



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:31 AM UTC

PDB ID : 6UQ3 / pdb_00006uq3
Title : RNA polymerase II elongation complex with 5-guanidinohydantoin lesion in state 5
Authors : Oh, J.; Wang, D.
Deposited on : 2019-10-18
Resolution : 3.47 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
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

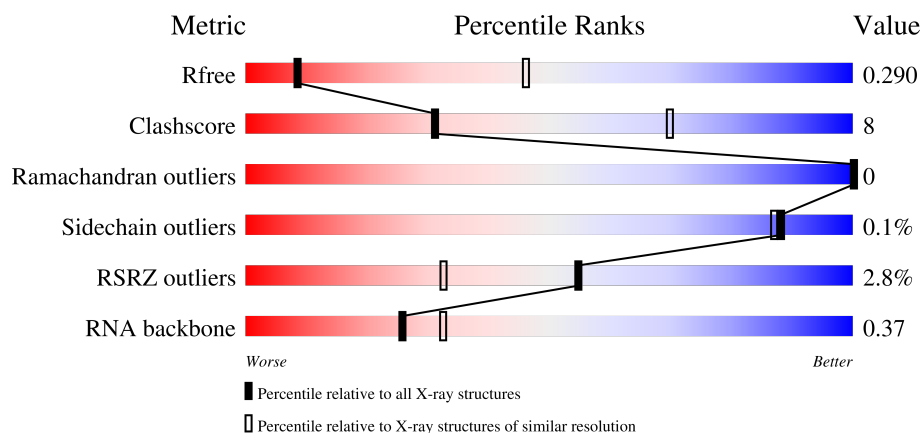
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.47 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)
RNA backbone	3983	1001 (3.94-3.02)

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	R	11	 64% 18% 9% 9%
2	T	29	 62% 24% 10%
3	N	18	 72% 17% 11%
4	A	1733	 2% 64% 16% 20%

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Mol	Chain	Length	Quality of chain
5	B	1224	3% 71% 20% 8%
6	C	318	% 63% 21% 16%
7	E	215	7% 77% 22% .
8	F	155	50% 6% 45%
9	H	146	2% 78% 13% 9%
10	I	122	% 74% 23% .
11	J	70	3% 74% 19% 7%
12	K	120	% 80% 15% 5%
13	L	70	40% 21% 39%

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29119 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			218	97	42	69	10			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	0	0
			519	248	81	164	26			

- Molecule 3 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	16	Total	C	N	O	P	0	0	0
			339	158	76	89	16			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1385	Total	C	N	O	S	0	0	0
			10837	6836	1898	2043	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1123	Total	C	N	O	S	0	0	0
			8859	5607	1552	1647	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	213	Total	C	N	O	S	0	0	0
			1740	1105	307	317	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			952	585	173	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

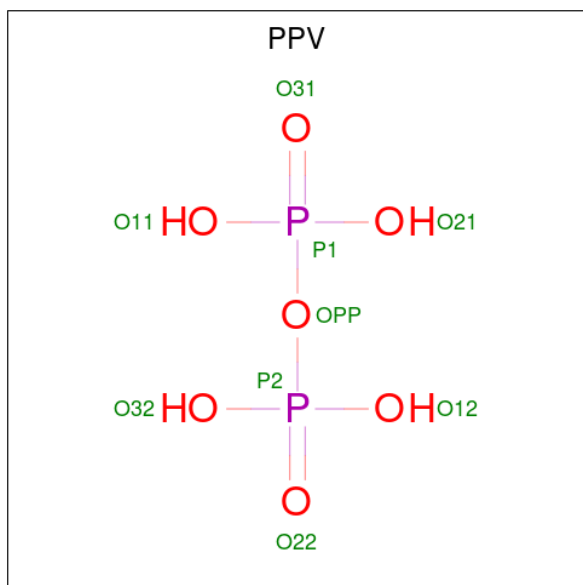
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	R	1	Total Mg 1 1	0	0

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	2	Total Zn 2 2	0	0
15	B	1	Total Zn 1 1	0	0
15	C	1	Total Zn 1 1	0	0
15	I	2	Total Zn 2 2	0	0
15	J	1	Total Zn 1 1	0	0
15	L	1	Total Zn 1 1	0	0

- Molecule 16 is PYROPHOSPHATE (CCD ID: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total O P 9 7 2	0	0

3 Residue-property plots

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

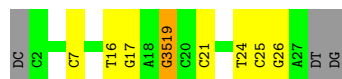
- Molecule 1: RNA

Chain R: 



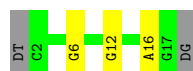
- Molecule 2: Template strand DNA

Chain T: 



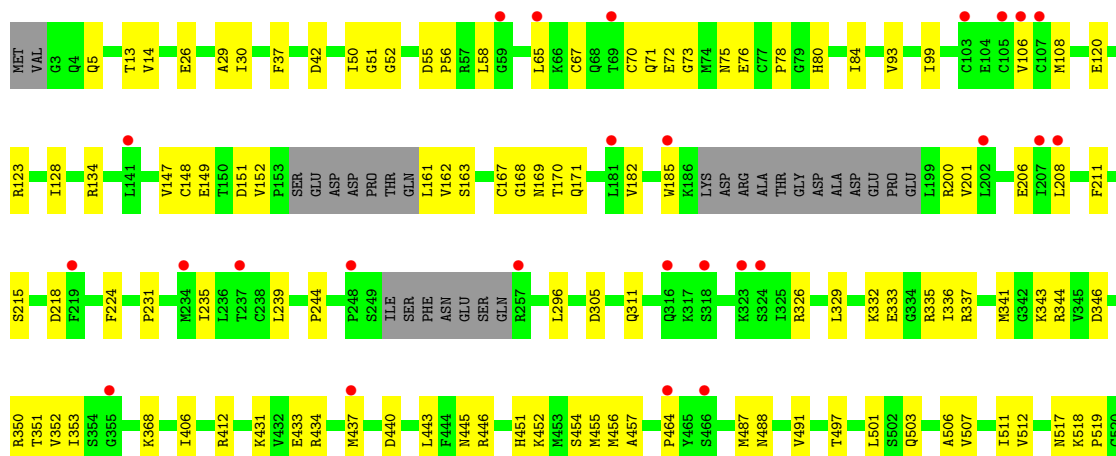
- Molecule 3: Non-template strand DNA

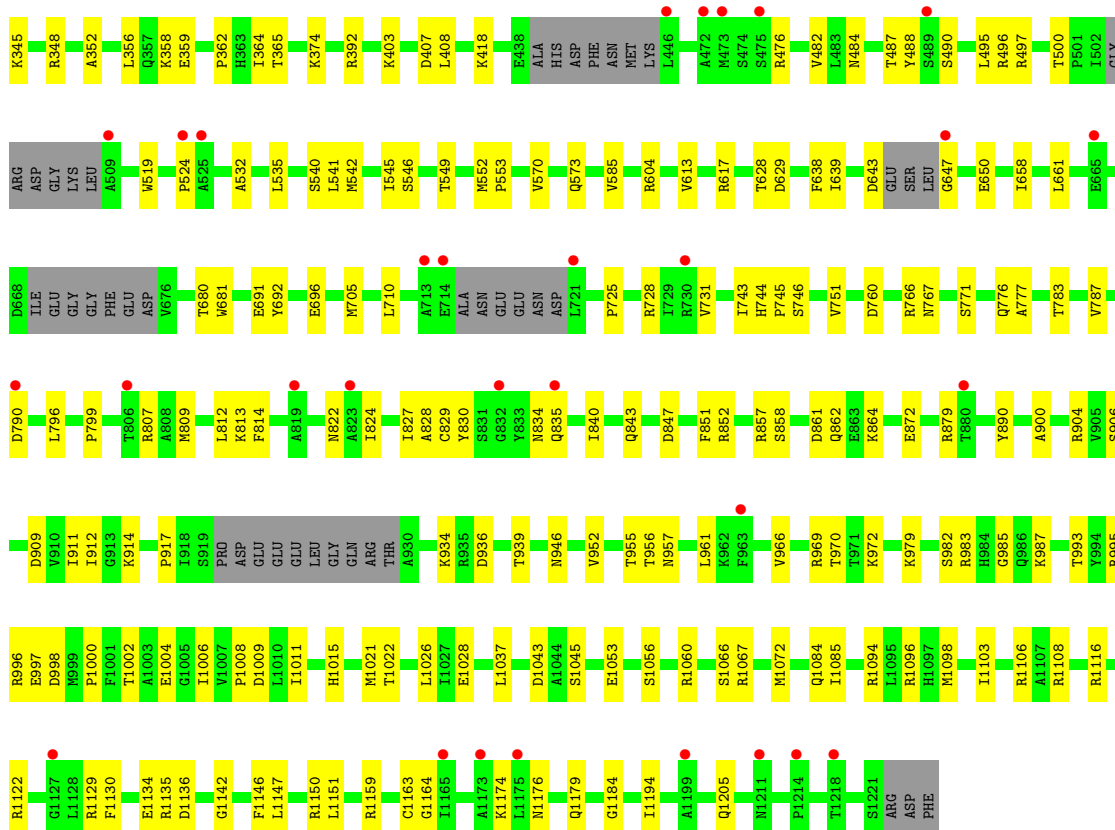
Chain N: 



