



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:35 AM UTC

PDB ID : 5F4H / pdb_00005f4h
Title : Archaeal RuvB-like Holiday junction helicase
Authors : Zhai, B.; DuPrez, K.T.; Doukov, T.I.; Shen, Y.; Fan, L.
Deposited on : 2015-12-03
Resolution : 2.70 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

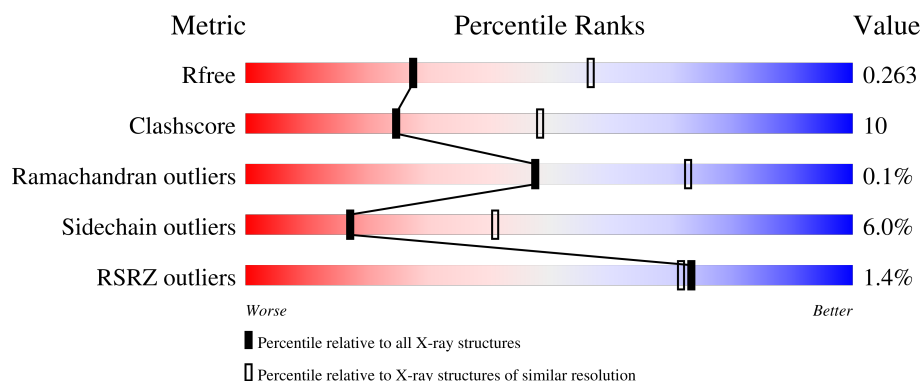
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	505	% 65% 18% • 13%
1	B	505	% 65% 18% • 14%
1	C	505	2% 66% 18% • 14%
1	D	505	2% 66% 18% • 14%
1	E	505	% 65% 18% • 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	505	% 64% 19% 14%

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
2	GOL	C	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20358 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 Nucleotide binding protein PINc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3329	2118	556	639	16			
1	B	435	Total	C	N	O	S	0	0	0
			3347	2132	556	644	15			
1	C	436	Total	C	N	O	S	0	0	0
			3274	2071	554	635	14			
1	D	436	Total	C	N	O	S	0	0	0
			3324	2110	557	642	15			
1	E	436	Total	C	N	O	S	0	0	0
			3334	2115	561	644	14			
1	F	436	Total	C	N	O	S	0	0	0
			3350	2131	565	638	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ALA	LYS	engineered mutation	UNP C3MQK6
B	261	ALA	LYS	engineered mutation	UNP C3MQK6
C	261	ALA	LYS	engineered mutation	UNP C3MQK6
D	261	ALA	LYS	engineered mutation	UNP C3MQK6
E	261	ALA	LYS	engineered mutation	UNP C3MQK6
F	261	ALA	LYS	engineered mutation	UNP C3MQK6

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

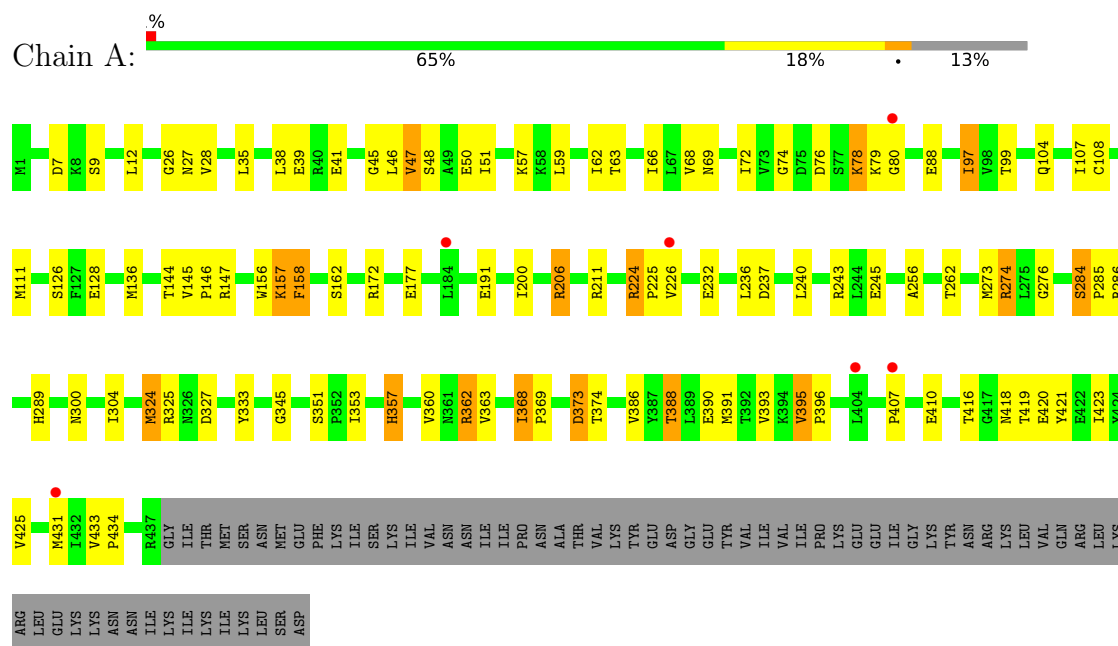
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	49	Total O 49 49	0	0
4	B	28	Total O 28 28	0	0
4	C	19	Total O 19 19	0	0
4	D	38	Total O 38 38	0	0
4	E	56	Total O 56 56	0	0
4	F	40	Total O 40 40	0	0

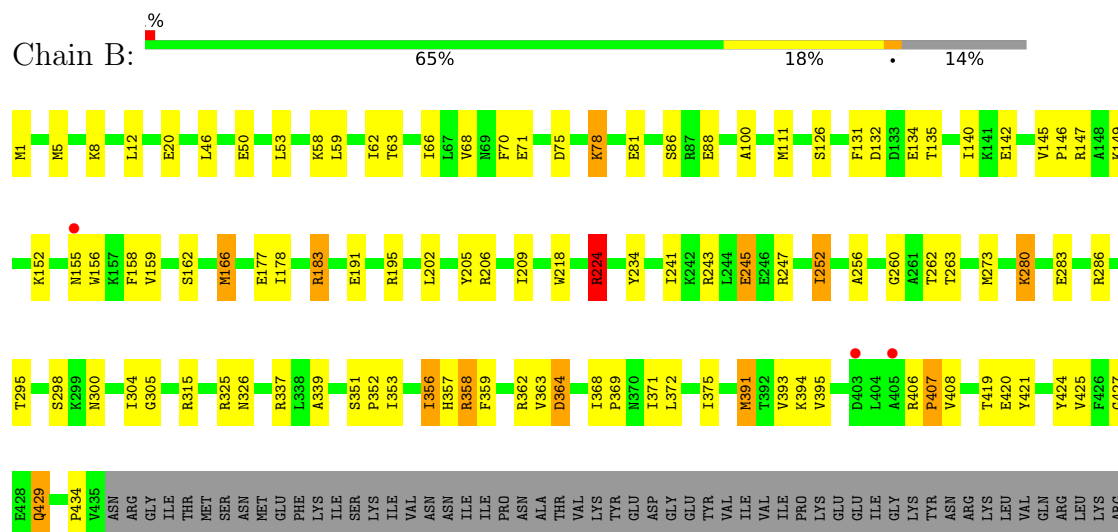
3 Residue-property plots

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: Nucleotide binding protein PINc



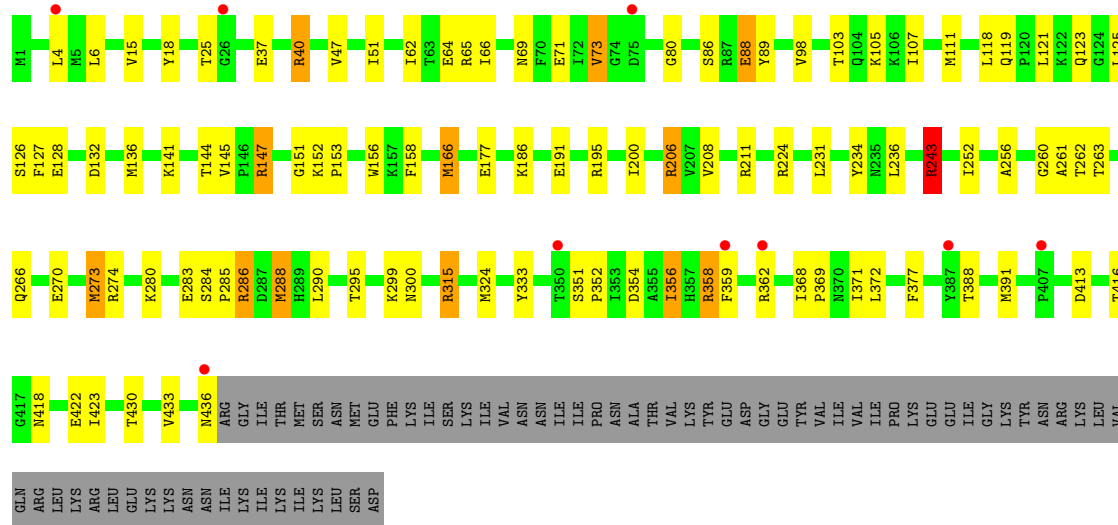
• Molecule 1: Nucleotide binding protein PINc



