



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:35 AM UTC

PDB ID : 4DPV / pdb_00004dpv
Title : PARVOVIRUS/DNA COMPLEX
Authors : Chapman, M.S.; Rossmann, M.G.
Deposited on : 1996-02-01
Resolution : 2.90 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
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

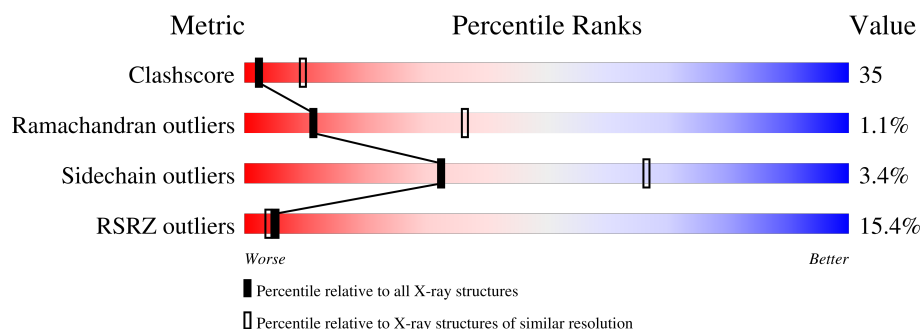
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	N	11	55% 27% 36% 36%
2	Z	584	14% 42% 40% 13% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4606 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 DNA chain called DNA (5'-D(*AP*TP*AP*CP*CP*TP*CP*TP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	11	Total	C	N	O	P	0	0	0
			212	101	31	69	11			

- Molecule 2 is a protein called PROTEIN (PARVOVIRUS COAT PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	559	Total	C	N	O	S	0	0	0
			4390	2780	753	841	16			

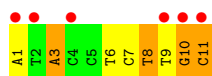
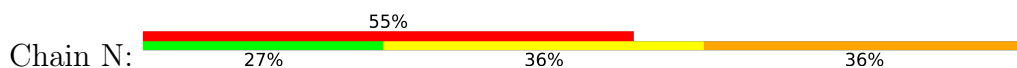
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	N	2	Total	Mg	0	0
			2	2		
3	Z	2	Total	Mg	0	0
			2	2		

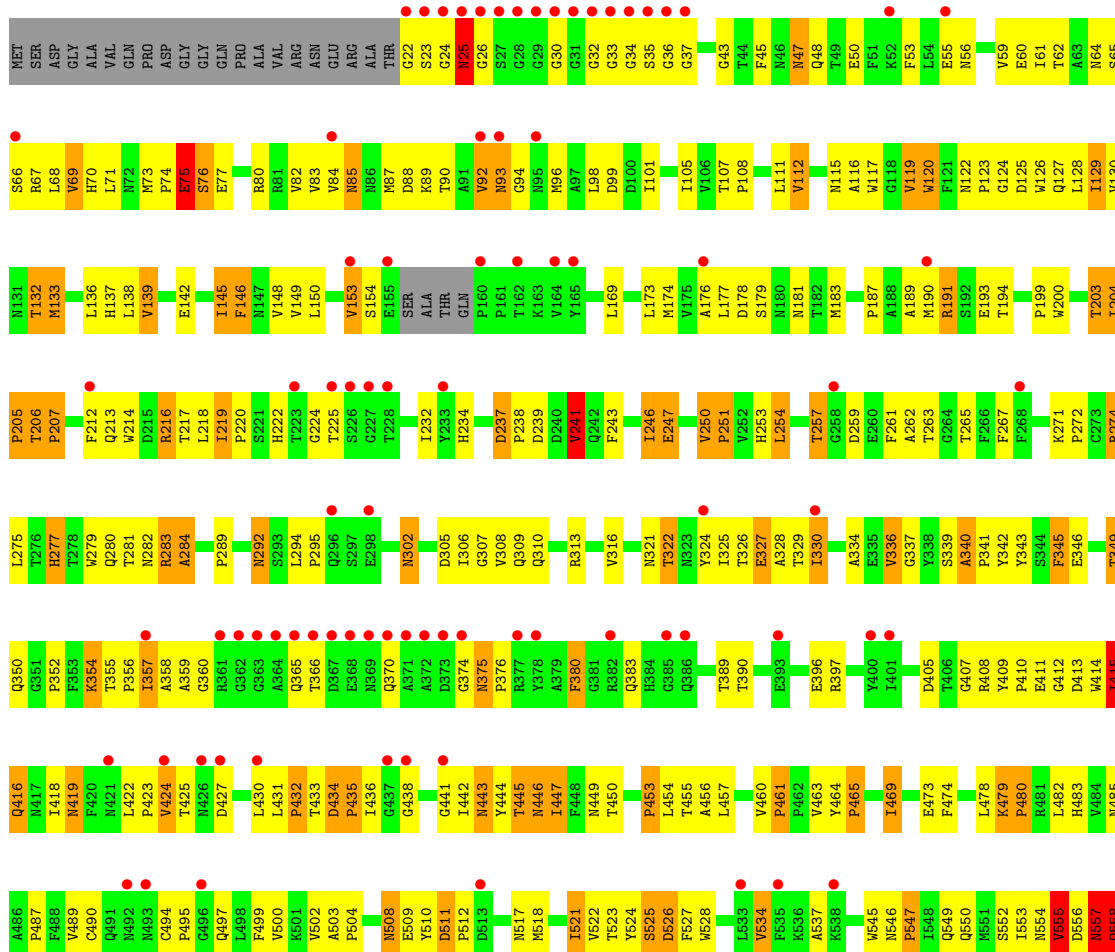
3 Residue-property plots

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: DNA (5'-D(*AP*TP*AP*CP*CP*TP*CP*TP*TP*GP*C)-3')



- Molecule 2: PROTEIN (PARVOVIRUS COAT PROTEIN)



F559	N560	Y561	V562	P563	S564	N565	I566	G567	G568	I571	V572	Y573	E574	L578	A579	P580	L583	Y584
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	263.21Å 349.01Å 267.32Å 90.00° 90.82° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90 200.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90) 99.9 (200.00-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.52Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , 0.283 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 109.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.018 for l,k,-h 0.023 for h,-k,-l 0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.22	EDS
Total number of atoms	4606	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	N	1.24	1/233 (0.4%)	1.58	8/354 (2.3%)
2	Z	1.79	60/4518 (1.3%)	2.04	153/6172 (2.5%)
All	All	1.76	61/4751 (1.3%)	2.01	161/6526 (2.5%)

