



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:10 PM UTC

PDB ID : 1UVK / pdb_00001uvk
Title : The structural basis for RNA specificity and Ca²⁺ inhibition of an RNA-dependent RNA polymerase phi6p2 dead-end complex
Authors : Salgado, P.S.; Makeyev, E.V.; Butcher, S.; Bamford, D.; Stuart, D.I.; Grimes, J.M.
Deposited on : 2004-01-21
Resolution : 2.45 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

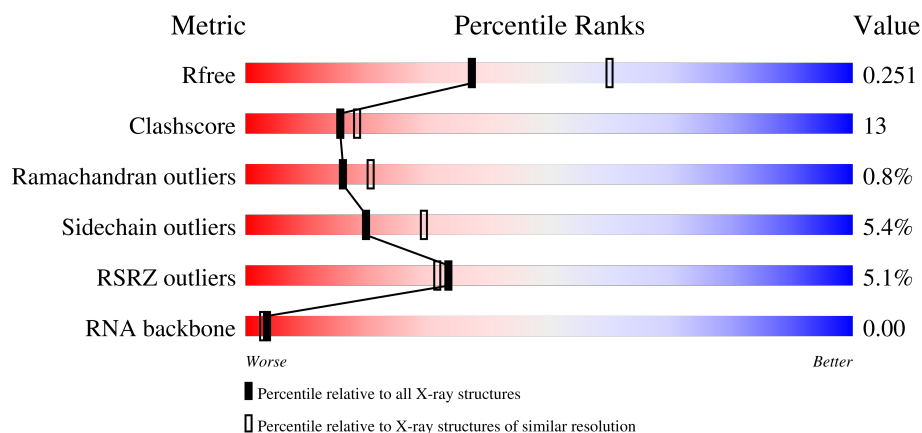
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)
RNA backbone	3983	1023 (2.72-2.20)

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	664	5% 70% 25% 5%
1	C	664	6% 70% 25% .
1	E	664	5% 71% 24% .
2	B	2	50% 50% 50%

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Mol	Chain	Length	Quality of chain
2	D	2	 50%50%
2	F	2	 50%50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16257 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	C	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	E	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	conflict	UNP P11124
C	456	MET	ILE	conflict	UNP P11124
E	456	MET	ILE	conflict	UNP P11124

- Molecule 2 is a RNA chain called RNA (pppGpG).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	P	0	0	0
			55	20	10	21	4			
2	D	2	Total	C	N	O	P	0	0	0
			55	20	10	21	4			
2	F	2	Total	C	N	O	P	0	0	0
			55	20	10	21	4			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

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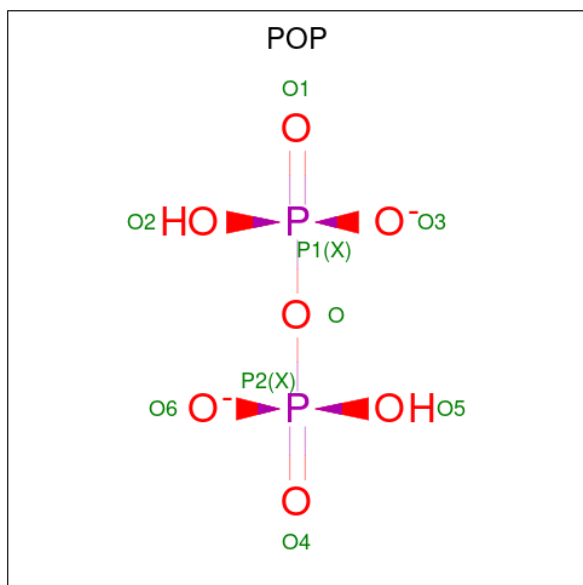
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Mn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			9	7	2		
5	C	1	Total	O	P	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	83	Total	O	0	0
			83	83		
6	C	86	Total	O	0	0
			86	86		
6	E	89	Total	O	0	0
			89	89		
6	B	1	Total	O	0	0
			1	1		
6	D	1	Total	O	0	0
			1	1		
6	F	1	Total	O	0	0
			1	1		

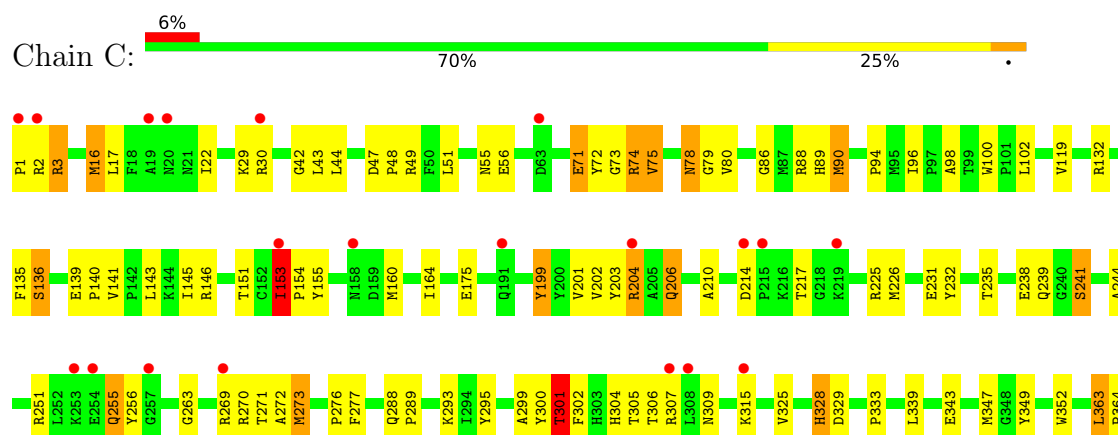
3 Residue-property plots

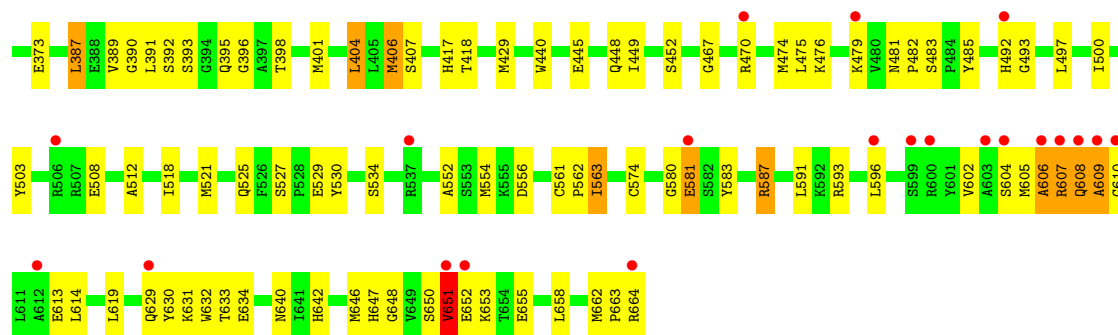
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: RNA-directed RNA polymerase

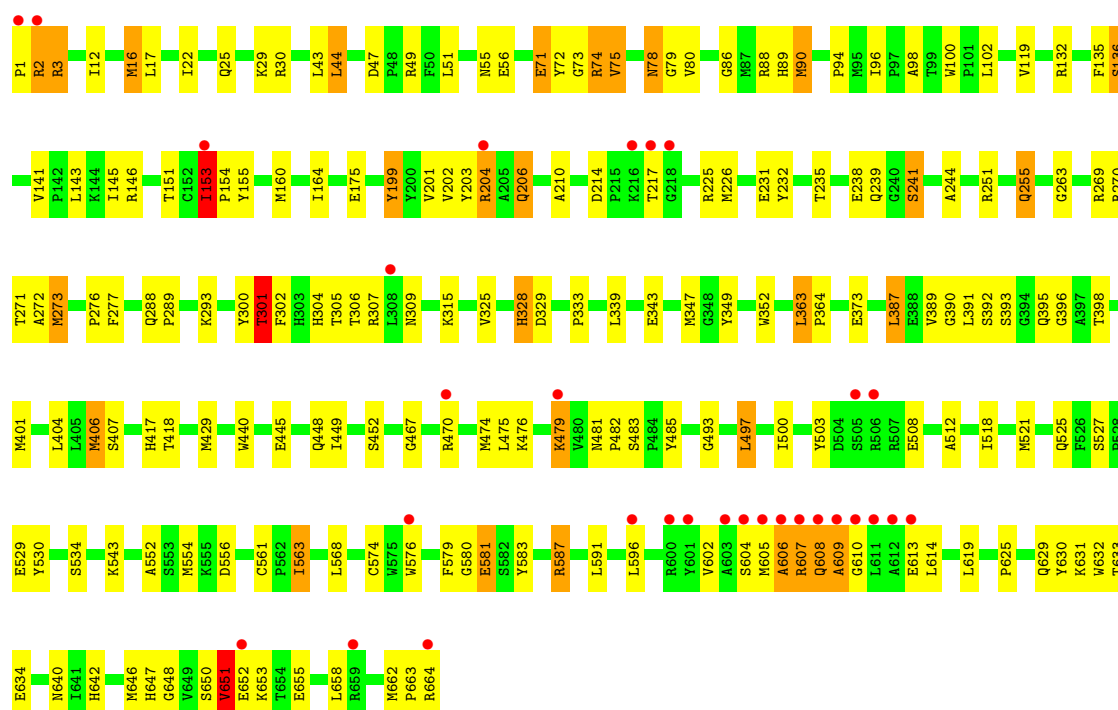


• Molecule 1: RNA-directed RNA polymerase





• Molecule 1: RNA-directed RNA polymerase



• Molecule 2: RNA (pppGpG)