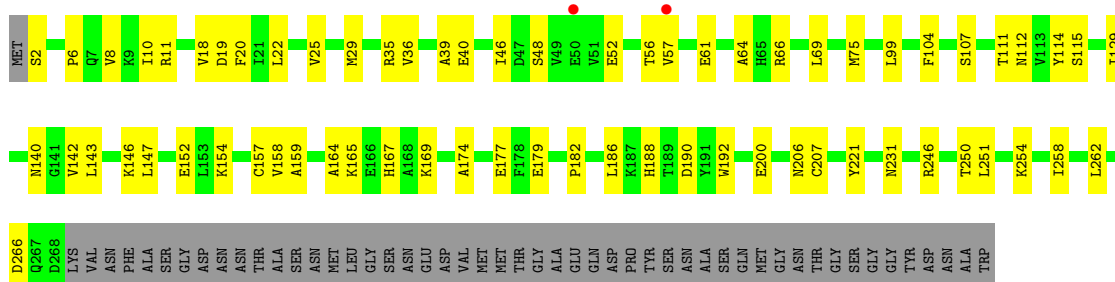
- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain A: 

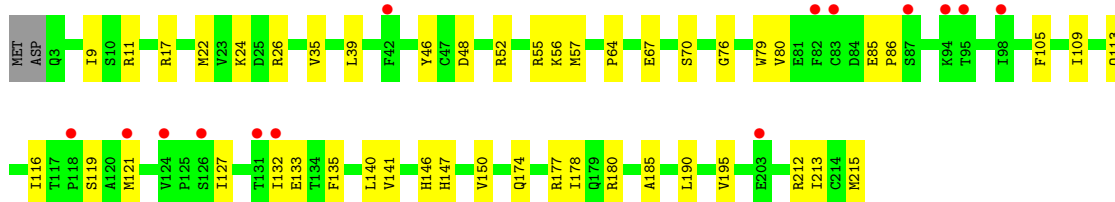
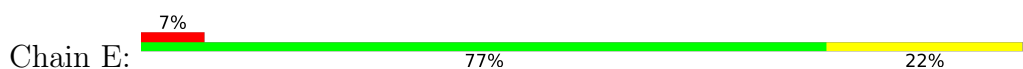




- Molecule 6: DNA-directed RNA polymerase II subunit RPB3

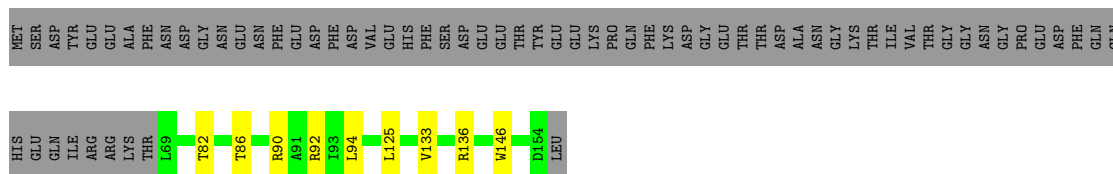


- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



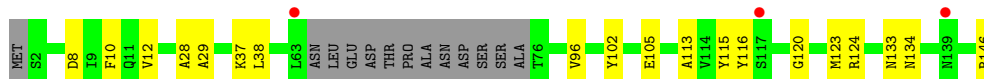
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  50% 6% 45%



- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  2% 78% 13% 9%



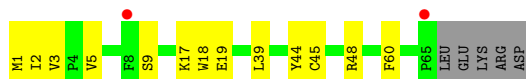
- Molecule 10: DNA-directed RNA polymerase II subunit RPB9

Chain I:  2% 74% 23% .



- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  3% 74% 19% 7%

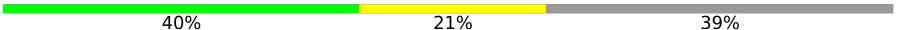


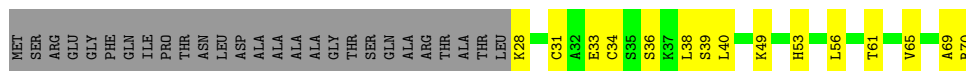
- Molecule 12: DNA-directed RNA polymerase II subunit RPB11

Chain K:  2% 80% 15% 5%



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  40% 21% 39%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.19Å 222.58Å 194.61Å 90.00° 101.34° 90.00°	Depositor
Resolution (Å)	49.27 – 3.47 49.27 – 3.47	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.27-3.47) 99.9 (49.27-3.47)	Depositor EDS
R_{merge}	0.58	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.234 , 0.286 0.235 , 0.290	Depositor DCC
R_{free} test set	2000 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 89.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	29119	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: G35, MG, PPV, ZN

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	R	0.15	0/244	0.33	0/379
2	T	0.29	0/550	0.55	0/841
3	N	0.24	0/384	0.50	0/592
4	A	0.20	0/11029	0.47	0/14919
5	B	0.18	0/9030	0.43	0/12186
6	C	0.16	0/2139	0.39	0/2899
7	E	0.18	0/1776	0.45	0/2390
8	F	0.18	0/696	0.42	0/943
9	H	0.20	0/1082	0.51	0/1466
10	I	0.19	0/970	0.43	0/1308
11	J	0.19	0/541	0.49	0/727
12	K	0.17	0/937	0.39	0/1265
13	L	0.20	0/339	0.53	0/450
All	All	0.19	0/29717	0.45	0/40365

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
4	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	311	GLN	Peptide
4	A	55	ASP	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	R	218	0	109	1	0
2	T	519	0	298	8	0
3	N	339	0	177	3	0
4	A	10837	0	10882	199	0
5	B	8859	0	8816	174	0
6	C	2101	0	2056	54	0
7	E	1740	0	1766	33	0
8	F	684	0	692	7	0
9	H	1064	0	1029	15	0
10	I	952	0	900	19	0
11	J	532	0	542	15	0
12	K	919	0	929	17	0
13	L	337	0	352	11	0
14	R	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	B	9	0	0	0	0
All	All	29119	0	28548	467	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 8.

