



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:41 PM UTC

PDB ID : 3DZF / pdb_00003dzf
Title : Crystal structure of human CD38 extracellular domain complexed with a covalent intermediate, ara-F-ribose-5'-phosphate
Authors : Liu, Q.; Kriksunov, I.A.; Jiang, H.; Graeff, R.; Lin, H.; Lee, H.C.; Hao, Q.
Deposited on : 2008-07-29
Resolution : 2.01 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

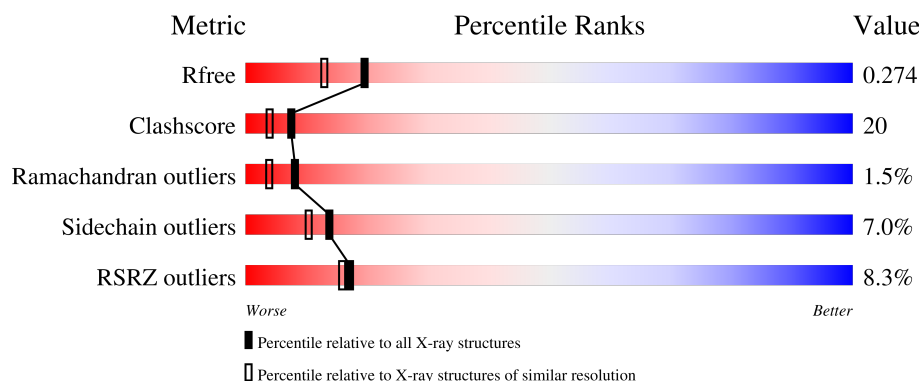
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	262	10% 60% 31% 6% .
1	B	262	5% 62% 30% 5% .
1	C	262	6% 58% 29% 8% .
1	D	262	11% 60% 31% 6% .
1	E	262	6% 61% 31% 5% .

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Mol	Chain	Length	Quality of chain
1	F	262	9% 56% 34% 5% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12987 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 ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	B	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	C	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	D	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	E	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	F	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	expression tag	UNP P28907
A	40	ARG	-	expression tag	UNP P28907
A	41	GLU	-	expression tag	UNP P28907
A	42	ALA	-	expression tag	UNP P28907
A	43	GLU	-	expression tag	UNP P28907
A	44	ALA	-	expression tag	UNP P28907
A	49	THR	GLN	engineered mutation	UNP P28907
A	100	ASP	ASN	engineered mutation	UNP P28907
A	164	ASP	ASN	engineered mutation	UNP P28907
A	209	ASP	ASN	engineered mutation	UNP P28907
A	219	ASP	ASN	engineered mutation	UNP P28907
B	39	LYS	-	expression tag	UNP P28907
B	40	ARG	-	expression tag	UNP P28907
B	41	GLU	-	expression tag	UNP P28907
B	42	ALA	-	expression tag	UNP P28907
B	43	GLU	-	expression tag	UNP P28907
B	44	ALA	-	expression tag	UNP P28907

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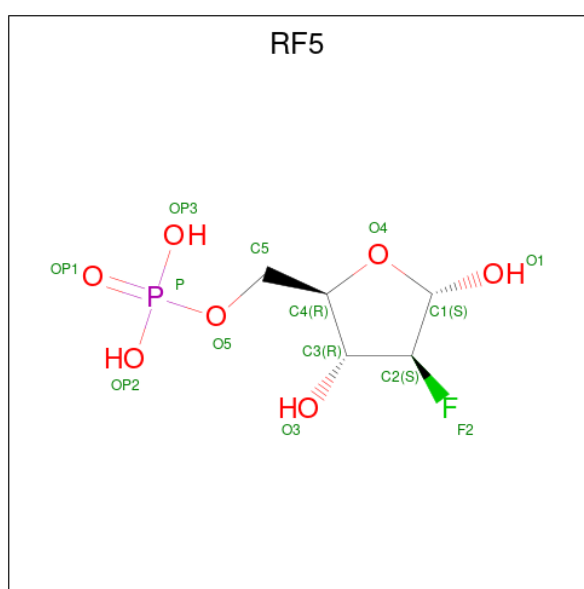
Chain	Residue	Modelled	Actual	Comment	Reference
B	49	THR	GLN	engineered mutation	UNP P28907
B	100	ASP	ASN	engineered mutation	UNP P28907
B	164	ASP	ASN	engineered mutation	UNP P28907
B	209	ASP	ASN	engineered mutation	UNP P28907
B	219	ASP	ASN	engineered mutation	UNP P28907
C	39	LYS	-	expression tag	UNP P28907
C	40	ARG	-	expression tag	UNP P28907
C	41	GLU	-	expression tag	UNP P28907
C	42	ALA	-	expression tag	UNP P28907
C	43	GLU	-	expression tag	UNP P28907
C	44	ALA	-	expression tag	UNP P28907
C	49	THR	GLN	engineered mutation	UNP P28907
C	100	ASP	ASN	engineered mutation	UNP P28907
C	164	ASP	ASN	engineered mutation	UNP P28907
C	209	ASP	ASN	engineered mutation	UNP P28907
C	219	ASP	ASN	engineered mutation	UNP P28907
D	39	LYS	-	expression tag	UNP P28907
D	40	ARG	-	expression tag	UNP P28907
D	41	GLU	-	expression tag	UNP P28907
D	42	ALA	-	expression tag	UNP P28907
D	43	GLU	-	expression tag	UNP P28907
D	44	ALA	-	expression tag	UNP P28907
D	49	THR	GLN	engineered mutation	UNP P28907
D	100	ASP	ASN	engineered mutation	UNP P28907
D	164	ASP	ASN	engineered mutation	UNP P28907
D	209	ASP	ASN	engineered mutation	UNP P28907
D	219	ASP	ASN	engineered mutation	UNP P28907
E	39	LYS	-	expression tag	UNP P28907
E	40	ARG	-	expression tag	UNP P28907
E	41	GLU	-	expression tag	UNP P28907
E	42	ALA	-	expression tag	UNP P28907
E	43	GLU	-	expression tag	UNP P28907
E	44	ALA	-	expression tag	UNP P28907
E	49	THR	GLN	engineered mutation	UNP P28907
E	100	ASP	ASN	engineered mutation	UNP P28907
E	164	ASP	ASN	engineered mutation	UNP P28907
E	209	ASP	ASN	engineered mutation	UNP P28907
E	219	ASP	ASN	engineered mutation	UNP P28907
F	39	LYS	-	expression tag	UNP P28907
F	40	ARG	-	expression tag	UNP P28907
F	41	GLU	-	expression tag	UNP P28907
F	42	ALA	-	expression tag	UNP P28907

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Chain	Residue	Modelled	Actual	Comment	Reference
F	43	GLU	-	expression tag	UNP P28907
F	44	ALA	-	expression tag	UNP P28907
F	49	THR	GLN	engineered mutation	UNP P28907
F	100	ASP	ASN	engineered mutation	UNP P28907
F	164	ASP	ASN	engineered mutation	UNP P28907
F	209	ASP	ASN	engineered mutation	UNP P28907
F	219	ASP	ASN	engineered mutation	UNP P28907

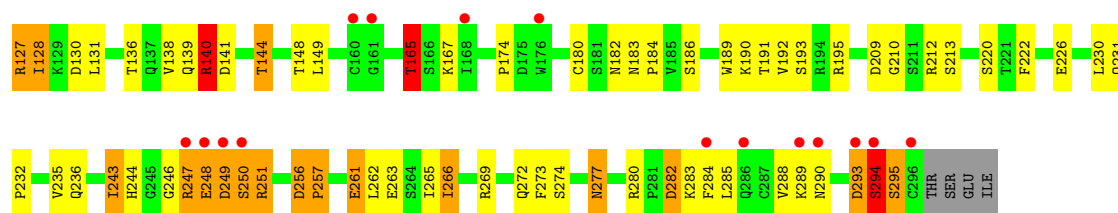
- Molecule 2 is 2-deoxy-2-fluoro-5-O-phosphono-alpha-D-arabinofuranose (CCD ID: RF5) (formula: $C_5H_{10}FO_7P$).



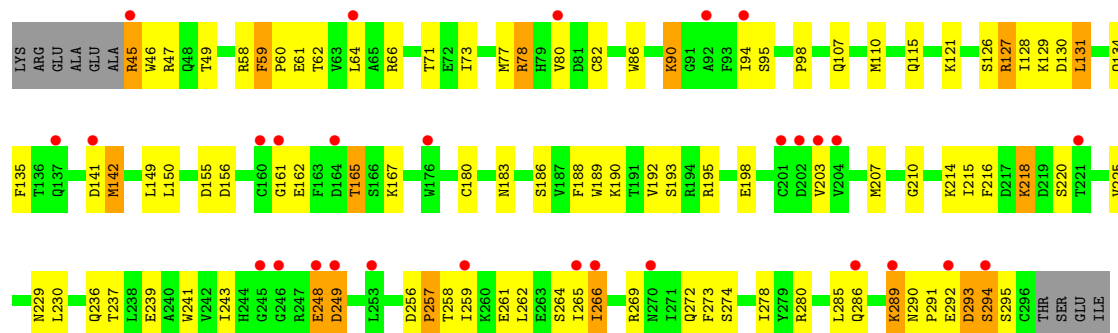
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	O	P	0	0
			13	5	1	6	1		
2	B	1	Total	C	F	O	P	0	0
			13	5	1	6	1		
2	C	1	Total	C	F	O	P	0	0
			13	5	1	6	1		
2	D	1	Total	C	F	O	P	0	0
			13	5	1	6	1		
2	E	1	Total	C	F	O	P	0	0
			13	5	1	6	1		
2	F	1	Total	C	F	O	P	0	0
			13	5	1	6	1		

- Molecule 3 is water.

