



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:05 AM UTC

PDB ID : 2OYQ / pdb_00002oyq
Title : Crystal structure of RB69 gp43 in complex with DNA with 5-NIMP opposite an abasic site analog
Authors : Zahn, K.E.; Belrhali, H.; Wallace, S.S.; Doublié, S.
Deposited on : 2007-02-22
Resolution : 2.86 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

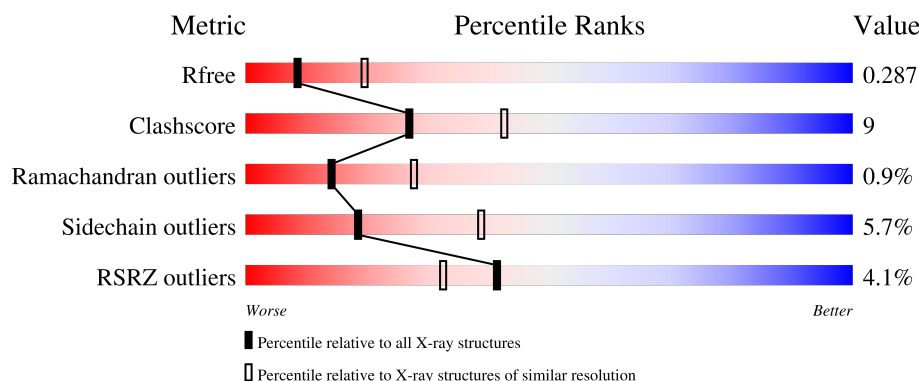
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	E	21	24% 52% 24%
1	G	21	14% 48% 5% 48%
1	I	21	5% 71% 24% 5%
1	K	21	48% 10% 43%
2	F	15	53% 47%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	15	7% 40% 53% 7%
2	J	15	47% 47% 7%
2	L	15	20% 67% 13%
3	A	903	% 73% 20% 6%
3	B	903	2% 61% 21% 16%
3	C	903	2% 76% 20% 2%
3	D	903	10% 73% 15% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28889 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	16	Total	C	N	O	P	0	0	0
			314	150	56	93	15			
1	G	11	Total	C	N	O	P	0	0	0
			223	106	44	63	10			
1	I	20	Total	C	N	O	P	0	0	0
			395	188	72	116	19			
1	K	12	Total	C	N	O	P	0	0	0
			244	116	49	68	11			

- Molecule 2 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			310	150	57	89	14			
2	H	14	Total	C	N	O	P	0	0	0
			287	137	55	82	13			
2	J	15	Total	C	N	O	P	0	0	0
			310	150	57	89	14			
2	L	13	Total	C	N	O	P	0	0	0
			265	127	50	76	12			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	848	Total	C	N	O	S	0	0	0
			6877	4423	1143	1280	31			
3	B	756	Total	C	N	O	S	0	0	0
			6045	3883	1001	1134	27			
3	C	891	Total	C	N	O	S	0	0	0
			7150	4583	1182	1352	33			
3	D	807	Total	C	N	O	S	0	0	0
			5688	3586	953	1125	24			

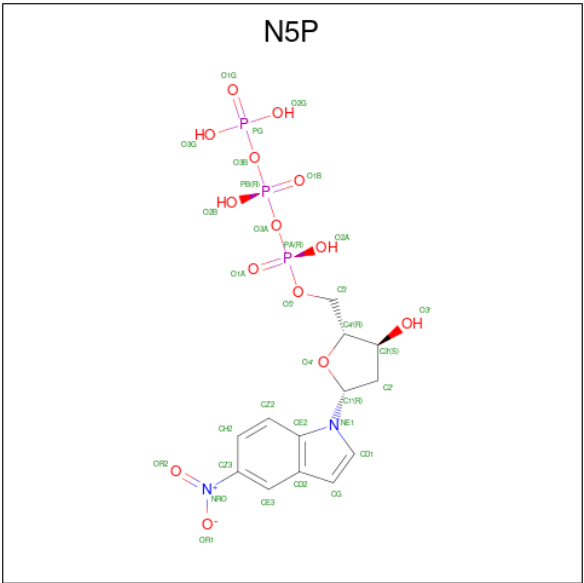
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0

- Molecule 5 is 1-{2-DEOXY-5-O-[(R)-HYDROXY{[(R)-HYDROXY(PHOSPHONOOXY)P HOSPHORYL]OXY}PHOSPHORYL]-BETA-D-ERYTHRO-PENTOFURANOSYL}-5-NI TRO -1H-INDOLE (CCD ID: N5P) (formula: C₁₃H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C N O P 32 13 2 14 3	0	0
5	A	1	Total C N O P 32 13 2 14 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	13	2	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	13	2	14	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	5	Total	O	0	0
			5	5		
6	F	8	Total	O	0	0
			8	8		
6	G	2	Total	O	0	0
			2	2		
6	H	3	Total	O	0	0
			3	3		
6	I	22	Total	O	0	0
			22	22		
6	J	19	Total	O	0	0
			19	19		
6	K	3	Total	O	0	0
			3	3		
6	L	3	Total	O	0	0
			3	3		
6	A	235	Total	O	0	0
			235	235		
6	B	125	Total	O	0	0
			125	125		
6	C	185	Total	O	0	0
			185	185		
6	D	41	Total	O	0	0
			41	41		

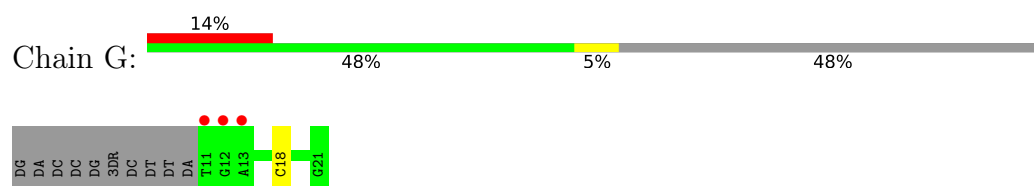
3 Residue-property plots [i](#)

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.

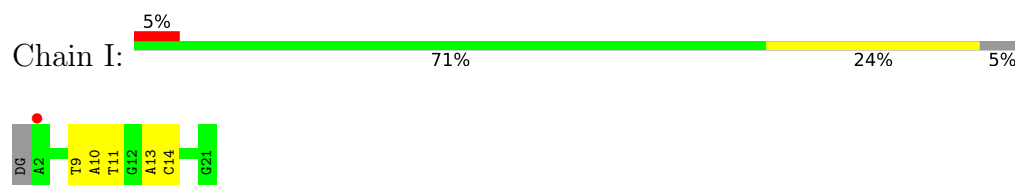
- Molecule 1: Template DNA



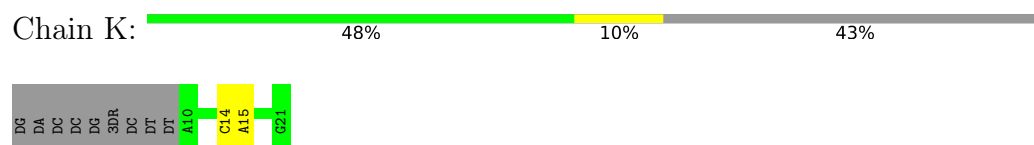
- Molecule 1: Template DNA



- Molecule 1: Template DNA



- Molecule 1: Template DNA



- Molecule 2: Primer DNA



- Molecule 2: Primer DNA





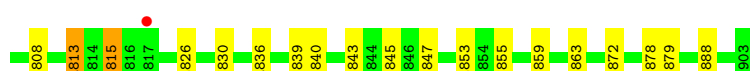
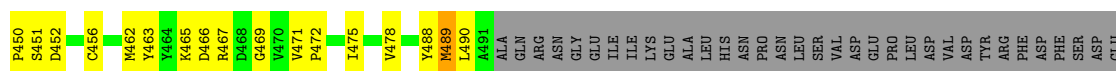
• Molecule 2: Primer DNA



