



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 07:57 AM EDT

PDB ID : 4FF4 / pdb_00004ff4
Title : N4 mini-vRNAP transcription initiation complex, 4 min after soaking GTP, ATP and Mn
Authors : Murakami, K.S.
Deposited on : 2012-05-31
Resolution : 2.03 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

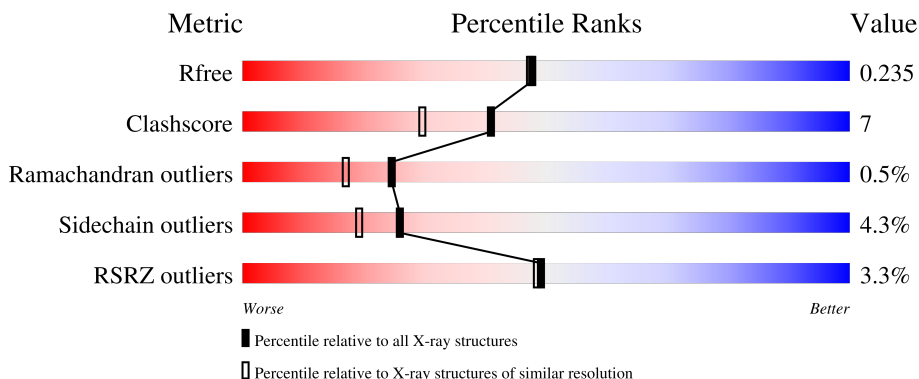
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

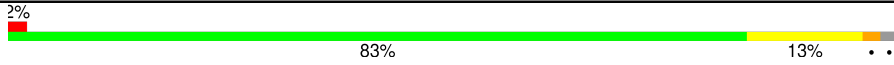

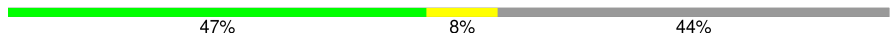
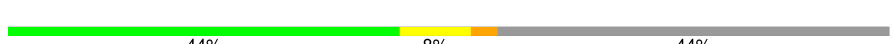
The reported resolution of this entry is 2.03 Å.

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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	1118	 2% 83% 13% ..
1	B	1118	 5% 81% 15% ..
2	C	36	 47% 8% 44%
2	D	36	 44% 8% 44%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 18998 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
			Total	C	N	O	S			
1	A	1095	8454	5306	1435	1672	41	0	0	0
1	B	1095	8454	5306	1435	1672	41	0	0	0

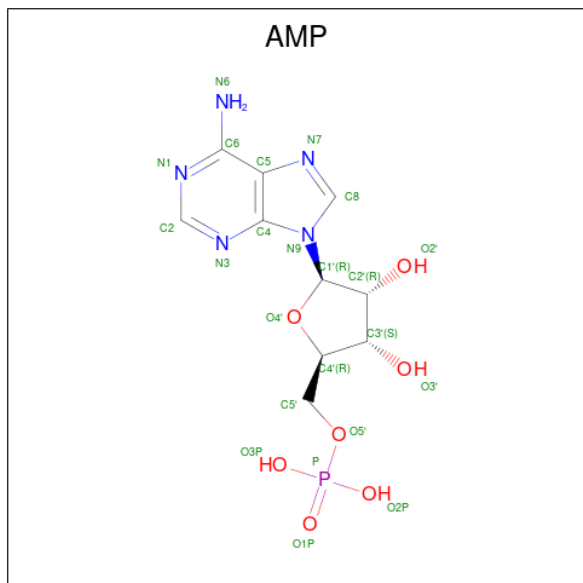
There are 24 discrepancies between the modelled and reference sequences:

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 Bacteriophage N4 P2 promoter.

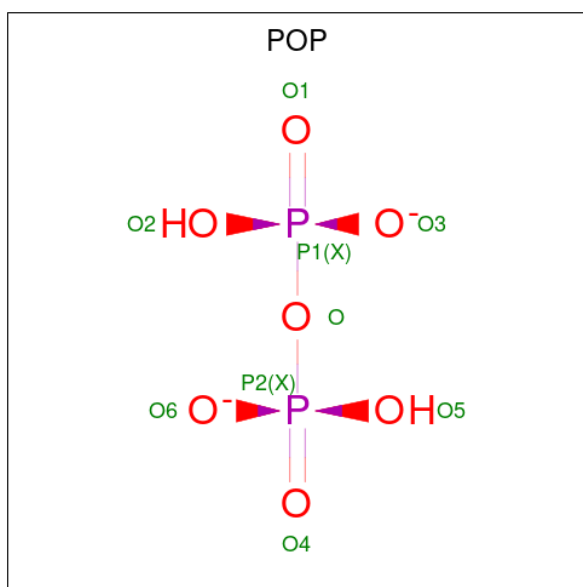
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	20	Total 413	196	80	117	20	0	0	0
2	D	20	Total 413	196	80	117	20	0	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 22	10	5	6	1	0	0

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).

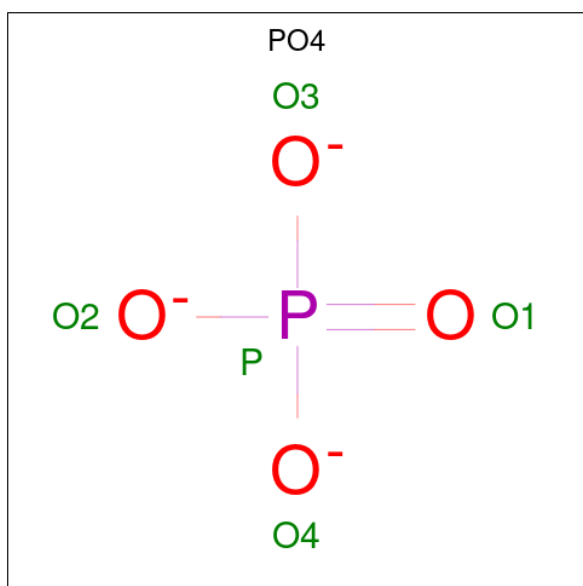


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 9 7 2	0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