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
2	Z	0	2

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	35	SER	C-N	9.26	1.43	1.33
2	Z	24	GLY	C-N	9.18	1.46	1.33
2	Z	33	GLY	C-O	8.00	1.32	1.23
2	Z	33	GLY	C-N	7.91	1.43	1.33
2	Z	26	GLY	C-O	7.70	1.33	1.23
2	Z	107	THR	C-N	-7.62	1.26	1.33
2	Z	34	GLY	CA-C	7.45	1.60	1.52
1	N	1	DA	OP3-P	7.35	1.63	1.48
2	Z	30	GLY	C-N	7.00	1.43	1.33
2	Z	34	GLY	N-CA	6.72	1.54	1.45
2	Z	75	GLU	CD-OE2	6.67	1.38	1.25
2	Z	133	MET	CA-CB	-6.57	1.43	1.53
2	Z	37	GLY	N-CA	6.41	1.51	1.45
2	Z	36	GLY	N-CA	6.41	1.51	1.45
2	Z	34	GLY	C-N	6.32	1.42	1.33
2	Z	26	GLY	CA-C	6.26	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	129	ILE	CA-CB	-6.17	1.47	1.54
2	Z	500	VAL	CA-C	-6.13	1.46	1.52
2	Z	24	GLY	C-O	6.08	1.31	1.24
2	Z	461	PRO	CA-C	-6.02	1.46	1.52
2	Z	447	ILE	CA-CB	-6.00	1.48	1.54
2	Z	37	GLY	CA-C	5.94	1.58	1.51
2	Z	23	SER	C-N	5.92	1.43	1.33
2	Z	22	GLY	C-N	5.89	1.41	1.33
2	Z	23	SER	C-O	5.88	1.31	1.23
2	Z	34	GLY	C-O	5.80	1.30	1.23
2	Z	61	ILE	CA-CB	-5.79	1.47	1.54
2	Z	30	GLY	C-O	5.72	1.31	1.23
2	Z	237	ASP	CG-OD2	5.71	1.36	1.25
2	Z	35	SER	CA-C	5.62	1.61	1.52
2	Z	32	GLY	C-N	5.55	1.40	1.33
2	Z	534	VAL	CA-CB	-5.55	1.47	1.54
2	Z	205	PRO	CA-C	-5.54	1.47	1.53
2	Z	36	GLY	CA-C	5.49	1.57	1.51
2	Z	33	GLY	CA-C	5.44	1.60	1.52
2	Z	274	ARG	CA-C	-5.44	1.45	1.52
2	Z	521	ILE	CA-CB	-5.42	1.48	1.54
2	Z	69	VAL	CA-CB	-5.41	1.47	1.54
2	Z	499	PHE	CA-C	-5.39	1.46	1.52
2	Z	206	THR	C-N	-5.38	1.27	1.33
2	Z	200	TRP	NE1-CE2	-5.36	1.31	1.37
2	Z	139	VAL	CA-CB	-5.34	1.50	1.55
2	Z	178	ASP	CA-C	-5.34	1.47	1.53
2	Z	250	VAL	CA-CB	-5.32	1.49	1.55
2	Z	194	THR	CA-C	-5.29	1.47	1.53
2	Z	23	SER	CA-C	5.24	1.60	1.53
2	Z	509	GLU	CD-OE2	5.21	1.35	1.25
2	Z	207	PRO	N-CA	-5.20	1.41	1.47
2	Z	500	VAL	CA-CB	-5.19	1.47	1.54
2	Z	133	MET	CA-C	-5.18	1.46	1.52
2	Z	434	ASP	CA-C	-5.18	1.47	1.53
2	Z	510	TYR	C-N	-5.17	1.29	1.33
2	Z	108	PRO	N-CA	-5.14	1.41	1.47
2	Z	25	ASN	CA-CB	5.10	1.62	1.53
2	Z	461	PRO	C-N	-5.09	1.27	1.33
2	Z	435	PRO	N-CA	-5.07	1.41	1.47
2	Z	145	ILE	CA-CB	-5.06	1.48	1.54
2	Z	129	ILE	N-CA	-5.06	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	460	VAL	C-N	-5.04	1.27	1.33
2	Z	25	ASN	CA-C	5.02	1.59	1.52
2	Z	36	GLY	C-N	5.01	1.38	1.33

