



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2016 – 07:45 PM EDT

PDB ID : 3DZF
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027674

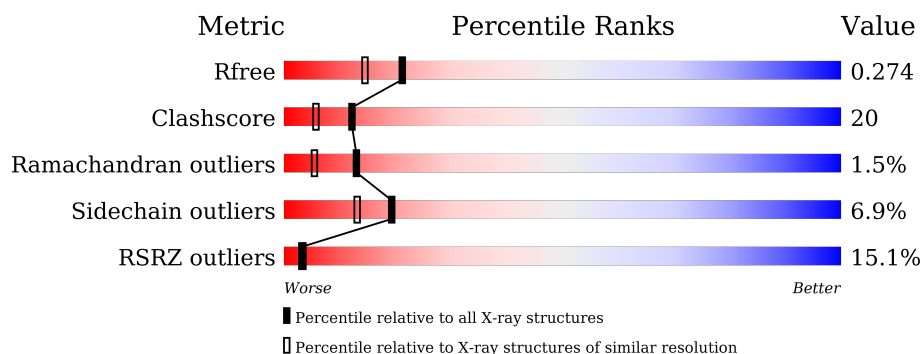
1 Overall quality at a glance

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>10%</div> <div>63%</div> <div>30%</div> <div>• •</div> </div>
1	B	262	<div> <div>9%</div> <div>65%</div> <div>29%</div> <div>• •</div> </div>
1	C	262	<div> <div>13%</div> <div>62%</div> <div>26%</div> <div>7% • •</div> </div>
1	D	262	<div> <div>24%</div> <div>59%</div> <div>32%</div> <div>5% •</div> </div>
1	E	262	<div> <div>7%</div> <div>66%</div> <div>26%</div> <div>• •</div> </div>
1	F	262	<div> <div>25%</div> <div>60%</div> <div>30%</div> <div>6% •</div> </div>

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	UNP P28907
A	100	ASP	ASN	ENGINEERED	UNP P28907
A	164	ASP	ASN	ENGINEERED	UNP P28907
A	209	ASP	ASN	ENGINEERED	UNP P28907
A	219	ASP	ASN	ENGINEERED	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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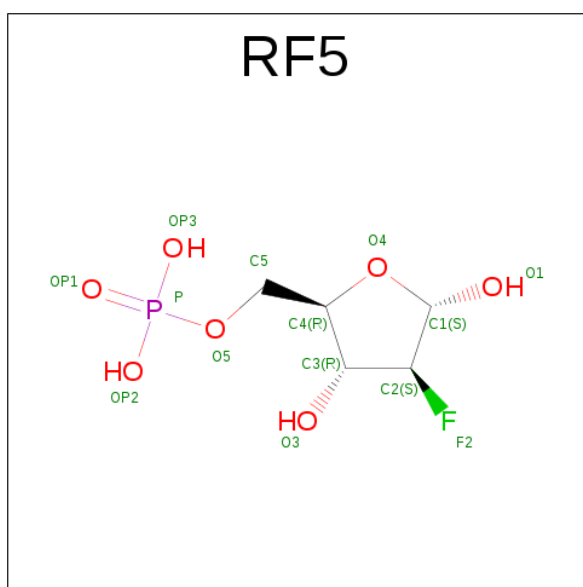
Chain	Residue	Modelled	Actual	Comment	Reference
B	49	THR	GLN	ENGINEERED	UNP P28907
B	100	ASP	ASN	ENGINEERED	UNP P28907
B	164	ASP	ASN	ENGINEERED	UNP P28907
B	209	ASP	ASN	ENGINEERED	UNP P28907
B	219	ASP	ASN	ENGINEERED	UNP P28907
C	39	LYS	-	EXPRESSION TAG	UNP P28907
C	40	ARG	-	EXPRESSION TAG	UNP P28907
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	UNP P28907
C	100	ASP	ASN	ENGINEERED	UNP P28907
C	164	ASP	ASN	ENGINEERED	UNP P28907
C	209	ASP	ASN	ENGINEERED	UNP P28907
C	219	ASP	ASN	ENGINEERED	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	UNP P28907
D	100	ASP	ASN	ENGINEERED	UNP P28907
D	164	ASP	ASN	ENGINEERED	UNP P28907
D	209	ASP	ASN	ENGINEERED	UNP P28907
D	219	ASP	ASN	ENGINEERED	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	UNP P28907
E	100	ASP	ASN	ENGINEERED	UNP P28907
E	164	ASP	ASN	ENGINEERED	UNP P28907
E	209	ASP	ASN	ENGINEERED	UNP P28907
E	219	ASP	ASN	ENGINEERED	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	UNP P28907
F	100	ASP	ASN	ENGINEERED	UNP P28907
F	164	ASP	ASN	ENGINEERED	UNP P28907
F	209	ASP	ASN	ENGINEERED	UNP P28907
F	219	ASP	ASN	ENGINEERED	UNP P28907

- Molecule 2 is SUGAR (2-DEOXY-2-FLUORO-5-O-PHOSPHONO-ALPHA-D-ARABINOF URANOSE) (three-letter code: RF5) (formula: C₅H₁₀FO₇P).