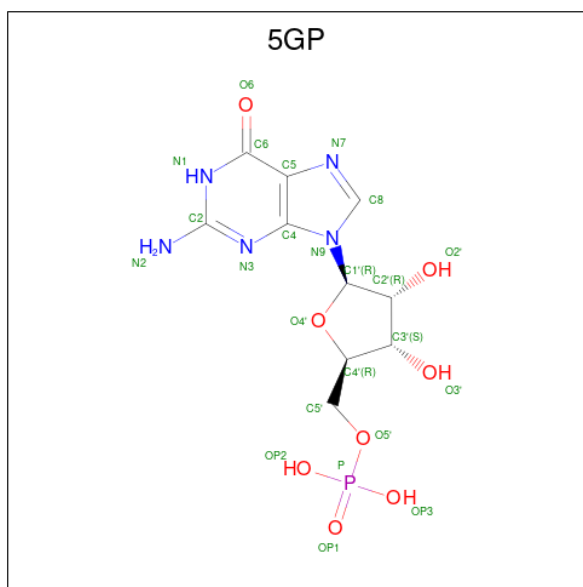
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mn 1 1	0	0

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 7 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C N O P 24 10 5 8 1	0	0

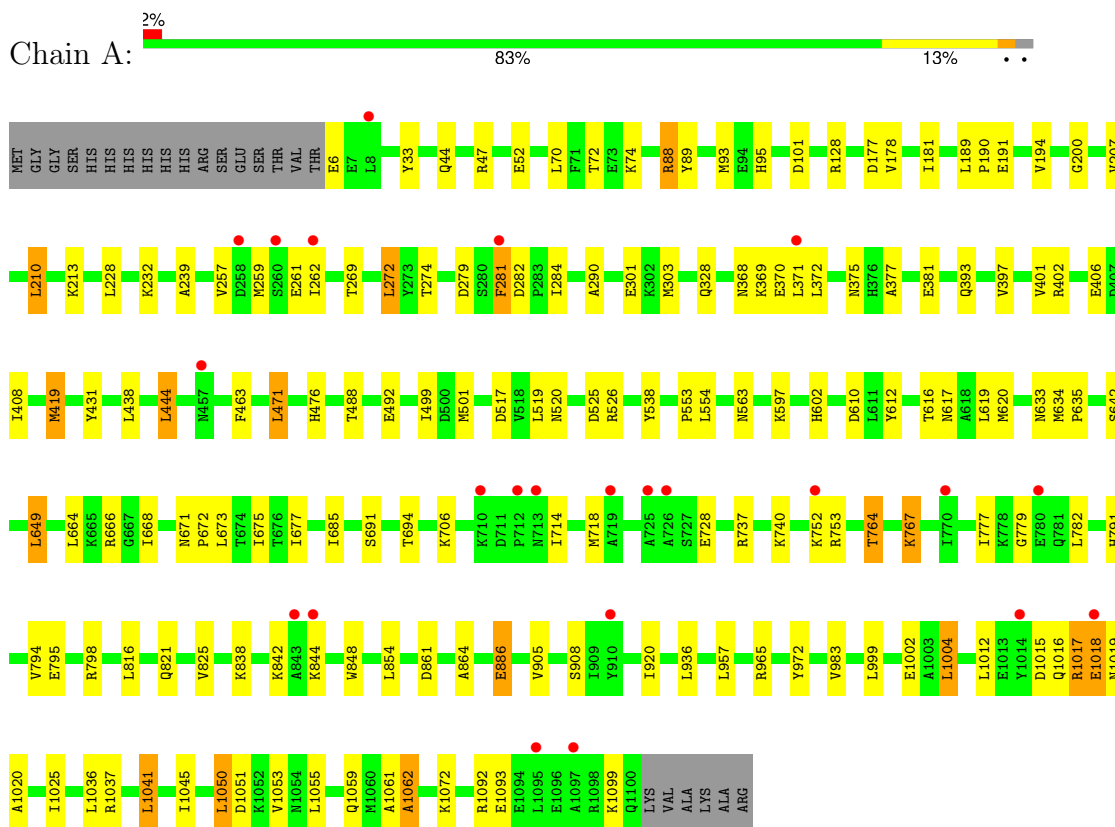
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	546	Total O 546 546	0	0
8	C	39	Total O 39 39	0	0
8	B	572	Total O 572 572	0	0
8	D	41	Total O 41 41	0	0

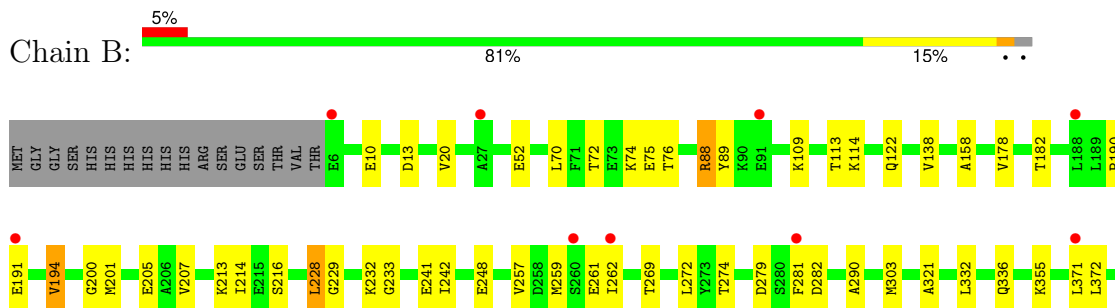
3 Residue-property plots [i](#)