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	25	ASN	CA-CB-CG	16.65	129.25	112.60
2	Z	241	VAL	N-CA-C	9.47	121.39	108.89
2	Z	359	ALA	N-CA-C	9.39	121.20	110.97
2	Z	30	GLY	CA-C-N	9.16	129.85	120.60
2	Z	30	GLY	C-N-CA	9.16	129.85	120.60
2	Z	345	PHE	CA-CB-CG	-8.93	104.87	113.80
2	Z	92	VAL	N-CA-C	8.69	119.49	110.36
2	Z	24	GLY	CA-C-N	8.58	137.93	121.54
2	Z	24	GLY	C-N-CA	8.58	137.93	121.54
1	N	3	DA	P-O5'-C5'	-8.42	107.37	120.00
2	Z	583	LEU	N-CA-C	-8.31	103.66	113.88
2	Z	133	MET	CA-CB-CG	-8.14	97.81	114.10
2	Z	480	PRO	CB-CA-C	-8.04	100.75	111.12
2	Z	499	PHE	CA-CB-CG	-8.03	105.77	113.80
2	Z	33	GLY	CA-C-N	8.02	128.82	120.00
2	Z	33	GLY	C-N-CA	8.02	128.82	120.00
2	Z	321	ASN	CB-CA-C	-7.95	97.44	110.79
2	Z	139	VAL	N-CA-C	7.88	118.88	111.48
2	Z	443	ASN	CA-CB-CG	-7.75	104.86	112.60
2	Z	375	ASN	CA-CB-CG	-7.69	104.91	112.60
2	Z	181	ASN	CA-CB-CG	-7.49	105.11	112.60
2	Z	241	VAL	CB-CA-C	-7.46	101.45	111.15
2	Z	133	MET	N-CA-C	7.31	120.88	110.14
2	Z	445	THR	CA-C-N	-7.24	108.47	121.14
2	Z	445	THR	C-N-CA	-7.24	108.47	121.14
2	Z	204	ILE	CA-C-N	7.07	128.49	120.85
2	Z	204	ILE	C-N-CA	7.07	128.49	120.85
2	Z	479	LYS	N-CA-C	7.01	119.48	108.55
2	Z	26	GLY	CA-C-O	6.92	128.26	122.24
2	Z	432	PRO	N-CA-C	-6.83	105.63	114.03
2	Z	53	PHE	CA-CB-CG	-6.79	107.01	113.80
2	Z	453	PRO	CA-C-N	-6.79	111.34	122.54
2	Z	453	PRO	C-N-CA	-6.79	111.34	122.54
2	Z	526	ASP	CA-CB-CG	-6.75	105.84	112.60
2	Z	405	ASP	CA-CB-CG	6.71	119.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	243	PHE	N-CA-CB	-6.66	100.71	110.84
2	Z	284	ALA	CA-C-N	-6.65	113.83	123.00
2	Z	284	ALA	C-N-CA	-6.65	113.83	123.00
2	Z	534	VAL	N-CA-C	6.62	117.37	108.11
2	Z	251	PRO	CA-C-N	-6.48	115.16	123.19
2	Z	251	PRO	C-N-CA	-6.48	115.16	123.19
2	Z	527	PHE	CA-CB-CG	-6.48	107.32	113.80
1	N	11	DC	P-O5'-C5'	6.43	129.65	120.00
2	Z	510	TYR	CA-C-N	-6.42	115.07	122.52
2	Z	510	TYR	C-N-CA	-6.42	115.07	122.52
2	Z	336	VAL	CB-CA-C	-6.39	102.27	111.34
2	Z	534	VAL	CB-CA-C	-6.37	101.20	110.63
2	Z	322	THR	CB-CA-C	-6.33	98.08	113.15
2	Z	120	TRP	CA-C-N	-6.32	112.89	122.81
2	Z	120	TRP	C-N-CA	-6.32	112.89	122.81
2	Z	316	VAL	N-CA-C	6.30	117.85	108.46
2	Z	259	ASP	CA-CB-CG	-6.30	106.30	112.60
2	Z	434	ASP	CA-CB-CG	-6.30	106.30	112.60
2	Z	36	GLY	N-CA-C	6.27	119.90	110.75
2	Z	567	GLY	CA-C-O	6.24	124.63	118.77
2	Z	199	PRO	CA-C-N	-6.17	111.94	122.56
2	Z	199	PRO	C-N-CA	-6.17	111.94	122.56
1	N	3	DA	N9-C1'-C2'	6.16	122.73	113.50
2	Z	292	ASN	CA-CB-CG	-6.14	106.46	112.60
2	Z	153	VAL	CB-CA-C	-6.13	102.50	110.84
2	Z	572	VAL	CB-CA-C	-6.09	104.89	111.59
2	Z	112	VAL	CB-CA-C	-6.02	103.56	111.81
2	Z	289	PRO	CB-CA-C	-6.01	103.22	111.21
2	Z	30	GLY	O-C-N	6.00	130.50	122.70
2	Z	334	ALA	CA-C-N	-6.00	113.51	122.39
2	Z	334	ALA	C-N-CA	-6.00	113.51	122.39
2	Z	419	ASN	CA-CB-CG	-5.99	106.61	112.60
2	Z	557	ASN	CA-CB-CG	-5.96	106.64	112.60
1	N	8	DT	O3'-P-O5'	-5.95	95.08	104.00
2	Z	129	ILE	N-CA-CB	-5.95	103.91	110.51
2	Z	247	GLU	CA-C-N	-5.92	112.78	122.54
2	Z	247	GLU	C-N-CA	-5.92	112.78	122.54
2	Z	119	VAL	CB-CA-C	-5.84	102.80	112.26
2	Z	169	LEU	CA-C-N	-5.83	113.32	122.65
2	Z	169	LEU	C-N-CA	-5.83	113.32	122.65
2	Z	558	GLN	CA-C-N	-5.83	111.83	122.38
2	Z	558	GLN	C-N-CA	-5.83	111.83	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	203	THR	CA-CB-CG2	-5.79	100.65	110.50
2	Z	489	VAL	CB-CA-C	-5.79	102.51	110.96
2	Z	132	THR	CA-C-N	-5.77	112.71	123.05
2	Z	132	THR	C-N-CA	-5.77	112.71	123.05
2	Z	139	VAL	CB-CA-C	-5.76	106.82	111.71
2	Z	349	THR	CA-C-N	-5.74	113.53	122.37
2	Z	349	THR	C-N-CA	-5.74	113.53	122.37
2	Z	525	SER	N-CA-C	5.72	117.88	109.24
2	Z	194	THR	CA-C-N	-5.71	110.69	121.66
2	Z	194	THR	C-N-CA	-5.71	110.69	121.66
2	Z	340	ALA	O-C-N	5.71	125.37	121.71
2	Z	380	PHE	N-CA-C	5.71	116.94	108.60
2	Z	145	ILE	CB-CA-C	-5.71	102.12	110.62
2	Z	559	PHE	CA-CB-CG	-5.69	108.11	113.80
2	Z	461	PRO	CB-CA-C	-5.68	103.99	110.92
2	Z	325	ILE	CA-C-N	-5.67	113.69	122.59
2	Z	325	ILE	C-N-CA	-5.67	113.69	122.59
2	Z	146	PHE	N-CA-C	5.62	115.66	108.24
2	Z	85	ASN	N-CA-C	5.61	118.99	107.37
2	Z	250	VAL	C-N-CD	-5.60	102.05	125.00
2	Z	283	ARG	CA-C-N	-5.58	114.32	122.86
2	Z	283	ARG	C-N-CA	-5.58	114.32	122.86
2	Z	578	LEU	N-CA-C	5.56	117.14	111.14
2	Z	132	THR	CA-CB-OG1	-5.54	101.28	109.60
2	Z	254	LEU	CA-C-N	-5.53	114.91	122.93
2	Z	254	LEU	C-N-CA	-5.53	114.91	122.93
2	Z	257	THR	CB-CA-C	-5.52	101.62	110.79
2	Z	246	ILE	CB-CA-C	-5.52	104.91	111.97
2	Z	94	GLY	N-CA-C	-5.51	107.06	115.00
2	Z	547	PRO	CB-CA-C	-5.51	102.90	111.22
2	Z	343	TYR	CA-C-N	-5.47	114.50	122.65
2	Z	343	TYR	C-N-CA	-5.47	114.50	122.65
2	Z	511	ASP	CA-CB-CG	-5.46	107.14	112.60
2	Z	469	ILE	CA-C-N	-5.45	114.04	122.59
2	Z	469	ILE	C-N-CA	-5.45	114.04	122.59
2	Z	357	ILE	CA-CB-CG1	-5.44	101.14	110.40
2	Z	487	PRO	CA-C-N	-5.42	115.46	123.05
2	Z	487	PRO	C-N-CA	-5.42	115.46	123.05
2	Z	194	THR	CA-CB-OG1	-5.42	101.47	109.60
2	Z	25	ASN	CB-CA-C	5.40	121.17	110.42
1	N	8	DT	P-O3'-C3'	5.39	128.29	120.20
2	Z	138	LEU	CA-C-N	-5.38	117.70	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	138	LEU	C-N-CA	-5.38	117.70	122.97
2	Z	277	HIS	CA-CB-CG	-5.36	108.44	113.80
2	Z	357	ILE	N-CA-CB	-5.36	105.69	112.60
2	Z	274	ARG	CA-CB-CG	-5.35	103.39	114.10
2	Z	567	GLY	N-CA-C	-5.31	107.30	116.01
2	Z	508	ASN	CA-C-N	-5.29	115.41	122.72
2	Z	508	ASN	C-N-CA	-5.29	115.41	122.72
2	Z	219	ILE	N-CA-C	5.29	113.18	108.63
2	Z	225	THR	CA-C-N	5.29	129.06	121.50
2	Z	225	THR	C-N-CA	5.29	129.06	121.50
2	Z	101	ILE	N-CA-C	5.28	116.83	109.80
2	Z	465	PRO	CA-C-N	-5.26	112.86	122.38
2	Z	465	PRO	C-N-CA	-5.26	112.86	122.38
1	N	1	DA	P-O3'-C3'	5.26	128.09	120.20
2	Z	107	THR	CB-CA-C	-5.25	102.09	109.96
2	Z	446	ASN	CA-CB-CG	-5.25	107.35	112.60
2	Z	508	ASN	CA-CB-CG	-5.25	107.36	112.60
2	Z	302	ASN	CA-CB-CG	-5.22	107.38	112.60
2	Z	322	THR	N-CA-C	5.22	117.95	109.86
2	Z	415	ILE	CA-C-N	-5.20	114.03	122.36
2	Z	415	ILE	C-N-CA	-5.20	114.03	122.36
2	Z	205	PRO	CB-CA-C	-5.18	102.64	110.20
1	N	10	DG	P-O3'-C3'	5.18	127.97	120.20
2	Z	479	LYS	CA-C-N	5.13	125.41	119.92
2	Z	479	LYS	C-N-CA	5.13	125.41	119.92
2	Z	179	SER	CA-C-N	-5.12	111.60	121.58
2	Z	179	SER	C-N-CA	-5.12	111.60	121.58
2	Z	26	GLY	N-CA-C	-5.10	106.31	112.48
2	Z	108	PRO	N-CA-C	-5.09	107.57	114.80
2	Z	560	ASN	CA-C-N	-5.09	114.58	122.67
2	Z	560	ASN	C-N-CA	-5.09	114.58	122.67
2	Z	447	ILE	CB-CA-C	-5.08	105.45	111.65
2	Z	310	GLN	CA-C-N	-5.08	114.56	122.73
2	Z	310	GLN	C-N-CA	-5.08	114.56	122.73
2	Z	187	PRO	CB-CA-C	-5.08	105.25	111.64
2	Z	219	ILE	CB-CA-C	-5.06	106.23	110.94
2	Z	212	PHE	CA-CB-CG	-5.06	108.74	113.80
2	Z	416	GLN	N-CA-C	5.05	116.67	109.14
2	Z	424	VAL	N-CA-C	5.03	116.49	109.55
1	N	1	DA	P-O5'-C5'	5.02	127.53	120.00
2	Z	555	VAL	CB-CA-C	-5.01	104.39	112.16
2	Z	504	PRO	CB-CA-C	-5.01	105.33	111.64