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

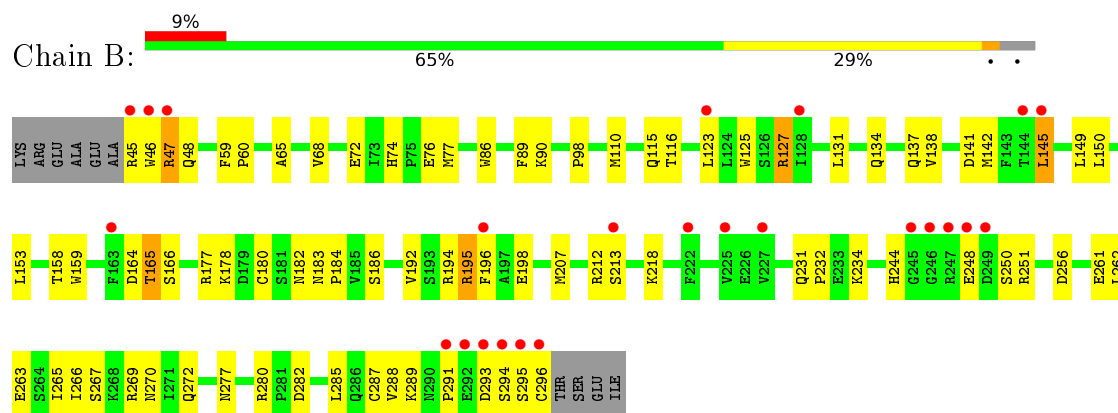
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