All (467) 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)
4:A:567:LYS:HB2	9:H:96:VAL:HG12	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:26:GLU:O	4:A:30:ILE:HD13	1.64	0.98
7:E:55:ARG:NH1	7:E:113:GLN:OE1	2.02	0.92
2:T:21:DC:OP1	4:A:344:ARG:NH2	2.05	0.90
5:B:1072:MET:HE2	5:B:1085:ILE:HG13	1.55	0.87
5:B:613:VAL:HG23	5:B:628:THR:HG22	1.66	0.77
4:A:344:ARG:CZ	5:B:1129:ARG:HG3	2.16	0.75
6:C:40:GLU:OE1	6:C:254:LYS:HE3	1.88	0.74
4:A:75:ASN:HA	5:B:1116:ARG:HH22	1.53	0.73
6:C:66:ARG:NH2	11:J:3:VAL:O	2.23	0.72
5:B:213:ILE:HD11	5:B:497:ARG:HB3	1.73	0.71
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.71	0.71
6:C:6:PRO:HB3	6:C:25:VAL:HG22	1.73	0.70
12:K:7:PHE:HB2	12:K:11:LEU:HD13	1.74	0.70
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.74	0.70
2:T:21:DC:P	4:A:344:ARG:HH22	2.15	0.69
5:B:552:MET:HG3	5:B:553:PRO:HD3	1.75	0.69
5:B:705:MET:HE2	5:B:745:PRO:HB3	1.74	0.69
5:B:851:PHE:HB3	5:B:1094:ARG:HD2	1.76	0.68
4:A:567:LYS:CB	9:H:96:VAL:HG12	2.23	0.67
9:H:116:TYR:HB2	9:H:123:MET:HG2	1.76	0.67
6:C:57:VAL:HG21	11:J:60:PHE:HB3	1.76	0.67
4:A:596:THR:HG22	4:A:597:LEU:H	1.61	0.65
11:J:17:LYS:HB3	11:J:39:LEU:HD13	1.79	0.65
4:A:535:THR:O	4:A:575:LYS:NZ	2.30	0.65
4:A:346:ASP:HB3	5:B:1106:ARG:HE	1.62	0.65
4:A:65:LEU:HA	4:A:73:GLY:HA2	1.79	0.64
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.78	0.64
4:A:666:ILE:HG22	5:B:1026:LEU:HB3	1.78	0.63
4:A:51:GLY:HA2	4:A:56:PRO:HB3	1.78	0.63
4:A:147:VAL:HG23	4:A:149:GLU:HG2	1.82	0.62
9:H:10:PHE:CD2	9:H:38:LEU:HD22	2.34	0.62
5:B:847:ASP:OD2	12:K:6:ARG:NH2	2.32	0.61
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.81	0.61
4:A:13:THR:OG1	4:A:1432:GLN:NE2	2.31	0.61
4:A:412:ARG:NH1	4:A:433:GLU:OE2	2.33	0.61
2:T:24:DT:OP1	5:B:857:ARG:NH2	2.33	0.61
4:A:1107:VAL:HG22	4:A:1383:SER:HB3	1.80	0.61
4:A:526:ASP:OD1	5:B:835:GLN:NE2	2.34	0.61
5:B:995:ARG:NH1	5:B:997:GLU:OE2	2.34	0.61
5:B:766:ARG:HG2	5:B:1022:THR:HG22	1.83	0.61
9:H:10:PHE:CE2	9:H:38:LEU:HD22	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:7:DC:H42	3:N:12:DG:H22	1.48	0.60
4:A:106:VAL:O	4:A:171:GLN:NE2	2.34	0.60
5:B:643:ASP:HB3	5:B:647:GLY:HA2	1.82	0.60
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.34	0.60
4:A:898:ARG:O	4:A:1029:ARG:NH2	2.34	0.60
4:A:590:ARG:NH1	4:A:592:ASP:OD1	2.35	0.60
5:B:218:SER:O	5:B:241:ARG:NH2	2.35	0.60
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.84	0.60
4:A:108:MET:SD	4:A:108:MET:N	2.71	0.60
4:A:525:GLN:O	5:B:1015:HIS:NE2	2.35	0.60
4:A:167:CYS:SG	4:A:168:GLY:N	2.74	0.60
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.35	0.60
7:E:85:GLU:C	7:E:113:GLN:HE21	2.11	0.59
4:A:350:ARG:NH1	4:A:488:ASN:OD1	2.36	0.59
4:A:344:ARG:NH1	5:B:1129:ARG:HG3	2.17	0.59
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.35	0.59
4:A:37:PHE:H	4:A:52:GLY:HA2	1.67	0.59
4:A:128:ILE:HG23	4:A:134:ARG:HB2	1.84	0.59
4:A:900:ASP:OD1	4:A:926:GLN:NE2	2.36	0.59
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.82	0.59
5:B:969:ARG:NH1	6:C:61:GLU:OE1	2.34	0.58
4:A:443:LEU:HG	4:A:501:LEU:HD11	1.83	0.58
6:C:112:ASN:ND2	11:J:19:GLU:OE2	2.36	0.58
4:A:1363:VAL:HB	4:A:1368:MET:HE2	1.85	0.58
5:B:1072:MET:HE2	5:B:1085:ILE:HG21	1.85	0.58
5:B:203:PHE:HE1	5:B:212:LEU:HG	1.67	0.58
5:B:952:VAL:HG22	5:B:966:VAL:HG13	1.86	0.58
4:A:575:LYS:HE2	9:H:120:GLY:HA3	1.86	0.58
5:B:617:ARG:NH2	10:I:61:ASP:OD2	2.36	0.57
6:C:143:LEU:HD21	6:C:146:LYS:HE3	1.85	0.57
4:A:503:GLN:OE1	8:F:90:ARG:NH2	2.37	0.57
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.84	0.57
4:A:50:ILE:HD13	4:A:52:GLY:H	1.69	0.57
4:A:795:GLU:HG2	5:B:731:VAL:HG11	1.86	0.57
6:C:169:LYS:NZ	13:L:69:ALA:O	2.37	0.57
4:A:445:ASN:HD21	5:B:1134:GLU:HG2	1.67	0.57
4:A:1397:LEU:HB2	4:A:1426:GLU:HG3	1.85	0.57
5:B:1009:ASP:OD2	11:J:48:ARG:NH2	2.37	0.57
7:E:79:TRP:HB2	7:E:105:PHE:HD1	1.69	0.57
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.87	0.57
4:A:999:VAL:HG12	4:A:1000:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1281:ARG:HG2	4:A:1309:ASP:HB2	1.86	0.57
5:B:260:GLY:O	5:B:267:ARG:NH1	2.38	0.57
12:K:91:CYS:HA	12:K:94:ILE:HD12	1.87	0.57
5:B:364:ILE:HD13	5:B:585:VAL:HG13	1.86	0.56
5:B:852:ARG:NH2	13:L:70:ARG:O	2.36	0.56
6:C:66:ARG:HH21	11:J:2:ILE:HG23	1.70	0.56
2:T:25:DC:H2"	2:T:26:DG:H5"	1.87	0.56
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.88	0.56
5:B:208:SER:OG	5:B:210:LYS:NZ	2.37	0.56
5:B:62:ILE:HG23	5:B:418:LYS:HG2	1.87	0.56
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.69	0.56
7:E:9:ILE:HG22	7:E:39:LEU:HD11	1.88	0.56
6:C:56:THR:HG22	6:C:147:LEU:HD21	1.88	0.56
4:A:42:ASP:HB2	4:A:50:ILE:HG23	1.88	0.55
4:A:351:THR:OG1	4:A:352:VAL:N	2.39	0.55
7:E:177:ARG:O	7:E:212:ARG:NH2	2.39	0.55
4:A:337:ARG:HA	4:A:341:MET:HB2	1.89	0.55
4:A:456:MET:HE3	4:A:507:VAL:HG22	1.89	0.55
4:A:663:SER:O	4:A:742:ASN:ND2	2.39	0.55
5:B:1037:LEU:HD21	11:J:44:TYR:HD2	1.71	0.55
4:A:877:HIS:HB2	4:A:1056:SER:HB3	1.88	0.55
5:B:41:LYS:NZ	5:B:692:TYR:OH	2.39	0.55
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.87	0.55
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.40	0.55
5:B:298:LEU:HD22	5:B:314:LEU:HD13	1.88	0.55
6:C:52:GLU:HB3	6:C:154:LYS:HB3	1.89	0.54
4:A:523:ILE:HG23	4:A:527:THR:HB	1.90	0.54
5:B:307:ASP:OD2	5:B:392:ARG:NH1	2.40	0.54
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.89	0.54
4:A:549:MET:HG2	4:A:652:VAL:HG13	1.89	0.54
4:A:992:ASP:O	4:A:996:ASN:ND2	2.40	0.54
12:K:100:ALA:O	12:K:104:ASN:ND2	2.36	0.54
4:A:662:PHE:HB3	5:B:829:CYS:HB2	1.88	0.54
5:B:243:ALA:HB2	5:B:251:ILE:HG13	1.88	0.54
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.88	0.54
2:T:19:G35:OP1	4:A:332:LYS:NZ	2.37	0.54
4:A:903:ASN:O	4:A:907:THR:OG1	2.26	0.54
5:B:54:PHE:HA	5:B:58:THR:HB	1.89	0.54
5:B:112:LEU:HD21	5:B:117:ALA:HB2	1.90	0.54
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.41	0.54
5:B:983:ARG:NH2	5:B:1028:GLU:OE1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:613:VAL:CG2	5:B:628:THR:HG22	2.37	0.54
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.89	0.54
6:C:165:LYS:NZ	12:K:39:ASP:OD2	2.34	0.54
4:A:898:ARG:NH1	4:A:930:ASP:OD1	2.34	0.53
6:C:46:ILE:HA	6:C:159:ALA:HA	1.89	0.53
4:A:588:LEU:HB3	4:A:607:ILE:HB	1.90	0.53
4:A:598:LEU:HD21	9:H:124:ARG:HB2	1.90	0.53
4:A:1155:ASP:HB3	4:A:1241:ARG:HH21	1.74	0.53
5:B:484:ASN:OD1	5:B:490:SER:OG	2.24	0.53
5:B:985:GLY:O	5:B:987:LYS:NZ	2.39	0.53
10:I:80:SER:OG	10:I:103:CYS:SG	2.63	0.53
4:A:170:THR:HB	4:A:185:TRP:HE1	1.73	0.53
5:B:28:GLU:OE1	5:B:807:ARG:NH2	2.41	0.53
5:B:259:TYR:OH	5:B:279:ASP:OD2	2.27	0.53
5:B:549:THR:HB	5:B:628:THR:HB	1.90	0.53
4:A:663:SER:OG	5:B:827:ILE:O	2.22	0.53
4:A:71:GLN:OE1	5:B:1176:ASN:N	2.36	0.53
4:A:808:LEU:O	5:B:728:ARG:NH1	2.42	0.53
11:J:9:SER:OG	11:J:48:ARG:NH2	2.41	0.53
5:B:232:SER:O	5:B:261:ARG:NH2	2.40	0.53
5:B:403:LYS:NZ	5:B:696:GLU:OE1	2.38	0.53
4:A:1325:THR:OG1	7:E:146:HIS:O	2.27	0.53
2:T:25:DC:H5"	5:B:482:VAL:HG21	1.91	0.53
4:A:569:LYS:HD2	6:C:221:TYR:HB2	1.91	0.53
5:B:604:ARG:NH2	5:B:613:VAL:O	2.41	0.53
5:B:334:ILE:HG21	5:B:352:ALA:HB2	1.91	0.53
7:E:121:MET:SD	7:E:121:MET:N	2.82	0.53
4:A:879:GLU:OE1	4:A:962:ARG:NH2	2.31	0.52
4:A:913:LEU:HD22	4:A:915:SER:H	1.74	0.52
4:A:1288:ASP:OD2	4:A:1288:ASP:N	2.39	0.52
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.91	0.52
7:E:177:ARG:NH1	7:E:215:MET:SD	2.82	0.52
5:B:1084:GLN:OE1	6:C:192:TRP:N	2.40	0.52
5:B:1174:LYS:HD2	5:B:1179:GLN:HG3	1.90	0.52
4:A:67:CYS:O	4:A:70:CYS:N	2.39	0.52
4:A:541:ILE:HG21	4:A:549:MET:HE1	1.91	0.52
4:A:800:VAL:HG13	4:A:812:GLU:HB3	1.90	0.52
9:H:133:ASN:ND2	9:H:134:ASN:OD1	2.34	0.52
11:J:9:SER:HB2	11:J:45:CYS:HB2	1.91	0.52