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Z	241	VAL	Mainchain
2	Z	25	ASN	Peptide

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	N	212	0	121	12	0
2	Z	4390	0	4172	306	0
3	N	2	0	0	0	0
3	Z	2	0	0	0	0
All	All	4606	0	4293	314	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 35.

All (314) 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)
2:Z:557:ASN:HD22	2:Z:558:GLN:N	1.49	1.09
2:Z:75:GLU:HG3	2:Z:76:SER:N	1.77	1.00
1:N:3:DA:N6	2:Z:267:PHE:H	1.60	0.99
1:N:3:DA:H61	2:Z:267:PHE:H	1.03	0.98
2:Z:554:ASN:H	2:Z:557:ASN:HD21	0.97	0.93
2:Z:366:THR:HA	2:Z:370:GLN:HB2	1.52	0.91
2:Z:193:GLU:HB3	2:Z:206:THR:HG21	1.51	0.90
2:Z:425:THR:HG22	2:Z:427:ASP:H	1.36	0.88
2:Z:173:LEU:HD12	2:Z:174:MET:N	1.88	0.88
2:Z:354:LYS:HD2	2:Z:355:THR:N	1.90	0.87
2:Z:557:ASN:HD22	2:Z:558:GLN:H	1.19	0.86
2:Z:479:LYS:HB3	2:Z:480:PRO:HD2	1.58	0.85
2:Z:204:ILE:HB	2:Z:205:PRO:HD2	1.59	0.84
2:Z:360:GLY:HA2	2:Z:374:GLY:HA3	1.58	0.84
2:Z:122:ASN:HB2	2:Z:123:PRO:HD2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:148:VAL:O	2:Z:257:THR:HG23	1.78	0.83
1:N:6:DT:H2''	1:N:7:DC:H5'	1.61	0.82
2:Z:554:ASN:N	2:Z:557:ASN:HD21	1.79	0.80
1:N:10:DG:H3'	1:N:11:DC:H5''	1.65	0.78
2:Z:73:MET:HB2	2:Z:74:PRO:HD2	1.65	0.78
2:Z:562:VAL:CG1	2:Z:563:PRO:HD2	2.14	0.78
1:N:3:DA:H61	2:Z:267:PHE:N	1.83	0.76
2:Z:562:VAL:HG13	2:Z:563:PRO:HD2	1.65	0.76
2:Z:232:ILE:HD11	2:Z:234:HIS:CE1	2.21	0.76
2:Z:431:LEU:HB3	2:Z:432:PRO:HD2	1.68	0.75
2:Z:430:LEU:C	2:Z:431:LEU:HD23	2.12	0.75
2:Z:422:LEU:HB2	2:Z:423:PRO:HA	1.68	0.75
2:Z:77:GLU:HG3	2:Z:518:MET:CE	2.17	0.73
2:Z:173:LEU:HD12	2:Z:174:MET:H	1.49	0.73
2:Z:366:THR:HA	2:Z:370:GLN:CB	2.19	0.72
2:Z:366:THR:O	2:Z:370:GLN:HG2	1.89	0.72
2:Z:557:ASN:ND2	2:Z:558:GLN:N	2.32	0.72
2:Z:271:LYS:HB3	2:Z:272:PRO:HD2	1.72	0.71
2:Z:322:THR:HB	2:Z:324:TYR:H	1.55	0.71
2:Z:354:LYS:HD2	2:Z:354:LYS:C	2.16	0.71
2:Z:457:LEU:N	2:Z:457:LEU:HD23	2.06	0.71
2:Z:494:CYS:HB3	2:Z:495:PRO:HD2	1.73	0.70
2:Z:422:LEU:HA	2:Z:423:PRO:C	2.15	0.70
2:Z:219:ILE:CG2	2:Z:220:PRO:HD2	2.21	0.70
2:Z:422:LEU:HD23	2:Z:422:LEU:N	2.05	0.70
2:Z:149:VAL:C	2:Z:150:LEU:HD12	2.16	0.70
2:Z:68:LEU:HD12	2:Z:69:VAL:N	2.08	0.69
2:Z:111:LEU:HD12	2:Z:112:VAL:N	2.08	0.69
1:N:3:DA:N6	2:Z:267:PHE:N	2.40	0.69
2:Z:250:VAL:HG12	2:Z:251:PRO:N	2.08	0.68
2:Z:326:THR:O	2:Z:329:THR:N	2.26	0.68
2:Z:340:ALA:HB1	2:Z:341:PRO:HD2	1.75	0.68
2:Z:422:LEU:HD23	2:Z:422:LEU:H	1.58	0.68
2:Z:409:TYR:CE2	2:Z:411:GLU:HB2	2.29	0.68
2:Z:583:LEU:C	2:Z:583:LEU:HD23	2.20	0.67
2:Z:92:VAL:O	2:Z:93:ASN:HB2	1.95	0.66
1:N:10:DG:H2'	1:N:11:DC:O4'	1.96	0.66
2:Z:583:LEU:HD23	2:Z:583:LEU:O	1.95	0.66
2:Z:206:THR:HB	2:Z:207:PRO:HD2	1.77	0.66
2:Z:150:LEU:HD12	2:Z:150:LEU:N	2.11	0.65
2:Z:425:THR:HG22	2:Z:427:ASP:N	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:203:THR:OG1	2:Z:204:ILE:N	2.27	0.65
2:Z:422:LEU:HA	2:Z:423:PRO:O	1.96	0.65
2:Z:43:GLY:HA3	2:Z:146:PHE:CD2	2.32	0.65
2:Z:66:SER:C	2:Z:67:ARG:HG2	2.21	0.65
2:Z:326:THR:H	2:Z:329:THR:HB	1.61	0.65
2:Z:557:ASN:ND2	2:Z:557:ASN:H	1.94	0.65
2:Z:422:LEU:HB2	2:Z:423:PRO:CA	2.26	0.64
1:N:3:DA:H5'	1:N:9:DT:H5''	1.79	0.64
2:Z:485:ASN:OD1	2:Z:485:ASN:N	2.25	0.64
2:Z:204:ILE:CB	2:Z:205:PRO:HD2	2.22	0.63
2:Z:366:THR:HA	2:Z:370:GLN:CG	2.29	0.63
2:Z:150:LEU:HG	2:Z:525:SER:HB2	1.80	0.63
2:Z:357:ILE:HG22	2:Z:358:ALA:N	2.13	0.63
2:Z:557:ASN:HD22	2:Z:557:ASN:C	2.02	0.62
2:Z:396:GLU:HG3	2:Z:397:ARG:N	2.14	0.62
2:Z:525:SER:OG	2:Z:526:ASP:N	2.31	0.62
2:Z:59:VAL:HG12	2:Z:60:GLU:N	2.12	0.62
2:Z:579:ALA:HB1	2:Z:580:PRO:HD2	1.82	0.61
2:Z:96:MET:HG2	2:Z:220:PRO:HA	1.82	0.61
2:Z:193:GLU:HB3	2:Z:206:THR:CG2	2.29	0.61
2:Z:219:ILE:HG23	2:Z:220:PRO:HD2	1.83	0.60
2:Z:111:LEU:HD12	2:Z:112:VAL:H	1.66	0.59
2:Z:365:GLN:O	2:Z:370:GLN:HG3	2.02	0.59
2:Z:204:ILE:HG13	2:Z:204:ILE:O	2.01	0.59
2:Z:132:THR:C	2:Z:133:MET:HG3	2.26	0.59
2:Z:183:MET:HE3	2:Z:246:ILE:HD13	1.83	0.59
2:Z:206:THR:HB	2:Z:207:PRO:CD	2.31	0.59
2:Z:302:ASN:OD1	2:Z:302:ASN:N	2.35	0.59
2:Z:554:ASN:O	2:Z:557:ASN:ND2	2.35	0.58
2:Z:410:PRO:HA	2:Z:413:ASP:OD2	2.04	0.58
2:Z:557:ASN:ND2	2:Z:557:ASN:N	2.47	0.58
2:Z:47:ASN:C	2:Z:47:ASN:HD22	2.11	0.58
2:Z:336:VAL:O	2:Z:408:ARG:NH2	2.36	0.58
2:Z:217:THR:HG22	2:Z:218:LEU:N	2.17	0.57
2:Z:494:CYS:HB3	2:Z:495:PRO:CD	2.35	0.57
2:Z:422:LEU:CA	2:Z:423:PRO:C	2.78	0.57
2:Z:563:PRO:HA	2:Z:568:GLY:O	2.05	0.57
2:Z:75:GLU:CG	2:Z:76:SER:N	2.60	0.56
2:Z:177:LEU:HD22	2:Z:263:THR:HG22	1.88	0.56
2:Z:349:THR:HG22	2:Z:350:GLN:HG3	1.87	0.56
2:Z:483:HIS:HB3	2:Z:485:ASN:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:219:ILE:HG22	2:Z:220:PRO:HD2	1.86	0.56
2:Z:250:VAL:CG1	2:Z:251:PRO:N	2.69	0.55
2:Z:473:GLU:HA	2:Z:473:GLU:OE1	2.06	0.55
