



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:29 PM UTC

PDB ID : 7Y7S / pdb_00007y7s
Title : QDE-1 in complex with DNA template, RNA primer and AMPNPP
Authors : Cui, R.X.; Gan, J.H.; Ma, J.B.
Deposited on : 2022-06-22
Resolution : 2.70 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:

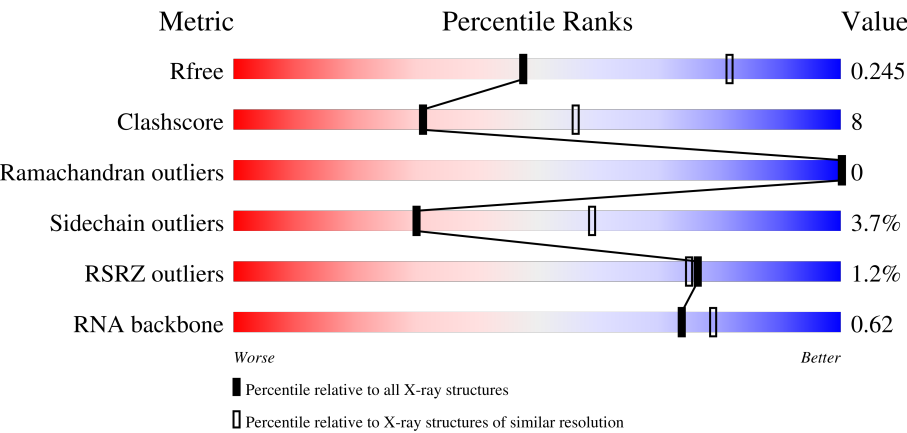
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	1026	73%18%9%
1	B	1026	71%18%10%
2	C	14	50%21%29%
2	I	14	86%14%

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Mol	Chain	Length	Quality of chain
3	D	7	71% 29%
3	J	7	29% 43% 14% 14%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15570 atoms, of which 10 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	937	Total	C	N	O	S	0	0	0
			7349	4699	1259	1358	33			
1	B	920	Total	C	N	O	S	0	0	0
			7231	4627	1249	1323	32			

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*AP*CP*TP*AP*TP*GP*GP*TP*CP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			209	99	39	61	10			
2	I	14	Total	C	N	O	P	0	0	0
			289	138	57	81	13			

- Molecule 3 is a RNA chain called RNA (5'-R(*UP*CP*CP*GP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	7	Total	C	N	O	P	0	0	0
			142	65	24	47	6			
3	J	6	Total	C	N	O	P	0	0	0
			125	56	22	41	6			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

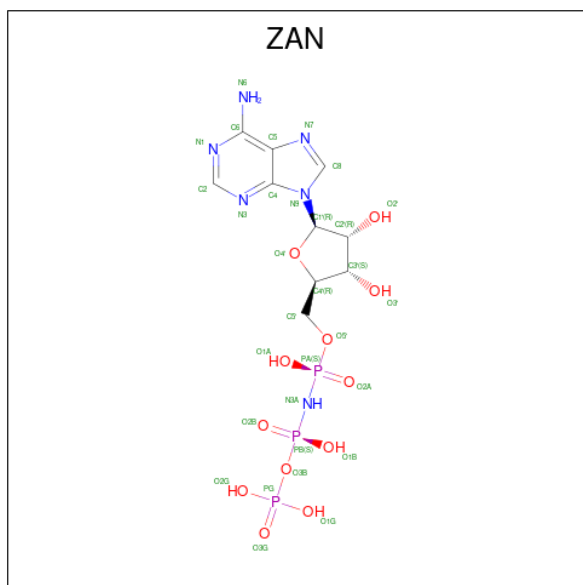
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	B	2	Total	Ca	0	0
			2	2		
4	C	1	Total	Ca	0	0
			1	1		