4:A:806:ARG:NH2	5:B:725:PRO:O	2.43	0.52
4:A:563:PRO:HG2	4:A:566:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1012:ARG:O	4:A:1016:THR:OG1	2.28	0.52
11:J:3:VAL:HG11	11:J:18:TRP:HB2	1.92	0.52
13:L:39:SER:H	13:L:40:LEU:HD22	1.74	0.52
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.43	0.52
4:A:888:GLY:O	4:A:940:ARG:NH2	2.43	0.52
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.45	0.52
4:A:455:MET:HE1	5:B:1130:PHE:HE1	1.75	0.51
4:A:491:VAL:O	5:B:1150:ARG:NH2	2.43	0.51
4:A:14:VAL:HG23	5:B:1194:ILE:HG21	1.93	0.51
4:A:72:GLU:HB3	4:A:76:GLU:HB3	1.92	0.51
5:B:356:LEU:O	5:B:374:LYS:NZ	2.40	0.51
5:B:1053:GLU:OE2	5:B:1067:ARG:NH1	2.43	0.51
4:A:517:ASN:OD1	4:A:1364:ASN:ND2	2.39	0.51
7:E:46:TYR:OH	7:E:56:LYS:N	2.39	0.51
5:B:216:GLU:OE1	5:B:500:THR:OG1	2.25	0.51
4:A:78:PRO:O	5:B:1205:GLN:NE2	2.43	0.51
4:A:1276:VAL:HB	4:A:1279:ILE:HD13	1.93	0.51
4:A:346:ASP:HB2	5:B:1108:ARG:H	1.76	0.51
4:A:758:ILE:O	4:A:762:SER:OG	2.28	0.51
4:A:1350:LYS:O	4:A:1354:ASN:ND2	2.36	0.51
10:I:56:ALA:O	10:I:89:GLN:NE2	2.41	0.51
4:A:445:ASN:OD1	4:A:446:ARG:N	2.44	0.50
5:B:1072:MET:HE2	5:B:1085:ILE:CG1	2.33	0.50
5:B:1072:MET:CE	5:B:1085:ILE:HG13	2.36	0.50
6:C:11:ARG:NH1	6:C:19:ASP:OD2	2.45	0.50
4:A:550:LEU:HD12	4:A:556:TRP:CE2	2.46	0.50
5:B:487:THR:OG1	5:B:777:ALA:O	2.28	0.50
4:A:93:VAL:HG21	4:A:305:ASP:HB3	1.93	0.50
4:A:434:ARG:NH2	4:A:440:ASP:OD2	2.44	0.50
5:B:760:ASP:OD1	5:B:760:ASP:N	2.39	0.50
5:B:955:THR:OG1	5:B:956:THR:N	2.45	0.50
12:K:18:LYS:HD3	12:K:18:LYS:O	2.11	0.50
4:A:1143:LEU:O	4:A:1147:THR:OG1	2.28	0.50
5:B:1043:ASP:OD1	5:B:1045:SER:OG	2.25	0.50
10:I:32:CYS:SG	10:I:33:SER:N	2.85	0.50
5:B:861:ASP:OD1	5:B:914:LYS:NZ	2.40	0.50
3:N:16:DA:OP1	7:E:119:SER:OG	2.29	0.50
5:B:258:LEU:HD13	5:B:269:ILE:HG12	1.94	0.50
4:A:446:ARG:HG3	4:A:487:MET:HE2	1.94	0.49
5:B:904:ARG:HG3	13:L:65:VAL:HG21	1.93	0.49
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:518:LYS:NZ	4:A:624:SER:O	2.41	0.49
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.45	0.49
4:A:875:ALA:HA	4:A:878:ILE:HD12	1.95	0.49
5:B:193:LYS:HB3	5:B:787:VAL:HG11	1.94	0.49
4:A:451:HIS:HB2	4:A:454:SER:HB2	1.94	0.49
4:A:900:ASP:HA	4:A:926:GLN:HE22	1.76	0.49
5:B:790:ASP:OD2	5:B:790:ASP:N	2.40	0.49
5:B:834:ASN:HB3	5:B:840:ILE:HG13	1.94	0.49
5:B:972:LYS:HD2	5:B:1098:MET:HE3	1.94	0.49
6:C:165:LYS:O	12:K:6:ARG:NH1	2.46	0.49
4:A:1025:ARG:O	4:A:1035:TYR:OH	2.30	0.49
5:B:828:ALA:O	5:B:834:ASN:ND2	2.44	0.49
6:C:258:ILE:HG23	12:K:19:LEU:HD11	1.95	0.49
9:H:102:TYR:CZ	9:H:115:TYR:HB3	2.47	0.49
13:L:28:LYS:N	13:L:38:LEU:O	2.46	0.49
5:B:996:ARG:NH2	6:C:174:ALA:O	2.46	0.49
6:C:36:VAL:HG11	6:C:251:LEU:HB2	1.95	0.49
7:E:127:ILE:HD13	7:E:132:ILE:HD11	1.95	0.49
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.95	0.49
4:A:858:ASN:HD21	4:A:862:ASN:HB2	1.78	0.48
9:H:29:ALA:HA	9:H:37:LYS:HA	1.94	0.48
10:I:55:THR:HG21	10:I:109:ILE:HD13	1.93	0.48
5:B:542:MET:HE1	5:B:743:ILE:HG21	1.95	0.48
5:B:946:ASN:O	5:B:970:THR:OG1	2.23	0.48
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.79	0.48
4:A:850:VAL:HG21	4:A:1058:VAL:HG11	1.96	0.48
4:A:1395:GLY:O	4:A:1399:ARG:NE	2.35	0.48
7:E:135:PHE:HD2	7:E:140:LEU:HD21	1.77	0.48
6:C:246:ARG:O	6:C:250:THR:OG1	2.28	0.48
4:A:596:THR:HG22	4:A:597:LEU:N	2.27	0.48
5:B:358:LYS:HG3	5:B:359:GLU:HG2	1.95	0.48
5:B:917:PRO:HA	5:B:934:LYS:HA	1.95	0.48
5:B:957:ASN:HD21	5:B:961:LEU:HB2	1.77	0.48
4:A:58:LEU:HD21	4:A:80:HIS:H	1.78	0.48
4:A:1025:ARG:HA	4:A:1030:ARG:HH11	1.78	0.48
5:B:496:ARG:NH1	5:B:540:SER:O	2.47	0.48
13:L:34:CYS:SG	13:L:36:SER:OG	2.66	0.48
5:B:364:ILE:HG22	5:B:365:THR:HG22	1.96	0.47
5:B:957:ASN:OD1	5:B:961:LEU:N	2.44	0.47
5:B:215:GLN:HB3	5:B:407:ASP:HB2	1.96	0.47
5:B:345:LYS:HA	5:B:348:ARG:HE	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:195:VAL:HG22	7:E:213:ILE:HG13	1.96	0.47
12:K:18:LYS:HD3	12:K:18:LYS:C	2.39	0.47
4:A:1428:VAL:HG22	5:B:1147:LEU:HD11	1.97	0.47
4:A:1436:ILE:HG22	5:B:1142:GLY:HA2	1.97	0.47
6:C:29:MET:HB2	6:C:29:MET:HE3	1.77	0.47
4:A:437:MET:HE3	4:A:437:MET:HB2	1.78	0.47
5:B:890:TYR:OH	5:B:936:ASP:OD2	2.32	0.47
6:C:115:SER:H	6:C:142:VAL:H	1.61	0.47
8:F:94:LEU:HD21	8:F:125:LEU:HD22	1.96	0.47
4:A:868:TYR:HD2	4:A:1058:VAL:HG21	1.80	0.47
5:B:1094:ARG:NH1	5:B:1098:MET:SD	2.88	0.47
4:A:344:ARG:NH1	4:A:344:ARG:HG2	2.29	0.47
6:C:254:LYS:NZ	12:K:38:GLU:OE1	2.47	0.47
7:E:178:ILE:N	7:E:213:ILE:O	2.46	0.47
5:B:102:VAL:HG22	5:B:112:LEU:HB2	1.97	0.46
5:B:982:SER:OG	5:B:983:ARG:N	2.48	0.46
5:B:843:GLN:HB2	5:B:993:THR:HB	1.98	0.46
4:A:344:ARG:HG2	5:B:1129:ARG:CG	2.45	0.46
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.97	0.46
10:I:78:CYS:SG	10:I:80:SER:OG	2.73	0.46
4:A:151:ASP:OD2	4:A:163:SER:N	2.48	0.46
4:A:671:ALA:HB3	4:A:676:MET:HE2	1.97	0.46
5:B:100:PRO:O	5:B:180:TYR:OH	2.33	0.46
4:A:208:LEU:HD23	4:A:235:ILE:HD11	1.97	0.46
5:B:240:ILE:HG23	5:B:254:LEU:HB3	1.98	0.46
6:C:22:LEU:HG	6:C:25:VAL:HG21	1.97	0.46
7:E:80:VAL:HA	7:E:109:ILE:HB	1.97	0.46
10:I:5:ARG:NH2	10:I:36:GLU:OE2	2.49	0.46
10:I:7:CYS:SG	10:I:9:ASP:N	2.88	0.46
4:A:883:LEU:H	4:A:952:ALA:HB1	1.80	0.46
5:B:118:ARG:NH2	5:B:194:GLU:OE1	2.48	0.46
5:B:195:CYS:SG	5:B:783:THR:OG1	2.69	0.46
7:E:17:ARG:HG3	7:E:35:VAL:HG13	1.98	0.46
5:B:408:LEU:HD23	5:B:545:ILE:HG21	1.98	0.46
4:A:1152:ILE:HB	10:I:44:TYR:HB3	1.97	0.46
6:C:69:LEU:HD12	11:J:5:VAL:HG23	1.98	0.46
10:I:84:VAL:HG12	10:I:102:VAL:HB	1.97	0.46
13:L:33:GLU:HB2	13:L:53:HIS:ND1	2.31	0.46
4:A:353:ILE:HD13	4:A:487:MET:HE3	1.98	0.46
4:A:1166:ASP:OD1	4:A:1194:ARG:NH2	2.41	0.45
5:B:276:ILE:HD11	5:B:334:ILE:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:107:SER:OG	6:C:111:THR:OG1	2.33	0.45
7:E:11:ARG:HD2	7:E:141:VAL:HG11	1.99	0.45
4:A:329:LEU:HA	4:A:335:ARG:H	1.81	0.45
4:A:1393:ASN:OD1	4:A:1393:ASN:N	2.44	0.45
5:B:215:GLN:HG2	5:B:476:ARG:HH11	1.81	0.45
4:A:886:ILE:HD13	4:A:944:ARG:HG3	1.97	0.45
7:E:48:ASP:OD2	7:E:52:ARG:N	2.48	0.45
2:T:16:DT:H2'	2:T:17:DG:C8	2.52	0.45
4:A:1282:VAL:HG22	4:A:1308:THR:HG22	1.98	0.45
7:E:86:PRO:HA	7:E:113:GLN:HG3	1.98	0.45
4:A:151:ASP:OD2	4:A:162:VAL:N	2.49	0.45
4:A:711:ARG:NH2	10:I:87:GLN:OE1	2.49	0.45
3:N:6:DG:OP2	4:A:1109:LYS:NZ	2.43	0.45
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.50	0.45
4:A:148:CYS:O	4:A:168:GLY:N	2.43	0.45
4:A:592:ASP:H	4:A:595:THR:HG21	1.82	0.45
5:B:235:SER:OG	5:B:236:HIS:ND1	2.39	0.45
6:C:104:PHE:CD1	6:C:152:GLU:HB3	2.52	0.45
12:K:57:LEU:HD12	12:K:76:GLN:HG2	1.99	0.45
4:A:821:ARG:NH1	5:B:524:PRO:O	2.49	0.45
4:A:848:ILE:HG21	4:A:1370:LEU:HD21	1.98	0.45
5:B:790:ASP:O	5:B:858:SER:OG	2.33	0.45
6:C:167:HIS:CD2	13:L:70:ARG:HB2	2.51	0.45
4:A:781:ASP:OD1	10:I:91:ARG:NH2	2.50	0.45
5:B:680:THR:OG1	5:B:681:TRP:N	2.50	0.45
5:B:1060:ARG:HH12	6:C:200:GLU:HA	1.82	0.45
12:K:114:LEU:HD23	12:K:114:LEU:HA	1.80	0.45
4:A:848:ILE:HG22	4:A:1064:VAL:HG23	1.99	0.45
5:B:59:LEU:HG	5:B:95:ILE:HD13	1.98	0.45
6:C:40:GLU:CD	6:C:254:LYS:HE3	2.41	0.45
4:A:452:LYS:HD2	4:A:1067:LEU:HD13	1.99	0.45
5:B:185:THR:OG1	5:B:188:ASP:OD1	2.35	0.45
9:H:10:PHE:CD2	9:H:38:LEU:CD2	2.98	0.45
4:A:443:LEU:HD12	5:B:1146:PHE:CZ	2.52	0.44
4:A:711:ARG:NH1	10:I:95:THR:O	2.50	0.44
6:C:10:ILE:HG12	6:C:20:PHE:HB3	1.99	0.44
4:A:457:ALA:HB2	4:A:501:LEU:HD12	2.00	0.44
5:B:270:LYS:HA	5:B:281:PRO:HA	2.00	0.44
7:E:116:ILE:HG13	7:E:121:MET:HE1	1.98	0.44
6:C:48:SER:HB3	6:C:158:VAL:HB	1.99	0.44
13:L:49:LYS:H	13:L:49:LYS:HG3	1.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1202:MET:HE1	4:A:1212:VAL:HG21	1.98	0.44
6:C:262:LEU:HD11	12:K:87:LEU:HD23	1.99	0.44
5:B:532:ALA:HB1	5:B:535:LEU:HB2	1.98	0.44
6:C:61:GLU:HA	6:C:64:ALA:HB3	1.99	0.44
1:R:10:A:OP1	5:B:979:LYS:NZ	2.33	0.44