LEU
GLU
LYS
LYS
ASN
ASN
ILE
LYS
LYS
ILE
LYS
LYS
LEU
SER
ASP

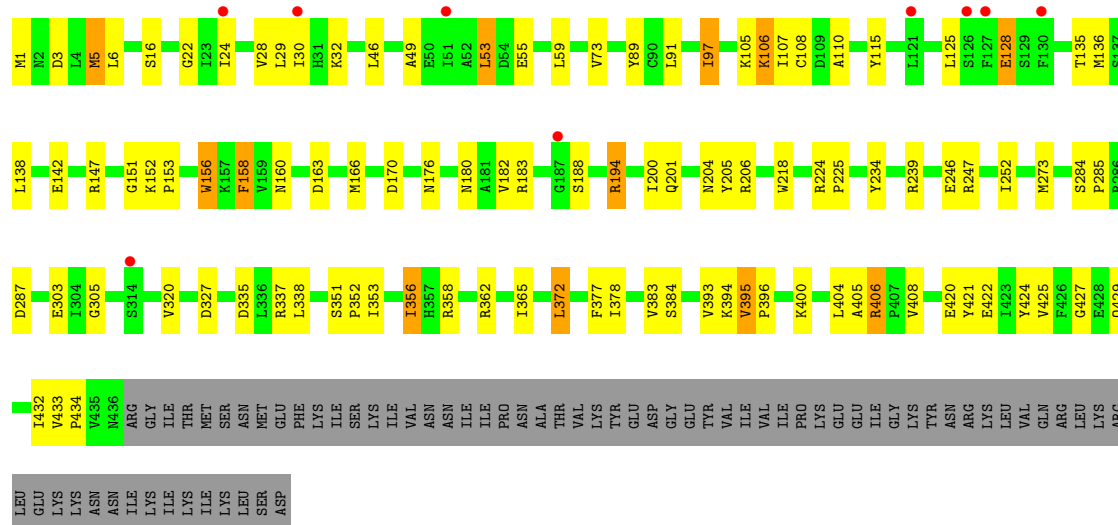
• Molecule 1: Nucleotide binding protein PINc

Chain C: 



• Molecule 1: Nucleotide binding protein PINc

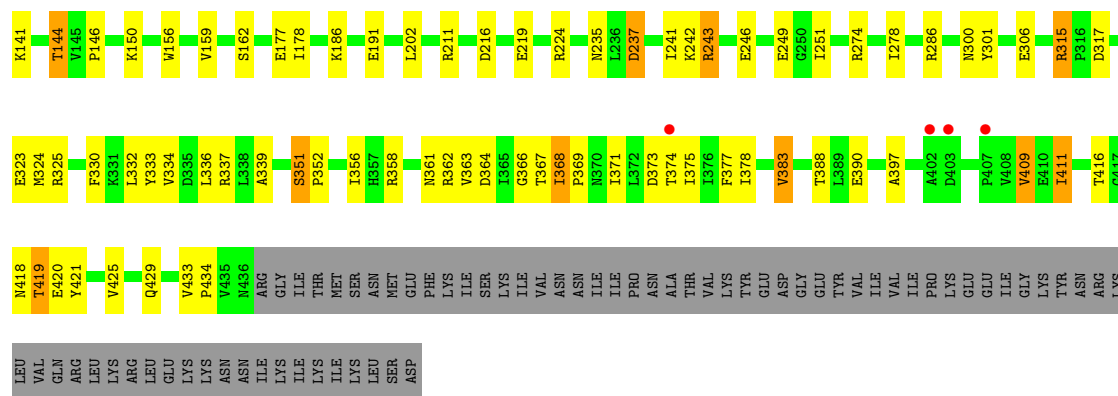
Chain D: 



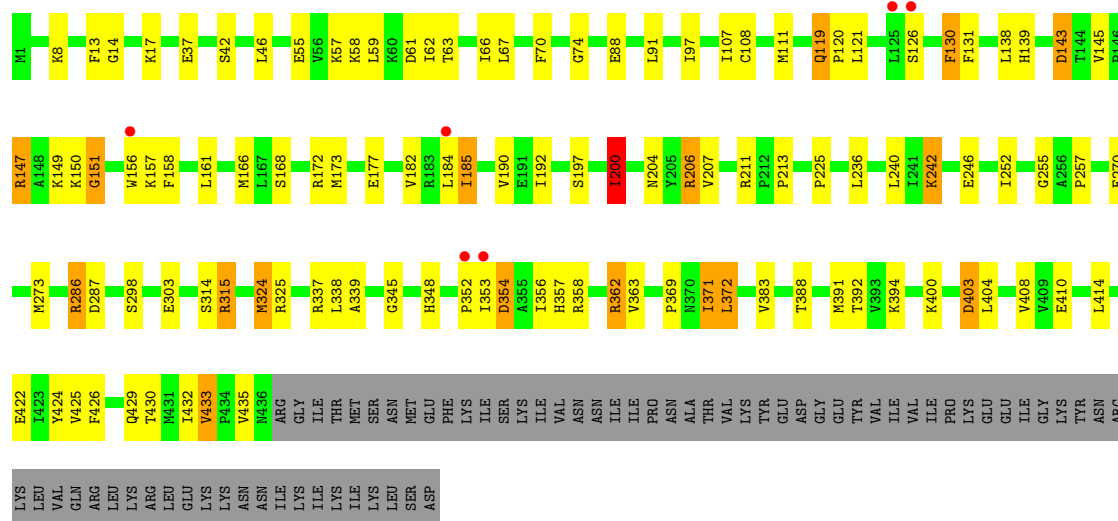
• Molecule 1: Nucleotide binding protein PINc

Chain E: 





• Molecule 1: Nucleotide binding protein PINc



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.72Å 148.98Å 122.13Å 90.00° 104.07° 90.00°	Depositor
Resolution (Å)	39.19 – 2.70 39.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.19-2.70) 97.6 (39.19-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.227 , 0.265 0.227 , 0.263	Depositor DCC
R_{free} test set	4732 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20358	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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 ⓘ

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

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	1.29	1/3381 (0.0%)	1.25	20/4585 (0.4%)
1	B	1.22	4/3401 (0.1%)	1.23	18/4610 (0.4%)
1	C	1.21	2/3326 (0.1%)	1.28	26/4515 (0.6%)
1	D	1.22	3/3376 (0.1%)	1.27	17/4577 (0.4%)
1	E	1.30	4/3384 (0.1%)	1.27	21/4587 (0.5%)
1	F	1.32	4/3402 (0.1%)	1.29	24/4604 (0.5%)
All	All	1.26	18/20270 (0.1%)	1.27	126/27478 (0.5%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	224	ARG	CA-C	-6.51	1.47	1.52
1	E	219	GLU	CD-OE1	6.26	1.37	1.25
1	A	38	LEU	N-CA	-6.24	1.38	1.46
1	D	406	ARG	N-CA	6.24	1.50	1.46
1	D	427	GLY	N-CA	6.15	1.54	1.45
1	D	320	VAL	CA-C	-5.93	1.45	1.52
1	E	76	ASP	CA-CB	5.83	1.62	1.53
1	B	155	ASN	CA-C	5.42	1.59	1.53
1	E	235	ASN	CA-C	-5.36	1.46	1.53
1	B	368	ILE	C-O	-5.33	1.20	1.24
1	C	436	ASN	N-CA	5.30	1.56	1.46
1	B	429	GLN	N-CA	5.30	1.52	1.46
1	F	354	ASP	CB-CG	5.25	1.65	1.52
1	C	286	ARG	C-O	-5.25	1.17	1.24
1	F	354	ASP	CA-CB	5.21	1.61	1.53
1	F	42	SER	C-O	-5.20	1.18	1.24
1	F	414	LEU	C-O	-5.16	1.18	1.24
1	B	209	ILE	N-CA	-5.05	1.40	1.46