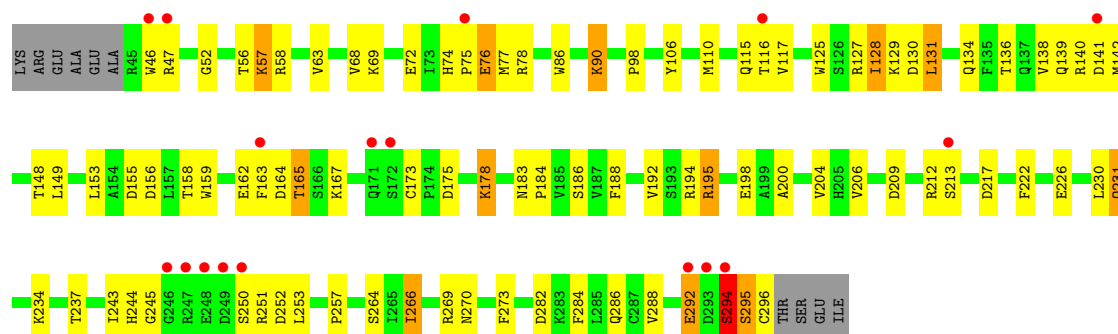
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total 98	O 98	0	0
3	B	112	Total 112	O 112	0	0
3	C	93	Total 93	O 93	0	0
3	D	81	Total 81	O 81	0	0
3	E	115	Total 115	O 115	0	0
3	F	110	Total 110	O 110	0	0



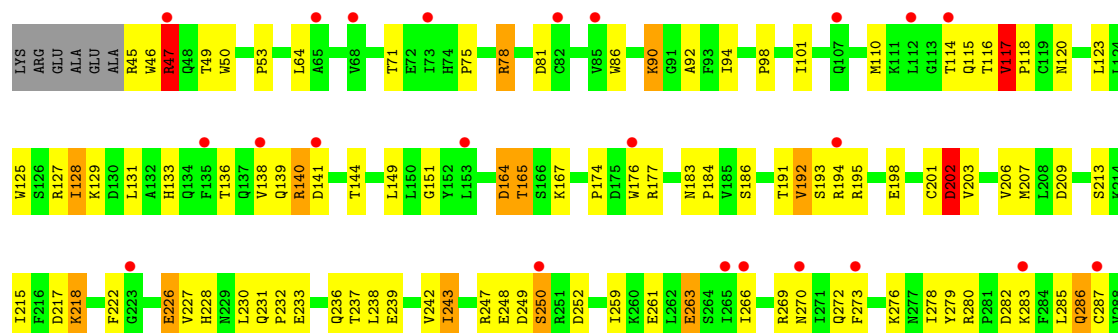
• Molecule 1: ADP-ribosyl cyclase 1



• Molecule 1: ADP-ribosyl cyclase 1



• Molecule 1: ADP-ribosyl cyclase 1



K289	K290	P291	E292	D293	S294	S295	C296	THR	SER	GLU	ILE

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.75Å 96.16Å 103.61Å 79.48° 82.72° 86.78°	Depositor
Resolution (Å)	20.00 – 2.01 20.00 – 2.01	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-2.01) 86.2 (20.00-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.201 , 0.272 0.204 , 0.274	Depositor DCC
R_{free} test set	4495 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 61.1	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	0.94	EDS
Total number of atoms	12987	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0517e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: RF5

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	1.39	9/2101 (0.4%)	1.32	15/2846 (0.5%)
1	B	1.36	14/2101 (0.7%)	1.27	7/2846 (0.2%)
1	C	1.17	2/2101 (0.1%)	1.28	17/2846 (0.6%)
1	D	1.11	1/2101 (0.0%)	1.16	3/2846 (0.1%)
1	E	1.31	4/2101 (0.2%)	1.26	9/2846 (0.3%)
1	F	1.21	5/2101 (0.2%)	1.23	12/2846 (0.4%)
All	All	1.26	35/12606 (0.3%)	1.25	63/17076 (0.4%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	ARG	N-CA	9.89	1.58	1.46
1	B	153	LEU	N-CA	8.92	1.57	1.46
1	A	153	LEU	N-CA	7.74	1.55	1.46
1	A	206	VAL	CA-CB	7.36	1.64	1.54
1	B	128	ILE	CA-CB	7.33	1.64	1.54
1	F	206	VAL	C-O	6.49	1.30	1.24
1	A	235	VAL	CA-CB	-6.45	1.46	1.54
1	E	206	VAL	CA-CB	6.26	1.62	1.54
1	A	197	ALA	CA-CB	6.14	1.62	1.53
1	B	280	ARG	C-O	-5.96	1.18	1.24
1	E	63	VAL	CA-CB	-5.84	1.47	1.54
1	C	94	ILE	C-O	-5.83	1.17	1.24
1	B	122	ILE	CA-CB	5.76	1.61	1.54
1	F	192	VAL	CA-CB	-5.66	1.47	1.54
1	B	63	VAL	CA-CB	-5.66	1.47	1.54
1	A	154	ALA	CA-CB	-5.63	1.44	1.53
1	B	206	VAL	CA-CB	5.58	1.61	1.54
1	A	128	ILE	C-O	5.57	1.30	1.24
1	A	173	CYS	N-CA	5.54	1.50	1.45
1	B	128	ILE	C-O	5.54	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	153	LEU	N-CA	5.45	1.52	1.46
1	F	53	PRO	N-CA	-5.44	1.40	1.47
1	B	231	GLN	CA-C	-5.43	1.46	1.52
1	B	240	ALA	CA-C	-5.43	1.45	1.52
1	B	126	SER	C-O	-5.34	1.18	1.23
1	F	242	VAL	CA-CB	5.34	1.59	1.53
1	A	280	ARG	C-O	-5.30	1.20	1.24
1	F	92	ALA	CA-CB	5.23	1.61	1.53
1	B	202	ASP	CA-C	-5.21	1.48	1.53
1	E	237	THR	CA-C	-5.17	1.46	1.52
1	B	235	VAL	CA-CB	-5.16	1.47	1.54
1	C	94	ILE	CA-CB	5.11	1.59	1.54
1	B	128	ILE	CA-C	5.09	1.59	1.52
1	B	202	ASP	C-O	-5.08	1.19	1.24
1	D	59	PHE	C-O	-5.04	1.19	1.24

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ARG	N-CA-C	9.54	123.95	108.41
1	F	202	ASP	CB-CA-C	-8.37	105.85	117.23
1	E	138	VAL	N-CA-C	8.27	118.30	110.53
1	C	290	ASN	CA-C-N	7.99	128.01	119.78
1	C	290	ASN	C-N-CA	7.99	128.01	119.78
1	E	231	GLN	CA-C-N	7.68	128.38	119.47
1	E	231	GLN	C-N-CA	7.68	128.38	119.47
1	C	256	ASP	CA-C-N	7.47	129.18	119.84
1	C	256	ASP	C-N-CA	7.47	129.18	119.84
1	A	290	ASN	CA-C-N	7.47	129.18	119.84
1	A	290	ASN	C-N-CA	7.47	129.18	119.84
1	A	129	LYS	N-CA-C	7.39	120.39	111.82
1	F	117	VAL	CA-C-N	-7.32	111.92	119.83
1	F	117	VAL	C-N-CA	-7.32	111.92	119.83
1	E	222	PHE	N-CA-C	-7.03	103.55	111.07
1	B	46	TRP	N-CA-C	-6.67	103.45	112.26
1	C	144	THR	N-CA-C	-6.67	100.10	110.17
1	C	261	GLU	N-CA-C	-6.57	104.05	111.14
1	D	293	ASP	N-CA-C	6.17	118.78	109.23
1	A	95	SER	N-CA-C	6.08	120.02	112.47
1	C	235	VAL	CB-CA-C	-6.07	103.62	110.96
1	B	133	HIS	N-CA-C	5.98	117.47	111.07
1	B	249	ASP	N-CA-C	5.97	118.94	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	THR	CB-CA-C	-5.87	101.62	110.90
1	C	243	ILE	CB-CA-C	-5.87	104.95	111.35
1	C	130	ASP	N-CA-C	5.84	117.32	111.07
1	A	173	CYS	CA-C-N	-5.79	113.82	119.90
1	A	173	CYS	C-N-CA	-5.79	113.82	119.90
1	D	73	ILE	CB-CA-C	-5.75	103.25	112.16
1	C	243	ILE	N-CA-C	5.70	115.76	108.12
1	C	182	ASN	N-CA-C	5.66	118.55	110.68
1	E	136	THR	N-CA-C	5.66	118.22	111.71
1	B	141	ASP	N-CA-C	-5.59	105.72	112.54
1	D	161	GLY	N-CA-C	-5.48	106.21	112.79
1	E	266	ILE	N-CA-C	5.46	117.91	111.09
1	A	211	SER	N-CA-C	-5.34	106.81	113.38
1	F	243	ILE	N-CA-C	5.34	115.27	108.12
1	E	282	ASP	N-CA-C	-5.30	105.42	111.14
1	B	130	ASP	N-CA-C	5.29	116.73	111.07
1	A	277	ASN	CA-C-N	-5.27	116.42	122.95
1	A	277	ASN	C-N-CA	-5.27	116.42	122.95
1	A	80	VAL	N-CA-C	5.26	115.87	109.30
1	F	151	GLY	N-CA-C	-5.25	106.34	113.37
1	C	165	THR	CA-C-N	-5.24	114.30	122.73
1	C	165	THR	C-N-CA	-5.24	114.30	122.73
1	F	259	ILE	N-CA-C	-5.21	105.46	110.72
1	F	47	ARG	N-CA-C	5.20	118.06	109.85
1	F	215	ILE	N-CA-C	-5.17	105.45	110.42
1	A	141	ASP	N-CA-C	-5.17	106.48	112.89
1	C	210	GLY	CA-C-N	-5.14	114.43	122.65
1	C	210	GLY	C-N-CA	-5.14	114.43	122.65
1	A	247	ARG	N-CA-C	5.11	117.84	110.28
1	E	128	ILE	N-CA-C	5.10	119.96	109.34
1	C	95	SER	CB-CA-C	-5.07	103.50	111.51
1	F	193	SER	CA-C-N	5.06	127.02	120.44
1	F	193	SER	C-N-CA	5.06	127.02	120.44
1	C	277	ASN	CB-CA-C	-5.05	101.80	109.89
1	A	90	LYS	CB-CA-C	-5.04	102.74	110.81
1	B	265	ILE	N-CA-C	5.04	115.26	110.42
1	E	245	GLY	N-CA-C	-5.03	106.31	113.86
1	B	117	VAL	CB-CA-C	5.00	120.46	111.36
1	F	249	ASP	CA-C-N	-5.00	115.96	124.31
1	F	249	ASP	C-N-CA	-5.00	115.96	124.31

