1:B:78:LEU:O	1:B:78:LEU:HD12	1.91	0.69
1:A:11:ALA:HB2	1:A:54:ILE:HD13	1.74	0.69
1:A:110:GLY:N	2:A:414:HOH:O	2.25	0.69
1:B:80:ALA:CB	1:B:84:LYS:HE3	2.21	0.69
1:B:19:GLY:HA3	1:B:31:LYS:HD2	1.75	0.68
1:A:107[B]:VAL:HG21	1:A:125:VAL:CG2	2.24	0.67
1:B:78:LEU:HD11	1:B:82:LEU:HD11	1.76	0.67
1:A:297:GLU:HB3	2:A:485:HOH:O	1.93	0.67
1:B:24:PRO:HD2	1:D:38:ASP:O	1.95	0.67
1:C:111:LEU:HG	1:D:74:THR:HG21	1.75	0.67
1:D:251:LYS:HD2	1:D:251:LYS:N	2.08	0.67
1:A:6:THR:HB	1:A:160:ASP:OD2	1.95	0.67
1:B:178:TYR:O	1:B:202:LYS:HA	1.94	0.67
1:D:241:LEU:HG	1:D:245:ILE:CD1	2.24	0.67
1:A:284:ASN:OD1	2:A:476:HOH:O	2.12	0.66
1:B:79:GLU:HA	1:B:82:LEU:HD12	1.77	0.66
1:C:270:LEU:O	1:C:274:GLN:HG3	1.95	0.66
1:A:270:LEU:O	1:A:274:GLN:HG3	1.95	0.66
1:C:19:GLY:HA3	1:C:31:LYS:HD3	1.76	0.66
1:D:296:GLU:O	1:D:297:GLU:C	2.38	0.66
1:C:143:TYR:CE1	1:C:282:ARG:HD2	2.30	0.65
1:B:7:LYS:HB3	1:B:130:PRO:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LYS:O	1:B:295:GLU:HG3	1.97	0.65
1:D:151:ASN:O	1:D:155:MET:HG3	1.96	0.65
1:B:129:GLU:HB3	1:B:130:PRO:HD2	1.79	0.65
1:B:15:VAL:O	1:B:62[A]:HIS:NE2	2.31	0.64
1:D:154:GLU:O	1:D:158:ARG:HG3	1.97	0.64
1:A:188:LEU:CD2	1:A:194:VAL:HG23	2.27	0.64
1:B:268:ASN:HD21	1:B:271:GLY:HA3	1.61	0.64
1:C:189:ALA:HB3	1:C:192:GLU:OE2	1.98	0.64
1:D:61:THR:HG21	1:D:106:GLN:HG3	1.79	0.63
1:C:143:TYR:CD1	1:C:282:ARG:HD2	2.33	0.63
1:A:83:GLU:HG2	1:A:91:LEU:HD22	1.78	0.63
1:C:22:MET:CE	1:C:269:LYS:HG2	2.28	0.63
1:C:91:LEU:O	1:C:91:LEU:HD12	1.99	0.62
1:D:91:LEU:HD12	1:D:91:LEU:O	2.00	0.62
1:A:16:ALA:HB2	1:A:61:THR:CA	2.28	0.62
1:B:7:LYS:HE2	1:B:7:LYS:HA	1.81	0.62
1:B:188:LEU:HD22	1:B:192:GLU:HB2	1.78	0.62
1:B:73:ASP:OD1	1:B:74:THR:N	2.30	0.62
1:C:203:PRO:C	1:C:204:LYS:O	2.35	0.62
1:A:220:LEU:HB3	1:A:224:ILE:HG12	1.81	0.62
2:A:496:HOH:O	1:C:22:MET:HE2	1.99	0.62
1:B:16:ALA:O	2:B:389:HOH:O	2.16	0.62
1:C:83:GLU:HG2	1:C:91:LEU:HD21	1.82	0.62
1:B:27:LYS:HE2	1:D:75:SER:OG	2.00	0.61
1:D:188:LEU:HD13	1:D:258:HIS:HB2	1.82	0.61
1:B:9:LYS:O	2:B:387:HOH:O	2.16	0.61
1:D:171:PRO:HA	1:D:211:ASN:O	2.00	0.61
1:A:211:ASN:OD1	2:A:483:HOH:O	2.16	0.61
1:B:78:LEU:HD12	1:B:78:LEU:C	2.26	0.60
1:B:293:TRP:O	1:B:297:GLU:HB2	2.01	0.60
1:C:78:LEU:HD23	1:C:82:LEU:HD12	1.84	0.60
1:A:169:VAL:HA	1:A:213:ALA:O	2.01	0.60
1:B:80:ALA:HB1	1:B:84:LYS:NZ	2.15	0.60
1:A:188:LEU:HD22	1:A:192:GLU:O	2.02	0.60
1:C:90:LEU:HD23	1:C:90:LEU:N	2.15	0.60
1:B:62[B]:HIS:ND1	1:B:64:SER:N	2.44	0.60
1:C:22:MET:HE1	1:C:269:LYS:HG2	1.82	0.60
1:A:78:LEU:HG	1:A:82:LEU:CD1	2.32	0.60
1:A:292:ALA:O	1:A:296:GLU:HG3	2.02	0.60
1:C:157:ARG:NH1	2:C:470:HOH:O	2.35	0.60
1:A:91:LEU:O	1:A:95:GLN:HG3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:SER:O	1:A:76:PHE:C	2.44	0.59
1:D:180:VAL:CG2	1:D:209:PRO:HD2	2.32	0.59
1:A:269:LYS:HB3	1:A:273:MET:HE3	1.83	0.59
1:D:115:LEU:HD21	1:D:241:LEU:HD22	1.84	0.59
1:A:298:MET:HE2	1:C:294:LEU:CB	2.29	0.59
1:C:241:LEU:HG	1:C:245:ILE:HD12	1.85	0.59