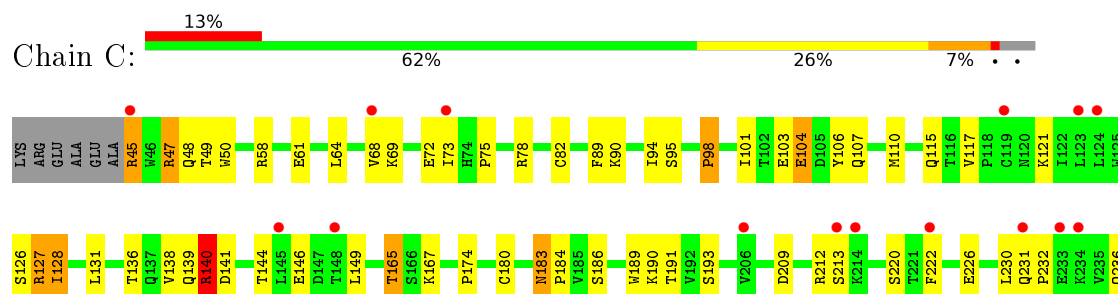
• Molecule 1: ADP-ribosyl cyclase 1

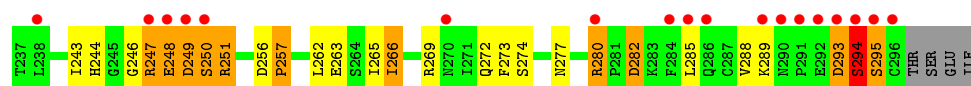


• Molecule 1: ADP-ribosyl cyclase 1

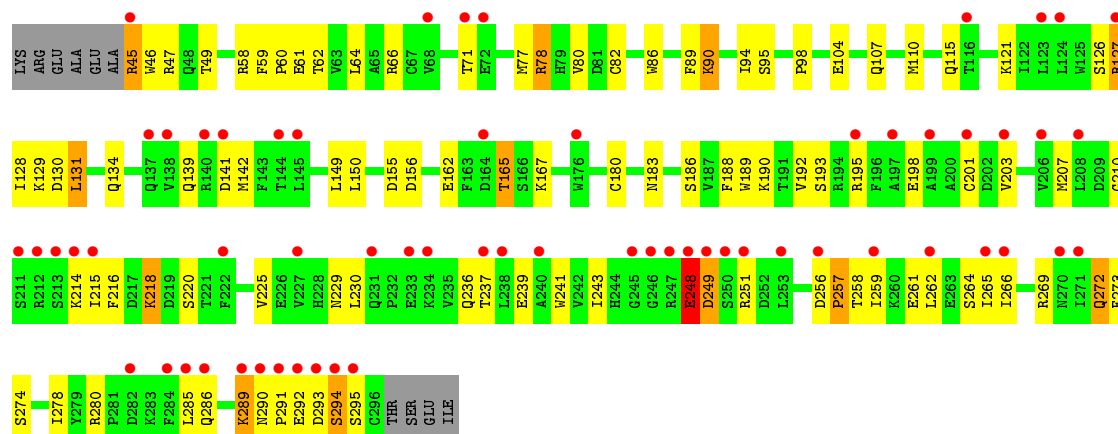


• Molecule 1: ADP-ribosyl cyclase 1

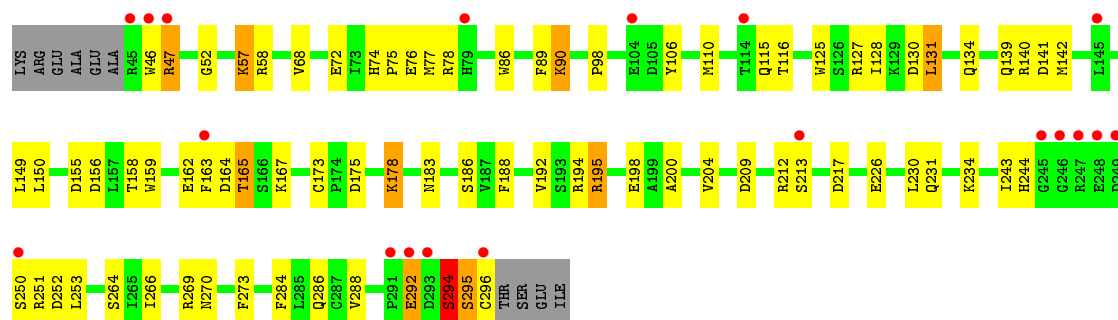




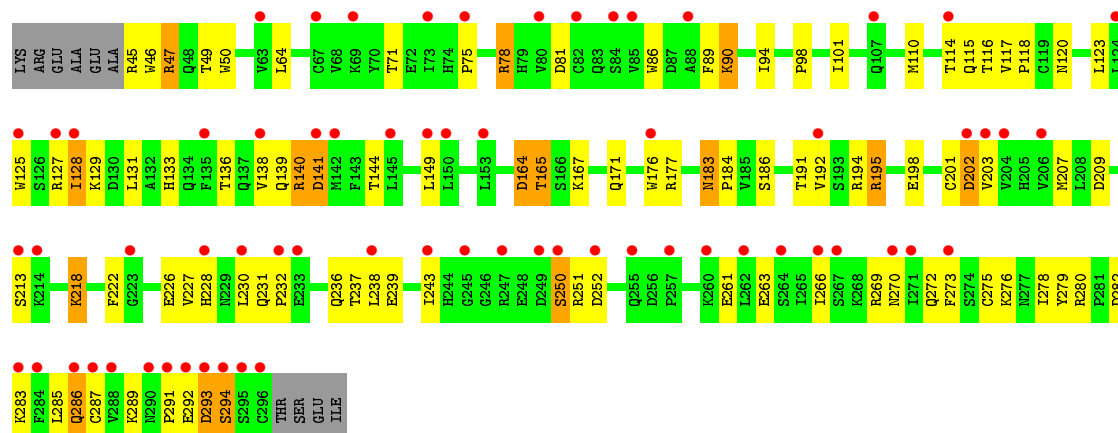
• Molecule 1: ADP-ribosyl cyclase 1



• Molecule 1: ADP-ribosyl cyclase 1



• Molecule 1: ADP-ribosyl cyclase 1



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 30.11 – 2.01	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-2.01) 81.8 (30.11-2.01)	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 0.203 , 0.274	Depositor DCC
R_{free} test set	4493 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.5	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	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	1.11	4/2101 (0.2%)	1.00	4/2846 (0.1%)
1	B	1.11	2/2101 (0.1%)	0.98	2/2846 (0.1%)
1	C	0.95	2/2101 (0.1%)	0.92	0/2846
1	D	0.92	2/2101 (0.1%)	0.86	0/2846
1	E	1.08	0/2101	0.97	0/2846
1	F	1.01	2/2101 (0.1%)	0.92	3/2846 (0.1%)
All	All	1.03	12/12606 (0.1%)	0.94	9/17076 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	VAL	CB-CG1	6.66	1.66	1.52
1	D	248	GLU	CG-CD	5.88	1.60	1.51
1	A	187	VAL	CB-CG2	5.86	1.65	1.52
1	A	47	ARG	N-CA	5.83	1.58	1.46
1	B	125	TRP	CE3-CZ3	5.42	1.47	1.38
1	B	153	LEU	N-CA	5.40	1.57	1.46
1	D	104	GLU	CG-CD	5.37	1.60	1.51
1	F	275	CYS	CB-SG	5.34	1.91	1.82
1	C	146	GLU	CD-OE2	-5.34	1.19	1.25
1	F	171	GLN	CG-CD	5.27	1.63	1.51
1	C	104	GLU	CG-CD	5.21	1.59	1.51
1	A	206	VAL	CB-CG2	5.07	1.63	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	145	LEU	CB-CG-CD2	-6.10	100.62	111.00
1	A	66	ARG	NE-CZ-NH2	5.77	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	251	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	131	LEU	CB-CG-CD1	5.65	120.61	111.00
1	F	141	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	B	256	ASP	CB-CG-OD1	5.25	123.02	118.30
1	F	251	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	66	ARG	NE-CZ-NH1	-5.03	117.78	120.30