• Molecule 2: Primer DNA

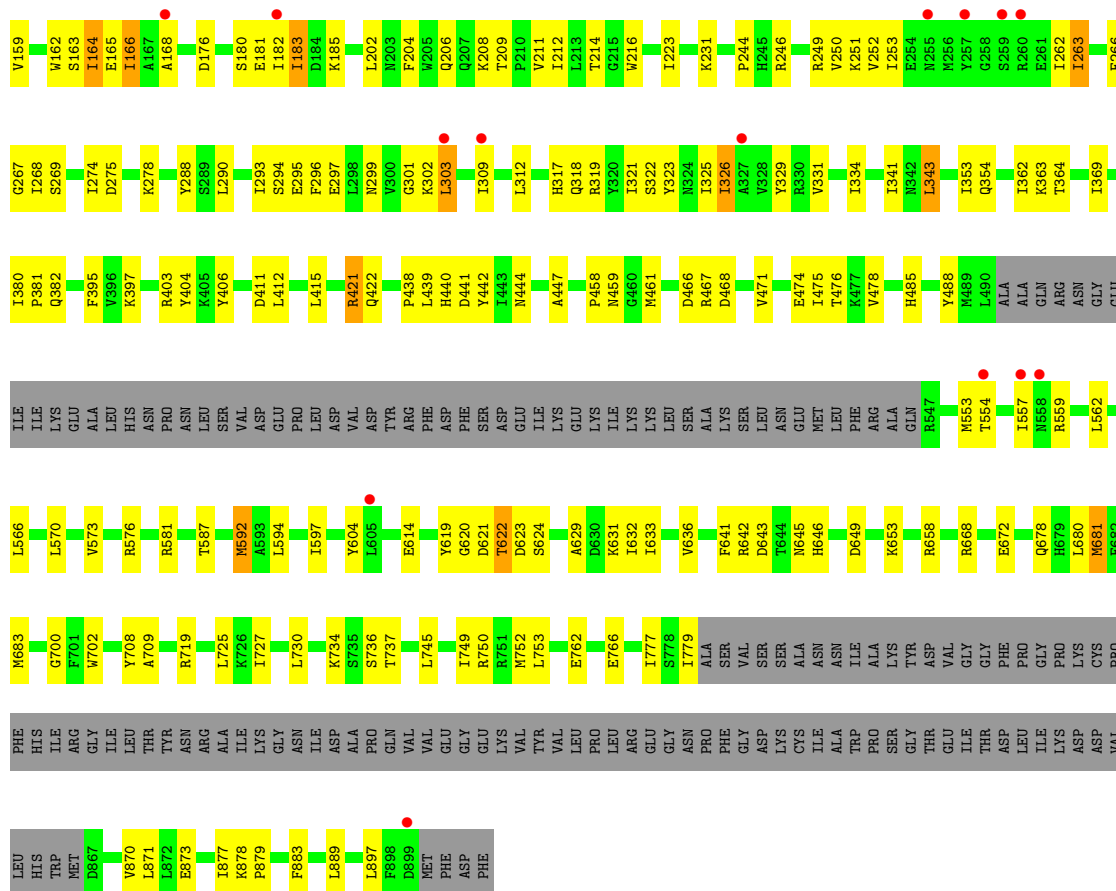


• Molecule 3: DNA polymerase

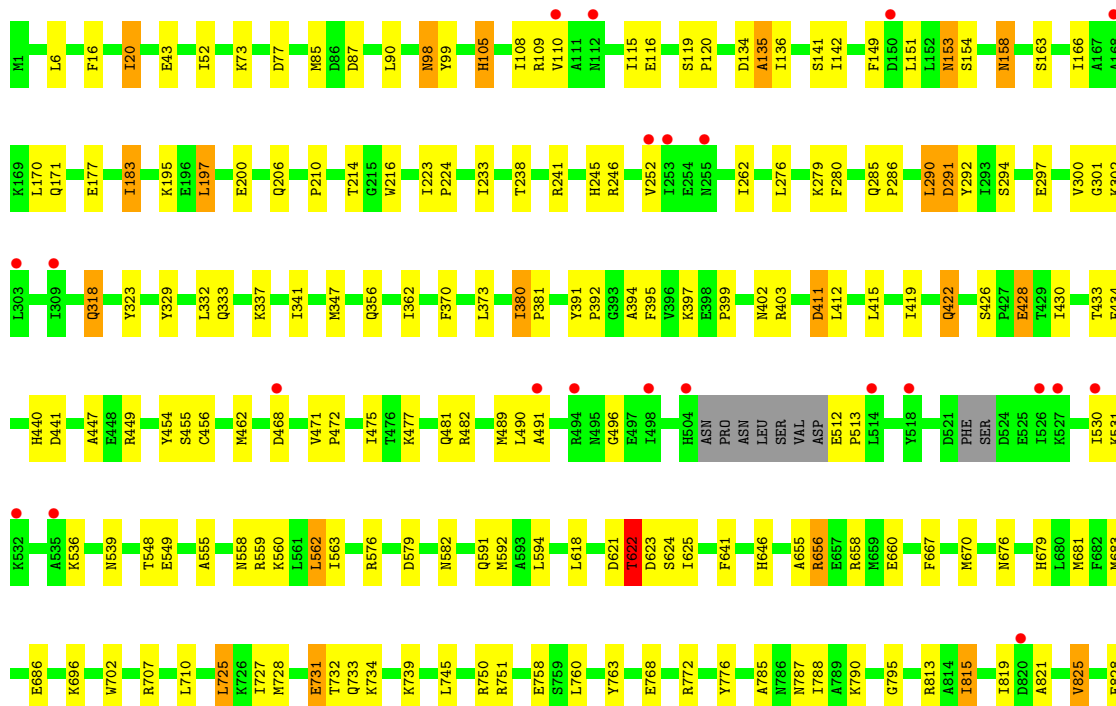
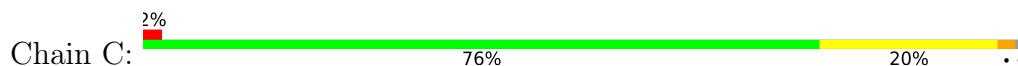


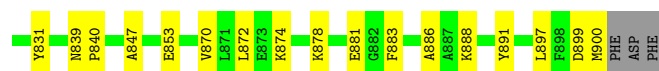
• Molecule 3: DNA polymerase



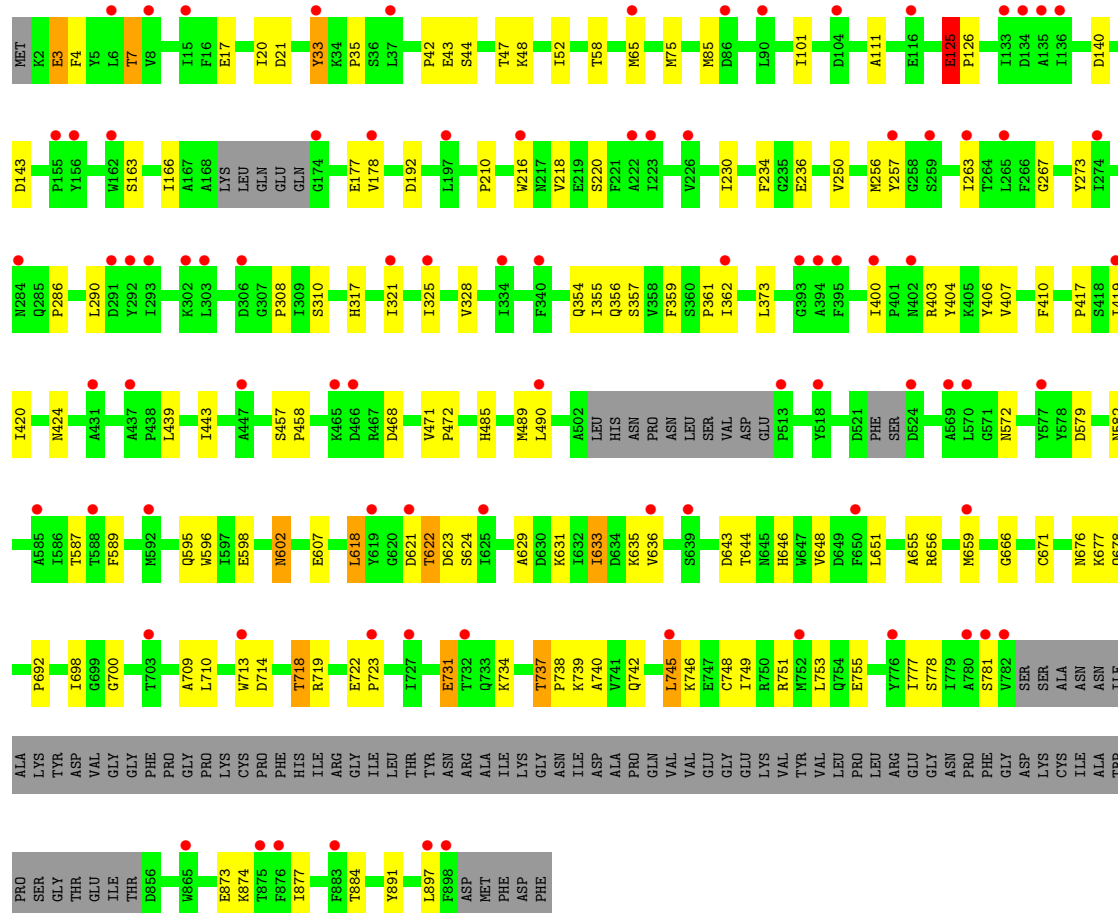
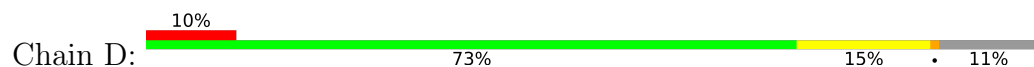


• Molecule 3: DNA polymerase





• Molecule 3: DNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.59Å 123.48Å 164.33Å 90.00° 96.22° 90.00°	Depositor
Resolution (Å)	30.00 – 2.86 30.00 – 2.86	Depositor EDS
% Data completeness (in resolution range)	91.2 (30.00-2.86) 91.1 (30.00-2.86)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.228 , 0.294 0.227 , 0.287	Depositor DCC
R_{free} test set	23125 reflections (9.68%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.8	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	0.92	EDS
Total number of atoms	28889	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: N5P, MG, N5I, 3DR

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	E	0.19	0/342	0.53	0/525
1	G	0.28	0/250	0.76	0/384
1	I	0.32	0/429	0.98	0/657
1	K	0.25	0/274	0.79	0/421
2	F	0.26	0/322	0.86	0/496
2	H	0.28	0/322	0.87	0/496
2	J	0.27	0/322	0.88	0/496
2	L	0.27	0/297	0.85	0/457
3	A	0.51	0/7049	0.84	1/9536 (0.0%)
3	B	0.49	0/6193	0.83	0/8393
3	C	0.49	0/7324	0.82	2/9912 (0.0%)
3	D	0.47	0/5812	0.84	4/7955 (0.1%)
All	All	0.48	0/28936	0.83	7/39728 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	737	THR	CA-C-N	5.55	125.56	119.90
3	D	737	THR	C-N-CA	5.55	125.56	119.90
3	D	125	GLU	CA-C-N	5.53	126.75	119.84
3	D	125	GLU	C-N-CA	5.53	126.75	119.84
3	C	449	ARG	CA-C-N	5.36	125.43	119.32
3	C	449	ARG	C-N-CA	5.36	125.43	119.32
3	A	164	ILE	CB-CA-C	-5.00	105.39	112.14

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	E	314	0	177	19	0
1	G	223	0	124	2	0
1	I	395	0	222	4	0
1	K	244	0	135	3	0
2	F	310	0	171	6	0
2	H	287	0	159	11	0
2	J	310	0	171	13	0
2	L	265	0	148	6	0
3	A	6877	0	6731	123	0
3	B	6045	0	5799	130	0
3	C	7150	0	6884	124	0
3	D	5688	0	4707	68	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	A	64	0	26	1	0
5	C	32	0	13	0	0
5	I	32	0	13	0	0
6	A	235	0	0	4	0
6	B	125	0	0	7	0
6	C	185	0	0	3	0
6	D	41	0	0	1	0
6	E	5	0	0	1	0
6	F	8	0	0	1	0
6	G	2	0	0	0	0
6	H	3	0	0	1	0
6	I	22	0	0	1	0
6	J	19	0	0	0	0
6	K	3	0	0	0	0
6	L	3	0	0	0	0
All	All	28889	0	25480	494	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 9.

