



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:51 PM UTC

PDB ID : 2EF5 / pdb_00002ef5
Title : Crystal structure of the arginase from thermus thermophilus
Authors : Kumarevel, T.S.; Karthe, P.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-02-20
Resolution : 2.00 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
Mogul : 2022.3.0, CSD as543be (2022)
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

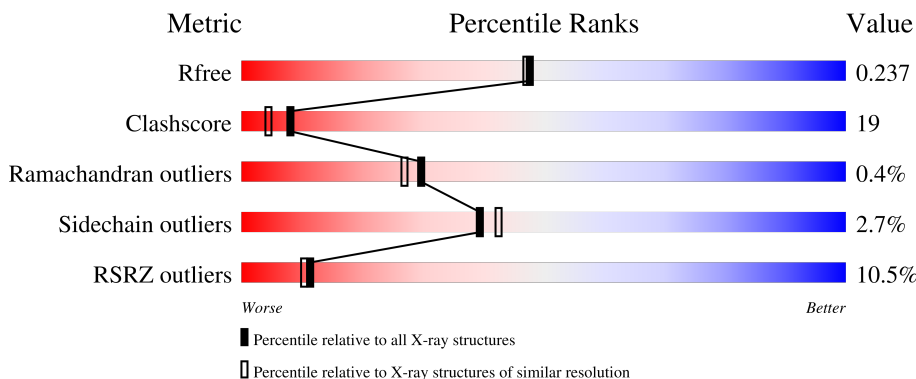
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	290	 7% 67% 25% • 6%
1	B	290	 10% 69% 23% • 6%
1	D	290	 10% 68% 23% • 6%
1	E	290	 9% 68% 23% • 6%
1	F	290	 12% 68% 23% • 6%

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Mol	Chain	Length	Quality of chain
1	G	290	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LYS	A	3001	-	X	X	-
4	LYS	E	3003	-	X	X	-
4	LYS	F	3004	-	X	X	-
4	LYS	G	3005	-	X	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13060 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.

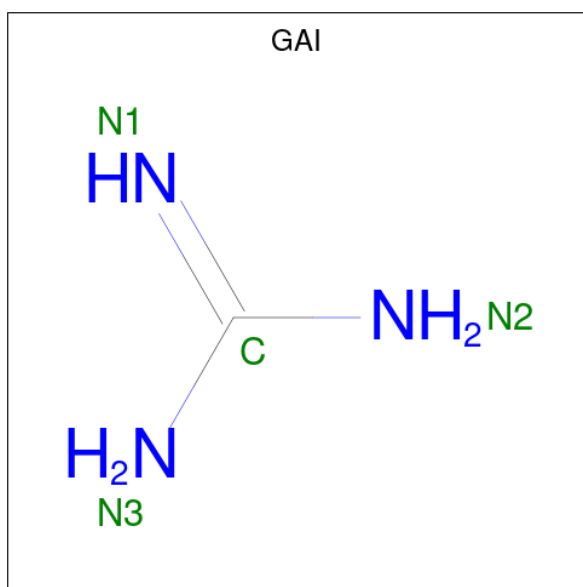
- Molecule 1 is a protein called Arginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	2052	1300	363	382	7	0	0	0
1	B	273	2052	1300	363	382	7	0	0	0
1	D	273	2052	1300	363	382	7	0	0	0
1	E	273	2052	1300	363	382	7	0	0	0
1	F	273	2052	1300	363	382	7	0	0	0
1	G	273	2052	1300	363	382	7	0	0	0

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

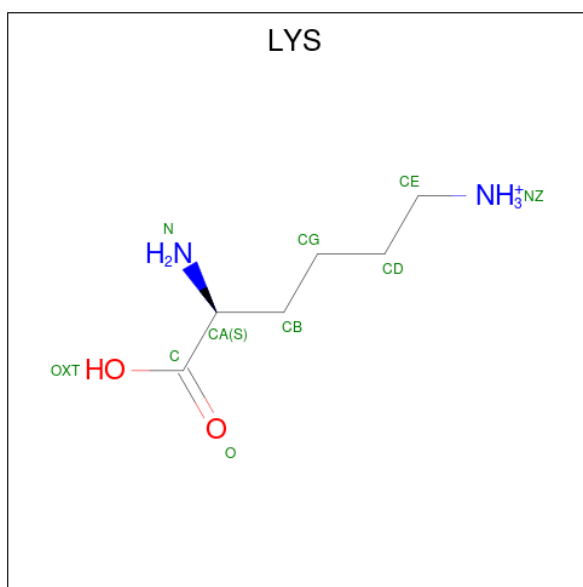
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mn 2	0	0
2	B	2	Total 2	Mn 2	0	0
2	D	2	Total 2	Mn 2	0	0
2	E	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0
2	G	2	Total 2	Mn 2	0	0

- Molecule 3 is GUANIDINE (CCD ID: GAI) (formula: CH₅N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	4	1	3	0	0
3	A	1	4	1	3	0	0
3	B	1	4	1	3	0	0
3	D	1	4	1	3	0	0
3	E	1	4	1	3	0	0
3	G	1	4	1	3	0	0

- Molecule 4 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total 10	C 6	N 2	O 2	0	0
4	B	1	Total 10	C 6	N 2	O 2	0	0
4	D	1	Total 10	C 6	N 2	O 2	0	0
4	E	1	Total 10	C 6	N 2	O 2	0	0
4	F	1	Total 10	C 6	N 2	O 2	0	0
4	G	1	Total 10	C 6	N 2	O 2	0	0

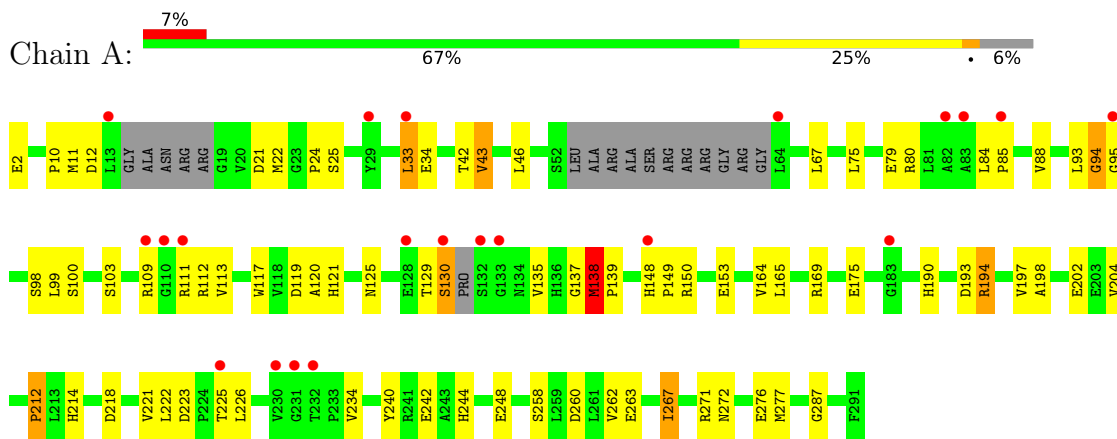
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	100	Total 100	O 100	0	0
5	B	116	Total 116	O 116	0	0
5	D	91	Total 91	O 91	0	0
5	E	132	Total 132	O 132	0	0
5	F	103	Total 103	O 103	0	0
5	G	110	Total 110	O 110	0	0

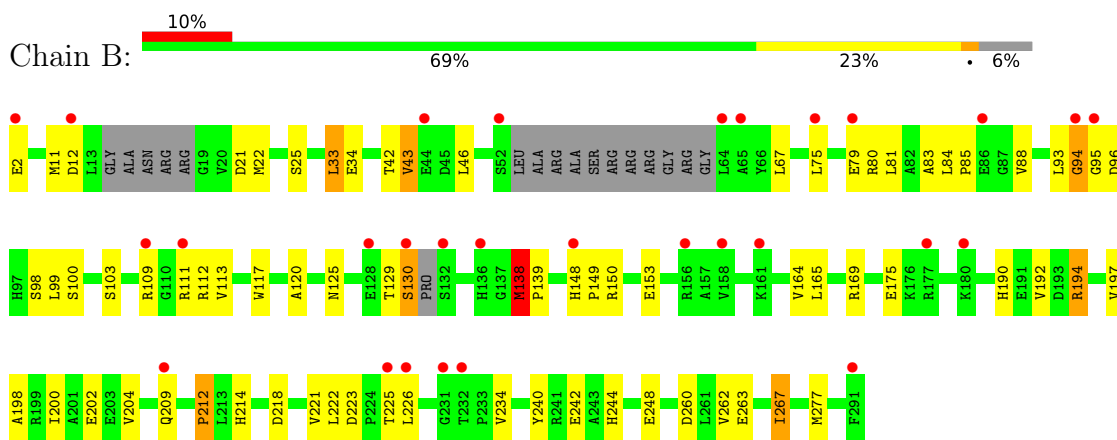
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