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	83	0
1	B	2050	0	1976	84	0
1	C	2050	0	1976	85	0
1	D	2050	0	1976	72	0
1	E	2050	0	1976	84	0
1	F	2050	0	1976	81	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	9	0
3	F	110	0	0	5	0
All	All	12987	0	11892	480	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 (480) 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
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:A:110:MET:HE1	1:A:192:VAL:HG12	1.30	1.08
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:C:128:ILE:HD13	1:C:243:ILE:CD1	1.87	1.04
1:C:47:ARG:CG	1:C:47:ARG:HH11	1.69	1.04
1:C:165:THR:HG23	1:C:167:LYS:H	1.17	1.03
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: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:E:110:MET:HE1	1:E:192:VAL:HG12	1.48	0.93
1:A:141:ASP:OD1	1:C:47:ARG:HD3	1.70	0.92
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:F:139:GLN:C	1:F:141:ASP:H	1.75	0.90
1:A:64:LEU:HA	3:A:398:HOH:O	1.72	0.90
1:B:110:MET:HE1	1:B:192:VAL:HG12	1.52	0.89
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:A:110:MET:CE	1:A:192:VAL:CG1	2.55	0.85
1:C:246:GLY:O	1:C:247:ARG:HB2	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	1:C:47:ARG:HH11	1.44	0.81
1:E:183:ASN:HD21	1:E:186:SER:H	1.25	0.81
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:B:115:GLN:HE22	1:B:149:LEU:H	1.30	0.77
1:B:47:ARG:HG3	1:B:47:ARG:O	1.83	0.77
1:A:110:MET:HE1	1:A:192:VAL:CG1	2.11	0.77
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:HG2	1:C:47:ARG:HH11	1.53	0.74
1:F:238:LEU:HB3	1:F:266:ILE:HD13	1.70	0.73
1:E:57:LYS:O	1:E:57:LYS:HG3	1.89	0.73
1:C:226:GLU:CD	2:C:301:RF5:C1	2.56	0.73
1:C:236:GLN:HB2	3:C:354:HOH:O	1.88	0.72
1:E:110:MET:HE1	1:E:192:VAL:CG1	2.19	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:A:289:LYS:C	1:A:290:ASN:HD22	1.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ARG:HG2	1:E:212:ARG:NH1	2.06	0.70
1:E:110:MET:CE	1:E:192:VAL:CG1	2.70	0.69
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
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:HB2	1:C:47:ARG:NH1	2.04	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:B:164:ASP:C	1:B:165:THR:CG2	2.61	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:F:285:LEU:O	1:F:289:LYS:HG3	1.93	0.67
1:A:110:MET:HE3	1:A:192:VAL:CG1	2.23	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:E:226:GLU:CD	2:E:301:RF5:C1	2.61	0.66
1:F:98:PRO:O	1:F:183:ASN:HA	1.96	0.66
1:B:110:MET:HE1	1:B:192:VAL:CG1	2.24	0.66
1:E:74:HIS:CE1	3:E:367:HOH:O	2.40	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:B:110:MET:CE	1:B:192:VAL:CG1	2.72	0.64
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:HD3	1:A:251:ARG:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:139:GLN:C	1:C:141:ASP:H	2.00	0.63
1:D:266:ILE:HD11	1:D:273:PHE:HB2	1.79	0.63
1:F:291:PRO:C	1:F:293:ASP:H	2.01	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:A:290:ASN:C	1:A:292:GLU:H	1.99	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: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: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:HH11	1:E:195:ARG:HB3	1.65	0.61
1:E:128:ILE:CD1	1:E:243:ILE:CD1	2.76	0.61
1:F:139:GLN:C	1:F:141:ASP:N	2.49	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:CG	1:B:47:ARG:O	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:B:110:MET:HE1	1:B:150:LEU:HD13	1.81	0.60
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:F:138:VAL:HG21	1:F:289:LYS:HG2	1.83	0.60
1:F:86:TRP:NE1	1:F:90:LYS:HE2	2.16	0.60
1:C:251:ARG:HD3	1:C:251:ARG:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	1:A:128:ILE:HG12	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:195:ARG:HH11	1:B:195:ARG:CB	2.16	0.59
1:B:86:TRP:CZ2	1:B:90:LYS:HG3	2.37	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:HD2	1:A:178:LYS:H	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:162:GLU:OE2	1:E:165:THR:HG21	2.03	0.58
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: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:195:ARG:HG3	3:E:403:HOH:O	2.03	0.56
1:E:75:PRO:O	1:E:78:ARG:NE	2.37	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:HB3	1:A:268:LYS:NZ	2.20	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:E:57:LYS:HZ2	1:E:58:ARG:HD3	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:O	1:A:72:GLU:HG3	2.07	0.54
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:N	1:C:282:ASP:OD1	2.33	0.54
1:A:268:LYS:HZ3	1:A:268:LYS:HB3	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:286:GLN:HA	1:E:286:GLN:OE1	2.07	0.53
1:E:52:GLY:HA3	1:E:173:CYS:O	2.08	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:F:291:PRO:C	1:F:293:ASP:N	2.62	0.52
1:A:145:LEU:HD13	1:A:196:PHE:CG	2.45	0.52
1:B:46:TRP:N	1:B:46:TRP:CD2	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:B:164:ASP:O	1:B:165:THR:CG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:110:MET:HE1	1:A:150:LEU:HD13	1.93	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: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:E:127:ARG:HG2	1:E:212:ARG:HH12	1.76	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:B:145:LEU:HD13	1:B:196:PHE:CG	2.48	0.49
1:A:282:ASP:OD2	1:F:78:ARG:NH2	2.46	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:290:ASN:N	1:A:290:ASN:HD22	2.09	0.48
1:A:48:GLN:HA	1:A:48:GLN:NE2	2.28	0.48
1:C:140:ARG:NH1	1:C:140:ARG:HG3	2.27	0.48