• Molecule 2: RNA (pppGpG)



- Molecule 2: RNA (pppGpG)

Chain F:  50% 50%

G706
G707

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.29Å 93.80Å 140.77Å 90.00° 101.35° 90.00°	Depositor
Resolution (Å)	19.98 – 2.45 19.98 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.98-2.45) 97.3 (19.98-2.45)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.68 (at 2.47Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.265 0.228 , 0.251	Depositor DCC
R_{free} test set	4874 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16257	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	7/5396 (0.1%)	1.32	60/7297 (0.8%)
1	C	0.91	7/5396 (0.1%)	1.32	59/7297 (0.8%)
1	E	0.91	7/5396 (0.1%)	1.32	59/7297 (0.8%)
2	B	0.47	0/25	0.58	0/37
2	D	0.47	0/25	0.58	0/37
2	F	0.48	0/25	0.58	0/37
All	All	0.91	21/16263 (0.1%)	1.32	178/22002 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
All	All	0	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	153	ILE	CA-CB	-16.69	1.32	1.54
1	C	153	ILE	CA-CB	-16.68	1.32	1.54
1	A	153	ILE	CA-CB	-16.66	1.32	1.54
1	E	90	MET	SD-CE	-6.72	1.62	1.79
1	A	90	MET	SD-CE	-6.71	1.62	1.79
1	C	90	MET	SD-CE	-6.70	1.62	1.79
1	E	554	MET	SD-CE	5.73	1.93	1.79
1	C	554	MET	SD-CE	5.72	1.93	1.79
1	A	554	MET	SD-CE	5.71	1.93	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	96	ILE	CA-CB	5.58	1.58	1.54
1	A	96	ILE	CA-CB	5.52	1.58	1.54
1	C	96	ILE	CA-CB	5.44	1.58	1.54
1	E	347	MET	SD-CE	5.33	1.92	1.79
1	A	347	MET	SD-CE	5.33	1.92	1.79
1	C	347	MET	SD-CE	5.33	1.92	1.79
1	A	301	THR	CA-CB	5.20	1.62	1.53
1	E	301	THR	CA-CB	5.19	1.61	1.53
1	C	301	THR	CA-CB	5.18	1.61	1.53
1	C	406	MET	SD-CE	5.07	1.92	1.79
1	E	406	MET	SD-CE	5.04	1.92	1.79
1	A	406	MET	SD-CE	5.03	1.92	1.79