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	362	ARG	N-CA-C	10.78	123.03	111.28
1	F	74	GLY	N-CA-C	-9.82	102.03	112.04
1	A	80	GLY	N-CA-C	-9.72	96.56	110.75
1	E	80	GLY	N-CA-C	-9.62	99.36	112.25
1	F	131	PHE	N-CA-C	9.46	121.60	111.28
1	E	300	ASN	N-CA-CB	-8.55	97.05	110.22
1	C	356	ILE	N-CA-C	8.20	121.29	111.05
1	D	406	ARG	CA-C-N	-7.11	112.65	119.76
1	D	406	ARG	C-N-CA	-7.11	112.65	119.76
1	C	86	SER	CA-CB-OG	-6.93	97.24	111.10
1	E	274	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	F	130	PHE	N-CA-C	6.76	120.79	112.54
1	F	315	ARG	CA-C-N	-6.76	113.83	120.52
1	F	315	ARG	C-N-CA	-6.76	113.83	120.52
1	D	395	VAL	N-CA-C	-6.70	102.39	108.95
1	A	74	GLY	N-CA-C	-6.67	97.38	113.18
1	F	119	GLN	CA-C-N	-6.61	112.86	119.93
1	F	119	GLN	C-N-CA	-6.61	112.86	119.93
1	C	211	ARG	CA-C-N	-6.55	114.88	119.66
1	C	211	ARG	C-N-CA	-6.55	114.88	119.66
1	E	77	SER	N-CA-C	-6.55	105.83	113.88
1	E	419	THR	CB-CA-C	6.52	119.55	110.16
1	F	211	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	A	224	ARG	CA-C-N	-6.41	113.37	119.85
1	A	224	ARG	C-N-CA	-6.41	113.37	119.85
1	E	397	ALA	N-CA-C	-6.39	100.23	110.14
1	E	79	LYS	CA-C-N	6.39	129.36	121.06
1	E	79	LYS	C-N-CA	6.39	129.36	121.06
1	F	151	GLY	N-CA-C	6.33	118.68	110.45
1	B	395	VAL	N-CA-C	-6.32	102.75	108.95
1	E	224	ARG	CA-C-N	-6.31	113.47	119.85
1	E	224	ARG	C-N-CA	-6.31	113.47	119.85
1	A	47	VAL	N-CA-C	6.29	116.97	110.36
1	C	121	LEU	N-CA-C	-6.25	101.85	110.35
1	D	176	ASN	N-CA-CB	6.21	119.25	110.12
1	C	166	MET	CG-SD-CE	-6.20	87.25	100.90
1	D	337	ARG	NE-CZ-NH2	6.18	124.77	119.20
1	D	194	ARG	N-CA-C	-6.07	101.21	109.95
1	D	239	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	C	73	VAL	N-CA-C	6.04	118.93	108.90
1	E	74	GLY	N-CA-C	6.03	121.87	114.69
1	A	351	SER	CA-C-N	-6.01	112.38	119.05
1	A	351	SER	C-N-CA	-6.01	112.38	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	ASP	CB-CA-C	-5.95	99.65	109.65
1	A	274	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	B	183	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	E	211	ARG	CA-C-N	-5.82	115.47	119.66
1	E	211	ARG	C-N-CA	-5.82	115.47	119.66
1	E	47	VAL	CB-CA-C	-5.80	104.55	111.97
1	B	359	PHE	N-CA-C	5.77	117.65	111.36
1	F	372	LEU	CB-CA-C	-5.77	99.26	109.70
1	C	80	GLY	N-CA-C	5.75	119.39	110.88
1	F	206	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	F	206	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	C	206	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	C	206	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	F	177	GLU	N-CA-C	-5.63	104.52	111.33
1	E	366	GLY	N-CA-C	-5.62	106.75	114.67
1	F	432	ILE	N-CA-C	-5.60	100.52	108.58
1	A	200	ILE	N-CA-C	5.58	116.78	108.46
1	D	246	GLU	N-CA-C	5.58	121.11	113.97
1	A	363	VAL	N-CA-C	5.57	116.72	108.65
1	C	119	GLN	CA-C-N	-5.55	114.04	119.76
1	C	119	GLN	C-N-CA	-5.55	114.04	119.76
1	C	200	ILE	N-CA-C	5.55	116.72	108.46
1	C	288	MET	CG-SD-CE	5.54	113.09	100.90
1	B	234	TYR	N-CA-C	-5.52	100.81	109.25
1	D	356	ILE	N-CA-C	-5.52	104.99	110.62
1	E	362	ARG	N-CA-C	5.51	118.22	111.82
1	F	242	LYS	N-CA-C	-5.50	105.28	111.28
1	A	28	VAL	CB-CA-C	5.50	118.32	110.84
1	C	299	LYS	N-CA-CB	5.48	118.66	110.22
1	F	362	ARG	N-CA-C	5.45	118.14	111.82
1	B	337	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	B	252	ILE	CB-CA-C	5.43	118.27	110.33
1	B	256	ALA	CA-C-N	-5.43	114.33	119.76
1	B	256	ALA	C-N-CA	-5.43	114.33	119.76
1	C	243	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	C	368	ILE	CB-CA-C	-5.41	108.56	113.70
1	C	65	ARG	N-CA-CB	5.39	119.19	110.40
1	D	224	ARG	N-CA-C	-5.39	102.85	110.29
1	C	64	GLU	CB-CA-C	-5.38	102.43	110.88
1	D	395	VAL	CA-C-N	-5.37	114.42	119.90
1	D	395	VAL	C-N-CA	-5.37	114.42	119.90
1	B	429	GLN	N-CA-C	5.36	118.28	109.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ALA	CA-C-N	-5.36	114.24	119.76
1	A	256	ALA	C-N-CA	-5.36	114.24	119.76
1	A	368	ILE	CB-CA-C	-5.35	108.61	113.70
1	F	314	SER	CB-CA-C	-5.34	101.77	110.85
1	A	360	VAL	N-CA-C	5.33	116.06	110.62
1	B	286	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	B	286	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	C	234	TYR	N-CA-C	-5.30	101.14	109.25
1	A	395	VAL	N-CA-C	-5.28	103.77	108.95
1	B	427	GLY	CA-C-O	-5.27	115.79	120.53
1	F	200	ILE	CA-CB-CG2	5.27	119.45	110.50
1	C	430	THR	N-CA-C	-5.26	100.67	109.24
1	F	185	ILE	N-CA-C	-5.23	100.85	109.12
1	C	256	ALA	CA-C-N	-5.22	114.38	119.76
1	C	256	ALA	C-N-CA	-5.22	114.38	119.76
1	A	97	ILE	N-CA-CB	5.22	117.41	110.26
1	E	79	LYS	N-CA-C	-5.22	106.50	112.86
1	B	224	ARG	CA-C-N	-5.18	114.62	119.85
1	B	224	ARG	C-N-CA	-5.18	114.62	119.85
1	F	286	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	D	234	TYR	N-CA-C	5.16	117.80	111.82
1	D	200	ILE	N-CA-C	5.14	116.12	108.46
1	B	326	ASN	N-CA-C	5.13	118.12	110.52
1	A	395	VAL	CA-C-N	-5.12	114.45	119.93
1	A	395	VAL	C-N-CA	-5.12	114.45	119.93
1	C	315	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	E	383	VAL	N-CA-CB	5.11	117.59	111.31
1	D	135	THR	N-CA-C	5.10	118.26	110.20
1	C	351	SER	CA-C-N	-5.10	113.56	119.47
1	C	351	SER	C-N-CA	-5.10	113.56	119.47
1	D	372	LEU	CB-CA-C	-5.09	100.48	109.70
1	E	351	SER	CA-C-N	-5.07	113.32	118.85
1	E	351	SER	C-N-CA	-5.07	113.32	118.85
1	E	368	ILE	CB-CA-C	-5.07	107.36	114.00
1	F	337	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	D	384	SER	CB-CA-C	-5.05	102.92	110.90
1	F	145	VAL	CA-C-N	-5.04	114.72	119.76
1	F	145	VAL	C-N-CA	-5.04	114.72	119.76
1	B	298	SER	CA-C-O	5.04	125.78	120.54
1	B	364	ASP	CB-CA-C	5.03	118.63	109.62
1	F	119	GLN	CA-C-O	-5.03	115.47	120.66

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	3329	0	3283	69	0
1	B	3347	0	3303	67	0
1	C	3274	0	3126	64	0
1	D	3324	0	3234	66	1
1	E	3334	0	3295	77	0
1	F	3350	0	3334	70	1
2	A	18	0	24	2	0
2	B	12	0	16	2	0
2	C	6	0	8	6	0
2	D	36	0	48	3	0
2	E	30	0	40	0	0
2	F	24	0	32	0	0
3	A	8	0	12	3	0
3	B	16	0	24	1	0
3	C	4	0	6	0	0
3	D	8	0	12	0	0
3	F	8	0	12	1	0
4	A	49	0	0	0	0
4	B	28	0	0	0	0
4	C	19	0	0	0	0
4	D	38	0	0	0	0
4	E	56	0	0	0	0
4	F	40	0	0	0	0
All	All	20358	0	19809	390	1

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 10.