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	2050	0	1976	84	0
1	B	2050	0	1976	84	0
1	C	2050	0	1976	90	0
1	D	2050	0	1976	74	0
1	E	2050	0	1976	86	0
1	F	2050	0	1976	83	0
2	A	13	0	6	1	0
2	B	13	0	6	0	0
2	C	13	0	6	5	0
2	D	13	0	6	1	0
2	E	13	0	6	3	0
2	F	13	0	6	3	0
3	A	98	0	0	7	0
3	B	112	0	0	9	0
3	C	93	0	0	5	0
3	D	81	0	0	6	0
3	E	115	0	0	10	0
3	F	110	0	0	4	0
All	All	12987	0	11892	492	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (492) 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:E:226:GLU:OE2	2:E:301:RF5:C1	1.63	1.45
1:C:226:GLU:OE2	2:C:301:RF5:C1	1.75	1.35
1:F:226:GLU:OE2	2:F:301:RF5:C1	1.74	1.34
1:A:180:CYS:HB2	3:A:397:HOH:O	1.43	1.19
1:C:47:ARG:CB	1:C:47:ARG:HH11	1.57	1.17
1:B:195:ARG:CG	1:B:195:ARG:HH11	1.59	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:THR:O	1:F:78:ARG:HD3	1.44	1.16
1:A:110:MET:CE	1:A:192:VAL:HG12	1.77	1.13
1:E:128:ILE:HD13	1:E:243:ILE:HD12	1.31	1.11
1:E:110:MET:HE1	1:E:192:VAL:HG12	1.16	1.10
1:B:110:MET:HE1	1:B:192:VAL:HG12	1.20	1.10
1:A:110:MET:HE1	1:A:192:VAL:CG1	1.81	1.09
1:B:195:ARG:HH11	1:B:195:ARG:HG2	0.95	1.07
1:A:268:LYS:HD2	1:B:166:SER:OG	1.52	1.07
1:E:110:MET:HE1	1:E:192:VAL:CG1	1.85	1.07
1:C:128:ILE:HD13	1:C:243:ILE:CD1	1.87	1.04
1:C:47:ARG:HH11	1:C:47:ARG:CG	1.69	1.04
1:C:165:THR:HG23	1:C:167:LYS:H	1.17	1.03
1:B:110:MET:HE1	1:B:192:VAL:CG1	1.89	1.02
1:B:195:ARG:HG2	1:B:195:ARG:NH1	1.59	1.02
1:E:292:GLU:HA	1:E:296:CYS:CB	1.88	1.02
1:E:292:GLU:HA	1:E:296:CYS:HB2	1.03	1.00
1:A:110:MET:HE1	1:A:192:VAL:HG12	1.00	0.98
1:E:110:MET:CE	1:E:192:VAL:HG12	1.94	0.97
1:D:165:THR:HG23	1:D:167:LYS:H	1.29	0.96
1:D:115:GLN:HE22	1:D:149:LEU:H	1.06	0.95
1:B:110:MET:CE	1:B:192:VAL:HG12	1.97	0.94
1:A:141:ASP:OD1	1:C:47:ARG:HD3	1.70	0.92
1:F:139:GLN:C	1:F:141:ASP:H	1.75	0.91
1:F:194:ARG:O	1:F:198:GLU:HG3	1.69	0.91
1:D:210:GLY:HA2	1:D:215:ILE:HG12	1.51	0.91
1:A:64:LEU:HA	3:A:398:HOH:O	1.72	0.90
1:C:128:ILE:HD13	1:C:243:ILE:HD12	1.53	0.89
1:C:128:ILE:HD13	1:C:243:ILE:HD13	1.53	0.89
1:E:165:THR:CG2	1:E:167:LYS:H	1.85	0.88
1:A:115:GLN:HE22	1:A:149:LEU:H	1.17	0.87
1:E:292:GLU:CA	1:E:296:CYS:HB2	1.99	0.86
1:C:115:GLN:HE22	1:C:149:LEU:H	1.21	0.86
1:A:127:ARG:HG2	1:A:212:ARG:NH1	1.90	0.86
1:E:128:ILE:HD13	1:E:243:ILE:CD1	2.06	0.86
1:C:165:THR:CG2	1:C:167:LYS:H	1.89	0.85
1:C:47:ARG:CB	1:C:47:ARG:NH1	2.40	0.85
1:C:246:GLY:O	1:C:247:ARG:HB2	1.79	0.83
1:D:248:GLU:O	1:D:249:ASP:HB2	1.78	0.82
1:D:165:THR:CG2	1:D:167:LYS:H	1.91	0.81
1:C:47:ARG:HH11	1:C:47:ARG:HB2	1.44	0.81
1:E:183:ASN:HD21	1:E:186:SER:H	1.25	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ILE:CD1	1:C:243:ILE:HD13	2.10	0.80
1:C:246:GLY:O	1:C:247:ARG:CB	2.30	0.80
1:E:74:HIS:HE1	3:E:367:HOH:O	1.64	0.80
1:F:218:LYS:HG2	1:F:261:GLU:OE1	1.82	0.80
1:A:134:GLN:HE21	1:A:285:LEU:HD11	1.46	0.80
1:B:127:ARG:HG2	1:B:212:ARG:NH1	1.97	0.79
1:E:165:THR:HG22	1:E:167:LYS:H	1.46	0.79
1:F:222:PHE:HA	1:F:226:GLU:HG3	1.64	0.78
1:E:128:ILE:CD1	1:E:243:ILE:HD12	2.11	0.78
1:F:266:ILE:HD11	1:F:273:PHE:HB2	1.65	0.78
1:C:226:GLU:CD	2:C:301:RF5:C1	2.56	0.77
1:B:115:GLN:HE22	1:B:149:LEU:H	1.30	0.77
1:B:47:ARG:O	1:B:47:ARG:HG3	1.83	0.77
1:A:289:LYS:C	1:A:290:ASN:HD22	1.92	0.76
1:B:164:ASP:O	1:B:165:THR:HG22	1.86	0.76
1:D:115:GLN:NE2	1:D:149:LEU:H	1.82	0.76
1:B:178:LYS:HD2	3:B:340:HOH:O	1.86	0.76
1:C:58:ARG:NH1	1:C:61:GLU:HG2	2.01	0.75
1:F:266:ILE:HD11	1:F:273:PHE:CB	2.15	0.75
1:D:86:TRP:CZ2	1:D:90:LYS:HG3	2.22	0.74
1:F:165:THR:CG2	1:F:167:LYS:H	2.01	0.74
1:B:289:LYS:O	1:B:291:PRO:HD3	1.88	0.74
1:C:47:ARG:HH11	1:C:47:ARG:HG2	1.53	0.74
1:F:238:LEU:HB3	1:F:266:ILE:HD13	1.70	0.73
1:B:164:ASP:C	1:B:165:THR:CG2	2.61	0.73
1:E:57:LYS:HG3	1:E:57:LYS:O	1.89	0.73
1:C:236:GLN:HB2	3:C:354:HOH:O	1.88	0.72
1:F:115:GLN:HE22	1:F:149:LEU:H	1.35	0.72
1:B:127:ARG:CG	1:B:212:ARG:HH12	2.02	0.72
1:C:262:LEU:O	1:C:266:ILE:HG23	1.90	0.72
1:C:226:GLU:OE2	2:C:301:RF5:C2	2.38	0.72
1:F:201:CYS:SG	1:F:202:ASP:OD2	2.48	0.71
1:E:116:THR:HA	3:E:399:HOH:O	1.90	0.71
1:C:285:LEU:O	1:C:289:LYS:HG3	1.91	0.71
1:E:226:GLU:CD	2:E:301:RF5:C1	2.61	0.70
1:F:286:GLN:HG3	1:F:287:CYS:N	2.06	0.70
1:C:115:GLN:NE2	1:C:149:LEU:H	1.90	0.70
1:E:127:ARG:HG2	1:E:212:ARG:NH1	2.06	0.70
1:C:45:ARG:HD3	1:C:47:ARG:H	1.57	0.69
1:D:58:ARG:NH1	1:D:61:GLU:HG2	2.08	0.69
1:B:195:ARG:CG	1:B:195:ARG:NH1	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:THR:HG23	1:C:167:LYS:N	1.99	0.69
1:C:47:ARG:CG	1:C:47:ARG:NH1	2.40	0.68
1:C:47:ARG:NH1	1:C:47:ARG:HB2	2.04	0.68
1:C:139:GLN:C	1:C:141:ASP:H	2.00	0.68
1:D:121:LYS:HE3	1:D:141:ASP:OD2	1.94	0.68
1:B:116:THR:HG23	3:B:348:HOH:O	1.94	0.68
1:F:120:ASN:HB3	1:F:202:ASP:OD2	1.94	0.68
1:F:198:GLU:O	1:F:231:GLN:NE2	2.26	0.68
1:F:291:PRO:C	1:F:293:ASP:H	2.01	0.68
1:B:194:ARG:O	1:B:198:GLU:HG3	1.94	0.68
1:D:46:TRP:HE1	1:D:47:ARG:HH11	1.39	0.68
1:E:75:PRO:HA	1:E:78:ARG:HG3	1.76	0.68
1:C:47:ARG:NH1	1:C:47:ARG:HG2	2.06	0.67
1:E:115:GLN:HE22	1:E:149:LEU:H	1.40	0.67
1:E:57:LYS:NZ	1:E:58:ARG:HD3	2.09	0.67
1:B:178:LYS:CD	3:B:340:HOH:O	2.41	0.67
1:D:77:MET:HE3	1:D:80:VAL:HG21	1.74	0.67
1:A:290:ASN:C	1:A:292:GLU:H	1.99	0.67
1:F:285:LEU:O	1:F:289:LYS:HG3	1.93	0.67
1:D:115:GLN:HE22	1:D:149:LEU:N	1.88	0.67
1:C:190:LYS:HD2	3:C:372:HOH:O	1.96	0.66
1:E:163:PHE:CG	1:E:163:PHE:O	2.48	0.66
1:F:98:PRO:O	1:F:183:ASN:HA	1.96	0.66
1:A:268:LYS:HD2	1:B:166:SER:HG	1.61	0.66
1:E:74:HIS:CE1	3:E:367:HOH:O	2.40	0.66
1:A:110:MET:CE	1:A:192:VAL:CG1	2.55	0.66
1:A:138:VAL:HG11	1:A:288:VAL:HG12	1.77	0.65
