



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:25 AM UTC

PDB ID : 3C46 / pdb_00003c46
Title : X-ray crystal structure of the N4 mini-vRNAP P2_7a promoter complex soaked with MgCl₂
Authors : Gleghorn, M.L.; Murakami, K.S.
Deposited on : 2008-01-29
Resolution : 2.00 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

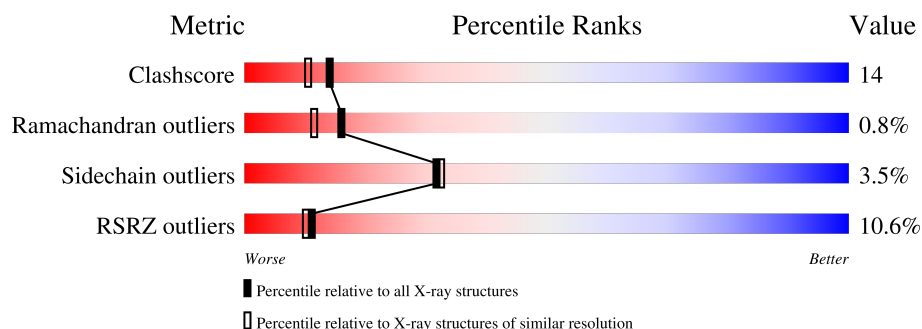
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1117	11% 68% 26% ..
1	B	1117	9% 72% 23% ..
2	C	36	17% 39% 17% 44%
2	D	36	8% 42% 17% 42%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18696 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 Virion RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1095	Total	C	N	O	S	0	0	0
			8454	5306	1435	1672	41			
1	B	1094	Total	C	N	O	S	0	0	0
			8443	5299	1432	1671	41			

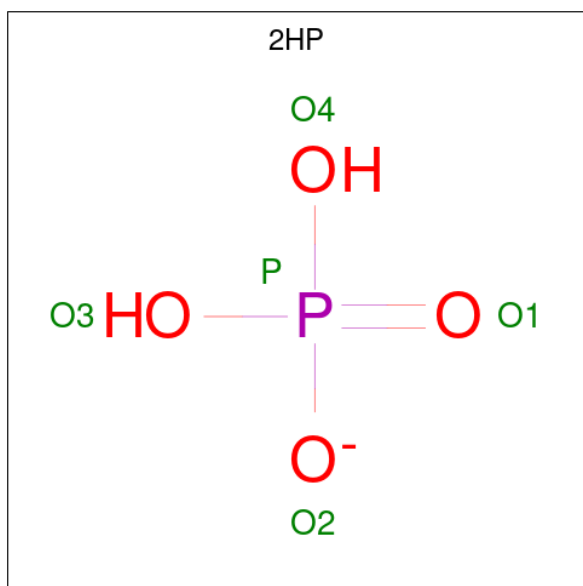
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q859P9
A	-10	GLY	-	expression tag	UNP Q859P9
A	-9	GLY	-	expression tag	UNP Q859P9
A	-8	SER	-	expression tag	UNP Q859P9
A	-7	HIS	-	expression tag	UNP Q859P9
A	-6	HIS	-	expression tag	UNP Q859P9
A	-5	HIS	-	expression tag	UNP Q859P9
A	-4	HIS	-	expression tag	UNP Q859P9
A	-3	HIS	-	expression tag	UNP Q859P9
A	-2	HIS	-	expression tag	UNP Q859P9
A	-1	ARG	-	expression tag	UNP Q859P9
A	0	SER	-	expression tag	UNP Q859P9
B	-11	MET	-	expression tag	UNP Q859P9
B	-10	GLY	-	expression tag	UNP Q859P9
B	-9	GLY	-	expression tag	UNP Q859P9
B	-8	SER	-	expression tag	UNP Q859P9
B	-7	HIS	-	expression tag	UNP Q859P9
B	-6	HIS	-	expression tag	UNP Q859P9
B	-5	HIS	-	expression tag	UNP Q859P9
B	-4	HIS	-	expression tag	UNP Q859P9
B	-3	HIS	-	expression tag	UNP Q859P9
B	-2	HIS	-	expression tag	UNP Q859P9
B	-1	ARG	-	expression tag	UNP Q859P9
B	0	SER	-	expression tag	UNP Q859P9

- Molecule 2 is a DNA chain called P2_7a Promoter DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			393	185	79	110	19			
2	D	21	Total	C	N	O	P	0	0	0
			429	205	83	121	20			

- Molecule 3 is DIHYDROGENPHOSPHATE ION (CCD ID: 2HP) (formula: $\text{H}_2\text{O}_4\text{P}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

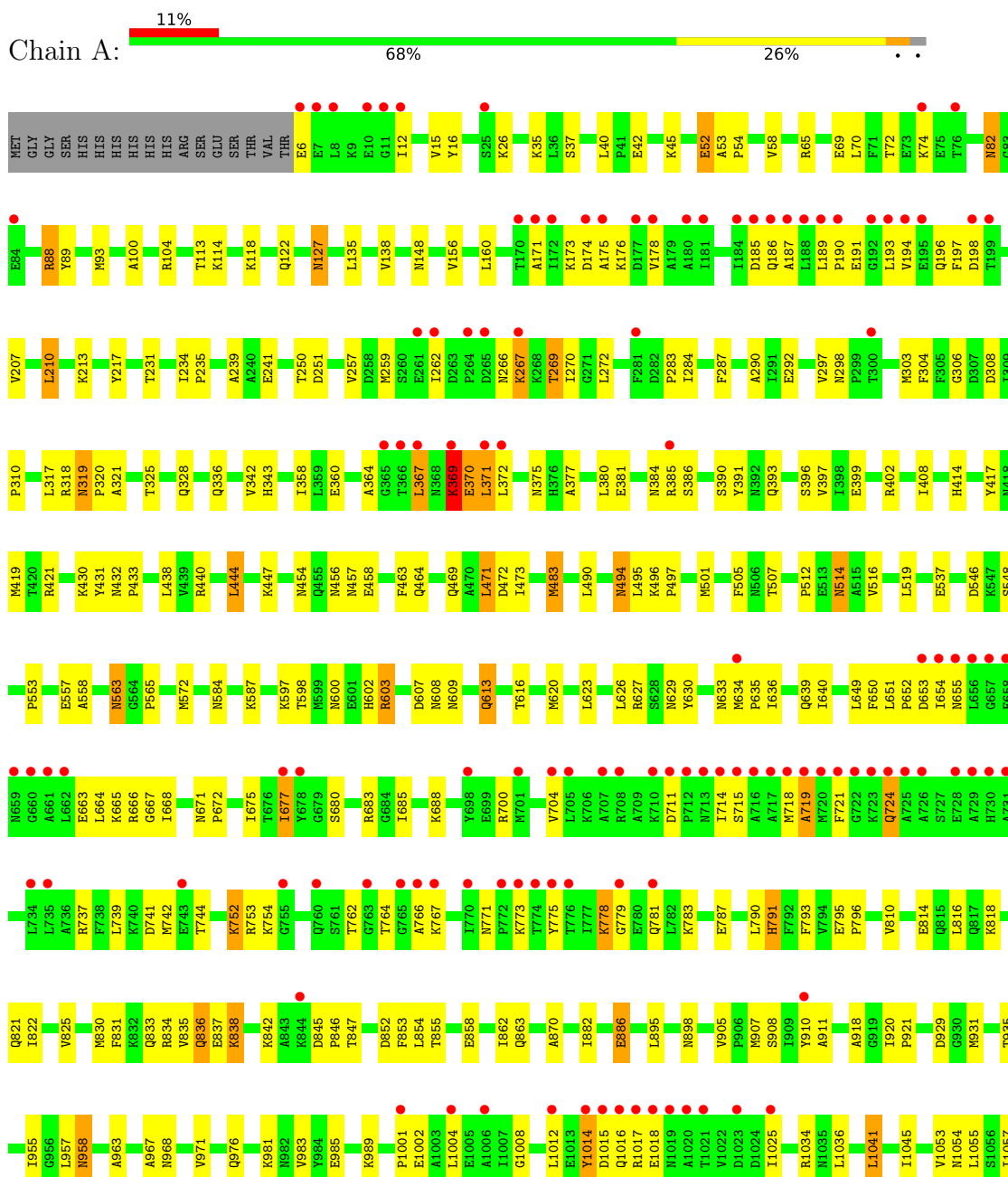
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	433	Total	O	0	0
			433	433		
4	C	27	Total	O	0	0
			27	27		
4	B	475	Total	O	0	0
			475	475		
4	D	32	Total	O	0	0
			32	32		