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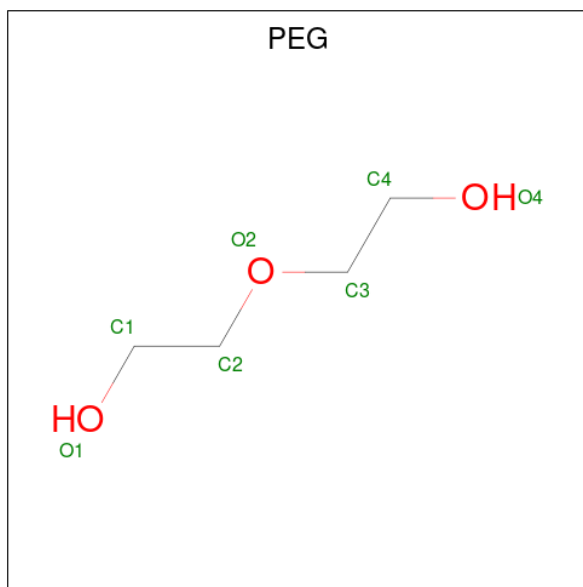
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]adenosine (CCD ID: ZAN) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		

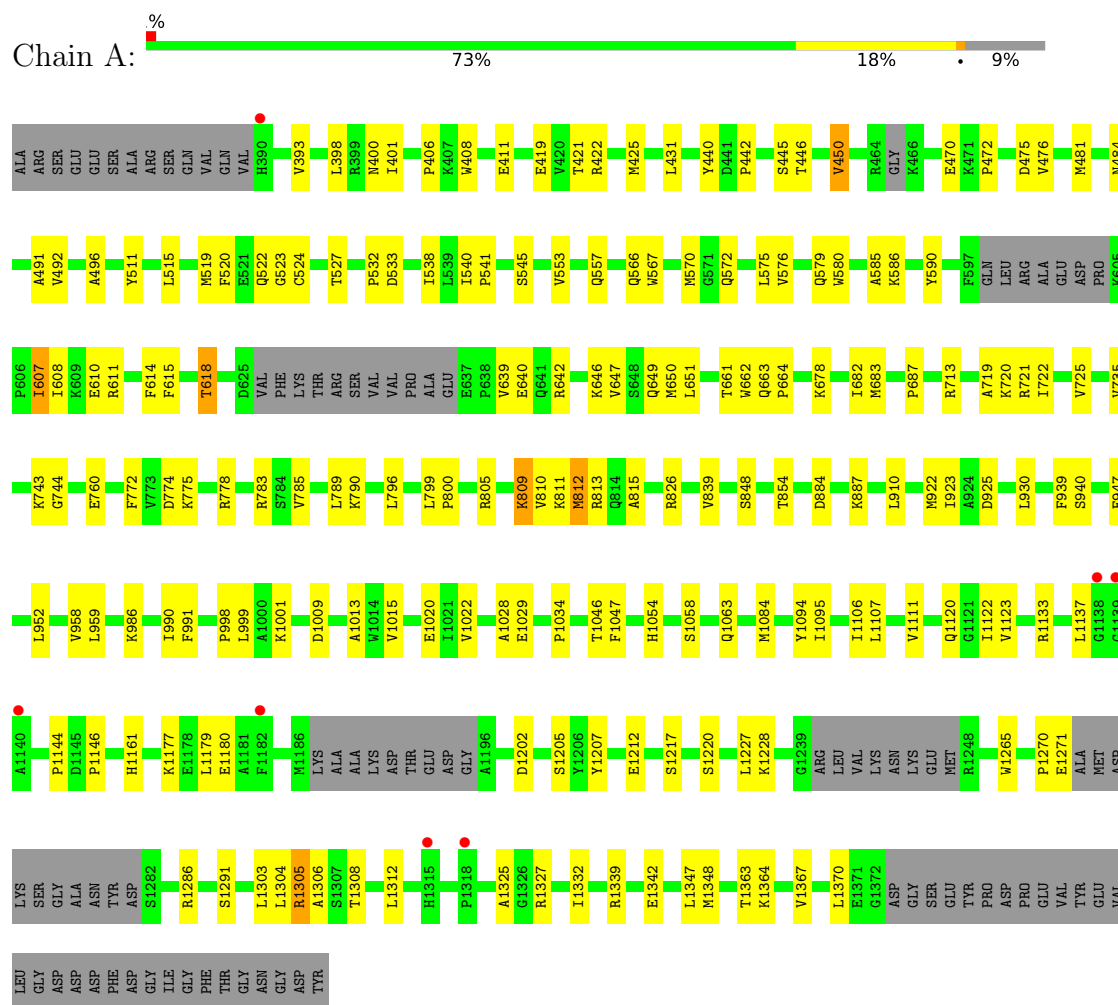
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	54	Total	O	0	0
			54	54		
8	B	67	Total	O	0	0
			67	67		
8	C	9	Total	O	0	0
			9	9		
8	I	6	Total	O	0	0
			6	6		
8	J	2	Total	O	0	0
			2	2		