1:D:131:LEU:HD13	1:D:207:MET:HE1	1.95	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:HB2	1:F:218:LYS:HE3	1.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:243:ILE:CD1	1:F:278:ILE:HD12	2.43	0.48
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: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:195:ARG:HG3	3:A:391:HOH:O	2.12	0.48
1:A:86:TRP:CE2	1:A:90:LYS:HG3	2.49	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:A:292:GLU:O	1:A:293:ASP:HB2	2.14	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:F:90:LYS:HG2	1:F:94:ILE:CG1	2.44	0.47
1:A:268:LYS:HD2	1:B:166:SER:HG	1.71	0.47
1:A:243:ILE:CD1	1:A:278:ILE:HD12	2.44	0.47
1:A:86:TRP:CZ2	1:A:90:LYS:HG2	2.48	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:N	1:D:243:ILE:HD13	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:164:ASP:C	1:B:165:THR:HG22	2.28	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:182:ASN:HB2	3:B:357:HOH:O	2.15	0.47
1:D:292:GLU:HB3	3:D:339:HOH:O	2.15	0.47
1:E:128:ILE:HG12	1:E:128:ILE:O	2.15	0.47
1:F:167:LYS:NZ	3:F:406:HOH:O	2.47	0.47
1:B:76:GLU:HG2	1:B:77:MET:HG2	1.97	0.47
1:C:47:ARG:HG3	1:C:48:GLN:N	2.28	0.47
1:E:158:THR:HG22	1:E:159:TRP:N	2.28	0.47
1:E:110:MET:SD	1:E:195:ARG:CD	3.03	0.47
1:B:244:HIS:HE1	1:B:277:ASN:OD1	1.98	0.47
1:B:98:PRO:O	1:B:183:ASN:HA	2.15	0.47
1:D:294:SER:OG	1:D:295:SER:N	2.45	0.47
1:E:194:ARG:HG2	1:E:194:ARG:HH11	1.80	0.47
1:A:104:GLU:HA	1:A:107:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:115:GLN:HE22	1:B:149:LEU:N	2.06	0.46
1:B:164:ASP:C	1:B:165:THR:HG23	2.36	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:N	1:A:251:ARG:HD3	2.29	0.46
1:B:141:ASP:O	1:B:142:MET:CG	2.63	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:C:128:ILE:HG23	1:C:128:ILE:O	2.16	0.46
1:A:268:LYS:CD	1:B:166:SER:OG	2.43	0.46
1:B:127:ARG:HG3	1:B:212:ARG:HH12	1.81	0.46
1:B:74:HIS:CE1	3:B:353:HOH:O	2.69	0.46
1:D:241:TRP:HB3	1:D:278:ILE:HD12	1.97	0.46
1:E:195:ARG:NH1	1:E:195:ARG:HB3	2.28	0.46
1:D:220:SER:HB2	2:D:301:RF5:OP1	2.16	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:291:PRO:C	1:B:293:ASP:H	2.20	0.45
1:B:48:GLN:HE21	1:B:48:GLN:HA	1.81	0.45
1:C:75:PRO:HA	1:C:78:ARG:HG3	1.99	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:218:LYS:HG3	1:D:218:LYS:H	1.23	0.45
1:D:198:GLU:HG3	1:D:229:ASN:HB3	1.98	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:B:294:SER:C	1:B:296:CYS:H	2.16	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
1:B:212:ARG:HA	1:B:212:ARG:HD3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:252:ASP:C	1:E:252:ASP:OD1	2.54	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: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:256:ASP:OD2	1:C:257:PRO:HD2	2.18	0.44
1:C:230:LEU:H	1:C:269:ARG:HH22	1.66	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:CD	1:A:178:LYS:H	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:A:164:ASP:N	1:A:164:ASP:OD1	2.51	0.43
1:D:77:MET:HE3	1:D:80:VAL:HG21	2.00	0.43
1:C:167:LYS:HE3	3:C:336:HOH:O	2.18	0.43
1:A:193:SER:HB2	1:A:226:GLU:OE2	2.18	0.43
1:A:131:LEU:HD13	1:A:207:MET:CE	2.48	0.43
1:B:244:HIS:HD2	1:B:250:SER:HB2	1.83	0.43
1:E:110:MET:HE1	1:E:150:LEU:HD13	2.00	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:121:LYS:HD2	1:C:121:LYS:HA	1.76	0.43
1:C:98:PRO:HB2	1:C:174:PRO:HG2	2.00	0.43
1:C:64:LEU:HD12	1:C:82:CYS:HB3	2.00	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ARG:CD	1:C:251:ARG:H	2.30	0.43
1:C:68:VAL:O	1:C:72:GLU:HG3	2.19	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:123:LEU:HD11	1:F:207:MET:HG3	2.02	0.42
1:F:75:PRO:HA	1:F:78:ARG:CG	2.49	0.42
1:B:218:LYS:HD3	1:B:261:GLU:OE1	2.20	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:D:47:ARG:NE	3:D:373:HOH:O	2.52	0.42
1:E:46:TRP:N	1:E:46:TRP:CD2	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:E:106:TYR:CZ	1:E:188:PHE:HB2	2.54	0.42
1:E:47:ARG:HG3	1:E:47:ARG:O	2.18	0.42
1:B:294:SER:C	1:B:296:CYS:N	2.73	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:D:286:GLN:O	1:D:290:ASN:N	2.51	0.41
1:E:110:MET:HE3	1:E:192:VAL:CG1	2.47	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
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:D:139:GLN:HG2	1:D:142:MET:HE2	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASP:O	1:A:156:ASP:HB2	2.21	0.41
1:A:162:GLU:CD	1:A:165:THR:HG21	2.41	0.41
1:E:110:MET:SD	1:E:192:VAL:HG12	2.61	0.41
1:B:263:GLU:O	1:B:267:SER:OG	2.29	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:D:110:MET:CE	1:D:150:LEU:HD13	2.51	0.41
1:D:264:SER:O	1:D:265:ILE:C	2.57	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:HD3	1:E:212:ARG:HA	1.86	0.41
1:F:237:THR:HA	1:F:272:GLN:O	2.20	0.41
1:F:49:THR:HB	1:F:50:TRP:CD1	2.56	0.41
1:B:158:THR:HG22	1:B:159:TRP:N	2.36	0.41
1:C:139:GLN:C	1:C:141:ASP:N	2.71	0.41
1:C:244:HIS:CD2	1:C:250:SER:HB3	2.55	0.41
1:C:127:ARG:HG3	1:C:212:ARG:NH2	2.36	0.41
1:E:183:ASN:ND2	1:E:183:ASN:C	2.74	0.41
1:A:51:SER:HB2	1:A:179:ASP:OD2	2.20	0.41
1:B:110:MET:HE3	1:B:192:VAL:CG1	2.49	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: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:F:117:VAL:O	1:F:118:PRO:C	2.58	0.40
1:A:141:ASP:O	1:A:142:MET:CG	2.69	0.40
1:E:57:LYS:O	1:E:58:ARG:HB2	2.22	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%)	16	8
1	B	250/262 (95%)	233 (93%)	15 (6%)	2 (1%)	24	15
1	C	250/262 (95%)	232 (93%)	10 (4%)	8 (3%)	5	1
1	D	250/262 (95%)	235 (94%)	11 (4%)	4 (2%)	12	5
1	E	250/262 (95%)	234 (94%)	14 (6%)	2 (1%)	24	15
1	F	250/262 (95%)	234 (94%)	13 (5%)	3 (1%)	16	8
All	All	1500/1572 (95%)	1398 (93%)	80 (5%)	22 (2%)	13	5