1:D:75:SER:O	1:D:78:LEU:HB3	2.02	0.59
1:D:250:GLU:C	1:D:251:LYS:HD2	2.27	0.59
1:A:113:LYS:HB2	1:A:117:HIS:CG	2.38	0.59
1:D:180:VAL:HG23	1:D:209:PRO:HD2	1.83	0.59
1:A:107[B]:VAL:HG21	1:A:125:VAL:HG21	1.84	0.59
1:D:268:ASN:ND2	1:D:271:GLY:H	2.01	0.59
1:C:143:TYR:CD1	1:C:282:ARG:CD	2.86	0.58
1:A:38:ASP:O	1:C:24:PRO:HD2	2.03	0.58
1:B:225:TRP:HB2	1:B:226:PRO:HD3	1.85	0.58
1:B:62[B]:HIS:ND1	1:B:63:SER:N	2.51	0.58
1:B:247:MET:HG3	2:B:490:HOH:O	2.03	0.58
1:A:47:ASN:ND2	2:A:316:HOH:O	2.28	0.58
1:B:76:PHE:HE1	1:C:81:MET:HE2	1.68	0.58
1:B:6:THR:HB	1:B:160:ASP:OD2	2.03	0.58
1:B:265:ASP:HB2	2:B:427:HOH:O	2.04	0.58
1:C:224:ILE:HD12	1:C:224:ILE:N	2.18	0.58
1:D:224:ILE:HA	1:D:227:LEU:HD12	1.86	0.57
1:A:99:PRO:HB2	1:A:101[B]:HIS:CE1	2.39	0.57
1:B:123:HIS:HB3	1:B:124:PRO:HD3	1.86	0.57
1:B:298:MET:HE3	1:D:295:GLU:HA	1.86	0.57
1:B:223:ASP:HB3	2:B:374:HOH:O	2.03	0.57
1:C:99:PRO:HB3	1:C:101:HIS:CE1	2.39	0.57
1:A:61:THR:HG23	1:A:62:HIS:N	2.19	0.57
1:A:136:PRO:HD2	2:A:395:HOH:O	2.03	0.57
1:A:273:MET:HE1	1:C:286:LEU:HD13	1.85	0.57
1:A:36:LEU:O	2:A:495:HOH:O	2.18	0.57
1:A:91:LEU:O	1:A:91:LEU:HD12	2.05	0.56
1:D:174:ASP:OD1	1:D:177:ALA:HB2	2.06	0.56
1:A:21:ARG:NH2	2:A:422:HOH:O	2.28	0.56
1:A:221:SER:O	1:A:224:ILE:HG13	2.04	0.56
1:C:22:MET:HE1	1:C:269:LYS:HA	1.87	0.56
1:C:150:ASP:CG	1:C:260:LYS:HE3	2.31	0.56
1:D:7:LYS:HD3	1:D:130:PRO:CG	2.35	0.56
1:B:188:LEU:HD13	1:B:258:HIS:HB2	1.87	0.56
1:D:115:LEU:CD2	1:D:241:LEU:HD22	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:CD1	1:B:94:VAL:HG21	2.36	0.56
1:A:61:THR:OG1	1:A:62:HIS:N	2.36	0.55
1:B:76:PHE:CE1	1:C:77:GLU:HG3	2.41	0.55
1:D:274:GLN:O	1:D:278:GLU:HG3	2.06	0.55
1:D:16:ALA:HB2	1:D:61:THR:HA	1.87	0.55
1:B:18:LEU:HD12	1:B:18:LEU:H	1.72	0.55
1:B:170:GLU:HB2	1:B:171:PRO:HD2	1.89	0.55
1:C:203:PRO:N	2:C:424:HOH:O	2.39	0.55
1:A:224:ILE:HD12	1:A:225:TRP:N	2.21	0.55
1:C:99:PRO:CB	1:C:101:HIS:CE1	2.89	0.55
1:A:239:ILE:HD12	1:A:239:ILE:N	2.15	0.55
1:D:82:LEU:C	1:D:91:LEU:HD22	2.32	0.55
1:B:7:LYS:HE2	1:B:7:LYS:CA	2.36	0.55
1:D:140:LEU:CD1	1:D:168:MET:HE1	2.37	0.55
1:D:7:LYS:HD2	1:D:159:PHE:HE2	1.72	0.54
1:A:27:LYS:NZ	1:C:73:ASP:O	2.29	0.54
1:C:20:THR:HB	1:C:21:ARG:HH11	1.72	0.54
1:D:145:SER:OG	1:D:260:LYS:O	2.26	0.54
1:A:78:LEU:O	1:A:81:MET:HB3	2.08	0.54
1:C:82:LEU:HB3	1:C:91:LEU:HD22	1.90	0.54
1:C:296:GLU:O	1:C:297:GLU:C	2.50	0.54
1:D:182:ASP:OD1	1:D:182:ASP:C	2.51	0.54
1:D:234:GLY:HA3	1:D:238:GLU:O	2.08	0.54
1:C:236:GLY:O	1:C:237:ASP:HB2	2.07	0.53
1:A:188:LEU:HD21	1:A:194:VAL:HG23	1.89	0.53
1:D:182:ASP:OD1	1:D:184:LYS:N	2.37	0.53
1:A:44:TYR:HE2	2:A:495:HOH:O	1.91	0.53
1:D:92:ASP:HB2	1:D:93:GLU:OE2	2.08	0.53
1:A:107[B]:VAL:CG2	1:A:125:VAL:HG21	2.39	0.53
1:D:180:VAL:C	1:D:199:VAL:HG13	2.33	0.53
1:D:10:LYS:HE3	1:D:126:VAL:HA	1.91	0.53
1:A:15:VAL:HG23	1:A:15:VAL:O	2.07	0.53
1:D:247:MET:HA	1:D:250:GLU:OE2	2.08	0.53
1:B:200:VAL:O	1:B:200:VAL:HG13	2.08	0.53