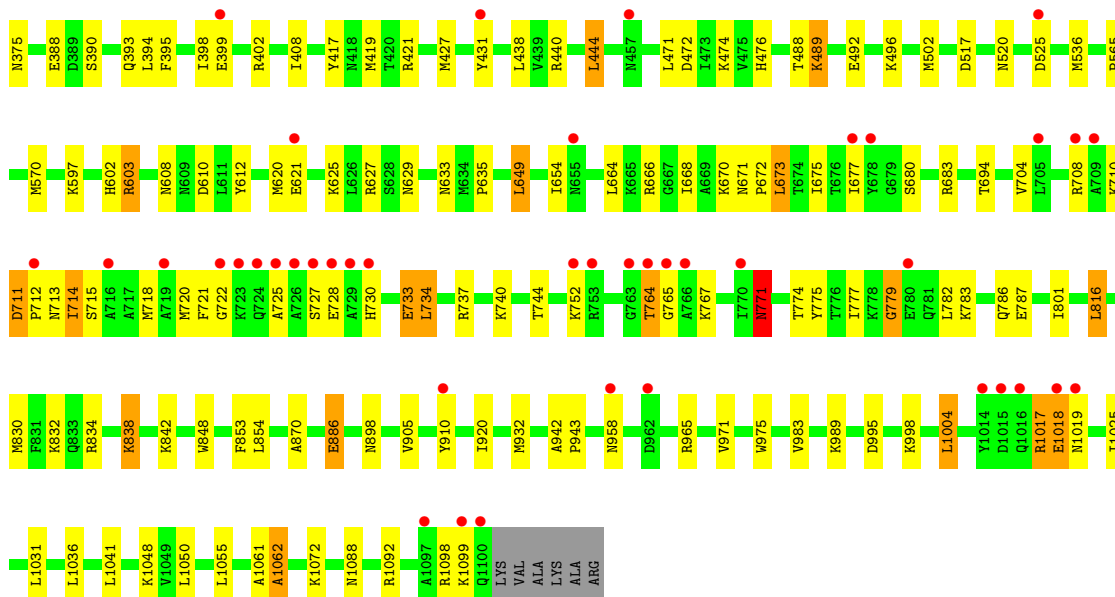
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

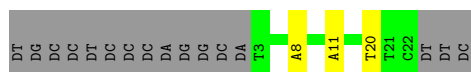


- Molecule 1: Virion RNA polymerase

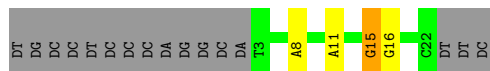




• Molecule 2: Bacteriophage N4 P2 promoter



• Molecule 2: Bacteriophage N4 P2 promoter



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.40Å 111.78Å 276.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.87 – 2.03 43.87 – 2.03	Depositor EDS
% Data completeness (in resolution range)	94.1 (43.87-2.03) 90.5 (43.87-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.03Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.191 , 0.239 0.186 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtrriage
Anisotropy	0.257	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18998	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 5GP, AMP, MN, POP

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	0.73	2/11609 (0.0%)
1	B	0.42	0/8583	0.73	3/11609 (0.0%)
2	C	0.20	0/464	0.73	0/714
2	D	0.21	0/464	0.77	1/714 (0.1%)
All	All	0.41	0/18094	0.73	6/24646 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	15	DG	C4'-C3'-O3'	-6.54	100.19	110.00
1	B	771	ASN	CA-C-N	5.63	125.74	119.32
1	B	771	ASN	C-N-CA	5.63	125.74	119.32
1	B	371	LEU	N-CA-C	-5.58	105.78	112.59
1	A	371	LEU	N-CA-C	-5.46	105.23	112.94
1	A	563	ASN	N-CA-C	5.35	116.79	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8454	0	8479	123	0
2	C	413	0	225	3	0
2	D	413	0	225	4	0
3	A	22	0	12	1	0
4	A	9	0	0	1	0
5	A	1	0	0	0	0
6	A	5	0	0	1	0
6	B	5	0	0	1	0
7	C	24	0	11	0	0
8	A	546	0	0	14	0
8	B	572	0	0	17	0
8	C	39	0	0	1	0
8	D	41	0	0	0	0
All	All	18998	0	17431	230	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 7.