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
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%)	219 (94%)	14 (6%)	24	17
1	B	233/241 (97%)	223 (96%)	10 (4%)	35	30
1	C	233/241 (97%)	213 (91%)	20 (9%)	13	7
1	D	233/241 (97%)	216 (93%)	17 (7%)	17	11
1	E	233/241 (97%)	219 (94%)	14 (6%)	24	17
1	F	233/241 (97%)	211 (91%)	22 (9%)	11	6
All	All	1398/1446 (97%)	1301 (93%)	97 (7%)	19	13

All (97) 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	89	PHE
1	A	117	VAL
1	A	131	LEU
1	A	140	ARG
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	B	47	ARG
1	B	89	PHE
1	B	127	ARG
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	C	45	ARG
1	C	47	ARG
1	C	89	PHE
1	C	98	PRO

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Mol	Chain	Res	Type
1	C	117	VAL
1	C	127	ARG
1	C	131	LEU
1	C	140	ARG
1	C	165	THR
1	C	183	ASN
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	280	ARG
1	C	282	ASP
1	C	294	SER
1	D	45	ARG
1	D	49	THR
1	D	78	ARG
1	D	89	PHE
1	D	90	LYS
1	D	127	ARG
1	D	131	LEU
1	D	165	THR
1	D	201	CYS
1	D	218	LYS
1	D	248	GLU
1	D	251	ARG
1	D	257	PRO
1	D	272	GLN
1	D	280	ARG
1	D	285	LEU
1	D	293	ASP
1	E	47	ARG
1	E	57	LYS
1	E	89	PHE
1	E	90	LYS
1	E	131	LEU
1	E	140	ARG
1	E	165	THR
1	E	178	LYS
1	E	195	ARG

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Mol	Chain	Res	Type
1	E	213	SER
1	E	250	SER
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	89	PHE
1	F	90	LYS
1	F	114	THR
1	F	116	THR
1	F	131	LEU
1	F	140	ARG
1	F	164	ASP
1	F	165	THR
1	F	183	ASN
1	F	195	ARG
1	F	202	ASP
1	F	213	SER
1	F	218	LYS
1	F	227	VAL
1	F	250	SER
1	F	280	ARG
1	F	286	GLN
1	F	292	GLU
1	F	293	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) 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	183	ASN
1	A	231	GLN
1	A	272	GLN
1	A	290	ASN
1	B	48	GLN
1	B	115	GLN
1	B	134	GLN