All (390) 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:A:191:GLU:OE1	1:A:206:ARG:NH1	1.63	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:394:LYS:NZ	1:F:422:GLU:OE2	1.65	1.29
1:B:325:ARG:O	1:B:358:ARG:NH2	1.76	1.18
1:D:206:ARG:NH1	1:D:287:ASP:OD2	1.78	1.16
1:A:243:ARG:HH12	1:A:388:THR:HB	0.97	1.13
1:F:57:LYS:NZ	1:F:61:ASP:OD1	1.89	1.05
1:A:206:ARG:NH2	1:A:286:ARG:O	1.93	1.01
1:A:243:ARG:NH1	1:A:388:THR:HB	1.76	1.00
1:F:425:VAL:HA	1:F:430:THR:HA	1.48	0.95
1:A:99:THR:HG21	1:A:104:GLN:HG2	1.49	0.93
1:A:324:MET:HE2	1:A:345:GLY:HA3	1.54	0.88
1:E:243:ARG:NH2	1:E:388:THR:HB	1.88	0.87
1:D:55:GLU:O	1:D:59:LEU:HD13	1.76	0.85
1:A:369:PRO:HG2	1:A:391:MET:HB2	1.57	0.84
1:D:421:TYR:HA	1:D:434:PRO:HD3	1.60	0.84
1:A:243:ARG:HH12	1:A:388:THR:CB	1.89	0.81
1:D:305:GLY:H	2:D:604:GOL:H2	1.46	0.81
1:F:66:ILE:HG22	1:F:66:ILE:O	1.82	0.77
1:F:149:LYS:HG3	1:F:158:PHE:CZ	2.20	0.77
1:C:266:GLN:HA	1:C:288:MET:HE3	1.67	0.77
1:C:369:PRO:HG2	1:C:391:MET:CB	2.16	0.76
1:B:146:PRO:HD2	1:B:162:SER:HB3	1.68	0.75
1:F:324:MET:HE2	1:F:345:GLY:HA3	1.69	0.75
1:F:190:VAL:HA	1:F:200:ILE:HG22	1.69	0.74
1:E:390:GLU:O	1:E:409:VAL:HB	1.87	0.73
1:A:126:SER:HB3	1:A:177:GLU:OE1	1.89	0.73
1:C:352:PRO:HG3	1:C:377:PHE:CD1	2.23	0.73
1:B:352:PRO:HG2	1:B:421:TYR:CE2	2.25	0.72
1:F:150:LYS:O	1:F:157:LYS:N	2.22	0.72
1:F:13:PHE:HE1	1:F:184:LEU:CD1	2.03	0.71
1:E:63:THR:HG23	1:E:68:VAL:O	1.91	0.71
1:E:243:ARG:HH21	1:E:388:THR:HB	1.55	0.71
1:F:168:SER:OG	1:F:172:ARG:NH2	2.24	0.70
1:C:288:MET:HE2	1:C:290:LEU:HD11	1.72	0.70
1:B:100:ALA:O	1:B:183:ARG:NH2	2.26	0.69
1:B:262:THR:HB	2:B:601:GOL:H31	1.74	0.69
1:D:425:VAL:HA	1:D:429:GLN:HA	1.75	0.69
1:F:138:LEU:HD11	1:F:161:LEU:HD21	1.73	0.69
1:A:27:ASN:HA	1:A:68:VAL:CG1	2.23	0.69
1:D:204:ASN:O	1:D:225:PRO:HD3	1.94	0.68
1:D:351:SER:HB2	1:D:353:ILE:CD1	2.24	0.68
1:A:232:GLU:CD	1:A:274:ARG:HH12	2.01	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:ILE:HG12	1:F:147:ARG:HH12	1.58	0.68
1:D:338:LEU:HD12	1:E:325:ARG:HD2	1.74	0.67
1:F:14:GLY:HA2	1:F:55:GLU:OE2	1.93	0.67
1:F:139:HIS:HB3	1:F:147:ARG:HE	1.60	0.66
1:C:62:ILE:O	1:C:66:ILE:HG12	1.96	0.66
1:E:35:LEU:HD22	1:E:72:ILE:HD13	1.76	0.65
1:B:280:LYS:HE2	1:B:295:THR:HG21	1.79	0.65
1:E:278:ILE:HD11	1:F:158:PHE:CE2	2.31	0.65
1:F:151:GLY:HA3	1:F:156:TRP:HA	1.77	0.65
1:A:35:LEU:HD22	1:A:72:ILE:HD13	1.79	0.65
1:B:394:LYS:N	1:B:406:ARG:O	2.29	0.65
1:F:206:ARG:NH2	1:F:287:ASP:OD2	2.30	0.65
1:C:263:THR:H	2:C:601:GOL:H31	1.60	0.64
1:B:59:LEU:O	1:B:63:THR:HG23	1.98	0.64
1:B:241:ILE:HG22	1:B:245:GLU:OE1	1.97	0.64
1:A:410:GLU:CD	1:A:419:THR:HG21	2.23	0.64
1:F:13:PHE:CE1	1:F:184:LEU:CD1	2.80	0.64
1:C:145:VAL:O	1:C:147:ARG:HD2	1.98	0.63
1:B:352:PRO:HG2	1:B:421:TYR:HE2	1.62	0.63
1:C:191:GLU:CD	1:C:206:ARG:HH11	2.06	0.63
1:C:416:THR:HG22	1:C:418:ASN:CB	2.29	0.63
1:B:280:LYS:CE	1:B:295:THR:HG21	2.27	0.63
1:D:305:GLY:N	2:D:604:GOL:H2	2.12	0.63
1:B:408:VAL:HG12	1:B:424:TYR:HB3	1.78	0.62
1:A:240:LEU:HD12	1:A:386:VAL:HG21	1.81	0.62
1:C:260:GLY:H	2:C:601:GOL:H12	1.63	0.62
1:F:149:LYS:HG3	1:F:158:PHE:CE1	2.34	0.62
1:D:394:LYS:C	1:D:405:ALA:HB1	2.26	0.61
1:E:63:THR:HG21	1:E:70:PHE:HB2	1.82	0.61
1:B:146:PRO:HG3	1:B:166:MET:HE1	1.82	0.61
1:E:32:LYS:HD2	1:E:75:ASP:HA	1.84	0.60
1:A:35:LEU:HD23	1:F:111:MET:HE3	1.84	0.60
1:B:20:GLU:HG3	1:B:62:ILE:HD12	1.83	0.60
1:D:97:ILE:HG21	1:D:108:CYS:SG	2.40	0.60
1:B:140:ILE:HG23	1:B:166:MET:HE3	1.81	0.60
1:C:6:LEU:CD2	1:C:15:VAL:HG21	2.32	0.60
1:A:327:ASP:HB3	1:A:362:ARG:HH22	1.67	0.60
1:B:295:THR:HB	1:C:141:LYS:HE2	1.85	0.59
1:B:369:PRO:HG2	1:B:391:MET:HB2	1.84	0.59
1:F:286:ARG:HH21	1:F:298:SER:HB2	1.68	0.59
1:A:97:ILE:HG12	1:A:108:CYS:SG	2.42	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:GLU:O	1:D:434:PRO:HD2	2.03	0.59
1:B:135:THR:HG23	1:B:135:THR:O	2.03	0.59
1:E:356:ILE:O	1:E:356:ILE:HG22	2.03	0.58
1:C:126:SER:HB3	1:C:177:GLU:OE2	2.02	0.58
1:A:97:ILE:HD12	1:A:99:THR:HG23	1.85	0.58
1:B:5:MET:HE3	1:B:86:SER:HA	1.84	0.58
1:D:335:ASP:OD1	1:E:325:ARG:NH2	2.30	0.58
1:F:13:PHE:HE1	1:F:184:LEU:HD11	1.66	0.58
1:C:422:GLU:N	1:C:433:VAL:O	2.36	0.58
1:C:260:GLY:HA2	2:C:601:GOL:H32	1.86	0.58
1:D:147:ARG:HD3	1:D:160:ASN:OD1	2.04	0.58
1:D:351:SER:HB2	1:D:353:ILE:HD13	1.86	0.57
1:F:59:LEU:O	1:F:63:THR:HG23	2.04	0.57
1:F:13:PHE:CE1	1:F:184:LEU:HD13	2.39	0.57
1:C:358:ARG:HG3	1:C:358:ARG:HH11	1.69	0.57
1:D:394:LYS:HE3	1:D:395:VAL:O	2.05	0.57
1:B:131:PHE:CD1	1:B:135:THR:CG2	2.88	0.57
1:B:363:VAL:HG11	1:B:371:ILE:HD12	1.85	0.57
1:D:201:GLN:HA	1:D:201:GLN:OE1	2.05	0.57
1:A:39:GLU:HB2	1:F:107:ILE:HD11	1.87	0.56
1:C:206:ARG:NH2	1:C:286:ARG:O	2.38	0.56
1:A:410:GLU:OE1	1:A:419:THR:HG21	2.05	0.56
1:C:356:ILE:CD1	1:C:372:LEU:HD22	2.35	0.56
1:B:63:THR:HG21	1:B:70:PHE:HB2	1.87	0.56
1:D:156:TRP:HE3	1:D:156:TRP:O	1.87	0.56
1:B:260:GLY:HA2	2:B:601:GOL:H32	1.88	0.56
1:C:191:GLU:CD	1:C:206:ARG:NH1	2.63	0.56
1:A:324:MET:HE2	1:A:345:GLY:CA	2.29	0.56
1:B:243:ARG:NH1	1:B:247:ARG:HE	2.03	0.56
1:C:141:LYS:O	1:C:144:THR:HB	2.05	0.56
1:D:6:LEU:CD1	1:D:28:VAL:HG13	2.36	0.56
1:A:136:MET:HE1	1:A:156:TRP:CD1	2.41	0.56
1:C:37:GLU:HA	1:C:40:ARG:HD2	1.87	0.56
1:E:351:SER:C	1:E:377:PHE:HZ	2.14	0.56
1:B:66:ILE:HG12	1:B:66:ILE:O	2.05	0.55
1:B:371:ILE:HG22	1:B:372:LEU:HD12	1.88	0.55
1:C:136:MET:HE1	1:C:153:PRO:HA	1.88	0.55
1:D:396:PRO:HB3	1:D:424:TYR:CE2	2.40	0.55
1:D:394:LYS:HE2	1:D:422:GLU:OE2	2.07	0.55
1:E:334:VAL:HG13	1:E:371:ILE:HD12	1.89	0.55
1:F:57:LYS:NZ	1:F:61:ASP:CG	2.63	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:HD13	1:C:127:PHE:CE1	2.42	0.55
1:A:76:ASP:OD1	1:A:78:LYS:HB3	2.07	0.54
1:B:145:VAL:O	1:B:147:ARG:HG3	2.07	0.54
1:C:252:ILE:HD11	1:C:359:PHE:CE2	2.42	0.54
1:B:280:LYS:CE	1:B:295:THR:CG2	2.85	0.54
1:C:18:TYR:CE2	1:C:118:LEU:HG	2.43	0.54
1:E:126:SER:HB3	1:E:177:GLU:OE1	2.08	0.54
1:F:58:LYS:O	1:F:62:ILE:HG12	2.08	0.54
1:F:236:LEU:CD2	1:F:383:VAL:HG21	2.37	0.54
1:B:353:ILE:O	1:B:357:HIS:HB3	2.07	0.54
1:C:4:LEU:HD23	1:C:98:VAL:HG21	1.90	0.54
1:F:139:HIS:CB	1:F:147:ARG:HH21	2.21	0.54
1:F:426:PHE:N	1:F:429:GLN:O	2.41	0.54
1:C:88:GLU:OE2	1:D:32:LYS:NZ	2.42	0.54
1:E:186:LYS:HE3	1:F:143:ASP:OD2	2.08	0.53
1:E:334:VAL:HG13	1:E:371:ILE:CD1	2.38	0.53
1:D:16:SER:CB	1:D:55:GLU:OE1	2.56	0.53
1:F:13:PHE:CE1	1:F:184:LEU:HD11	2.43	0.53
1:B:75:ASP:OD1	1:B:78:LYS:HB2	2.08	0.53
1:F:67:LEU:HD12	1:F:67:LEU:N	2.23	0.53
1:C:69:ASN:HB3	1:C:71:GLU:OE1	2.08	0.53
1:F:358:ARG:O	1:F:362:ARG:HG3	2.09	0.53
1:A:353:ILE:O	1:A:357:HIS:HB3	2.08	0.53
1:D:353:ILE:HD12	1:D:353:ILE:H	1.73	0.53
1:D:358:ARG:O	1:D:362:ARG:HG3	2.09	0.52
1:E:332:LEU:HD21	1:E:336:LEU:HD11	1.92	0.52
1:E:251:ILE:HG12	1:E:374:THR:CG2	2.38	0.52
1:C:266:GLN:HA	1:C:288:MET:CE	2.38	0.52
1:D:49:ALA:O	1:D:53:LEU:HB2	2.09	0.52
1:E:132:ASP:OD2	1:E:150:LYS:NZ	2.40	0.52
1:B:295:THR:HB	1:C:141:LYS:CE	2.40	0.52
1:C:158:PHE:CD1	1:C:158:PHE:C	2.88	0.52
1:A:7:ASP:OD1	1:A:9:SER:HB3	2.09	0.52
1:B:131:PHE:HD1	1:B:135:THR:CG2	2.22	0.52
1:E:146:PRO:HD2	1:E:162:SER:HB3	1.92	0.52
1:E:286:ARG:NH2	1:F:213:PRO:O	2.43	0.52
1:F:8:LYS:NZ	1:F:37:GLU:OE2	2.38	0.52
1:E:7:ASP:OD2	1:E:104:GLN:OE1	2.28	0.52
1:C:252:ILE:CD1	1:C:359:PHE:CE2	2.93	0.51
1:D:106:LYS:HE2	1:E:54:ASP:OD1	2.09	0.51
1:E:332:LEU:HD23	1:E:332:LEU:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASP:OD2	1:A:99:THR:HB	2.10	0.51
1:A:41:GLU:HB3	1:A:46:LEU:HD12	1.90	0.51
1:E:278:ILE:HD11	1:F:158:PHE:CZ	2.45	0.51
1:E:324:MET:HE1	1:E:333:TYR:HB2	1.91	0.51
1:D:16:SER:HB2	1:D:55:GLU:OE1	2.10	0.51
1:E:332:LEU:HD23	1:E:332:LEU:C	2.36	0.51
1:F:252:ILE:CG1	1:F:372:LEU:HD21	2.41	0.51
1:D:421:TYR:CA	1:D:434:PRO:HD3	2.38	0.51
1:E:20:GLU:HB2	1:E:62:ILE:HD13	1.91	0.51
1:C:273:MET:HG3	1:C:274:ARG:N	2.22	0.51
1:E:141:LYS:O	1:E:144:THR:HG22	2.10	0.51
1:E:243:ARG:NH1	1:E:374:THR:HB	2.25	0.51
1:C:262:THR:HB	2:C:601:GOL:H31	1.93	0.51
1:A:368:ILE:HB	1:A:369:PRO:HD3	1.93	0.50
1:A:391:MET:HE2	1:A:407:PRO:HB2	1.93	0.50
1:F:66:ILE:O	1:F:66:ILE:CG2	2.52	0.50
1:A:224:ARG:HG3	1:A:225:PRO:HD2	1.93	0.50
1:C:266:GLN:CA	1:C:288:MET:HE3	2.39	0.50
1:C:324:MET:HE1	1:C:333:TYR:HB2	1.92	0.50
1:A:423:ILE:HG12	1:A:431:MET:HG3	1.92	0.50
1:E:141:LYS:NZ	1:E:216:ASP:OD1	2.44	0.50
1:E:74:GLY:O	1:E:75:ASP:C	2.54	0.50
1:D:395:VAL:HA	1:D:405:ALA:HA	1.93	0.50
1:D:125:LEU:HD12	1:D:128:GLU:OE1	2.11	0.50
1:B:241:ILE:CG2	1:B:245:GLU:OE1	2.60	0.50
1:F:315:ARG:NH1	1:F:339:ALA:O	2.45	0.50
1:A:7:ASP:OD2	1:A:99:THR:CG2	2.60	0.49
1:B:252:ILE:HD11	1:B:356:ILE:HG22	1.92	0.49
1:F:352:PRO:O	1:F:356:ILE:HG13	2.12	0.49