2:Z:482:LEU:N	2:Z:482:LEU:HD23	2.20	0.55
2:Z:294:LEU:HB3	2:Z:295:PRO:HD2	1.88	0.55
2:Z:441:GLY:O	2:Z:442:ILE:HD13	2.05	0.55
2:Z:431:LEU:HB3	2:Z:432:PRO:CD	2.35	0.54
2:Z:122:ASN:HB2	2:Z:123:PRO:CD	2.33	0.54
2:Z:237:ASP:OD1	2:Z:238:PRO:HD2	2.07	0.54
2:Z:432:PRO:O	2:Z:443:ASN:ND2	2.37	0.54
2:Z:380:PHE:CD1	2:Z:380:PHE:N	2.75	0.54
2:Z:139:VAL:HB	2:Z:534:VAL:HG12	1.88	0.54
2:Z:339:SER:O	2:Z:449:ASN:HA	2.08	0.54
2:Z:410:PRO:HD2	2:Z:411:GLU:OE1	2.08	0.54
2:Z:564:SER:C	2:Z:566:ILE:H	2.16	0.54
2:Z:203:THR:C	2:Z:204:ILE:HG23	2.33	0.54
2:Z:218:LEU:HD12	2:Z:219:ILE:N	2.22	0.54
2:Z:271:LYS:HB3	2:Z:272:PRO:CD	2.38	0.54
2:Z:572:VAL:CG1	2:Z:573:TYR:N	2.71	0.54
2:Z:173:LEU:HD12	2:Z:173:LEU:C	2.31	0.54
2:Z:345:PHE:N	2:Z:345:PHE:CD1	2.73	0.53
2:Z:431:LEU:HD23	2:Z:431:LEU:N	2.22	0.53
2:Z:119:VAL:HB	2:Z:120:TRP:CD1	2.43	0.53
2:Z:357:ILE:CG2	2:Z:358:ALA:N	2.71	0.53
2:Z:432:PRO:C	2:Z:443:ASN:HD22	2.17	0.53
2:Z:422:LEU:N	2:Z:422:LEU:CD2	2.72	0.53
2:Z:561:TYR:C	2:Z:562:VAL:HG23	2.34	0.53
2:Z:572:VAL:HG12	2:Z:573:TYR:N	2.24	0.53
2:Z:442:ILE:HG22	2:Z:443:ASN:N	2.22	0.53
2:Z:578:LEU:N	2:Z:578:LEU:CD1	2.72	0.53
2:Z:68:LEU:HD12	2:Z:68:LEU:C	2.34	0.52
2:Z:443:ASN:H	2:Z:446:ASN:HD22	1.56	0.52
2:Z:218:LEU:HD12	2:Z:218:LEU:C	2.33	0.52
2:Z:119:VAL:HG12	2:Z:119:VAL:O	2.08	0.52
1:N:3:DA:H5'	1:N:9:DT:C5'	2.39	0.52
2:Z:73:MET:HB2	2:Z:74:PRO:CD	2.37	0.52
2:Z:360:GLY:HA2	2:Z:374:GLY:CA	2.35	0.52
2:Z:546:ASN:HB2	2:Z:547:PRO:HD2	1.90	0.52
2:Z:555:VAL:HG23	2:Z:556:ASP:N	2.24	0.52
2:Z:554:ASN:OD1	2:Z:556:ASP:N	2.42	0.52
2:Z:553:ILE:HG12	2:Z:554:ASN:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:572:VAL:HG12	2:Z:573:TYR:O	2.09	0.52
2:Z:142:GLU:HB3	2:Z:265:THR:HA	1.92	0.52
2:Z:565:ASN:O	2:Z:566:ILE:HD13	2.10	0.52
2:Z:274:ARG:O	2:Z:275:LEU:HD23	2.10	0.51
2:Z:407:GLY:O	2:Z:408:ARG:HD3	2.09	0.51
2:Z:479:LYS:CB	2:Z:480:PRO:HD2	2.28	0.51
2:Z:511:ASP:OD1	2:Z:512:PRO:HD2	2.11	0.51
2:Z:68:LEU:HD12	2:Z:69:VAL:H	1.76	0.51
2:Z:523:THR:HG22	2:Z:524:TYR:N	2.26	0.51
2:Z:117:TRP:HA	2:Z:469:ILE:HD11	1.93	0.51
2:Z:206:THR:CB	2:Z:207:PRO:CD	2.86	0.51
2:Z:502:VAL:HG12	2:Z:503:ALA:N	2.24	0.51
2:Z:247:GLU:H	2:Z:247:GLU:CD	2.19	0.50
2:Z:139:VAL:HB	2:Z:534:VAL:O	2.11	0.50
2:Z:552:SER:OG	2:Z:553:ILE:N	2.42	0.50
2:Z:99:ASP:CG	2:Z:216:ARG:HH21	2.19	0.50
2:Z:463:VAL:O	2:Z:463:VAL:HG12	2.07	0.50
2:Z:360:GLY:CA	2:Z:374:GLY:HA3	2.37	0.50
2:Z:66:SER:O	2:Z:67:ARG:HG2	2.12	0.49
2:Z:122:ASN:OD1	2:Z:122:ASN:C	2.56	0.49
2:Z:241:VAL:O	2:Z:241:VAL:HG12	2.09	0.49
2:Z:436:ILE:HG12	2:Z:443:ASN:HA	1.94	0.49
2:Z:125:ASP:O	2:Z:126:TRP:C	2.52	0.49
2:Z:281:THR:O	2:Z:283:ARG:N	2.45	0.49
2:Z:281:THR:O	2:Z:282:ASN:C	2.52	0.49
2:Z:123:PRO:O	2:Z:124:GLY:C	2.54	0.49
2:Z:217:THR:CG2	2:Z:218:LEU:N	2.75	0.49
2:Z:281:THR:C	2:Z:283:ARG:N	2.69	0.49
2:Z:203:THR:CB	2:Z:383:GLN:HE22	2.25	0.49
2:Z:455:THR:HG22	2:Z:456:ALA:N	2.28	0.49
2:Z:253:HIS:C	2:Z:254:LEU:HD23	2.37	0.49
2:Z:354:LYS:HD2	2:Z:355:THR:C	2.38	0.48
2:Z:203:THR:CB	2:Z:383:GLN:NE2	2.76	0.48
2:Z:149:VAL:HG12	2:Z:150:LEU:N	2.29	0.48
2:Z:55:GLU:O	2:Z:56:ASN:HB2	2.13	0.48
2:Z:326:THR:O	2:Z:328:ALA:N	2.46	0.48
2:Z:564:SER:C	2:Z:566:ILE:N	2.71	0.48
2:Z:82:VAL:HG12	2:Z:83:VAL:N	2.28	0.48
2:Z:528:TRP:CD1	2:Z:528:TRP:N	2.81	0.48
2:Z:85:ASN:OD1	2:Z:87:MET:HB2	2.14	0.48
2:Z:444:TYR:O	2:Z:447:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:579:ALA:HB1	2:Z:580:PRO:CD	2.44	0.47
2:Z:176:ALA:HB1	2:Z:250:VAL:HG11	1.96	0.47
2:Z:473:GLU:HG3	2:Z:474:PHE:N	2.29	0.47
2:Z:69:VAL:HG12	2:Z:70:HIS:N	2.29	0.47
2:Z:326:THR:C	2:Z:328:ALA:N	2.68	0.47
2:Z:554:ASN:OD1	2:Z:554:ASN:C	2.57	0.47
2:Z:578:LEU:N	2:Z:578:LEU:HD12	2.29	0.47
1:N:10:DG:H3'	1:N:11:DC:C5'	2.38	0.47
1:N:7:DC:H2'	1:N:8:DT:C6	2.49	0.47
2:Z:562:VAL:HG12	2:Z:563:PRO:HD2	1.94	0.47
2:Z:557:ASN:HD22	2:Z:557:ASN:N	2.12	0.47
2:Z:444:TYR:O	2:Z:445:THR:C	2.54	0.47
2:Z:357:ILE:HD13	2:Z:357:ILE:HA	1.31	0.47
2:Z:408:ARG:HD3	2:Z:408:ARG:HA	1.52	0.47
2:Z:557:ASN:O	2:Z:559:PHE:N	2.48	0.47
2:Z:508:ASN:OD1	2:Z:508:ASN:N	2.46	0.46
2:Z:59:VAL:CG1	2:Z:60:GLU:N	2.76	0.46
2:Z:148:VAL:HG12	2:Z:149:VAL:N	2.30	0.46
2:Z:213:GLN:CD	2:Z:214:TRP:N	2.73	0.46
2:Z:117:TRP:CE2	2:Z:469:ILE:HG12	2.49	0.46
2:Z:204:ILE:HB	2:Z:205:PRO:CD	2.36	0.46
2:Z:330:ILE:HG23	2:Z:330:ILE:O	2.15	0.46
2:Z:562:VAL:CG1	2:Z:563:PRO:CD	2.90	0.46
2:Z:337:GLY:C	2:Z:408:ARG:NH2	2.73	0.46
2:Z:116:ALA:O	2:Z:117:TRP:C	2.58	0.46
2:Z:479:LYS:HB3	2:Z:480:PRO:CD	2.39	0.46
2:Z:554:ASN:H	2:Z:557:ASN:ND2	1.83	0.46
2:Z:128:LEU:O	2:Z:129:ILE:C	2.57	0.46
2:Z:146:PHE:CD1	2:Z:146:PHE:N	2.84	0.46
2:Z:346:GLU:HG3	2:Z:355:THR:OG1	2.16	0.46
2:Z:455:THR:CG2	2:Z:456:ALA:N	2.79	0.46
2:Z:465:PRO:HG3	2:Z:571:ILE:CG2	2.45	0.45