3 Residue-property plots

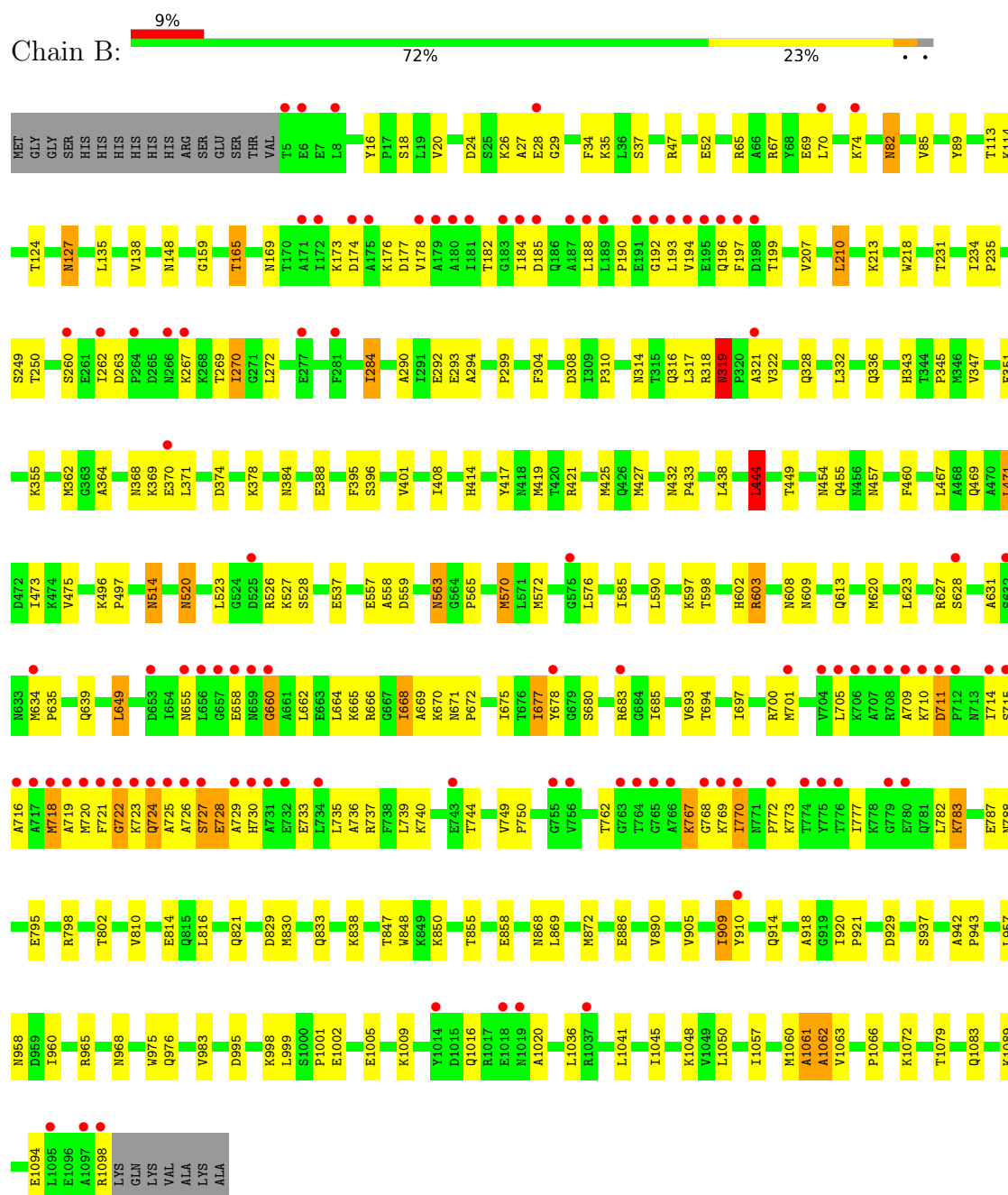
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Virion RNA polymerase

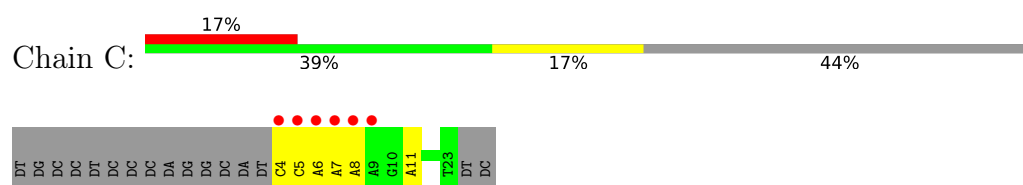




• Molecule 1: Virion RNA polymerase



• Molecule 2: P2_7a Promoter DNA



● Molecule 2: P2_7a Promoter DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.62Å 111.42Å 276.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	82.3 (50.00-2.00) 82.3 (50.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.242 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18696	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: 2HP

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	0.41	0/8583	0.90	26/11609 (0.2%)
1	B	0.41	0/8572	0.89	27/11596 (0.2%)
2	C	0.27	0/442	0.62	0/681
2	D	0.27	0/482	0.66	0/742
All	All	0.40	0/18079	0.88	53/24628 (0.2%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	852	ASP	N-CA-C	-10.41	95.81	110.50
1	B	660	GLY	N-CA-C	-8.97	102.94	115.32
1	B	148	ASN	N-CA-C	-8.61	96.93	109.59
1	A	148	ASN	N-CA-C	-8.33	97.35	109.59
1	B	1061	ALA	N-CA-C	7.88	121.19	110.55
1	B	722	GLY	N-CA-C	-7.87	106.01	114.67
1	A	558	ALA	N-CA-C	-7.87	96.48	108.67
1	A	1061	ALA	N-CA-C	7.57	120.30	110.53
1	B	396	SER	N-CA-C	-7.41	103.28	111.36
1	B	718	MET	N-CA-C	-6.54	105.45	113.50
1	A	396	SER	N-CA-C	-6.54	103.99	112.23
1	A	572	MET	N-CA-C	6.43	120.77	112.41
1	B	563	ASN	N-CA-C	6.32	118.69	111.11
1	B	473	ILE	N-CA-C	-6.22	99.62	108.58
1	B	558	ALA	N-CA-C	-6.20	97.56	108.23
1	A	852	ASP	CA-C-N	-6.13	116.57	123.13
1	A	852	ASP	C-N-CA	-6.13	116.57	123.13
1	A	494	ASN	N-CA-C	5.98	118.59	111.71
1	B	976	GLN	N-CA-C	-5.93	105.81	113.16
1	A	719	ALA	N-CA-C	-5.89	107.33	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	GLU	N-CA-C	-5.83	105.01	111.36
1	A	251	ASP	N-CA-C	-5.82	105.67	112.89
1	B	18	SER	N-CA-C	5.82	120.38	113.16
1	A	270	ILE	N-CA-C	5.77	116.25	108.17
1	A	473	ILE	N-CA-C	-5.75	100.29	108.58
1	B	218	TRP	N-CA-C	-5.73	105.55	112.54
1	A	1063	VAL	N-CA-C	5.67	116.45	110.72
1	B	475	VAL	N-CA-C	5.65	118.11	111.05
1	A	563	ASN	N-CA-C	5.65	117.91	111.02
1	B	576	LEU	N-CA-C	-5.62	103.28	110.53
1	A	269	THR	N-CA-C	-5.54	99.26	108.34
1	A	976	GLN	N-CA-C	-5.52	106.21	113.17
1	A	791	HIS	N-CA-C	5.45	119.09	112.23
1	B	960	ILE	N-CA-C	5.43	116.16	110.62
1	B	1072	LYS	N-CA-C	5.42	119.61	112.89
1	B	957	LEU	N-CA-C	5.36	118.91	112.38
1	A	882	ILE	N-CA-C	5.34	116.07	110.62
1	A	53	ALA	CA-C-N	5.32	124.78	119.24
1	A	53	ALA	C-N-CA	5.32	124.78	119.24
1	B	1063	VAL	N-CA-C	5.32	116.10	110.72
1	B	270	ILE	N-CA-C	5.32	115.62	108.17
1	A	911	ALA	N-CA-C	5.26	112.95	108.22
1	B	1089	LYS	N-CA-C	-5.21	105.60	111.28
1	A	1071	GLY	N-CA-C	-5.18	105.45	112.14
1	B	319	ASN	CA-C-N	5.13	125.42	119.47
1	B	319	ASN	C-N-CA	5.13	125.42	119.47
1	A	287	PHE	CA-C-N	5.12	126.13	120.45
1	A	287	PHE	C-N-CA	5.12	126.13	120.45
1	B	34	PHE	N-CA-C	-5.09	105.19	111.40
1	B	559	ASP	N-CA-C	5.07	117.24	109.07
1	B	572	MET	N-CA-C	5.07	121.21	113.61
1	B	444	LEU	N-CA-C	5.04	116.42	108.55
1	B	165	THR	N-CA-C	5.03	121.11	114.12

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	8454	0	8479	276	0
1	B	8443	0	8465	222	0
2	C	393	0	212	10	0
2	D	429	0	237	10	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	433	0	0	3	0
4	B	475	0	0	3	0
4	C	27	0	0	1	0
4	D	32	0	0	1	0
All	All	18696	0	17393	502	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 14.