1:A:369:PRO:CG	1:A:391:MET:HB2	2.38	0.49
1:A:240:LEU:CD1	1:A:386:VAL:HG21	2.43	0.49
1:E:363:VAL:HG23	1:E:368:ILE:CD1	2.42	0.49
1:A:262:THR:HB	2:A:601:GOL:H11	1.95	0.49
1:A:420:GLU:O	1:A:434:PRO:HD2	2.12	0.49
1:B:149:LYS:HG2	1:B:156:TRP:CD1	2.48	0.49
1:B:191:GLU:OE2	1:B:206:ARG:NH2	2.46	0.49
1:C:371:ILE:HG22	1:C:372:LEU:HD12	1.95	0.49
1:D:182:VAL:HA	1:D:188:SER:OG	2.13	0.49
1:D:425:VAL:CA	1:D:429:GLN:HA	2.43	0.48
1:B:420:GLU:O	1:B:434:PRO:HD2	2.14	0.48
1:D:105:LYS:HG3	1:D:115:TYR:CE2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:SER:HB3	1:B:177:GLU:OE1	2.13	0.48
1:D:152:LYS:CB	1:D:153:PRO:HD2	2.43	0.48
1:A:158:PHE:C	1:A:158:PHE:CD1	2.91	0.48
1:F:408:VAL:HG12	1:F:424:TYR:HB3	1.93	0.48
1:C:263:THR:N	2:C:601:GOL:H31	2.27	0.48
1:C:152:LYS:O	1:C:156:TRP:HD1	1.96	0.48
1:E:278:ILE:HD12	1:E:317:ASP:OD2	2.12	0.48
1:E:420:GLU:O	1:E:433:VAL:HG23	2.14	0.48
1:A:157:LYS:HE2	3:A:604:EDO:C1	2.44	0.48
1:E:191:GLU:OE1	1:E:301:TYR:OH	2.19	0.48
1:B:146:PRO:HG3	1:B:166:MET:CE	2.42	0.48
1:F:139:HIS:HB2	1:F:147:ARG:HH21	1.77	0.48
1:F:424:TYR:CE1	1:F:433:VAL:HG11	2.49	0.48
1:D:352:PRO:O	1:D:356:ILE:HG13	2.13	0.47
1:E:352:PRO:HB3	1:E:377:PHE:HE2	1.79	0.47
1:D:424:TYR:OH	1:D:432:ILE:HG21	2.14	0.47
1:E:390:GLU:O	1:E:409:VAL:CB	2.59	0.47
1:D:136:MET:HG3	1:D:151:GLY:O	2.14	0.47
1:D:378:ILE:HD13	1:D:383:VAL:HG12	1.96	0.47
1:B:152:LYS:O	1:B:156:TRP:N	2.47	0.47
1:C:4:LEU:HD11	1:C:25:THR:O	2.15	0.47
1:D:252:ILE:CG1	1:D:372:LEU:HD21	2.45	0.47
1:B:260:GLY:O	1:B:263:THR:HG22	2.15	0.47
1:B:364:ASP:OD2	1:C:354:ASP:HB3	2.14	0.47
1:E:411:ILE:N	1:E:411:ILE:HD12	2.30	0.47
1:E:416:THR:CG2	1:E:418:ASN:CB	2.93	0.47
1:A:12:LEU:HD22	1:A:48:SER:HB3	1.96	0.47
1:D:107:ILE:HD11	1:E:39:GLU:HB2	1.96	0.47
1:B:419:THR:O	1:B:419:THR:HG23	2.15	0.47
1:A:26:GLY:O	1:A:68:VAL:HG11	2.14	0.46
1:B:166:MET:HE2	1:B:166:MET:HB2	1.78	0.46
1:B:75:ASP:OD1	1:B:78:LYS:N	2.46	0.46
1:B:205:TYR:CE1	1:B:224:ARG:HG3	2.50	0.46
1:D:73:VAL:HG21	1:D:89:TYR:CE2	2.50	0.46
1:E:306:GLU:OE2	1:F:197:SER:CB	2.63	0.46
1:F:130:PHE:CD1	1:F:130:PHE:N	2.83	0.46
1:B:132:ASP:O	1:B:135:THR:HG22	2.16	0.46
1:A:50:GLU:CB	1:A:172:ARG:HH12	2.29	0.46
1:A:107:ILE:CG2	1:A:111:MET:HE3	2.45	0.46
1:B:58:LYS:O	1:B:62:ILE:HG12	2.14	0.46
1:E:63:THR:CG2	1:E:68:VAL:O	2.61	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:LYS:HG2	1:E:80:GLY:CA	2.46	0.46
1:E:105:LYS:HG3	1:E:115:TYR:CE2	2.51	0.46
1:E:156:TRP:CD1	1:E:156:TRP:C	2.94	0.46
1:E:5:MET:HE1	1:E:89:TYR:CD1	2.50	0.46
1:A:7:ASP:CG	1:A:99:THR:HG22	2.41	0.46
1:A:146:PRO:HD2	1:A:162:SER:HB3	1.98	0.46
1:E:242:LYS:O	1:E:246:GLU:HB2	2.15	0.45
1:E:330:PHE:CD2	1:E:358:ARG:HG2	2.51	0.45
1:B:280:LYS:HE3	1:B:295:THR:CG2	2.46	0.45
1:B:140:ILE:HG23	1:B:166:MET:CE	2.47	0.45
1:C:261:ALA:N	2:C:601:GOL:H11	2.31	0.45
1:C:352:PRO:HG3	1:C:377:PHE:CG	2.51	0.45
1:E:315:ARG:NH2	1:E:315:ARG:HG2	2.31	0.45
1:E:416:THR:HG22	1:E:418:ASN:CB	2.47	0.45
1:F:63:THR:HG21	1:F:70:PHE:HB2	1.97	0.45
1:F:369:PRO:HG2	1:F:391:MET:HB2	1.98	0.45
1:B:135:THR:O	1:B:135:THR:CG2	2.65	0.45
1:A:324:MET:HE1	1:A:333:TYR:CD2	2.51	0.45
1:C:151:GLY:HA3	1:C:156:TRP:HA	1.98	0.45
1:B:8:LYS:HE3	1:B:12:LEU:HD11	1.98	0.45
1:C:252:ILE:HD11	1:C:359:PHE:CZ	2.52	0.45
1:D:142:GLU:OE2	1:D:218:TRP:HD1	2.00	0.45
1:D:352:PRO:HD3	1:D:377:PHE:CE2	2.52	0.45
1:E:315:ARG:CG	1:E:315:ARG:HH21	2.30	0.45
1:E:421:TYR:CE2	1:E:433:VAL:HB	2.52	0.45
1:A:39:GLU:HB2	1:F:107:ILE:CD1	2.47	0.45
1:D:166:MET:HE2	1:D:170:ASP:HB3	1.99	0.45
1:E:178:ILE:HG23	1:E:202:LEU:HD22	1.97	0.45
1:E:332:LEU:CD2	1:E:336:LEU:HD11	2.47	0.45
1:C:103:THR:O	1:C:107:ILE:HD13	2.17	0.45
1:A:157:LYS:HE2	3:A:604:EDO:H12	1.99	0.45
1:B:146:PRO:C	1:B:147:ARG:HG3	2.42	0.45
1:B:66:ILE:HG23	1:B:68:VAL:HG13	1.99	0.44
1:D:284:SER:HA	1:D:285:PRO:HA	1.69	0.44
1:B:363:VAL:CG1	1:B:371:ILE:HD12	2.48	0.44
1:A:243:ARG:NH1	1:A:374:THR:HG22	2.32	0.44
1:C:132:ASP:O	1:C:224:ARG:NH2	2.49	0.44
1:C:358:ARG:HG3	1:C:358:ARG:NH1	2.33	0.44
1:D:393:VAL:HG23	1:D:406:ARG:C	2.42	0.44
1:E:62:ILE:O	1:E:66:ILE:HG12	2.17	0.44
1:F:236:LEU:HD23	1:F:383:VAL:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:PHE:CD1	1:B:135:THR:HG21	2.52	0.44
1:A:126:SER:CB	1:A:177:GLU:OE1	2.62	0.44
1:A:78:LYS:O	1:A:79:LYS:C	2.58	0.44
1:A:325:ARG:HD3	1:F:338:LEU:HD12	2.00	0.44
1:C:103:THR:O	1:C:107:ILE:CD1	2.66	0.44
1:A:62:ILE:O	1:A:66:ILE:HG12	2.18	0.43
1:C:125:LEU:HD13	1:C:127:PHE:HE1	1.83	0.43
1:E:249:GLU:HG3	1:E:337:ARG:NH2	2.33	0.43
1:A:144:THR:HG22	1:A:145:VAL:O	2.19	0.43
1:C:191:GLU:OE1	1:C:206:ARG:NH1	2.51	0.43
1:D:147:ARG:NH1	1:D:158:PHE:CD2	2.87	0.43
1:D:252:ILE:HG13	1:D:372:LEU:HD21	2.00	0.43
1:D:420:GLU:C	1:D:434:PRO:CD	2.92	0.43
1:F:400:LYS:O	1:F:403:ASP:N	2.50	0.43
1:B:131:PHE:CD1	1:B:135:THR:HG23	2.52	0.43
1:B:425:VAL:HG23	1:B:429:GLN:CA	2.48	0.43
1:C:280:LYS:HD3	1:C:295:THR:HB	2.01	0.43
1:F:182:VAL:O	1:F:185:ILE:O	2.37	0.43
1:A:393:VAL:HA	1:A:407:PRO:HA	2.00	0.43
1:C:126:SER:HB2	1:C:177:GLU:OE1	2.17	0.43
1:D:408:VAL:CG1	1:D:422:GLU:HG2	2.48	0.43
1:A:68:VAL:HG12	1:A:69:ASN:N	2.33	0.43
1:C:243:ARG:HH22	1:C:388:THR:CB	2.31	0.43
1:A:276:GLY:O	1:B:158:PHE:HB3	2.19	0.43
1:A:421:TYR:HA	1:A:433:VAL:HA	1.99	0.43
1:D:147:ARG:CZ	1:D:158:PHE:CD2	3.02	0.43
1:E:243:ARG:HH12	1:E:373:ASP:C	2.25	0.43
1:C:6:LEU:HD23	1:C:15:VAL:HG21	2.00	0.43
1:E:306:GLU:OE2	1:F:197:SER:HB2	2.19	0.43
1:B:356:ILE:HG21	1:B:375:ILE:HD11	2.00	0.43
1:E:332:LEU:CD2	1:E:336:LEU:CD1	2.97	0.43
1:E:339:ALA:HB2	1:F:257:PRO:HB2	1.99	0.43
1:F:204:ASN:O	1:F:225:PRO:HD3	2.18	0.43
1:C:4:LEU:HD23	1:C:98:VAL:CG2	2.48	0.43
1:D:110:ALA:HB1	1:E:72:ILE:HD11	2.00	0.43
1:E:132:ASP:HB2	1:E:135:THR:OG1	2.18	0.43
1:E:364:ASP:O	1:E:367:THR:HB	2.19	0.43
1:D:5:MET:HE2	1:D:30:ILE:HA	2.00	0.42
1:E:421:TYR:HA	1:E:434:PRO:HD2	2.00	0.42
1:A:262:THR:HB	2:A:601:GOL:H31	2.00	0.42
1:C:47:VAL:O	1:C:51:ILE:HD12	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:ILE:HB	1:E:369:PRO:HD3	2.00	0.42
1:E:132:ASP:CG	1:E:150:LYS:NZ	2.77	0.42
1:F:242:LYS:HG2	1:F:246:GLU:OE1	2.19	0.42
1:A:226:VAL:O	1:A:289:HIS:ND1	2.52	0.42
1:D:3:ASP:HB3	1:D:29:LEU:HD11	2.02	0.42
1:E:60:LYS:O	1:E:63:THR:HB	2.19	0.42
1:E:88:GLU:O	1:E:92:GLU:HG3	2.20	0.42
1:F:424:TYR:CZ	1:F:433:VAL:HG11	2.55	0.42
1:B:315:ARG:NH1	1:B:339:ALA:O	2.52	0.42
1:F:252:ILE:HG12	1:F:372:LEU:HD21	2.02	0.42
1:A:59:LEU:O	1:A:63:THR:HG23	2.20	0.42
1:C:284:SER:HA	1:C:285:PRO:HA	1.71	0.42
1:E:378:ILE:HD13	1:E:383:VAL:HG12	2.01	0.42
1:D:147:ARG:NH1	1:D:158:PHE:HB3	2.35	0.42
1:F:70:PHE:CD1	1:F:70:PHE:C	2.98	0.42
1:B:178:ILE:HG23	1:B:202:LEU:HD22	2.01	0.41
1:A:97:ILE:CD1	1:A:99:THR:HG23	2.50	0.41
1:A:107:ILE:HG22	1:A:111:MET:HE3	2.02	0.41
1:D:105:LYS:HE3	1:D:115:TYR:OH	2.20	0.41
1:B:305:GLY:C	3:B:605:EDO:H21	2.45	0.41
1:C:73:VAL:HG21	1:C:89:TYR:CZ	2.55	0.41
1:D:247:ARG:HB3	2:D:605:GOL:O2	2.20	0.41
1:E:125:LEU:HB2	1:E:128:GLU:HG3	2.00	0.41
1:F:392:THR:HG21	1:F:410:GLU:OE1	2.20	0.41
1:A:144:THR:HG21	1:A:147:ARG:NH2	2.35	0.41
1:C:422:GLU:O	1:C:433:VAL:N	2.40	0.41
1:D:5:MET:HE3	1:D:29:LEU:C	2.46	0.41
1:D:180:ASN:O	1:D:183:ARG:HG3	2.20	0.41
1:D:46:LEU:HD23	1:D:46:LEU:HA	1.90	0.41
1:D:138:LEU:HD12	1:D:138:LEU:HA	1.84	0.41
1:B:142:GLU:OE2	1:B:218:TRP:HD1	2.03	0.41
1:D:201:GLN:OE1	1:D:205:TYR:O	2.39	0.41
1:E:315:ARG:NH2	1:E:315:ARG:CG	2.84	0.41
1:F:166:MET:HE1	3:F:605:EDO:H12	2.01	0.41
1:A:416:THR:CG2	1:A:418:ASN:CB	2.99	0.41
1:C:358:ARG:CD	1:C:358:ARG:H	2.34	0.41
1:F:236:LEU:HD22	1:F:240:LEU:HD23	2.02	0.41
1:A:145:VAL:HG12	1:A:146:PRO:O	2.20	0.41
1:C:88:GLU:OE1	1:C:88:GLU:HA	2.20	0.41
1:D:5:MET:HE3	1:D:29:LEU:HB2	2.03	0.41
1:F:91:LEU:HD23	1:F:91:LEU:HA	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HD23	1:B:53:LEU:HA	1.87	0.40
1:D:107:ILE:CD1	1:E:39:GLU:HB2	2.51	0.40
1:E:237:ASP:OD1	1:E:237:ASP:N	2.52	0.40
1:F:255:GLY:O	1:F:348:HIS:HA	2.20	0.40
1:A:284:SER:O	3:A:605:EDO:H12	2.21	0.40
1:E:79:LYS:C	1:E:80:GLY:O	2.63	0.40
1:E:356:ILE:HD11	1:E:375:ILE:CD1	2.51	0.40
1:F:119:GLN:O	1:F:120:PRO:C	2.64	0.40
1:F:200:ILE:HG13	1:F:207:VAL:HB	2.03	0.40
1:A:284:SER:HA	1:A:285:PRO:HA	1.73	0.40
1:A:395:VAL:O	1:A:396:PRO:C	2.64	0.40
1:C:273:MET:CG	1:C:274:ARG:N	2.82	0.40
1:F:13:PHE:CZ	1:F:184:LEU:HD13	2.56	0.40
1:A:45:GLY:O	1:A:211:ARG:NH2	2.42	0.40
1:F:97:ILE:HD12	1:F:108:CYS:SG	2.61	0.40
1:B:132:ASP:OD1	1:B:135:THR:HB	2.21	0.40
1:B:393:VAL:HA	1:B:407:PRO:HA	2.03	0.40
1:C:413:ASP:HB3	1:C:416:THR:HB	2.03	0.40
1:D:327:ASP:OD1	1:D:358:ARG:NH2	2.54	0.40
1:F:363:VAL:HG11	1:F:371:ILE:HD13	2.04	0.40