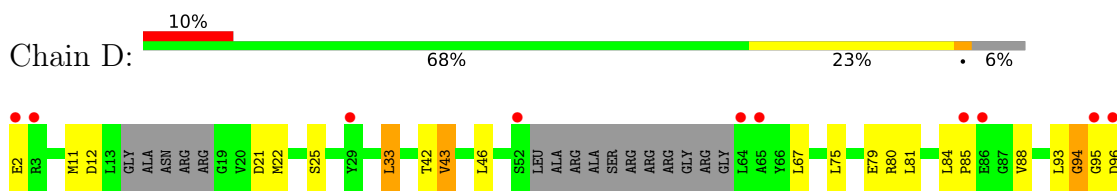
- Molecule 1: Arginase

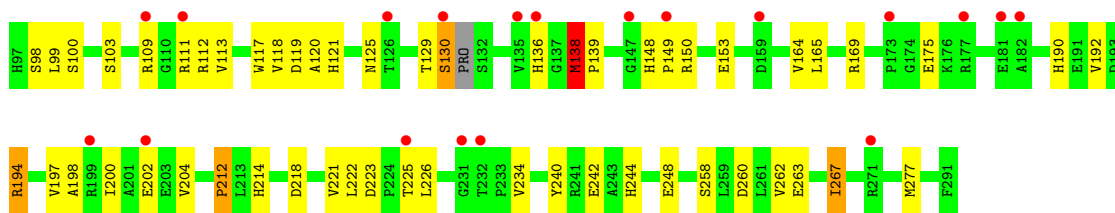


- Molecule 1: Arginase

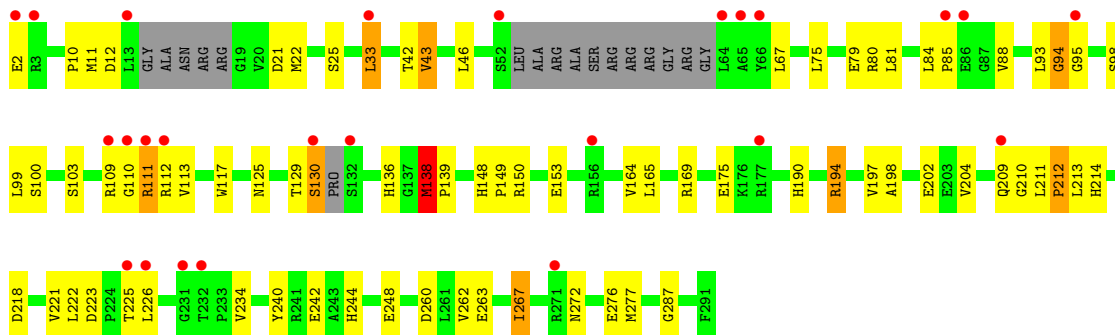


- Molecule 1: Arginase

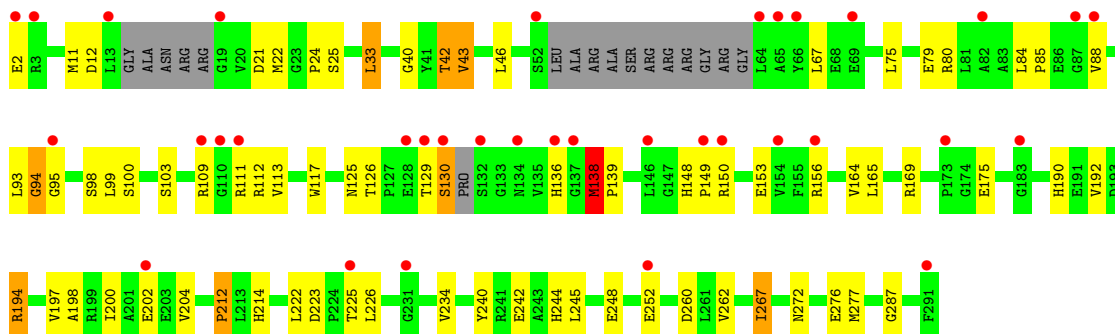




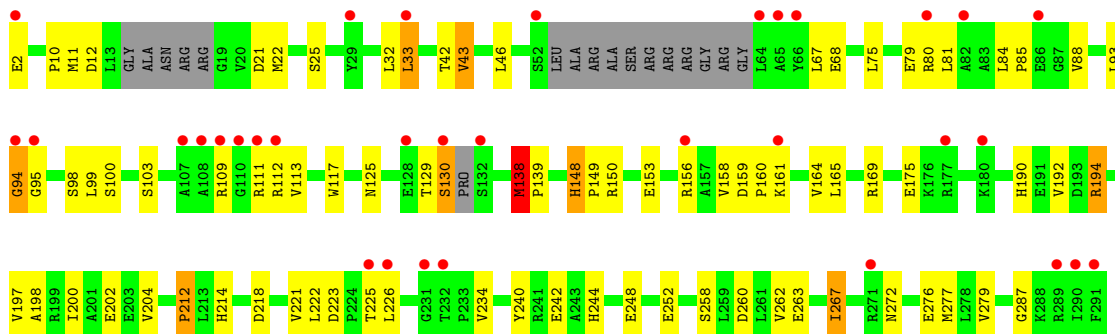
• Molecule 1: Arginase



• Molecule 1: Arginase



• Molecule 1: Arginase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.79Å 97.48Å 126.46Å 90.00° 108.66° 90.00°	Depositor
Resolution (Å)	19.98 – 2.00 19.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.98-2.00) 99.0 (19.98-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.00Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.236 0.233 , 0.237	Depositor DCC
R_{free} test set	1150 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtrriage
Anisotropy	0.553	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13060	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/2083	0.97	10/2828 (0.4%)
1	B	0.46	0/2083	0.99	9/2828 (0.3%)
1	D	0.40	0/2083	0.96	9/2828 (0.3%)
1	E	0.46	0/2083	1.02	10/2828 (0.4%)
1	F	0.39	0/2083	0.97	9/2828 (0.3%)
1	G	0.45	0/2083	0.99	11/2828 (0.4%)
All	All	0.43	0/12498	0.98	58/16968 (0.3%)

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	93	LEU	CA-C-N	-9.01	114.15	122.17
1	E	93	LEU	C-N-CA	-9.01	114.15	122.17
1	F	95	GLY	N-CA-C	-8.60	92.81	113.18
1	E	95	GLY	N-CA-C	-8.45	93.16	113.18
1	G	95	GLY	N-CA-C	-8.09	94.00	113.18
1	A	93	LEU	CA-C-N	-8.06	114.99	122.17
1	A	93	LEU	C-N-CA	-8.06	114.99	122.17
1	B	95	GLY	N-CA-C	-7.97	94.30	113.18
1	A	95	GLY	N-CA-C	-7.96	94.30	113.18
1	D	95	GLY	N-CA-C	-7.70	94.93	113.18
1	D	94	GLY	N-CA-C	7.59	122.43	111.12
1	E	94	GLY	N-CA-C	7.58	122.18	111.42
1	F	94	GLY	N-CA-C	7.18	121.81	111.12
1	G	94	GLY	N-CA-C	7.14	121.77	111.12
1	A	94	GLY	N-CA-C	7.13	121.54	111.42
1	F	262	VAL	N-CA-C	7.06	118.99	108.96
1	G	262	VAL	N-CA-C	7.06	118.98	108.96
1	B	94	GLY	N-CA-C	6.97	121.50	111.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	VAL	N-CA-C	6.70	118.47	108.96
1	A	262	VAL	N-CA-C	6.68	118.45	108.96
1	E	262	VAL	N-CA-C	6.68	118.45	108.96
1	D	262	VAL	N-CA-C	6.67	118.43	108.96
1	B	212	PRO	N-CA-C	-6.38	101.23	111.38
1	E	42	THR	N-CA-C	-6.33	98.96	109.46
1	G	43	VAL	N-CA-C	6.25	117.60	108.53
1	F	42	THR	N-CA-C	-6.12	99.30	109.46
1	A	43	VAL	N-CA-C	6.08	117.24	108.48
1	D	42	THR	N-CA-C	-6.06	98.85	108.73
1	E	212	PRO	N-CA-C	-6.02	102.38	111.41
1	G	212	PRO	N-CA-C	-5.90	102.00	111.38
1	D	43	VAL	N-CA-C	5.89	116.96	108.48
1	G	287	GLY	N-CA-C	5.89	122.57	114.92
1	D	120	ALA	N-CA-C	-5.88	105.59	112.89
1	A	212	PRO	N-CA-C	-5.84	102.09	111.38
1	G	93	LEU	CA-C-N	-5.78	114.63	122.03
1	G	93	LEU	C-N-CA	-5.78	114.63	122.03
1	B	42	THR	N-CA-C	-5.67	99.48	108.73
1	B	93	LEU	CA-C-N	-5.62	114.83	122.03
1	B	93	LEU	C-N-CA	-5.62	114.83	122.03
1	A	42	THR	N-CA-C	-5.60	99.61	108.73
1	F	93	LEU	CA-C-N	-5.57	114.90	122.03
1	F	93	LEU	C-N-CA	-5.57	114.90	122.03
1	E	287	GLY	N-CA-C	5.50	121.30	114.37
1	B	43	VAL	N-CA-C	5.49	116.38	108.48
1	D	212	PRO	N-CA-C	-5.39	102.81	111.38
1	E	43	VAL	N-CA-C	5.36	116.20	108.48
1	G	42	THR	N-CA-C	-5.30	100.08	108.73
1	D	93	LEU	CA-C-N	-5.30	115.25	122.03
1	D	93	LEU	C-N-CA	-5.30	115.25	122.03
1	A	120	ALA	N-CA-C	-5.27	106.35	112.89
1	A	287	GLY	N-CA-C	5.24	121.97	114.64
1	F	212	PRO	N-CA-C	-5.21	103.10	111.38
1	F	287	GLY	N-CA-C	5.17	121.88	114.64
1	B	120	ALA	N-CA-C	-5.12	106.54	112.89
1	G	148	HIS	CA-C-N	5.06	124.67	119.05
1	G	148	HIS	C-N-CA	5.06	124.67	119.05
1	E	213	LEU	N-CA-C	5.01	117.07	108.90
1	F	43	VAL	N-CA-C	5.01	115.69	108.48

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	2052	0	2101	74	0
1	B	2052	0	2101	72	2
1	D	2052	0	2101	62	0
1	E	2052	0	2101	121	0
1	F	2052	0	2101	80	0
1	G	2052	0	2101	141	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
3	A	8	0	8	0	0
3	B	4	0	4	0	0
3	D	4	0	4	0	0
3	E	4	0	4	0	0
3	G	4	0	4	0	0
4	A	10	0	12	17	0
4	B	10	0	12	4	0
4	D	10	0	12	3	0
4	E	10	0	12	9	0
4	F	10	0	12	12	2
4	G	10	0	12	12	2
5	A	100	0	0	6	0
5	B	116	0	0	2	0
5	D	91	0	0	1	0
5	E	132	0	0	5	0
5	F	103	0	0	6	0
5	G	110	0	0	3	0
All	All	13060	0	12702	489	4

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 19.