All (502) 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:B:701:MET:HE1	1:B:720:MET:HE2	1.39	1.03
1:B:680:SER:HA	2:D:4:DC:H5'	1.41	1.00
1:B:364:ALA:H	1:B:384:ASN:HD21	1.00	0.99
1:A:336:GLN:HE21	1:A:417:TYR:H	1.09	0.99
1:A:688:LYS:HD2	2:C:4:DC:H41	1.27	0.98
1:B:336:GLN:HE21	1:B:417:TYR:H	1.11	0.97
1:B:769:LYS:HG3	1:B:770:ILE:H	1.28	0.95
1:B:364:ALA:H	1:B:384:ASN:ND2	1.65	0.94
1:A:469:GLN:HE22	1:A:557:GLU:H	0.94	0.92
1:A:364:ALA:H	1:A:384:ASN:HD21	1.12	0.90
2:D:5:DC:H2''	2:D:6:DA:H5'	1.55	0.88
1:B:603:ARG:HH11	1:B:603:ARG:HB3	1.38	0.88
1:A:680:SER:HA	2:C:4:DC:H5'	1.55	0.87
1:B:469:GLN:NE2	1:B:557:GLU:H	1.74	0.86
1:B:469:GLN:HE22	1:B:557:GLU:H	0.90	0.86
1:B:718:MET:HE3	1:B:722:GLY:HA2	1.56	0.86
1:A:364:ALA:H	1:A:384:ASN:ND2	1.73	0.85
1:A:469:GLN:NE2	1:A:557:GLU:H	1.75	0.85
1:A:603:ARG:HH11	1:A:603:ARG:HB3	1.41	0.84
1:B:769:LYS:HG3	1:B:770:ILE:N	1.90	0.83
1:B:449:THR:H	1:B:958:ASN:HD21	1.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:VAL:HG22	1:B:872:MET:HE1	1.61	0.83
1:B:24:ASP:HB3	1:B:27:ALA:HB2	1.59	0.81
1:B:769:LYS:CG	1:B:770:ILE:H	1.91	0.81
1:A:1072:LYS:HE2	1:A:1072:LYS:HA	1.63	0.81
1:A:838:LYS:O	1:A:842:LYS:HG2	1.81	0.80
1:A:958:ASN:HD22	1:A:958:ASN:H	1.28	0.80
1:A:790:LEU:O	1:A:795:GLU:HG2	1.81	0.80
1:A:724:GLN:H	1:A:724:GLN:NE2	1.81	0.79
1:A:863:GLN:HA	1:A:863:GLN:HE21	1.47	0.79
1:A:52:GLU:CD	1:A:52:GLU:H	1.90	0.79
1:A:469:GLN:HE22	1:A:557:GLU:N	1.78	0.79
1:A:920:ILE:HB	1:A:921:PRO:HD3	1.65	0.78
1:B:267:LYS:HE2	1:B:267:LYS:HA	1.64	0.78
1:B:705:LEU:HD11	1:B:773:LYS:HA	1.67	0.77
1:B:725:ALA:O	1:B:730:HIS:HB3	1.86	0.76
1:A:724:GLN:H	1:A:724:GLN:HE21	1.30	0.76
1:A:454:ASN:HB3	1:A:457:ASN:HD21	1.50	0.75
1:A:303:MET:HE1	1:A:397:VAL:HG13	1.68	0.75
1:B:783:LYS:O	1:B:787:GLU:HG2	1.86	0.74
1:B:127:ASN:H	1:B:127:ASN:HD22	1.32	0.74
1:A:688:LYS:HD2	2:C:4:DC:N4	2.03	0.74
1:B:26:LYS:HG2	1:B:847:THR:HG21	1.69	0.74
1:A:127:ASN:HD22	1:A:127:ASN:H	1.35	0.73
1:A:1001:PRO:HG2	1:A:1002:GLU:OE2	1.88	0.73
1:B:469:GLN:HE22	1:B:557:GLU:N	1.76	0.72
2:C:5:DC:H2''	2:C:6:DA:H5'	1.70	0.72
1:B:995:ASP:CG	1:B:998:LYS:HG2	2.14	0.72
1:A:367:LEU:HD23	1:A:367:LEU:H	1.54	0.72
1:A:714:ILE:HG22	1:A:719:ALA:HB2	1.70	0.72
1:A:603:ARG:HB3	1:A:603:ARG:NH1	2.05	0.71
1:B:570:MET:HE3	1:B:975:TRP:HB3	1.72	0.71
1:B:523:LEU:O	1:B:526:ARG:HG3	1.91	0.70
1:B:65:ARG:O	1:B:69:GLU:HG3	1.92	0.70
1:B:213:LYS:HE3	1:B:292:GLU:OE2	1.91	0.70
1:B:700:ARG:NE	1:B:723:LYS:HE3	2.07	0.69
1:A:1091:PHE:HE2	1:A:1095:LEU:HD23	1.58	0.69
1:B:769:LYS:O	1:B:770:ILE:HB	1.90	0.69
1:A:267:LYS:HD3	1:A:267:LYS:N	2.07	0.69
1:A:752:LYS:HZ2	1:A:752:LYS:HB2	1.57	0.68
1:A:931:MET:HE3	1:A:935:THR:OG1	1.94	0.68
1:B:918:ALA:O	1:B:921:PRO:HD2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:ARG:CZ	1:B:723:LYS:HG3	2.25	0.67
1:B:830:MET:HE3	1:B:999:LEU:HD23	1.75	0.67
1:A:597:LYS:NZ	1:A:602:HIS:HD2	1.91	0.67
1:A:454:ASN:HB3	1:A:457:ASN:ND2	2.09	0.67
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.76	0.67
1:A:267:LYS:HD3	1:A:267:LYS:H	1.61	0.66
1:A:360:GLU:HG2	1:A:516:VAL:HG11	1.78	0.66
1:A:968:ASN:HD21	1:A:1060:MET:H	1.44	0.65
1:A:1099:LYS:C	1:A:1099:LYS:HD3	2.21	0.65
1:A:454:ASN:HD22	1:A:457:ASN:ND2	1.93	0.65
1:A:724:GLN:NE2	1:A:724:GLN:N	2.43	0.65
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.77	0.65
1:B:920:ILE:HB	1:B:921:PRO:HD3	1.78	0.65
1:A:546:ASP:OD2	1:A:548:SER:HB3	1.97	0.65
1:A:584:ASN:HA	1:A:587:LYS:HD2	1.78	0.65
1:B:700:ARG:HE	1:B:723:LYS:HE3	1.61	0.65
1:B:868:ASN:OD1	1:B:869:LEU:HD22	1.96	0.65
1:B:603:ARG:HB3	1:B:603:ARG:NH1	2.09	0.64
1:B:336:GLN:HE21	1:B:417:TYR:N	1.91	0.64
1:B:401:VAL:HG12	1:B:408:ILE:HG13	1.78	0.64
1:B:336:GLN:NE2	1:B:417:TYR:H	1.90	0.63
1:A:654:ILE:C	1:A:655:ASN:HD22	2.06	0.63
1:B:767:LYS:HD2	1:B:768:GLY:H	1.62	0.63
1:B:234:ILE:HB	1:B:235:PRO:HD3	1.79	0.63
1:A:616:THR:HG23	1:A:668:ILE:HD11	1.80	0.63
1:A:830:MET:O	1:A:834:ARG:HG2	1.99	0.63
1:A:855:THR:OG1	1:A:858:GLU:HG3	1.99	0.63
1:A:496:LYS:HB3	1:A:497:PRO:HD3	1.80	0.62
1:B:421:ARG:HD2	2:D:7:DA:H5"	1.82	0.62
1:A:653:ASP:CB	1:A:668:ILE:HG23	2.30	0.62
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.81	0.62
1:B:89:TYR:CZ	1:B:284:ILE:HD11	2.35	0.62
1:A:371:LEU:C	1:A:372:LEU:HD12	2.25	0.62
1:A:791:HIS:HA	1:A:795:GLU:HG3	1.82	0.62
1:A:791:HIS:HA	1:A:795:GLU:CG	2.29	0.62
1:B:1045:ILE:HD11	1:B:1098:ARG:NH2	2.14	0.61
1:A:178:VAL:HG21	1:A:194:VAL:HG13	1.82	0.61
1:A:402:ARG:HA	1:A:408:ILE:HG22	1.82	0.61
1:A:1091:PHE:CE2	1:A:1095:LEU:HD23	2.36	0.61
1:B:514:ASN:H	1:B:514:ASN:HD22	1.48	0.61
1:B:127:ASN:HD22	1:B:127:ASN:N	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:SER:HB3	1:B:718:MET:HB3	1.83	0.61
1:B:848:TRP:CH2	1:B:850:LYS:HA	2.35	0.61
1:A:778:LYS:CE	1:A:778:LYS:H	2.12	0.61
2:C:4:DC:H2''	2:C:5:DC:OP2	2.00	0.61
1:A:958:ASN:H	1:A:958:ASN:ND2	1.98	0.61
1:B:597:LYS:NZ	1:B:602:HIS:HD2	1.99	0.61
1:B:715:SER:HB3	1:B:718:MET:CB	2.31	0.61
1:A:895:LEU:HD13	1:A:907:MET:HE3	1.82	0.60
1:B:304:PHE:CD2	1:B:310:PRO:HG3	2.37	0.60
1:B:449:THR:H	1:B:958:ASN:ND2	1.97	0.60
1:B:675:ILE:HD11	1:B:685:ILE:HG12	1.82	0.60
1:A:1015:ASP:OD1	1:A:1016:GLN:HG3	2.01	0.60
1:B:250:THR:HG22	1:B:250:THR:O	2.01	0.60
1:B:421:ARG:HD2	2:D:7:DA:C5'	2.32	0.60
1:B:1045:ILE:HD12	1:B:1094:GLU:HG3	1.84	0.60
1:B:178:VAL:HG21	1:B:194:VAL:HG13	1.84	0.60
1:A:189:LEU:HD22	1:A:193:LEU:HD23	1.85	0.59
1:A:1025:ILE:C	1:A:1025:ILE:HD12	2.27	0.59
1:A:336:GLN:HE21	1:A:417:TYR:N	1.92	0.59
1:B:173:LYS:HD2	1:B:197:PHE:O	2.03	0.59
1:A:393:GLN:HG2	1:A:431:TYR:HB2	1.84	0.58
1:A:430:LYS:HE3	1:A:431:TYR:CE2	2.39	0.58
1:A:724:GLN:HE21	1:A:724:GLN:N	2.01	0.58
1:B:603:ARG:NH1	1:B:608:ASN:OD1	2.37	0.58
1:B:725:ALA:C	1:B:727:SER:H	2.11	0.58
1:A:297:VAL:HG12	1:A:298:ASN:ND2	2.19	0.58
1:A:82:ASN:HD22	1:A:82:ASN:C	2.10	0.58
1:A:88:ARG:HG3	1:A:283:PRO:HB2	1.86	0.58
1:B:364:ALA:N	1:B:384:ASN:HD21	1.85	0.58
1:B:496:LYS:HB3	1:B:497:PRO:HD3	1.85	0.57
1:B:918:ALA:C	1:B:921:PRO:HD2	2.29	0.57
1:B:159:GLY:HA2	1:B:210:LEU:HD21	1.85	0.57
1:A:267:LYS:N	1:A:267:LYS:CD	2.67	0.57
1:A:328:GLN:HB3	1:A:419:MET:HE3	1.86	0.56
1:A:633:ASN:CG	1:A:636:ILE:HG12	2.30	0.56
1:B:260:SER:HA	1:B:263:ASP:O	2.05	0.56
1:B:995:ASP:OD2	1:B:998:LYS:HG2	2.04	0.56
1:A:267:LYS:H	1:A:267:LYS:CD	2.18	0.56
1:A:336:GLN:NE2	1:A:417:TYR:H	1.92	0.56
1:B:598:THR:HG22	1:B:1066:PRO:HD3	1.88	0.56
1:B:810:VAL:O	1:B:814:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.41	0.56
1:A:778:LYS:H	1:A:778:LYS:HE3	1.69	0.56
1:B:603:ARG:HH11	1:B:603:ARG:CB	2.14	0.56
1:B:1016:GLN:O	1:B:1020:ALA:HB2	2.06	0.56
1:A:464:GLN:CB	1:A:483:MET:HE1	2.36	0.56
1:B:82:ASN:C	1:B:82:ASN:HD22	2.12	0.55
1:A:113:THR:HG22	1:A:114:LYS:HG3	1.89	0.55
2:D:4:DC:H2''	2:D:5:DC:OP2	2.07	0.55
1:A:234:ILE:HB	1:A:235:PRO:HD3	1.88	0.55
1:A:399:GLU:OE1	1:A:399:GLU:HA	2.07	0.55
1:B:317:LEU:HG	1:B:318:ARG:NH1	2.22	0.55
1:A:213:LYS:HE3	1:A:292:GLU:OE1	2.07	0.55
1:A:1096:GLU:OE2	1:A:1096:GLU:HA	2.07	0.55
1:A:649:LEU:HB3	1:A:650:PHE:CD1	2.41	0.55
1:A:52:GLU:N	1:A:52:GLU:OE1	2.40	0.55
1:A:464:GLN:HB3	1:A:483:MET:HE1	1.88	0.54
1:A:653:ASP:HB3	1:A:668:ILE:HG23	1.90	0.54
1:B:328:GLN:HB3	1:B:419:MET:HE3	1.89	0.54
1:A:778:LYS:H	1:A:778:LYS:CD	2.20	0.54
1:B:332:LEU:O	1:B:336:GLN:HG3	2.07	0.54
1:B:705:LEU:HD11	1:B:773:LYS:CA	2.34	0.54
1:B:735:LEU:O	1:B:739:LEU:HD13	2.06	0.54
1:A:603:ARG:NH1	1:A:608:ASN:OD1	2.41	0.54
1:B:620:MET:HG3	1:B:664:LEU:HD12	1.90	0.54