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Mol	Chain	Res	Type
1	B	183	ASN
1	B	244	HIS
1	B	272	GLN
1	C	115	GLN
1	C	134	GLN
1	C	183	ASN
1	C	244	HIS
1	C	272	GLN
1	C	290	ASN
1	D	115	GLN
1	D	183	ASN
1	D	205	HIS
1	E	48	GLN
1	E	107	GLN
1	E	115	GLN
1	E	137	GLN
1	E	183	ASN
1	E	272	GLN
1	F	79	HIS
1	F	115	GLN
1	F	183	ASN
1	F	231	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	301	-	13,13,14	0.86	0	16,19,21	2.31	5 (31%)
2	RF5	B	301	-	13,13,14	1.06	1 (7%)	16,19,21	2.16	7 (43%)
2	RF5	C	301	-	13,13,14	1.11	0	16,19,21	2.50	5 (31%)
2	RF5	D	301	-	13,13,14	0.62	0	16,19,21	1.88	1 (6%)
2	RF5	E	301	-	13,13,14	0.72	0	16,19,21	2.90	3 (18%)
2	RF5	F	301	-	13,13,14	0.96	0	16,19,21	1.96	5 (31%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	RF5	P-OP3	-2.14	1.47	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	RF5	F2-C2-C3	-4.26	104.75	108.64
2	B	301	RF5	O3-C3-C2	-3.43	102.85	112.27
2	B	301	RF5	C1-O4-C4	-3.24	99.82	108.11
2	F	301	RF5	O5-P-OP1	-3.24	98.94	107.08
2	A	301	RF5	O4-C4-C3	-2.82	99.43	104.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	RF5	O3-C3-C2	-2.64	105.02	112.27
2	C	301	RF5	OP3-P-O5	-2.56	99.25	106.72
2	A	301	RF5	O5-P-OP1	-2.50	100.81	107.08
2	A	301	RF5	O3-C3-C2	-2.48	105.44	112.27
2	F	301	RF5	OP3-P-O5	-2.27	100.09	106.72
2	B	301	RF5	OP3-P-O5	-2.25	100.14	106.72
2	F	301	RF5	OP2-P-OP1	2.34	118.26	110.63
2	F	301	RF5	O3-C3-C4	2.43	118.25	111.01
2	B	301	RF5	O3-C3-C4	2.49	118.44	111.01
2	B	301	RF5	C1-C2-C3	2.58	107.52	104.23
2	B	301	RF5	OP3-P-OP2	2.59	116.93	107.44
2	C	301	RF5	O4-C4-C3	2.73	109.03	104.31
2	C	301	RF5	C1-C2-C3	2.84	107.86	104.23
2	A	301	RF5	OP3-P-OP1	3.21	121.11	110.63
2	C	301	RF5	OP3-P-OP2	3.27	119.44	107.44
2	E	301	RF5	OP3-P-OP2	3.31	119.60	107.44
2	B	301	RF5	F2-C2-C3	4.04	112.32	108.64
2	A	301	RF5	F2-C2-C3	6.68	114.74	108.64
2	D	301	RF5	F2-C2-C3	6.76	114.81	108.64
2	C	301	RF5	F2-C2-C3	7.60	115.58	108.64
2	E	301	RF5	F2-C2-C3	10.06	117.83	108.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RF5	1	0
2	C	301	RF5	5	0
2	D	301	RF5	1	0
2	E	301	RF5	3	0
2	F	301	RF5	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.75	25 (9%) 9 10	28, 37, 53, 68	0
1	B	252/262 (96%)	0.66	24 (9%) 10 11	27, 36, 52, 71	0
1	C	252/262 (96%)	0.89	33 (13%) 5 5	25, 37, 50, 61	0
1	D	252/262 (96%)	1.30	62 (24%) 1 1	27, 39, 54, 57	0
1	E	252/262 (96%)	0.73	19 (7%) 17 18	28, 36, 53, 68	0
1	F	252/262 (96%)	1.36	66 (26%) 1 1	26, 37, 48, 55	0
All	All	1512/1572 (96%)	0.95	229 (15%) 3 3	25, 37, 53, 71	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	ASP	16.1
1	C	248	GLU	10.7
1	E	248	GLU	10.7
1	A	249	ASP	10.4
1	D	245	GLY	10.3
1	E	292	GLU	10.3
1	B	292	GLU	9.7
1	C	293	ASP	9.3
1	B	249	ASP	8.8
1	E	249	ASP	8.1
1	F	283	LYS	7.6
1	A	247	ARG	7.0
1	D	249	ASP	6.9
1	A	293	ASP	6.6
1	B	46	TRP	6.5
1	F	85	VAL	6.3
1	A	248	GLU	6.0
1	A	295	SER	5.9
1	A	246	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	292	GLU	5.8
1	D	286	GLN	5.7
1	D	253	LEU	5.5
1	B	247	ARG	5.5
1	D	289	LYS	5.4
1	E	47	ARG	5.3
1	F	270	ASN	5.3
1	B	291	PRO	5.3
1	D	270	ASN	5.2
1	D	295	SER	5.2
1	F	290	ASN	5.0
1	A	294	SER	5.0
1	F	82	CYS	5.0
1	F	295	SER	5.0
1	E	246	GLY	4.9
1	B	248	GLU	4.8
1	F	294	SER	4.8
1	F	284	PHE	4.7
1	A	46	TRP	4.7
1	E	293	ASP	4.6
1	B	47	ARG	4.6
1	D	294	SER	4.6
1	E	291	PRO	4.6
1	D	248	GLU	4.6
1	D	290	ASN	4.4
1	F	202	ASP	4.4
1	E	247	ARG	4.4
1	F	107	GLN	4.4
1	C	289	LYS	4.3
1	E	245	GLY	4.3
1	A	290	ASN	4.3
1	B	246	GLY	4.3
1	F	292	GLU	4.2