All (230) 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:718:MET:HE3	1:B:728:GLU:HA	1.57	0.86
1:B:476:HIS:ND1	6:B:1201:PO4:O2	2.10	0.81
1:A:767:LYS:NZ	1:A:767:LYS:HA	1.95	0.81
1:A:861:ASP:OD2	8:A:1625:HOH:O	2.02	0.76
1:A:6:GLU:N	8:A:1361:HOH:O	2.18	0.76
1:A:393:GLN:HG3	1:A:431:TYR:CD2	2.21	0.75
1:B:1018:GLU:HG3	1:B:1019:ASN:H	1.52	0.75
1:B:228:LEU:HD12	1:B:232:LYS:HD2	1.69	0.75
1:A:844:LYS:NZ	8:A:1717:HOH:O	2.20	0.74
1:B:1017:ARG:O	1:B:1019:ASN:N	2.20	0.74
1:A:228:LEU:HD12	1:A:232:LYS:HD2	1.70	0.73
1:B:711:ASP:C	1:B:713:ASN:H	1.98	0.71
1:B:1072:LYS:HA	1:B:1072:LYS:HE2	1.72	0.71
1:B:402:ARG:HA	1:B:408:ILE:HG22	1.71	0.71
1:B:610:ASP:OD2	1:B:666:ARG:NH1	2.25	0.70
1:A:999:LEU:HB2	1:A:1004:LEU:HD23	1.73	0.70
1:A:718:MET:HE2	1:A:728:GLU:HA	1.72	0.70
1:A:191:GLU:HG3	1:A:375:ASN:HB3	1.74	0.69
1:B:612:TYR:HD1	1:B:666:ARG:NH1	1.89	0.69
1:A:190:PRO:HG2	1:A:262:ILE:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:LEU:HD13	1:B:737:ARG:NH2	2.08	0.69
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.75	0.68
1:A:1018:GLU:HG3	1:A:1019:ASN:H	1.60	0.67
1:B:720:MET:HE2	1:B:721:PHE:CZ	2.29	0.67
1:A:1017:ARG:O	1:A:1019:ASN:N	2.28	0.67
2:C:20:DT:O4	8:C:217:HOH:O	2.12	0.66
1:A:612:TYR:HD1	1:A:666:ARG:NH1	1.92	0.66
1:B:711:ASP:O	1:B:713:ASN:N	2.29	0.66
1:B:393:GLN:HG3	1:B:431:TYR:CD2	2.30	0.65
1:B:694:THR:HG22	1:B:777:ILE:HD12	1.78	0.65
1:A:1072:LYS:HE2	1:A:1072:LYS:HA	1.79	0.65
1:A:419:MET:HE3	8:A:1309:HOH:O	1.96	0.64
1:B:570:MET:HE2	1:B:975:TRP:HB3	1.78	0.64
1:B:870:ALA:HB2	1:B:989:LYS:HD3	1.79	0.64
1:A:328:GLN:HG2	1:A:419:MET:HE2	1.80	0.64
1:A:886:GLU:O	2:C:8:DA:H4'	1.98	0.64
1:A:617:ASN:HA	1:A:620:MET:HE2	1.80	0.63
1:B:783:LYS:O	1:B:787:GLU:HG2	1.97	0.63
1:B:958:ASN:ND2	8:B:1799:HOH:O	2.32	0.63
1:B:355:LYS:HD2	1:B:388:GLU:HG3	1.80	0.62
1:B:191:GLU:HG3	1:B:375:ASN:HB3	1.82	0.62
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.82	0.61
1:A:767:LYS:HA	1:A:767:LYS:HZ3	1.64	0.60
1:B:417:TYR:OH	1:B:427:MET:HE3	2.02	0.60
1:B:764:THR:OG1	1:B:765:GLY:N	2.31	0.60
1:A:303:MET:HE1	1:A:397:VAL:HG13	1.84	0.60
1:B:496:LYS:NZ	8:B:1687:HOH:O	2.31	0.59
1:B:740:LYS:O	1:B:744:THR:HG22	2.02	0.59
1:B:332:LEU:O	1:B:336:GLN:HG3	2.02	0.59
1:A:767:LYS:HA	1:A:767:LYS:HZ2	1.67	0.58
1:B:771:ASN:OD1	1:B:774:THR:OG1	2.18	0.58
1:A:402:ARG:HA	1:A:408:ILE:HG22	1.84	0.58
1:A:714:ILE:HD11	1:A:718:MET:HB3	1.86	0.58
1:B:670:LYS:NZ	8:B:1607:HOH:O	2.36	0.58
1:B:1048:LYS:HD2	1:B:1098:ARG:HH21	1.69	0.57
1:B:830:MET:O	1:B:834:ARG:HG3	2.04	0.57
1:A:444:LEU:HG	1:A:553:PRO:HB2	1.87	0.57
1:B:710:LYS:O	1:B:711:ASP:HB3	2.04	0.56
1:B:597:LYS:HE2	1:B:602:HIS:HB2	1.87	0.56
1:A:1002:GLU:OE1	1:A:1002:GLU:N	2.29	0.56
1:A:965:ARG:HD2	8:A:1702:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:PRO:HG2	1:B:262:ILE:HG23	1.88	0.56
1:B:621:GLU:OE1	8:B:1730:HOH:O	2.17	0.56
1:A:88:ARG:HD3	1:A:282:ASP:OD1	2.06	0.56
1:B:52:GLU:H	1:B:52:GLU:CD	2.14	0.56
1:B:158:ALA:HB1	1:B:213:LYS:HG3	1.88	0.55
1:B:207:VAL:HG11	1:B:905:VAL:HG21	1.88	0.55
1:B:257:VAL:HG12	1:B:259:MET:HE3	1.88	0.55
1:B:842:LYS:NZ	8:B:1385:HOH:O	2.25	0.55
1:B:421:ARG:HG3	8:B:1312:HOH:O	2.05	0.55
1:B:965:ARG:NH2	8:B:1724:HOH:O	2.35	0.55
1:B:259:MET:HA	1:B:259:MET:HE2	1.88	0.54
1:A:47:ARG:NH1	8:A:1533:HOH:O	2.41	0.54
1:B:673:LEU:HD22	1:B:801:ILE:HG12	1.89	0.54
1:A:842:LYS:HB3	1:A:848:TRP:CD2	2.43	0.54
1:A:1004:LEU:HD13	1:A:1025:ILE:HG13	1.90	0.54
1:B:671:ASN:HB3	1:B:672:PRO:HD3	1.89	0.53
1:A:612:TYR:CD1	1:A:666:ARG:NH1	2.74	0.53
1:B:1018:GLU:HG3	1:B:1019:ASN:N	2.23	0.53
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.89	0.53
1:B:257:VAL:HG12	1:B:259:MET:CE	2.39	0.53
1:B:727:SER:OG	1:B:730:HIS:HB2	2.09	0.53
1:B:201:MET:HE2	1:B:205:GLU:HG2	1.91	0.52
1:B:88:ARG:HD3	1:B:282:ASP:OD1	2.10	0.52
1:A:488:THR:O	1:A:492:GLU:HG2	2.09	0.52
1:B:114:LYS:NZ	2:D:15:DG:N7	2.56	0.52
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.09	0.52
1:A:257:VAL:HG12	1:A:259:MET:CE	2.41	0.51
1:B:625:LYS:O	1:B:629:ASN:ND2	2.43	0.51
1:B:965:ARG:NE	8:B:1724:HOH:O	2.36	0.51
1:A:274:THR:HG23	8:A:1387:HOH:O	2.09	0.51
1:B:402:ARG:HA	1:B:408:ILE:CG2	2.40	0.51
1:A:95:HIS:HA	1:B:248:GLU:O	2.11	0.51
1:A:377:ALA:O	1:A:381:GLU:HG3	2.11	0.51
1:B:816:LEU:HD13	1:B:983:VAL:HG21	1.93	0.51
1:B:182:THR:HB	1:B:259:MET:SD	2.51	0.51
1:B:603:ARG:NH1	1:B:608:ASN:OD1	2.44	0.51
1:A:471:LEU:O	1:A:526:ARG:HD3	2.11	0.51
1:A:1061:ALA:O	1:A:1062:ALA:CB	2.58	0.51
1:A:190:PRO:HG2	1:A:262:ILE:CG2	2.40	0.50
1:B:677:ILE:O	1:B:920:ILE:HG21	2.11	0.50
1:B:777:ILE:HG22	1:B:782:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLY:HA2	1:A:274:THR:HG22	1.94	0.49
1:A:753:ARG:NH2	8:A:1796:HOH:O	2.45	0.49
1:B:965:ARG:NH1	8:B:1673:HOH:O	2.32	0.49
1:B:395:PHE:O	1:B:399:GLU:HG2	2.13	0.49
1:A:463:PHE:HA	1:A:957:LEU:HD13	1.95	0.49
1:A:821:GLN:O	1:A:825:VAL:HG23	2.13	0.49
1:A:675:ILE:HD11	1:A:685:ILE:HG12	1.94	0.48
1:B:229:GLY:O	1:B:233:GLY:HA3	2.13	0.48
1:B:842:LYS:HB3	1:B:848:TRP:CD2	2.48	0.48
1:A:972:TYR:OH	1:A:1051:ASP:OD1	2.27	0.48
1:B:1061:ALA:O	1:B:1062:ALA:HB2	2.14	0.48
1:B:995:ASP:CG	1:B:998:LYS:HG3	2.38	0.48
1:B:675:ILE:O	1:B:680:SER:HB3	2.13	0.48
1:A:1018:GLU:HG3	1:A:1019:ASN:N	2.26	0.48
1:B:886:GLU:O	2:D:8:DA:H4'	2.13	0.48
1:A:368:ASN:O	1:A:370:GLU:N	2.47	0.47
1:B:1017:ARG:O	1:B:1018:GLU:C	2.58	0.47