1:B:829:ASP:O	1:B:833:GLN:HG3	2.07	0.54
1:A:1034:ARG:NH1	1:A:1034:ARG:HB2	2.22	0.54
1:A:653:ASP:HB2	1:A:668:ILE:HG23	1.89	0.54
1:A:886:GLU:O	2:C:8:DA:H4'	2.08	0.54
1:B:1001:PRO:HG2	1:B:1002:GLU:OE2	2.08	0.54
1:A:600:ASN:ND2	1:A:600:ASN:H	2.06	0.53
1:A:127:ASN:HD22	1:A:127:ASN:N	1.98	0.53
1:A:1014:TYR:HA	1:A:1017:ARG:CZ	2.39	0.53
1:A:259:MET:CB	1:A:266:ASN:HD22	2.21	0.53
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.08	0.53
1:B:597:LYS:HE2	1:B:602:HIS:HB2	1.91	0.53
1:A:714:ILE:CG2	1:A:719:ALA:HB2	2.38	0.53
1:A:863:GLN:HA	1:A:863:GLN:NE2	2.19	0.53
1:B:1005:GLU:HG2	1:B:1009:LYS:NZ	2.24	0.53
1:A:649:LEU:HD13	1:A:737:ARG:NH2	2.24	0.53
1:B:749:VAL:HG13	1:B:762:THR:CG2	2.39	0.53
1:B:769:LYS:O	1:B:770:ILE:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.38	0.52
1:A:700:ARG:O	1:A:704:VAL:HG23	2.09	0.52
1:A:818:LYS:O	1:A:822:ILE:HG13	2.10	0.52
1:B:639:GLN:NE2	1:B:744:THR:CG2	2.73	0.52
1:B:655:ASN:HD21	1:B:665:LYS:HE3	1.75	0.52
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.91	0.52
1:A:795:GLU:HB2	1:A:796:PRO:CD	2.40	0.52
1:B:700:ARG:NH2	1:B:723:LYS:HG3	2.25	0.52
1:A:603:ARG:HH11	1:A:603:ARG:CB	2.16	0.52
1:B:520:ASN:HD21	1:B:527:LYS:NZ	2.09	0.51
1:B:668:ILE:HD12	1:B:669:ALA:N	2.25	0.51
1:A:175:ALA:HB1	1:A:186:GLN:HG3	1.91	0.51
1:B:347:VAL:O	1:B:351:GLU:HG3	2.11	0.51
1:A:739:LEU:HB3	1:A:767:LYS:HZ1	1.76	0.51
1:B:830:MET:HA	1:B:830:MET:HE2	1.93	0.51
1:A:1012:LEU:HD11	1:A:1025:ILE:HG22	1.92	0.51
1:A:15:VAL:HG21	1:A:40:LEU:HD21	1.91	0.51
1:A:858:GLU:O	1:A:862:ILE:HG13	2.11	0.51
1:B:701:MET:HE1	1:B:720:MET:CE	2.25	0.51
1:A:752:LYS:HA	1:A:752:LYS:HZ1	1.75	0.51
1:B:767:LYS:CE	1:B:769:LYS:HE2	2.41	0.51
1:A:440:ARG:O	1:A:444:LEU:HD13	2.11	0.51
1:A:563:ASN:HD21	1:A:929:ASP:HB3	1.76	0.51
1:A:185:ASP:OD2	1:A:187:ALA:HB3	2.10	0.50
1:B:678:TYR:O	1:B:921:PRO:HG3	2.11	0.50
1:B:816:LEU:HD13	1:B:983:VAL:HG21	1.92	0.50
1:B:855:THR:OG1	1:B:858:GLU:HG3	2.11	0.50
1:B:293:GLU:HA	1:B:299:PRO:CG	2.41	0.50
1:A:1061:ALA:O	1:A:1062:ALA:CB	2.60	0.50
1:B:185:ASP:HB3	1:B:188:LEU:HD12	1.94	0.50
1:A:463:PHE:HA	1:A:957:LEU:HD13	1.94	0.50
1:B:190:PRO:HD2	1:B:193:LEU:HD22	1.92	0.50
1:B:269:THR:O	2:D:11:DA:H5'	2.12	0.50
1:A:587:LYS:NZ	1:A:607:ASP:OD2	2.45	0.49
1:B:514:ASN:HD22	1:B:514:ASN:N	2.09	0.49
1:B:671:ASN:HB3	1:B:672:PRO:HD3	1.94	0.49
1:B:1079:THR:O	1:B:1083:GLN:HG3	2.12	0.49
1:A:454:ASN:HD21	1:A:456:ASN:HB2	1.76	0.49
1:A:968:ASN:ND2	1:A:1060:MET:H	2.08	0.49
1:B:47:ARG:HD2	1:B:294:ALA:O	2.12	0.49
1:B:750:PRO:HD3	1:B:788:ASN:OD1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LYS:NZ	1:A:369:LYS:HB3	2.27	0.49
1:A:371:LEU:HD13	1:A:371:LEU:O	2.12	0.49
1:B:351:GLU:HG2	1:B:395:PHE:CE2	2.46	0.49
1:B:767:LYS:HE2	1:B:769:LYS:HE2	1.94	0.49
1:A:342:VAL:HG11	1:A:408:ILE:HD12	1.93	0.49
1:B:249:SER:O	1:B:250:THR:HB	2.11	0.49
1:B:777:ILE:HG22	1:B:782:LEU:HG	1.93	0.49
1:B:1061:ALA:O	1:B:1062:ALA:HB2	2.13	0.49
1:B:730:HIS:O	1:B:733:GLU:HB3	2.13	0.49
1:A:358:ILE:HD12	1:A:391:TYR:CE1	2.47	0.49
1:A:65:ARG:O	1:A:69:GLU:HG3	2.12	0.49
1:A:88:ARG:HD3	1:A:283:PRO:HD2	1.94	0.49
1:A:269:THR:O	2:C:11:DA:H5'	2.12	0.49
1:A:370:GLU:O	1:A:370:GLU:HG3	2.12	0.49
1:A:367:LEU:HB2	1:A:372:LEU:CD2	2.42	0.48
1:A:633:ASN:OD1	1:A:636:ILE:HG12	2.13	0.48
1:A:721:PHE:HA	1:A:724:GLN:NE2	2.28	0.48
1:B:16:TYR:O	1:B:35:LYS:CE	2.61	0.48
1:B:649:LEU:HD13	1:B:737:ARG:NH2	2.28	0.48
1:B:714:ILE:CG1	1:B:719:ALA:HB2	2.42	0.48
1:A:176:LYS:HD2	2:C:5:DC:OP2	2.13	0.48
1:A:190:PRO:HG2	1:A:193:LEU:HB2	1.96	0.48
1:B:701:MET:HA	1:B:701:MET:HE2	1.95	0.48
1:B:737:ARG:HA	1:B:740:LYS:HE2	1.95	0.48
1:B:968:ASN:HD21	1:B:1060:MET:H	1.62	0.48
1:B:767:LYS:HD2	1:B:768:GLY:N	2.27	0.48
1:B:69:GLU:HB3	1:B:74:LYS:O	2.12	0.48
1:B:113:THR:HG22	1:B:114:LYS:HG3	1.96	0.48
1:B:284:ILE:HD13	1:B:284:ILE:O	2.14	0.48
1:B:316:GLN:NE2	1:B:421:ARG:HA	2.29	0.48
1:A:6:GLU:O	1:A:6:GLU:HG2	2.13	0.48
1:A:665:LYS:O	1:A:668:ILE:HG12	2.14	0.48
1:B:597:LYS:HZ1	1:B:602:HIS:HD2	1.60	0.48
1:B:767:LYS:HE2	1:B:769:LYS:HG2	1.95	0.48
1:A:304:PHE:HB3	1:A:308:ASP:O	2.14	0.48
1:A:259:MET:HB3	1:A:266:ASN:HD22	1.79	0.48
1:B:417:TYR:OH	1:B:427:MET:HE3	2.14	0.48
1:B:802:THR:HG23	1:B:810:VAL:HG21	1.96	0.48
1:A:262:ILE:N	1:A:262:ILE:HD12	2.29	0.47
1:A:639:GLN:NE2	1:A:744:THR:OG1	2.47	0.47
1:B:304:PHE:CG	1:B:310:PRO:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ASN:HB2	1:A:663:GLU:HB3	1.96	0.47
1:B:207:VAL:HG11	1:B:905:VAL:HG21	1.96	0.47
1:B:438:LEU:C	1:B:438:LEU:HD23	2.38	0.47
1:A:766:ALA:HB2	1:A:781:GLN:CD	2.40	0.47
1:B:182:THR:HA	1:B:270:ILE:CD1	2.45	0.47
1:B:694:THR:HG21	1:B:782:LEU:HD21	1.97	0.47
1:A:72:THR:O	1:A:74:LYS:HG3	2.14	0.47
1:A:653:ASP:OD1	1:A:667:GLY:HA3	2.14	0.47
1:A:319:ASN:HD22	1:A:319:ASN:HA	1.56	0.47
1:A:1014:TYR:HA	1:A:1017:ARG:NE	2.30	0.47
1:A:1094:GLU:OE2	1:A:1098:ARG:NH1	2.47	0.47
1:B:565:PRO:HA	1:B:677:ILE:HG12	1.97	0.47
1:A:565:PRO:HA	1:A:677:ILE:HG12	1.97	0.47
1:A:627:ARG:NH2	1:A:640:ILE:HG22	2.30	0.47
1:B:82:ASN:ND2	1:B:85:VAL:H	2.12	0.47
1:A:343:HIS:HE1	1:A:537:GLU:OE2	1.98	0.47
1:A:739:LEU:CB	1:A:767:LYS:HZ1	2.28	0.47
1:B:444:LEU:N	1:B:444:LEU:HD23	2.30	0.47
1:A:325:THR:OG1	1:A:328:GLN:HG3	2.15	0.47
1:A:600:ASN:H	1:A:600:ASN:HD22	1.63	0.47
1:B:683:ARG:HH21	2:D:3:DT:H5"	1.80	0.47
1:A:367:LEU:HD23	1:A:367:LEU:N	2.27	0.46
1:A:778:LYS:H	1:A:778:LYS:HD2	1.80	0.46
1:A:833:GLN:O	1:A:837:GLU:HG3	2.16	0.46
1:B:70:LEU:HD13	1:B:70:LEU:O	2.14	0.46
1:B:725:ALA:C	1:B:727:SER:N	2.71	0.46
1:A:620:MET:HG2	1:A:664:LEU:HD12	1.96	0.46
1:A:1099:LYS:HD3	1:A:1099:LYS:O	2.15	0.46
1:A:377:ALA:O	1:A:381:GLU:HG3	2.15	0.46
1:A:793:PHE:O	1:A:796:PRO:HG2	2.15	0.46
1:A:767:LYS:HD2	1:A:767:LYS:HA	1.77	0.46
1:B:628:SER:O	1:B:631:ALA:HB2	2.16	0.46
1:B:693:VAL:O	1:B:697:ILE:HG13	2.16	0.46
1:B:701:MET:O	1:B:772:PRO:HB2	2.14	0.46
1:A:210:LEU:HB3	1:A:239:ALA:HB1	1.98	0.46
1:A:385:ARG:HD3	1:A:386:SER:N	2.30	0.46
1:A:778:LYS:HZ2	1:A:781:GLN:NE2	2.13	0.46
1:A:633:ASN:OD1	1:A:635:PRO:HD2	2.15	0.46
1:B:176:LYS:HE3	2:D:5:DC:OP2	2.16	0.46
1:B:178:VAL:CG2	1:B:194:VAL:HG13	2.45	0.46
1:A:171:ALA:HB2	2:C:7:DA:N7	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:O	1:A:250:THR:HG22	2.16	0.46
1:A:597:LYS:HZ3	1:A:602:HIS:HD2	1.62	0.46
1:A:664:LEU:HB3	1:A:668:ILE:CD1	2.46	0.46
1:B:1057:ILE:HD12	1:B:1057:ILE:N	2.30	0.46
1:A:629:ASN:N	1:A:629:ASN:HD22	2.12	0.46
1:B:304:PHE:HB3	1:B:308:ASP:O	2.16	0.46
1:B:421:ARG:HG3	4:D:152:HOH:O	2.16	0.46
1:B:127:ASN:H	1:B:127:ASN:ND2	2.09	0.46
1:B:368:ASN:C	1:B:368:ASN:ND2	2.73	0.46
1:B:816:LEU:CD1	1:B:983:VAL:HG21	2.46	0.46
1:A:810:VAL:O	1:A:814:GLU:HG3	2.16	0.45
1:B:965:ARG:HG2	4:B:1333:HOH:O	2.16	0.45
1:B:1061:ALA:O	1:B:1062:ALA:CB	2.64	0.45
1:A:778:LYS:NZ	1:A:781:GLN:NE2	2.64	0.45
1:A:836:GLN:HA	1:A:836:GLN:OE1	2.16	0.45
1:A:981:LYS:O	1:A:985:GLU:HG3	2.16	0.45
1:B:368:ASN:C	1:B:368:ASN:HD22	2.23	0.45
1:A:364:ALA:N	1:A:384:ASN:HD21	1.96	0.45
1:A:791:HIS:HA	1:A:795:GLU:HG2	1.97	0.45
1:A:1008:GLY:O	1:A:1012:LEU:HB2	2.16	0.45
1:A:1091:PHE:C	1:A:1091:PHE:CD2	2.95	0.45
1:A:514:ASN:HD22	1:A:514:ASN:H	1.65	0.45
1:B:336:GLN:O	1:B:414:HIS:HD2	1.99	0.45
1:A:191:GLU:HG2	1:A:375:ASN:HB3	1.98	0.45
1:A:421:ARG:HD2	2:C:7:DA:H5"	1.98	0.45
1:A:783:LYS:O	1:A:787:GLU:HG2	2.16	0.45
1:A:1053:VAL:HG12	1:A:1054:ASN:N	2.30	0.45
1:B:715:SER:O	1:B:716:ALA:HB3	2.16	0.45
1:B:343:HIS:CD2	1:B:345:PRO:HD2	2.52	0.45