All (1) 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:D:22:GLY:O	1:F:121:LEU:O[2_356]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	435/505 (86%)	426 (98%)	9 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	433/505 (86%)	423 (98%)	9 (2%)	1 (0%)	43	68
1	C	434/505 (86%)	428 (99%)	6 (1%)	0	100	100
1	D	434/505 (86%)	423 (98%)	11 (2%)	0	100	100
1	E	434/505 (86%)	426 (98%)	7 (2%)	1 (0%)	43	68
1	F	434/505 (86%)	425 (98%)	9 (2%)	0	100	100
All	All	2604/3030 (86%)	2551 (98%)	51 (2%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	75	ASP
1	B	407	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/447 (78%)	325 (93%)	23 (7%)	15	36
1	B	351/447 (78%)	328 (93%)	23 (7%)	15	36
1	C	328/447 (73%)	306 (93%)	22 (7%)	15	36
1	D	340/447 (76%)	322 (95%)	18 (5%)	20	46
1	E	350/447 (78%)	334 (95%)	16 (5%)	24	51
1	F	352/447 (79%)	329 (94%)	23 (6%)	15	37
All	All	2069/2682 (77%)	1944 (94%)	125 (6%)	17	41

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	51	ILE
1	A	57	LYS
1	A	78	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	88	GLU
1	A	128	GLU
1	A	157	LYS
1	A	158	PHE
1	A	206	ARG
1	A	236	LEU
1	A	237	ASP
1	A	245	GLU
1	A	273	MET
1	A	284	SER
1	A	300	ASN
1	A	304	ILE
1	A	324	MET
1	A	357	HIS
1	A	362	ARG
1	A	373	ASP
1	A	388	THR
1	A	390	GLU
1	A	425	VAL
1	B	1	MET
1	B	46	LEU
1	B	50	GLU
1	B	71	GLU
1	B	78	LYS
1	B	81	GLU
1	B	88	GLU
1	B	111	MET
1	B	134	GLU
1	B	159	VAL
1	B	166	MET
1	B	195	ARG
1	B	224	ARG
1	B	245	GLU
1	B	273	MET
1	B	280	LYS
1	B	283	GLU
1	B	300	ASN
1	B	304	ILE
1	B	351	SER
1	B	356	ILE
1	B	358	ARG
1	B	391	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	40	ARG
1	C	88	GLU
1	C	105	LYS
1	C	111	MET
1	C	123	GLN
1	C	128	GLU
1	C	147	ARG
1	C	166	MET
1	C	186	LYS
1	C	195	ARG
1	C	208	VAL
1	C	231	LEU
1	C	236	LEU
1	C	243	ARG
1	C	270	GLU
1	C	273	MET
1	C	283	GLU
1	C	300	ASN
1	C	315	ARG
1	C	358	ARG
1	C	362	ARG
1	C	423	ILE
1	D	1	MET
1	D	5	MET
1	D	24	ILE
1	D	53	LEU
1	D	91	LEU
1	D	97	ILE
1	D	106	LYS
1	D	128	GLU
1	D	156	TRP
1	D	158	PHE
1	D	163	ASP
1	D	194	ARG
1	D	273	MET
1	D	303	GLU
1	D	365	ILE
1	D	400	LYS
1	D	404	LEU
1	D	433	VAL
1	E	63	THR
1	E	88	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	111	MET
1	E	144	THR
1	E	159	VAL
1	E	237	ASP
1	E	241	ILE
1	E	243	ARG
1	E	315	ARG
1	E	323	GLU
1	E	361	ASN
1	E	409	VAL
1	E	411	ILE
1	E	419	THR
1	E	425	VAL
1	E	429	GLN
1	F	17	LYS
1	F	46	LEU
1	F	88	GLU
1	F	126	SER
1	F	143	ASP
1	F	147	ARG
1	F	173	MET
1	F	192	ILE
1	F	200	ILE
1	F	270	GLU
1	F	273	MET
1	F	303	GLU
1	F	324	MET
1	F	325	ARG
1	F	353	ILE
1	F	354	ASP
1	F	357	HIS
1	F	371	ILE
1	F	388	THR
1	F	403	ASP
1	F	404	LEU
1	F	433	VAL
1	F	435	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	116	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	379	ASN
1	C	27	ASN
1	C	116	ASN
1	C	123	GLN
1	C	201	GLN
1	C	289	HIS
1	D	180	ASN
1	E	104	GLN
1	E	116	ASN
1	E	361	ASN
1	E	370	ASN
1	F	69	ASN
1	F	348	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](#)