1:D:126:SER:O	1:D:127:ARG:HB2	1.96	0.65
1:F:263:GLU:HB2	1:F:273:PHE:CD2	2.32	0.65
1:A:69:LYS:HE2	1:A:73:ILE:HD11	1.79	0.64
1:B:45:ARG:HD2	1:B:47:ARG:O	1.96	0.64
1:B:231:GLN:HG3	1:B:234:LYS:HE2	1.80	0.64
1:D:162:GLU:OE2	1:D:165:THR:HG21	1.97	0.64
1:A:251:ARG:H	1:A:251:ARG:HD3	1.63	0.64
1:D:216:PHE:CD1	1:D:262:LEU:HD13	2.33	0.64
1:F:191:THR:O	1:F:195:ARG:HG3	1.98	0.64
1:E:183:ASN:ND2	1:E:186:SER:H	1.96	0.64
1:E:269:ARG:NH1	3:E:449:HOH:O	2.31	0.63
1:C:115:GLN:HE22	1:C:149:LEU:N	1.96	0.63
1:D:257:PRO:HD3	3:D:357:HOH:O	1.97	0.63
1:D:131:LEU:HD13	1:D:207:MET:HE1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:GLN:C	1:F:141:ASP:N	2.49	0.63
1:D:266:ILE:HD11	1:D:273:PHE:HB2	1.79	0.63
1:A:63:VAL:HG12	3:A:398:HOH:O	1.99	0.63
1:B:180:CYS:HB2	3:B:357:HOH:O	1.99	0.63
1:B:280:ARG:HH12	1:D:78:ARG:HH12	1.47	0.63
1:D:45:ARG:HD3	1:D:47:ARG:H	1.64	0.63
1:E:230:LEU:O	1:E:269:ARG:NH2	2.31	0.63
1:F:165:THR:HG22	1:F:167:LYS:H	1.63	0.63
1:A:127:ARG:HG2	1:A:212:ARG:HH12	1.62	0.62
1:C:249:ASP:O	1:C:250:SER:O	2.17	0.62
1:C:98:PRO:O	1:C:183:ASN:HA	1.99	0.62
1:D:218:LYS:HD2	1:D:261:GLU:OE2	1.99	0.62
1:D:135:PHE:HE1	1:D:142:MET:HE2	1.65	0.62
1:C:180:CYS:HB2	3:C:355:HOH:O	1.99	0.62
1:F:266:ILE:HD11	1:F:273:PHE:CA	2.29	0.62
1:A:176:TRP:CD1	1:A:186:SER:HG	2.17	0.62
1:F:291:PRO:O	1:F:293:ASP:N	2.29	0.61
1:B:251:ARG:H	1:B:251:ARG:HD3	1.65	0.61
1:E:195:ARG:HB3	1:E:195:ARG:HH11	1.65	0.61
1:E:128:ILE:CD1	1:E:243:ILE:CD1	2.76	0.61
1:F:90:LYS:HG2	1:F:94:ILE:HG13	1.83	0.61
1:B:183:ASN:ND2	1:B:186:SER:H	1.99	0.61
1:F:110:MET:SD	1:F:192:VAL:HG12	2.41	0.61
1:F:269:ARG:O	1:F:270:ASN:HB2	2.00	0.61
1:B:47:ARG:O	1:B:47:ARG:CG	2.49	0.61
1:D:107:GLN:OE1	1:D:195:ARG:NH2	2.34	0.61
1:D:130:ASP:O	1:D:134:GLN:HG3	2.01	0.61
1:C:126:SER:O	1:C:127:ARG:HB2	2.00	0.60
1:D:214:LYS:HA	1:D:258:THR:HG21	1.82	0.60
1:E:165:THR:HG23	1:E:167:LYS:H	1.65	0.60
1:D:77:MET:HE3	1:D:80:VAL:CG2	2.32	0.60
1:F:86:TRP:NE1	1:F:90:LYS:HE2	2.16	0.60
1:F:138:VAL:HG21	1:F:289:LYS:HG2	1.83	0.60
1:C:251:ARG:H	1:C:251:ARG:HD3	1.67	0.60
1:F:176:TRP:CE3	1:F:177:ARG:HG2	2.35	0.60
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.84	0.60
1:F:136:THR:HG21	1:F:144:THR:HG23	1.84	0.59
1:E:251:ARG:H	1:E:251:ARG:HD3	1.65	0.59
1:A:127:ARG:CG	1:A:212:ARG:HH12	2.15	0.59
1:B:183:ASN:HD21	1:B:186:SER:H	1.48	0.59
1:C:103:GLU:HG2	1:C:191:THR:OG1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ASN:ND2	1:D:186:SER:H	2.00	0.59
1:F:125:TRP:CZ3	2:F:301:RF5:H5A	2.38	0.59
1:A:128:ILE:HG12	1:A:128:ILE:O	2.02	0.59
1:E:194:ARG:NH1	3:E:403:HOH:O	2.33	0.59
1:A:127:ARG:CG	1:A:212:ARG:NH1	2.65	0.59
1:B:86:TRP:CZ2	1:B:90:LYS:HG3	2.37	0.59
1:B:195:ARG:HH11	1:B:195:ARG:CB	2.16	0.59
1:A:74:HIS:HE1	3:A:360:HOH:O	1.85	0.58
1:D:216:PHE:CE1	1:D:262:LEU:HD13	2.39	0.58
1:A:178:LYS:H	1:A:178:LYS:HD2	1.69	0.58
1:A:134:GLN:NE2	1:A:285:LEU:HD11	2.15	0.58
1:F:139:GLN:O	1:F:141:ASP:N	2.34	0.58
1:E:57:LYS:HZ1	1:E:58:ARG:HD3	1.69	0.58
1:E:162:GLU:OE2	1:E:165:THR:HG21	2.03	0.58
1:A:110:MET:HE2	1:A:150:LEU:HD13	1.85	0.57
1:D:248:GLU:O	1:D:249:ASP:CB	2.49	0.57
1:A:48:GLN:HB3	1:A:172:SER:HB3	1.86	0.57
1:D:239:GLU:HA	1:D:274:SER:O	2.04	0.57
1:D:165:THR:HG23	1:D:167:LYS:N	2.11	0.57
1:F:291:PRO:C	1:F:293:ASP:N	2.62	0.57
1:F:129:LYS:HG3	1:F:133:HIS:CE1	2.40	0.56
1:B:127:ARG:HD2	1:B:127:ARG:N	2.18	0.56
1:C:90:LYS:HG3	1:C:94:ILE:HG13	1.87	0.56
1:E:75:PRO:O	1:E:78:ARG:NE	2.37	0.56
1:E:195:ARG:HG3	3:E:403:HOH:O	2.03	0.56
1:A:176:TRP:HD1	1:A:186:SER:HG	1.52	0.56
1:B:287:CYS:O	1:B:291:PRO:HA	2.05	0.56
1:A:268:LYS:NZ	1:A:268:LYS:HB3	2.20	0.56
1:B:164:ASP:C	1:B:165:THR:HG22	2.28	0.56
1:E:155:ASP:O	1:E:156:ASP:HB2	2.05	0.56
1:B:294:SER:O	1:B:296:CYS:N	2.30	0.56
1:C:58:ARG:HH12	1:C:61:GLU:HG2	1.71	0.56
1:F:165:THR:HG23	1:F:167:LYS:H	1.69	0.56
1:C:248:GLU:HG2	1:C:280:ARG:HH21	1.70	0.55
1:B:218:LYS:HG3	1:B:261:GLU:OE1	2.06	0.55
1:F:47:ARG:HD2	3:F:394:HOH:O	2.05	0.55
1:C:293:ASP:HB2	3:C:391:HOH:O	2.06	0.55
1:E:47:ARG:HG2	1:E:47:ARG:HH11	1.72	0.55
1:B:65:ALA:HB1	1:D:292:GLU:OE2	2.07	0.55
1:C:222:PHE:HA	1:C:226:GLU:HG3	1.89	0.54
1:A:68:VAL:O	1:A:72:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ARG:HG3	1:C:140:ARG:HH11	1.72	0.54
1:D:236:GLN:O	1:D:272:GLN:HB2	2.07	0.54
1:A:104:GLU:OE1	1:A:104:GLU:N	2.38	0.54
1:A:48:GLN:NE2	1:A:171:GLN:HB3	2.23	0.54
1:C:230:LEU:N	1:C:269:ARG:HH22	2.05	0.54
1:B:47:ARG:HG2	1:B:47:ARG:HH11	1.73	0.54
1:A:230:LEU:O	1:A:269:ARG:NH1	2.40	0.54
1:C:265:ILE:O	1:C:269:ARG:HG3	2.07	0.54
1:B:86:TRP:CE2	1:B:90:LYS:HG3	2.43	0.54
1:C:183:ASN:ND2	1:C:186:SER:H	2.06	0.54
1:C:282:ASP:OD1	1:C:282:ASP:N	2.33	0.54
1:A:268:LYS:HB3	1:A:268:LYS:HZ3	1.71	0.53
1:F:266:ILE:HD11	1:F:273:PHE:HA	1.90	0.53
1:E:231:GLN:HG3	1:E:234:LYS:HD3	1.91	0.53
1:B:127:ARG:HG2	1:B:212:ARG:HH12	1.60	0.53
1:E:52:GLY:HA3	1:E:173:CYS:O	2.08	0.53
1:E:286:GLN:HA	1:E:286:GLN:OE1	2.07	0.53
1:D:289:LYS:O	1:D:291:PRO:HD3	2.09	0.53
1:C:232:PRO:HG3	1:C:269:ARG:O	2.09	0.53
1:B:110:MET:SD	1:B:195:ARG:NE	2.82	0.53
1:B:127:ARG:CG	1:B:212:ARG:NH1	2.64	0.53
1:A:110:MET:SD	1:A:195:ARG:CD	2.97	0.53
1:D:62:THR:O	1:D:66:ARG:HG3	2.08	0.53
1:D:129:LYS:HE3	1:D:155:ASP:OD2	2.09	0.52
1:F:183:ASN:HD21	1:F:186:SER:H	1.56	0.52
1:D:155:ASP:O	1:D:156:ASP:HB2	2.08	0.52
1:A:145:LEU:HD13	1:A:196:PHE:CG	2.45	0.52
1:B:46:TRP:CD2	1:B:46:TRP:N	2.78	0.52
1:D:90:LYS:HG2	1:D:94:ILE:HG13	1.90	0.52
1:A:266:ILE:HD11	1:A:273:PHE:HB2	1.91	0.52
1:A:110:MET:CE	1:A:150:LEU:HD13	2.40	0.52
1:F:283:LYS:HA	1:F:286:GLN:HG2	1.91	0.51