All (494) 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:E:13:DA:H2''	1:E:14:DC:H5''	1.29	1.07
3:B:442:TYR:HB3	3:B:592:MET:HE2	1.36	1.06
1:E:9:DT:H71	6:E:210:HOH:O	1.59	1.00
3:A:356:GLN:H	3:A:356:GLN:HE21	1.02	0.98
3:B:597:ILE:HG21	3:B:683:MET:HE1	1.48	0.95
1:E:8:DT:O4	2:F:113:DA:N6	2.03	0.91
1:E:13:DA:C2'	1:E:14:DC:H5''	2.00	0.91
1:E:8:DT:H4'	1:E:9:DT:OP1	1.70	0.91
3:A:395:PHE:HB2	3:A:591:GLN:HG3	1.55	0.88
1:E:13:DA:H2''	1:E:14:DC:C5'	2.04	0.86
3:D:700:GLY:H	3:D:753:LEU:HD22	1.42	0.85
3:A:208:LYS:HG3	6:A:924:HOH:O	1.78	0.83
3:C:656:ARG:HH11	3:C:656:ARG:HG3	1.44	0.82
3:C:394:ALA:HB1	3:C:622:THR:HB	1.62	0.82
2:J:105:DC:H5'	2:J:105:DC:H6	1.45	0.81
3:B:317:HIS:CE1	3:B:321:ILE:HD11	2.15	0.81
3:D:655:ALA:HA	3:D:659:MET:HB2	1.63	0.81
3:B:441:ASP:HB3	3:B:447:ALA:HB2	1.61	0.81
3:B:734:LYS:HB3	3:B:737:THR:HG22	1.62	0.80
3:B:442:TYR:HB3	3:B:592:MET:CE	2.13	0.79
3:A:441:ASP:HB3	3:A:447:ALA:HB2	1.64	0.78
3:A:813:ARG:HG3	3:A:813:ARG:HH11	1.50	0.77
2:H:105:DC:N4	6:H:380:HOH:O	2.17	0.77
3:C:825:VAL:HB	3:C:828:GLU:HG3	1.67	0.77
2:J:105:DC:H2''	2:J:106:DT:H5'	1.67	0.76
3:A:303:LEU:HD13	3:A:326:ILE:HG13	1.67	0.76
3:C:85:MET:HE2	3:C:87:ASP:HB3	1.68	0.75
3:C:395:PHE:HB2	3:C:591:GLN:HG3	1.67	0.75
3:A:23:ASN:HD22	3:A:25:ARG:NH2	1.85	0.74
3:A:8:VAL:HG23	3:A:15:ILE:HD11	1.68	0.74
3:B:362:ILE:HD13	6:B:1161:HOH:O	1.88	0.73
3:C:151:LEU:HD21	3:C:154:SER:HB3	1.71	0.73
1:I:9:DT:H2''	1:I:10:DA:H5''	1.71	0.72
3:A:548:THR:C	3:A:550:VAL:H	1.96	0.72
3:D:403:ARG:HB2	3:D:698:ILE:HG21	1.70	0.72
6:I:818:HOH:O	3:C:707:ARG:HD3	1.90	0.71
3:D:656:ARG:HB3	6:D:925:HOH:O	1.92	0.70
3:A:356:GLN:H	3:A:356:GLN:NE2	1.84	0.70
3:A:422:GLN:NE2	3:A:680:LEU:H	1.90	0.70
3:A:582:ASN:O	3:A:586:ILE:HD12	1.92	0.70
3:C:592:MET:HE3	3:C:670:MET:SD	2.32	0.70
3:C:370:PHE:HB2	3:C:380:ILE:HD11	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:411:ASP:HB2	3:C:686:GLU:HG2	1.73	0.69
3:B:614:GLU:OE2	3:B:631:LYS:HE2	1.93	0.69
3:C:641:PHE:HD1	3:C:646:HIS:HD1	1.41	0.69
3:A:422:GLN:HE22	3:A:681:MET:HG2	1.58	0.68
1:E:9:DT:H1'	1:E:10:DA:H5'	1.74	0.68
3:C:110:VAL:H	3:C:141:SER:HB3	1.59	0.68
2:J:105:DC:H5'	2:J:105:DC:C6	2.27	0.68
3:B:362:ILE:H	3:B:362:ILE:HD12	1.58	0.68
3:C:471:VAL:HB	3:C:472:PRO:HD3	1.76	0.67
1:G:18:DC:H42	2:H:103:DG:H1	1.42	0.67
1:E:10:DA:H2''	1:E:11:DT:OP2	1.95	0.67
1:E:19:DG:H2''	1:E:20:DC:H5''	1.76	0.67
3:C:477:LYS:HG2	3:C:481:GLN:HE21	1.60	0.67
1:I:13:DA:H2''	1:I:14:DC:O5'	1.96	0.66
3:A:785:ALA:HB2	3:A:808:ILE:HD11	1.77	0.65
3:B:115:ILE:HG22	3:B:136:ILE:HD13	1.78	0.65
3:B:206:GLN:HE22	3:B:246:ARG:HH22	1.42	0.65
3:C:395:PHE:HD2	3:C:594:LEU:HD23	1.61	0.65
2:H:110:DA:H2''	2:H:111:DT:O5'	1.97	0.65
3:B:168:ALA:HB2	3:B:183:ILE:HG21	1.79	0.65
3:A:579:ASP:OD2	6:A:985:HOH:O	2.15	0.65
2:H:114:DG:OP1	3:B:290:LEU:HB2	1.97	0.64
3:B:211:VAL:HG12	3:B:212:ILE:HD12	1.78	0.64
3:A:356:GLN:HE21	3:A:356:GLN:N	1.85	0.64
2:F:113:DA:H5''	6:F:118:HOH:O	1.97	0.64
3:C:433:THR:H	3:C:462:MET:HE2	1.63	0.64
3:A:199:MET:HE3	3:A:234:PHE:CE2	2.33	0.64
3:D:579:ASP:HB3	3:D:582:ASN:HB2	1.80	0.63
3:B:214:THR:HG21	3:B:341:ILE:HD11	1.80	0.63
3:B:312:LEU:HD11	3:B:319:ARG:HG2	1.79	0.63
3:D:740:ALA:HB2	3:D:778:SER:HB2	1.81	0.63
3:B:322:SER:HA	3:B:325:ILE:HD12	1.81	0.63
3:C:412:LEU:HG	3:C:683:MET:HE3	1.81	0.62
3:B:76:GLU:HG2	3:B:382:GLN:HE22	1.64	0.62
3:A:768:GLU:HG3	3:A:872:LEU:HD21	1.80	0.62
3:D:419:ILE:HD12	3:D:589:PHE:HD2	1.65	0.62
2:J:104:DG:H1'	2:J:105:DC:H5''	1.81	0.62
1:I:11:DT:H4'	3:C:707:ARG:HD2	1.82	0.62
3:D:700:GLY:HA3	3:D:710:LEU:HD23	1.79	0.61
2:L:103:DG:H2'	2:L:104:DG:C8	2.36	0.61
3:A:113:PHE:CE1	3:A:213:LEU:HD11	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:126:PRO:HB2	3:A:224:PRO:HB2	1.82	0.60
2:J:105:DC:C2'	2:J:106:DT:H5'	2.31	0.60
3:B:159:VAL:HG11	3:B:317:HIS:HB2	1.83	0.60
2:L:108:DT:H2''	2:L:109:DC:O4'	2.00	0.60
3:D:417:PRO:HA	3:D:420:ILE:HD12	1.83	0.60
3:C:825:VAL:HB	3:C:828:GLU:CG	2.31	0.60
2:L:102:DC:H2''	2:L:103:DG:H5''	1.82	0.60
2:H:109:DC:H2''	2:H:110:DA:C8	2.37	0.60
3:B:290:LEU:HD13	3:B:302:LYS:HE3	1.82	0.60
3:C:732:THR:HG23	3:C:733:GLN:OE1	2.02	0.60
2:J:111:DT:H2''	2:J:112:DA:H8	1.65	0.60
3:B:294:SER:HB2	3:B:301:GLY:HA2	1.84	0.60
3:C:667:PHE:HB3	3:C:679:HIS:HE1	1.67	0.60
3:C:731:GLU:CD	3:C:731:GLU:H	2.09	0.59
3:C:116:GLU:HB2	3:C:135:ALA:HB3	1.82	0.59
3:B:442:TYR:CB	3:B:592:MET:HE2	2.23	0.59
3:C:579:ASP:HB3	3:C:582:ASN:HB2	1.85	0.59
3:D:35:PRO:HG2	3:D:65:MET:HA	1.85	0.59
3:A:245:HIS:HE1	6:A:973:HOH:O	1.85	0.59
3:C:727:ILE:HG21	3:C:732:THR:HG21	1.85	0.59
3:A:449:ARG:HH12	3:A:452:ASP:HB3	1.68	0.58
3:B:249:ARG:HD2	3:B:251:LYS:HE3	1.83	0.58
3:A:604:TYR:OH	3:A:658:ARG:HB3	2.04	0.58
3:A:664:ASP:O	3:A:668:ARG:HG3	2.02	0.58
3:B:653:LYS:NZ	6:B:1097:HOH:O	2.33	0.58
3:A:449:ARG:NH1	3:A:452:ASP:HB3	2.17	0.58
3:A:555:ALA:O	3:A:559:ARG:HG2	2.05	0.57
3:D:739:LYS:HA	3:D:742:GLN:HE21	1.69	0.57
3:C:702:TRP:CH2	3:C:710:LEU:HD21	2.39	0.57
3:B:288:TYR:HA	3:B:293:ILE:HD11	1.87	0.57
3:B:204:PHE:CE1	3:B:208:LYS:HD2	2.40	0.56
3:C:6:LEU:HD11	3:C:20:ILE:CD1	2.35	0.56
2:H:104:DG:H2''	2:H:105:DC:O5'	2.05	0.56
3:A:17:GLU:OE2	3:A:97:TYR:OH	2.17	0.56
3:A:466:ASP:OD1	3:A:467:ARG:NH1	2.38	0.56
3:A:294:SER:OG	3:A:330:ARG:HG3	2.06	0.56
3:A:878:LYS:HB3	3:A:879:PRO:HD3	1.87	0.56
3:C:297:GLU:O	3:C:337:LYS:HE3	2.05	0.56
3:A:214:THR:HG21	3:A:341:ILE:HD11	1.88	0.56
3:A:422:GLN:HE21	3:A:680:LEU:H	1.54	0.56
3:C:477:LYS:HG2	3:C:481:GLN:NE2	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:209:THR:HG21	3:B:244:PRO:HG3	1.88	0.55
3:D:738:PRO:HD3	3:D:781:SER:HB2	1.87	0.55
3:C:394:ALA:CB	3:C:622:THR:HB	2.34	0.55
3:D:407:VAL:HG11	3:D:710:LEU:HD22	1.87	0.55
1:E:18:DC:H2''	1:E:19:DG:H5'	1.89	0.55
3:D:731:GLU:HG3	3:D:734:LYS:HG3	1.88	0.55
3:B:303:LEU:HD23	3:B:326:ILE:HD13	1.89	0.55
3:C:656:ARG:HG3	3:C:656:ARG:NH1	2.13	0.55
3:D:749:ILE:O	3:D:753:LEU:HG	2.06	0.55
3:B:727:ILE:HG23	3:B:730:LEU:HD12	1.89	0.54
3:A:120:PRO:HG3	3:A:156:TYR:CE1	2.41	0.54
3:D:714:ASP:HA	3:D:718:THR:O	2.07	0.54
3:B:700:GLY:N	3:B:753:LEU:HD22	2.23	0.54
3:C:329:TYR:O	3:C:333:GLN:HG3	2.08	0.54
3:D:631:LYS:O	3:D:635:LYS:HB2	2.07	0.54
3:C:411:ASP:O	3:C:683:MET:HA	2.08	0.54
3:D:884:THR:HG21	3:D:891:TYR:HB3	1.90	0.54
3:A:15:ILE:HG22	3:A:31:VAL:O	2.08	0.54
3:A:548:THR:C	3:A:550:VAL:N	2.66	0.53
3:A:777:ILE:HD11	3:A:853:GLU:HA	1.89	0.53
3:C:347:MET:HE2	3:C:558:ASN:ND2	2.23	0.53
3:C:870:VAL:O	3:C:874:LYS:HB2	2.08	0.53
3:A:422:GLN:NE2	3:A:681:MET:HG2	2.22	0.53
3:B:223:ILE:HG22	3:B:263:ILE:HD11	1.89	0.53
3:B:395:PHE:HD2	3:B:594:LEU:HD23	1.72	0.53
3:B:702:TRP:CD1	3:B:708:TYR:HB3	2.43	0.53
3:B:730:LEU:HB3	3:B:883:PHE:CE1	2.43	0.53
3:A:788:ILE:HD13	3:A:826:GLU:HA	1.91	0.53
3:B:3:GLU:HG2	3:B:21:ASP:HA	1.90	0.53
3:C:170:LEU:HA	3:C:177:GLU:HG3	1.91	0.53
2:J:111:DT:H2''	2:J:112:DA:C8	2.44	0.53
2:L:112:DA:H2'	2:L:113:DA:C8	2.44	0.53
3:B:87:ASP:OD2	3:B:363:LYS:HE3	2.09	0.53
2:F:103:DG:H2''	2:F:104:DG:OP2	2.09	0.52
3:B:897:LEU:HD13	3:D:636:VAL:HG21	1.91	0.52
3:A:830:VAL:CG1	3:A:847:ALA:HB1	2.39	0.52
3:C:110:VAL:HB	3:C:141:SER:HB2	1.91	0.52
3:A:115:ILE:HG22	3:A:136:ILE:HG12	1.90	0.52
3:C:73:LYS:O	3:C:77:ASP:HB2	2.08	0.52
3:C:621:ASP:O	3:C:623:ASP:N	2.43	0.52
3:B:468:ASP:HA	6:B:1154:HOH:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:114:DG:H5'	3:B:216:TRP:HD1	1.75	0.51