32 ligands are modelled in this entry.

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	$\# Z > 2$
2	GOL	D	603	-	5,5,5	0.62	0	5,5,5	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	F	605	-	3,3,3	0.78	0	2,2,2	0.13	0
2	GOL	E	603	-	5,5,5	0.74	0	5,5,5	0.33	0
2	GOL	A	603	-	5,5,5	0.82	0	5,5,5	0.64	0
2	GOL	E	601	-	5,5,5	0.57	0	5,5,5	0.39	0
3	EDO	F	606	-	3,3,3	0.65	0	2,2,2	0.19	0
2	GOL	F	602	-	5,5,5	0.88	0	5,5,5	0.81	0
2	GOL	D	601	-	5,5,5	0.28	0	5,5,5	0.41	0
3	EDO	D	608	-	3,3,3	0.74	0	2,2,2	0.31	0
2	GOL	E	604	-	5,5,5	0.88	0	5,5,5	0.97	0
3	EDO	B	605	-	3,3,3	0.58	0	2,2,2	0.72	0
3	EDO	A	605	-	3,3,3	0.69	0	2,2,2	0.10	0
2	GOL	E	602	-	5,5,5	0.44	0	5,5,5	0.58	0
3	EDO	B	603	-	3,3,3	0.58	0	2,2,2	0.32	0
2	GOL	D	605	-	5,5,5	0.45	0	5,5,5	0.32	0
2	GOL	A	602	-	5,5,5	0.73	0	5,5,5	0.63	0
2	GOL	E	605	-	5,5,5	0.80	0	5,5,5	0.78	0
3	EDO	D	607	-	3,3,3	0.50	0	2,2,2	0.31	0
2	GOL	F	603	-	5,5,5	0.77	0	5,5,5	0.52	0
2	GOL	D	606	-	5,5,5	0.73	0	5,5,5	0.27	0
3	EDO	C	602	-	3,3,3	0.58	0	2,2,2	0.34	0
2	GOL	D	602	-	5,5,5	0.86	0	5,5,5	0.92	0
3	EDO	B	604	-	3,3,3	0.63	0	2,2,2	0.16	0
3	EDO	A	604	-	3,3,3	0.62	0	2,2,2	0.30	0
2	GOL	F	604	-	5,5,5	0.83	0	5,5,5	0.58	0
2	GOL	F	601	-	5,5,5	0.53	0	5,5,5	1.05	1 (20%)
2	GOL	B	602	-	5,5,5	0.81	0	5,5,5	0.74	0
2	GOL	B	601	-	5,5,5	0.19	0	5,5,5	1.12	1 (20%)
2	GOL	C	601	-	5,5,5	0.50	0	5,5,5	0.86	0
2	GOL	A	601	-	5,5,5	0.39	0	5,5,5	0.90	0
3	EDO	B	606	-	3,3,3	0.51	0	2,2,2	0.16	0
2	GOL	D	604	-	5,5,5	0.76	0	5,5,5	0.76	0