1:F:293:ASP:O	1:F:294:SER:CB	2.57	0.51
1:E:231:GLN:HB2	1:E:234:LYS:HD3	1.92	0.51
1:D:236:GLN:HB2	3:D:306:HOH:O	2.09	0.51
1:C:209:ASP:HB3	1:C:212:ARG:HG2	1.90	0.51
1:A:178:LYS:HD2	1:A:178:LYS:N	2.26	0.51
1:A:290:ASN:HB3	1:A:292:GLU:HG2	1.92	0.51
1:E:68:VAL:O	1:E:72:GLU:HG3	2.11	0.51
1:A:126:SER:O	1:A:127:ARG:HB2	2.10	0.51
1:C:45:ARG:NH1	1:C:47:ARG:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:PHE:O	1:D:192:VAL:HG22	2.11	0.51
1:F:183:ASN:ND2	1:F:186:SER:H	2.09	0.51
1:A:142:MET:HE1	1:A:241:TRP:CH2	2.46	0.51
1:E:195:ARG:HH11	1:E:195:ARG:CB	2.24	0.50
1:E:209:ASP:HB3	1:E:212:ARG:HG2	1.93	0.50
1:F:176:TRP:HE3	1:F:177:ARG:HG2	1.75	0.50
1:F:263:GLU:HB2	1:F:273:PHE:CE2	2.46	0.50
1:B:164:ASP:C	1:B:165:THR:HG23	2.36	0.50
1:F:90:LYS:CG	1:F:94:ILE:HG13	2.41	0.50
1:E:86:TRP:CE2	1:E:90:LYS:HG3	2.47	0.50
1:A:183:ASN:ND2	1:A:186:SER:H	2.10	0.50
1:A:194:ARG:O	1:A:198:GLU:HG3	2.11	0.50
1:F:164:ASP:HB2	3:F:369:HOH:O	2.11	0.50
1:D:98:PRO:O	1:D:183:ASN:HA	2.11	0.50
1:A:141:ASP:OD1	1:C:47:ARG:CD	2.54	0.50
1:F:110:MET:SD	1:F:195:ARG:HD2	2.52	0.50
1:D:203:VAL:HG22	1:D:237:THR:HB	1.94	0.50
1:B:291:PRO:C	1:B:293:ASP:H	2.20	0.50
1:E:127:ARG:HG2	1:E:212:ARG:HH12	1.76	0.49
1:B:294:SER:C	1:B:296:CYS:H	2.16	0.49
1:D:230:LEU:O	1:D:269:ARG:NH2	2.44	0.49
1:D:236:GLN:O	1:D:272:GLN:N	2.25	0.49
1:E:86:TRP:CZ2	1:E:90:LYS:CG	2.95	0.49
1:F:266:ILE:CD1	1:F:273:PHE:HB2	2.39	0.49
1:A:175:ASP:OD1	1:A:178:LYS:HD3	2.13	0.49
1:F:228:HIS:O	1:F:269:ARG:NH2	2.46	0.49
1:B:218:LYS:CG	1:B:261:GLU:OE1	2.61	0.49
1:D:241:TRP:HB3	1:D:278:ILE:CD1	2.42	0.49
1:E:252:ASP:C	1:E:252:ASP:OD1	2.54	0.49
1:A:282:ASP:OD2	1:F:78:ARG:NH2	2.46	0.49
1:B:145:LEU:HD13	1:B:196:PHE:CG	2.48	0.49
3:D:317:HOH:O	1:F:81:ASP:HB2	2.12	0.49
1:A:128:ILE:HD13	1:A:243:ILE:HG13	1.94	0.49
1:B:272:GLN:NE2	3:B:358:HOH:O	2.46	0.49
1:A:86:TRP:CZ2	1:A:90:LYS:CG	2.96	0.49
1:A:48:GLN:NE2	1:A:48:GLN:HA	2.28	0.48
1:C:140:ARG:HG3	1:C:140:ARG:NH1	2.27	0.48
1:F:232:PRO:HG3	1:F:269:ARG:O	2.14	0.48
1:C:139:GLN:O	1:C:141:ASP:N	2.47	0.48
1:F:218:LYS:HE3	1:F:218:LYS:HB2	1.58	0.48
1:F:243:ILE:CD1	1:F:278:ILE:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:VAL:HG12	1:C:288:VAL:HG12	1.96	0.48
1:D:95:SER:HA	1:D:165:THR:O	2.13	0.48
1:B:110:MET:CE	1:B:192:VAL:CG1	2.72	0.48
1:B:138:VAL:HG11	1:B:288:VAL:HG12	1.96	0.48
1:E:244:HIS:CE1	1:E:253:LEU:HG	2.48	0.48
1:A:86:TRP:CE2	1:A:90:LYS:HG3	2.49	0.48
1:A:195:ARG:HG3	3:A:391:HOH:O	2.12	0.48
1:E:125:TRP:CZ3	2:E:301:RF5:H5	2.48	0.48
1:D:131:LEU:CD1	1:D:207:MET:CE	2.92	0.48
1:A:195:ARG:HB3	3:A:375:HOH:O	2.13	0.48
1:B:74:HIS:HE1	3:B:353:HOH:O	1.96	0.48
1:F:218:LYS:CG	1:F:261:GLU:OE1	2.56	0.48
1:C:95:SER:HA	1:C:165:THR:O	2.14	0.47
1:C:230:LEU:O	1:C:269:ARG:NH2	2.47	0.47
1:E:110:MET:CE	1:E:192:VAL:CG1	2.70	0.47
1:F:90:LYS:HG2	1:F:94:ILE:CG1	2.44	0.47
1:A:86:TRP:CZ2	1:A:90:LYS:HG2	2.48	0.47
1:A:243:ILE:CD1	1:A:278:ILE:HD12	2.44	0.47
1:B:59:PHE:HB3	1:B:60:PRO:HD3	1.97	0.47
1:C:69:LYS:HE2	1:C:73:ILE:HD11	1.97	0.47
1:D:243:ILE:HD13	1:D:243:ILE:N	2.28	0.47
1:E:284:PHE:O	1:E:288:VAL:HG23	2.14	0.47
1:A:175:ASP:OD1	1:A:178:LYS:CD	2.63	0.47
1:A:59:PHE:HB3	1:A:60:PRO:HD3	1.97	0.47
1:B:134:GLN:NE2	1:B:285:LEU:HD11	2.29	0.47
1:C:244:HIS:HE1	1:C:277:ASN:OD1	1.98	0.47
1:B:76:GLU:HG2	1:B:77:MET:HG2	1.97	0.47
1:B:182:ASN:HB2	3:B:357:HOH:O	2.15	0.47
1:C:47:ARG:HG3	1:C:48:GLN:N	2.28	0.47
1:D:292:GLU:HB3	3:D:339:HOH:O	2.15	0.47
1:E:110:MET:SD	1:E:195:ARG:CD	3.03	0.47
1:E:158:THR:HG22	1:E:159:TRP:N	2.28	0.47
1:B:98:PRO:O	1:B:183:ASN:HA	2.15	0.47
1:B:244:HIS:HE1	1:B:277:ASN:OD1	1.98	0.47
1:C:77:MET:HE3	1:C:80:VAL:HG21	1.96	0.47
1:E:194:ARG:HH11	1:E:194:ARG:HG2	1.80	0.47
1:A:104:GLU:HA	1:A:107:GLN:HG2	1.97	0.47
1:E:128:ILE:HG12	1:E:128:ILE:O	2.15	0.47
1:F:230:LEU:O	1:F:269:ARG:NH2	2.47	0.47
1:A:183:ASN:HD21	1:A:186:SER:H	1.62	0.46
1:A:292:GLU:O	1:A:293:ASP:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:SER:OG	1:D:295:SER:N	2.45	0.46
1:B:115:GLN:HE22	1:B:149:LEU:N	2.06	0.46
1:E:269:ARG:CZ	3:E:449:HOH:O	2.61	0.46
1:A:195:ARG:NH1	3:A:375:HOH:O	2.46	0.46
1:E:141:ASP:O	1:E:142:MET:CG	2.63	0.46
1:A:251:ARG:HD3	1:A:251:ARG:N	2.29	0.46
1:B:141:ASP:O	1:B:142:MET:CG	2.63	0.46
1:B:294:SER:C	1:B:296:CYS:N	2.73	0.46
1:E:294:SER:HB2	1:E:295:SER:H	1.40	0.46
1:B:270:ASN:HB3	3:B:389:HOH:O	2.15	0.46
1:E:175:ASP:OD1	1:E:178:LYS:HD3	2.16	0.46
1:E:270:ASN:HB3	3:E:435:HOH:O	2.15	0.46
1:A:162:GLU:CD	1:A:165:THR:HG21	2.41	0.46
1:A:268:LYS:CD	1:B:166:SER:OG	2.43	0.46
1:B:74:HIS:CE1	3:B:353:HOH:O	2.69	0.46
1:B:127:ARG:HG3	1:B:212:ARG:HH12	1.81	0.46
1:C:128:ILE:HG23	1:C:128:ILE:O	2.16	0.46
1:D:241:TRP:HB3	1:D:278:ILE:HD12	1.97	0.46
1:E:195:ARG:HB3	1:E:195:ARG:NH1	2.28	0.46
1:D:220:SER:HB2	2:D:301:RF5:OP1	2.16	0.46
1:D:264:SER:O	1:D:265:ILE:C	2.57	0.46
1:E:47:ARG:HG2	1:E:47:ARG:NH1	2.31	0.45
1:A:98:PRO:O	1:A:183:ASN:HA	2.17	0.45
1:B:48:GLN:HA	1:B:48:GLN:HE21	1.81	0.45
1:C:75:PRO:HA	1:C:78:ARG:HG3	1.99	0.45
1:E:183:ASN:ND2	1:E:183:ASN:C	2.74	0.45
1:A:290:ASN:HD22	1:A:290:ASN:N	2.09	0.45
1:B:86:TRP:CZ2	1:B:90:LYS:CG	2.98	0.45
1:D:189:TRP:O	1:D:193:SER:HB2	2.17	0.45
1:D:198:GLU:HG3	1:D:229:ASN:HB3	1.98	0.45
1:D:218:LYS:H	1:D:218:LYS:HG3	1.23	0.45
1:E:98:PRO:O	1:E:183:ASN:HA	2.16	0.45
1:F:127:ARG:HD2	2:F:301:RF5:OP2	2.16	0.45
1:D:180:CYS:HB2	3:D:351:HOH:O	2.15	0.45
1:B:123:LEU:HD11	1:B:207:MET:HG3	1.98	0.45
1:B:244:HIS:CD2	1:B:250:SER:HB2	2.52	0.45
1:C:236:GLN:O	1:C:272:GLN:HB2	2.17	0.45
1:B:46:TRP:N	1:B:46:TRP:CE3	2.85	0.45