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ILE	CA-C-N	-26.88	86.24	119.84
1	A	153	ILE	C-N-CA	-26.88	86.24	119.84
1	E	153	ILE	CA-C-N	-26.88	86.24	119.84
1	E	153	ILE	C-N-CA	-26.88	86.24	119.84
1	C	153	ILE	CA-C-N	-26.84	86.29	119.84
1	C	153	ILE	C-N-CA	-26.84	86.29	119.84
1	A	141	VAL	CA-C-N	-13.42	107.16	120.31
1	A	141	VAL	C-N-CA	-13.42	107.16	120.31
1	E	141	VAL	CA-C-N	-13.40	107.17	120.31
1	E	141	VAL	C-N-CA	-13.40	107.17	120.31
1	C	141	VAL	CA-C-N	-13.38	107.20	120.31
1	C	141	VAL	C-N-CA	-13.38	107.20	120.31
1	A	153	ILE	N-CA-C	11.54	133.80	108.88
1	C	153	ILE	N-CA-C	11.53	133.79	108.88
1	E	153	ILE	N-CA-C	11.53	133.78	108.88
1	A	136	SER	N-CA-C	8.81	122.61	111.24
1	C	136	SER	N-CA-C	8.80	122.59	111.24
1	E	136	SER	N-CA-C	8.79	122.58	111.24
1	E	136	SER	CA-C-N	-8.00	112.16	123.20
1	E	136	SER	C-N-CA	-8.00	112.16	123.20
1	A	136	SER	CA-C-N	-7.99	112.18	123.20
1	A	136	SER	C-N-CA	-7.99	112.18	123.20
1	C	136	SER	CA-C-N	-7.99	112.18	123.20
1	C	136	SER	C-N-CA	-7.99	112.18	123.20
1	A	363	LEU	N-CA-C	7.85	120.91	110.08
1	C	363	LEU	N-CA-C	7.83	120.89	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	363	LEU	N-CA-C	7.83	120.89	110.08
1	A	206	GLN	N-CA-C	-7.50	92.84	107.62
1	C	206	GLN	N-CA-C	-7.49	92.86	107.62
1	E	206	GLN	N-CA-C	-7.49	92.87	107.62
1	A	153	ILE	CB-CA-C	-7.40	97.89	111.36
1	E	153	ILE	CB-CA-C	-7.40	97.89	111.36
1	C	153	ILE	CB-CA-C	-7.39	97.91	111.36
1	C	155	TYR	N-CA-C	7.31	122.47	112.90
1	A	155	TYR	N-CA-C	7.30	122.47	112.90
1	E	100	TRP	N-CA-C	-7.29	100.60	109.72
1	E	155	TYR	N-CA-C	7.29	122.45	112.90
1	A	100	TRP	N-CA-C	-7.29	100.61	109.72
1	C	100	TRP	N-CA-C	-7.27	100.64	109.72
1	E	153	ILE	CG1-CB-CG2	7.17	132.22	110.70
1	A	153	ILE	CG1-CB-CG2	7.17	132.21	110.70
1	C	153	ILE	CG1-CB-CG2	7.17	132.21	110.70
1	C	485	TYR	N-CA-C	6.94	122.09	112.45
1	A	485	TYR	N-CA-C	6.93	122.09	112.45
1	E	485	TYR	N-CA-C	6.92	122.06	112.45
1	A	153	ILE	C-N-CD	6.85	153.08	125.00
1	E	153	ILE	C-N-CD	6.85	153.09	125.00
1	C	153	ILE	C-N-CD	6.85	153.07	125.00
1	E	277	PHE	N-CA-C	6.83	119.59	111.33
1	A	396	GLY	N-CA-C	6.81	121.96	114.40
1	C	277	PHE	N-CA-C	6.81	119.57	111.33
1	C	396	GLY	N-CA-C	6.81	121.96	114.40
1	E	396	GLY	N-CA-C	6.81	121.96	114.40
1	A	277	PHE	N-CA-C	6.81	119.57	111.33
1	E	98	ALA	N-CA-C	-6.77	101.80	110.53
1	A	98	ALA	N-CA-C	-6.74	101.84	110.53
1	C	98	ALA	N-CA-C	-6.73	101.85	110.53
1	C	3	ARG	N-CA-C	-6.70	100.57	110.48
1	E	3	ARG	N-CA-C	-6.69	100.57	110.48
1	A	3	ARG	N-CA-C	-6.68	100.59	110.48
1	E	201	VAL	CB-CA-C	-6.61	102.96	110.96
1	A	201	VAL	CB-CA-C	-6.58	102.99	110.96
1	C	201	VAL	CB-CA-C	-6.58	102.99	110.96
1	C	393	SER	N-CA-C	6.34	119.00	111.71
1	C	153	ILE	CA-CB-CG1	-6.29	99.71	110.40
1	E	153	ILE	CA-CB-CG1	-6.28	99.72	110.40
1	A	153	ILE	CA-CB-CG1	-6.28	99.72	110.40
1	E	393	SER	N-CA-C	6.27	118.92	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	SER	N-CA-C	6.27	118.92	111.71
1	E	521	MET	N-CA-C	-6.25	104.39	111.14
1	A	521	MET	N-CA-C	-6.24	104.40	111.14
1	C	521	MET	N-CA-C	-6.24	104.40	111.14
1	E	647	HIS	CA-C-N	-6.21	116.60	121.82
1	E	647	HIS	C-N-CA	-6.21	116.60	121.82
1	E	201	VAL	N-CA-C	6.19	117.69	108.23
1	C	201	VAL	N-CA-C	6.18	117.69	108.23
1	A	201	VAL	N-CA-C	6.18	117.68	108.23
1	A	647	HIS	CA-C-N	-6.18	116.63	121.82
1	A	647	HIS	C-N-CA	-6.18	116.63	121.82
1	C	647	HIS	CA-C-N	-6.17	116.64	121.82
1	C	647	HIS	C-N-CA	-6.17	116.64	121.82
1	E	199	TYR	N-CA-C	-6.13	100.57	110.32
1	A	199	TYR	N-CA-C	-6.12	100.58	110.32
1	C	199	TYR	N-CA-C	-6.12	100.59	110.32
1	A	390	GLY	N-CA-C	-5.99	104.08	111.45
1	E	390	GLY	N-CA-C	-5.99	104.08	111.45
1	C	390	GLY	N-CA-C	-5.98	104.10	111.45
1	E	302	PHE	N-CA-C	5.96	121.60	113.97
1	C	302	PHE	N-CA-C	5.96	121.59	113.97
1	A	302	PHE	N-CA-C	5.94	121.58	113.97
1	C	614	LEU	N-CA-C	5.92	119.55	110.20
1	E	614	LEU	N-CA-C	5.91	119.54	110.20
1	A	614	LEU	N-CA-C	5.90	119.52	110.20
1	A	449	ILE	N-CA-C	-5.86	99.68	108.12
1	E	449	ILE	N-CA-C	-5.86	99.68	108.12
1	C	449	ILE	N-CA-C	-5.85	99.70	108.12
1	E	333	PRO	N-CA-C	5.77	124.36	112.47
1	C	452	SER	CB-CA-C	-5.77	109.91	116.54
1	C	333	PRO	N-CA-C	5.77	124.35	112.47
1	E	452	SER	CB-CA-C	-5.76	109.91	116.54
1	A	333	PRO	N-CA-C	5.76	124.33	112.47
1	A	452	SER	CB-CA-C	-5.75	109.93	116.54
1	C	527	SER	CA-C-N	-5.75	113.77	119.92
1	C	527	SER	C-N-CA	-5.75	113.77	119.92
1	A	527	SER	CA-C-N	-5.74	113.78	119.92
1	A	527	SER	C-N-CA	-5.74	113.78	119.92
1	E	527	SER	CA-C-N	-5.74	113.78	119.92
1	E	527	SER	C-N-CA	-5.74	113.78	119.92
1	E	307	ARG	N-CA-C	-5.73	105.12	111.36
1	A	307	ARG	N-CA-C	-5.72	105.13	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	ARG	N-CA-C	-5.71	105.14	111.36
1	C	613	GLU	N-CA-C	5.67	119.92	112.89
1	A	613	GLU	N-CA-C	5.64	119.89	112.89
1	E	613	GLU	N-CA-C	5.62	119.86	112.89
1	C	151	THR	N-CA-C	-5.61	106.42	113.20
1	C	389	VAL	CA-C-N	-5.60	117.10	121.86
1	C	389	VAL	C-N-CA	-5.60	117.10	121.86
1	A	389	VAL	CA-C-N	-5.59	117.11	121.86
1	A	389	VAL	C-N-CA	-5.59	117.11	121.86
1	A	151	THR	N-CA-C	-5.58	106.45	113.20
1	E	389	VAL	CA-C-N	-5.55	117.14	121.86
1	E	389	VAL	C-N-CA	-5.55	117.14	121.86
1	E	563	ILE	N-CA-C	5.53	116.83	111.91
1	E	151	THR	N-CA-C	-5.53	106.51	113.20
1	C	563	ILE	N-CA-C	5.52	116.82	111.91
1	A	563	ILE	N-CA-C	5.51	116.82	111.91
1	E	648	GLY	N-CA-C	5.48	119.14	111.14
1	C	648	GLY	N-CA-C	5.46	119.12	111.14
1	A	606	ALA	N-CA-C	-5.46	103.28	110.43
1	C	606	ALA	N-CA-C	-5.46	103.28	110.43
1	A	648	GLY	N-CA-C	5.46	119.11	111.14
1	E	606	ALA	N-CA-C	-5.45	103.29	110.43
1	E	563	ILE	CB-CA-C	-5.37	106.02	112.19
1	C	255	GLN	N-CA-C	5.36	116.92	111.14
1	C	563	ILE	CB-CA-C	-5.35	106.04	112.19
1	A	563	ILE	CB-CA-C	-5.34	106.05	112.19
1	E	255	GLN	N-CA-C	5.33	116.90	111.14
1	A	255	GLN	N-CA-C	5.33	116.90	111.14
1	E	651	VAL	CB-CA-C	-5.32	103.91	112.16
1	A	328	HIS	N-CA-C	5.31	117.49	111.11
1	A	651	VAL	CB-CA-C	-5.30	103.95	112.16
1	E	328	HIS	N-CA-C	5.30	117.47	111.11
1	E	22	ILE	N-CA-C	5.29	116.01	110.62
1	C	651	VAL	CB-CA-C	-5.28	103.97	112.16
1	C	328	HIS	N-CA-C	5.27	117.44	111.11
1	C	22	ILE	N-CA-C	5.27	116.00	110.62
1	A	22	ILE	N-CA-C	5.25	115.98	110.62
1	A	479	LYS	N-CA-C	-5.23	107.28	113.97
1	C	479	LYS	N-CA-C	-5.22	107.29	113.97
1	E	479	LYS	N-CA-C	-5.22	107.29	113.97
1	E	241	SER	N-CA-C	5.20	117.10	109.24
1	A	241	SER	N-CA-C	5.19	117.08	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	SER	N-CA-C	5.17	117.04	109.24
1	C	609	ALA	N-CA-C	-5.16	102.74	110.23
1	C	508	GLU	CA-C-N	5.16	125.20	119.32
1	C	508	GLU	C-N-CA	5.16	125.20	119.32
1	E	73	GLY	CA-C-N	-5.15	114.47	122.09
1	E	73	GLY	C-N-CA	-5.15	114.47	122.09
1	C	153	ILE	CB-CG1-CD1	-5.15	102.99	113.80
1	A	609	ALA	N-CA-C	-5.15	102.77	110.23
1	E	609	ALA	N-CA-C	-5.15	102.77	110.23
1	A	153	ILE	CB-CG1-CD1	-5.14	103.00	113.80
1	A	73	GLY	CA-C-N	-5.14	114.48	122.09
1	A	73	GLY	C-N-CA	-5.14	114.48	122.09
1	E	210	ALA	N-CA-C	5.13	117.78	110.24
1	A	508	GLU	CA-C-N	5.13	125.16	119.32
1	A	508	GLU	C-N-CA	5.13	125.16	119.32
1	A	210	ALA	N-CA-C	5.12	117.77	110.24
1	E	153	ILE	CB-CG1-CD1	-5.12	103.04	113.80
1	C	73	GLY	CA-C-N	-5.12	114.51	122.09
1	C	73	GLY	C-N-CA	-5.12	114.51	122.09
1	C	210	ALA	N-CA-C	5.12	117.77	110.24
1	E	508	GLU	CA-C-N	5.10	125.14	119.32
1	E	508	GLU	C-N-CA	5.10	125.14	119.32
1	E	610	GLY	N-CA-C	5.07	120.24	111.98
1	C	610	GLY	N-CA-C	5.06	120.23	111.98
1	A	610	GLY	N-CA-C	5.06	120.23	111.98
1	A	95	MET	N-CA-C	-5.00	103.44	110.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TYR	Sidechain
1	C	199	TYR	Sidechain
1	E	199	TYR	Sidechain

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	5265	0	5165	144	2
1	C	5265	0	5165	142	1
1	E	5265	0	5165	139	7
2	B	55	0	23	5	0
2	D	55	0	23	5	0
2	F	55	0	23	5	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	9	0	0	0	0
5	C	9	0	0	0	0
5	E	9	0	0	0	0
6	A	83	0	0	4	1
6	B	1	0	0	0	0
6	C	86	0	0	6	2
6	D	1	0	0	0	0
6	E	89	0	0	11	1
6	F	1	0	0	0	0
All	All	16257	0	15564	422	9

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 13.