1:A:75:SER:O	1:A:78:LEU:N	2.42	0.53
1:D:156:ILE:HG13	1:D:219:VAL:HG21	1.90	0.52
1:D:91:LEU:CD1	1:D:95:GLN:NE2	2.72	0.52
1:B:80:ALA:O	1:B:84:LYS:HE3	2.08	0.52
1:B:223:ASP:OD2	1:B:252:GLU:OE2	2.28	0.52
1:C:55:THR:C	1:C:56:GLU:HG3	2.35	0.52
1:B:164:HIS:CE1	1:B:253:THR:HB	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:VAL:O	1:B:50:ILE:HG13	2.10	0.52
1:B:178:TYR:O	1:B:202:LYS:N	2.42	0.52
1:A:76:PHE:N	2:A:505:HOH:O	2.31	0.52
1:C:174:ASP:OD1	1:C:176:THR:OG1	2.23	0.52
1:B:76:PHE:CG	1:C:77:GLU:HG3	2.45	0.51
1:D:251:LYS:N	1:D:251:LYS:CD	2.73	0.51
1:B:178:TYR:O	1:B:202:LYS:CA	2.58	0.51
1:D:61:THR:CG2	1:D:106:GLN:HG3	2.40	0.51
1:D:246:ASP:HA	1:D:249:ILE:HD12	1.93	0.51
1:A:60:VAL:HG22	1:A:107[A]:VAL:CG1	2.40	0.51
1:B:61:THR:HG22	1:B:106:GLN:CG	2.40	0.51
1:D:75:SER:HB2	1:D:78:LEU:HB3	1.92	0.51
1:D:11:ALA:HB2	1:D:54:ILE:HD12	1.92	0.51
1:A:108:ARG:NH1	1:B:73:ASP:OD2	2.39	0.51
1:B:293:TRP:HA	2:B:455:HOH:O	2.10	0.51
1:A:269:LYS:HB3	1:A:273:MET:HE1	1.91	0.51
1:B:40:PRO:O	1:B:41:LEU:C	2.53	0.51
1:C:77:GLU:O	1:C:80:ALA:HB3	2.10	0.51
1:C:218:TYR:N	1:C:218:TYR:CD1	2.78	0.51
1:D:225:TRP:N	1:D:226:PRO:CD	2.74	0.51
1:D:226:PRO:HD2	1:D:227:LEU:H	1.75	0.50
1:D:77:GLU:O	1:D:80:ALA:HB3	2.10	0.50
1:A:36:LEU:N	2:A:495:HOH:O	2.30	0.50
1:B:122:ALA:O	1:B:123:HIS:C	2.53	0.50
1:B:298:MET:CE	1:D:295:GLU:N	2.75	0.50
1:A:16:ALA:HB2	1:A:61:THR:C	2.35	0.50
1:A:199:VAL:HG21	1:A:245:ILE:HG22	1.93	0.50
1:B:82:LEU:HD13	1:B:94:VAL:HG21	1.93	0.50
1:A:178:TYR:O	1:A:202:LYS:N	2.38	0.50
1:B:74:THR:C	2:B:464:HOH:O	2.54	0.50
1:B:154:GLU:O	1:B:158[A]:ARG:HG3	2.11	0.50
1:C:24:PRO:O	1:C:25:ALA:C	2.55	0.50
1:A:76:PHE:CE2	1:D:77:GLU:HA	2.47	0.50
1:C:90:LEU:N	1:C:90:LEU:CD2	2.75	0.50
1:C:189:ALA:O	1:C:190:PRO:C	2.54	0.50
1:C:223:ASP:OD2	1:C:252:GLU:OE2	2.30	0.50
1:A:61:THR:CG2	1:A:106:GLN:CD	2.85	0.50
1:A:214:ILE:O	2:A:545:HOH:O	2.20	0.50
1:B:115:LEU:O	1:B:119:VAL:HG23	2.11	0.50
1:C:224:ILE:HD12	1:C:225:TRP:N	2.26	0.50
1:D:62:HIS:HB3	1:D:65:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:GLU:O	1:B:202:LYS:C	2.56	0.49
1:D:162:THR:CG2	1:D:164:HIS:HB2	2.43	0.49
1:A:76:PHE:CD2	1:D:77:GLU:HB2	2.47	0.49
1:B:7:LYS:HB3	1:B:130:PRO:CG	2.42	0.49
1:B:182:ASP:HA	1:B:209:PRO:HB2	1.93	0.49
1:B:61:THR:CG2	1:B:106:GLN:CG	2.91	0.49
1:D:199:VAL:HG21	1:D:214:ILE:HD11	1.95	0.49
1:C:21:ARG:N	1:C:21:ARG:CD	2.71	0.49
1:D:140:LEU:N	1:D:140:LEU:HD23	2.25	0.49
1:A:105:MET:HG2	1:B:125:VAL:HG22	1.94	0.49
1:D:225:TRP:N	1:D:226:PRO:HD3	2.28	0.49
1:D:242:THR:O	1:D:246:ASP:OD1	2.31	0.49
1:B:7:LYS:CB	1:B:130:PRO:HG3	2.43	0.49
1:B:77:GLU:HA	1:C:76:PHE:CE2	2.48	0.49
1:A:56:GLU:HB3	1:A:105:MET:HE1	1.95	0.48
1:D:129:GLU:C	1:D:222:ALA:HB2	2.38	0.48
1:A:63:SER:HB3	1:A:108:ARG:NH1	2.28	0.48
1:B:16:ALA:HB2	1:B:31:LYS:HD3	1.90	0.48
1:D:123:HIS:HB3	1:D:124:PRO:HD3	1.93	0.48
1:D:169:VAL:HA	1:D:213:ALA:O	2.13	0.48
1:B:130:PRO:HA	1:B:220:LEU:O	2.13	0.48
1:D:16:ALA:HB2	1:D:61:THR:C	2.39	0.48