1:F:45:ARG:HG3	1:F:46:TRP:N	2.32	0.45
1:D:256:ASP:HB3	1:D:259:ILE:HG12	1.99	0.45
1:E:86:TRP:CZ2	1:E:90:LYS:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:VAL:O	1:F:118:PRO:C	2.58	0.45
1:B:212:ARG:HA	1:B:212:ARG:HD3	1.79	0.45
1:F:110:MET:HE2	1:F:110:MET:HA	1.99	0.45
1:A:115:GLN:NE2	1:A:149:LEU:H	1.98	0.44
1:E:76:GLU:HG2	1:E:77:MET:N	2.31	0.44
1:A:110:MET:HE2	1:A:110:MET:HA	1.99	0.44
1:B:131:LEU:HD13	1:B:207:MET:HE1	1.98	0.44
1:C:101:ILE:HG13	1:C:184:PRO:HG3	1.99	0.44
1:D:190:LYS:HE3	1:D:225:VAL:HG22	1.99	0.44
1:E:231:GLN:CD	3:E:430:HOH:O	2.59	0.44
1:F:128:ILE:HB	1:F:209:ASP:HB2	1.98	0.44
1:D:59:PHE:HB3	1:D:60:PRO:HD3	2.00	0.44
1:B:289:LYS:C	1:B:291:PRO:HD3	2.43	0.44
1:D:135:PHE:CE1	1:D:142:MET:HE2	2.47	0.44
1:A:110:MET:SD	1:A:195:ARG:HD2	2.57	0.44
1:E:131:LEU:HD12	1:E:243:ILE:HD13	2.00	0.44
1:F:90:LYS:HB3	1:F:90:LYS:HE3	1.60	0.44
1:B:262:LEU:O	1:B:266:ILE:HG23	2.18	0.44
1:D:218:LYS:CD	1:D:261:GLU:OE2	2.65	0.44
1:F:90:LYS:NZ	3:F:370:HOH:O	2.49	0.44
1:C:230:LEU:H	1:C:269:ARG:HH22	1.66	0.44
1:C:256:ASP:OD2	1:C:257:PRO:HD2	2.18	0.44
1:F:218:LYS:H	1:F:218:LYS:HG3	1.51	0.44
1:A:125:TRP:CZ3	2:A:301:RF5:H5	2.52	0.43
1:C:263:GLU:HG3	1:C:273:PHE:CD2	2.52	0.43
1:F:239:GLU:OE2	1:F:276:LYS:HE2	2.18	0.43
1:A:178:LYS:H	1:A:178:LYS:CD	2.29	0.43
1:B:68:VAL:O	1:B:72:GLU:HG3	2.17	0.43
1:C:104:GLU:HA	1:C:107:GLN:HG2	2.00	0.43
1:D:45:ARG:HD3	1:D:47:ARG:HG2	1.99	0.43
1:C:167:LYS:HE3	3:C:336:HOH:O	2.18	0.43
1:A:131:LEU:HD13	1:A:207:MET:CE	2.48	0.43
1:A:193:SER:HB2	1:A:226:GLU:OE2	2.18	0.43
1:B:244:HIS:HD2	1:B:250:SER:HB2	1.83	0.43
1:A:128:ILE:O	1:A:128:ILE:HG23	2.18	0.43
1:B:164:ASP:OD1	1:B:164:ASP:N	2.52	0.43
1:F:165:THR:HG23	1:F:167:LYS:HG3	2.01	0.43
1:A:130:ASP:O	1:A:134:GLN:HG3	2.19	0.43
1:C:98:PRO:HB2	1:C:174:PRO:HG2	2.00	0.43
1:C:121:LYS:HA	1:C:121:LYS:HD2	1.76	0.43
1:C:64:LEU:HD12	1:C:82:CYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LEU:HD13	1:D:207:MET:CE	2.48	0.43
1:F:293:ASP:O	1:F:294:SER:HB2	2.17	0.43
1:C:68:VAL:O	1:C:72:GLU:HG3	2.19	0.43
1:C:189:TRP:O	1:C:193:SER:HB2	2.18	0.43
1:C:220:SER:HB2	2:C:301:RF5:OP1	2.18	0.43
1:C:251:ARG:H	1:C:251:ARG:CD	2.30	0.43
1:C:102:THR:O	1:C:103:GLU:C	2.61	0.43
1:E:130:ASP:O	1:E:134:GLN:HG3	2.18	0.43
1:F:236:GLN:O	1:F:272:GLN:HB2	2.19	0.42
1:F:286:GLN:HG3	1:F:287:CYS:H	1.79	0.42
1:B:282:ASP:OD1	1:B:282:ASP:N	2.53	0.42
1:F:75:PRO:HA	1:F:78:ARG:CG	2.49	0.42
1:F:123:LEU:HD11	1:F:207:MET:HG3	2.02	0.42
1:B:61:GLU:CD	1:B:61:GLU:H	2.26	0.42
1:B:218:LYS:HD3	1:B:261:GLU:OE1	2.20	0.42
1:D:47:ARG:NE	3:D:373:HOH:O	2.52	0.42
1:D:216:PHE:HB3	1:D:258:THR:O	2.18	0.42
1:D:289:LYS:O	1:D:291:PRO:CD	2.68	0.42
1:E:46:TRP:CD2	1:E:46:TRP:N	2.88	0.42
1:C:106:TYR:O	1:C:110:MET:HG2	2.19	0.42
1:D:64:LEU:HD12	1:D:82:CYS:HB3	2.00	0.42
1:A:53:PRO:O	1:A:173:CYS:HB2	2.20	0.42
1:D:59:PHE:N	1:D:60:PRO:CD	2.83	0.42
1:E:127:ARG:NH1	1:E:217:ASP:OD2	2.51	0.42
1:A:60:PRO:HB3	1:A:86:TRP:CZ2	2.55	0.42
1:C:49:THR:HB	1:C:50:TRP:CD1	2.54	0.42
1:C:110:MET:HE1	1:C:192:VAL:HG12	2.01	0.42
1:E:47:ARG:O	1:E:47:ARG:HG3	2.18	0.42
1:E:106:TYR:CZ	1:E:188:PHE:HB2	2.54	0.42
1:B:110:MET:SD	1:B:192:VAL:HG12	2.60	0.42
1:C:183:ASN:HD21	1:C:186:SER:H	1.68	0.42
1:A:228:HIS:O	1:A:269:ARG:NH2	2.53	0.42
1:A:266:ILE:HD12	1:A:271:ILE:HG22	2.02	0.42
1:C:293:ASP:O	1:C:295:SER:N	2.53	0.42
1:E:266:ILE:HD11	1:E:273:PHE:HB2	2.01	0.42
1:B:232:PRO:HD3	1:B:269:ARG:HH21	1.85	0.41
1:C:261:GLU:O	1:C:262:LEU:C	2.63	0.41
1:D:286:GLN:O	1:D:290:ASN:N	2.51	0.41
1:E:56:THR:O	1:E:57:LYS:C	2.63	0.41
1:F:176:TRP:CZ3	1:F:177:ARG:HG2	2.55	0.41
1:C:293:ASP:HB3	1:C:294:SER:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:THR:O	1:E:149:LEU:C	2.62	0.41
1:E:269:ARG:NE	3:E:449:HOH:O	2.52	0.41
1:F:252:ASP:N	3:F:382:HOH:O	2.53	0.41
1:C:226:GLU:OE2	2:C:301:RF5:H2	2.18	0.41
1:D:47:ARG:NH2	1:E:139:GLN:OE1	2.50	0.41
1:E:129:LYS:NZ	1:E:155:ASP:OD2	2.48	0.41
1:D:45:ARG:NH1	1:D:47:ARG:O	2.53	0.41
1:E:164:ASP:OD1	1:E:164:ASP:N	2.54	0.41
1:E:110:MET:SD	1:E:192:VAL:HG12	2.61	0.41
1:C:136:THR:HG21	1:C:144:THR:HG23	2.03	0.41
1:F:282:ASP:OD1	1:F:282:ASP:N	2.53	0.41
1:A:155:ASP:O	1:A:156:ASP:HB2	2.21	0.41
1:D:110:MET:CE	1:D:150:LEU:HD13	2.51	0.41
1:E:194:ARG:O	1:E:198:GLU:HG3	2.20	0.41
1:E:200:ALA:HB1	1:E:204:VAL:HG22	2.01	0.41
1:E:212:ARG:HA	1:E:212:ARG:HD3	1.86	0.41
1:F:49:THR:HB	1:F:50:TRP:CD1	2.56	0.41
1:F:237:THR:HA	1:F:272:GLN:O	2.20	0.41
1:B:158:THR:HG22	1:B:159:TRP:N	2.36	0.41
1:C:127:ARG:HG3	1:C:212:ARG:NH2	2.36	0.41
1:C:244:HIS:CD2	1:C:250:SER:HB3	2.55	0.41
1:C:283:LYS:O	1:C:284:PHE:C	2.64	0.41
1:F:247:ARG:O	1:F:248:GLU:C	2.61	0.41
1:A:51:SER:HB2	1:A:179:ASP:OD2	2.20	0.41
1:F:125:TRP:HA	1:F:207:MET:O	2.21	0.41
1:F:202:ASP:HB2	1:F:203:VAL:H	1.45	0.41
1:F:101:ILE:HG13	1:F:184:PRO:HG3	2.04	0.40
1:B:110:MET:CE	1:B:150:LEU:HD13	2.52	0.40
1:B:265:ILE:HD13	1:B:265:ILE:HG21	1.76	0.40
1:D:71:THR:O	1:D:78:ARG:HG3	2.20	0.40
1:A:141:ASP:O	1:A:142:MET:CG	2.69	0.40
1:C:148:THR:O	1:C:149:LEU:C	2.62	0.40
1:E:57:LYS:O	1:E:58:ARG:HB2	2.22	0.40
1:F:217:ASP:OD1	1:F:217:ASP:C	2.62	0.40
1:F:250:SER:HA	1:F:279:TYR:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	250/262 (95%)	230 (92%)	17 (7%)	3 (1%)	10	6
1	B	250/262 (95%)	233 (93%)	15 (6%)	2 (1%)	16	11
1	C	250/262 (95%)	232 (93%)	10 (4%)	8 (3%)	3	1
1	D	250/262 (95%)	235 (94%)	11 (4%)	4 (2%)	7	3
1	E	250/262 (95%)	234 (94%)	14 (6%)	2 (1%)	16	11
1	F	250/262 (95%)	234 (94%)	13 (5%)	3 (1%)	10	6
All	All	1500/1572 (95%)	1398 (93%)	80 (5%)	22 (2%)	8	4