All (422) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ILE:HG23	1:C:154:PRO:CD	1.50	1.41
1:A:153:ILE:HG23	1:A:154:PRO:CD	1.50	1.39
1:E:153:ILE:HG23	1:E:154:PRO:CD	1.50	1.38
1:A:608:GLN:HE22	1:C:593:ARG:CZ	1.58	1.14
1:A:206:GLN:NE2	1:A:270:ARG:HE	1.51	1.09
1:C:206:GLN:NE2	1:C:270:ARG:HE	1.51	1.09
1:A:153:ILE:HG23	1:A:154:PRO:HD2	1.35	1.08
1:E:576:TRP:CE3	6:E:873:HOH:O	2.03	1.08
1:E:206:GLN:NE2	1:E:270:ARG:HE	1.51	1.07
1:E:153:ILE:HG23	1:E:154:PRO:N	1.61	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ILE:HG23	1:C:154:PRO:HD2	1.34	1.05
1:A:153:ILE:HG23	1:A:154:PRO:N	1.61	1.05
1:E:153:ILE:HG23	1:E:154:PRO:HD2	1.34	1.04
1:C:153:ILE:HG23	1:C:154:PRO:N	1.61	1.03
1:E:153:ILE:CG2	1:E:154:PRO:CD	2.37	1.03
1:C:153:ILE:CG2	1:C:154:PRO:CD	2.37	1.03
1:A:153:ILE:CG2	1:A:154:PRO:CD	2.37	1.02
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.12	0.95
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.12	0.95
1:C:581:GLU:OE1	6:C:801:HOH:O	1.89	0.90
1:E:576:TRP:HB3	6:E:873:HOH:O	1.71	0.90
1:A:561:CYS:HB3	6:A:850:HOH:O	1.73	0.89
1:C:561:CYS:HB3	6:C:850:HOH:O	1.73	0.89
1:E:251:ARG:HH11	1:E:255:GLN:HE22	1.12	0.89
1:E:561:CYS:HB3	6:E:852:HOH:O	1.73	0.89
1:C:153:ILE:CG2	1:C:154:PRO:N	2.37	0.88
1:A:555:LYS:NZ	6:A:801:HOH:O	2.01	0.87
1:A:153:ILE:CG2	1:A:154:PRO:N	2.37	0.87
1:E:576:TRP:HE3	6:E:873:HOH:O	1.45	0.86
1:E:206:GLN:HE21	1:E:270:ARG:HE	1.23	0.85
1:E:364:PRO:HA	1:E:387:LEU:HD22	1.59	0.84
1:C:206:GLN:HE21	1:C:270:ARG:HE	1.23	0.84
1:A:206:GLN:HE21	1:A:270:ARG:HE	1.23	0.84
1:C:364:PRO:HA	1:C:387:LEU:HD22	1.59	0.83
1:A:364:PRO:HA	1:A:387:LEU:HD22	1.59	0.83
1:A:608:GLN:NE2	1:C:593:ARG:CZ	2.40	0.83
2:F:706:GTP:N7	2:F:706:GTP:O1G	2.12	0.82
2:B:706:GTP:N7	2:B:706:GTP:O1G	2.12	0.82
2:D:706:GTP:N7	2:D:706:GTP:O1G	2.12	0.82
1:E:49:ARG:NH1	6:E:801:HOH:O	2.14	0.79
1:E:153:ILE:CG2	1:E:154:PRO:N	2.37	0.79
1:A:226:MET:HE1	1:A:244:ALA:HB2	1.65	0.78
1:E:226:MET:HE1	1:E:244:ALA:HB2	1.65	0.78
1:C:226:MET:HE1	1:C:244:ALA:HB2	1.65	0.78
1:A:74:ARG:HB3	1:A:503:TYR:CD2	2.19	0.77
1:E:74:ARG:HB3	1:E:503:TYR:CD2	2.19	0.77
1:C:74:ARG:HB3	1:C:503:TYR:CD2	2.19	0.77
1:C:132:ARG:HH11	1:C:429:MET:HE2	1.50	0.77
1:C:301:THR:HG23	1:C:440:TRP:O	1.85	0.76
1:A:301:THR:HG23	1:A:440:TRP:O	1.85	0.76
1:A:132:ARG:HH11	1:A:429:MET:HE2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ARG:HH11	1:E:429:MET:HE2	1.50	0.76
1:E:301:THR:HG23	1:E:440:TRP:O	1.85	0.75
1:C:55:ASN:OD1	1:C:88:ARG:NH2	2.19	0.75
1:A:55:ASN:OD1	1:A:88:ARG:NH2	2.19	0.75
1:C:401:MET:HE2	1:C:401:MET:HA	1.69	0.75
1:E:55:ASN:OD1	1:E:88:ARG:NH2	2.19	0.75
1:C:90:MET:HA	1:C:90:MET:HE2	1.69	0.74
1:A:90:MET:HA	1:A:90:MET:HE2	1.69	0.74
1:C:629:GLN:O	1:C:629:GLN:HG2	1.87	0.74
1:E:401:MET:HA	1:E:401:MET:HE2	1.69	0.74
1:A:629:GLN:O	1:A:629:GLN:HG2	1.87	0.74
1:E:325:VAL:HG21	1:E:406:MET:HE2	1.70	0.73
1:A:401:MET:HE2	1:A:401:MET:HA	1.69	0.73
1:C:325:VAL:HG21	1:C:406:MET:HE2	1.70	0.73
1:E:90:MET:HE2	1:E:90:MET:HA	1.69	0.73
1:E:629:GLN:O	1:E:629:GLN:HG2	1.87	0.73
1:A:325:VAL:HG21	1:A:406:MET:HE2	1.70	0.72
1:C:529:GLU:OE2	2:D:706:GTP:O2G	2.08	0.71
1:A:529:GLU:OE2	2:B:706:GTP:O2G	2.08	0.71
1:E:529:GLU:OE2	2:F:706:GTP:O2G	2.08	0.70
1:A:206:GLN:NE2	1:A:270:ARG:NE	2.35	0.69
1:E:153:ILE:CG2	1:E:154:PRO:HD2	2.17	0.69
1:C:153:ILE:CG2	1:C:154:PRO:HD2	2.17	0.68
1:C:206:GLN:NE2	1:C:270:ARG:NE	2.35	0.68
1:A:206:GLN:HE21	1:A:270:ARG:NE	1.92	0.68
1:C:206:GLN:HE21	1:C:270:ARG:NE	1.92	0.68
1:C:417:HIS:ND1	1:C:474:MET:HE1	2.10	0.67
1:A:417:HIS:ND1	1:A:474:MET:HE1	2.10	0.67
1:E:325:VAL:CG2	1:E:406:MET:HE2	2.25	0.67
1:C:325:VAL:CG2	1:C:406:MET:HE2	2.25	0.66
1:A:325:VAL:CG2	1:A:406:MET:HE2	2.25	0.66
2:F:706:GTP:O2G	2:F:707:G:O6	2.14	0.66
1:E:417:HIS:ND1	1:E:474:MET:HE1	2.10	0.66
2:D:706:GTP:O2G	2:D:707:G:O6	2.14	0.66
2:B:706:GTP:O2G	2:B:707:G:O6	2.14	0.65
1:E:206:GLN:HE21	1:E:270:ARG:NE	1.92	0.65
1:E:206:GLN:HE22	1:E:270:ARG:HE	1.41	0.65
1:E:78:ASN:ND2	1:E:80:VAL:H	1.94	0.65
1:C:206:GLN:HE22	1:C:270:ARG:HE	1.41	0.64
1:C:78:ASN:ND2	1:C:80:VAL:H	1.94	0.64
1:E:206:GLN:NE2	1:E:270:ARG:NE	2.35	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:CD	1:A:71:GLU:H	2.06	0.64
1:C:288:GLN:HB3	1:C:289:PRO:HD3	1.80	0.64
1:A:78:ASN:ND2	1:A:80:VAL:H	1.94	0.64
1:A:206:GLN:HE22	1:A:270:ARG:HE	1.41	0.63
1:C:71:GLU:CD	1:C:71:GLU:H	2.06	0.63
1:E:71:GLU:CD	1:E:71:GLU:H	2.06	0.63
1:A:153:ILE:CG2	1:A:154:PRO:HD2	2.17	0.62
1:A:288:GLN:HB3	1:A:289:PRO:HD3	1.80	0.62
1:E:288:GLN:HB3	1:E:289:PRO:HD3	1.80	0.62
1:C:581:GLU:CG	6:C:801:HOH:O	2.47	0.62
1:E:78:ASN:HD22	1:E:79:GLY:N	1.98	0.61
1:A:418:THR:HG22	1:A:467:GLY:C	2.26	0.61
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.36	0.61
1:E:418:THR:HG22	1:E:467:GLY:C	2.26	0.61
1:A:606:ALA:C	1:A:608:GLN:H	2.09	0.60
1:C:78:ASN:HD22	1:C:79:GLY:N	1.98	0.60
1:C:418:THR:HG22	1:C:467:GLY:C	2.26	0.60
1:E:203:TYR:CE1	1:E:271:THR:HG22	2.36	0.60
1:A:78:ASN:HD22	1:A:79:GLY:N	1.98	0.60
1:A:153:ILE:CG2	1:A:154:PRO:HD3	2.32	0.60
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.36	0.60
1:C:75:VAL:HG12	1:C:493:GLY:HA2	1.84	0.60
1:E:658:LEU:HG	1:E:662:MET:HE2	1.83	0.60
1:C:606:ALA:C	1:C:608:GLN:H	2.09	0.60
1:A:427:LYS:HE3	1:E:12:ILE:HG21	1.84	0.59
1:E:606:ALA:C	1:E:608:GLN:H	2.09	0.59
1:A:608:GLN:HE22	1:C:593:ARG:NE	1.98	0.59
1:A:75:VAL:HG12	1:A:493:GLY:HA2	1.84	0.59
1:A:658:LEU:HG	1:A:662:MET:HE2	1.83	0.59
1:C:642:HIS:CE1	1:C:646:MET:HG3	2.38	0.59
1:E:75:VAL:HG12	1:E:493:GLY:HA2	1.84	0.59
1:A:642:HIS:CE1	1:A:646:MET:HG3	2.38	0.59
1:E:642:HIS:CE1	1:E:646:MET:HG3	2.38	0.59
1:C:658:LEU:HG	1:C:662:MET:HE2	1.83	0.58
1:A:608:GLN:HE22	1:C:593:ARG:NH1	1.99	0.58
1:E:579:PHE:HE2	6:E:801:HOH:O	1.86	0.58
1:A:608:GLN:NE2	1:C:593:ARG:NH1	2.50	0.58
1:C:203:TYR:HE1	1:C:271:THR:HG22	1.69	0.58
1:A:119:VAL:O	1:E:25:GLN:HG3	2.04	0.57
1:E:576:TRP:CD2	6:E:873:HOH:O	2.43	0.57
1:E:203:TYR:HE1	1:E:271:THR:HG22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HB	1:A:448:GLN:O	2.06	0.56
1:A:304:HIS:HA	1:A:309:ASN:HD21	1.71	0.56
1:E:304:HIS:HA	1:E:309:ASN:HD21	1.71	0.56
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.69	0.56
1:C:304:HIS:HA	1:C:309:ASN:HD21	1.70	0.56
1:C:301:THR:HB	1:C:448:GLN:O	2.06	0.56
1:E:78:ASN:HD22	1:E:78:ASN:C	2.14	0.55
1:C:606:ALA:HB3	1:C:609:ALA:HB2	1.88	0.55