4:A:215:SER:HB2	4:A:218:ASP:HB2	2.00	0.44
4:A:346:ASP:N	4:A:346:ASP:OD1	2.46	0.44
4:A:497:THR:HG23	5:B:1146:PHE:HA	1.99	0.44
5:B:242:SER:OG	5:B:252:SER:O	2.33	0.44
5:B:287:ARG:HG3	5:B:292:ILE:HA	1.99	0.44
5:B:570:VAL:HG23	5:B:573:GLN:HB3	2.00	0.44
5:B:1084:GLN:NE2	6:C:190:ASP:O	2.40	0.44
6:C:266:ASP:N	6:C:266:ASP:OD1	2.50	0.44
10:I:74:GLU:OE1	10:I:81:ARG:NH1	2.51	0.44
4:A:982:THR:N	4:A:985:ASP:OD2	2.50	0.44
4:A:1381:LEU:HD23	4:A:1381:LEU:HA	1.86	0.44
5:B:751:VAL:HG23	5:B:812:LEU:HD22	2.00	0.44
9:H:105:GLU:O	9:H:113:ALA:N	2.51	0.44
4:A:84:ILE:HG23	4:A:239:LEU:HB3	2.00	0.44
5:B:101:MET:HE3	5:B:101:MET:HB2	1.86	0.44
4:A:642:CYS:HA	4:A:645:LEU:HB3	1.99	0.44
4:A:768:GLN:HG2	4:A:816:HIS:HA	1.99	0.44
6:C:2:SER:N	12:K:104:ASN:OD1	2.51	0.44
7:E:46:TYR:HH	7:E:57:MET:H	1.63	0.44
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.99	0.44
4:A:152:VAL:O	4:A:161:LEU:N	2.51	0.43
6:C:6:PRO:HB2	12:K:101:LEU:HG	2.01	0.43
7:E:177:ARG:HD3	7:E:215:MET:HG3	1.99	0.43
4:A:742:ASN:OD1	4:A:742:ASN:N	2.51	0.43
4:A:1215:ARG:O	4:A:1219:THR:OG1	2.35	0.43
4:A:1444:MET:O	8:F:133:VAL:N	2.40	0.43
5:B:728:ARG:NH2	5:B:760:ASP:OD2	2.38	0.43
4:A:884:ASP:OD2	4:A:884:ASP:N	2.50	0.43
4:A:1348:LEU:HD23	4:A:1372:VAL:HG13	2.00	0.43
5:B:232:SER:OG	5:B:234:ILE:O	2.28	0.43
5:B:912:ILE:HB	5:B:939:THR:HB	2.01	0.43
7:E:22:MET:SD	7:E:26:ARG:NH2	2.77	0.43
5:B:830:TYR:OH	5:B:998:ASP:O	2.23	0.43
6:C:8:VAL:HG22	6:C:22:LEU:HD12	2.00	0.43
6:C:114:TYR:CG	6:C:140:ASN:HB3	2.53	0.43
4:A:200:ARG:NH2	4:A:206:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:224:PHE:CD1	4:A:231:PRO:HG3	2.54	0.43
4:A:1059:HIS:HB3	8:F:86:THR:HB	2.01	0.43
11:J:1:MET:HB2	11:J:60:PHE:HE2	1.84	0.43
4:A:1267:MET:HE2	4:A:1267:MET:HB3	1.75	0.43
6:C:115:SER:HB3	6:C:142:VAL:HB	2.01	0.43
6:C:179:GLU:OE1	6:C:206:ASN:ND2	2.52	0.43
7:E:64:PRO:HD3	7:E:76:GLY:HA2	2.00	0.43
5:B:242:SER:HB2	5:B:362:PRO:HD2	2.00	0.43
5:B:345:LYS:HE3	5:B:345:LYS:HB3	1.80	0.43
5:B:776:GLN:HB2	5:B:1096:ARG:HG2	2.01	0.43
5:B:33:VAL:HG11	5:B:638:PHE:HE2	1.82	0.43
5:B:488:TYR:HE2	5:B:813:LYS:HB2	1.83	0.43
6:C:186:LEU:HD23	6:C:188:HIS:CE1	2.53	0.43
7:E:133:GLU:HB3	7:E:135:PHE:HE1	1.83	0.43
4:A:1009:ASN:OD1	4:A:1012:ARG:NH2	2.51	0.42
5:B:906:SER:N	5:B:909:ASP:OD2	2.52	0.42
8:F:136:ARG:HD2	8:F:146:TRP:CD1	2.53	0.42
4:A:550:LEU:HD22	4:A:577:ILE:HD13	2.01	0.42
4:A:1118:VAL:HG13	4:A:1327:ILE:HD11	2.00	0.42
4:A:861:GLY:O	7:E:174:GLN:NE2	2.44	0.42
5:B:546:SER:OG	5:B:629:ASP:O	2.32	0.42
7:E:24:LYS:HE3	7:E:24:LYS:HB2	1.80	0.42
10:I:29:CYS:SG	10:I:30:ARG:N	2.93	0.42
4:A:351:THR:HB	5:B:1103:ILE:HD13	2.01	0.42
4:A:1095:THR:HG21	4:A:1112:LYS:HB2	2.01	0.42
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	2.02	0.42
9:H:146:ARG:H	9:H:146:ARG:HG3	1.49	0.42
10:I:61:ASP:OD1	10:I:61:ASP:N	2.53	0.42
4:A:977:LYS:HE3	4:A:977:LYS:HB2	1.83	0.42
6:C:69:LEU:HD12	11:J:5:VAL:CG2	2.50	0.42
5:B:1006:ILE:HG23	11:J:45:CYS:HB3	2.01	0.42
7:E:147:HIS:HB3	7:E:150:VAL:HG23	2.01	0.42
4:A:58:LEU:HD13	4:A:244:PRO:HD3	2.02	0.42
4:A:368:LYS:HE3	4:A:368:LYS:HB2	1.78	0.42
4:A:761:MET:HG3	5:B:1021:MET:HG2	2.02	0.42
4:A:1153:TYR:HB2	4:A:1192:LEU:HD23	2.01	0.42
4:A:1232:ASN:OD1	4:A:1232:ASN:N	2.50	0.42
7:E:55:ARG:HH22	7:E:113:GLN:HB3	1.83	0.42
4:A:336:ILE:HG21	4:A:1401:SER:HA	2.02	0.42
4:A:900:ASP:O	4:A:907:THR:OG1	2.38	0.42
4:A:1166:ASP:OD1	4:A:1166:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1438:THR:HG23	8:F:92:ARG:HB2	2.01	0.42
7:E:67:GLU:O	7:E:70:SER:OG	2.35	0.42
10:I:99:LEU:HB2	10:I:101:PHE:CE1	2.55	0.42
4:A:29:ALA:HB1	5:B:1184:GLY:HA2	2.02	0.41
4:A:120:GLU:HB2	4:A:123:ARG:HH21	1.84	0.41
4:A:455:MET:HE1	5:B:1130:PHE:CE1	2.54	0.41
4:A:512:VAL:HG21	4:A:635:ARG:HH21	1.85	0.41
6:C:75:MET:HE2	6:C:75:MET:HB2	1.90	0.41
4:A:182:VAL:HG12	4:A:201:VAL:HA	2.02	0.41
4:A:512:VAL:HA	4:A:519:PRO:HA	2.02	0.41
4:A:691:LEU:HD22	4:A:695:LYS:HE2	2.02	0.41
4:A:511:ILE:HA	4:A:521:MET:HE3	2.02	0.41
4:A:527:THR:HG23	4:A:653:VAL:HB	2.01	0.41
5:B:496:ARG:HH12	5:B:541:LEU:HA	1.85	0.41
4:A:679:ILE:HG23	4:A:729:ALA:HB1	2.01	0.41
5:B:209:GLU:H	5:B:209:GLU:HG2	1.59	0.41
5:B:864:LYS:NZ	5:B:872:GLU:OE2	2.42	0.41
4:A:746:MET:SD	5:B:1015:HIS:ND1	2.93	0.41
4:A:915:SER:O	4:A:919:ILE:HB	2.20	0.41
5:B:824:ILE:HG22	5:B:1008:PRO:HA	2.03	0.41
4:A:147:VAL:HG12	4:A:170:THR:HA	2.02	0.41
6:C:18:VAL:HG12	6:C:20:PHE:HD2	1.86	0.41
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.53	0.41
10:I:94:ASP:OD1	10:I:94:ASP:N	2.51	0.41
4:A:343:LYS:HE3	5:B:1151:LEU:HG	2.02	0.41
4:A:1268:LEU:HD23	4:A:1268:LEU:HA	1.91	0.41
5:B:744:HIS:ND1	5:B:746:SER:OG	2.37	0.41
10:I:103:CYS:SG	10:I:104:LEU:N	2.93	0.41
4:A:705:LYS:NZ	4:A:717:ASN:OD1	2.54	0.41
4:A:846:GLU:HA	4:A:1066:VAL:HG22	2.02	0.41
5:B:29:ASP:HB3	5:B:658:ILE:HG12	2.02	0.41
5:B:767:ASN:O	5:B:771:SER:OG	2.37	0.41
5:B:1163:CYS:SG	5:B:1164:GLY:N	2.94	0.41
7:E:180:ARG:N	7:E:215:MET:OXT	2.52	0.41
8:F:82:THR:O	8:F:136:ARG:NH1	2.33	0.41
9:H:12:VAL:HA	9:H:28:ALA:HB2	2.03	0.41
4:A:99:ILE:HD12	4:A:211:PHE:HE2	1.84	0.41
5:B:44:VAL:HG11	5:B:495:LEU:HD13	2.03	0.41
5:B:658:ILE:HA	5:B:661:LEU:HD12	2.03	0.41
6:C:129:ILE:HD13	6:C:129:ILE:HA	1.99	0.41
13:L:31:CYS:HA	13:L:56:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:116:GLU:OE2	5:B:120:ARG:NH1	2.46	0.40
6:C:177:GLU:HB2	6:C:231:ASN:HB3	2.03	0.40
6:C:182:PRO:HB2	6:C:207:CYS:SG	2.61	0.40
4:A:296:LEU:HD23	4:A:296:LEU:HA	1.79	0.40
5:B:809:MET:HG2	5:B:814:PHE:HB3	2.02	0.40
4:A:169:ASN:OD1	4:A:170:THR:N	2.53	0.40
5:B:650:GLU:HA	5:B:710:LEU:HD23	2.02	0.40
5:B:822:ASN:O	11:J:48:ARG:NH1	2.54	0.40
9:H:8:ASP:HB3	9:H:10:PHE:CE1	2.56	0.40
4:A:901:LEU:HA	4:A:907:THR:HG23	2.03	0.40
4:A:977:LYS:HA	4:A:978:PRO:HD3	1.97	0.40
4:A:1195:LEU:HD11	4:A:1267:MET:HE1	2.01	0.40
5:B:862:GLN:O	5:B:914:LYS:NZ	2.48	0.40
4:A:464:PRO:O	12:K:2:ASN:HB3	2.21	0.40
4:A:1209:MET:HE3	4:A:1228:TRP:HB2	2.04	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	
4	A	1371/1733 (79%)	1298 (95%)	73 (5%)	0	100	100
5	B	1103/1224 (90%)	1055 (96%)	48 (4%)	0	100	100
6	C	265/318 (83%)	252 (95%)	13 (5%)	0	100	100
7	E	211/215 (98%)	197 (93%)	14 (7%)	0	100	100
8	F	84/155 (54%)	79 (94%)	5 (6%)	0	100	100
9	H	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
10	I	116/122 (95%)	110 (95%)	6 (5%)	0	100	100
11	J	63/70 (90%)	59 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	K	112/120 (93%)	108 (96%)	4 (4%)	0	100	100
13	L	41/70 (59%)	38 (93%)	3 (7%)	0	100	100
All	All	3495/4173 (84%)	3318 (95%)	177 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	
4	A	1195/1520 (79%)	1194 (100%)	1 (0%)	88	87
5	B	955/1061 (90%)	953 (100%)	2 (0%)	87	84
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	194/197 (98%)	194 (100%)	0	100	100
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	116/128 (91%)	116 (100%)	0	100	100
10	I	110/116 (95%)	110 (100%)	0	100	100
11	J	60/65 (92%)	60 (100%)	0	100	100
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3074/3657 (84%)	3071 (100%)	3 (0%)	88	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	333	GLU
5	B	879	ARG
5	B	911	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	4	GLN
4	A	64	ASN
4	A	358	ASN
4	A	390	GLN
4	A	399	HIS
4	A	447	GLN
4	A	626	ASN
4	A	767	GLN
4	A	768	GLN
4	A	968	GLN
4	A	994	GLN
4	A	1278	ASN
4	A	1427	ASN
5	B	309	GLN
5	B	538	ASN
5	B	733	HIS
5	B	761	HIS
5	B	951	GLN
5	B	984	HIS
5	B	1176	ASN
6	C	112	ASN
6	C	188	HIS
6	C	267	GLN
7	E	8	ASN
7	E	174	GLN
9	H	11	GLN
10	I	51	ASN
10	I	60	GLN
10	I	79	HIS
10	I	90	GLN
12	K	92	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/11 (81%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	4	G
1	R	8	G