1:A:26:LYS:HD3	1:A:847:THR:HG21	1.99	0.45
1:A:918:ALA:C	1:A:921:PRO:HD2	2.42	0.45
1:B:355:LYS:HD2	1:B:388:GLU:HG3	1.98	0.45
1:B:890:VAL:HG11	1:B:909:ILE:HD11	1.98	0.45
1:A:217:TYR:OH	1:A:292:GLU:HA	2.17	0.45
1:A:257:VAL:HG12	1:A:259:MET:CE	2.47	0.45
1:B:196:GLN:O	1:B:199:THR:HG22	2.17	0.45
1:B:639:GLN:NE2	1:B:744:THR:HG22	2.32	0.45
1:B:749:VAL:HG13	1:B:762:THR:HG21	1.99	0.45
1:A:54:PRO:O	1:A:58:VAL:HG23	2.17	0.45
1:A:135:LEU:O	1:A:138:VAL:HG22	2.17	0.45
1:A:89:TYR:CZ	1:A:290:ALA:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:TYR:O	1:B:35:LYS:HE2	2.17	0.44
1:A:194:VAL:O	1:A:198:ASP:HB2	2.17	0.44
1:A:918:ALA:O	1:A:921:PRO:HD2	2.17	0.44
1:A:1017:ARG:HG2	1:A:1017:ARG:HH11	1.82	0.44
1:A:318:ARG:O	1:A:421:ARG:NH1	2.50	0.44
1:A:598:THR:HG22	1:A:1066:PRO:HD3	1.99	0.44
1:A:651:LEU:HA	1:A:652:PRO:HD3	1.86	0.44
1:B:715:SER:HB3	1:B:718:MET:HB2	2.00	0.44
1:A:174:ASP:OD1	1:A:176:LYS:HB3	2.17	0.44
1:A:654:ILE:HD11	1:A:668:ILE:HG21	2.00	0.44
1:A:821:GLN:O	1:A:825:VAL:HG23	2.17	0.44
1:B:197:PHE:CD1	1:B:272:LEU:HD21	2.53	0.44
1:A:336:GLN:O	1:A:414:HIS:HD2	2.01	0.44
1:A:609:ASN:HB3	1:A:613:GLN:HB3	1.99	0.44
1:B:724:GLN:HA	1:B:724:GLN:OE1	2.17	0.44
1:A:196:GLN:O	1:A:272:LEU:HD21	2.18	0.44
1:A:317:LEU:HB3	4:C:29:HOH:O	2.17	0.44
1:B:135:LEU:O	1:B:138:VAL:HG22	2.18	0.44
1:B:563:ASN:HD21	1:B:929:ASP:HB3	1.81	0.44
1:A:37:SER:HB3	1:A:231:THR:HG22	1.99	0.44
1:A:501:MET:HE1	1:A:519:LEU:HG	2.00	0.44
1:A:45:LYS:HE3	4:A:1232:HOH:O	2.18	0.44
1:A:1057:ILE:N	1:A:1057:ILE:HD12	2.32	0.44
1:A:1053:VAL:HG11	1:A:1075:LEU:HD12	1.99	0.43
1:A:100:ALA:O	1:A:104:ARG:HG3	2.18	0.43
1:A:118:LYS:O	1:A:122:GLN:HG3	2.18	0.43
1:A:444:LEU:HG	1:A:553:PRO:HB2	2.00	0.43
1:A:471:LEU:O	1:A:472:ASP:HB2	2.18	0.43
1:B:722:GLY:O	1:B:723:LYS:C	2.61	0.43
1:A:12:ILE:HA	1:A:40:LEU:HD11	1.99	0.43
1:A:370:GLU:HA	1:A:773:LYS:HE2	1.99	0.43
1:A:372:LEU:HD23	1:A:380:LEU:HD12	2.00	0.43
1:B:444:LEU:HB3	4:B:1167:HOH:O	2.17	0.43
1:B:725:ALA:HB1	1:B:730:HIS:CD2	2.52	0.43
1:A:386:SER:O	1:A:390:SER:HB2	2.19	0.43
1:A:762:THR:HB	1:A:764:THR:HG22	2.01	0.43
1:B:455:GLN:HG2	1:B:460:PHE:CZ	2.53	0.43
1:B:714:ILE:HG12	1:B:719:ALA:HB2	2.00	0.43
1:B:942:ALA:HA	1:B:943:PRO:HD3	1.90	0.43
1:A:671:ASN:HB3	1:A:672:PRO:HD3	2.01	0.43
1:A:1058:ASP:HB2	1:A:1066:PRO:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ALA:HB2	1:B:910:TYR:HE2	1.84	0.43
1:A:752:LYS:NZ	1:A:752:LYS:CB	2.81	0.43
1:B:425:MET:HE1	1:B:937:SER:OG	2.19	0.43
1:B:520:ASN:HD21	1:B:527:LYS:HZ2	1.66	0.43
1:B:585:ILE:HG12	1:B:590:LEU:HD23	2.01	0.43
1:B:725:ALA:O	1:B:727:SER:N	2.52	0.43
1:B:1005:GLU:HG2	1:B:1009:LYS:HZ3	1.84	0.43
1:A:89:TYR:O	1:A:93:MET:HG2	2.19	0.43
1:A:304:PHE:CD2	1:A:310:PRO:HG3	2.53	0.43
1:A:319:ASN:N	1:A:320:PRO:HD3	2.33	0.43
1:A:711:ASP:OD1	1:A:714:ILE:HG12	2.18	0.43
1:A:1034:ARG:HG3	4:A:1249:HOH:O	2.18	0.43
1:B:318:ARG:NE	2:D:7:DA:C5	2.87	0.43
1:B:721:PHE:C	1:B:723:LYS:N	2.76	0.43
1:B:848:TRP:CZ3	1:B:850:LYS:HA	2.53	0.43
1:A:432:ASN:HB2	1:A:433:PRO:CD	2.49	0.43
1:A:664:LEU:HB3	1:A:668:ILE:HD11	2.01	0.43
1:B:174:ASP:O	1:B:177:ASP:HB2	2.18	0.43
1:B:369:LYS:O	1:B:371:LEU:N	2.52	0.43
1:A:156:VAL:O	1:A:160:LEU:HG	2.19	0.43
1:A:967:ALA:O	1:A:971:VAL:HG23	2.19	0.43
1:A:1053:VAL:O	1:A:1055:LEU:HD13	2.17	0.43
1:B:609:ASN:OD1	1:B:613:GLN:HG2	2.19	0.43
1:A:505:PHE:C	1:A:507:THR:H	2.26	0.43
1:B:362:MET:HE1	1:B:528:SER:HA	2.01	0.43
1:A:454:ASN:ND2	1:A:457:ASN:ND2	2.64	0.42
1:B:384:ASN:HD22	1:B:384:ASN:HA	1.64	0.42
1:A:514:ASN:HD22	1:A:514:ASN:N	2.17	0.42
1:A:752:LYS:HZ2	1:A:752:LYS:CB	2.27	0.42
1:A:955:ILE:HD13	1:A:963:ALA:HB3	2.01	0.42
1:B:685:ILE:HD12	1:B:798:ARG:HD3	2.01	0.42
1:A:771:ASN:C	1:A:773:LYS:H	2.28	0.42
1:B:705:LEU:O	1:B:709:ALA:HB2	2.20	0.42
1:A:367:LEU:HB2	1:A:372:LEU:HD21	2.02	0.42
1:B:343:HIS:HE1	1:B:537:GLU:OE2	2.02	0.42
1:B:627:ARG:NH1	1:B:627:ARG:HG2	2.35	0.42
1:A:306:GLY:O	1:A:414:HIS:HE1	2.03	0.42
1:B:728:GLU:OE2	1:B:728:GLU:HA	2.18	0.42
1:B:767:LYS:CE	1:B:769:LYS:HG2	2.50	0.42
1:A:752:LYS:HA	1:A:752:LYS:NZ	2.35	0.42
1:A:795:GLU:HB2	1:A:796:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:MET:HB2	1:B:635:PRO:HD3	2.01	0.42
1:A:742:MET:HE2	1:A:775:TYR:OH	2.20	0.42
1:B:620:MET:CG	1:B:664:LEU:HD12	2.50	0.42
1:B:710:LYS:O	1:B:711:ASP:HB2	2.20	0.42
1:B:821:GLN:HE22	1:B:914:GLN:NE2	2.18	0.42
1:A:369:LYS:O	1:A:370:GLU:HB3	2.20	0.41
1:A:399:GLU:OE1	1:A:402:ARG:NH1	2.53	0.41
1:B:37:SER:HB3	1:B:231:THR:HG22	2.02	0.41
1:B:165:THR:O	1:B:169:ASN:ND2	2.53	0.41
1:B:192:GLY:HA3	1:B:378:LYS:HB3	2.02	0.41
1:B:292:GLU:HG3	1:B:299:PRO:HB3	2.01	0.41
1:A:321:ALA:HB2	1:A:910:TYR:HE1	1.85	0.41
1:A:675:ILE:HD11	1:A:685:ILE:HG12	2.01	0.41
1:A:514:ASN:C	1:A:514:ASN:ND2	2.78	0.41
1:B:374:ASP:O	1:B:378:LYS:HG2	2.20	0.41
1:B:1048:LYS:HE2	1:B:1048:LYS:HB3	1.91	0.41
1:A:432:ASN:HB2	1:A:433:PRO:HD2	2.03	0.41
1:A:438:LEU:HD23	1:A:438:LEU:C	2.46	0.41
1:B:20:VAL:HG23	1:B:138:VAL:O	2.20	0.41
1:B:432:ASN:HB2	1:B:433:PRO:CD	2.50	0.41
1:A:1098:ARG:NE	1:A:1098:ARG:HA	2.36	0.41
1:B:184:ILE:HG12	4:B:1445:HOH:O	2.19	0.41
1:A:241:GLU:OE2	1:A:898:ASN:HB2	2.20	0.41
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.21	0.41
1:B:319:ASN:HD22	1:B:319:ASN:HA	1.51	0.41
1:A:118:LYS:HE3	1:A:118:LYS:HB2	1.93	0.41
1:A:343:HIS:CE1	1:A:537:GLU:OE2	2.74	0.41
1:A:1053:VAL:HG21	1:A:1087:LEU:HD21	2.03	0.41
1:B:127:ASN:N	1:B:127:ASN:ND2	2.67	0.41
1:B:467:LEU:O	1:B:471:LEU:HD23	2.21	0.41
1:B:728:GLU:O	1:B:729:ALA:C	2.64	0.41
1:A:512:PRO:HB2	1:A:514:ASN:ND2	2.36	0.41
1:A:1053:VAL:HG13	1:A:1075:LEU:HG	2.03	0.41
1:B:184:ILE:HD13	1:B:262:ILE:HG21	2.02	0.41
1:B:369:LYS:C	1:B:371:LEU:H	2.28	0.41
1:B:454:ASN:HB3	1:B:457:ASN:ND2	2.35	0.41
1:A:741:ASP:HA	1:A:744:THR:HG22	2.02	0.41
1:A:1041:LEU:HD22	1:A:1041:LEU:HA	1.91	0.41
1:B:733:GLU:O	1:B:736:ALA:HB3	2.21	0.41
1:A:52:GLU:CD	1:A:52:GLU:N	2.64	0.41
1:A:173:LYS:HD2	1:A:197:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:ALA:HB2	1:A:989:LYS:HD3	2.03	0.41
1:B:173:LYS:HA	1:B:177:ASP:OD1	2.20	0.41
1:B:250:THR:O	1:B:250:THR:CG2	2.69	0.41
1:B:322:VAL:HG22	1:B:872:MET:CE	2.41	0.41
1:A:16:TYR:O	1:A:35:LYS:CE	2.69	0.40
1:A:683:ARG:HG3	1:A:683:ARG:HH11	1.86	0.40
1:B:28:GLU:CD	1:B:29:GLY:N	2.79	0.40
1:A:385:ARG:HD3	1:A:385:ARG:C	2.47	0.40
1:A:626:LEU:O	1:A:630:TYR:HD1	2.04	0.40
1:A:655:ASN:HD22	1:A:655:ASN:N	2.15	0.40
1:A:715:SER:OG	1:A:718:MET:HB2	2.22	0.40
1:A:369:LYS:HE2	1:A:377:ALA:HB1	2.03	0.40
1:A:845:ASP:HA	1:A:846:PRO:HD2	1.85	0.40
1:A:886:GLU:HG3	1:A:908:SER:HB3	2.04	0.40
1:A:1074:ASP:OD1	1:A:1074:ASP:C	2.64	0.40
1:B:24:ASP:HB3	1:B:27:ALA:CB	2.42	0.40
1:B:293:GLU:HA	1:B:299:PRO:HG2	2.03	0.40
1:B:317:LEU:HD21	1:B:318:ARG:HH12	1.86	0.40
1:B:421:ARG:HD2	2:D:7:DA:H5'	2.01	0.40
1:B:658:GLU:C	1:B:660:GLY:N	2.79	0.40
1:A:267:LYS:HE2	1:A:267:LYS:HB2	1.76	0.40
1:A:471:LEU:HD12	1:A:471:LEU:HA	1.96	0.40
1:A:753:ARG:O	1:A:754:LYS:HB2	2.22	0.40
1:A:1034:ARG:HB2	1:A:1034:ARG:HH11	1.86	0.40
1:A:1075:LEU:HD21	1:A:1086:GLU:HG2	2.03	0.40
1:A:178:VAL:CG2	1:A:194:VAL:HG13	2.51	0.40
1:A:490:LEU:HD23	1:A:495:LEU:HD11	2.03	0.40
1:A:652:PRO:HD3	4:A:1481:HOH:O	2.21	0.40
1:A:831:PHE:O	1:A:835:VAL:HG23	2.21	0.40
1:A:853:PHE:CG	1:A:854:LEU:N	2.89	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	1093/1117 (98%)	1050 (96%)	35 (3%)	8 (1%)	18	14
1	B	1092/1117 (98%)	1053 (96%)	30 (3%)	9 (1%)	16	11
All	All	2185/2234 (98%)	2103 (96%)	65 (3%)	17 (1%)	16	11