All (489) 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)
4:A:3001:LYS:CE	4:A:3001:LYS:NZ	1.69	1.52
1:E:111:ARG:HH22	1:G:161:LYS:N	0.99	1.40
4:E:3003:LYS:NZ	4:E:3003:LYS:CE	1.81	1.40
1:E:111:ARG:NH2	1:G:161:LYS:N	1.77	1.32
1:E:21:ASP:O	4:E:3003:LYS:HE2	1.42	1.20
1:E:211:LEU:HG	1:G:156:ARG:NH2	1.57	1.19
1:F:21:ASP:O	4:F:3004:LYS:HE2	1.44	1.18
1:G:22:MET:HA	4:G:3005:LYS:HD2	1.25	1.18
1:G:21:ASP:O	4:G:3005:LYS:HE2	1.42	1.16
1:B:25:SER:OG	4:B:3006:LYS:HG2	1.47	1.13
1:A:21:ASP:O	4:A:3001:LYS:CE	2.00	1.09
1:B:111:ARG:HD3	1:B:112:ARG:N	1.67	1.08
1:E:111:ARG:NH2	1:G:161:LYS:H	1.41	1.07
1:B:111:ARG:HD3	1:B:112:ARG:H	0.90	1.05
1:E:111:ARG:CZ	1:G:161:LYS:H	1.73	1.02
1:A:22:MET:HA	4:A:3001:LYS:HD2	1.38	1.01
1:E:111:ARG:NH2	1:G:161:LYS:HG3	1.76	1.01
1:B:111:ARG:CD	1:B:112:ARG:H	1.73	1.01
1:E:111:ARG:HH22	1:G:161:LYS:CA	1.75	0.99
1:E:209:GLN:OE1	1:G:153:GLU:O	1.81	0.97
1:A:21:ASP:O	4:A:3001:LYS:HE3	1.60	0.96
1:E:111:ARG:CD	1:G:159:ASP:OD1	2.14	0.96
1:A:21:ASP:O	4:A:3001:LYS:HE2	1.66	0.96
1:D:25:SER:OG	4:D:3002:LYS:HG2	1.64	0.96
1:E:211:LEU:HG	1:G:156:ARG:CZ	1.96	0.95
1:E:111:ARG:HG2	1:E:111:ARG:HH11	1.32	0.94
1:E:111:ARG:CZ	1:G:159:ASP:OD1	2.17	0.93
1:E:209:GLN:O	1:G:156:ARG:NH2	2.02	0.93
1:E:111:ARG:CD	1:E:112:ARG:H	1.81	0.92
1:A:21:ASP:C	4:A:3001:LYS:HE3	1.96	0.90
1:G:21:ASP:O	4:G:3005:LYS:CE	2.20	0.89
1:E:111:ARG:HD2	1:G:159:ASP:OD1	1.70	0.89
4:F:3004:LYS:C	5:F:3097:HOH:O	2.15	0.89
1:A:129:THR:O	1:A:130:SER:HB2	1.70	0.89
1:E:129:THR:O	1:E:130:SER:HB2	1.73	0.88
1:D:129:THR:O	1:D:130:SER:HB2	1.74	0.88
1:E:111:ARG:HD3	1:E:112:ARG:N	1.88	0.87
1:G:129:THR:O	1:G:130:SER:HB2	1.74	0.86
1:G:111:ARG:HD3	1:G:112:ARG:H	1.41	0.85
1:F:129:THR:O	1:F:130:SER:HB2	1.74	0.84
1:G:22:MET:HA	4:G:3005:LYS:CD	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:THR:O	1:B:130:SER:HB2	1.76	0.84
1:E:111:ARG:NH2	1:G:161:LYS:CG	2.38	0.84
1:E:111:ARG:HD2	1:G:159:ASP:CG	2.02	0.83
1:E:111:ARG:HD3	1:E:112:ARG:H	1.38	0.83
1:D:111:ARG:HD3	1:D:112:ARG:H	1.42	0.83
1:E:111:ARG:NH1	1:G:161:LYS:H	1.76	0.82
1:F:111:ARG:HD3	1:F:112:ARG:H	1.44	0.81
1:E:211:LEU:HG	1:G:156:ARG:HH22	1.44	0.81
1:A:111:ARG:HD3	1:A:112:ARG:H	1.43	0.81
1:E:111:ARG:HG3	1:G:159:ASP:OD2	1.80	0.80
1:F:2:GLU:CD	1:G:150:ARG:HD3	2.07	0.80
1:F:22:MET:HG2	4:F:3004:LYS:HD2	1.64	0.79
1:E:111:ARG:NH1	1:G:159:ASP:OD1	2.15	0.79
1:E:21:ASP:O	4:E:3003:LYS:CE	2.26	0.79
1:E:111:ARG:NE	1:G:159:ASP:OD1	2.16	0.78
1:D:84:LEU:O	1:D:109:ARG:NH2	2.16	0.78
1:E:111:ARG:CD	1:G:159:ASP:CG	2.56	0.78
1:E:111:ARG:HG2	1:E:111:ARG:NH1	1.98	0.77
1:E:84:LEU:O	1:E:109:ARG:NH2	2.19	0.76
1:F:21:ASP:C	4:F:3004:LYS:HE2	2.11	0.75
1:E:111:ARG:HH11	1:E:111:ARG:CG	1.98	0.75
1:A:22:MET:HA	4:A:3001:LYS:CD	2.15	0.75
1:B:209:GLN:CD	1:F:156:ARG:HH22	1.95	0.75
1:E:111:ARG:NH2	1:G:161:LYS:CB	2.50	0.75
1:B:75:LEU:O	1:B:79:GLU:HG3	1.87	0.74
1:E:111:ARG:CG	1:G:159:ASP:CG	2.60	0.74
1:E:111:ARG:NH1	1:G:161:LYS:HB2	2.02	0.74
1:B:209:GLN:NE2	1:F:156:ARG:HH22	1.86	0.73
1:E:209:GLN:O	1:G:156:ARG:CZ	2.34	0.73
1:A:117:TRP:HB3	1:A:165:LEU:HD23	1.71	0.72
1:E:117:TRP:HB3	1:E:165:LEU:HD23	1.70	0.72
1:G:159:ASP:OD1	1:G:160:PRO:HD2	1.90	0.72
1:A:22:MET:CA	4:A:3001:LYS:HD2	2.16	0.71
1:E:111:ARG:CZ	1:G:161:LYS:HB2	2.21	0.70
1:G:117:TRP:HB3	1:G:165:LEU:HD23	1.71	0.70
1:F:2:GLU:OE2	1:G:150:ARG:NH1	2.23	0.70
1:F:84:LEU:O	1:F:109:ARG:NH2	2.25	0.69
1:E:111:ARG:CD	1:E:112:ARG:N	2.51	0.69
1:E:209:GLN:NE2	1:G:153:GLU:HA	2.08	0.69
1:G:22:MET:CA	4:G:3005:LYS:HD2	2.15	0.69
4:F:3004:LYS:CA	5:F:3097:HOH:O	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:ARG:HD2	1:G:159:ASP:OD2	1.93	0.69
1:F:117:TRP:HB3	1:F:165:LEU:HD23	1.75	0.69
1:B:84:LEU:O	1:B:109:ARG:NH2	2.27	0.68
1:B:25:SER:OG	4:B:3006:LYS:CG	2.36	0.68
1:A:11:MET:CE	1:A:98:SER:HB2	2.24	0.68
1:B:25:SER:HG	4:B:3006:LYS:HG2	1.58	0.67
4:E:3003:LYS:HG2	5:E:3084:HOH:O	1.94	0.67
1:A:84:LEU:O	1:A:109:ARG:NH2	2.27	0.67
1:D:117:TRP:HB3	1:D:165:LEU:HD23	1.76	0.67
1:G:84:LEU:O	1:G:109:ARG:NH2	2.28	0.67
1:A:164:VAL:HG11	1:A:204:VAL:HG22	1.76	0.66
1:E:111:ARG:HH22	1:G:160:PRO:C	1.94	0.66
1:A:94:GLY:HA3	1:A:99:LEU:HD21	1.77	0.66
1:A:148:HIS:HD2	1:A:150:ARG:H	1.44	0.65
1:E:111:ARG:HG3	1:G:159:ASP:CG	2.22	0.65
1:G:21:ASP:O	4:G:3005:LYS:HD2	1.96	0.65
1:G:21:ASP:O	4:G:3005:LYS:CD	2.44	0.65
1:B:190:HIS:HE1	1:B:194:ARG:HE	1.45	0.65
4:G:3005:LYS:HG3	5:G:3038:HOH:O	1.94	0.65
1:E:111:ARG:CZ	1:G:161:LYS:CB	2.75	0.65
1:E:111:ARG:HD2	1:E:112:ARG:H	1.59	0.65
1:F:198:ALA:O	1:F:202:GLU:HG2	1.97	0.65
1:B:198:ALA:O	1:B:202:GLU:HG2	1.97	0.64
1:A:169:ARG:HG3	1:A:234:VAL:HG11	1.77	0.64
1:G:11:MET:CE	1:G:98:SER:HB2	2.27	0.64
1:B:11:MET:CE	1:B:98:SER:HB2	2.28	0.64
1:D:11:MET:CE	1:D:98:SER:HB2	2.27	0.64
1:G:75:LEU:O	1:G:79:GLU:HG3	1.98	0.64
1:E:94:GLY:HA3	1:E:99:LEU:HD21	1.79	0.63
1:B:117:TRP:HB3	1:B:165:LEU:HD23	1.80	0.63
1:E:111:ARG:HH21	1:G:161:LYS:HG3	1.62	0.63
1:E:211:LEU:HD23	1:G:156:ARG:NH1	2.13	0.63
1:F:129:THR:O	1:F:130:SER:CB	2.46	0.63
1:G:129:THR:O	1:G:130:SER:CB	2.46	0.63
1:D:149:PRO:O	1:D:153:GLU:HG2	1.99	0.63
1:G:169:ARG:HG3	1:G:234:VAL:HG11	1.80	0.63
1:G:198:ALA:O	1:G:202:GLU:HG2	1.98	0.63
1:E:110:GLY:O	1:G:161:LYS:NZ	2.31	0.63
1:E:129:THR:O	1:E:130:SER:CB	2.47	0.63
1:E:169:ARG:HG3	1:E:234:VAL:HG11	1.80	0.62
4:F:3004:LYS:HA	5:F:3097:HOH:O	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:HG3	1:B:234:VAL:HG11	1.81	0.62
1:B:209:GLN:OE1	1:F:156:ARG:NH1	2.31	0.62
1:F:94:GLY:HA3	1:F:99:LEU:HD21	1.82	0.62
1:D:169:ARG:HG3	1:D:234:VAL:HG11	1.82	0.62
1:B:129:THR:O	1:B:130:SER:CB	2.48	0.62
1:D:129:THR:O	1:D:130:SER:CB	2.46	0.62
1:G:22:MET:SD	1:G:267:ILE:HD13	2.40	0.62
1:A:129:THR:O	1:A:130:SER:CB	2.45	0.62
1:B:22:MET:SD	1:B:267:ILE:HD13	2.40	0.62
1:A:94:GLY:HA3	1:A:99:LEU:CD2	2.30	0.62
1:B:209:GLN:NE2	1:F:156:ARG:NH2	2.48	0.61
1:D:138:MET:N	1:D:139:PRO:HD2	2.16	0.61
1:F:169:ARG:HG3	1:F:234:VAL:HG11	1.81	0.61
1:A:149:PRO:O	1:A:153:GLU:HG2	2.00	0.61
1:E:2:GLU:HG3	5:E:3124:HOH:O	1.98	0.61
1:E:164:VAL:HG11	1:E:204:VAL:HG22	1.82	0.61
1:E:223:ASP:OD2	1:E:225:THR:HG22	2.00	0.61
1:D:164:VAL:HG11	1:D:204:VAL:HG22	1.82	0.61
1:E:111:ARG:CG	1:G:159:ASP:OD2	2.47	0.61
1:F:11:MET:CE	1:F:98:SER:HB2	2.30	0.61
1:F:138:MET:N	1:F:139:PRO:HD2	2.16	0.61
1:B:94:GLY:HA3	1:B:99:LEU:HD21	1.82	0.60
1:E:75:LEU:O	1:E:79:GLU:HG3	2.01	0.60
1:F:42:THR:HG21	1:G:68:GLU:OE2	2.01	0.60
1:E:190:HIS:HE1	1:E:194:ARG:HE	1.49	0.60
1:F:138:MET:N	1:F:139:PRO:CD	2.65	0.60
1:B:209:GLN:CD	1:F:156:ARG:NH2	2.59	0.60
1:D:138:MET:N	1:D:139:PRO:CD	2.65	0.60
1:B:111:ARG:HH11	1:B:111:ARG:HG2	1.67	0.60
1:F:244:HIS:O	1:F:248:GLU:HG3	2.02	0.60
1:D:198:ALA:O	1:D:202:GLU:HG2	2.01	0.60
1:F:2:GLU:CD	1:G:150:ARG:CD	2.74	0.60
4:E:3003:LYS:CA	5:E:3121:HOH:O	2.49	0.60
1:D:94:GLY:HA3	1:D:99:LEU:HD21	1.84	0.59
1:E:209:GLN:CD	1:G:153:GLU:O	2.45	0.59
1:B:149:PRO:O	1:B:153:GLU:HG2	2.02	0.59
1:F:149:PRO:O	1:F:153:GLU:HG2	2.00	0.59
1:G:148:HIS:HD2	1:G:150:ARG:H	1.50	0.59
1:E:149:PRO:O	1:E:153:GLU:HG2	2.02	0.59
1:E:138:MET:N	1:E:139:PRO:CD	2.66	0.58
1:F:190:HIS:HE1	1:F:194:ARG:HE	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:SER:HG	4:G:3005:LYS:N	2.00	0.58