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Mol	Chain	Res	Type
1	R	10	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G35	T	19	2	18,23,24	4.78	15 (83%)	18,33,36	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G35	T	19	2	-	2/11/41/42	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	G35	C2-N3	9.10	1.48	1.33
2	T	19	G35	O4'-C4'	7.88	1.62	1.45
2	T	19	G35	C3'-C4'	-7.43	1.33	1.53
2	T	19	G35	C8-N9	6.84	1.46	1.37
2	T	19	G35	C5-N7	6.17	1.45	1.37
2	T	19	G35	O4'-C1'	-5.07	1.31	1.42
2	T	19	G35	C8-N7	4.93	1.47	1.38
2	T	19	G35	C2-N12	4.50	1.48	1.32
2	T	19	G35	C4-N3	3.25	1.48	1.44
2	T	19	G35	O8-C8	-3.09	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	G35	O3'-C3'	3.01	1.49	1.43
2	T	19	G35	C1'-N9	2.94	1.49	1.45
2	T	19	G35	O5-C5	-2.69	1.18	1.23
2	T	19	G35	C2-N11	-2.42	1.25	1.34
2	T	19	G35	C2'-C1'	2.02	1.57	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	G35	O4'-C1'-N9-C4
2	T	19	G35	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	19	G35	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	$\# Z > 2$
16	PPV	B	1401	-	6,8,8	0.77	0	12,13,13	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PPV	B	1401	-	-	3/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