1:C:78:ASN:HD22	1:C:78:ASN:C	2.14	0.55
1:E:153:ILE:CG2	1:E:154:PRO:HD3	2.32	0.55
1:A:606:ALA:HB3	1:A:609:ALA:HB2	1.88	0.55
1:C:153:ILE:CG2	1:C:154:PRO:HD3	2.32	0.55
1:E:301:THR:HB	1:E:448:GLN:O	2.06	0.55
1:A:78:ASN:HD22	1:A:78:ASN:C	2.14	0.55
1:C:300:TYR:HD1	1:C:301:THR:HG22	1.71	0.54
1:E:606:ALA:HB3	1:E:609:ALA:HB2	1.88	0.54
1:C:339:LEU:C	1:C:339:LEU:HD23	2.33	0.54
1:E:300:TYR:HD1	1:E:301:THR:HG22	1.71	0.54
1:A:300:TYR:HD1	1:A:301:THR:HG22	1.71	0.54
1:A:17:LEU:O	1:A:153:ILE:O	2.26	0.54
1:A:339:LEU:C	1:A:339:LEU:HD23	2.33	0.53
1:E:339:LEU:C	1:E:339:LEU:HD23	2.33	0.53
1:E:576:TRP:CG	6:E:873:HOH:O	2.61	0.53
1:C:17:LEU:O	1:C:153:ILE:O	2.26	0.53
1:A:407:SER:HA	1:A:448:GLN:HE22	1.74	0.53
1:C:475:LEU:HD21	1:C:482:PRO:HG3	1.91	0.53
1:C:251:ARG:NH1	1:C:255:GLN:HE22	1.95	0.52
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.45	0.52
1:C:401:MET:HE2	1:C:401:MET:CA	2.39	0.52
1:E:17:LEU:O	1:E:153:ILE:O	2.26	0.52
1:A:136:SER:OG	1:A:293:LYS:NZ	2.43	0.52
1:C:136:SER:OG	1:C:293:LYS:NZ	2.43	0.52
1:E:587:ARG:NH1	6:E:804:HOH:O	2.43	0.52
1:A:401:MET:HE2	1:A:401:MET:CA	2.39	0.52
1:A:475:LEU:HD21	1:A:482:PRO:HG3	1.91	0.52
1:E:136:SER:OG	1:E:293:LYS:NZ	2.43	0.52
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.45	0.52
1:E:175:GLU:HA	1:E:352:TRP:CE3	2.45	0.52
1:A:88:ARG:HD3	1:A:263:GLY:O	2.10	0.52
1:C:88:ARG:HD3	1:C:263:GLY:O	2.10	0.52
1:E:364:PRO:HA	1:E:387:LEU:CD2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:475:LEU:HD21	1:E:482:PRO:HG3	1.91	0.52
1:E:407:SER:HA	1:E:448:GLN:HE22	1.74	0.52
1:E:88:ARG:HD3	1:E:263:GLY:O	2.10	0.51
1:A:2:ARG:HD2	1:A:2:ARG:O	2.11	0.51
1:C:407:SER:HA	1:C:448:GLN:HE22	1.74	0.51
1:A:587:ARG:NH1	6:A:803:HOH:O	2.43	0.51
1:C:481:ASN:ND2	1:C:483:SER:O	2.44	0.51
1:C:587:ARG:NH1	6:C:803:HOH:O	2.43	0.51
1:C:175:GLU:HA	1:C:352:TRP:CD2	2.46	0.51
1:E:481:ASN:ND2	1:E:483:SER:O	2.44	0.51
1:A:481:ASN:ND2	1:A:483:SER:O	2.44	0.51
1:C:2:ARG:HD2	1:C:2:ARG:O	2.11	0.51
1:E:576:TRP:CB	6:E:873:HOH:O	2.41	0.51
1:C:602:VAL:HG11	1:C:605:MET:HG3	1.93	0.50
1:A:175:GLU:HA	1:A:352:TRP:CD2	2.46	0.50
1:E:2:ARG:HD2	1:E:2:ARG:O	2.11	0.50
1:E:401:MET:HE2	1:E:401:MET:CA	2.39	0.50
1:C:581:GLU:HG3	6:C:801:HOH:O	2.11	0.50
1:E:175:GLU:HA	1:E:352:TRP:CD2	2.46	0.49
1:C:72:TYR:CZ	1:C:476:LYS:HD3	2.47	0.49
1:A:47:ASP:OD1	1:A:49:ARG:HD3	2.12	0.49
1:E:72:TYR:CZ	1:E:476:LYS:HD3	2.47	0.49
1:A:593:ARG:CG	1:C:42:GLY:HA2	2.43	0.49
1:C:1:PRO:HD2	1:C:238:GLU:OE2	2.13	0.49
1:A:534:SER:O	1:C:48:PRO:HG2	2.13	0.49
1:E:47:ASP:OD1	1:E:49:ARG:HD3	2.12	0.49
2:D:706:GTP:N7	2:D:706:GTP:PG	2.85	0.49
1:E:251:ARG:NH1	1:E:255:GLN:HE22	1.95	0.49
1:E:602:VAL:HG11	1:E:605:MET:HG3	1.93	0.49
1:A:72:TYR:CZ	1:A:476:LYS:HD3	2.47	0.49
1:E:90:MET:HE2	1:E:90:MET:CA	2.42	0.49
1:A:1:PRO:HD2	1:A:238:GLU:OE2	2.13	0.49
1:E:1:PRO:HD2	1:E:238:GLU:OE2	2.13	0.49
2:B:706:GTP:N7	2:B:706:GTP:PG	2.85	0.48
1:A:602:VAL:HG11	1:A:605:MET:HG3	1.94	0.48
2:F:706:GTP:N7	2:F:706:GTP:PG	2.85	0.48
1:E:652:GLU:H	1:E:652:GLU:CD	2.21	0.48
1:A:72:TYR:CE1	1:A:476:LYS:HD3	2.48	0.48
1:E:72:TYR:CE1	1:E:476:LYS:HD3	2.48	0.48
1:C:47:ASP:OD1	1:C:49:ARG:HD3	2.12	0.48
1:A:29:LYS:O	1:A:30:ARG:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:GLU:H	1:C:652:GLU:CD	2.21	0.48
1:E:56:GLU:HG2	1:E:574:CYS:SG	2.54	0.48
1:C:56:GLU:HG2	1:C:574:CYS:SG	2.54	0.48
1:A:56:GLU:HG2	1:A:574:CYS:SG	2.54	0.48
1:E:273:MET:HE3	1:E:392:SER:OG	2.14	0.48
1:A:364:PRO:HA	1:A:387:LEU:CD2	2.37	0.47
1:A:273:MET:HE3	1:A:392:SER:OG	2.14	0.47
1:C:72:TYR:CE1	1:C:476:LYS:HD3	2.48	0.47
1:C:273:MET:HE3	1:C:392:SER:OG	2.14	0.47
1:A:305:THR:OG1	1:A:306:THR:N	2.47	0.47
1:C:29:LYS:O	1:C:30:ARG:C	2.57	0.47
1:E:602:VAL:CG1	1:E:605:MET:HG3	2.45	0.47
1:A:602:VAL:CG1	1:A:605:MET:HG3	2.45	0.47
1:A:652:GLU:CD	1:A:652:GLU:H	2.21	0.47
1:C:602:VAL:CG1	1:C:605:MET:HG3	2.45	0.47
1:C:633:THR:O	1:C:634:GLU:C	2.58	0.47
1:A:153:ILE:HA	1:A:153:ILE:HD12	1.41	0.47
1:A:401:MET:HA	1:A:401:MET:CE	2.43	0.47
1:C:86:GLY:O	1:C:89:HIS:HD2	1.98	0.47
1:E:633:THR:O	1:E:634:GLU:C	2.58	0.47
1:A:427:LYS:HE3	1:E:12:ILE:CG2	2.45	0.47
1:A:633:THR:O	1:A:634:GLU:C	2.58	0.47
1:C:235:THR:O	1:C:238:GLU:HG3	2.15	0.47
1:E:305:THR:OG1	1:E:306:THR:N	2.47	0.47
1:C:606:ALA:O	1:C:608:GLN:N	2.45	0.47
1:A:235:THR:O	1:A:238:GLU:HG3	2.15	0.46
1:E:235:THR:O	1:E:238:GLU:HG3	2.14	0.46
1:E:29:LYS:O	1:E:30:ARG:C	2.57	0.46
1:C:226:MET:HE1	1:C:244:ALA:CB	2.42	0.46
1:E:145:ILE:HD12	1:E:164:ILE:HD13	1.98	0.46
1:E:606:ALA:O	1:E:608:GLN:N	2.45	0.46
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.98	0.46
1:C:401:MET:HA	1:C:401:MET:CE	2.43	0.46
1:A:90:MET:HE2	1:A:90:MET:CA	2.42	0.46
1:E:204:ARG:HD2	1:E:530:TYR:OH	2.15	0.46
1:C:304:HIS:HA	1:C:309:ASN:ND2	2.30	0.46
1:E:86:GLY:O	1:E:89:HIS:HD2	1.98	0.46
1:E:226:MET:HE1	1:E:244:ALA:CB	2.42	0.46
1:C:51:LEU:CD2	1:C:90:MET:HE1	2.46	0.46
1:E:304:HIS:HA	1:E:309:ASN:ND2	2.30	0.46
1:A:51:LEU:CD2	1:A:90:MET:HE1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.77	0.46
1:E:51:LEU:CD2	1:E:90:MET:HE1	2.46	0.46
1:A:86:GLY:O	1:A:89:HIS:HD2	1.98	0.46
1:C:145:ILE:HD12	1:C:164:ILE:HD13	1.98	0.46
1:E:232:TYR:HA	1:E:239:GLN:O	2.15	0.46
1:A:232:TYR:HA	1:A:239:GLN:O	2.15	0.45
1:A:304:HIS:HA	1:A:309:ASN:ND2	2.30	0.45
1:A:132:ARG:HH12	1:A:429:MET:HG3	1.82	0.45
1:C:2:ARG:O	1:C:2:ARG:CD	2.65	0.45
1:C:90:MET:HE2	1:C:90:MET:CA	2.42	0.45
1:C:204:ARG:HD2	1:C:530:TYR:OH	2.15	0.45
1:C:305:THR:OG1	1:C:306:THR:N	2.47	0.45
1:C:395:GLN:HB3	1:C:398:THR:HG22	1.98	0.45
1:E:640:ASN:OD1	1:E:640:ASN:N	2.48	0.45
1:C:662:MET:HB3	1:C:663:PRO:CD	2.47	0.45
1:E:395:GLN:HB3	1:E:398:THR:HG22	1.98	0.45
1:C:232:TYR:HA	1:C:239:GLN:O	2.15	0.45
1:A:204:ARG:HD2	1:A:530:TYR:OH	2.15	0.45
1:A:315:LYS:HE3	1:A:512:ALA:O	2.17	0.45
1:A:395:GLN:HB3	1:A:398:THR:HG22	1.98	0.45
1:A:607:ARG:O	1:A:608:GLN:HG3	2.16	0.45
1:C:132:ARG:HH12	1:C:429:MET:HG3	1.82	0.45
1:E:132:ARG:HH12	1:E:429:MET:HG3	1.82	0.45
1:E:607:ARG:O	1:E:608:GLN:HG3	2.16	0.45
1:E:315:LYS:HE3	1:E:512:ALA:O	2.17	0.45
1:C:135:PHE:HB3	1:C:349:TYR:OH	2.16	0.44
1:E:135:PHE:HB3	1:E:349:TYR:OH	2.16	0.44
1:A:135:PHE:HB3	1:A:349:TYR:OH	2.16	0.44
1:A:662:MET:HB3	1:A:663:PRO:CD	2.47	0.44
1:C:587:ARG:HA	1:C:587:ARG:HD2	1.77	0.44
1:E:2:ARG:O	1:E:2:ARG:CD	2.64	0.44
1:E:662:MET:HB3	1:E:663:PRO:CD	2.47	0.44