1:E:138:MET:N	1:E:139:PRO:HD2	2.18	0.58
1:G:94:GLY:HA3	1:G:99:LEU:HD21	1.86	0.58
1:A:75:LEU:O	1:A:79:GLU:HG3	2.02	0.58
1:E:111:ARG:HH12	1:G:161:LYS:H	1.48	0.58
1:A:138:MET:N	1:A:139:PRO:CD	2.66	0.58
1:G:158:VAL:HG22	1:G:159:ASP:N	2.17	0.58
1:A:148:HIS:CD2	1:A:150:ARG:HB2	2.39	0.58
1:G:138:MET:N	1:G:139:PRO:HD2	2.18	0.58
1:E:11:MET:CE	1:E:98:SER:HB2	2.34	0.58
1:G:11:MET:HE3	1:G:98:SER:HB2	1.85	0.58
1:A:148:HIS:CD2	1:A:150:ARG:H	2.22	0.57
1:D:109:ARG:NH1	1:D:109:ARG:HG2	2.18	0.57
1:G:138:MET:N	1:G:139:PRO:CD	2.67	0.57
1:A:223:ASP:OD2	1:A:225:THR:HG22	2.04	0.57
1:B:164:VAL:HG11	1:B:204:VAL:HG22	1.87	0.57
1:F:75:LEU:O	1:F:79:GLU:HG3	2.04	0.57
1:B:138:MET:N	1:B:139:PRO:CD	2.67	0.57
1:D:11:MET:HE3	1:D:98:SER:HB2	1.87	0.57
1:E:210:GLY:C	1:G:156:ARG:HH12	2.13	0.57
4:F:3004:LYS:O	5:F:3097:HOH:O	2.17	0.57
1:G:10:PRO:HB2	4:G:3005:LYS:NZ	2.20	0.57
1:G:190:HIS:HE1	1:G:194:ARG:HE	1.53	0.57
1:E:111:ARG:NH2	1:G:160:PRO:C	2.59	0.56
1:E:111:ARG:NH1	1:G:159:ASP:CG	2.63	0.56
1:A:198:ALA:O	1:A:202:GLU:HG2	2.06	0.56
1:D:25:SER:CB	4:D:3002:LYS:HG2	2.34	0.56
1:D:75:LEU:O	1:D:79:GLU:HG3	2.04	0.56
1:F:12:ASP:HB2	1:F:21:ASP:HB3	1.87	0.56
1:B:138:MET:N	1:B:139:PRO:HD2	2.20	0.56
1:D:148:HIS:HD2	1:D:150:ARG:H	1.54	0.56
1:F:94:GLY:HA3	1:F:99:LEU:CD2	2.36	0.56
1:A:169:ARG:NH2	1:A:221:VAL:O	2.35	0.56
1:E:94:GLY:HA3	1:E:99:LEU:CD2	2.35	0.56
1:E:111:ARG:HH11	1:G:159:ASP:CG	2.14	0.56
1:G:244:HIS:O	1:G:248:GLU:HG3	2.05	0.56
1:A:99:LEU:C	1:A:99:LEU:HD12	2.31	0.56
1:B:12:ASP:HB2	1:B:21:ASP:HB3	1.88	0.56
1:A:138:MET:N	1:A:139:PRO:HD2	2.21	0.55
1:E:210:GLY:C	1:G:156:ARG:NH1	2.65	0.55
1:F:2:GLU:OE1	1:G:150:ARG:HD2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:HIS:CE1	1:B:194:ARG:HE	2.22	0.55
1:B:209:GLN:HE22	1:F:156:ARG:HH22	1.55	0.55
1:D:109:ARG:HG2	1:D:109:ARG:HH11	1.70	0.55
1:F:21:ASP:O	4:F:3004:LYS:CE	2.37	0.55
1:G:190:HIS:CE1	1:G:194:ARG:HE	2.25	0.55
1:A:11:MET:HE3	1:A:98:SER:HB2	1.87	0.55
1:B:94:GLY:HA3	1:B:99:LEU:CD2	2.37	0.55
1:B:148:HIS:HD2	1:B:150:ARG:H	1.54	0.55
1:G:21:ASP:C	4:G:3005:LYS:HE2	2.25	0.55
1:B:85:PRO:HG2	1:B:88:VAL:HG21	1.89	0.55
1:D:22:MET:SD	1:D:267:ILE:HD13	2.47	0.55
1:D:94:GLY:HA3	1:D:99:LEU:CD2	2.37	0.55
1:E:10:PRO:HB2	4:E:3003:LYS:NZ	2.21	0.55
1:F:109:ARG:NH1	1:F:109:ARG:HG2	2.21	0.55
1:E:22:MET:SD	1:E:267:ILE:HD13	2.46	0.55
1:D:12:ASP:HB2	1:D:21:ASP:HB3	1.89	0.55
1:F:24:PRO:HD2	5:F:3034:HOH:O	2.06	0.55
1:F:25:SER:OG	4:F:3004:LYS:HA	2.07	0.55
1:F:164:VAL:HG11	1:F:204:VAL:HG22	1.89	0.55
1:F:67:LEU:C	1:F:67:LEU:HD23	2.33	0.54
1:E:211:LEU:CD2	1:G:156:ARG:NH1	2.70	0.54
1:A:11:MET:HE1	1:A:98:SER:HB2	1.89	0.54
1:E:11:MET:HE3	1:E:98:SER:HB2	1.89	0.54
1:G:67:LEU:C	1:G:67:LEU:HD23	2.32	0.54
1:D:111:ARG:CD	1:D:112:ARG:H	2.18	0.54
1:B:111:ARG:HG2	1:B:111:ARG:NH1	2.21	0.54
1:D:226:LEU:HD21	1:D:240:TYR:HB2	1.90	0.54
1:G:148:HIS:CD2	1:G:150:ARG:HB2	2.43	0.54
1:A:111:ARG:CD	1:A:112:ARG:H	2.19	0.54
1:F:148:HIS:HD2	1:F:150:ARG:H	1.56	0.54
1:G:94:GLY:HA3	1:G:99:LEU:CD2	2.37	0.54
1:B:197:VAL:HG21	1:B:242:GLU:HB3	1.90	0.53
1:D:67:LEU:HD23	1:D:67:LEU:C	2.34	0.53
1:A:109:ARG:NH1	1:A:109:ARG:HG2	2.22	0.53
1:D:125:ASN:ND2	1:D:175:GLU:HG3	2.24	0.53
1:E:109:ARG:NH1	1:E:109:ARG:HG2	2.23	0.53
1:G:111:ARG:HD3	1:G:112:ARG:N	2.19	0.53
1:A:67:LEU:C	1:A:67:LEU:HD23	2.33	0.53
4:E:3003:LYS:C	5:E:3121:HOH:O	2.51	0.53
1:E:111:ARG:NH2	1:G:161:LYS:CA	2.49	0.53
1:A:190:HIS:HE1	1:A:194:ARG:HE	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:MET:HE3	1:B:98:SER:HB2	1.88	0.53
1:G:223:ASP:OD2	1:G:225:THR:HG22	2.08	0.53
1:B:226:LEU:HD21	1:B:240:TYR:HB2	1.89	0.53
1:E:148:HIS:HD2	1:E:150:ARG:H	1.55	0.53
1:A:10:PRO:HB2	4:A:3001:LYS:NZ	2.24	0.53
1:F:11:MET:HE3	1:F:98:SER:HB2	1.90	0.53
1:B:111:ARG:CD	1:B:112:ARG:N	2.48	0.53
1:F:125:ASN:ND2	1:F:175:GLU:HG3	2.24	0.53
1:E:85:PRO:HG2	1:E:88:VAL:HG21	1.91	0.52
1:E:209:GLN:C	1:G:156:ARG:NH2	2.67	0.52
1:G:148:HIS:CD2	1:G:150:ARG:H	2.26	0.52
1:G:109:ARG:NH1	1:G:109:ARG:HG2	2.24	0.52
1:G:164:VAL:HG11	1:G:204:VAL:HG22	1.89	0.52
1:B:109:ARG:NH1	1:B:109:ARG:HG2	2.23	0.52
1:B:125:ASN:O	1:B:138:MET:HB3	2.10	0.52
1:B:67:LEU:C	1:B:67:LEU:HD23	2.35	0.52
1:E:211:LEU:CG	1:G:156:ARG:HH22	2.19	0.52
1:F:222:LEU:HD13	1:F:277:MET:HE2	1.91	0.52
1:B:223:ASP:OD2	1:B:225:THR:HG22	2.10	0.52
1:G:169:ARG:NH2	1:G:221:VAL:O	2.37	0.52
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.75	0.52
1:F:272:ASN:O	1:F:276:GLU:HG3	2.09	0.52
1:B:99:LEU:C	1:B:99:LEU:HD12	2.35	0.52
1:E:67:LEU:C	1:E:67:LEU:HD23	2.35	0.52
1:D:25:SER:OG	4:D:3002:LYS:CG	2.50	0.51
1:G:226:LEU:HD21	1:G:240:TYR:HB2	1.92	0.51
1:E:222:LEU:HD13	1:E:277:MET:HE2	1.91	0.51
1:E:198:ALA:O	1:E:202:GLU:HG2	2.10	0.51
1:A:22:MET:HG2	4:A:3001:LYS:HD2	1.92	0.51
1:B:209:GLN:OE1	1:F:156:ARG:NH2	2.44	0.51
1:E:125:ASN:ND2	1:E:175:GLU:HG3	2.25	0.51
1:B:169:ARG:NH2	1:B:221:VAL:O	2.34	0.51
1:D:148:HIS:CD2	1:D:150:ARG:HB2	2.45	0.51
4:A:3001:LYS:C	5:A:3076:HOH:O	2.53	0.51
1:D:190:HIS:HE1	1:D:194:ARG:HE	1.58	0.51
1:E:111:ARG:CD	1:G:159:ASP:OD2	2.57	0.51
1:F:190:HIS:CE1	1:F:194:ARG:HE	2.28	0.51
1:F:214:HIS:HE1	1:F:260:ASP:OD2	1.94	0.51
1:F:21:ASP:C	4:F:3004:LYS:CE	2.82	0.50
1:F:226:LEU:HD21	1:F:240:TYR:HB2	1.94	0.50
1:E:99:LEU:HD12	1:E:99:LEU:C	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:MET:HE1	1:D:98:SER:HB2	1.93	0.50
4:E:3003:LYS:HA	5:E:3121:HOH:O	2.11	0.50
1:A:244:HIS:O	1:A:248:GLU:HG3	2.11	0.50
1:F:99:LEU:C	1:F:99:LEU:HD12	2.36	0.50
1:F:109:ARG:HG2	1:F:109:ARG:HH11	1.75	0.50
1:G:149:PRO:O	1:G:153:GLU:HG2	2.10	0.50
1:D:222:LEU:HD13	1:D:277:MET:HE2	1.93	0.50
1:E:111:ARG:CZ	1:G:161:LYS:CG	2.90	0.50
1:B:222:LEU:HD13	1:B:277:MET:HE2	1.92	0.50
1:A:12:ASP:HB2	1:A:21:ASP:HB3	1.93	0.50
1:D:148:HIS:CD2	1:D:150:ARG:H	2.30	0.50
1:E:226:LEU:HD21	1:E:240:TYR:HB2	1.94	0.50
1:A:148:HIS:HD2	1:A:150:ARG:HB2	1.76	0.50
1:D:169:ARG:NH2	1:D:221:VAL:O	2.37	0.49
1:E:190:HIS:CE1	1:E:194:ARG:HE	2.27	0.49
1:F:2:GLU:OE1	1:G:150:ARG:CD	2.60	0.49
1:G:159:ASP:OD1	1:G:160:PRO:CD	2.58	0.49
1:D:99:LEU:C	1:D:99:LEU:HD12	2.37	0.49
1:D:223:ASP:OD2	1:D:225:THR:HG22	2.12	0.49
1:E:109:ARG:HG2	1:E:109:ARG:HH11	1.76	0.49
1:F:248:GLU:O	1:F:252:GLU:HG3	2.12	0.49
1:A:214:HIS:HD2	1:A:258:SER:OG	1.96	0.49
1:F:138:MET:H	1:F:139:PRO:CD	2.25	0.49
1:G:109:ARG:HG2	1:G:109:ARG:HH11	1.78	0.49
1:A:2:GLU:HG3	5:A:3079:HOH:O	2.10	0.49
1:D:2:GLU:HG3	5:D:3084:HOH:O	2.11	0.49
1:B:33:LEU:HG	1:B:43:VAL:HG11	1.93	0.49
1:E:148:HIS:CD2	1:E:150:ARG:H	2.30	0.49
1:F:85:PRO:HG2	1:F:88:VAL:HG21	1.94	0.49
1:A:24:PRO:HD2	5:A:3009:HOH:O	2.12	0.49
1:F:148:HIS:CD2	1:F:150:ARG:HB2	2.47	0.49
1:A:190:HIS:CE1	1:A:194:ARG:HE	2.30	0.49
1:G:33:LEU:HG	1:G:43:VAL:HG11	1.95	0.49
1:B:148:HIS:CD2	1:B:150:ARG:H	2.30	0.49
1:D:85:PRO:HG2	1:D:88:VAL:HG21	1.94	0.49
1:G:12:ASP:HB2	1:G:21:ASP:HB3	1.93	0.49
1:E:211:LEU:HG	1:G:156:ARG:NH1	2.27	0.48
1:B:244:HIS:O	1:B:248:GLU:HG3	2.13	0.48
1:D:244:HIS:O	1:D:248:GLU:HG3	2.13	0.48
1:F:113:VAL:HG12	1:F:212:PRO:HG2	1.96	0.48
1:B:125:ASN:ND2	1:B:175:GLU:HG3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD21	1:A:240:TYR:HB2	1.96	0.48