2:Z:153:VAL:HG12	2:Z:154:SER:N	2.27	0.45
1:N:6:DT:C2'	1:N:7:DC:H5'	2.40	0.45
2:Z:557:ASN:O	2:Z:558:GLN:C	2.55	0.45
2:Z:443:ASN:H	2:Z:446:ASN:ND2	2.15	0.45
2:Z:465:PRO:HG3	2:Z:571:ILE:HG22	1.98	0.45
2:Z:88:ASP:CG	2:Z:89:LYS:N	2.75	0.45
2:Z:356:PRO:O	2:Z:357:ILE:HD13	2.16	0.45
2:Z:443:ASN:N	2:Z:443:ASN:OD1	2.48	0.45
2:Z:549:GLN:O	2:Z:550:GLN:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:573:TYR:C	2:Z:574:GLU:HG2	2.42	0.45
2:Z:415:ILE:HG22	2:Z:416:GLN:N	2.32	0.45
2:Z:126:TRP:O	2:Z:127:GLN:C	2.60	0.44
2:Z:246:ILE:O	2:Z:247:GLU:C	2.60	0.44
2:Z:410:PRO:O	2:Z:411:GLU:C	2.60	0.44
2:Z:45:PHE:CD1	2:Z:45:PHE:C	2.95	0.44
2:Z:237:ASP:OD1	2:Z:239:ASP:OD2	2.35	0.44
2:Z:219:ILE:CG2	2:Z:220:PRO:CD	2.95	0.44
2:Z:342:TYR:O	2:Z:342:TYR:CG	2.69	0.44
2:Z:566:ILE:HD13	2:Z:566:ILE:HA	1.54	0.44
2:Z:579:ALA:HA	2:Z:580:PRO:HD3	1.62	0.44
2:Z:98:LEU:HD23	2:Z:98:LEU:HA	1.72	0.44
2:Z:340:ALA:HB1	2:Z:341:PRO:CD	2.45	0.44
2:Z:261:PHE:CG	2:Z:262:ALA:N	2.85	0.44
2:Z:277:HIS:CD2	2:Z:277:HIS:C	2.95	0.44
2:Z:307:GLY:C	2:Z:308:VAL:HG23	2.42	0.44
2:Z:431:LEU:C	2:Z:433:THR:H	2.25	0.44
2:Z:431:LEU:C	2:Z:433:THR:N	2.75	0.44
2:Z:565:ASN:OD1	2:Z:566:ILE:HG12	2.18	0.44
2:Z:45:PHE:CE2	2:Z:66:SER:HB2	2.53	0.43
2:Z:237:ASP:O	2:Z:238:PRO:C	2.60	0.43
2:Z:434:ASP:HA	2:Z:435:PRO:HD3	1.49	0.43
2:Z:545:TRP:CD1	2:Z:545:TRP:C	2.96	0.43
2:Z:115:ASN:OD1	2:Z:469:ILE:N	2.41	0.43
2:Z:189:ALA:C	2:Z:191:ARG:N	2.77	0.43
2:Z:478:LEU:C	2:Z:479:LYS:HG3	2.42	0.43
2:Z:139:VAL:HB	2:Z:534:VAL:CG1	2.49	0.43
2:Z:424:VAL:HG22	2:Z:425:THR:N	2.34	0.43
2:Z:277:HIS:O	2:Z:580:PRO:HA	2.19	0.43
2:Z:430:LEU:O	2:Z:431:LEU:HD23	2.18	0.43
2:Z:560:ASN:N	2:Z:560:ASN:ND2	2.67	0.43
2:Z:561:TYR:C	2:Z:562:VAL:CG2	2.91	0.43
2:Z:130:VAL:O	2:Z:130:VAL:HG12	2.18	0.42
2:Z:308:VAL:HG12	2:Z:309:GLN:N	2.33	0.42
2:Z:422:LEU:CB	2:Z:423:PRO:CA	2.94	0.42
2:Z:136:LEU:HD12	2:Z:537:ALA:HB2	2.01	0.42
2:Z:203:THR:C	2:Z:204:ILE:CG2	2.92	0.42
2:Z:280:GLN:HB3	2:Z:284:ALA:HB3	2.01	0.42
2:Z:555:VAL:H	2:Z:555:VAL:HG22	1.35	0.42
2:Z:430:LEU:HD12	2:Z:430:LEU:HA	1.75	0.42
2:Z:521:ILE:HG22	2:Z:522:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:443:ASN:O	2:Z:444:TYR:C	2.61	0.42
2:Z:464:TYR:CD1	2:Z:465:PRO:HA	2.54	0.42
2:Z:366:THR:CA	2:Z:370:GLN:HB2	2.36	0.42
2:Z:564:SER:O	2:Z:566:ILE:N	2.52	0.42
2:Z:346:GLU:O	2:Z:352:PRO:HA	2.19	0.42
2:Z:83:VAL:CG1	2:Z:84:VAL:N	2.81	0.42
2:Z:279:TRP:CE3	2:Z:280:GLN:HA	2.55	0.42
2:Z:309:GLN:O	2:Z:313:ARG:HG3	2.20	0.42
2:Z:549:GLN:CG	2:Z:550:GLN:N	2.83	0.42
2:Z:77:GLU:HG3	2:Z:518:MET:HE2	1.99	0.41
2:Z:90:THR:C	2:Z:92:VAL:N	2.75	0.41
2:Z:222:HIS:ND1	2:Z:224:GLY:N	2.68	0.41
2:Z:444:TYR:C	2:Z:446:ASN:N	2.77	0.41
2:Z:464:TYR:HA	2:Z:465:PRO:HA	1.80	0.41
2:Z:96:MET:HE2	2:Z:96:MET:HB2	1.81	0.41
2:Z:137:HIS:CE1	2:Z:272:PRO:HB3	2.55	0.41
2:Z:517:ASN:HD22	2:Z:517:ASN:HA	1.64	0.41
2:Z:216:ARG:NH2	2:Z:218:LEU:HD22	2.36	0.41
2:Z:261:PHE:CD1	2:Z:261:PHE:C	2.97	0.41
2:Z:337:GLY:HA3	2:Z:408:ARG:HH21	1.86	0.41
2:Z:478:LEU:C	2:Z:479:LYS:CG	2.93	0.41
2:Z:453:PRO:C	2:Z:454:LEU:HD23	2.45	0.41
2:Z:177:LEU:HD12	2:Z:497:GLN:O	2.20	0.41
2:Z:389:THR:HG23	2:Z:568:GLY:HA2	2.03	0.41
2:Z:445:THR:H	2:Z:445:THR:HG23	1.48	0.41
2:Z:473:GLU:OE1	2:Z:473:GLU:CA	2.68	0.41
2:Z:204:ILE:HA	2:Z:205:PRO:HD3	1.69	0.41
2:Z:216:ARG:O	2:Z:216:ARG:HG3	2.13	0.41
2:Z:214:TRP:CD1	2:Z:214:TRP:C	2.96	0.41
2:Z:105:ILE:HG23	2:Z:105:ILE:HD12	1.78	0.41
2:Z:145:ILE:HG22	2:Z:146:PHE:N	2.30	0.41
2:Z:203:THR:OG1	2:Z:383:GLN:NE2	2.49	0.41
2:Z:326:THR:O	2:Z:327:GLU:C	2.62	0.41
2:Z:396:GLU:C	2:Z:397:ARG:HG3	2.46	0.41
2:Z:502:VAL:CG1	2:Z:503:ALA:N	2.82	0.41
2:Z:48:GLN:H	2:Z:64:ASN:HB2	1.86	0.41
2:Z:50:GLU:HB2	2:Z:62:THR:HB	2.03	0.41
2:Z:305:ASP:OD1	2:Z:306:ILE:N	2.54	0.41
2:Z:414:TRP:CD1	2:Z:414:TRP:C	2.98	0.41
2:Z:70:HIS:O	2:Z:204:ILE:HG22	2.21	0.40
2:Z:75:GLU:HG3	2:Z:76:SER:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:410:PRO:C	2:Z:412:GLY:N	2.76	0.40
2:Z:557:ASN:C	2:Z:559:PHE:N	2.79	0.40
2:Z:237:ASP:C	2:Z:239:ASP:N	2.76	0.40
2:Z:246:ILE:HD13	2:Z:246:ILE:HA	1.77	0.40
2:Z:375:ASN:HA	2:Z:376:PRO:HD3	1.83	0.40
2:Z:436:ILE:C	2:Z:438:GLY:N	2.77	0.40
2:Z:549:GLN:C	2:Z:550:GLN:HG2	2.46	0.40
2:Z:292:ASN:HB2	2:Z:306:ILE:O	2.22	0.40
2:Z:418:ILE:HG23	2:Z:419:ASN:N	2.36	0.40
2:Z:565:ASN:OD1	2:Z:565:ASN:N	2.54	0.40
2:Z:579:ALA:CB	2:Z:580:PRO:CD	2.95	0.40
2:Z:47:ASN:CG	2:Z:65:SER:HA	2.46	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	
2	Z	555/584 (95%)	499 (90%)	50 (9%)	6 (1%)	11	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Z	25	ASN
2	Z	558	GLN
2	Z	93	ASN
2	Z	327	GLU
2	Z	330	ILE
2	Z	461	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	Z	477/495 (96%)	461 (97%)	16 (3%)	32 66