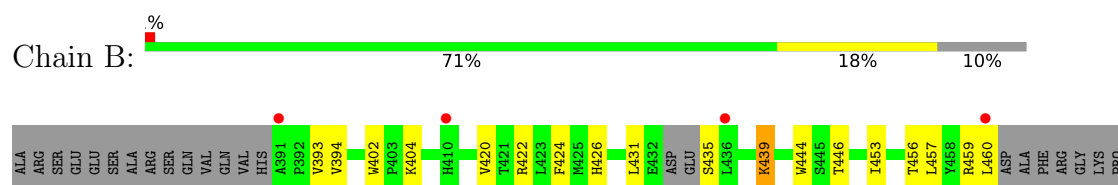
3 Residue-property plots

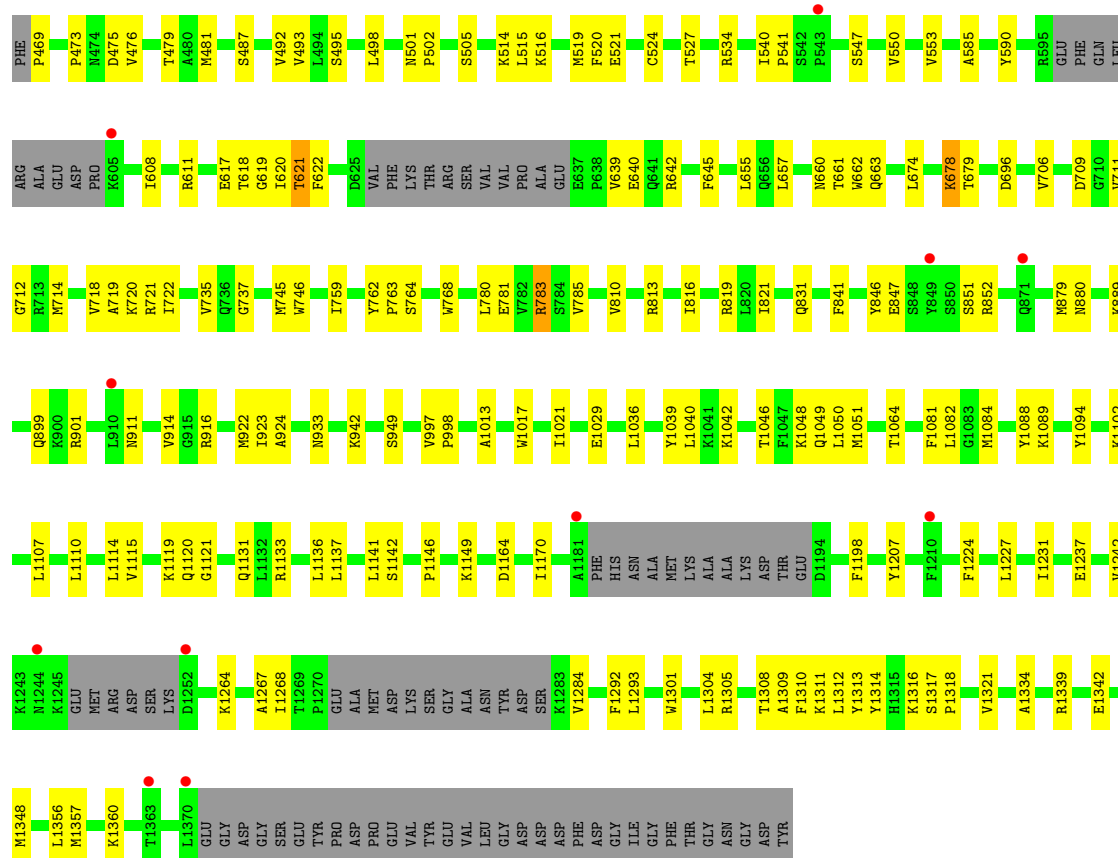
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: RNA-dependent RNA polymerase

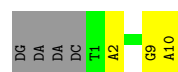


• Molecule 1: RNA-dependent RNA polymerase

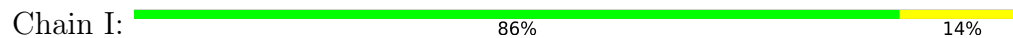




- Molecule 2: DNA (5'-D(*GP*AP*AP*CP*TP*AP*TP*GP*GP*TP*CP*GP*GP*A)-3')