3:C:776:TYR:OH	3:C:853:GLU:OE1	2.27	0.51
3:A:440:HIS:CE1	3:A:444:ASN:ND2	2.78	0.51
3:D:359:PHE:O	3:D:361:PRO:HD3	2.10	0.51
3:B:422:GLN:HG3	3:B:678:GLN:O	2.11	0.51
3:B:439:LEU:HD11	3:B:592:MET:HB2	1.91	0.51
3:D:400:ILE:HG13	3:D:404:TYR:OH	2.10	0.51
3:C:555:ALA:O	3:C:559:ARG:HD3	2.10	0.51
3:A:166:ILE:HA	3:A:169:LYS:HE2	1.93	0.51
3:A:645:ASN:HD21	3:A:719:ARG:HE	1.59	0.51
3:C:402:ASN:HA	3:C:886:ALA:O	2.11	0.51
3:C:646:HIS:HD2	6:C:1057:HOH:O	1.93	0.51
3:B:749:ILE:O	3:B:753:LEU:HG	2.11	0.51
3:D:33:TYR:O	3:D:35:PRO:HD3	2.11	0.51
3:A:488:TYR:C	3:A:490:LEU:H	2.19	0.51
3:B:629:ALA:HA	3:B:632:ILE:HD12	1.92	0.51
3:C:785:ALA:HB1	3:C:788:ILE:HD11	1.94	0.50
3:B:132:PRO:HG2	3:B:155:PRO:HD2	1.92	0.50
3:A:170:LEU:HA	3:A:177:GLU:HG2	1.93	0.50
3:A:283:THR:O	3:A:285:GLN:HG2	2.10	0.50
3:C:329:TYR:HA	3:C:332:LEU:HD12	1.93	0.50
2:J:112:DA:H5'	3:C:734:LYS:HG2	1.93	0.50
3:B:440:HIS:CE1	3:B:444:ASN:HD21	2.29	0.50
3:C:787:ASN:HB3	3:C:790:LYS:HB3	1.92	0.50
3:D:419:ILE:HD12	3:D:589:PHE:CD2	2.47	0.50
2:J:114:DG:H4'	3:C:622:THR:HG23	1.94	0.50
3:A:85:MET:HE3	3:A:85:MET:HA	1.93	0.50
3:A:645:ASN:ND2	3:A:719:ARG:HE	2.09	0.50
3:B:296:PHE:HD1	3:B:297:GLU:HG2	1.77	0.50
3:B:397:LYS:HD3	3:B:619:TYR:HA	1.94	0.50
3:B:441:ASP:CB	3:B:447:ALA:HB2	2.36	0.50
3:A:787:ASN:HB3	3:A:790:LYS:CB	2.42	0.49
3:C:831:TYR:O	3:C:847:ALA:HA	2.11	0.49
3:A:408:MET:HE3	3:A:688:ILE:HG12	1.93	0.49
3:A:436:VAL:HG12	3:A:437:ALA:O	2.12	0.49
3:B:622:THR:HG23	3:B:623:ASP:H	1.76	0.49
3:C:214:THR:HG21	3:C:341:ILE:HD11	1.94	0.49
3:D:250:VAL:HA	3:D:263:ILE:HA	1.95	0.49
1:E:19:DG:C6	1:E:20:DC:N4	2.80	0.49
3:A:11:ILE:HD12	3:A:16:PHE:CD1	2.47	0.49
3:A:408:MET:HE2	3:A:685:ARG:HD2	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:294:SER:HB2	3:C:301:GLY:HA2	1.94	0.49
3:A:547:ARG:HG3	3:A:548:THR:N	2.27	0.49
3:B:412:LEU:HD13	3:B:415:LEU:HD13	1.94	0.49
3:B:421:ARG:HB3	3:B:680:LEU:HD12	1.95	0.49
3:A:178:VAL:HA	3:A:326:ILE:HD11	1.93	0.49
3:B:145:ARG:NH1	3:B:185:LYS:HA	2.27	0.49
3:C:380:ILE:HG23	3:C:381:PRO:O	2.13	0.49
3:C:621:ASP:OD1	3:C:622:THR:HG22	2.13	0.49
3:B:471:VAL:HG11	3:B:570:LEU:HD11	1.94	0.49
3:B:642:ARG:H	3:B:646:HIS:HD2	1.60	0.49
3:D:3:GLU:HG3	3:D:21:ASP:HA	1.94	0.49
3:A:83:LEU:H	3:A:83:LEU:HD23	1.77	0.49
3:B:47:THR:HG23	3:B:49:TYR:H	1.77	0.49
1:E:8:DT:H2''	1:E:9:DT:H72	1.95	0.48
2:F:101:DG:H4'	2:F:102:DC:H5'	1.95	0.48
3:B:700:GLY:H	3:B:753:LEU:HD22	1.78	0.48
3:D:4:PHE:HA	3:D:101:ILE:HD11	1.95	0.48
3:A:238:THR:HA	3:A:241:ARG:HH21	1.78	0.48
3:A:547:ARG:HG3	3:A:548:THR:H	1.78	0.48
3:C:412:LEU:HD13	3:C:415:LEU:HD13	1.96	0.48
3:D:140:ASP:HB2	3:D:143:ASP:HB2	1.96	0.48
3:B:182:ILE:HD11	3:B:329:TYR:CD2	2.49	0.48
3:B:331:VAL:HA	3:B:334:ILE:HD12	1.95	0.48
3:C:105:HIS:HA	3:C:108:ILE:HG13	1.96	0.48
3:D:75:MET:HA	3:D:75:MET:HE2	1.95	0.48
3:B:381:PRO:HG2	3:B:576:ARG:HG2	1.96	0.48
3:B:421:ARG:HD2	3:B:476:THR:OG1	2.12	0.48
3:B:681:MET:HA	3:B:681:MET:HE3	1.95	0.48
3:C:115:ILE:HG22	3:C:136:ILE:HG12	1.94	0.48
3:D:622:THR:HG23	3:D:623:ASP:H	1.78	0.48
2:J:103:DG:H2''	2:J:104:DG:C8	2.49	0.48
3:B:421:ARG:HB3	3:B:680:LEU:CD1	2.44	0.48
3:B:641:PHE:HA	3:B:646:HIS:HD2	1.79	0.48
3:D:648:VAL:HB	3:D:719:ARG:NH2	2.29	0.48
3:D:111:ALA:HB3	3:D:210:PRO:HB3	1.96	0.47
3:D:873:GLU:HA	3:D:877:ILE:HB	1.96	0.47
3:A:813:ARG:HH11	3:A:813:ARG:CG	2.21	0.47
3:C:426:SER:C	3:C:582:ASN:HD21	2.22	0.47
3:C:815:ILE:HG23	3:C:821:ALA:HB3	1.96	0.47
3:A:121:ASP:N	3:A:121:ASP:OD1	2.48	0.47
3:A:412:LEU:HD13	3:A:415:LEU:HD13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:466:ASP:OD2	3:B:467:ARG:HG3	2.13	0.47
3:C:285:GLN:HG3	3:C:286:PRO:HD2	1.95	0.47
3:D:218:VAL:C	3:D:220:SER:H	2.22	0.47
2:H:113:DA:OP1	3:B:288:TYR:HB2	2.14	0.47
3:A:172:GLU:H	3:A:172:GLU:CD	2.22	0.47
3:A:426:SER:HB2	3:A:472:PRO:HD3	1.96	0.47
3:B:397:LYS:HB3	3:B:620:GLY:H	1.78	0.47
3:C:900:MET:SD	3:C:900:MET:N	2.88	0.47
3:B:643:ASP:HB2	6:B:1157:HOH:O	2.13	0.47
3:C:52:ILE:HD12	3:C:428:GLU:HG2	1.97	0.47
3:C:151:LEU:CD2	3:C:154:SER:HB3	2.43	0.47
3:C:163:SER:HB3	3:C:166:ILE:HD12	1.97	0.47
3:D:216:TRP:CD2	3:D:290:LEU:HD13	2.50	0.47
3:D:629:ALA:HB1	3:D:651:LEU:HD21	1.96	0.47
3:A:428:GLU:OE2	3:A:469:GLY:HA2	2.15	0.47
3:B:668:ARG:O	3:B:672:GLU:HG3	2.14	0.47
3:C:136:ILE:HB	3:C:149:PHE:HB2	1.97	0.47
3:A:803:PHE:CZ	3:A:845:CYS:HB3	2.50	0.47
3:D:485:HIS:O	3:D:489:MET:HB2	2.15	0.47
3:C:291:ASP:OD2	3:C:302:LYS:HB2	2.15	0.46
3:A:75:MET:HG2	3:A:82:ALA:HB2	1.97	0.46
3:C:433:THR:HG22	3:C:434:PHE:N	2.30	0.46
3:C:454:TYR:HB3	3:C:462:MET:HB3	1.97	0.46
2:H:103:DG:H2"	2:H:104:DG:C8	2.50	0.46
1:I:14:DC:OP1	3:C:874:LYS:HD3	2.15	0.46
3:A:176:ASP:O	3:A:303:LEU:HD11	2.15	0.46
3:B:752:MET:HE3	3:B:889:LEU:HD12	1.95	0.46
3:A:725:LEU:HD22	3:A:753:LEU:HD12	1.98	0.46
1:K:14:DC:H2"	1:K:15:DA:C8	2.50	0.46
3:A:395:PHE:CB	3:A:591:GLN:HG3	2.36	0.46
3:A:423:VAL:O	3:A:424:ASN:CB	2.62	0.46
3:D:745:LEU:HA	3:D:748:CYS:HB2	1.97	0.46
3:A:787:ASN:HB3	3:A:790:LYS:HB3	1.97	0.46
3:C:881:GLU:HG2	3:C:891:TYR:CE2	2.51	0.46
3:D:739:LYS:HA	3:D:742:GLN:HB2	1.98	0.46
3:A:471:VAL:HB	3:A:472:PRO:HD3	1.98	0.46
3:A:597:ILE:O	3:A:601:VAL:HG23	2.16	0.46
3:A:788:ILE:H	3:A:788:ILE:HD12	1.79	0.46
3:C:380:ILE:HG23	3:C:576:ARG:HD3	1.97	0.46
1:E:8:DT:O4	2:F:113:DA:C6	2.68	0.46
3:A:429:THR:HG22	3:A:463:TYR:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:75:MET:HE3	3:B:75:MET:HA	1.96	0.46
3:A:302:LYS:HE3	3:A:327:ALA:HB2	1.98	0.46
3:A:661:PRO:O	3:A:665:ARG:HB2	2.15	0.46
3:C:223:ILE:HB	3:C:224:PRO:HD3	1.98	0.46
3:D:410:PHE:O	3:D:624:SER:HA	2.15	0.46
3:B:10:GLN:HG3	3:B:65:MET:HE1	1.97	0.46
3:B:458:PRO:HG3	3:B:592:MET:CE	2.46	0.46
3:D:230:ILE:O	3:D:234:PHE:N	2.46	0.46
3:D:407:VAL:HG23	3:D:618:LEU:HD21	1.98	0.46
3:B:421:ARG:HD3	3:B:475:ILE:HG23	1.97	0.45
3:C:482:ARG:CZ	3:C:560:LYS:HB2	2.46	0.45
3:C:134:ASP:O	3:C:135:ALA:HB2	2.17	0.45
3:A:68:ALA:O	3:A:72:ILE:HG13	2.16	0.45
3:C:391:TYR:HB2	3:C:392:PRO:HD2	1.99	0.45
3:C:434:PHE:HE2	3:C:456:CYS:HB3	1.82	0.45
3:B:404:TYR:HA	6:B:1043:HOH:O	2.17	0.45
3:B:745:LEU:HD22	3:B:883:PHE:HE2	1.82	0.45
3:D:439:LEU:O	3:D:443:ILE:HG12	2.15	0.45
3:B:162:TRP:HB2	3:B:321:ILE:CD1	2.47	0.45
3:C:562:LEU:HD12	3:C:562:LEU:HA	1.85	0.45
3:C:667:PHE:HB3	3:C:679:HIS:CE1	2.50	0.45
3:A:440:HIS:CE1	3:A:444:ASN:HD21	2.35	0.45
3:B:725:LEU:HD11	3:B:750:ARG:HB2	1.98	0.45
3:C:302:LYS:HD3	3:C:323:TYR:CE1	2.52	0.45
3:A:472:PRO:HA	3:A:475:ILE:HG22	1.98	0.45
3:A:752:MET:HG3	3:A:760:LEU:HD13	1.99	0.44
3:C:276:LEU:HD12	3:C:276:LEU:HA	1.83	0.44
3:C:300:VAL:HG13	3:C:301:GLY:H	1.82	0.44
1:E:10:DA:N1	2:F:112:DA:C6	2.86	0.44
1:E:15:DA:C6	1:E:16:DG:C6	3.05	0.44
1:E:18:DC:H2''	1:E:19:DG:C5'	2.47	0.44
2:H:113:DA:P	3:B:288:TYR:H	2.40	0.44
1:K:14:DC:P	3:D:874:LYS:HD3	2.57	0.44
3:B:144:ASP:CG	3:B:144:ASP:O	2.60	0.44
3:C:641:PHE:HD1	3:C:646:HIS:ND1	2.12	0.44
3:A:839:ASN:HB2	3:A:840:PRO:HD2	1.99	0.44
3:B:85:MET:HA	3:B:380:ILE:HD11	1.99	0.44
3:B:302:LYS:HD3	3:B:323:TYR:OH	2.17	0.44
3:B:406:TYR:CD2	3:B:633:ILE:HG13	2.52	0.44
3:A:785:ALA:HB1	3:A:788:ILE:HD11	1.98	0.44
3:B:176:ASP:OD2	3:B:318:GLN:HG3	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:471:VAL:HB	3:D:472:PRO:HD3	2.00	0.44
3:A:330:ARG:HD2	3:A:330:ARG:HA	1.85	0.44
3:A:408:MET:CE	3:A:655:ALA:HB2	2.48	0.44
3:C:454:TYR:CB	3:C:462:MET:HB3	2.46	0.44