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Z	25	ASN
2	Z	47	ASN
2	Z	71	LEU
2	Z	75	GLU
2	Z	76	SER
2	Z	80	ARG
2	Z	190	MET
2	Z	191	ARG
2	Z	216	ARG
2	Z	354	LYS
2	Z	390	THR
2	Z	415	ILE
2	Z	450	THR
2	Z	490	CYS
2	Z	555	VAL
2	Z	557	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	Z	25	ASN
2	Z	104	GLN
2	Z	242	GLN
2	Z	309	GLN
2	Z	323	ASN
2	Z	350	GLN
2	Z	383	GLN
2	Z	428	ASN
2	Z	446	ASN

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Mol	Chain	Res	Type
2	Z	466	ASN
2	Z	491	GLN
2	Z	492	ASN
2	Z	517	ASN
2	Z	543	HIS
2	Z	549	GLN
2	Z	557	ASN
2	Z	560	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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	N	11/11 (100%)	2.07	6 (54%) 0 0	24, 36, 69, 73	0
2	Z	559/584 (95%)	1.32	82 (14%) 6 4	1, 16, 45, 85	13 (2%)
All	All	570/595 (95%)	1.33	88 (15%) 5 4	1, 16, 46, 85	13 (2%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	30	GLY	8.0
2	Z	28	GLY	7.9
2	Z	363	GLY	6.8
2	Z	362	GLY	6.3
2	Z	368	GLU	6.1
2	Z	365	GLN	6.0
2	Z	364	ALA	5.8
2	Z	33	GLY	5.4
2	Z	32	GLY	5.1
2	Z	492	ASN	4.9
2	Z	370	GLN	4.7
2	Z	225	THR	4.7
2	Z	227	GLY	4.5
2	Z	369	ASN	4.5
2	Z	27	SER	4.5
2	Z	371	ALA	4.4
2	Z	361	ARG	4.4
2	Z	25	ASN	4.3
2	Z	226	SER	4.3
2	Z	29	GLY	4.1
2	Z	373	ASP	3.9
2	Z	367	ASP	3.8
2	Z	22	GLY	3.8
1	N	1	DA	3.8