1	C	247	ARG	4.2
1	F	230	LEU	4.2
1	C	295	SER	4.2
1	F	114	THR	4.1
1	F	73	ILE	4.1
1	D	285	LEU	4.1
1	D	271	ILE	4.1
1	F	247	ARG	4.0
1	D	265	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	266	ILE	3.9
1	C	286	GLN	3.8
1	D	233	GLU	3.8
1	D	211	SER	3.8
1	A	47	ARG	3.8
1	B	293	ASP	3.7
1	D	201	CYS	3.7
1	F	291	PRO	3.7
1	C	294	SER	3.7
1	D	214	LYS	3.7
1	C	270	ASN	3.6
1	D	212	ARG	3.6
1	F	127	ARG	3.6
1	F	141	ASP	3.5
1	F	296	CYS	3.5
1	C	290	ASN	3.5
1	F	250	SER	3.5
1	C	296	CYS	3.4
1	D	284	PHE	3.4
1	F	203	VAL	3.4
1	F	213	SER	3.4
1	E	46	TRP	3.4
1	C	292	GLU	3.4
1	B	296	CYS	3.3
1	B	145	LEU	3.3
1	A	145	LEU	3.3
1	F	204	VAL	3.3
1	D	234	LYS	3.3
1	F	232	PRO	3.3
1	D	68	VAL	3.3
1	F	287	CYS	3.2
1	F	75	PRO	3.2
1	C	233	GLU	3.2
1	F	223	GLY	3.2
1	B	294	SER	3.2
1	A	245	GLY	3.1
1	D	206	VAL	3.1
1	D	237	THR	3.1
1	E	163	PHE	3.1
1	F	128	ILE	3.1
1	D	247	ARG	3.1
1	F	176	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	67	CYS	3.1
1	C	284	PHE	3.1
1	D	282	ASP	3.1
1	F	135	PHE	3.1
1	F	153	LEU	3.1
1	D	203	VAL	3.1
1	A	213	SER	3.0
1	D	127	ARG	3.0
1	D	213	SER	3.0
1	D	164	ASP	3.0
1	F	262	LEU	2.9
1	D	208	LEU	2.9
1	D	199	ALA	2.9
1	C	124	LEU	2.9
1	F	286	GLN	2.8
1	C	250	SER	2.8
1	F	238	LEU	2.8
1	B	295	SER	2.8
1	C	291	PRO	2.8
1	F	243	ILE	2.8
1	E	114	THR	2.8
1	D	123	LEU	2.8
1	D	141	ASP	2.8
1	D	231	GLN	2.8
1	F	288	VAL	2.8
1	A	292	GLU	2.8
1	F	293	ASP	2.8
1	C	206	VAL	2.7
1	E	79	HIS	2.7
1	D	116	THR	2.7
1	F	249	ASP	2.7
1	F	149	LEU	2.7
1	F	88	ALA	2.7
1	A	296	CYS	2.7
1	D	227	VAL	2.7
1	F	264	SER	2.7
1	D	124	LEU	2.7
1	E	45	ARG	2.6
1	A	225	VAL	2.6
1	D	251	ARG	2.6
1	F	267	SER	2.6
1	D	137	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	259	ILE	2.6
1	D	293	ASP	2.6
1	F	150	LEU	2.6
1	F	214	LYS	2.6
1	A	124	LEU	2.6
1	F	266	ILE	2.6
1	F	233	GLU	2.5
1	D	144	THR	2.5
1	C	123	LEU	2.5
1	D	140	ARG	2.5
1	F	142	MET	2.5
1	C	145	LEU	2.5
1	D	176	TRP	2.5
1	D	240	ALA	2.5
1	F	228	HIS	2.5
1	B	123	LEU	2.4
1	D	262	LEU	2.4
1	F	69	LYS	2.4
1	B	222	PHE	2.4
1	F	255	GLN	2.4
1	C	285	LEU	2.4
1	C	73	ILE	2.4
1	B	144	THR	2.4
1	A	123	LEU	2.4
1	F	245	GLY	2.4
1	F	124	LEU	2.4
1	F	257	PRO	2.4
1	F	271	ILE	2.3
1	B	245	GLY	2.3
1	D	138	VAL	2.3
1	C	119	CYS	2.3
1	F	138	VAL	2.3
1	C	148	THR	2.3
1	C	214	LYS	2.3
1	D	72	GLU	2.3
1	C	234	LYS	2.2
1	D	238	LEU	2.2
1	E	145	LEU	2.2
1	B	163	PHE	2.2
1	D	291	PRO	2.2
1	E	250	SER	2.2
1	F	273	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	222	PHE	2.2
1	D	45	ARG	2.2
1	F	125	TRP	2.2
1	E	296	CYS	2.2
1	A	206	VAL	2.2
1	B	227	VAL	2.2
1	B	45	ARG	2.2
1	C	280	ARG	2.2
1	D	250	SER	2.2
1	C	45	ARG	2.2
1	F	260	LYS	2.2
1	D	145	LEU	2.1
1	A	154	ALA	2.1
1	D	197	ALA	2.1
1	F	84	SER	2.1
1	E	104	GLU	2.1
1	F	252	ASP	2.1
1	D	71	THR	2.1
1	B	128	ILE	2.1
1	A	222	PHE	2.1
1	D	195	ARG	2.1
1	A	150	LEU	2.1
1	E	213	SER	2.1
1	F	63	VAL	2.1
1	F	80	VAL	2.1
1	A	162	GLU	2.1
1	D	215	ILE	2.1
1	B	225	VAL	2.1
1	F	192	VAL	2.1
1	C	238	LEU	2.0
1	A	148	THR	2.0
1	A	165	THR	2.0
1	C	68	VAL	2.0
1	C	222	PHE	2.0
1	C	213	SER	2.0
1	F	145	LEU	2.0
1	B	196	PHE	2.0
1	D	246	GLY	2.0
1	B	213	SER	2.0
1	C	231	GLN	2.0
1	D	256	ASP	2.0
1	F	206	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	RF5	F	301	13/14	0.94	0.12	-1.44	43,51,54,54	0
2	RF5	D	301	13/14	0.95	0.12	-1.73	48,51,57,59	0
2	RF5	C	301	13/14	0.96	0.10	-1.74	40,45,51,55	0
2	RF5	A	301	13/14	0.97	0.07	-2.54	24,29,38,41	0
2	RF5	E	301	13/14	0.98	0.07	-2.58	23,31,37,44	0
2	RF5	B	301	13/14	0.98	0.07	-3.11	19,28,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.