1:D:76:PHE:O	1:D:80:ALA:N	2.42	0.48
1:D:253:THR:HB	2:D:388:HOH:O	2.12	0.48
1:C:175:VAL:O	1:C:203:PRO:HD2	2.14	0.48
1:A:74:THR:HG23	1:A:79:GLU:OE1	2.14	0.48
1:C:295:GLU:O	1:C:296:GLU:C	2.56	0.48
1:C:76:PHE:HB3	2:C:462:HOH:O	2.14	0.48
1:D:16:ALA:HB2	1:D:61:THR:CA	2.44	0.48
1:D:242:THR:HG23	2:D:372:HOH:O	2.13	0.48
1:B:62[B]:HIS:CE1	1:B:64:SER:N	2.75	0.47
1:D:15:VAL:O	1:D:15:VAL:HG23	2.12	0.47
1:B:78:LEU:HD11	1:B:82:LEU:CD1	2.43	0.47
1:D:151:ASN:HB3	1:D:168:MET:CE	2.43	0.47
1:A:83:GLU:HG2	1:A:91:LEU:HD21	1.94	0.47
1:C:78:LEU:O	1:C:82:LEU:HB2	2.14	0.47
1:C:169:VAL:HA	1:C:213:ALA:O	2.15	0.47
1:A:10:LYS:HD2	1:A:126:VAL:HA	1.97	0.47
1:C:17:GLY:O	1:C:65:LYS:NZ	2.35	0.47
1:A:239:ILE:H	1:A:239:ILE:CD1	2.18	0.47
1:B:223:ASP:O	1:B:227:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:THR:HB	1:D:79:GLU:OE2	2.14	0.47
1:B:146:ASP:OD1	1:B:146:ASP:C	2.58	0.47
1:C:22:MET:HE3	1:C:269:LYS:HG2	1.97	0.47
1:A:152:LEU:O	1:A:156:ILE:HG13	2.14	0.47
1:D:121:CYS:O	1:D:124:PRO:HD2	2.15	0.47
1:C:91:LEU:O	1:C:95:GLN:HG3	2.15	0.46
1:C:164:HIS:HD2	1:C:255:GLU:OE2	1.97	0.46
1:B:171:PRO:HA	1:B:211:ASN:O	2.15	0.46
1:B:17:GLY:O	1:B:65:LYS:NZ	2.46	0.46
1:B:274:GLN:O	1:B:278:GLU:HG3	2.15	0.46
1:A:113:LYS:HB2	1:A:117:HIS:ND1	2.30	0.46
1:D:124:PRO:HD3	2:D:352:HOH:O	2.14	0.46
1:A:207:VAL:O	1:A:207:VAL:HG22	2.16	0.46
1:B:62[B]:HIS:CE1	1:B:64:SER:OG	2.69	0.46
1:D:223:ASP:O	1:D:226:PRO:HD2	2.15	0.46
1:A:22:MET:HE2	1:A:22:MET:HB3	1.86	0.46
1:C:6:THR:OG1	1:C:7:LYS:N	2.49	0.46
1:D:174:ASP:OD2	1:D:176:THR:CB	2.64	0.46
1:C:99:PRO:HB3	1:C:101:HIS:HE1	1.81	0.46
1:A:91:LEU:HD12	1:A:91:LEU:C	2.40	0.46
1:C:34:LEU:HA	1:C:34:LEU:HD23	1.69	0.46
1:C:221:SER:O	1:C:224:ILE:HG13	2.15	0.46
1:A:188:LEU:HD23	1:A:194:VAL:HG23	1.96	0.45
1:C:22:MET:CE	1:C:269:LYS:CG	2.94	0.45
1:C:99:PRO:HB2	1:C:101:HIS:CE1	2.50	0.45
1:C:203:PRO:CD	2:C:424:HOH:O	2.64	0.45
1:C:224:ILE:HD12	1:C:225:TRP:H	1.81	0.45
1:D:74:THR:HG22	2:D:436:HOH:O	2.15	0.45
1:D:246:ASP:O	1:D:250:GLU:HG3	2.16	0.45
1:A:227:LEU:HD22	1:A:247:MET:CE	2.42	0.45
1:A:22:MET:CE	1:A:269:LYS:CG	2.92	0.45
1:B:69:GLU:CD	1:B:106:GLN:HE21	2.25	0.45
1:C:269:LYS:O	1:C:273:MET:HG3	2.16	0.45
1:B:78:LEU:C	1:B:78:LEU:CD1	2.88	0.45
1:B:107[B]:VAL:HG21	1:B:125:VAL:HG21	1.98	0.45
1:D:140:LEU:HD11	1:D:168:MET:HE1	1.97	0.45
1:C:91:LEU:O	1:C:95:GLN:HB2	2.16	0.45
1:D:6:THR:HG22	1:D:6:THR:O	2.16	0.45
1:D:162:THR:HG23	1:D:164:HIS:HB2	1.97	0.45
1:A:132:ALA:HA	1:A:218:TYR:O	2.17	0.45
1:B:107[B]:VAL:HG21	1:B:125:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:MET:HE1	1:C:20:THR:OG1	2.17	0.45
1:B:69:GLU:OE1	2:B:402:HOH:O	2.20	0.45
1:A:79:GLU:O	1:A:83:GLU:HG3	2.16	0.45
1:B:7:LYS:HA	1:B:7:LYS:CE	2.40	0.45
1:B:109:GLN:O	1:B:110:GLY:C	2.60	0.45
1:D:39:LYS:HE3	2:D:323:HOH:O	2.17	0.45
1:A:225:TRP:HB2	1:A:226:PRO:HD3	1.99	0.45
1:B:80:ALA:O	1:B:84:LYS:CE	2.65	0.45
1:D:91:LEU:HD12	1:D:95:GLN:NE2	2.32	0.45
1:A:129:GLU:HG2	2:A:420:HOH:O	2.17	0.44