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Mol	Chain	Res	Type	RSRZ
2	Z	24	GLY	3.7
2	Z	228	THR	3.6
2	Z	372	ALA	3.5
1	N	10	DG	3.4
1	N	11	DC	3.3
2	Z	441	GLY	3.1
2	Z	223	THR	3.1
2	Z	374	GLY	3.0
1	N	9	DT	3.0
2	Z	93	ASN	3.0
2	Z	26	GLY	2.9
2	Z	430	LEU	2.9
2	Z	533	LEU	2.9
2	Z	385	GLY	2.8
2	Z	155	GLU	2.8
2	Z	493	ASN	2.8
2	Z	37	GLY	2.8
2	Z	164	VAL	2.7
2	Z	268	PHE	2.7
2	Z	23	SER	2.7
2	Z	36	GLY	2.7
2	Z	393	GLU	2.7
2	Z	176	ALA	2.6
1	N	2	DT	2.6
2	Z	95	ASN	2.6
2	Z	233	TYR	2.5
2	Z	427	ASP	2.5
2	Z	382	ARG	2.5
2	Z	31	GLY	2.4
2	Z	190	MET	2.4
2	Z	162	THR	2.4
2	Z	330	ILE	2.4
2	Z	153	VAL	2.4
2	Z	378	TYR	2.4
2	Z	55	GLU	2.3
2	Z	165	TYR	2.3
2	Z	66	SER	2.3
2	Z	513	ASP	2.3
2	Z	496	GLY	2.2
2	Z	84	VAL	2.2
2	Z	258	GLY	2.2
2	Z	400	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	Z	52	LYS	2.2
1	N	4	DC	2.2
2	Z	401	ILE	2.1
2	Z	366	THR	2.1
2	Z	538	LYS	2.1
2	Z	357	ILE	2.1
2	Z	386	GLN	2.1
2	Z	426	ASN	2.1
2	Z	92	VAL	2.1
2	Z	34	GLY	2.1
2	Z	35	SER	2.1
2	Z	298	GLU	2.1
2	Z	535	PHE	2.1
2	Z	296	GLN	2.1
2	Z	437	GLY	2.1
2	Z	438	GLY	2.1
2	Z	160	PRO	2.0
2	Z	212	PHE	2.0
2	Z	377	ARG	2.0
2	Z	324	TYR	2.0
2	Z	424	VAL	2.0
2	Z	421	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	N	13	1/1	0.90	0.18	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	N	12	1/1	0.99	0.06	1,1,1,1	0
3	MG	Z	585	1/1	0.99	0.06	1,1,1,1	0
3	MG	Z	586	1/1	0.99	0.17	6,6,6,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.