1:A:228:LEU:HD23	1:A:854:LEU:O	2.14	0.47
1:A:259:MET:HE2	1:A:259:MET:HA	1.97	0.47
1:B:502:MET:CE	1:B:536:MET:HE2	2.44	0.47
1:A:694:THR:HG22	1:A:777:ILE:HD12	1.97	0.47
1:A:1016:GLN:O	1:A:1020:ALA:HB2	2.15	0.47
1:B:72:THR:O	1:B:74:LYS:HG2	2.14	0.47
1:A:499:ILE:HD12	1:A:538:TYR:HD2	1.80	0.47
1:A:1092:ARG:HG2	1:A:1092:ARG:HH11	1.80	0.47
1:B:488:THR:O	1:B:492:GLU:HG2	2.15	0.47
1:A:368:ASN:C	1:A:370:GLU:H	2.23	0.47
1:B:321:ALA:HB2	1:B:910:TYR:HE1	1.80	0.47
1:B:722:GLY:N	8:B:1796:HOH:O	2.36	0.47
1:A:33:TYR:OH	1:A:128:ARG:CZ	2.63	0.47
1:B:710:LYS:HE2	1:B:710:LYS:HB3	1.67	0.47
1:B:438:LEU:C	1:B:438:LEU:HD23	2.40	0.46
1:A:1004:LEU:CD1	1:A:1025:ILE:HG13	2.44	0.46
1:B:1088:ASN:O	1:B:1092:ARG:HG3	2.16	0.46
1:B:725:ALA:HB3	8:B:1744:HOH:O	2.14	0.46
1:A:89:TYR:CZ	1:A:290:ALA:HB3	2.51	0.46
1:B:279:ASP:HB3	1:B:281:PHE:CE1	2.51	0.46
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.16	0.46
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.98	0.46
1:A:554:LEU:HD23	1:A:957:LEU:HD11	1.98	0.46
1:A:1015:ASP:CG	1:A:1016:GLN:N	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:GLY:O	1:B:783:LYS:HG3	2.16	0.46
1:A:93:MET:HE2	1:A:93:MET:HA	1.98	0.45
1:A:328:GLN:HG2	1:A:419:MET:CE	2.45	0.45
1:A:597:LYS:HE2	1:A:602:HIS:HB2	1.97	0.45
1:B:832:LYS:HG3	8:B:1786:HOH:O	2.15	0.45
1:B:995:ASP:OD1	1:B:998:LYS:HG3	2.15	0.45
1:B:711:ASP:C	1:B:713:ASN:N	2.66	0.45
1:B:113:THR:HG22	1:B:114:LYS:HG3	1.98	0.45
1:B:214:ILE:HD11	1:B:242:ILE:HD12	1.99	0.45
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.81	0.45
1:A:619:LEU:O	1:A:619:LEU:HD12	2.17	0.45
1:A:642:SER:OG	1:A:740:LYS:NZ	2.50	0.45
1:B:710:LYS:O	1:B:711:ASP:CB	2.65	0.45
1:B:1061:ALA:O	1:B:1062:ALA:CB	2.65	0.45
1:B:694:THR:HG22	1:B:777:ILE:CD1	2.45	0.45
1:B:1072:LYS:HE2	1:B:1072:LYS:CA	2.44	0.45
1:B:1048:LYS:HD2	1:B:1098:ARG:NH2	2.31	0.45
1:A:101:ASP:OD1	1:B:109:LYS:HE3	2.18	0.44
1:B:489:LYS:NZ	8:B:1606:HOH:O	2.50	0.44
1:A:397:VAL:O	1:A:401:VAL:HG23	2.17	0.44
1:B:654:ILE:HD13	1:B:664:LEU:HD22	1.99	0.44
1:B:708:ARG:HA	1:B:714:ILE:HG21	1.98	0.44
1:B:774:THR:O	1:B:775:TYR:C	2.60	0.44
1:A:649:LEU:HD13	1:A:737:ARG:NH2	2.32	0.44
1:B:269:THR:O	2:D:11:DA:H5'	2.18	0.44
1:A:616:THR:CG2	1:A:664:LEU:HB2	2.48	0.43
1:A:706:LYS:HB2	1:A:706:LYS:HE3	1.68	0.43
1:A:791:HIS:ND1	1:A:795:GLU:OE2	2.50	0.43
1:B:259:MET:CE	1:B:262:ILE:HD12	2.48	0.43
1:B:633:ASN:OD1	1:B:635:PRO:HD2	2.18	0.43
1:B:1004:LEU:CD1	1:B:1025:ILE:HG13	2.48	0.43
1:B:394:LEU:O	1:B:398:ILE:HG12	2.19	0.43
1:B:942:ALA:HA	1:B:943:PRO:HD3	1.89	0.43
1:B:20:VAL:HG23	1:B:138:VAL:O	2.18	0.43
3:A:1201:AMP:P	4:A:1202:POP:O3	2.77	0.43
1:B:673:LEU:HD13	1:B:673:LEU:O	2.19	0.43
1:B:853:PHE:CG	1:B:854:LEU:N	2.87	0.43
1:A:438:LEU:HD23	1:A:438:LEU:C	2.44	0.43
1:A:476:HIS:ND1	6:A:1204:PO4:O1	2.34	0.43
1:B:627:ARG:NE	8:B:1716:HOH:O	2.50	0.43
1:B:565:PRO:HG3	1:B:673:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ASN:OD1	1:A:635:PRO:HD2	2.19	0.42
1:A:279:ASP:HB3	1:A:281:PHE:CE1	2.53	0.42
1:A:764:THR:HG23	8:A:1596:HOH:O	2.20	0.42
1:B:259:MET:HE2	1:B:262:ILE:HD12	2.01	0.42
1:B:816:LEU:HD12	1:B:816:LEU:O	2.20	0.42
1:A:671:ASN:HB3	1:A:672:PRO:HD3	2.02	0.42
1:B:721:PHE:O	8:B:1744:HOH:O	2.21	0.42
1:B:13:ASP:HB2	8:B:1671:HOH:O	2.18	0.42
1:A:189:LEU:HA	1:A:190:PRO:HD3	1.93	0.42
1:A:1050:LEU:HD12	1:A:1050:LEU:HA	1.87	0.42
1:B:440:ARG:O	1:B:444:LEU:HD13	2.19	0.42
1:A:213:LYS:NZ	1:A:301:GLU:OE2	2.28	0.42
1:A:1037:ARG:HG3	8:A:1811:HOH:O	2.19	0.42
1:A:1092:ARG:HG2	1:A:1092:ARG:NH1	2.35	0.41
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.46	0.41
1:A:1012:LEU:O	1:A:1017:ARG:NH1	2.51	0.41
1:B:75:GLU:HG3	1:B:76:THR:N	2.35	0.41
1:A:52:GLU:CD	1:A:52:GLU:H	2.29	0.41
1:A:471:LEU:HD12	1:A:471:LEU:HA	1.92	0.41
1:B:303:MET:HE2	1:B:303:MET:HB3	1.98	0.41
1:A:610:ASP:OD1	1:A:610:ASP:C	2.64	0.41
1:B:838:LYS:HA	1:B:838:LYS:HD3	1.78	0.41
1:A:44:GLN:NE2	8:A:1458:HOH:O	2.24	0.41
1:A:210:LEU:HB3	1:A:239:ALA:HB1	2.03	0.41
1:A:393:GLN:HG2	8:A:1783:HOH:O	2.20	0.41
1:B:474:LYS:HD3	1:B:474:LYS:HA	1.90	0.41
1:A:864:ALA:HB3	8:A:1826:HOH:O	2.21	0.41
1:A:965:ARG:NH2	8:A:1488:HOH:O	2.37	0.41
1:A:177:ASP:O	1:A:181:ILE:HG13	2.21	0.41
1:A:634:MET:N	1:A:635:PRO:CD	2.84	0.41
1:A:677:ILE:O	1:A:920:ILE:HG21	2.21	0.41
1:A:794:VAL:O	1:A:798:ARG:HG2	2.20	0.41
1:B:241:GLU:OE2	1:B:898:ASN:HB2	2.21	0.41
1:B:965:ARG:CZ	8:B:1724:HOH:O	2.69	0.41
1:A:269:THR:O	2:C:11:DA:H5'	2.21	0.41
1:B:200:GLY:HA2	1:B:274:THR:HG22	2.01	0.40
1:B:683:ARG:HG2	1:B:786:GLN:HE21	1.86	0.40
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.56	0.40
1:A:1015:ASP:C	1:A:1017:ARG:H	2.30	0.40
1:B:733:GLU:HG2	1:B:734:LEU:N	2.34	0.40
1:B:932:MET:HE2	1:B:971:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:THR:O	1:A:74:LYS:HE3	2.21	0.40
2:D:15:DG:H2''	2:D:16:DG:C8	2.57	0.40
1:A:501:MET:HE1	1:A:519:LEU:HG	2.03	0.40
1:A:764:THR:O	1:A:764:THR:OG1	2.29	0.40
1:B:620:MET:HG3	1:B:664:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1093/1118 (98%)	1065 (97%)	23 (2%)	5 (0%)	24 17
1	B	1093/1118 (98%)	1057 (97%)	30 (3%)	6 (0%)	24 17
All	All	2186/2236 (98%)	2122 (97%)	53 (2%)	11 (0%)	24 17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1018	GLU
1	B	711	ASP
1	B	1018	GLU
1	A	369	LYS
1	A	779	GLY
1	A	1017	ARG
1	A	1062	ALA
1	B	1017	ARG
1	B	1062	ALA
1	B	712	PRO
1	B	779	GLY