1:A:270:ARG:NH2	2:B:707:G:O2'	2.50	0.44
1:E:270:ARG:NH2	2:F:707:G:O2'	2.50	0.44
1:C:607:ARG:O	1:C:608:GLN:HG3	2.16	0.44
1:A:2:ARG:O	1:A:2:ARG:CD	2.65	0.44
1:A:160:MET:O	1:A:164:ILE:HG12	2.18	0.44
1:E:650:SER:OG	1:E:653:LYS:CG	2.66	0.44
1:A:525:GLN:NE2	1:A:583:TYR:OH	2.51	0.44
1:C:270:ARG:NH2	2:D:707:G:O2'	2.50	0.44
1:C:315:LYS:HE3	1:C:512:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:PRO:HA	1:C:387:LEU:CD2	2.37	0.44
1:C:640:ASN:OD1	1:C:640:ASN:N	2.48	0.44
1:E:328:HIS:HD2	1:E:329:ASP:OD1	2.01	0.44
1:E:417:HIS:CE1	1:E:474:MET:HE1	2.53	0.44
1:C:16:MET:HE2	1:C:16:MET:HB3	1.79	0.44
1:A:328:HIS:HD2	1:A:329:ASP:OD1	2.01	0.43
1:A:407:SER:OG	1:A:448:GLN:NE2	2.51	0.43
1:C:204:ARG:HE	1:C:204:ARG:HB3	1.56	0.43
1:C:417:HIS:CE1	1:C:474:MET:HE1	2.53	0.43
1:C:650:SER:OG	1:C:653:LYS:CG	2.66	0.43
1:E:160:MET:O	1:E:164:ILE:HG12	2.18	0.43
1:C:407:SER:OG	1:C:448:GLN:NE2	2.51	0.43
1:E:202:VAL:CG2	1:E:272:ALA:HB3	2.48	0.43
1:A:640:ASN:OD1	1:A:640:ASN:N	2.48	0.43
1:C:328:HIS:HD2	1:C:329:ASP:OD1	2.01	0.43
1:A:75:VAL:HG21	1:A:500:ILE:HG21	2.01	0.43
1:A:251:ARG:NH1	1:A:255:GLN:HE22	1.95	0.43
1:C:251:ARG:HB2	1:C:255:GLN:NE2	2.33	0.43
1:C:525:GLN:NE2	1:C:583:TYR:OH	2.51	0.43
1:E:387:LEU:HD12	1:E:387:LEU:HA	1.75	0.43
1:A:214:ASP:HB3	1:A:217:THR:OG1	2.18	0.43
1:E:525:GLN:NE2	1:E:583:TYR:OH	2.51	0.43
1:E:587:ARG:HA	1:E:587:ARG:HD2	1.77	0.43
1:A:650:SER:OG	1:A:653:LYS:HG3	2.18	0.43
1:C:160:MET:O	1:C:164:ILE:HG12	2.18	0.43
1:C:251:ARG:HB2	1:C:255:GLN:HE21	1.84	0.43
1:E:75:VAL:HG21	1:E:500:ILE:HG21	2.01	0.43
1:E:214:ASP:HB3	1:E:217:THR:OG1	2.18	0.43
1:E:407:SER:OG	1:E:448:GLN:NE2	2.51	0.43
1:E:650:SER:OG	1:E:653:LYS:HG3	2.19	0.43
1:E:251:ARG:HB2	1:E:255:GLN:NE2	2.34	0.43
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.77	0.43
1:A:251:ARG:HB2	1:A:255:GLN:NE2	2.34	0.43
1:A:305:THR:H	1:A:309:ASN:ND2	2.17	0.43
1:C:214:ASP:HB3	1:C:217:THR:OG1	2.18	0.43
1:E:78:ASN:HD22	1:E:80:VAL:H	1.64	0.43
1:A:651:VAL:O	1:A:655:GLU:HB2	2.19	0.43
1:C:202:VAL:CG2	1:C:272:ALA:HB3	2.48	0.43
1:C:663:PRO:HD2	1:C:664:ARG:H	1.83	0.43
1:E:663:PRO:HD2	1:E:664:ARG:H	1.83	0.43
1:A:251:ARG:HB2	1:A:255:GLN:HE21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:HIS:CE1	1:A:474:MET:HE1	2.53	0.43
1:A:650:SER:OG	1:A:653:LYS:CG	2.66	0.43
1:E:305:THR:H	1:E:309:ASN:ND2	2.17	0.43
1:A:16:MET:HE2	1:A:16:MET:HB3	1.79	0.42
1:A:78:ASN:HD22	1:A:80:VAL:H	1.64	0.42
1:E:16:MET:HE2	1:E:16:MET:HB3	1.79	0.42
1:E:251:ARG:HB2	1:E:255:GLN:HE21	1.84	0.42
1:A:663:PRO:HD2	1:A:664:ARG:H	1.83	0.42
1:E:132:ARG:CZ	1:E:343:GLU:OE2	2.67	0.42
1:A:132:ARG:CZ	1:A:343:GLU:OE2	2.68	0.42
1:A:42:GLY:O	1:C:256:TYR:HB3	2.20	0.42
1:E:518:ILE:HG21	1:E:563:ILE:HD11	2.01	0.42
1:E:568:LEU:HA	1:E:568:LEU:HD23	1.82	0.42
1:A:202:VAL:CG2	1:A:272:ALA:HB3	2.48	0.42
1:C:580:GLY:C	1:C:581:GLU:HG2	2.44	0.42
1:C:651:VAL:O	1:C:655:GLU:HB2	2.19	0.42
1:A:86:GLY:O	1:A:89:HIS:CD2	2.73	0.42
1:A:554:MET:HE2	1:A:554:MET:HB3	1.93	0.42
1:A:631:LYS:HE3	1:A:632:TRP:CZ2	2.55	0.42
1:E:606:ALA:C	1:E:608:GLN:N	2.78	0.42
1:E:651:VAL:O	1:E:655:GLU:HB2	2.19	0.42
1:A:593:ARG:HG2	1:C:42:GLY:HA2	2.02	0.42
1:A:606:ALA:O	1:A:608:GLN:N	2.45	0.42
1:C:153:ILE:HB	1:C:276:PRO:HB3	2.02	0.42
1:E:226:MET:HE2	1:E:244:ALA:HA	2.01	0.42
1:C:305:THR:H	1:C:309:ASN:ND2	2.17	0.42
1:E:153:ILE:HD12	1:E:153:ILE:HA	1.41	0.42
1:A:153:ILE:HB	1:A:276:PRO:HB3	2.02	0.42
1:C:132:ARG:CZ	1:C:343:GLU:OE2	2.67	0.42
1:C:650:SER:OG	1:C:653:LYS:HG3	2.19	0.42
1:E:225:ARG:HD3	1:E:225:ARG:HA	1.87	0.42
1:C:86:GLY:O	1:C:89:HIS:CD2	2.73	0.41
1:C:225:ARG:HA	1:C:225:ARG:HD3	1.87	0.41
1:E:631:LYS:HE3	1:E:632:TRP:CZ2	2.55	0.41
1:A:226:MET:HE2	1:A:244:ALA:HA	2.01	0.41
1:C:518:ILE:HG21	1:C:563:ILE:HD11	2.01	0.41
1:C:631:LYS:HE3	1:C:632:TRP:CZ2	2.55	0.41
1:C:75:VAL:HG21	1:C:500:ILE:HG21	2.01	0.41
1:E:94:PRO:CB	1:E:269:ARG:HG3	2.51	0.41
1:E:580:GLY:C	1:E:581:GLU:HG2	2.44	0.41
1:E:49:ARG:CZ	6:E:801:HOH:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:HA	1:A:225:ARG:HD3	1.87	0.41
1:A:552:ALA:HB3	1:A:619:LEU:HD13	2.03	0.41
1:A:580:GLY:C	1:A:581:GLU:HG2	2.44	0.41
1:C:226:MET:HE2	1:C:244:ALA:HA	2.01	0.41
1:C:552:ALA:HB3	1:C:619:LEU:HD13	2.03	0.41
1:C:561:CYS:O	1:C:562:PRO:C	2.64	0.41
1:C:596:LEU:CD2	1:C:608:GLN:HG2	2.51	0.41
1:E:153:ILE:HB	1:E:276:PRO:HB3	2.02	0.41
1:E:300:TYR:CD1	1:E:300:TYR:C	2.99	0.41
1:A:3:ARG:HH22	1:A:231:GLU:CD	2.29	0.41
1:A:404:LEU:C	1:A:404:LEU:CD1	2.94	0.41
1:A:492:HIS:HB2	6:A:875:HOH:O	2.21	0.41
1:A:606:ALA:C	1:A:608:GLN:N	2.78	0.41
1:C:3:ARG:HH22	1:C:231:GLU:CD	2.29	0.41
1:A:94:PRO:CB	1:A:269:ARG:HG3	2.51	0.41
1:A:518:ILE:HG21	1:A:563:ILE:HD11	2.01	0.41
1:C:51:LEU:HD22	1:C:90:MET:HE1	2.03	0.41
1:C:202:VAL:O	1:C:202:VAL:HG23	2.21	0.41
1:C:295:TYR:O	1:C:299:ALA:HB2	2.21	0.41
1:E:2:ARG:CD	1:E:2:ARG:C	2.94	0.41
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.92	0.41
1:A:596:LEU:CD2	1:A:608:GLN:HG2	2.51	0.41
1:C:392:SER:O	1:C:398:THR:HG21	2.21	0.41
1:C:404:LEU:CD1	1:C:404:LEU:C	2.94	0.41
1:C:492:HIS:HB2	6:C:876:HOH:O	2.21	0.41
1:C:650:SER:HG	1:C:653:LYS:CG	2.34	0.41
1:A:51:LEU:HD22	1:A:90:MET:HE1	2.03	0.40
1:A:392:SER:O	1:A:398:THR:HG21	2.21	0.40
1:A:543:LYS:O	1:A:625:PRO:HD2	2.21	0.40
1:E:202:VAL:O	1:E:202:VAL:HG23	2.21	0.40
1:A:561:CYS:O	1:A:562:PRO:C	2.64	0.40
1:A:568:LEU:HA	1:A:568:LEU:HD23	1.81	0.40
1:C:78:ASN:HD22	1:C:80:VAL:H	1.64	0.40
1:C:153:ILE:HD12	1:C:153:ILE:HA	1.41	0.40
1:E:51:LEU:HD22	1:E:90:MET:HE1	2.03	0.40
1:E:552:ALA:HB3	1:E:619:LEU:HD13	2.03	0.40
1:E:596:LEU:CD2	1:E:608:GLN:HG2	2.51	0.40
1:C:94:PRO:CB	1:C:269:ARG:HG3	2.51	0.40
1:C:139:GLU:HA	1:C:140:PRO:HD3	1.96	0.40
1:A:2:ARG:CD	1:A:2:ARG:C	2.94	0.40
1:A:226:MET:HE1	1:A:244:ALA:CB	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:ARG:HH22	1:E:231:GLU:CD	2.29	0.40
1:E:543:LYS:O	1:E:625:PRO:HD2	2.21	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:860:HOH:O	6:C:804:HOH:O[2_646]	0.65	1.55
6:C:861:HOH:O	6:E:805:HOH:O[2_555]	1.48	0.72
1:E:479:LYS:NZ	1:E:607:ARG:C[2_445]	1.70	0.50
1:E:479:LYS:NZ	1:E:608:GLN:N[2_445]	1.93	0.27
1:A:569:GLU:OE2	1:E:1:PRO:CB[2_555]	2.08	0.12
1:C:607:ARG:CD	1:E:44:LEU:CD1[1_655]	2.12	0.08
1:E:479:LYS:CD	1:E:608:GLN:CB[2_445]	2.12	0.08
1:A:652:GLU:OE2	1:E:664:ARG:NH2[2_545]	2.15	0.05
1:E:479:LYS:NZ	1:E:607:ARG:O[2_445]	2.19	0.01