1:G:148:HIS:HD2	1:G:150:ARG:HB2	1.79	0.48
1:A:169:ARG:HG3	1:A:234:VAL:CG1	2.42	0.48
1:E:111:ARG:HH12	1:G:161:LYS:N	2.10	0.48
1:F:111:ARG:CD	1:F:112:ARG:H	2.21	0.48
1:B:113:VAL:HG12	1:B:212:PRO:HG2	1.96	0.48
1:F:148:HIS:CD2	1:F:150:ARG:H	2.32	0.48
1:D:190:HIS:CE1	1:D:194:ARG:HE	2.32	0.48
1:A:214:HIS:CD2	1:A:258:SER:OG	2.67	0.48
1:B:109:ARG:HG2	1:B:109:ARG:HH11	1.78	0.48
1:B:248:GLU:OE1	1:E:190:HIS:HD2	1.97	0.48
1:D:197:VAL:HG21	1:D:242:GLU:HB3	1.96	0.48
1:G:85:PRO:HG2	1:G:88:VAL:HG21	1.95	0.48
1:G:99:LEU:C	1:G:99:LEU:HD12	2.39	0.48
1:A:22:MET:CG	4:A:3001:LYS:HD2	2.43	0.48
1:B:100:SER:HA	1:B:103:SER:OG	2.14	0.48
1:B:148:HIS:CD2	1:B:150:ARG:HB2	2.49	0.48
1:B:11:MET:HE1	1:B:98:SER:HB2	1.95	0.47
1:E:209:GLN:NE2	1:G:153:GLU:CA	2.75	0.47
1:G:214:HIS:HE1	1:G:260:ASP:OD2	1.97	0.47
1:E:209:GLN:O	1:E:209:GLN:HG3	2.14	0.47
1:F:223:ASP:OD2	1:F:225:THR:HG22	2.14	0.47
1:G:111:ARG:CD	1:G:112:ARG:H	2.17	0.47
1:G:11:MET:HE1	1:G:98:SER:HB2	1.96	0.47
1:G:272:ASN:O	1:G:276:GLU:HG3	2.14	0.47
1:A:25:SER:OG	4:A:3001:LYS:CA	2.62	0.47
1:A:46:LEU:HD22	1:A:80:ARG:NH2	2.30	0.47
1:A:125:ASN:ND2	1:A:175:GLU:HG3	2.29	0.47
1:F:169:ARG:HG3	1:F:234:VAL:CG1	2.44	0.47
1:G:2:GLU:HG3	5:G:3105:HOH:O	2.14	0.47
1:E:12:ASP:HB2	1:E:21:ASP:HB3	1.96	0.47
1:A:111:ARG:HD3	1:A:112:ARG:N	2.22	0.46
1:E:148:HIS:CD2	1:E:150:ARG:HB2	2.51	0.46
1:F:22:MET:SD	1:F:267:ILE:HD13	2.55	0.46
1:G:125:ASN:ND2	1:G:175:GLU:HG3	2.30	0.46
1:D:138:MET:H	1:D:139:PRO:CD	2.27	0.46
1:E:214:HIS:HE1	1:E:260:ASP:OD2	1.98	0.46
1:G:100:SER:HA	1:G:103:SER:OG	2.16	0.46
1:A:197:VAL:HG21	1:A:242:GLU:HB3	1.98	0.46
1:B:169:ARG:HG3	1:B:234:VAL:CG1	2.46	0.46
1:D:192:VAL:HA	1:D:200:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:LEU:HD13	1:G:277:MET:HE2	1.98	0.46
1:A:138:MET:H	1:A:139:PRO:CD	2.29	0.46
1:B:2:GLU:HG3	5:B:3112:HOH:O	2.15	0.46
1:D:214:HIS:HE1	1:D:260:ASP:OD2	1.99	0.46
1:A:271:ARG:N	5:A:3023:HOH:O	2.49	0.46
1:D:111:ARG:HD3	1:D:112:ARG:N	2.21	0.46
1:G:248:GLU:O	1:G:252:GLU:HG3	2.15	0.46
1:D:118:VAL:HG12	1:D:221:VAL:HG21	1.97	0.45
1:A:25:SER:OG	4:A:3001:LYS:CB	2.64	0.45
1:A:218:ASP:OD2	1:A:263:GLU:HG3	2.16	0.45
1:B:85:PRO:HG2	1:B:88:VAL:CG2	2.46	0.45
1:D:148:HIS:HD2	1:D:150:ARG:HB2	1.81	0.45
1:E:209:GLN:HE22	1:G:153:GLU:CA	2.30	0.45
1:G:218:ASP:OD2	1:G:263:GLU:HG3	2.16	0.45
1:D:81:LEU:HD12	1:D:103:SER:HA	1.98	0.45
1:E:98:SER:OG	1:E:136:HIS:HA	2.15	0.45
1:F:111:ARG:HD3	1:F:112:ARG:N	2.24	0.45
1:A:25:SER:OG	4:A:3001:LYS:HA	2.16	0.45
1:G:169:ARG:HG3	1:G:234:VAL:CG1	2.47	0.45
1:E:218:ASP:OD2	1:E:263:GLU:HG3	2.16	0.45
1:F:11:MET:HE1	1:F:98:SER:HB2	1.97	0.45
1:A:113:VAL:HG12	1:A:212:PRO:HG2	1.99	0.45
1:A:119:ASP:HB3	1:A:121:HIS:O	2.17	0.45
1:G:158:VAL:CG2	1:G:159:ASP:N	2.80	0.45
1:D:113:VAL:HG12	1:D:212:PRO:HG2	1.98	0.45
1:F:148:HIS:HD2	1:F:150:ARG:HB2	1.82	0.45
1:E:85:PRO:HG2	1:E:88:VAL:CG2	2.47	0.44
1:E:209:GLN:OE1	1:G:153:GLU:C	2.58	0.44
1:F:214:HIS:CE1	1:F:260:ASP:OD2	2.70	0.44
1:A:85:PRO:HG2	1:A:88:VAL:HG21	1.98	0.44
1:G:214:HIS:HD2	1:G:258:SER:OG	2.00	0.44
1:D:46:LEU:HD22	1:D:80:ARG:NH2	2.32	0.44
1:F:25:SER:OG	4:F:3004:LYS:CA	2.65	0.44
1:B:46:LEU:HD22	1:B:80:ARG:NH2	2.33	0.44
1:D:169:ARG:HG3	1:D:234:VAL:CG1	2.46	0.44
1:F:98:SER:OG	1:F:136:HIS:HA	2.18	0.44
1:F:100:SER:HA	1:F:103:SER:OG	2.18	0.44
1:F:33:LEU:HG	1:F:43:VAL:HG11	1.99	0.44
1:B:34:GLU:H	1:B:34:GLU:CD	2.25	0.44
1:G:156:ARG:NH2	5:G:3031:HOH:O	2.42	0.44
1:E:169:ARG:HG3	1:E:234:VAL:CG1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:VAL:HG21	1:F:242:GLU:HB3	2.00	0.44
1:E:197:VAL:HG21	1:E:242:GLU:HB3	2.00	0.43
1:F:2:GLU:HB2	1:G:150:ARG:HD3	1.99	0.43
1:G:22:MET:SD	1:G:267:ILE:CD1	3.06	0.43
1:G:214:HIS:CD2	1:G:258:SER:OG	2.71	0.43
1:A:169:ARG:HH22	1:A:221:VAL:C	2.25	0.43
1:A:272:ASN:O	1:A:276:GLU:HG3	2.19	0.43
1:D:33:LEU:HG	1:D:43:VAL:HG11	2.00	0.43
1:E:111:ARG:HD3	1:E:111:ARG:HA	1.31	0.43
4:A:3001:LYS:HE2	5:A:3009:HOH:O	2.18	0.43
1:E:33:LEU:HG	1:E:43:VAL:HG11	2.00	0.43
1:E:169:ARG:NH2	1:E:221:VAL:O	2.40	0.43
1:F:22:MET:HA	4:F:3004:LYS:HG3	2.00	0.43
1:F:40:GLY:O	1:G:148:HIS:HE1	2.01	0.43
1:E:211:LEU:N	1:G:156:ARG:HH22	2.16	0.43
1:F:277:MET:HG2	5:F:3026:HOH:O	2.19	0.43
1:B:81:LEU:HD12	1:B:103:SER:HA	2.00	0.43
1:D:214:HIS:HD2	1:D:258:SER:OG	2.01	0.43
1:E:25:SER:OG	4:E:3003:LYS:CG	2.67	0.43
1:D:100:SER:HA	1:D:103:SER:OG	2.18	0.43
1:G:192:VAL:HA	1:G:200:ILE:CD1	2.49	0.43
1:A:99:LEU:HD12	1:A:100:SER:N	2.34	0.43
1:A:193:ASP:HB3	1:F:245:LEU:HD22	2.01	0.43
1:D:218:ASP:OD2	1:D:263:GLU:HG3	2.19	0.43
1:E:113:VAL:HG12	1:E:212:PRO:HG2	2.00	0.42
1:D:85:PRO:HG2	1:D:88:VAL:CG2	2.49	0.42
1:G:214:HIS:CE1	1:G:260:ASP:OD2	2.72	0.42
1:E:272:ASN:O	1:E:276:GLU:HG3	2.19	0.42
1:G:85:PRO:HG2	1:G:88:VAL:CG2	2.50	0.42
1:A:33:LEU:HG	1:A:43:VAL:HG11	2.02	0.42
1:B:22:MET:SD	1:B:267:ILE:CD1	3.07	0.42
1:D:119:ASP:HB3	1:D:121:HIS:O	2.20	0.42
1:D:98:SER:OG	1:D:136:HIS:HA	2.20	0.42
1:D:214:HIS:CD2	1:D:258:SER:OG	2.73	0.42
1:E:100:SER:HA	1:E:103:SER:OG	2.18	0.42
1:E:138:MET:H	1:E:139:PRO:CD	2.32	0.42
1:E:211:LEU:CG	1:G:156:ARG:CZ	2.85	0.42
1:A:100:SER:HA	1:A:103:SER:OG	2.19	0.42
1:B:218:ASP:OD2	1:B:263:GLU:HG3	2.19	0.42
1:E:244:HIS:O	1:E:248:GLU:HG3	2.19	0.42
1:G:197:VAL:HG21	1:G:242:GLU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ASN:O	1:D:138:MET:HB3	2.19	0.42
1:F:126:THR:H	1:F:129:THR:HG1	1.68	0.41
1:G:81:LEU:HD12	1:G:103:SER:HA	2.01	0.41
1:G:113:VAL:HG12	1:G:212:PRO:HG2	2.02	0.41
1:B:148:HIS:HD2	1:B:150:ARG:HB2	1.84	0.41
1:E:81:LEU:HD12	1:E:103:SER:HA	2.03	0.41
1:A:214:HIS:HE1	1:A:260:ASP:OD2	2.04	0.41
4:A:3001:LYS:CA	5:A:3076:HOH:O	2.68	0.41
1:E:211:LEU:HD23	1:G:156:ARG:HH12	1.85	0.41
1:F:46:LEU:HD22	1:F:80:ARG:NH2	2.35	0.41
1:F:85:PRO:HG2	1:F:88:VAL:CG2	2.50	0.41
1:A:135:VAL:C	1:A:137:GLY:H	2.28	0.41
1:B:194:ARG:HD2	5:B:3121:HOH:O	2.20	0.41
1:F:125:ASN:O	1:F:138:MET:HB3	2.21	0.41
1:B:111:ARG:CG	1:B:112:ARG:N	2.84	0.41
1:B:138:MET:H	1:B:139:PRO:CD	2.33	0.41
1:B:192:VAL:HA	1:B:200:ILE:CD1	2.51	0.41
1:G:156:ARG:NH1	1:G:156:ARG:HG2	2.34	0.41
1:A:125:ASN:O	1:A:138:MET:HB3	2.21	0.41
1:E:46:LEU:HD22	1:E:80:ARG:NH2	2.34	0.41
1:E:211:LEU:N	1:G:156:ARG:HH12	2.18	0.41
1:G:46:LEU:HD22	1:G:80:ARG:NH2	2.36	0.41
1:A:22:MET:SD	1:A:267:ILE:HD13	2.61	0.41
1:A:34:GLU:H	1:A:34:GLU:CD	2.28	0.41
1:A:222:LEU:HD13	1:A:277:MET:HE2	2.01	0.41
1:D:277:MET:HE3	1:D:277:MET:HB3	1.89	0.41
1:D:11:MET:HE3	1:D:96:ASP:HB2	2.03	0.41
1:G:32:LEU:HB2	1:G:279:VAL:HG22	2.03	0.41
1:B:214:HIS:HE1	1:B:260:ASP:OD2	2.04	0.40
1:A:148:HIS:HA	1:A:149:PRO:HD3	1.92	0.40
1:F:192:VAL:HA	1:F:200:ILE:CD1	2.51	0.40
1:B:11:MET:HE3	1:B:96:ASP:HB2	2.04	0.40
1:E:211:LEU:CG	1:G:156:ARG:NH1	2.85	0.40
1:F:148:HIS:HA	1:F:149:PRO:HD3	1.90	0.40
1:G:192:VAL:HA	1:G:200:ILE:HD11	2.03	0.40
1:B:25:SER:OG	4:B:3006:LYS:HA	2.21	0.40
1:E:148:HIS:HD2	1:E:150:ARG:HB2	1.84	0.40
1:G:21:ASP:C	4:G:3005:LYS:CE	2.91	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLU:O	1:B:111:ARG:NH2[2_555]	1.79	0.41
1:B:83:ALA:N	1:B:111:ARG:NH2[2_555]	1.91	0.29
4:F:3004:LYS:NZ	4:G:3005:LYS:OXT[2_556]	2.08	0.12
4:F:3004:LYS:CB	4:G:3005:LYS:CB[2_556]	2.10	0.10