3:B:9:GLU:OE1	3:B:267:GLY:N	2.43	0.44
3:B:485:HIS:HA	3:B:488:TYR:CD2	2.53	0.44
3:B:553:MET:O	3:B:557:ILE:HG12	2.18	0.44
3:B:649:ASP:OD1	3:B:719:ARG:NH2	2.48	0.44
3:B:672:GLU:HB3	6:B:1122:HOH:O	2.17	0.44
3:C:655:ALA:O	3:C:660:GLU:HG3	2.17	0.44
2:J:114:DG:H2'	2:J:115:N5I:HD1	1.99	0.44
3:C:16:PHE:HB3	3:C:245:HIS:CE1	2.53	0.44
3:C:881:GLU:HG2	3:C:891:TYR:HE2	1.81	0.44
3:B:730:LEU:HB3	3:B:883:PHE:HE1	1.82	0.44
2:L:106:DT:H2''	2:L:107:DG:H5'	1.99	0.43
3:A:813:ARG:HG3	3:A:813:ARG:NH1	2.27	0.43
3:C:433:THR:O	3:C:462:MET:HE2	2.17	0.43
3:D:325:ILE:O	3:D:328:VAL:HG22	2.17	0.43
3:A:290:LEU:HD11	3:A:330:ARG:HB3	2.00	0.43
3:B:411:ASP:O	3:B:683:MET:HA	2.18	0.43
3:D:596:TRP:NE1	3:D:666:GLY:O	2.45	0.43
3:D:598:GLU:O	3:D:602:ASN:HB2	2.19	0.43
3:A:408:MET:HE1	3:A:651:LEU:O	2.18	0.43
3:A:449:ARG:HA	3:A:450:PRO:HD3	1.88	0.43
3:B:17:GLU:OE1	3:B:29:ARG:NH1	2.49	0.43
3:B:119:SER:HA	3:B:120:PRO:HD2	1.92	0.43
3:C:725:LEU:HD21	3:C:750:ARG:HB2	2.00	0.43
3:A:362:ILE:HD11	3:A:572:ASN:HB3	2.01	0.43
3:B:274:ILE:HG23	3:B:275:ASP:N	2.33	0.43
3:C:768:GLU:HG2	3:C:872:LEU:HD21	2.00	0.43
3:A:4:PHE:CZ	3:A:20:ILE:HG13	2.54	0.43
3:B:478:VAL:HG13	3:B:559:ARG:HG3	2.01	0.43
3:D:42:PRO:C	3:D:44:SER:H	2.25	0.43
3:B:459:ASN:HD21	3:B:461:MET:HG2	1.84	0.43
3:B:645:ASN:OD1	3:B:719:ARG:NH1	2.52	0.43
3:C:216:TRP:CD2	3:C:290:LEU:HD23	2.54	0.43
3:C:455:SER:OG	3:C:676:ASN:HA	2.19	0.43
3:C:795:GLY:O	3:C:813:ARG:NH1	2.52	0.43
2:J:104:DG:C1'	2:J:105:DC:H5''	2.47	0.43
3:A:815:ILE:HD12	3:A:815:ILE:HA	1.83	0.43
3:C:727:ILE:O	3:C:728:MET:HE2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:751:ARG:CZ	3:C:763:TYR:HB2	2.49	0.43
3:D:47:THR:HB	3:D:48:LYS:H	1.64	0.43
3:D:777:ILE:HG13	3:D:778:SER:N	2.33	0.43
3:A:277:TYR:CE2	3:A:293:ILE:HD12	2.54	0.43
3:A:424:ASN:O	3:A:429:THR:HG21	2.19	0.43
3:B:362:ILE:H	3:B:362:ILE:CD1	2.30	0.43
3:B:878:LYS:N	3:B:879:PRO:HD2	2.34	0.43
3:B:604:TYR:OH	3:B:658:ARG:HB3	2.19	0.43
3:C:85:MET:CE	3:C:87:ASP:H	2.32	0.43
3:C:163:SER:HB3	3:C:318:GLN:OE1	2.19	0.43
3:C:415:LEU:CD1	3:C:681:MET:HE1	2.49	0.43
3:C:98:ASN:HD22	3:C:98:ASN:H	1.66	0.43
3:B:317:HIS:CE1	3:B:321:ILE:CD1	2.96	0.42
3:B:458:PRO:HB3	3:B:592:MET:HE3	2.01	0.42
3:C:475:ILE:HD11	3:C:563:ILE:HA	2.00	0.42
3:A:478:VAL:HG13	3:A:559:ARG:HD2	2.02	0.42
3:A:813:ARG:CG	3:A:813:ARG:NH1	2.82	0.42
3:C:216:TRP:CE3	3:C:290:LEU:HD23	2.53	0.42
3:C:489:MET:C	3:C:491:ALA:H	2.27	0.42
3:D:125:GLU:HA	3:D:126:PRO:HD3	1.87	0.42
3:D:457:SER:OG	3:D:458:PRO:HD2	2.19	0.42
3:A:836:ARG:NH1	3:A:836:ARG:HB2	2.34	0.42
3:A:135:ALA:HA	3:A:149:PHE:O	2.20	0.42
3:B:268:ILE:HG22	3:B:269:SER:N	2.34	0.42
3:B:438:PRO:HG2	3:B:441:ASP:OD2	2.19	0.42
3:B:873:GLU:HA	3:B:877:ILE:HB	2.00	0.42
3:C:109:ARG:HG2	3:C:210:PRO:HA	2.00	0.42
3:D:177:GLU:HB3	3:D:178:VAL:H	1.53	0.42
3:D:621:ASP:O	3:D:623:ASP:N	2.52	0.42
1:E:13:DA:C3'	1:E:14:DC:H5''	2.46	0.42
3:A:98:ASN:H	3:A:98:ASN:HD22	1.68	0.42
3:A:144:ASP:O	3:A:145:ARG:HD3	2.19	0.42
3:A:433:THR:N	3:A:462:MET:HE2	2.35	0.42
3:B:353:ILE:O	3:B:354:GLN:C	2.59	0.42
3:C:290:LEU:HD12	3:C:302:LYS:CE	2.50	0.42
3:A:113:PHE:CD1	3:A:213:LEU:HD11	2.54	0.42
3:B:364:THR:CG2	3:B:562:LEU:HD21	2.50	0.42
3:C:397:LYS:O	3:C:399:PRO:HD3	2.19	0.42
3:D:443:ILE:HD12	3:D:595:GLN:HB2	2.01	0.42
3:A:176:ASP:HA	3:A:319:ARG:HH21	1.84	0.42
3:B:573:VAL:HG22	6:B:1058:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:407:VAL:HG11	3:D:710:LEU:CD2	2.50	0.42
1:G:18:DC:N4	2:H:103:DG:H1	2.14	0.42
3:A:433:THR:H	3:A:462:MET:HE2	1.83	0.42
3:B:700:GLY:HA2	3:B:709:ALA:O	2.20	0.42
3:D:355:ILE:C	3:D:357:SER:H	2.28	0.42
3:D:424:ASN:HD21	3:D:468:ASP:HA	1.85	0.42
3:A:15:ILE:C	3:A:15:ILE:HD13	2.45	0.42
3:A:137:THR:HG22	3:A:328:VAL:HG21	2.02	0.42
3:A:747:GLU:HG3	3:A:751:ARG:HD2	2.01	0.42
3:A:776:TYR:CD1	3:A:863:LEU:HD11	2.55	0.42
3:B:164:ILE:H	3:B:164:ILE:HG13	1.67	0.42
3:B:295:GLU:O	3:B:299:ASN:HA	2.20	0.42
3:D:406:TYR:CE2	3:D:633:ILE:HG21	2.55	0.42
1:E:19:DG:C5	1:E:20:DC:C4	3.07	0.41
3:A:252:VAL:HA	3:A:260:ARG:O	2.20	0.41
3:B:415:LEU:HD12	3:B:681:MET:HE2	2.01	0.41
3:C:415:LEU:O	3:C:419:ILE:HG13	2.19	0.41
3:D:7:THR:HG21	3:D:267:GLY:C	2.45	0.41
3:D:621:ASP:O	3:D:624:SER:N	2.53	0.41
2:J:104:DG:C2'	2:J:105:DC:H5''	2.50	0.41
3:C:149:PHE:HB3	3:C:197:LEU:CD2	2.50	0.41
3:B:163:SER:HB3	3:B:166:ILE:HB	2.03	0.41
3:C:183:ILE:H	3:C:183:ILE:HG13	1.69	0.41
3:D:751:ARG:HB2	3:D:755:GLU:HB2	2.02	0.41
3:A:426:SER:HB3	3:A:429:THR:OG1	2.20	0.41
3:A:451:SER:HB3	3:A:456:CYS:SG	2.60	0.41
3:B:25:ARG:HA	3:B:25:ARG:HD2	1.78	0.41
3:B:302:LYS:HB3	3:B:323:TYR:HE1	1.85	0.41
3:B:369:ILE:HG12	3:B:474:GLU:HG3	2.01	0.41
3:C:403:ARG:NH2	3:C:888:LYS:O	2.53	0.41
3:D:700:GLY:HA2	3:D:709:ALA:O	2.21	0.41
3:A:6:LEU:CD1	3:A:26:GLU:HG3	2.51	0.41
3:A:408:MET:HE2	3:A:655:ALA:HB2	2.03	0.41
3:B:621:ASP:OD1	3:B:622:THR:HG22	2.20	0.41
3:D:737:THR:HA	3:D:738:PRO:HD2	1.81	0.41
3:A:270:VAL:HB	6:A:916:HOH:O	2.21	0.41
3:B:9:GLU:HG3	3:B:266:PHE:CD2	2.55	0.41
3:C:471:VAL:HB	3:C:472:PRO:CD	2.48	0.41
3:A:98:ASN:H	3:A:98:ASN:ND2	2.18	0.41
3:B:641:PHE:HA	3:B:646:HIS:CD2	2.55	0.41
3:C:206:GLN:NE2	3:C:241:ARG:HB3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:202:LEU:O	3:A:206:GLN:HG2	2.21	0.41
3:B:162:TRP:HB2	3:B:321:ILE:HD13	2.03	0.41
3:C:153:ASN:HA	3:C:158:ASN:HA	2.03	0.41
3:C:195:LYS:HE2	3:C:233:ILE:HG23	2.03	0.41
3:C:512:GLU:HA	3:C:513:PRO:HD3	1.86	0.41
3:D:317:HIS:O	3:D:321:ILE:HD12	2.20	0.41
3:D:644:THR:CG2	3:D:692:PRO:HA	2.51	0.41
3:A:216:TRP:O	3:A:217:ASN:HB2	2.20	0.41
3:A:302:LYS:HE2	3:A:323:TYR:CZ	2.56	0.41
3:A:799:PRO:O	3:A:800:LYS:HB2	2.21	0.41
3:B:251:LYS:HB3	3:B:253:ILE:HG12	2.03	0.41
3:C:739:LYS:NZ	6:C:946:HOH:O	2.52	0.41
3:C:745:LEU:HD22	3:C:883:PHE:CE2	2.56	0.41
3:D:713:TRP:CH2	3:D:723:PRO:HD3	2.56	0.41
3:A:34:LYS:HB2	5:A:905:N5P:O3'	2.21	0.41
3:B:364:THR:HG22	3:B:562:LEU:HD21	2.03	0.41
3:B:725:LEU:HD22	3:B:753:LEU:HD12	2.03	0.41
2:L:111:DT:H2''	2:L:112:DA:C8	2.56	0.40
3:A:785:ALA:CB	3:A:808:ILE:HD11	2.48	0.40
3:B:136:ILE:HB	3:B:149:PHE:HB2	2.04	0.40
3:B:475:ILE:HD13	3:B:566:LEU:HD22	2.02	0.40
3:B:622:THR:HG23	3:B:623:ASP:N	2.36	0.40
3:C:109:ARG:HD3	3:C:142:ILE:HD12	2.03	0.40
3:C:291:ASP:OD1	3:C:291:ASP:N	2.53	0.40
3:C:441:ASP:HB3	3:C:447:ALA:HB2	2.03	0.40
1:K:14:DC:H2''	1:K:15:DA:H8	1.86	0.40
3:B:9:GLU:CG	3:B:266:PHE:CD2	3.04	0.40
3:C:286:PRO:HD2	3:C:292:TYR:HE2	1.86	0.40
3:B:19:TYR:CE1	3:B:27:ARG:HB2	2.56	0.40
3:B:263:ILE:N	3:B:263:ILE:HD13	2.36	0.40
3:B:274:ILE:O	3:B:278:LYS:HB2	2.21	0.40
3:C:119:SER:HA	3:C:120:PRO:HD2	1.99	0.40
3:C:594:LEU:HD11	3:C:624:SER:O	2.22	0.40
3:D:671:CYS:SG	3:D:676:ASN:HB2	2.62	0.40
3:A:380:ILE:HD12	3:A:576:ARG:NE	2.36	0.40
3:A:397:LYS:HD3	3:A:619:TYR:HA	2.03	0.40
3:B:343:LEU:HD12	3:B:554:THR:HG23	2.03	0.40
3:C:839:ASN:HB2	3:C:840:PRO:HD2	2.02	0.40
1:E:9:DT:H6	1:E:9:DT:H2'	1.64	0.40
3:C:279:LYS:HD3	3:C:280:PHE:CZ	2.57	0.40
3:C:422:GLN:HE21	3:C:422:GLN:HB3	1.60	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:772:ARG:NH2	6:C:1041:HOH:O	2.52	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	
3	A	844/903 (94%)	794 (94%)	45 (5%)	5 (1%)	21	38
3	B	750/903 (83%)	697 (93%)	49 (6%)	4 (0%)	24	42
3	C	885/903 (98%)	817 (92%)	61 (7%)	7 (1%)	16	31
3	D	797/903 (88%)	701 (88%)	83 (10%)	13 (2%)	7	17
All	All	3276/3612 (91%)	3009 (92%)	238 (7%)	29 (1%)	14	28