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	662/664 (100%)	629 (95%)	28 (4%)	5 (1%)	16	20
1	C	662/664 (100%)	630 (95%)	27 (4%)	5 (1%)	16	20
1	E	662/664 (100%)	629 (95%)	27 (4%)	6 (1%)	14	17
All	All	1986/1992 (100%)	1888 (95%)	82 (4%)	16 (1%)	16	20

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ILE
1	A	608	GLN

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Mol	Chain	Res	Type
1	C	153	ILE
1	C	608	GLN
1	E	153	ILE
1	E	608	GLN
1	A	607	ARG
1	A	630	TYR
1	C	607	ARG
1	C	630	TYR
1	E	607	ARG
1	E	630	TYR
1	A	604	SER
1	C	604	SER
1	E	604	SER
1	E	2	ARG

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	557/557 (100%)	527 (95%)	30 (5%)	20	29
1	C	557/557 (100%)	527 (95%)	30 (5%)	20	29
1	E	557/557 (100%)	527 (95%)	30 (5%)	20	29
All	All	1671/1671 (100%)	1581 (95%)	90 (5%)	20	29

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	43	LEU
1	A	44	LEU
1	A	71	GLU
1	A	74	ARG
1	A	75	VAL
1	A	78	ASN
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	119	VAL
1	A	143	LEU
1	A	146	ARG
1	A	153	ILE
1	A	204	ARG
1	A	241	SER
1	A	273	MET
1	A	301	THR
1	A	363	LEU
1	A	373	GLU
1	A	387	LEU
1	A	391	LEU
1	A	404	LEU
1	A	445	GLU
1	A	470	ARG
1	A	497	LEU
1	A	534	SER
1	A	556	ASP
1	A	581	GLU
1	A	587	ARG
1	A	591	LEU
1	A	651	VAL
1	C	16	MET
1	C	43	LEU
1	C	44	LEU
1	C	71	GLU
1	C	74	ARG
1	C	75	VAL
1	C	78	ASN
1	C	102	LEU
1	C	119	VAL
1	C	143	LEU
1	C	146	ARG
1	C	153	ILE
1	C	204	ARG
1	C	241	SER
1	C	273	MET
1	C	301	THR
1	C	363	LEU
1	C	373	GLU
1	C	387	LEU
1	C	391	LEU