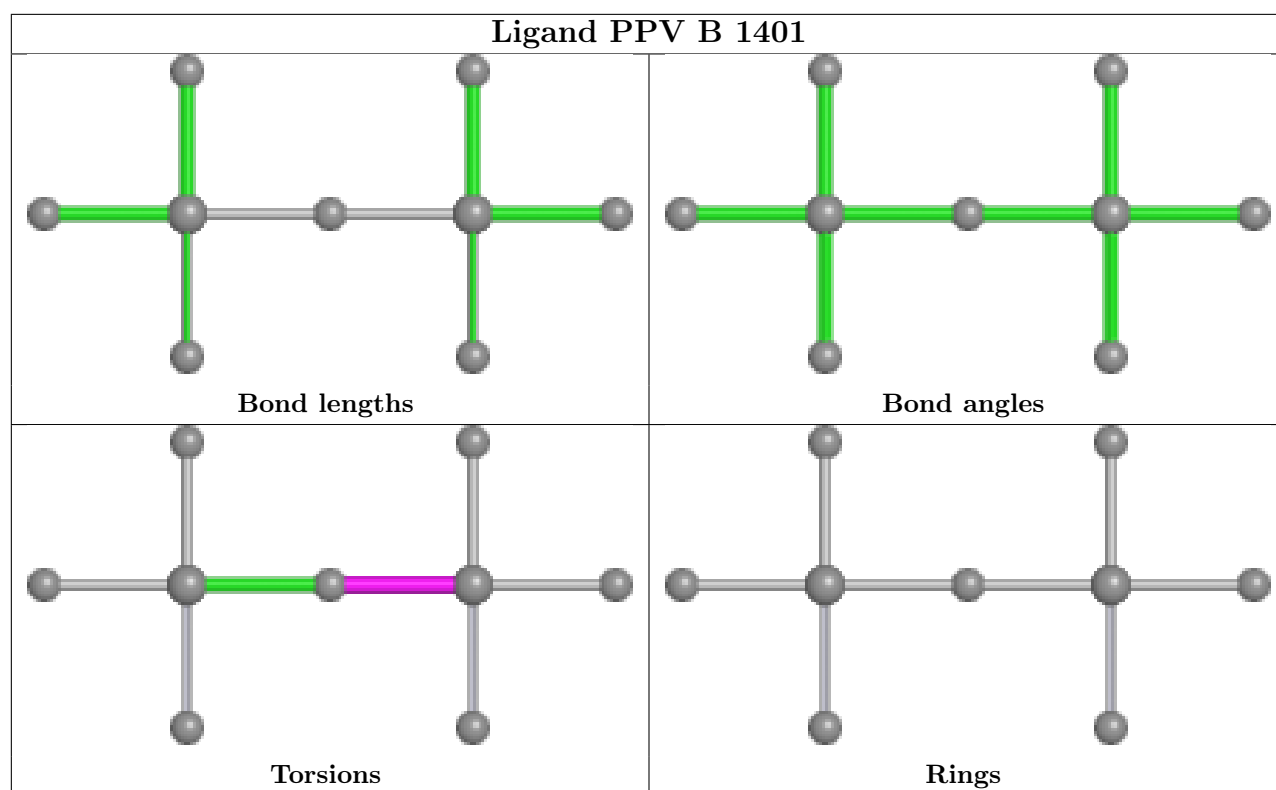
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	1401	PPV	P2-OPP-P1-O31
16	B	1401	PPV	P2-OPP-P1-O11
16	B	1401	PPV	P2-OPP-P1-O21