1:D:74:THR:H	1:D:74:THR:HG23	1.40	0.44
1:D:241:LEU:O	1:D:245:ILE:HD12	2.17	0.44
1:D:246:ASP:OD1	1:D:246:ASP:N	2.51	0.44
1:B:78:LEU:CD1	1:B:82:LEU:HD11	2.46	0.44
1:C:43:GLN:O	1:C:47:ASN:ND2	2.50	0.44
1:B:82:LEU:HB2	1:B:91:LEU:HD13	2.00	0.44
1:B:212:LEU:HA	1:B:212:LEU:HD23	1.61	0.44
1:A:115:LEU:CD2	1:A:241:LEU:CD2	2.95	0.44
1:A:201:GLU:HG2	1:A:202:LYS:CG	2.40	0.44
1:B:61:THR:HG21	1:B:106:GLN:HG3	2.00	0.44
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.58	0.44
1:A:154:GLU:HA	1:A:157:ARG:CZ	2.48	0.44
1:A:292:ALA:O	1:A:293:TRP:C	2.58	0.44
1:C:106:GLN:NE2	2:C:463:HOH:O	2.51	0.44
1:D:75:SER:O	1:D:79:GLU:HG3	2.18	0.44
1:A:22:MET:HE3	1:A:269:LYS:HG2	1.99	0.44
1:B:204:LYS:O	1:B:205:ALA:C	2.61	0.44
1:A:60:VAL:HG22	1:A:107[A]:VAL:HG12	1.99	0.44
1:C:69:GLU:H	1:C:69:GLU:HG2	1.65	0.44
1:A:36:LEU:CB	2:A:495:HOH:O	2.66	0.44
1:A:96:SER:O	1:A:97:ILE:C	2.58	0.44
1:B:79:GLU:OE2	2:B:341:HOH:O	2.20	0.44
1:C:285:THR:HG22	1:C:286:LEU:HG	2.00	0.44
1:D:92:ASP:O	1:D:96:SER:HB2	2.18	0.44
1:D:159:PHE:O	1:D:163:GLY:CA	2.65	0.44
1:D:298:MET:HE3	1:D:298:MET:HB3	1.40	0.44
1:C:135:LEU:HA	1:C:136:PRO:HD3	1.87	0.43
1:D:61:THR:CG2	1:D:106:GLN:CG	2.96	0.43
1:B:158[B]:ARG:CZ	1:B:162:THR:HG21	2.48	0.43
1:B:270:LEU:O	1:B:274:GLN:HG3	2.17	0.43
1:C:200:VAL:HG12	1:C:203:PRO:CG	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ASP:CG	1:B:74:THR:N	2.76	0.43
1:B:200:VAL:HG11	1:B:209:PRO:HD2	1.98	0.43
1:C:83:GLU:CG	1:C:91:LEU:HD21	2.46	0.43
1:B:241:LEU:HA	1:B:241:LEU:HD12	1.69	0.43
1:C:78:LEU:HD23	1:C:82:LEU:CD1	2.48	0.43
1:D:174:ASP:O	1:D:177:ALA:HB3	2.18	0.43
1:A:115:LEU:CD2	1:A:241:LEU:HD23	2.41	0.43
1:B:61:THR:CG2	1:B:106:GLN:HG3	2.48	0.43
1:D:223:ASP:O	1:D:227:LEU:HD12	2.18	0.43
1:A:289:GLU:HB2	2:A:479:HOH:O	2.19	0.43
1:C:78:LEU:CD2	1:C:94:VAL:HG11	2.49	0.43
1:A:107[B]:VAL:CG2	1:A:125:VAL:CG2	2.96	0.43
1:B:78:LEU:CD1	1:B:82:LEU:CD1	2.97	0.43
1:B:99:PRO:HA	1:B:100:PRO:HD3	1.82	0.43
1:C:262:LYS:HE3	1:C:278:GLU:OE1	2.18	0.43
1:A:252:GLU:HG2	2:A:386:HOH:O	2.19	0.42
1:B:131:VAL:HG22	1:B:132:ALA:N	2.33	0.42
1:B:180:VAL:HG12	1:B:210:SER:OG	2.19	0.42
1:C:283:HIS:CE1	1:C:285:THR:HB	2.55	0.42
1:D:288:THR:HB	2:D:421:HOH:O	2.19	0.42
1:B:61:THR:HG21	1:B:106:GLN:NE2	2.34	0.42
1:D:115:LEU:CD2	1:D:241:LEU:CD2	2.97	0.42
1:B:27:LYS:NZ	1:D:71:HIS:O	2.39	0.42
1:B:18:LEU:HD12	1:B:18:LEU:N	2.33	0.42
1:C:189:ALA:HB3	1:C:192:GLU:CD	2.44	0.42
1:A:231:THR:HA	1:A:232:PRO:HD3	1.65	0.42
1:B:89:GLN:H	1:B:89:GLN:HG2	1.55	0.42
1:B:200:VAL:CG1	1:B:209:PRO:CD	2.91	0.42
1:C:172:VAL:HG23	1:C:172:VAL:O	2.19	0.42
1:B:188:LEU:HD21	1:B:192:GLU:HB2	1.96	0.42
1:B:189:ALA:O	1:B:190:PRO:C	2.63	0.42
1:B:221:SER:O	1:B:224:ILE:HG13	2.19	0.42
1:B:259:MET:SD	1:B:263:SER:HB3	2.59	0.42
1:C:135:LEU:N	1:C:135:LEU:HD23	2.34	0.42
1:C:193:SER:HA	1:C:256:ALA:O	2.19	0.42
1:A:89:GLN:HE21	1:A:89:GLN:HB3	1.50	0.42
1:B:298:MET:HE1	1:D:295:GLU:HG3	1.95	0.42