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
2	GOL	D	603	-	-	0/4/4/4	-
3	EDO	F	605	-	-	0/1/1/1	-
2	GOL	E	603	-	-	4/4/4/4	-
2	GOL	A	603	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	E	601	-	-	2/4/4/4	-
3	EDO	F	606	-	-	1/1/1/1	-
2	GOL	F	602	-	-	4/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-
3	EDO	D	608	-	-	1/1/1/1	-
2	GOL	E	604	-	-	1/4/4/4	-
3	EDO	B	605	-	-	1/1/1/1	-
3	EDO	A	605	-	-	1/1/1/1	-
2	GOL	E	602	-	-	2/4/4/4	-
3	EDO	B	603	-	-	0/1/1/1	-
2	GOL	D	605	-	-	0/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	E	605	-	-	2/4/4/4	-
3	EDO	D	607	-	-	1/1/1/1	-
2	GOL	F	603	-	-	4/4/4/4	-
2	GOL	D	606	-	-	2/4/4/4	-
3	EDO	C	602	-	-	0/1/1/1	-
2	GOL	D	602	-	-	2/4/4/4	-
3	EDO	B	604	-	-	1/1/1/1	-
3	EDO	A	604	-	-	1/1/1/1	-
2	GOL	F	604	-	-	1/4/4/4	-
2	GOL	F	601	-	-	2/4/4/4	-
2	GOL	B	602	-	-	2/4/4/4	-
2	GOL	B	601	-	-	4/4/4/4	-
2	GOL	C	601	-	-	2/4/4/4	-
2	GOL	A	601	-	-	4/4/4/4	-
3	EDO	B	606	-	-	1/1/1/1	-
2	GOL	D	604	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	GOL	O2-C2-C1	2.15	118.08	109.18
2	B	601	GOL	O3-C3-C2	2.10	119.85	110.38

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	C1-C2-C3-O3
2	A	602	GOL	O1-C1-C2-C3
2	A	603	GOL	C1-C2-C3-O3
2	B	601	GOL	O1-C1-C2-C3
2	B	601	GOL	C1-C2-C3-O3
2	B	602	GOL	O1-C1-C2-C3
2	C	601	GOL	C1-C2-C3-O3
2	D	601	GOL	O1-C1-C2-C3
2	D	602	GOL	C1-C2-C3-O3
2	D	604	GOL	O1-C1-C2-O2
2	D	604	GOL	O1-C1-C2-C3
2	D	606	GOL	C1-C2-C3-O3
2	E	601	GOL	C1-C2-C3-O3
2	E	602	GOL	O1-C1-C2-C3
2	E	603	GOL	O1-C1-C2-C3
2	E	605	GOL	O1-C1-C2-C3
2	F	601	GOL	O1-C1-C2-C3
2	F	602	GOL	O1-C1-C2-C3
2	F	602	GOL	C1-C2-C3-O3
2	F	603	GOL	O1-C1-C2-C3
2	F	603	GOL	C1-C2-C3-O3
2	F	603	GOL	O2-C2-C3-O3
2	B	601	GOL	O2-C2-C3-O3
2	B	602	GOL	O1-C1-C2-O2
2	F	602	GOL	O1-C1-C2-O2
2	A	601	GOL	O1-C1-C2-C3
2	E	603	GOL	C1-C2-C3-O3
2	F	604	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2
2	A	601	GOL	O2-C2-C3-O3
2	A	602	GOL	O1-C1-C2-O2
2	D	601	GOL	O1-C1-C2-O2
2	D	602	GOL	O2-C2-C3-O3
2	D	606	GOL	O2-C2-C3-O3
2	E	601	GOL	O2-C2-C3-O3
2	E	603	GOL	O1-C1-C2-O2
2	E	603	GOL	O2-C2-C3-O3
2	E	605	GOL	O1-C1-C2-O2
2	F	601	GOL	O1-C1-C2-O2
2	F	602	GOL	O2-C2-C3-O3
3	A	604	EDO	O1-C1-C2-O2
3	B	604	EDO	O1-C1-C2-O2
3	B	605	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	602	GOL	O1-C1-C2-O2
2	F	603	GOL	O1-C1-C2-O2
2	A	603	GOL	O2-C2-C3-O3
3	B	606	EDO	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-O2
2	C	601	GOL	O2-C2-C3-O3
2	E	604	GOL	O2-C2-C3-O3
3	F	606	EDO	O1-C1-C2-O2
2	A	603	GOL	O1-C1-C2-O2
3	A	605	EDO	O1-C1-C2-O2
3	D	607	EDO	O1-C1-C2-O2
3	D	608	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	605	EDO	1	0
3	B	605	EDO	1	0
3	A	605	EDO	1	0
2	D	605	GOL	1	0
3	A	604	EDO	2	0
2	B	601	GOL	2	0
2	C	601	GOL	6	0
2	A	601	GOL	2	0
2	D	604	GOL	2	0

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	437/505 (86%)	0.01	6 (1%) 73 72	44, 72, 130, 185	0
1	B	435/505 (86%)	0.11	3 (0%) 84 83	47, 81, 147, 192	0
1	C	436/505 (86%)	0.25	9 (2%) 63 61	58, 95, 147, 179	0
1	D	436/505 (86%)	0.09	9 (2%) 63 61	40, 86, 136, 163	0
1	E	436/505 (86%)	-0.05	4 (0%) 81 80	42, 71, 143, 213	0
1	F	436/505 (86%)	-0.01	6 (1%) 73 72	42, 74, 127, 162	0
All	All	2616/3030 (86%)	0.06	37 (1%) 73 72	40, 80, 139, 213	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	374	THR	4.3
1	F	126	SER	3.7
1	B	155	ASN	3.4
1	E	403	ASP	3.3
1	A	184	LEU	3.2
1	C	75	ASP	3.2
1	D	126	SER	3.1
1	C	26	GLY	2.8
1	B	403	ASP	2.7
1	F	352	PRO	2.7
1	F	353	ILE	2.7
1	C	4	LEU	2.6
1	A	226	VAL	2.6
1	F	156	TRP	2.5
1	E	407	PRO	2.5
1	C	350	THR	2.4
1	D	30	ILE	2.4
1	A	404	LEU	2.3
1	D	314	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	51	ILE	2.3
1	C	359	PHE	2.3
1	C	362	ARG	2.2
1	B	405	ALA	2.2
1	A	407	PRO	2.2
1	F	125	LEU	2.2
1	C	436	ASN	2.1
1	C	387	TYR	2.1
1	D	187	GLY	2.1
1	A	431	MET	2.1
1	D	127	PHE	2.1
1	E	402	ALA	2.1
1	C	407	PRO	2.1
1	D	121	LEU	2.1
1	F	184	LEU	2.1
1	D	130	PHE	2.1
1	A	80	GLY	2.0
1	D	24	ILE	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(Å ²)	Q<0.9
2	GOL	D	602	6/6	0.51	0.11	107,109,114,119	0
2	GOL	B	601	6/6	0.64	0.17	86,88,91,109	0
3	EDO	C	602	4/4	0.65	0.19	89,96,100,103	0
3	EDO	A	604	4/4	0.68	0.12	83,85,85,89	0
2	GOL	C	601	6/6	0.69	0.19	73,77,86,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	B	606	4/4	0.73	0.10	90,97,100,105	0
2	GOL	E	604	6/6	0.74	0.20	96,105,111,114	0
2	GOL	A	603	6/6	0.77	0.13	86,94,102,102	0
2	GOL	F	604	6/6	0.78	0.19	86,104,111,111	0
2	GOL	B	602	6/6	0.78	0.16	85,91,95,98	0
2	GOL	D	601	6/6	0.79	0.17	83,87,90,91	0
2	GOL	F	601	6/6	0.79	0.14	71,80,84,88	0
2	GOL	F	602	6/6	0.80	0.14	74,88,93,95	0
2	GOL	A	601	6/6	0.81	0.17	63,74,82,95	0
2	GOL	F	603	6/6	0.81	0.09	95,101,103,107	0
3	EDO	D	607	4/4	0.81	0.17	92,92,93,94	0
3	EDO	B	604	4/4	0.82	0.09	88,90,91,93	0
2	GOL	E	603	6/6	0.82	0.13	93,95,104,105	0
2	GOL	D	605	6/6	0.83	0.14	97,103,111,111	0
2	GOL	A	602	6/6	0.84	0.10	94,103,108,109	0
2	GOL	D	603	6/6	0.84	0.11	96,101,105,108	0
3	EDO	F	606	4/4	0.84	0.17	78,84,89,90	0
2	GOL	D	604	6/6	0.85	0.12	70,86,94,95	0
2	GOL	D	606	6/6	0.86	0.11	88,101,104,106	0
2	GOL	E	605	6/6	0.86	0.17	78,90,92,97	0
3	EDO	D	608	4/4	0.87	0.12	73,82,84,85	0
2	GOL	E	602	6/6	0.88	0.12	96,102,105,106	0
3	EDO	B	605	4/4	0.89	0.15	67,75,76,76	0
3	EDO	F	605	4/4	0.89	0.16	72,79,81,84	0
2	GOL	E	601	6/6	0.89	0.13	64,79,86,88	0
3	EDO	A	605	4/4	0.90	0.15	68,75,77,81	0
3	EDO	B	603	4/4	0.90	0.15	70,72,75,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.