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	265/290 (91%)	258 (97%)	6 (2%)	1 (0%)	30 27
1	B	265/290 (91%)	259 (98%)	5 (2%)	1 (0%)	30 27
1	D	265/290 (91%)	258 (97%)	6 (2%)	1 (0%)	30 27
1	E	265/290 (91%)	260 (98%)	4 (2%)	1 (0%)	30 27
1	F	265/290 (91%)	259 (98%)	5 (2%)	1 (0%)	30 27
1	G	265/290 (91%)	258 (97%)	6 (2%)	1 (0%)	30 27
All	All	1590/1740 (91%)	1552 (98%)	32 (2%)	6 (0%)	30 27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	MET
1	B	138	MET
1	D	138	MET
1	F	138	MET
1	E	138	MET
1	G	138	MET

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	218/231 (94%)	213 (98%)	5 (2%)	44	49
1	B	218/231 (94%)	213 (98%)	5 (2%)	44	49
1	D	218/231 (94%)	213 (98%)	5 (2%)	44	49
1	E	218/231 (94%)	212 (97%)	6 (3%)	38	41
1	F	218/231 (94%)	213 (98%)	5 (2%)	44	49
1	G	218/231 (94%)	213 (98%)	5 (2%)	44	49
All	All	1308/1386 (94%)	1277 (98%)	31 (2%)	39	47