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	GLU
1	A	1062	ALA
1	B	770	ILE
1	B	1062	ALA
1	A	369	LYS
1	A	371	LEU
1	A	779	GLY
1	B	724	GLN
1	B	728	GLU
1	A	666	ARG
1	B	370	GLU
1	B	727	SER
1	B	666	ARG
1	B	726	ALA
1	A	1014	TYR
1	A	1018	GLU
1	B	711	ASP

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	916/934 (98%)	882 (96%)	34 (4%)	30	30
1	B	915/934 (98%)	885 (97%)	30 (3%)	33	34
All	All	1831/1868 (98%)	1767 (96%)	64 (4%)	32	32

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	52	GLU
1	A	70	LEU
1	A	82	ASN
1	A	88	ARG
1	A	127	ASN
1	A	210	LEU
1	A	267	LYS
1	A	284	ILE
1	A	319	ASN
1	A	367	LEU
1	A	369	LYS
1	A	444	LEU
1	A	447	LYS
1	A	471	LEU
1	A	483	MET
1	A	494	ASN
1	A	514	ASN
1	A	603	ARG
1	A	613	GLN
1	A	623	LEU
1	A	634	MET
1	A	677	ILE
1	A	724	GLN
1	A	752	LYS
1	A	778	LYS
1	A	836	GLN
1	A	838	LYS
1	A	886	GLU
1	A	958	ASN
1	A	1004	LEU
1	A	1036	LEU
1	A	1041	LEU
1	A	1095	LEU
1	B	52	GLU
1	B	67	ARG
1	B	82	ASN
1	B	124	THR
1	B	127	ASN
1	B	210	LEU
1	B	284	ILE
1	B	314	ASN