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	622	THR
3	B	736	SER
3	C	622	THR
3	D	622	THR
3	A	549	GLU
3	B	262	ILE
3	B	777	ILE
3	D	33	TYR
3	D	286	PRO
3	D	308	PRO
3	D	897	LEU
3	A	300	VAL
3	A	622	THR
3	C	496	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	531	LYS
3	D	310	SER
3	A	424	ASN
3	C	135	ALA
3	C	430	ILE
3	D	163	SER
3	D	256	MET
3	D	718	THR
3	A	489	MET
3	C	252	VAL
3	D	354	GLN
3	D	677	LYS
3	D	731	GLU
3	C	99	TYR
3	D	166	ILE

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	
3	A	738/800 (92%)	702 (95%)	36 (5%)	22	45
3	B	634/800 (79%)	598 (94%)	36 (6%)	18	39
3	C	755/800 (94%)	706 (94%)	49 (6%)	15	32
3	D	483/800 (60%)	454 (94%)	29 (6%)	17	36
All	All	2610/3200 (82%)	2460 (94%)	150 (6%)	18	39

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	15	ILE
3	A	83	LEU
3	A	85	MET
3	A	100	GLU
3	A	106	THR
3	A	145	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	154	SER
3	A	164	ILE
3	A	171	GLN
3	A	172	GLU
3	A	252	VAL
3	A	253	ILE
3	A	284	ASN
3	A	303	LEU
3	A	310	SER
3	A	356	GLN
3	A	403	ARG
3	A	433	THR
3	A	446	VAL
3	A	465	LYS
3	A	489	MET
3	A	614	GLU
3	A	645	ASN
3	A	672	GLU
3	A	677	LYS
3	A	719	ARG
3	A	726	LYS
3	A	739	LYS
3	A	746	LYS
3	A	805	ILE
3	A	813	ARG
3	A	815	ILE
3	A	843	ASP
3	A	855	THR
3	A	859	LYS
3	A	888	LYS
3	B	25	ARG
3	B	75	MET
3	B	112	ASN
3	B	114	ASP
3	B	117	VAL
3	B	134	ASP
3	B	136	ILE
3	B	137	THR
3	B	164	ILE
3	B	165	GLU
3	B	166	ILE
3	B	180	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	181	GLU
3	B	183	ILE
3	B	202	LEU
3	B	231	LYS
3	B	250	VAL
3	B	252	VAL
3	B	263	ILE
3	B	303	LEU
3	B	309	ILE
3	B	326	ILE
3	B	343	LEU
3	B	403	ARG
3	B	421	ARG
3	B	581	ARG
3	B	587	THR
3	B	592	MET
3	B	624	SER
3	B	636	VAL
3	B	681	MET
3	B	762	GLU
3	B	766	GLU
3	B	779	ILE
3	B	870	VAL
3	B	871	LEU
3	C	20	ILE
3	C	43	GLU
3	C	90	LEU
3	C	98	ASN
3	C	105	HIS
3	C	153	ASN
3	C	158	ASN
3	C	171	GLN
3	C	183	ILE
3	C	197	LEU
3	C	200	GLU
3	C	238	THR
3	C	246	ARG
3	C	262	ILE
3	C	290	LEU
3	C	291	ASP
3	C	318	GLN
3	C	356	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	362	ILE
3	C	373	LEU
3	C	380	ILE
3	C	411	ASP
3	C	422	GLN
3	C	428	GLU
3	C	440	HIS
3	C	468	ASP
3	C	490	LEU
3	C	530	ILE
3	C	536	LYS
3	C	539	ASN
3	C	548	THR
3	C	549	GLU
3	C	562	LEU
3	C	618	LEU
3	C	622	THR
3	C	625	ILE
3	C	656	ARG
3	C	658	ARG
3	C	696	LYS
3	C	725	LEU
3	C	731	GLU
3	C	758	GLU
3	C	760	LEU
3	C	815	ILE
3	C	819	ILE
3	C	825	VAL
3	C	878	LYS
3	C	897	LEU
3	C	899	ASP
3	D	3	GLU
3	D	7	THR
3	D	17	GLU
3	D	20	ILE
3	D	43	GLU
3	D	52	ILE
3	D	58	THR
3	D	85	MET
3	D	125	GLU
3	D	192	ASP
3	D	236	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	257	TYR
3	D	273	TYR
3	D	356	GLN
3	D	362	ILE
3	D	373	LEU
3	D	490	LEU
3	D	572	ASN
3	D	587	THR
3	D	602	ASN
3	D	607	GLU
3	D	618	LEU
3	D	633	ILE
3	D	643	ASP
3	D	646	HIS
3	D	678	GLN
3	D	722	GLU
3	D	745	LEU
3	D	746	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	ASN
3	A	98	ASN
3	A	112	ASN
3	A	171	GLN
3	A	228	ASN
3	A	324	ASN
3	A	342	ASN
3	A	356	GLN
3	A	422	GLN
3	A	485	HIS
3	A	564	ASN
3	A	645	ASN
3	A	679	HIS
3	A	787	ASN
3	A	823	GLN
3	B	10	GLN
3	B	23	ASN
3	B	70	GLN
3	B	285	GLN
3	B	317	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	324	ASN
3	B	339	GLN
3	B	354	GLN
3	B	371	ASN
3	B	440	HIS
3	B	444	ASN
3	B	595	GLN
3	B	646	HIS
3	B	678	GLN
3	C	10	GLN
3	C	40	HIS
3	C	64	ASN
3	C	98	ASN
3	C	112	ASN
3	C	171	GLN
3	C	217	ASN
3	C	228	ASN
3	C	245	HIS
3	C	316	ASN
3	C	324	ASN
3	C	339	GLN
3	C	354	GLN
3	C	376	GLN
3	C	480	ASN
3	C	485	HIS
3	C	539	ASN
3	C	556	GLN
3	C	558	ASN
3	C	564	ASN
3	C	591	GLN
3	C	606	ASN
3	C	645	ASN
3	C	679	HIS
3	D	10	GLN
3	D	112	ASN
3	D	342	ASN
3	D	354	GLN
3	D	371	ASN
3	D	386	HIS
3	D	402	ASN
3	D	481	GLN
3	D	572	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	595	GLN
3	D	645	ASN
3	D	678	GLN
3	D	742	GLN
3	D	754	GLN
3	D	761	GLN
3	D	773	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	3DR	I	6	1	8,11,12	0.47	0	7,14,17	0.81	0
2	N5I	J	115	2	22,25,26	0.84	0	29,36,39	0.99	1 (3%)
2	N5I	F	115	2	22,25,26	0.87	0	29,36,39	0.94	2 (6%)
1	3DR	E	6	1	8,8,12	0.43	0	9,10,17	0.81	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
1	3DR	I	6	1	-	2/3/15/16	0/1/1/1
2	N5I	J	115	2	-	0/9/25/26	0/3/3/3
2	N5I	F	115	2	-	0/9/25/26	0/3/3/3
1	3DR	E	6	1	-	2/2/12/16	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	115	N5I	CE2-NE1-CD1	2.21	109.49	107.77
2	F	115	N5I	CD2-CE3-CZ3	-2.07	118.06	120.47
2	J	115	N5I	CD2-CE3-CZ3	-2.03	118.12	120.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	6	3DR	C3'-C4'-C5'-O5'
1	E	6	3DR	O4'-C4'-C5'-O5'
1	I	6	3DR	O4'-C4'-C5'-O5'
1	I	6	3DR	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	115	N5I	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	N5P	A	905	4	33,34,34	1.00	3 (9%)	47,53,53	1.00	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	N5P	A	904	-	33,34,34	0.97	2 (6%)	47,53,53	0.95	2 (4%)
5	N5P	I	704	4	33,34,34	1.03	3 (9%)	47,53,53	0.93	2 (4%)
5	N5P	C	904	-	33,34,34	1.01	3 (9%)	47,53,53	0.94	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	N5P	A	905	4	-	4/24/38/38	0/3/3/3
5	N5P	A	904	-	-	4/24/38/38	0/3/3/3
5	N5P	I	704	4	-	4/24/38/38	0/3/3/3
5	N5P	C	904	-	-	1/24/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	904	N5P	PB-O3B	2.55	1.62	1.59
5	I	704	N5P	PA-O3A	2.45	1.62	1.59
5	I	704	N5P	PB-O3A	2.42	1.62	1.59
5	C	904	N5P	PB-O3A	2.33	1.62	1.59
5	A	905	N5P	PA-O3A	2.33	1.62	1.59
5	C	904	N5P	PA-O3A	2.30	1.62	1.59
5	A	905	N5P	PB-O3A	2.26	1.61	1.59
5	C	904	N5P	C1'-NE1	2.24	1.50	1.46
5	I	704	N5P	PB-O3B	2.23	1.61	1.59
5	A	905	N5P	PB-O3B	2.19	1.61	1.59
5	A	904	N5P	C1'-NE1	2.07	1.50	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	704	N5P	CE2-NE1-CD1	2.24	109.52	107.77
5	A	904	N5P	CE2-NE1-CD1	2.22	109.51	107.77
5	A	905	N5P	CD2-CE3-CZ3	-2.19	117.93	120.47
5	A	905	N5P	CE2-NE1-CD1	2.18	109.47	107.77
5	I	704	N5P	CD2-CE3-CZ3	-2.12	118.02	120.47
5	A	904	N5P	CD2-CE3-CZ3	-2.10	118.03	120.47
5	C	904	N5P	CD2-CE3-CZ3	-2.05	118.09	120.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	904	N5P	O4'-C4'-C5'-O5'
5	A	904	N5P	C3'-C4'-C5'-O5'
5	I	704	N5P	PA-O3A-PB-O1B
5	A	905	N5P	PA-O3A-PB-O1B
5	A	905	N5P	PB-O3A-PA-O1A
5	I	704	N5P	PA-O3A-PB-O2B
5	A	905	N5P	PB-O3A-PA-O2A
5	A	905	N5P	PA-O3A-PB-O2B
5	I	704	N5P	PB-O3A-PA-O1A
5	C	904	N5P	O4'-C1'-NE1-CE2
5	I	704	N5P	PB-O3A-PA-O2A
5	A	904	N5P	PB-O3A-PA-O1A
5	A	904	N5P	PB-O3A-PA-O2A