1:D:193:SER:HA	1:D:256:ALA:O	2.20	0.42
1:D:249:ILE:HG13	1:D:254:VAL:HG21	2.02	0.42
1:D:199:VAL:HG12	1:D:200:VAL:N	2.34	0.42
1:A:269:LYS:O	1:A:273:MET:HE3	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ALA:C	1:C:82:LEU:H	2.28	0.42
1:C:105:MET:SD	1:C:125:VAL:HG11	2.60	0.42
1:C:204:LYS:HG2	2:C:377:HOH:O	2.20	0.42
1:D:95:GLN:O	1:D:97:ILE:N	2.52	0.42
1:D:170:GLU:HG2	1:D:215:VAL:HG22	2.01	0.42
1:A:40:PRO:O	1:A:41:LEU:C	2.60	0.41
1:B:157:ARG:O	1:B:161:GLU:HG3	2.19	0.41
1:C:224:ILE:CD1	1:C:225:TRP:N	2.83	0.41
1:D:56:GLU:HB3	1:D:105:MET:HE3	2.02	0.41
1:D:162:THR:HG23	1:D:164:HIS:N	2.28	0.41
1:A:154:GLU:OE1	1:A:257:TYR:OH	2.38	0.41
1:A:259:MET:HE2	1:A:259:MET:HB3	1.90	0.41
1:B:188:LEU:HD23	1:B:192:GLU:HB2	1.92	0.41
1:C:33:MET:HE3	1:C:33:MET:HB3	1.86	0.41
1:D:72:PHE:CB	1:D:104:ILE:HD13	2.49	0.41
1:D:87:LYS:O	1:D:91:LEU:N	2.31	0.41
1:D:115:LEU:HD21	1:D:241:LEU:CD2	2.48	0.41
1:B:181:VAL:O	1:B:210:SER:OG	2.32	0.41
1:D:141:ASP:OD2	1:D:282:ARG:NH2	2.45	0.41
1:A:139:ILE:HD12	1:A:139:ILE:HG23	1.80	0.41
1:D:15:VAL:HG12	1:D:136:PRO:HG3	2.01	0.41
1:A:31:LYS:HE3	1:A:31:LYS:HB2	1.60	0.41
1:A:76:PHE:HB3	2:A:505:HOH:O	2.21	0.41
1:A:92:ASP:O	1:A:93:GLU:C	2.63	0.41
1:A:170:GLU:HG2	1:A:215:VAL:HG22	2.02	0.41
1:A:294:LEU:O	1:A:298:MET:HB2	2.20	0.41
1:B:65:LYS:HE2	2:B:389:HOH:O	2.21	0.41
1:C:141:ASP:OD2	1:C:282:ARG:NH2	2.53	0.41
1:D:180:VAL:O	1:D:199:VAL:HG13	2.20	0.41
1:B:15:VAL:O	1:B:62[A]:HIS:CD2	2.73	0.41
1:B:242:THR:HA	1:B:245:ILE:HB	2.03	0.41
1:B:298:MET:CE	1:D:295:GLU:HA	2.49	0.41
1:A:154:GLU:HA	1:A:157:ARG:NH2	2.36	0.41
1:B:230:LYS:O	1:B:231:THR:C	2.64	0.41
1:D:290:PHE:O	1:D:294:LEU:HB2	2.21	0.41
1:A:36:LEU:C	2:A:495:HOH:O	2.62	0.41
1:B:26:THR:HG21	1:B:31:LYS:HB3	2.03	0.41
1:B:81:MET:HA	1:B:84:LYS:HB2	2.01	0.41
1:B:240:GLN:HE21	1:B:240:GLN:HB2	1.71	0.41
1:D:123:HIS:N	1:D:124:PRO:CD	2.83	0.41
1:D:140:LEU:HD22	1:D:140:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:HG3	1:A:157:ARG:HE	1.86	0.40
1:B:47:ASN:HA	1:B:50:ILE:HD12	2.04	0.40
1:B:61:THR:HG22	1:B:106:GLN:HG2	2.02	0.40
1:C:151:ASN:O	1:C:152:LEU:C	2.64	0.40
1:D:39:LYS:HB2	1:D:44:TYR:CE2	2.56	0.40
1:B:31:LYS:H	1:B:31:LYS:HG2	1.73	0.40
1:B:82:LEU:CB	1:B:91:LEU:HD13	2.51	0.40
1:B:175:VAL:HG23	1:B:203:PRO:HG2	2.02	0.40
1:C:78:LEU:CD2	1:C:82:LEU:HD12	2.49	0.40
1:C:177:ALA:C	1:C:178:TYR:CD1	3.00	0.40
1:D:182:ASP:HA	1:D:209:PRO:HB2	2.03	0.40
1:A:224:ILE:HD12	1:A:224:ILE:C	2.46	0.40
1:B:294:LEU:HD13	1:D:298:MET:HG3	2.02	0.40
1:D:221:SER:C	1:D:223:ASP:N	2.78	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	282/302 (93%)	265 (94%)	14 (5%)	3 (1%)	11	4
1	B	276/302 (91%)	261 (95%)	13 (5%)	2 (1%)	18	10
1	C	282/302 (93%)	264 (94%)	15 (5%)	3 (1%)	11	4
1	D	268/302 (89%)	243 (91%)	22 (8%)	3 (1%)	11	4
All	All	1108/1208 (92%)	1033 (93%)	64 (6%)	11 (1%)	12	5

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	96	SER

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Mol	Chain	Res	Type