- Molecule 2: DNA (5'-D(*GP*AP*AP*CP*TP*AP*TP*GP*GP*TP*CP*GP*GP*A)-3')



- Molecule 3: RNA (5'-R(*UP*CP*CP*GP*AP*CP*C)-3')



- Molecule 3: RNA (5'-R(*UP*CP*CP*GP*AP*CP*C)-3')



U	C2	C3	G4	A5	C6	G7
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.95Å 120.41Å 114.99Å 90.00° 109.71° 90.00°	Depositor
Resolution (Å)	30.10 – 2.70 30.10 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.5 (30.10-2.70) 93.5 (30.10-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.72Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.208 , 0.245 0.208 , 0.245	Depositor DCC
R_{free} test set	3289 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtrriage
Anisotropy	0.558	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15570	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6646e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	1/7539 (0.0%)	0.85	0/10231
1	B	0.50	0/7414	0.77	0/10061
2	C	0.21	0/234	0.37	0/360
2	I	0.22	0/325	0.36	0/501
3	D	0.15	0/157	0.26	0/242
3	J	0.16	0/138	0.32	0/212
All	All	0.52	1/15807 (0.0%)	0.79	0/21607

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	ASN	C-N	6.14	1.41	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7349	0	7070	115	0
1	B	7231	0	7005	124	0
2	C	209	0	114	5	0
2	I	289	0	159	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	142	0	77	2	0
3	J	125	0	66	5	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	I	1	0	0	0	0
5	A	31	0	17	0	0
5	B	31	0	16	0	0
6	B	7	10	10	0	0
7	B	1	0	0	0	0
8	A	54	0	0	2	0
8	B	67	0	0	3	0
8	C	9	0	0	0	0
8	I	6	0	0	0	0
8	J	2	0	0	0	0
All	All	15560	10	14534	245	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 (245) 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:A:959:LEU:HG	1:A:1022:VAL:HG22	1.65	0.78
1:A:398:LEU:HD23	1:A:401:ILE:HD11	1.65	0.78
1:B:846:TYR:OH	1:B:1357:MET:HE2	1.85	0.76
1:A:540:ILE:HG13	1:A:541:PRO:HD2	1.67	0.76
1:A:682:ILE:HG22	1:A:683:MET:HG2	1.70	0.73
1:A:1054:HIS:HD1	1:A:1063:GLN:HB3	1.55	0.72
1:A:1348:MET:SD	1:B:1348:MET:HE2	2.31	0.71
1:B:1348:MET:HE1	1:B:1356:LEU:HD12	1.71	0.70
1:B:540:ILE:HG13	1:B:541:PRO:HD2	1.74	0.70
1:A:1286:ARG:HH12	1:A:1291:SER:H	1.39	0.69
1:B:1227:LEU:HD13	1:B:1301:TRP:CZ2	2.30	0.66
1:B:524:CYS:SG	1:B:527:THR:HG23	2.37	0.65
1:B:783:ARG:HD2	3:J:6:C:H4'	1.78	0.65
1:A:1034:PRO:HG3	1:A:1106:ILE:HG22	1.77	0.65
1:B:819:ARG:HH11	1:B:914:VAL:HA	1.62	0.65
2:C:9:DG:H4'	2:C:10:DA:H5'	1.78	0.65