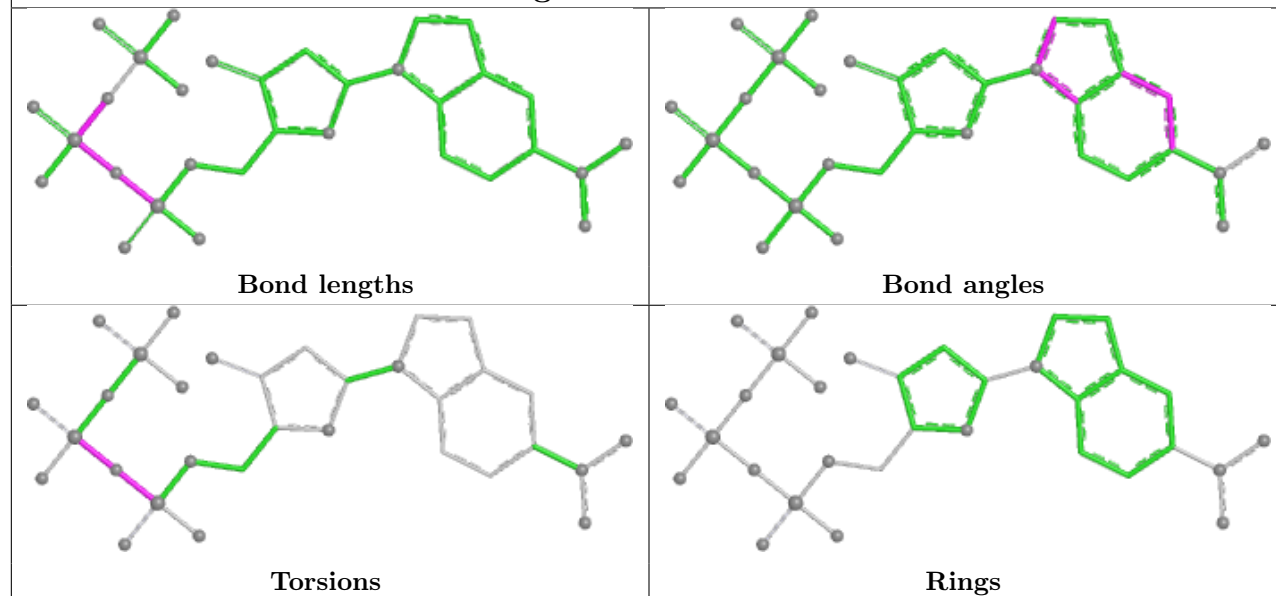
There are no ring outliers.

1 monomer is involved in 1 short contact:

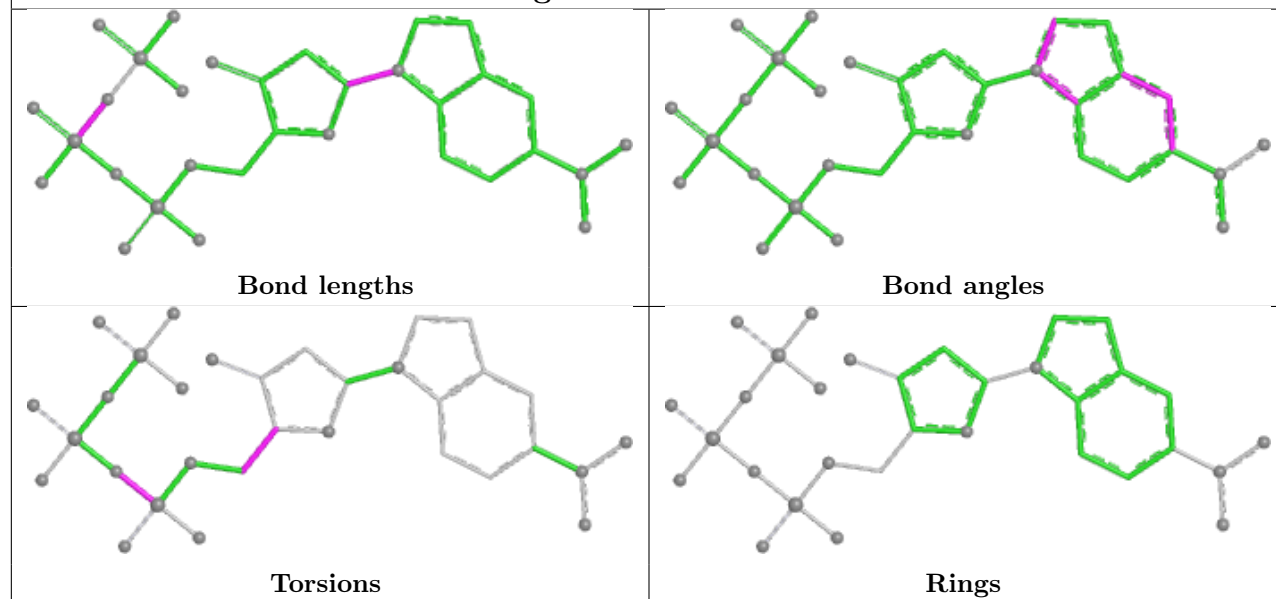
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	905	N5P	1	0

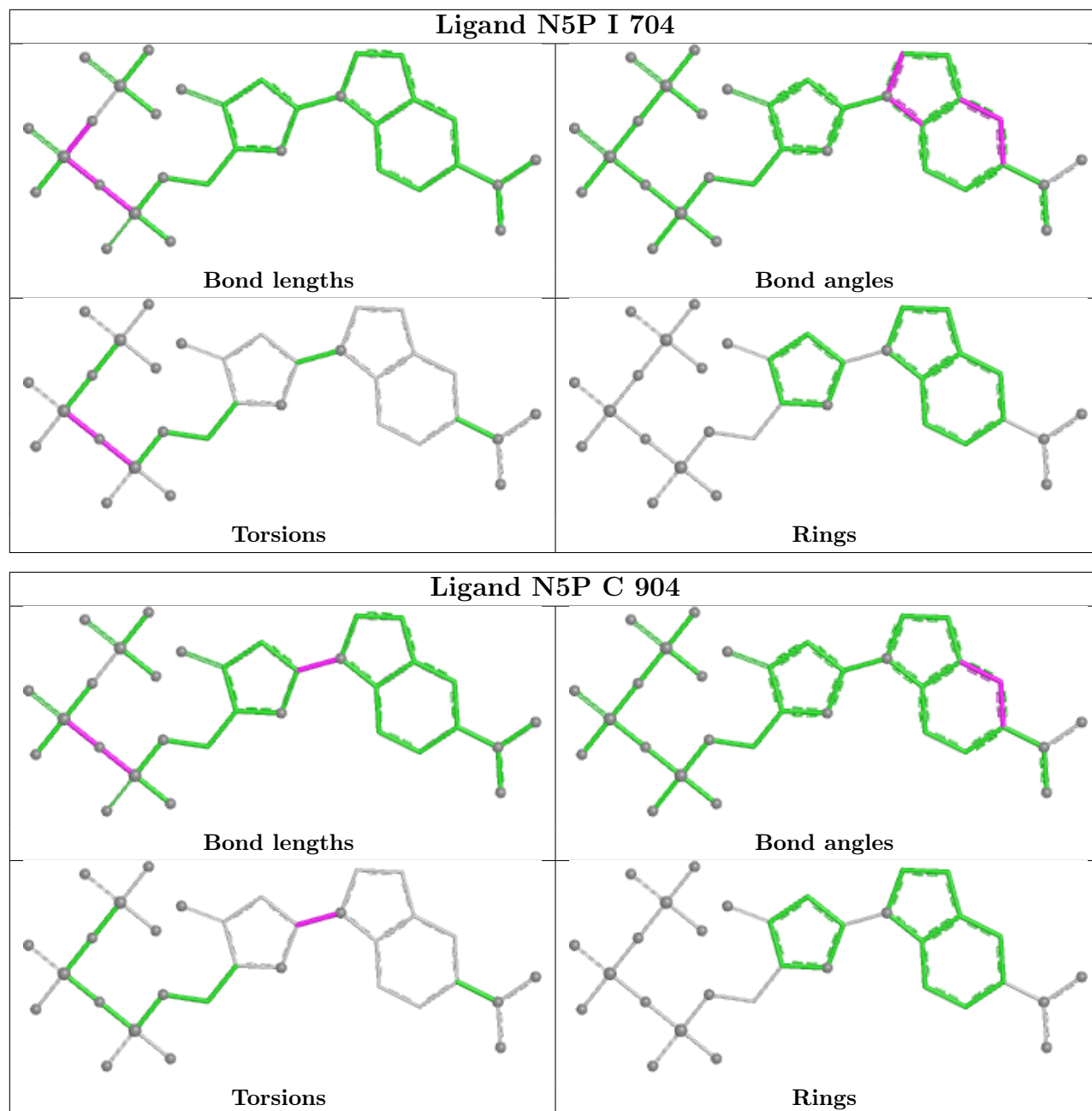
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand N5P A 905