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	130	SER
1	A	138	MET
1	A	194	ARG
1	A	267	ILE
1	B	33	LEU
1	B	130	SER
1	B	138	MET
1	B	194	ARG
1	B	267	ILE
1	D	33	LEU
1	D	130	SER
1	D	138	MET
1	D	194	ARG
1	D	267	ILE
1	E	33	LEU
1	E	111	ARG
1	E	130	SER
1	E	138	MET
1	E	194	ARG
1	E	267	ILE
1	F	33	LEU
1	F	130	SER
1	F	138	MET
1	F	194	ARG
1	F	267	ILE
1	G	33	LEU

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Mol	Chain	Res	Type
1	G	130	SER
1	G	138	MET
1	G	194	ARG
1	G	267	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	134	ASN
1	A	136	HIS
1	A	148	HIS
1	A	190	HIS
1	A	214	HIS
1	B	134	ASN
1	B	136	HIS
1	B	148	HIS
1	B	190	HIS
1	B	207	HIS
1	B	214	HIS
1	D	125	ASN
1	D	134	ASN
1	D	136	HIS
1	D	148	HIS
1	D	190	HIS
1	D	214	HIS
1	E	125	ASN
1	E	134	ASN
1	E	136	HIS
1	E	148	HIS
1	E	190	HIS
1	E	209	GLN
1	E	214	HIS
1	E	257	GLN
1	F	125	ASN
1	F	134	ASN
1	F	136	HIS
1	F	148	HIS
1	F	190	HIS
1	F	214	HIS
1	G	125	ASN
1	G	134	ASN

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Mol	Chain	Res	Type
1	G	136	HIS
1	G	148	HIS
1	G	190	HIS
1	G	214	HIS

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](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAI	D	1002	-	3,3,3	1.05	0	3,3,3	1.11	0
4	LYS	E	3003	4	8,9,9	2.99	4 (50%)	7,10,10	2.21	4 (57%)
3	GAI	E	1003	-	3,3,3	1.10	0	3,3,3	1.14	0
4	LYS	B	3006	-	8,9,9	0.84	0	7,10,10	2.77	4 (57%)
3	GAI	B	1006	-	3,3,3	1.01	0	3,3,3	1.08	0
4	LYS	D	3002	-	8,9,9	1.79	2 (25%)	7,10,10	2.30	2 (28%)
4	LYS	G	3005	4	8,9,9	2.82	5 (62%)	7,10,10	2.16	4 (57%)
3	GAI	A	1004	-	3,3,3	0.99	0	3,3,3	1.15	0
4	LYS	A	3001	4	8,9,9	2.68	5 (62%)	7,10,10	3.66	5 (71%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAI	A	1001	-	3,3,3	1.09	0	3,3,3	1.15	0
3	GAI	G	1005	-	3,3,3	0.96	0	3,3,3	1.11	0
4	LYS	F	3004	4	8,9,9	1.65	2 (25%)	7,10,10	1.36	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LYS	E	3003	4	-	8/9/9/9	-
4	LYS	B	3006	-	-	5/9/9/9	-
4	LYS	D	3002	-	-	4/9/9/9	-
4	LYS	G	3005	4	-	8/9/9/9	-
4	LYS	A	3001	4	-	6/9/9/9	-
4	LYS	F	3004	4	-	9/9/9/9	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3005	LYS	CG-CB	4.94	1.72	1.52
4	E	3003	LYS	CD-CE	4.67	1.73	1.51
4	E	3003	LYS	CE-NZ	4.65	1.81	1.46
4	E	3003	LYS	CD-CG	-3.79	1.32	1.51
4	A	3001	LYS	CD-CE	3.74	1.69	1.51
4	G	3005	LYS	CD-CE	3.65	1.68	1.51
4	A	3001	LYS	CG-CB	3.64	1.67	1.52
4	G	3005	LYS	CD-CG	3.45	1.68	1.51
4	D	3002	LYS	CG-CB	3.43	1.66	1.52
4	A	3001	LYS	CB-CA	3.40	1.60	1.53
4	A	3001	LYS	CE-NZ	3.04	1.69	1.46
4	F	3004	LYS	CD-CE	2.81	1.64	1.51
4	D	3002	LYS	O-C	2.77	1.30	1.22
4	A	3001	LYS	CA-N	2.73	1.62	1.48
4	G	3005	LYS	CE-NZ	2.66	1.66	1.46
4	F	3004	LYS	OXT-C	-2.62	1.22	1.30
4	E	3003	LYS	CG-CB	2.50	1.62	1.52
4	G	3005	LYS	O-C	2.26	1.28	1.22

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	LYS	CG-CB-CA	6.47	134.10	113.22
4	B	3006	LYS	CD-CG-CB	-4.94	95.02	113.62
4	D	3002	LYS	CD-CG-CB	-4.79	95.57	113.62
4	A	3001	LYS	OXT-C-O	-4.55	113.77	124.08
4	B	3006	LYS	OXT-C-O	3.83	132.76	124.08
4	A	3001	LYS	CD-CG-CB	3.61	127.23	113.62
4	G	3005	LYS	CD-CE-NZ	3.60	137.42	112.60
4	E	3003	LYS	OXT-C-O	3.19	131.33	124.08
4	B	3006	LYS	CG-CB-CA	-3.07	103.30	113.22
4	D	3002	LYS	OXT-C-O	2.98	130.85	124.08
4	E	3003	LYS	CD-CG-CB	-2.88	102.78	113.62
4	A	3001	LYS	CB-CA-N	-2.81	102.80	110.12
4	A	3001	LYS	CD-CE-NZ	2.61	130.55	112.60
4	G	3005	LYS	CB-CA-N	-2.54	103.50	110.12
4	E	3003	LYS	CG-CD-CE	2.39	129.82	113.42
4	F	3004	LYS	CD-CG-CB	-2.34	104.79	113.62
4	G	3005	LYS	OXT-C-O	-2.18	119.14	124.08
4	B	3006	LYS	CB-CA-N	-2.16	104.48	110.12
4	E	3003	LYS	CG-CB-CA	2.05	119.84	113.22
4	G	3005	LYS	CB-CA-C	2.01	115.78	110.45

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3006	LYS	O-C-CA-N
4	B	3006	LYS	N-CA-CB-CG
4	B	3006	LYS	C-CA-CB-CG
4	D	3002	LYS	O-C-CA-N
4	D	3002	LYS	N-CA-CB-CG
4	D	3002	LYS	C-CA-CB-CG
4	E	3003	LYS	O-C-CA-N
4	E	3003	LYS	N-CA-CB-CG
4	E	3003	LYS	C-CA-CB-CG
4	F	3004	LYS	O-C-CA-N
4	F	3004	LYS	N-CA-CB-CG
4	F	3004	LYS	C-CA-CB-CG
4	G	3005	LYS	O-C-CA-N
4	G	3005	LYS	N-CA-CB-CG
4	G	3005	LYS	C-CA-CB-CG
4	A	3001	LYS	OXT-C-CA-N
4	D	3002	LYS	OXT-C-CA-N
4	B	3006	LYS	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
4	E	3003	LYS	OXT-C-CA-N
4	F	3004	LYS	OXT-C-CA-N
4	G	3005	LYS	OXT-C-CA-N
4	E	3003	LYS	CA-CB-CG-CD
4	G	3005	LYS	CE-CD-CG-CB
4	G	3005	LYS	CG-CD-CE-NZ
4	F	3004	LYS	O-C-CA-CB
4	B	3006	LYS	CA-CB-CG-CD
4	A	3001	LYS	C-CA-CB-CG
4	A	3001	LYS	CG-CD-CE-NZ
4	F	3004	LYS	CG-CD-CE-NZ
4	G	3005	LYS	O-C-CA-CB
4	A	3001	LYS	CE-CD-CG-CB
4	A	3001	LYS	N-CA-CB-CG
4	E	3003	LYS	OXT-C-CA-CB
4	F	3004	LYS	CA-CB-CG-CD
4	E	3003	LYS	O-C-CA-CB
4	F	3004	LYS	OXT-C-CA-CB
4	G	3005	LYS	OXT-C-CA-CB
4	E	3003	LYS	CG-CD-CE-NZ
4	F	3004	LYS	CE-CD-CG-CB
4	A	3001	LYS	O-C-CA-N

There are no ring outliers.