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Mol	Chain	Res	Type
1	B	319	ASN
1	B	444	LEU
1	B	471	LEU
1	B	514	ASN
1	B	520	ASN
1	B	570	MET
1	B	603	ARG
1	B	623	LEU
1	B	649	LEU
1	B	662	LEU
1	B	668	ILE
1	B	670	LYS
1	B	677	ILE
1	B	767	LYS
1	B	783	LYS
1	B	795	GLU
1	B	838	LYS
1	B	886	GLU
1	B	909	ILE
1	B	1036	LEU
1	B	1041	LEU
1	B	1050	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	82	ASN
1	A	127	ASN
1	A	150	GLN
1	A	169	ASN
1	A	266	ASN
1	A	298	ASN
1	A	316	GLN
1	A	319	ASN
1	A	324	ASN
1	A	336	GLN
1	A	343	HIS
1	A	348	GLN
1	A	373	ASN
1	A	375	ASN
1	A	384	ASN

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Mol	Chain	Res	Type
1	A	414	HIS
1	A	454	ASN
1	A	455	GLN
1	A	457	ASN
1	A	469	GLN
1	A	494	ASN
1	A	506	ASN
1	A	514	ASN
1	A	520	ASN
1	A	563	ASN
1	A	600	ASN
1	A	602	HIS
1	A	613	GLN
1	A	629	ASN
1	A	639	GLN
1	A	655	ASN
1	A	671	ASN
1	A	724	GLN
1	A	771	ASN
1	A	781	GLN
1	A	815	GLN
1	A	817	GLN
1	A	823	GLN
1	A	863	GLN
1	A	867	ASN
1	A	954	ASN
1	A	958	ASN
1	A	968	ASN
1	A	982	ASN
1	A	1016	GLN
1	A	1035	ASN
1	A	1038	ASN
1	A	1047	HIS
1	A	1059	GLN
1	B	82	ASN
1	B	112	ASN
1	B	122	GLN
1	B	127	ASN
1	B	150	GLN
1	B	186	GLN
1	B	196	GLN
1	B	255	ASN

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Mol	Chain	Res	Type
1	B	316	GLN
1	B	319	ASN
1	B	324	ASN
1	B	336	GLN
1	B	343	HIS
1	B	348	GLN
1	B	376	HIS
1	B	384	ASN
1	B	414	HIS
1	B	457	ASN
1	B	469	GLN
1	B	514	ASN
1	B	520	ASN
1	B	563	ASN
1	B	602	HIS
1	B	613	GLN
1	B	629	ASN
1	B	639	GLN
1	B	655	ASN
1	B	771	ASN
1	B	781	GLN
1	B	786	GLN
1	B	791	HIS
1	B	815	GLN
1	B	817	GLN
1	B	833	GLN
1	B	856	GLN
1	B	892	ASN
1	B	893	GLN
1	B	914	GLN
1	B	954	ASN
1	B	958	ASN
1	B	968	ASN
1	B	1016	GLN
1	B	1019	ASN
1	B	1035	ASN
1	B	1059	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	2HP	A	1106	-	4,4,4	2.10	3 (75%)	6,6,6	0.34	0
3	2HP	B	1106	-	4,4,4	2.07	2 (50%)	6,6,6	0.47	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1106	2HP	P-O1	2.71	1.56	1.50
3	A	1106	2HP	P-O2	2.63	1.62	1.54
3	A	1106	2HP	P-O1	2.50	1.56	1.50
3	B	1106	2HP	P-O2	2.32	1.61	1.54
3	A	1106	2HP	P-O3	2.12	1.60	1.54