5.3.2 Protein sidechains [i](#)

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	916/935 (98%)	880 (96%)	36 (4%)	28	22
1	B	916/935 (98%)	874 (95%)	42 (5%)	24	17
All	All	1832/1870 (98%)	1754 (96%)	78 (4%)	26	19

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	88	ARG
1	A	210	LEU
1	A	261	GLU
1	A	272	LEU
1	A	281	PHE
1	A	284	ILE
1	A	372	LEU
1	A	406	GLU
1	A	419	MET
1	A	444	LEU
1	A	471	LEU
1	A	517	ASP
1	A	520	ASN
1	A	525	ASP
1	A	649	LEU
1	A	668	ILE
1	A	673	LEU
1	A	691	SER
1	A	752	LYS
1	A	764	THR
1	A	767	LYS
1	A	782	LEU
1	A	838	LYS
1	A	886	GLU
1	A	908	SER
1	A	936	LEU

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Mol	Chain	Res	Type
1	A	1004	LEU
1	A	1036	LEU
1	A	1041	LEU
1	A	1050	LEU
1	A	1053	VAL
1	A	1055	LEU
1	A	1059	GLN
1	A	1093	GLU
1	A	1099	LYS
1	B	10	GLU
1	B	70	LEU
1	B	88	ARG
1	B	122	GLN
1	B	194	VAL
1	B	216	SER
1	B	228	LEU
1	B	261	GLU
1	B	272	LEU
1	B	372	LEU
1	B	390	SER
1	B	419	MET
1	B	444	LEU
1	B	471	LEU
1	B	472	ASP
1	B	489	LYS
1	B	517	ASP
1	B	520	ASN
1	B	525	ASP
1	B	603	ARG
1	B	649	LEU
1	B	668	ILE
1	B	673	LEU
1	B	704	VAL
1	B	714	ILE
1	B	715	SER
1	B	733	GLU
1	B	734	LEU
1	B	752	LYS
1	B	764	THR
1	B	767	LYS
1	B	771	ASN
1	B	816	LEU