6 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	3003	LYS	9	0
4	B	3006	LYS	4	0
4	D	3002	LYS	3	0
4	G	3005	LYS	12	2
4	A	3001	LYS	17	0
4	F	3004	LYS	12	2

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	273/290 (94%)	0.50	21 (7%) 19 18	15, 27, 42, 52	0
1	B	273/290 (94%)	0.62	29 (10%) 11 10	12, 25, 43, 53	0
1	D	273/290 (94%)	0.67	29 (10%) 11 10	14, 28, 46, 55	0
1	E	273/290 (94%)	0.43	25 (9%) 14 13	12, 22, 40, 53	0
1	F	273/290 (94%)	0.89	35 (12%) 7 6	17, 31, 47, 54	0
1	G	273/290 (94%)	0.57	33 (12%) 8 8	13, 24, 41, 53	0
All	All	1638/1740 (94%)	0.61	172 (10%) 11 10	12, 26, 44, 55	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	291	PHE	9.0
1	B	111	ARG	6.9
1	E	110	GLY	6.7
1	E	111	ARG	6.6
1	B	52	SER	5.7
1	E	130	SER	5.5
1	B	65	ALA	5.0
1	G	132	SER	4.9
1	D	65	ALA	4.9
1	F	64	LEU	4.9
1	B	130	SER	4.9
1	B	291	PHE	4.8
1	F	2	GLU	4.6
1	B	64	LEU	4.6
1	G	156	ARG	4.5
1	E	64	LEU	4.5
1	G	64	LEU	4.5
1	E	2	GLU	4.5
1	F	156	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	109	ARG	4.3
1	G	82	ALA	4.3
1	B	79	GLU	4.3
1	B	231	GLY	4.2
1	G	110	GLY	4.2
1	F	111	ARG	4.2
1	B	86	GLU	4.1
1	F	95	GLY	4.1
1	E	86	GLU	4.1
1	D	231	GLY	4.0
1	E	209	GLN	4.0
1	D	2	GLU	4.0
1	E	132	SER	4.0
1	D	64	LEU	3.9
1	G	130	SER	3.9
1	G	231	GLY	3.9
1	F	52	SER	3.9
1	F	134	ASN	3.8
1	G	109	ARG	3.8
1	B	180	LYS	3.7
1	G	111	ARG	3.7
1	G	289	ARG	3.7
1	A	64	LEU	3.7
1	D	225	THR	3.7
1	F	128	GLU	3.6
1	F	65	ALA	3.6
1	G	112	ARG	3.6
1	F	69	GLU	3.6
1	F	231	GLY	3.6
1	B	44	GLU	3.5
1	B	225	THR	3.5
1	G	95	GLY	3.5
1	G	52	SER	3.5
1	D	86	GLU	3.5
1	G	2	GLU	3.4
1	G	86	GLU	3.4
1	F	66	TYR	3.4
1	B	2	GLU	3.4
1	G	232	THR	3.3
1	B	75	LEU	3.3
1	D	52	SER	3.3
1	B	136	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	29	TYR	3.2
1	E	226	LEU	3.1
1	A	83	ALA	3.1
1	F	136	HIS	3.0
1	G	161	LYS	3.0
1	E	65	ALA	3.0
1	G	65	ALA	3.0
1	F	173	PRO	3.0
1	F	154	VAL	2.9
1	D	109	ARG	2.9
1	D	177	ARG	2.9
1	B	132	SER	2.9
1	E	231	GLY	2.9
1	F	13	LEU	2.9
1	D	111	ARG	2.9
1	D	29	TYR	2.9
1	B	12	ASP	2.8
1	A	95	GLY	2.8
1	D	232	THR	2.8
1	F	202	GLU	2.8
1	B	232	THR	2.8
1	A	128	GLU	2.8
1	G	33	LEU	2.8
1	B	109	ARG	2.7
1	E	271	ARG	2.7
1	F	109	ARG	2.7
1	D	130	SER	2.7
1	G	225	THR	2.7
1	F	130	SER	2.7
1	B	95	GLY	2.7
1	D	95	GLY	2.7
1	A	132	SER	2.7
1	B	156	ARG	2.7
1	E	177	ARG	2.7
1	E	85	PRO	2.6
1	D	182	ALA	2.6
1	E	95	GLY	2.6
1	A	225	THR	2.6
1	G	177	ARG	2.6
1	A	230	VAL	2.6
1	F	82	ALA	2.6
1	E	52	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	111	ARG	2.5
1	F	110	GLY	2.5
1	G	226	LEU	2.5
1	B	209	GLN	2.5
1	F	132	SER	2.5
1	B	226	LEU	2.5
1	G	94	GLY	2.5
1	D	149	PRO	2.4
1	F	88	VAL	2.4
1	G	290	ILE	2.4
1	A	85	PRO	2.4
1	F	137	GLY	2.4
1	D	181	GLU	2.4
1	D	202	GLU	2.4
1	A	231	GLY	2.4
1	F	149	PRO	2.4
1	A	183	GLY	2.3
1	G	271	ARG	2.3
1	E	232	THR	2.3
1	D	159	ASP	2.3
1	E	13	LEU	2.3
1	E	66	TYR	2.3
1	F	3	ARG	2.3
1	F	291	PHE	2.3
1	G	128	GLU	2.3
1	D	135	VAL	2.3
1	A	232	THR	2.3
1	D	173	PRO	2.3
1	B	148	HIS	2.2
1	A	130	SER	2.2
1	D	3	ARG	2.2
1	F	19	GLY	2.2
1	B	128	GLU	2.2
1	A	109	ARG	2.2
1	E	112	ARG	2.2
1	G	108	ALA	2.2
1	E	156	ARG	2.2
1	D	126	THR	2.2
1	F	87	GLY	2.2
1	A	33	LEU	2.2
1	B	177	ARG	2.2
1	E	3	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	80	ARG	2.2
1	B	158	VAL	2.1
1	D	147	GLY	2.1
1	G	107	ALA	2.1
1	A	13	LEU	2.1
1	G	180	LYS	2.1
1	D	85	PRO	2.1
1	D	136	HIS	2.1
1	B	161	LYS	2.1
1	E	33	LEU	2.1
1	D	96	ASP	2.1
1	D	199	ARG	2.1
1	F	129	THR	2.1
1	F	150	ARG	2.1
1	G	66	TYR	2.1
1	A	133	GLY	2.1
1	A	148	HIS	2.0
1	F	183	GLY	2.0
1	G	29	TYR	2.0
1	F	252	GLU	2.0
1	A	82	ALA	2.0
1	F	146	LEU	2.0
1	D	271	ARG	2.0
1	E	225	THR	2.0
1	F	225	THR	2.0
1	A	110	GLY	2.0
1	B	94	GLY	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	LYS	D	3002	10/10	0.40	0.24	55,56,58,60	0
4	LYS	B	3006	10/10	0.45	0.23	54,56,57,57	0
4	LYS	F	3004	10/10	0.49	0.27	57,58,59,61	0
4	LYS	G	3005	10/10	0.52	0.26	56,57,59,59	0
4	LYS	E	3003	10/10	0.59	0.26	56,58,58,58	0
4	LYS	A	3001	10/10	0.64	0.26	54,55,57,57	0
3	GAI	A	1001	4/4	0.95	0.06	20,20,21,21	0
2	MN	E	1301	1/1	0.96	0.09	30,30,30,30	0
2	MN	B	1601	1/1	0.96	0.04	38,38,38,38	0
3	GAI	A	1004	4/4	0.96	0.06	20,20,21,22	0
3	GAI	B	1006	4/4	0.96	0.05	14,15,15,16	0
3	GAI	D	1002	4/4	0.96	0.06	19,20,20,21	0
3	GAI	G	1005	4/4	0.96	0.05	14,16,16,16	0
2	MN	F	1401	1/1	0.97	0.05	47,47,47,47	0
2	MN	G	1501	1/1	0.97	0.04	40,40,40,40	0
3	GAI	E	1003	4/4	0.97	0.05	12,13,13,15	0
2	MN	D	1201	1/1	0.97	0.04	43,43,43,43	0
2	MN	A	1102	1/1	0.97	0.04	28,28,28,28	0
2	MN	B	1602	1/1	0.98	0.10	32,32,32,32	0
2	MN	A	1101	1/1	0.98	0.04	42,42,42,42	0
2	MN	D	1202	1/1	0.98	0.03	30,30,30,30	0
2	MN	G	1502	1/1	0.98	0.12	36,36,36,36	0
2	MN	E	1302	1/1	0.99	0.08	16,16,16,16	0
2	MN	F	1402	1/1	0.99	0.03	31,31,31,31	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.