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

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	1095/1117 (98%)	0.51	124 (11%) 10 9	9, 25, 61, 75	0
1	B	1094/1117 (97%)	0.40	104 (9%) 14 12	10, 23, 58, 81	0
2	C	20/36 (55%)	0.96	6 (30%) 1 1	25, 36, 85, 86	0
2	D	21/36 (58%)	0.60	3 (14%) 6 5	19, 30, 70, 78	0
All	All	2230/2306 (96%)	0.46	237 (10%) 11 10	9, 24, 61, 86	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	725	ALA	8.4
1	B	726	ALA	6.5
1	A	714	ILE	6.0
1	B	716	ALA	5.9
1	B	719	ALA	5.6
2	C	4	DC	5.3
1	A	661	ALA	5.3
1	B	723	LYS	5.2
1	B	729	ALA	5.2
1	B	172	ILE	5.1
1	A	175	ALA	5.0
1	A	677	ILE	4.8
1	B	659	ASN	4.8
1	A	678	TYR	4.7
1	A	710	LYS	4.6
1	B	721	PHE	4.6
1	A	1014	TYR	4.5
1	A	755	GLY	4.5
1	B	766	ALA	4.4
1	B	191	GLU	4.3
1	A	1020	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	719	ALA	4.3
1	A	1019	ASN	4.2
1	B	184	ILE	4.2
1	A	766	ALA	4.1
1	A	656	LEU	4.1
1	B	1097	ALA	4.1
1	B	198	ASP	4.0
1	A	184	ILE	4.0
1	A	708	ARG	3.9
1	B	180	ALA	3.9
1	A	8	LEU	3.9
1	B	714	ILE	3.9
1	B	722	GLY	3.9
1	B	717	ALA	3.9
1	A	910	TYR	3.8
1	B	715	SER	3.8
1	A	767	LYS	3.8
1	B	194	VAL	3.8
1	A	707	ALA	3.7
1	A	716	ALA	3.7
1	A	1097	ALA	3.7
1	B	708	ARG	3.6
1	B	724	GLN	3.6
1	B	187	ALA	3.6
2	D	3	DT	3.6
1	A	265	ASP	3.5
1	B	707	ALA	3.5
1	A	722	GLY	3.5
1	B	5	THR	3.5
1	B	656	LEU	3.5
1	A	1100	GLN	3.5
1	B	770	ILE	3.4
1	A	367	LEU	3.4
1	A	718	MET	3.4
1	B	910	TYR	3.4
1	A	657	GLY	3.4
1	B	192	GLY	3.4
1	B	634	MET	3.4
1	B	28	GLU	3.4
1	A	369	LYS	3.4
1	A	172	ILE	3.4
1	A	189	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	185	ASP	3.3
2	D	4	DC	3.2
1	A	729	ALA	3.2
1	B	281	PHE	3.2
1	A	170	THR	3.2
1	A	658	GLU	3.2
1	B	731	ALA	3.2
1	A	705	LEU	3.2
1	A	730	HIS	3.2
1	B	657	GLY	3.2
1	A	712	PRO	3.2
1	B	711	ASP	3.1
1	A	726	ALA	3.1
1	B	171	ALA	3.1
1	A	372	LEU	3.1
1	B	764	THR	3.1
1	A	371	LEU	3.1
1	B	183	GLY	3.1
1	A	725	ALA	3.0
2	C	6	DA	3.0
1	A	704	VAL	3.0
1	B	704	VAL	3.0
1	A	772	PRO	3.0
1	A	1001	PRO	3.0
1	B	718	MET	3.0
1	A	1016	GLN	2.9
1	A	188	LEU	2.9
1	B	8	LEU	2.9
1	B	188	LEU	2.9
1	B	712	PRO	2.9
2	C	5	DC	2.9
1	B	709	ALA	2.9
1	A	198	ASP	2.8
1	B	763	GLY	2.9
1	A	1004	LEU	2.8
1	A	770	ILE	2.8
1	A	190	PRO	2.8
1	B	6	GLU	2.8
1	B	755	GLY	2.8
1	A	195	GLU	2.8
1	B	262	ILE	2.8
1	B	720	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	261	GLU	2.8
1	B	1018	GLU	2.8
1	A	76	THR	2.8
1	A	776	THR	2.8
1	A	186	GLN	2.8
1	B	195	GLU	2.8
1	B	658	GLU	2.8
1	A	763	GLY	2.8
1	B	705	LEU	2.8
1	A	281	PHE	2.7
1	B	193	LEU	2.7
1	A	262	ILE	2.7
1	A	724	GLN	2.7
1	A	1025	ILE	2.7
2	D	23	DT	2.7
1	B	575	GLY	2.7
1	A	662	LEU	2.7
1	B	264	PRO	2.7
1	B	780	GLU	2.7
1	A	74	LYS	2.7
1	A	844	LYS	2.7
1	A	187	ALA	2.7
1	B	727	SER	2.7
1	A	174	ASP	2.7
1	A	192	GLY	2.7
1	A	1017	ARG	2.7
1	B	779	GLY	2.7
1	A	781	GLN	2.6
1	B	655	ASN	2.6
1	A	765	GLY	2.6
1	A	264	PRO	2.6
1	B	734	LEU	2.6
1	B	1014	TYR	2.6
1	B	765	GLY	2.6
1	B	768	GLY	2.6
1	A	171	ALA	2.6
1	B	769	LYS	2.6
1	A	711	ASP	2.6
1	A	181	ILE	2.6
1	A	720	MET	2.6
1	B	74	LYS	2.6
1	A	199	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	181	ILE	2.5
1	A	659	ASN	2.5
1	A	774	THR	2.5
1	B	189	LEU	2.5
1	B	277	GLU	2.5
1	A	721	PHE	2.5
1	A	178	VAL	2.5
1	A	655	ASN	2.5
1	B	266	ASN	2.5
1	A	177	ASP	2.5
1	B	743	GLU	2.5
1	B	1098	ARG	2.5
1	A	185	ASP	2.5
1	B	772	PRO	2.5
1	B	197	PHE	2.5
1	B	706	LYS	2.5
1	B	1037	ARG	2.5
1	A	779	GLY	2.5
1	B	525	ASP	2.4
1	A	7	GLU	2.4
1	A	715	SER	2.4
1	B	776	THR	2.4
1	A	180	ALA	2.4
1	A	267	LYS	2.4
1	A	1095	LEU	2.4
1	A	6	GLU	2.4
1	A	743	GLU	2.4
1	B	196	GLN	2.4
1	A	194	VAL	2.4
1	B	70	LEU	2.4
1	A	10	GLU	2.4
1	A	728	GLU	2.4
1	A	660	GLY	2.4
1	B	1019	ASN	2.4
1	B	653	ASP	2.4
1	A	1021	THR	2.4
1	B	775	TYR	2.3
1	A	1023	ASP	2.3
1	B	732	GLU	2.3
1	A	193	LEU	2.3
1	A	1015	ASP	2.3
1	A	366	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	760	GLN	2.3
1	A	1098	ARG	2.3
1	A	1093	GLU	2.3
1	B	774	THR	2.3
1	A	365	GLY	2.3
1	A	775	TYR	2.3
1	A	1018	GLU	2.2
1	B	730	HIS	2.2
1	A	723	LYS	2.2
1	B	710	LYS	2.2
1	A	653	ASP	2.2
1	A	735	LEU	2.2
1	B	370	GLU	2.2
1	A	654	ILE	2.2
1	A	773	LYS	2.2
1	B	178	VAL	2.2
1	A	717	ALA	2.2
1	A	731	ALA	2.2
1	A	1006	ALA	2.2
1	A	734	LEU	2.2
1	B	1095	LEU	2.2
1	B	174	ASP	2.2
1	B	756	VAL	2.2
1	A	11	GLY	2.2
2	C	8	DA	2.2
2	C	9	DA	2.2
1	B	179	ALA	2.2
1	A	1012	LEU	2.2
1	B	678	TYR	2.2
1	A	701	MET	2.2
1	A	300	THR	2.2
1	B	260	SER	2.1
1	A	634	MET	2.1
1	B	660	GLY	2.1
1	B	267	LYS	2.1
1	B	628	SER	2.1
1	B	701	MET	2.1
1	A	84	GLU	2.1
1	A	12	ILE	2.1
1	B	175	ALA	2.1
1	A	25	SER	2.1
1	A	385	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	683	ARG	2.1
1	A	698	TYR	2.0
1	B	632	SER	2.0
1	B	321	ALA	2.0
1	A	713	ASN	2.0
2	C	7	DA	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($\text{\AA}^2$)	Q<0.9
3	2HP	B	1106	5/5	0.89	0.16	34,34,37,38	0
3	2HP	A	1106	5/5	0.94	0.10	27,28,30,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.