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Mol	Chain	Res	Type
1	B	838	LYS
1	B	886	GLU
1	B	1004	LEU
1	B	1031	LEU
1	B	1036	LEU
1	B	1041	LEU
1	B	1050	LEU
1	B	1055	LEU
1	B	1099	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	404	GLN
1	A	464	GLN
1	A	506	ASN
1	A	563	ASN
1	A	613	GLN
1	A	671	ASN
1	A	815	GLN
1	A	976	GLN
1	A	1035	ASN
1	A	1059	GLN
1	B	298	ASN
1	B	404	GLN
1	B	520	ASN
1	B	671	ASN
1	B	815	GLN
1	B	856	GLN
1	B	863	GLN
1	B	878	GLN
1	B	976	GLN
1	B	1016	GLN
1	B	1035	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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
3	AMP	A	1201	7	21,24,25	0.26	0	30,35,38	0.57	0
4	POP	A	1202	5	6,8,8	0.70	0	12,13,13	1.14	2 (16%)
6	PO4	A	1204	-	4,4,4	0.95	0	6,6,6	0.70	0
6	PO4	B	1201	-	4,4,4	0.89	0	6,6,6	0.52	0
7	5GP	C	101	3	26,26,26	1.00	2 (7%)	39,40,40	1.75	9 (23%)

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
3	AMP	A	1201	7	-	0/7/25/26	0/3/3/3
7	5GP	C	101	3	-	0/10/26/26	0/3/3/3
4	POP	A	1202	5	-	2/6/6/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	101	5GP	C6-N1	-2.12	1.34	1.38
7	C	101	5GP	C5-N7	-2.08	1.34	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	101	5GP	C5-C4-N3	-5.85	119.08	128.39
7	C	101	5GP	C2-N3-C4	4.47	119.99	112.30
7	C	101	5GP	N9-C4-N3	3.49	132.94	125.95
7	C	101	5GP	OP2-P-O5'	-3.05	98.71	106.67
4	A	1202	POP	O5-P2-O	2.35	112.53	104.64
7	C	101	5GP	C5-C6-N1	2.26	119.01	113.25
7	C	101	5GP	C2-N1-C6	-2.23	121.07	125.11
7	C	101	5GP	C4-C5-N7	-2.15	107.26	110.67
7	C	101	5GP	O6-C6-C5	-2.11	120.95	126.53
7	C	101	5GP	N9-C8-N7	-2.06	109.58	113.40
4	A	1202	POP	O2-P1-O	2.05	111.51	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

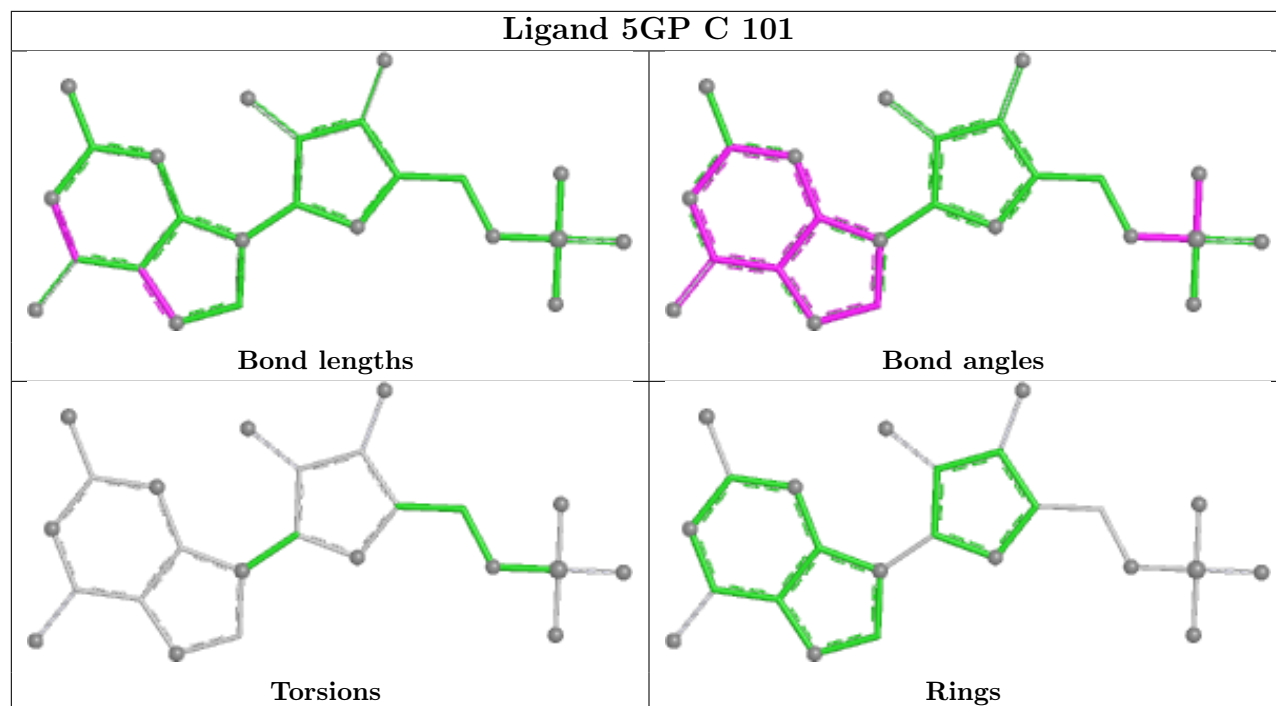
Mol	Chain	Res	Type	Atoms
4	A	1202	POP	P1-O-P2-O6
4	A	1202	POP	P1-O-P2-O4