Ligand N5P A 904





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	E	15/21 (71%)	0.25	0 100 100	58, 78, 115, 119	0
1	G	11/21 (52%)	1.48	3 (27%) 1 1	62, 115, 126, 132	0
1	I	19/21 (90%)	-0.19	1 (5%) 32 24	43, 56, 138, 144	0
1	K	12/21 (57%)	-0.04	0 100 100	42, 94, 107, 115	0
2	F	14/15 (93%)	0.22	0 100 100	73, 106, 124, 126	0
2	H	14/15 (93%)	1.29	1 (7%) 22 16	102, 129, 134, 137	0
2	J	14/15 (93%)	-0.35	0 100 100	44, 68, 85, 88	0
2	L	13/15 (86%)	0.55	0 100 100	85, 108, 113, 113	0
3	A	848/903 (93%)	-0.11	8 (0%) 81 76	36, 53, 79, 96	0
3	B	756/903 (83%)	0.22	19 (2%) 58 49	44, 68, 105, 116	0
3	C	891/903 (98%)	0.17	22 (2%) 58 49	36, 63, 110, 135	0
3	D	807/903 (89%)	0.94	86 (10%) 11 8	105, 121, 145, 147	0
All	All	3414/3756 (90%)	0.30	140 (4%) 41 32	36, 69, 138, 147	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	6	LEU	5.0
3	D	782	VAL	4.6
3	C	252	VAL	4.2
3	D	393	GLY	4.1
3	A	558	ASN	4.0
3	D	524	ASP	4.0
3	D	577	TYR	3.8
3	C	303	LEU	3.7
3	D	90	LEU	3.6
3	A	550	VAL	3.4
3	B	182	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	650	PHE	3.3
3	D	33	TYR	3.2
3	D	134	ASP	3.2
3	D	732	THR	3.2
3	D	216	TRP	3.2
3	A	773	GLN	3.1
3	C	535	ALA	3.1
3	C	468	ASP	3.1
3	B	554	THR	3.1
3	D	303	LEU	3.1
3	D	745	LEU	3.1
3	D	570	LEU	3.1
3	D	394	ALA	3.0
3	D	135	ALA	3.0
3	C	253	ILE	3.0
3	D	362	ILE	3.0
3	B	899	ASP	3.0
3	D	876	PHE	3.0
3	D	865	TRP	2.9
3	D	659	MET	2.9
3	D	752	MET	2.9
3	D	780	ALA	2.9
3	D	8	VAL	2.8
3	D	621	ASP	2.8
3	D	321	ILE	2.8
3	D	178	VAL	2.8
3	D	636	VAL	2.8
3	B	128	GLN	2.7
3	D	226	VAL	2.7
3	D	400	ILE	2.7
3	D	257	TYR	2.7
3	D	133	ILE	2.7
3	D	265	LEU	2.7
3	D	723	PRO	2.6
3	B	558	ASN	2.6
3	A	786	ASN	2.6
3	D	15	ILE	2.6
3	C	168	ALA	2.6
3	D	513	PRO	2.6
3	B	123	PHE	2.6
3	C	491	ALA	2.6
3	C	527	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	569	ALA	2.5
3	B	255	ASN	2.5
3	B	259	SER	2.5
3	D	325	ILE	2.5
3	D	395	PHE	2.5
1	G	13	DA	2.5
3	A	554	THR	2.5
3	B	132	PRO	2.5
3	D	727	ILE	2.5
1	G	11	DT	2.5
3	D	65	MET	2.4
3	C	530	ILE	2.4
3	B	257	TYR	2.4
3	D	156	TYR	2.4
3	D	776	TYR	2.4
3	D	490	LEU	2.4
3	D	619	TYR	2.4
3	B	309	ILE	2.4
1	G	12	DG	2.4
3	D	104	ASP	2.4
3	D	291	ASP	2.4
3	D	302	LYS	2.3
3	D	162	TRP	2.3
3	C	309	ILE	2.3
3	D	419	ILE	2.3
3	D	197	LEU	2.3
3	C	150	ASP	2.3
3	D	306	ASP	2.3
3	C	498	ILE	2.3
3	D	263	ILE	2.3
3	D	639	SER	2.3
3	B	260	ARG	2.3
3	C	518	TYR	2.3
3	A	817	GLY	2.3
3	D	402	ASN	2.2
3	B	605	LEU	2.2
3	D	713	TRP	2.2
3	D	781	SER	2.2
3	D	898	PHE	2.2
3	D	431	ALA	2.2
3	B	303	LEU	2.2
3	C	820	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	518	TYR	2.2
3	D	592	MET	2.2
3	C	514	LEU	2.2
3	D	37	LEU	2.2
3	D	897	LEU	2.2
3	C	504	HIS	2.2
3	D	588	THR	2.2
3	D	340	PHE	2.2
3	C	526	ILE	2.2
3	A	556	GLN	2.2
3	D	883	PHE	2.2
3	D	116	GLU	2.2
3	C	494	ARG	2.1
3	D	136	ILE	2.1
3	D	465	LYS	2.1
3	D	222	ALA	2.1
3	D	223	ILE	2.1
3	D	875	THR	2.1
3	D	447	ALA	2.1
3	D	259	SER	2.1
3	C	112	ASN	2.1
3	C	532	LYS	2.1
3	D	703	THR	2.1
3	A	551	ALA	2.1
3	B	133	ILE	2.1
3	D	274	ILE	2.1
3	D	292	TYR	2.1
3	D	293	ILE	2.1
3	D	437	ALA	2.1
3	B	117	VAL	2.1
3	D	284	ASN	2.1
3	D	86	ASP	2.1
3	D	466	ASP	2.1
3	B	557	ILE	2.1
3	D	334	ILE	2.1
3	D	155	PRO	2.0
1	I	2	DA	2.0
2	H	112	DA	2.0
3	D	174	GLY	2.0
3	D	625	ILE	2.0
3	B	327	ALA	2.0
3	C	255	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	168	ALA	2.0
3	D	585	ALA	2.0
3	C	110	VAL	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
1	3DR	E	6	8/12	0.43	0.16	123,124,124,124	0
2	N5I	F	115	23/24	0.76	0.16	127,128,128,128	0
2	N5I	J	115	23/24	0.88	0.12	83,89,89,89	0
1	3DR	I	6	11/12	0.90	0.11	104,108,115,115	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

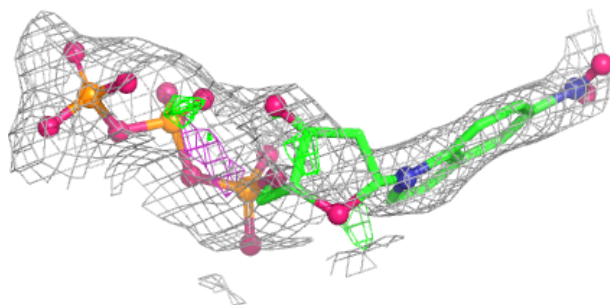
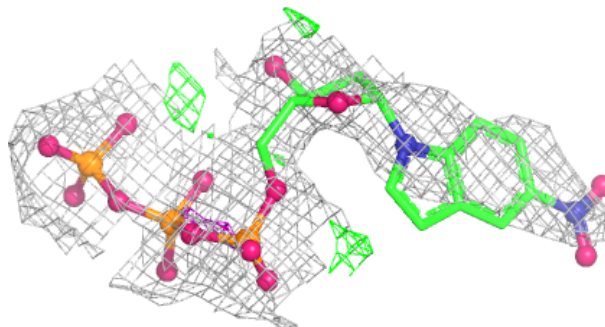
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	K	801	1/1	0.51	0.27	67,67,67,67	1
5	N5P	C	904	32/32	0.78	0.16	79,81,83,83	32
4	MG	I	802	1/1	0.85	0.29	82,82,82,82	1
5	N5P	I	704	32/32	0.86	0.18	78,80,84,84	32
5	N5P	A	904	32/32	0.88	0.13	74,76,88,88	32
5	N5P	A	905	32/32	0.91	0.13	61,65,75,76	32

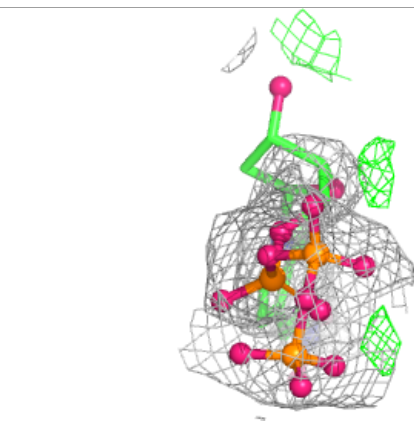
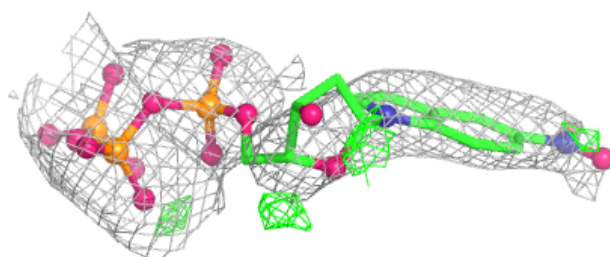
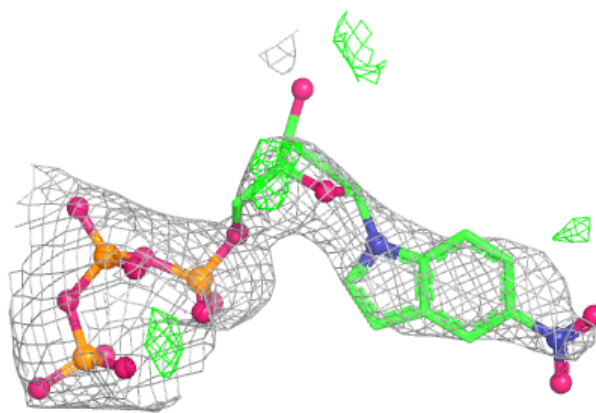
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around N5P C 904:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

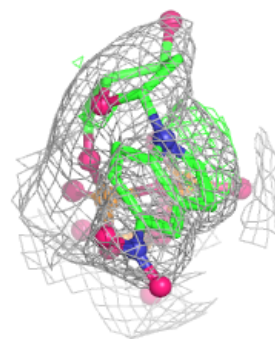
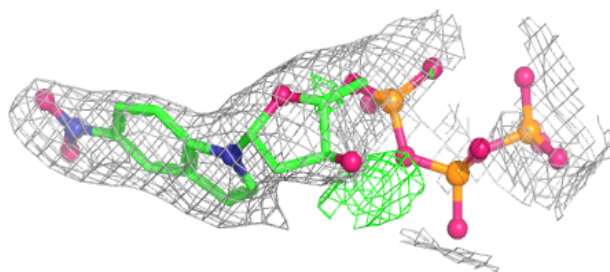
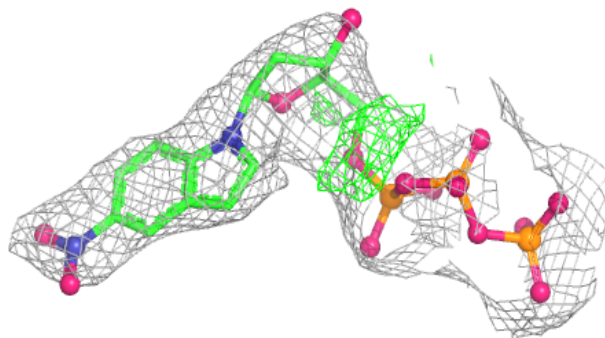
**Electron density around N5P I 704:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

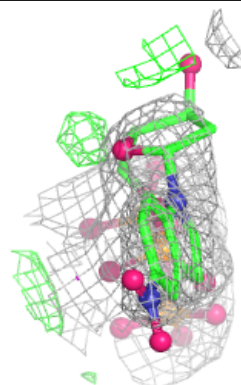
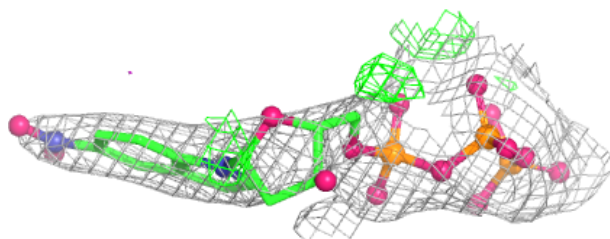
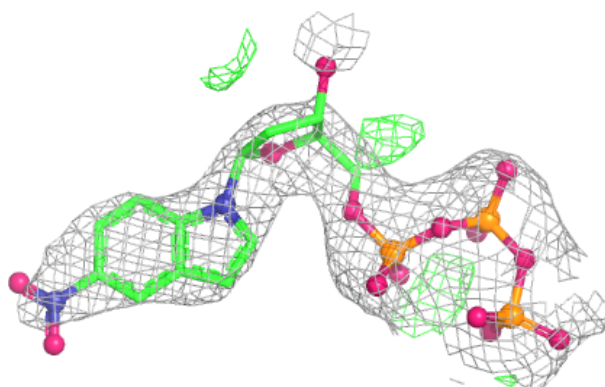


Electron density around N5P A 904:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around N5P A 905:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.