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	248	GLU
1	B	295	SER
1	C	247	ARG
1	C	250	SER
1	C	294	SER
1	C	295	SER
1	D	294	SER
1	F	294	SER
1	A	292	GLU
1	C	128	ILE
1	D	249	ASP
1	E	292	GLU
1	F	128	ILE
1	C	248	GLU
1	A	295	SER
1	C	140	ARG
1	C	293	ASP
1	D	289	LYS
1	F	140	ARG
1	A	246	GLY

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Mol	Chain	Res	Type
1	E	294	SER
1	D	128	ILE

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	233/241 (97%)	218 (94%)	15 (6%)	16	12
1	B	233/241 (97%)	222 (95%)	11 (5%)	23	22
1	C	233/241 (97%)	216 (93%)	17 (7%)	13	9
1	D	233/241 (97%)	218 (94%)	15 (6%)	16	12
1	E	233/241 (97%)	216 (93%)	17 (7%)	13	9
1	F	233/241 (97%)	210 (90%)	23 (10%)	7	4
All	All	1398/1446 (97%)	1300 (93%)	98 (7%)	14	10

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	51	SER
1	A	57	LYS
1	A	117	VAL
1	A	131	LEU
1	A	140	ARG
1	A	162	GLU
1	A	178	LYS
1	A	195	ARG
1	A	250	SER
1	A	251	ARG
1	A	264	SER
1	A	280	ARG
1	A	282	ASP
1	A	283	LYS
1	B	90	LYS

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Mol	Chain	Res	Type
1	B	117	VAL
1	B	131	LEU
1	B	137	GLN
1	B	165	THR
1	B	177	ARG
1	B	184	PRO
1	B	195	ARG
1	B	213	SER
1	B	266	ILE
1	B	282	ASP
1	C	45	ARG
1	C	47	ARG
1	C	117	VAL
1	C	127	ARG
1	C	131	LEU
1	C	140	ARG
1	C	165	THR
1	C	195	ARG
1	C	213	SER
1	C	231	GLN
1	C	249	ASP
1	C	251	ARG
1	C	257	PRO
1	C	266	ILE
1	C	274	SER
1	C	282	ASP
1	C	294	SER
1	D	45	ARG
1	D	49	THR
1	D	78	ARG
1	D	90	LYS
1	D	127	ARG
1	D	131	LEU
1	D	142	MET
1	D	165	THR
1	D	218	LYS
1	D	248	GLU
1	D	257	PRO
1	D	266	ILE
1	D	280	ARG
1	D	285	LEU
1	D	293	ASP

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Mol	Chain	Res	Type
1	E	57	LYS
1	E	69	LYS
1	E	76	GLU
1	E	90	LYS
1	E	117	VAL
1	E	131	LEU
1	E	140	ARG
1	E	165	THR
1	E	178	LYS
1	E	184	PRO
1	E	195	ARG
1	E	213	SER
1	E	250	SER
1	E	257	PRO
1	E	264	SER
1	E	294	SER
1	E	295	SER
1	F	47	ARG
1	F	64	LEU
1	F	78	ARG
1	F	90	LYS
1	F	114	THR
1	F	116	THR
1	F	117	VAL
1	F	131	LEU
1	F	140	ARG
1	F	164	ASP
1	F	165	THR
1	F	174	PRO
1	F	202	ASP
1	F	213	SER
1	F	218	LYS
1	F	226	GLU
1	F	227	VAL
1	F	233	GLU
1	F	250	SER
1	F	263	GLU
1	F	280	ARG
1	F	286	GLN
1	F	292	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	115	GLN
1	A	134	GLN
1	A	137	GLN
1	A	139	GLN
1	A	183	ASN
1	A	272	GLN
1	A	290	ASN
1	B	48	GLN
1	B	115	GLN
1	B	134	GLN
1	B	139	GLN
1	B	183	ASN
1	B	244	HIS
1	B	272	GLN
1	C	74	HIS
1	C	115	GLN
1	C	134	GLN
1	C	183	ASN
1	C	244	HIS
1	C	272	GLN
1	D	74	HIS
1	D	115	GLN
1	D	183	ASN
1	D	205	HIS
1	E	48	GLN
1	E	115	GLN
1	E	183	ASN
1	E	272	GLN
1	F	79	HIS
1	F	115	GLN
1	F	139	GLN
1	F	183	ASN
1	F	231	GLN
1	F	236	GLN
1	F	255	GLN
1	F	290	ASN

5.3.3 RNA ⓘ

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](#)

6 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	RF5	E	301	-	13,13,14	0.73	0	17,19,21	2.88	3 (17%)
2	RF5	A	301	-	13,13,14	0.95	0	17,19,21	2.81	7 (41%)
2	RF5	B	301	-	13,13,14	1.07	0	17,19,21	2.51	9 (52%)
2	RF5	F	301	-	13,13,14	1.04	1 (7%)	17,19,21	2.33	8 (47%)
2	RF5	C	301	-	13,13,14	1.15	0	17,19,21	2.70	6 (35%)
2	RF5	D	301	-	13,13,14	0.68	0	17,19,21	1.91	1 (5%)