1:B:1089:LYS:HA	1:B:1107:LEU:HD13	1.80	0.64
1:A:401:ILE:HD12	1:A:567:TRP:CZ2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:PHE:HB3	1:B:879:MET:HE1	1.79	0.63
1:B:444:TRP:CD1	1:B:453:ILE:HG23	2.33	0.63
1:B:1088:TYR:CE1	1:B:1137:LEU:HD23	2.34	0.62
1:B:735:VAL:HG12	1:B:785:VAL:HG12	1.80	0.62
2:C:9:DG:H4'	2:C:10:DA:C5'	2.29	0.62
1:B:997:VAL:HG13	1:B:998:PRO:HD2	1.82	0.62
1:A:1347:LEU:HD23	1:B:1334:ALA:HB3	1.82	0.62
1:B:1107:LEU:HD21	1:B:1137:LEU:HD21	1.83	0.61
1:B:674:LEU:HD12	1:B:768:TRP:HZ3	1.65	0.61
1:B:678:LYS:HG3	3:J:5:A:H4'	1.81	0.60
1:A:440:TYR:OH	1:A:445:SER:OG	2.18	0.60
1:A:662:TRP:CZ3	1:A:663:GLN:HG2	2.36	0.59
1:A:744:GLY:HA2	1:A:1009:ASP:HB2	1.83	0.59
1:B:1136:LEU:C	1:B:1137:LEU:HD12	2.28	0.59
1:B:1311:LYS:HD2	1:B:1311:LYS:O	2.03	0.59
1:A:476:VAL:HG13	1:A:492:VAL:HG22	1.84	0.59
1:B:662:TRP:CZ3	1:B:663:GLN:HG2	2.38	0.58
1:B:547:SER:O	1:B:550:VAL:HG12	2.02	0.58
1:A:839:VAL:HG22	1:A:1363:THR:HG23	1.85	0.58
1:A:735:VAL:HG12	1:A:785:VAL:HG12	1.86	0.58
1:B:759:ILE:CD1	1:B:780:LEU:HD13	2.34	0.57
1:A:789:LEU:HD12	1:A:939:PHE:CE1	2.39	0.57
1:A:1106:ILE:HD11	1:A:1137:LEU:CD2	2.33	0.57
2:C:9:DG:H2''	2:C:10:DA:OP2	2.04	0.57
1:A:1306:ALA:HB1	1:A:1325:ALA:HB1	1.87	0.56
1:B:1149:LYS:NZ	8:B:1603:HOH:O	2.37	0.56
1:B:402:TRP:O	1:B:404:LYS:HE3	2.06	0.56
1:A:1364:LYS:HA	1:A:1367:VAL:HG22	1.88	0.56
1:B:534:ARG:HD2	1:B:642:ARG:HD2	1.87	0.56
1:A:1029:GLU:OE2	1:A:1029:GLU:HA	2.05	0.56
1:B:1304:LEU:O	1:B:1308:THR:HG23	2.06	0.55
1:B:424:PHE:HB2	1:B:431:LEU:HD21	1.87	0.55
1:B:942:LYS:HG3	1:B:949:SER:HB3	1.88	0.55
1:A:421:THR:O	1:A:425:MET:HG3	2.06	0.54
1:B:1313:TYR:HB3	1:B:1317:SER:HB2	1.88	0.54
1:A:720:LYS:NZ	1:A:720:LYS:HB3	2.22	0.54
1:B:1046:THR:HG23	1:B:1049:GLN:H	1.72	0.54
1:A:401:ILE:HD13	1:A:511:TYR:HD2	1.71	0.54
1:A:580:TRP:HB3	1:A:614:PHE:HB3	1.88	0.54
1:B:1231:ILE:HD13	1:B:1309:ALA:HB2	1.89	0.54
1:A:1227:LEU:HD11	1:A:1305:ARG:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:PHE:CB	1:B:431:LEU:HD21	2.37	0.53
1:A:774:ASP:OD1	1:A:775:LYS:N	2.42	0.53
1:A:1348:MET:HE3	1:B:880:ASN:CG	2.34	0.53
1:A:884:ASP:HB3	1:A:887:LYS:HB2	1.90	0.53
1:A:572:GLN:OE1	1:A:579:GLN:HB3	2.09	0.52
1:A:958:VAL:HG11	1:A:1015:VAL:HG13	1.91	0.52
1:A:576:VAL:HG23	1:A:576:VAL:O	2.08	0.52
1:A:640:GLU:CD	1:A:640:GLU:H	2.16	0.52
1:A:650:MET:HE3	1:A:651:LEU:HD23	1.92	0.52
1:B:519:MET:HE3	1:B:521:GLU:OE2	2.10	0.52