There are no ring outliers.

No monomer is involved in short contacts.

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	R	10/11 (90%)	0.56	0	100	100	104, 114, 138, 151	0
2	T	25/29 (86%)	0.66	0	100	100	106, 188, 227, 239	0
3	N	16/18 (88%)	0.62	0	100	100	145, 181, 248, 281	0
4	A	1385/1733 (79%)	0.39	40 (2%)	53	31	43, 90, 162, 258	0
5	B	1123/1224 (91%)	0.44	38 (3%)	48	28	29, 81, 147, 248	0
6	C	267/318 (83%)	0.24	2 (0%)	84	63	46, 80, 122, 153	0
7	E	213/215 (99%)	0.45	14 (6%)	24	16	69, 120, 208, 265	0
8	F	86/155 (55%)	0.22	0	100	100	57, 94, 134, 159	0
9	H	133/146 (91%)	0.29	3 (2%)	61	37	64, 108, 160, 249	0
10	I	118/122 (96%)	0.24	1 (0%)	82	61	61, 96, 130, 181	0
11	J	65/70 (92%)	0.32	2 (3%)	51	30	41, 73, 123, 145	0
12	K	114/120 (95%)	0.12	1 (0%)	81	58	43, 80, 116, 138	0
13	L	43/70 (61%)	0.56	0	100	100	64, 113, 162, 196	0
All	All	3598/4231 (85%)	0.38	101 (2%)	55	32	29, 90, 164, 281	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	105	CYS	4.4
4	A	141	LEU	4.1
5	B	714	GLU	4.1
4	A	776	ALA	3.9
7	E	95	THR	3.6
5	B	819	ALA	3.6
5	B	472	ALA	3.6
5	B	1211	ASN	3.6
9	H	139	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
4	A	106	VAL	3.5
7	E	83	CYS	3.3
7	E	98	ILE	3.3
11	J	65	PRO	3.1
5	B	721	LEU	3.0
9	H	63	LEU	2.9
10	I	117	LYS	2.9
5	B	230	ALA	2.9
4	A	103	CYS	2.9
4	A	323	LYS	2.9
7	E	118	PRO	2.8
4	A	355	GLY	2.8
5	B	475	SER	2.8
4	A	1106	ASN	2.8
5	B	1214	PRO	2.8
7	E	82	PHE	2.7
5	B	509	ALA	2.7
4	A	466	SER	2.6
5	B	713	ALA	2.6
7	E	94	LYS	2.6
7	E	121	MET	2.6
5	B	74	LEU	2.6
5	B	1165	ILE	2.5
4	A	957	PRO	2.5
5	B	212	LEU	2.5
5	B	665	GLU	2.5
4	A	1271	ILE	2.5
5	B	1175	LEU	2.5
5	B	1127	GLY	2.5
4	A	1391	ARG	2.4
4	A	59	GLY	2.4
4	A	1330	ASN	2.4
4	A	464	PRO	2.4
5	B	335	GLY	2.4
4	A	687	LYS	2.4
6	C	57	VAL	2.4
5	B	647	GLY	2.3
5	B	1218	THR	2.3
4	A	437	MET	2.3
4	A	65	LEU	2.3
5	B	835	GLN	2.3
4	A	316	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
5	B	806	THR	2.3
7	E	87	SER	2.3
4	A	208	LEU	2.3
5	B	473	MET	2.3
5	B	162	SER	2.3
4	A	1176	LEU	2.3
5	B	525	ALA	2.3
5	B	832	GLY	2.3
4	A	248	PRO	2.2
4	A	234	MET	2.2
4	A	219	PHE	2.2
4	A	318	SER	2.2
4	A	324	SER	2.2
5	B	489	SER	2.2
5	B	823	ALA	2.2
5	B	730	ARG	2.2
4	A	202	LEU	2.2
4	A	1081	LEU	2.2
4	A	899	VAL	2.2
4	A	885	THR	2.1
5	B	880	THR	2.1
4	A	181	LEU	2.1
4	A	257	ARG	2.1
4	A	69	THR	2.1
5	B	524	PRO	2.1
6	C	50	GLU	2.1
9	H	117	SER	2.1
4	A	207	ILE	2.1
5	B	137	TYR	2.1
4	A	812	GLU	2.1
4	A	1332	PHE	2.1
7	E	126	SER	2.1
5	B	790	ASP	2.1
4	A	237	THR	2.1
7	E	203	GLU	2.1
11	J	8	PHE	2.1
5	B	178	ASN	2.1
5	B	446	LEU	2.1
5	B	106	ASP	2.1
4	A	107	CYS	2.1
7	E	42	PHE	2.1
4	A	1261	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
7	E	124	VAL	2.0
7	E	132	ILE	2.0
4	A	185	TRP	2.0
5	B	1173	ALA	2.0
5	B	1199	ALA	2.0
7	E	131	THR	2.0
5	B	963	PHE	2.0
12	K	91	CYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	G35	T	19	22/23	0.89	0.10	108,127,164,166	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

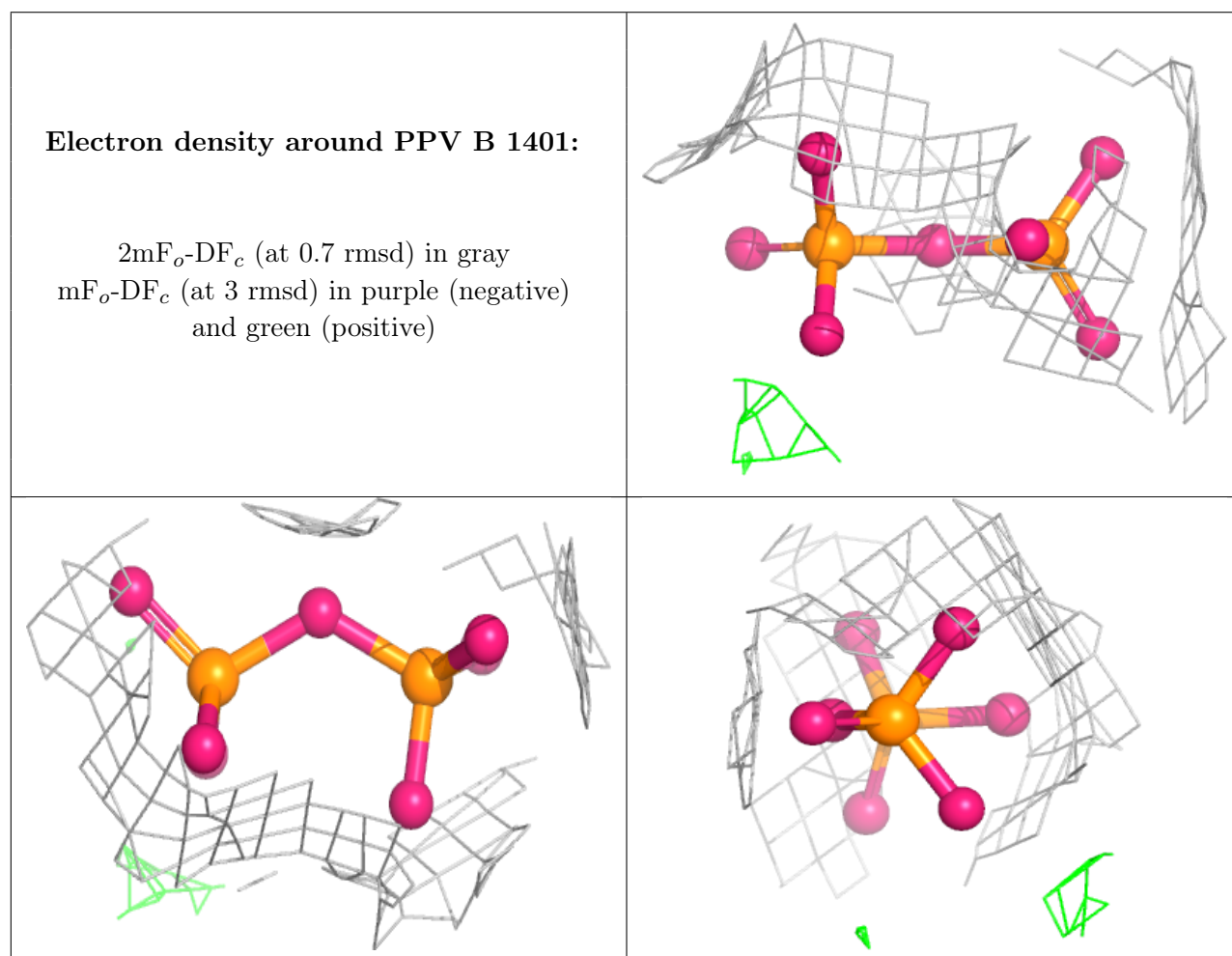
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	PPV	B	1401	9/9	0.57	0.13	132,151,169,169	0
15	ZN	A	1802	1/1	0.94	0.07	129,129,129,129	0
15	ZN	A	1801	1/1	0.94	0.07	244,244,244,244	0
15	ZN	C	401	1/1	0.97	0.06	94,94,94,94	0
15	ZN	J	101	1/1	0.98	0.14	148,148,148,148	0
15	ZN	B	1402	1/1	0.98	0.04	132,132,132,132	0
15	ZN	I	202	1/1	0.99	0.06	92,92,92,92	0
14	MG	R	101	1/1	0.99	0.04	35,35,35,35	0
15	ZN	L	101	1/1	0.99	0.03	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	ZN	I	201	1/1	0.99	0.08	101,101,101,101	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.