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	RF5	E	301	-	-	0/6/19/22	0/1/1/1
2	RF5	A	301	-	-	0/6/19/22	0/1/1/1
2	RF5	B	301	-	-	0/6/19/22	0/1/1/1
2	RF5	F	301	-	-	5/6/19/22	0/1/1/1
2	RF5	C	301	-	-	5/6/19/22	0/1/1/1
2	RF5	D	301	-	-	5/6/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	RF5	F2-C2	-2.33	1.35	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	RF5	F2-C2-C3	10.42	117.83	108.56
2	C	301	RF5	F2-C2-C3	7.89	115.58	108.56
2	D	301	RF5	F2-C2-C3	7.03	114.81	108.56
2	A	301	RF5	F2-C2-C3	6.94	114.74	108.56
2	A	301	RF5	O4-C4-C3	-5.64	99.43	104.63
2	B	301	RF5	C2-C3-C4	-5.27	95.34	102.38
2	C	301	RF5	O4-C4-C3	4.76	109.03	104.63
2	F	301	RF5	F2-C2-C1	4.69	115.70	109.75
2	F	301	RF5	F2-C2-C3	-4.29	104.75	108.56
2	B	301	RF5	F2-C2-C3	4.23	112.32	108.56
2	A	301	RF5	F2-C2-C1	-4.12	104.53	109.75
2	B	301	RF5	C1-O4-C4	-3.73	99.82	108.06
2	A	301	RF5	C2-C3-C4	-3.72	97.42	102.38
2	F	301	RF5	O4-C4-C3	3.23	107.62	104.63
2	E	301	RF5	OP3-P-OP2	3.15	119.60	107.80
2	C	301	RF5	OP3-P-OP2	3.10	119.44	107.80
2	C	301	RF5	C1-C2-C3	3.00	107.86	104.26
2	C	301	RF5	OP3-P-O5	-2.85	99.25	106.67
2	F	301	RF5	O5-P-OP1	-2.77	98.94	106.44
2	B	301	RF5	C1-C2-C3	2.72	107.52	104.26
2	B	301	RF5	O4-C4-C3	-2.71	102.13	104.63
2	A	301	RF5	OP3-P-OP1	2.64	121.11	110.83
2	B	301	RF5	O3-C3-C4	2.56	118.44	111.08
2	F	301	RF5	OP3-P-O5	-2.52	100.09	106.67
2	B	301	RF5	OP3-P-O5	-2.50	100.14	106.67
2	F	301	RF5	O3-C3-C4	2.50	118.25	111.08
2	B	301	RF5	O3-C3-C2	-2.45	102.85	111.63
2	B	301	RF5	OP3-P-OP2	2.44	116.93	107.80
2	F	301	RF5	C2-C3-C4	-2.31	99.29	102.38
2	E	301	RF5	C2-C3-C4	-2.25	99.38	102.38
2	C	301	RF5	C1-O4-C4	2.20	112.91	108.06
2	A	301	RF5	OP3-P-O5	-2.18	100.99	106.67
2	A	301	RF5	O5-P-OP1	-2.08	100.81	106.44
2	F	301	RF5	O5-C5-C4	-2.01	102.15	108.99

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	RF5	C5-O5-P-OP2
2	C	301	RF5	C5-O5-P-OP3
2	C	301	RF5	O4-C4-C5-O5
2	D	301	RF5	C5-O5-P-OP2
2	D	301	RF5	C5-O5-P-OP3
2	F	301	RF5	C5-O5-P-OP1
2	F	301	RF5	C5-O5-P-OP2
2	F	301	RF5	C5-O5-P-OP3
2	F	301	RF5	O4-C4-C5-O5
2	D	301	RF5	O4-C4-C5-O5
2	C	301	RF5	C3-C4-C5-O5
2	F	301	RF5	C3-C4-C5-O5
2	D	301	RF5	C3-C4-C5-O5
2	C	301	RF5	C5-O5-P-OP1
2	D	301	RF5	C5-O5-P-OP1

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	RF5	3	0
2	A	301	RF5	1	0
2	F	301	RF5	3	0
2	C	301	RF5	5	0
2	D	301	RF5	1	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	252/262 (96%)	0.91	25 (9%)	13 11	28, 37, 53, 68	0
1	B	252/262 (96%)	0.59	14 (5%)	30 29	27, 36, 52, 71	0
1	C	252/262 (96%)	0.93	17 (6%)	24 22	25, 37, 50, 61	0
1	D	252/262 (96%)	1.19	29 (11%)	9 8	27, 39, 54, 57	0
1	E	252/262 (96%)	0.66	17 (6%)	24 22	28, 36, 53, 68	0
1	F	252/262 (96%)	0.98	24 (9%)	14 12	26, 37, 48, 55	0
All	All	1512/1572 (96%)	0.87	126 (8%)	17 16	25, 37, 53, 71	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	ASP	9.8
1	E	292	GLU	6.0
1	B	249	ASP	5.3
1	C	250	SER	5.1
1	C	293	ASP	4.9
1	E	249	ASP	4.8
1	A	46	TRP	4.8
1	D	249	ASP	4.5
1	A	249	ASP	4.4
1	B	292	GLU	4.4
1	D	245	GLY	4.3
1	A	294	SER	4.2
1	C	294	SER	4.1
1	C	248	GLU	4.1
1	B	213	SER	3.9
1	E	293	ASP	3.7
1	B	128	ILE	3.7
1	F	266	ILE	3.6
1	D	164	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	292	GLU	3.5
1	B	293	ASP	3.4
1	E	250	SER	3.4
1	D	270	ASN	3.3
1	A	295	SER	3.3
1	A	293	ASP	3.3
1	A	250	SER	3.2
1	B	46	TRP	3.2
1	F	85	VAL	3.2
1	F	270	ASN	3.2
1	A	213	SER	3.1
1	F	82	CYS	3.1
1	D	294	SER	3.1
1	F	283	LYS	3.1
1	C	247	ARG	3.0
1	A	248	GLU	3.0
1	E	248	GLU	3.0
1	F	294	SER	3.0
1	D	221	THR	2.9
1	A	47	ARG	2.9
1	A	114	THR	2.8
1	A	290	ASN	2.8
1	C	119	CYS	2.8
1	D	266	ILE	2.8
1	D	203	VAL	2.8
1	A	164	ASP	2.8
1	D	248	GLU	2.8
1	C	176	TRP	2.8
1	E	163	PHE	2.7
1	D	94	ILE	2.7
1	E	294	SER	2.7
1	D	259	ILE	2.7
1	B	247	ARG	2.7
1	D	161	GLY	2.7
1	D	137	GLN	2.6
1	A	165	THR	2.6
1	D	141	ASP	2.6
1	F	141	ASP	2.6
1	F	250	SER	2.6
1	D	176	TRP	2.6
1	B	163	PHE	2.6
1	F	135	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	45	ARG	2.6
1	D	286	GLN	2.6
1	E	213	SER	2.5
1	B	245	GLY	2.5
1	A	95	SER	2.5
1	B	250	SER	2.5
1	A	128	ILE	2.5
1	F	138	VAL	2.4
1	D	253	LEU	2.4
1	B	248	GLU	2.4
1	C	161	GLY	2.4
1	F	107	GLN	2.4
1	E	116	THR	2.4
1	A	270	ASN	2.4
1	F	223	GLY	2.3
1	D	204	VAL	2.3
1	A	247	ARG	2.3
1	D	265	ILE	2.3
1	D	92	ALA	2.3
1	E	46	TRP	2.3
1	F	273	PHE	2.3
1	D	80	VAL	2.3
1	D	160	CYS	2.3
1	D	202	ASP	2.3
1	E	246	GLY	2.3
1	B	295	SER	2.2
1	E	75	PRO	2.2
1	E	247	ARG	2.2
1	A	82	CYS	2.2
1	A	162	GLU	2.2
1	A	176	TRP	2.2
1	C	289	LYS	2.2
1	A	245	GLY	2.2
1	E	172	SER	2.2
1	A	201	CYS	2.2
1	F	287	CYS	2.2
1	B	294	SER	2.2
1	E	141	ASP	2.2
1	F	114	THR	2.2
1	A	163	PHE	2.1
1	F	265	ILE	2.1
1	E	171	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	65	ALA	2.1
1	C	290	ASN	2.1
1	C	168	ILE	2.1
1	C	284	PHE	2.1
1	F	68	VAL	2.1
1	E	47	ARG	2.1
1	F	47	ARG	2.1
1	D	289	LYS	2.1
1	F	153	LEU	2.1
1	C	160	CYS	2.1
1	C	296	CYS	2.1
1	A	261	GLU	2.1
1	B	195	ARG	2.1
1	D	201	CYS	2.1
1	F	73	ILE	2.1
1	F	112	LEU	2.0
1	A	57	LYS	2.0
1	D	246	GLY	2.0
1	F	176	TRP	2.0
1	C	286	GLN	2.0
1	D	64	LEU	2.0
1	C	45	ARG	2.0
1	F	194	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RF5	D	301	13/14	0.89	0.11	48,51,57,59	0
2	RF5	C	301	13/14	0.92	0.10	40,45,51,55	0
2	RF5	F	301	13/14	0.92	0.11	43,51,54,54	0
2	RF5	A	301	13/14	0.94	0.10	24,29,38,41	0
2	RF5	E	301	13/14	0.95	0.09	23,31,37,44	0
2	RF5	B	301	13/14	0.96	0.08	19,28,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.