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Mol	Chain	Res	Type
1	C	404	LEU
1	C	445	GLU
1	C	470	ARG
1	C	497	LEU
1	C	534	SER
1	C	556	ASP
1	C	581	GLU
1	C	587	ARG
1	C	591	LEU
1	C	651	VAL
1	E	16	MET
1	E	43	LEU
1	E	44	LEU
1	E	71	GLU
1	E	74	ARG
1	E	75	VAL
1	E	78	ASN
1	E	102	LEU
1	E	119	VAL
1	E	143	LEU
1	E	146	ARG
1	E	153	ILE
1	E	204	ARG
1	E	241	SER
1	E	273	MET
1	E	301	THR
1	E	363	LEU
1	E	373	GLU
1	E	387	LEU
1	E	391	LEU
1	E	404	LEU
1	E	445	GLU
1	E	470	ARG
1	E	497	LEU
1	E	534	SER
1	E	556	ASP
1	E	581	GLU
1	E	587	ARG
1	E	591	LEU
1	E	651	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	26	GLN
1	A	64	HIS
1	A	78	ASN
1	A	89	HIS
1	A	91	ASN
1	A	191	GLN
1	A	206	GLN
1	A	255	GLN
1	A	309	ASN
1	A	328	HIS
1	A	448	GLN
1	A	519	ASN
1	A	525	GLN
1	A	608	GLN
1	A	626	ASN
1	C	26	GLN
1	C	64	HIS
1	C	78	ASN
1	C	89	HIS
1	C	91	ASN
1	C	191	GLN
1	C	206	GLN
1	C	255	GLN
1	C	309	ASN
1	C	328	HIS
1	C	448	GLN
1	C	519	ASN
1	C	525	GLN
1	C	626	ASN
1	E	26	GLN
1	E	78	ASN
1	E	89	HIS
1	E	91	ASN
1	E	191	GLN
1	E	206	GLN
1	E	255	GLN
1	E	309	ASN
1	E	328	HIS
1	E	448	GLN
1	E	519	ASN
1	E	525	GLN
1	E	626	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	0/2	-	-
2	D	0/2	-	-
2	F	0/2	-	-
All	All	0/6	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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	GTP	D	706	2,4	33,34,34	0.90	1 (3%)	50,54,54	0.70	1 (2%)
2	GTP	B	706	2,4	33,34,34	0.90	1 (3%)	50,54,54	0.70	1 (2%)
2	GTP	F	706	2,4	33,34,34	0.90	1 (3%)	50,54,54	0.70	1 (2%)

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	GTP	D	706	2,4	-	3/22/38/38	0/3/3/3
2	GTP	B	706	2,4	-	3/22/38/38	0/3/3/3
2	GTP	F	706	2,4	-	3/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	706	GTP	PB-O3B	4.09	1.63	1.59
2	B	706	GTP	PB-O3B	4.08	1.63	1.59
2	D	706	GTP	PB-O3B	4.08	1.63	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	706	GTP	O3A-PB-O1B	-2.53	103.11	110.70
2	D	706	GTP	O3A-PB-O1B	-2.52	103.12	110.70
2	F	706	GTP	O3A-PB-O1B	-2.52	103.13	110.70

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	706	GTP	C5'-O5'-PA-O3A
2	B	706	GTP	C5'-O5'-PA-O1A
2	B	706	GTP	C5'-O5'-PA-O2A
2	D	706	GTP	C5'-O5'-PA-O3A
2	D	706	GTP	C5'-O5'-PA-O1A
2	D	706	GTP	C5'-O5'-PA-O2A
2	F	706	GTP	C5'-O5'-PA-O3A
2	F	706	GTP	C5'-O5'-PA-O1A
2	F	706	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	706	GTP	4	0
2	B	706	GTP	4	0
2	F	706	GTP	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	POP	A	703	4	6,8,8	1.29	0	12,13,13	0.95	0
5	POP	E	701	4	6,8,8	1.29	0	12,13,13	0.95	0
5	POP	C	701	4	6,8,8	1.30	0	12,13,13	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POP	A	703	4	-	0/6/6/6	-
5	POP	E	701	4	-	0/6/6/6	-
5	POP	C	701	4	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	664/664 (100%)	0.26	30 (4%)	38	37	22, 38, 66, 119	0
1	C	664/664 (100%)	0.27	41 (6%)	26	24	22, 38, 66, 119	0
1	E	664/664 (100%)	0.31	30 (4%)	38	37	22, 38, 66, 119	0
2	B	1/2 (50%)	2.36	1 (100%)	0	0	74, 74, 74, 74	0
2	D	1/2 (50%)	1.74	0	100	100	74, 74, 74, 74	0
2	F	1/2 (50%)	1.24	0	100	100	74, 74, 74, 74	0
All	All	1995/1998 (99%)	0.28	102 (5%)	33	31	22, 38, 66, 119	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	609	ALA	8.3
1	C	607	ARG	7.3
1	A	606	ALA	6.6
1	C	609	ALA	6.4
1	A	610	GLY	6.0
1	A	609	ALA	5.8
1	E	608	GLN	5.7
1	E	1	PRO	5.7
1	E	606	ALA	5.6
1	A	603	ALA	5.3
1	C	1	PRO	5.2
1	C	2	ARG	5.0
1	E	612	ALA	4.9
1	C	537	ARG	4.9
1	E	610	GLY	4.9
1	A	1	PRO	4.7
1	C	603	ALA	4.6
1	E	576	TRP	4.4
1	E	605	MET	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	664	ARG	4.3
1	A	605	MET	4.2
1	E	664	ARG	4.1
1	A	608	GLN	4.0
1	A	204	ARG	4.0
1	A	607	ARG	4.0
1	C	608	GLN	4.0
1	E	2	ARG	3.9
1	E	611	LEU	3.9
1	A	611	LEU	3.9
1	E	607	ARG	3.8
1	C	610	GLY	3.8
1	C	470	ARG	3.7
1	A	257	GLY	3.6
1	C	204	ARG	3.4
1	A	158	ASN	3.3
1	E	479	LYS	3.3
1	E	470	ARG	3.3
1	E	308	LEU	3.2
1	A	604	SER	3.2
1	E	603	ALA	3.1
1	C	257	GLY	3.1
1	A	664	ARG	3.1
1	C	606	ALA	3.1
1	C	600	ARG	3.1
1	A	537	ARG	3.0
1	A	600	ARG	3.0
1	C	308	LEU	2.9
1	C	604	SER	2.9
1	C	581	GLU	2.9
1	C	599	SER	2.9
1	E	600	ARG	2.8
1	A	576	TRP	2.8
1	C	20	ASN	2.8
1	C	253	LYS	2.8
1	C	506	ARG	2.7
1	C	596	LEU	2.7
1	C	629	GLN	2.7
1	A	308	LEU	2.6
1	A	652	GLU	2.6
1	C	153	ILE	2.6
1	E	204	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	602	VAL	2.6
1	A	629	GLN	2.6
1	C	219	LYS	2.6
1	A	153	ILE	2.6
1	A	612	ALA	2.5
1	C	19	ALA	2.5
1	A	630	TYR	2.5
1	C	651	VAL	2.5
1	C	254	GLU	2.5
1	A	651	VAL	2.5
1	C	307	ARG	2.5
1	C	652	GLU	2.4
1	A	599	SER	2.4
1	A	149	SER	2.4
1	E	613	GLU	2.4
2	B	707	G	2.4
1	E	596	LEU	2.3
1	C	479	LYS	2.3
1	C	492	HIS	2.3
1	C	315	LYS	2.3
1	C	215	PRO	2.3
1	C	191	GLN	2.3
1	E	505	SER	2.3
1	C	158	ASN	2.2
1	E	506	ARG	2.3
1	C	612	ALA	2.2
1	E	604	SER	2.2
1	C	214	ASP	2.2
1	C	63	ASP	2.2
1	E	601	TYR	2.2
1	E	217	THR	2.1
1	C	269	ARG	2.1
1	E	216	LYS	2.1
1	A	492	HIS	2.1
1	A	2	ARG	2.1
1	E	153	ILE	2.1
1	E	659	ARG	2.0
1	E	652	GLU	2.0
1	C	30	ARG	2.0
1	E	218	GLY	2.0
1	A	601	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GTP	B	706	32/32	0.87	0.12	53,63,70,74	0
2	GTP	F	706	32/32	0.89	0.12	53,63,70,74	0
2	GTP	D	706	32/32	0.90	0.12	53,63,70,74	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	C	702	1/1	0.58	0.21	58,58,58,58	0
4	MG	E	702	1/1	0.59	0.19	58,58,58,58	0
5	POP	A	703	9/9	0.71	0.13	108,111,113,113	0
5	POP	E	701	9/9	0.73	0.16	108,111,113,113	0
5	POP	C	701	9/9	0.78	0.17	108,111,113,113	0
4	MG	A	702	1/1	0.82	0.11	58,58,58,58	0
4	MG	F	801	1/1	0.87	0.09	35,35,35,35	0
4	MG	B	801	1/1	0.90	0.09	35,35,35,35	0
4	MG	D	801	1/1	0.90	0.11	35,35,35,35	0
3	MN	E	703	1/1	0.94	0.05	50,50,50,50	0
3	MN	A	701	1/1	0.98	0.05	50,50,50,50	0
3	MN	C	703	1/1	0.98	0.08	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.