1	A	37	VAL
1	B	37	VAL
1	D	37	VAL
1	C	37	VAL
1	C	19	GLY
1	B	205	ALA
1	C	296	GLU
1	D	76	PHE
1	A	110	GLY
1	A	97	ILE

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	246/254 (97%)	219 (89%)	27 (11%)	6	1
1	B	242/254 (95%)	212 (88%)	30 (12%)	4	1
1	C	243/254 (96%)	216 (89%)	27 (11%)	6	1
1	D	227/254 (89%)	190 (84%)	37 (16%)	2	0
All	All	958/1016 (94%)	837 (87%)	121 (13%)	4	1

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	9	LYS
1	A	18	LEU
1	A	22	MET
1	A	31	LYS
1	A	57	ILE
1	A	65	LYS
1	A	69	GLU
1	A	74	THR
1	A	89	GLN
1	A	90	LEU

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Mol	Chain	Res	Type
1	A	94	VAL
1	A	106	GLN
1	A	115	LEU
1	A	145	SER
1	A	157	ARG
1	A	190	PRO
1	A	197	VAL
1	A	221	SER
1	A	224	ILE
1	A	239	ILE
1	A	251	LYS
1	A	260	LYS
1	A	281	ILE
1	A	282	ARG
1	A	294	LEU
1	A	298	MET
1	B	6	THR
1	B	7	LYS
1	B	10	LYS
1	B	18	LEU
1	B	29	ILE
1	B	54	ILE
1	B	56	GLU
1	B	61	THR
1	B	69	GLU
1	B	78	LEU
1	B	81	MET
1	B	89	GLN
1	B	92	ASP
1	B	175	VAL
1	B	184	LYS
1	B	188	LEU
1	B	190	PRO
1	B	195	PRO
1	B	196	MET
1	B	201	GLU
1	B	207	VAL
1	B	221	SER
1	B	224	ILE
1	B	230	LYS
1	B	240	GLN
1	B	251	LYS

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Mol	Chain	Res	Type
1	B	252	GLU
1	B	268	ASN
1	B	269	LYS
1	B	297	GLU
1	C	9	LYS
1	C	20	THR
1	C	21	ARG
1	C	22	MET
1	C	36	LEU
1	C	54	ILE
1	C	57	ILE
1	C	69	GLU
1	C	81	MET
1	C	90	LEU
1	C	91	LEU
1	C	93	GLU
1	C	106	GLN
1	C	107	VAL
1	C	117	HIS
1	C	134	ILE
1	C	140	LEU
1	C	184	LYS
1	C	194	VAL
1	C	224	ILE
1	C	245	ILE
1	C	249	ILE
1	C	251	LYS
1	C	284	ASN
1	C	285	THR
1	C	296	GLU
1	C	297	GLU
1	D	7	LYS
1	D	9	LYS
1	D	10	LYS
1	D	54	ILE
1	D	61	THR
1	D	69	GLU
1	D	74	THR
1	D	89	GLN
1	D	91	LEU
1	D	93	GLU
1	D	94	VAL

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Mol	Chain	Res	Type
1	D	106	GLN
1	D	107	VAL
1	D	120	LEU
1	D	136	PRO
1	D	140	LEU
1	D	156	ILE
1	D	157	ARG
1	D	188	LEU
1	D	196	MET
1	D	214	ILE
1	D	220	LEU
1	D	221	SER
1	D	224	ILE
1	D	240	GLN
1	D	241	LEU
1	D	242	THR
1	D	245	ILE
1	D	246	ASP
1	D	250	GLU
1	D	251	LYS
1	D	268	ASN
1	D	284	ASN
1	D	285	THR
1	D	288	THR
1	D	294	LEU
1	D	297	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	109	GLN
1	A	211	ASN
1	A	274	GLN
1	B	5	ASN
1	B	89	GLN
1	B	106	GLN
1	B	109	GLN
1	B	164	HIS
1	B	240	GLN
1	B	268	ASN
1	C	89	GLN

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Mol	Chain	Res	Type
1	C	109	GLN
1	C	149	GLN
1	C	274	GLN
1	D	47	ASN
1	D	89	GLN
1	D	109	GLN
1	D	117	HIS
1	D	268	ASN
1	D	274	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 oligosaccharides 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, 95th 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	286/302 (94%)	0.45	34 (11%) 9 10	6, 21, 72, 98	2 (0%)
1	B	281/302 (93%)	0.52	35 (12%) 8 9	5, 23, 74, 100	3 (1%)
1	C	288/302 (95%)	0.49	38 (13%) 7 8	5, 21, 72, 92	0
1	D	278/302 (92%)	0.86	53 (19%) 3 3	4, 29, 79, 100	0