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1201	AMP	1	0
4	A	1202	POP	1	0
6	A	1204	PO4	1	0
6	B	1201	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	1095/1118 (97%)	-0.08	23 (2%) 63 63	16, 34, 72, 106	0
1	B	1095/1118 (97%)	0.01	51 (4%) 36 35	15, 33, 75, 147	0
2	C	20/36 (55%)	-0.40	0 100 100	34, 41, 70, 71	0
2	D	20/36 (55%)	-0.29	0 100 100	28, 41, 69, 96	0
All	All	2230/2308 (96%)	-0.04	74 (3%) 49 48	15, 33, 72, 147	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	729	ALA	6.0
1	B	725	ALA	5.1
1	B	726	ALA	5.0
1	A	262	ILE	4.6
1	B	764	THR	4.6
1	B	1018	GLU	4.3
1	B	1014	TYR	4.2
1	B	1019	ASN	3.9
1	B	728	GLU	3.9
1	B	281	PHE	3.6
1	B	727	SER	3.4
1	B	709	ALA	3.3
1	A	910	TYR	3.3
1	B	752	LYS	3.3
1	A	726	ALA	3.2
1	B	457	ASN	3.2
1	A	1014	TYR	3.2
1	B	371	LEU	3.1
1	B	766	ALA	3.1
1	B	723	LYS	3.1
1	B	730	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	958	ASN	3.0
1	B	1100	GLN	2.9
1	B	1099	LYS	2.9
1	B	910	TYR	2.9
1	B	262	ILE	2.8
1	B	708	ARG	2.7
1	A	260	SER	2.7
1	B	763	GLY	2.7
1	B	716	ALA	2.7
1	B	962	ASP	2.6
1	B	770	ILE	2.6
1	B	1097	ALA	2.6
1	B	1015	ASP	2.6
1	B	6	GLU	2.6
1	A	713	ASN	2.6
1	A	725	ALA	2.5
1	B	678	TYR	2.5
1	A	719	ALA	2.5
1	A	843	ALA	2.5
1	B	191	GLU	2.5
1	A	281	PHE	2.5
1	A	1097	ALA	2.5
1	B	27	ALA	2.4
1	A	1095	LEU	2.4
1	A	371	LEU	2.3
1	B	724	GLN	2.3
1	A	770	ILE	2.3
1	B	677	ILE	2.3
1	B	525	ASP	2.3
1	B	91	GLU	2.3
1	B	719	ALA	2.3
1	B	765	GLY	2.3
1	B	188	LEU	2.2
1	B	753	ARG	2.2
1	B	780	GLU	2.2
1	A	8	LEU	2.2
1	B	1016	GLN	2.2
1	A	752	LYS	2.2
1	A	712	PRO	2.2
1	B	712	PRO	2.2
1	A	258	ASP	2.2
1	B	655	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	705	LEU	2.1
1	A	1018	GLU	2.1
1	A	844	LYS	2.1
1	B	722	GLY	2.1
1	A	710	LYS	2.1
1	A	780	GLU	2.1
1	B	399	GLU	2.1
1	B	621	GLU	2.1
1	A	457	ASN	2.1
1	B	431	TYR	2.1
1	B	260	SER	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](#)

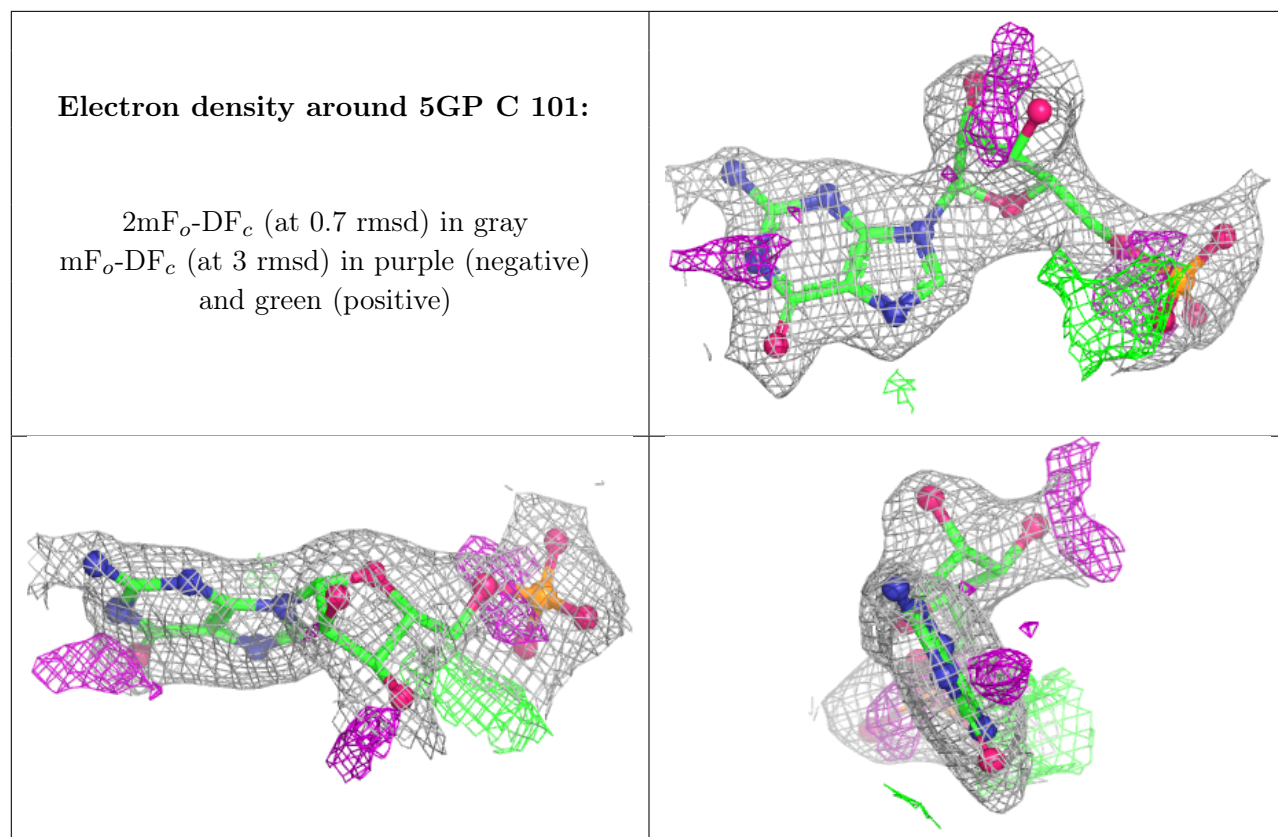
There are no oligosaccharides in this entry.

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(\AA^2)	Q<0.9
4	POP	A	1202	9/9	0.81	0.15	36,69,75,240	0
7	5GP	C	101	24/24	0.83	0.11	36,43,61,72	0
5	MN	A	1203	1/1	0.89	0.21	92,92,92,92	0
6	PO4	B	1201	5/5	0.91	0.17	49,50,57,58	0
3	AMP	A	1201	22/23	0.91	0.08	33,36,53,59	0
6	PO4	A	1204	5/5	0.95	0.11	43,47,49,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.