All	All	1133/1208 (93%)	0.58	160 (14%) 6 7	4, 23, 75, 100	5 (0%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	235	ALA	6.7
1	D	239	ILE	6.2
1	A	239	ILE	6.2
1	C	100	PRO	6.1
1	A	111	LEU	5.8
1	C	237	ASP	5.6
1	D	16	ALA	5.4
1	C	111	LEU	5.0
1	A	19	GLY	5.0
1	C	205	ALA	4.9
1	B	18	LEU	4.9
1	B	76	PHE	4.8
1	C	4	ILE	4.6
1	D	78	LEU	4.6
1	A	18	LEU	4.5
1	C	78	LEU	4.5
1	B	84	LYS	4.3
1	D	76	PHE	4.3
1	B	81	MET	4.3
1	C	236	GLY	4.3
1	B	82	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	89	GLN	4.2
1	D	173	ALA	4.1
1	B	88	ARG	4.1
1	D	82	LEU	4.1
1	D	199	VAL	4.0
1	D	94	VAL	3.9
1	A	110	GLY	3.9
1	A	233	PRO	3.8
1	D	6	THR	3.8
1	C	90	LEU	3.7
1	D	87	LYS	3.7
1	D	245	ILE	3.7
1	B	110	GLY	3.7
1	D	110	GLY	3.7
1	A	76	PHE	3.7
1	A	81	MET	3.6
1	C	94	VAL	3.6
1	D	95	GLN	3.6
1	D	18	LEU	3.6
1	D	178	TYR	3.6
1	A	62	HIS	3.5
1	A	113	LYS	3.5
1	B	95	GLN	3.5
1	C	76	PHE	3.5
1	A	82	LEU	3.5
1	D	251	LYS	3.5
1	D	9	LYS	3.4
1	D	198	GLY	3.4
1	C	200	VAL	3.4
1	D	161	GLU	3.3
1	A	88	ARG	3.3
1	A	112	ALA	3.3
1	C	238	GLU	3.3
1	D	231	THR	3.3
1	B	298	MET	3.3
1	D	184	LYS	3.3
1	B	16	ALA	3.3
1	C	62	HIS	3.2
1	D	292	ALA	3.2
1	B	199	VAL	3.2
1	D	201	GLU	3.2
1	D	90	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	64	SER	3.1
1	D	7	LYS	3.1
1	D	200	VAL	3.0
1	A	63	SER	3.0
1	B	200	VAL	3.0
1	D	197	VAL	3.0
1	B	83	GLU	2.9
1	D	77	GLU	2.9
1	C	5	ASN	2.9
1	B	90	LEU	2.9
1	D	128	ASP	2.9
1	D	175	VAL	2.9
1	D	224	ILE	2.9
1	A	5	ASN	2.8
1	B	5	ASN	2.8
1	C	235	ALA	2.8
1	C	18	LEU	2.8
1	B	231	THR	2.8
1	D	164	HIS	2.8
1	D	298	MET	2.8
1	C	96	SER	2.7
1	D	96	SER	2.7
1	A	296	GLU	2.7
1	D	237	ASP	2.7
1	C	112	ALA	2.7
1	B	240	GLN	2.7
1	B	230	LYS	2.7
1	B	17	GLY	2.6
1	C	17	GLY	2.6
1	D	92	ASP	2.6
1	C	88	ARG	2.6
1	D	75	SER	2.6
1	C	207	VAL	2.6
1	D	236	GLY	2.6
1	D	250	GLU	2.6
1	C	184	LYS	2.6
1	C	81	MET	2.6
1	D	179	GLY	2.6
1	C	95	GLN	2.5
1	B	204	LYS	2.5
1	A	75	SER	2.5
1	D	64	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	177	ALA	2.5
1	C	178	TYR	2.5
1	A	188	LEU	2.5
1	A	238	GLU	2.5
1	A	6	THR	2.5
1	D	240	GLN	2.4
1	C	282	ARG	2.4
1	A	79	GLU	2.4
1	A	95	GLN	2.4
1	A	161	GLU	2.4
1	A	297	GLU	2.4
1	B	79	GLU	2.4
1	D	246	ASP	2.4
1	A	91	LEU	2.3
1	B	250	GLU	2.3
1	A	284	ASN	2.3
1	B	247	MET	2.3
1	B	96	SER	2.3
1	A	83	GLU	2.3
1	D	106	GLN	2.3
1	D	176	THR	2.3
1	C	284	ASN	2.3
1	C	234	GLY	2.3
1	D	252	GLU	2.3
1	C	101	HIS	2.3
1	C	21	ARG	2.3
1	D	8	VAL	2.3
1	A	251	LYS	2.3
1	A	93	GLU	2.2
1	B	246	ASP	2.2
1	C	176	THR	2.2
1	D	91	LEU	2.2
1	A	101[A]	HIS	2.2
1	D	81	MET	2.2
1	B	77	GLU	2.2
1	C	83	GLU	2.2
1	B	78	LEU	2.2
1	C	19	GLY	2.2
1	B	92	ASP	2.2
1	A	90	LEU	2.2
1	D	80	ALA	2.2
1	A	250	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	297	GLU	2.1
1	C	245	ILE	2.1
1	B	206	ASP	2.1
1	A	96	SER	2.1
1	B	157	ARG	2.1
1	C	20	THR	2.1
1	B	94	VAL	2.1
1	C	172	VAL	2.1
1	B	205	ALA	2.1
1	C	75	SER	2.0
1	D	117	HIS	2.0
1	B	175	VAL	2.0
1	A	157	ARG	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 oligosaccharides 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.