1:A:1054:HIS:HD1	1:A:1063:GLN:CB	2.21	0.52
1:A:1054:HIS:ND1	1:A:1063:GLN:HB3	2.22	0.52
1:B:456:THR:OG1	1:B:457:LEU:HD22	2.10	0.52
1:B:479:THR:HG21	1:B:487:SER:HB3	1.92	0.52
1:B:1316:LYS:HD2	1:B:1316:LYS:O	2.09	0.52
1:A:646:LYS:HB2	1:A:649:GLN:HG3	1.92	0.51
1:A:1054:HIS:ND1	1:A:1063:GLN:OE1	2.42	0.51
1:B:620:ILE:HG13	1:B:621:THR:HG23	1.91	0.51
1:B:459:ARG:O	1:B:460:LEU:HB2	2.10	0.51
1:B:759:ILE:HD12	1:B:780:LEU:HD13	1.93	0.51
1:B:1051:MET:HG3	1:B:1064:THR:OG1	2.11	0.51
1:A:491:ALA:HB1	1:A:532:PRO:HB3	1.92	0.51
1:A:575:LEU:HG	1:A:576:VAL:HG13	1.92	0.51
1:A:1227:LEU:HD21	1:A:1305:ARG:HA	1.91	0.51
3:J:5:A:C2'	3:J:6:C:H5'	2.41	0.51
1:B:706:VAL:O	1:B:998:PRO:HG3	2.10	0.50
1:B:821:ILE:HG13	1:B:1170:ILE:CG2	2.41	0.50
1:A:422:ARG:HG2	1:A:515:LEU:HB2	1.93	0.50
1:A:639:VAL:HG22	1:A:642:ARG:HH21	1.76	0.50
1:A:1306:ALA:CB	1:A:1325:ALA:HB1	2.41	0.50
1:A:1265:TRP:CZ2	1:A:1305:ARG:HD2	2.46	0.50
3:J:5:A:H2'	3:J:6:C:H5'	1.94	0.49
1:A:713:ARG:HB2	1:A:760:GLU:OE2	2.12	0.49
1:A:783:ARG:HD2	3:D:6:C:H4'	1.94	0.49
1:B:1042:LYS:HA	1:B:1121:GLY:O	2.12	0.49
1:A:923:ILE:O	1:A:990:ILE:HA	2.11	0.49
1:B:662:TRP:CD1	1:B:662:TRP:H	2.31	0.49
1:B:1133:ARG:HA	1:B:1137:LEU:HB2	1.93	0.49
1:B:1141:LEU:HD23	1:B:1142:SER:N	2.27	0.49
1:A:796:LEU:HD21	1:A:910:LEU:HB2	1.93	0.49
1:A:1207:TYR:HD2	1:A:1308:THR:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:ASP:HB2	1:A:930:LEU:HD12	1.94	0.49
1:B:620:ILE:HG13	1:B:621:THR:N	2.28	0.49
1:B:933:ASN:OD1	8:B:1601:HOH:O	2.20	0.48
1:A:1202:ASP:O	1:A:1205:SER:OG	2.29	0.48
1:A:1339:ARG:HB2	1:A:1342:GLU:OE1	2.14	0.48
1:B:426:HIS:ND1	1:B:469:PRO:HB3	2.28	0.48
1:B:709:ASP:OD1	1:B:764:SER:HB2	2.13	0.48
1:B:745:MET:HE2	1:B:923:ILE:HD11	1.95	0.48
1:B:889:LYS:HB3	1:B:1198:PHE:CE1	2.48	0.48
1:B:1050:LEU:HB3	1:B:1064:THR:HG23	1.95	0.48
1:B:1316:LYS:HD2	1:B:1316:LYS:C	2.37	0.48
1:A:575:LEU:O	1:A:576:VAL:HG22	2.14	0.48
1:B:473:PRO:HB2	1:B:475:ASP:OD1	2.13	0.48
1:A:566:GLN:O	1:A:570:MET:HB3	2.14	0.47
1:A:1304:LEU:O	1:A:1308:THR:HG23	2.14	0.47
1:B:1339:ARG:HD3	1:B:1339:ARG:HA	1.68	0.47
1:A:1106:ILE:HG13	1:A:1107:LEU:N	2.29	0.47
1:B:661:THR:O	1:B:1048:LYS:HG3	2.14	0.47
1:A:947:GLU:OE2	1:A:947:GLU:HA	2.15	0.47
1:A:533:ASP:CG	1:A:639:VAL:HG13	2.39	0.47
1:B:473:PRO:HG2	1:B:476:VAL:HG21	1.97	0.47
1:B:655:LEU:HB2	1:B:657:LEU:CD2	2.44	0.47
1:B:889:LYS:HB3	1:B:1198:PHE:CD1	2.50	0.47
2:C:9:DG:H4'	2:C:10:DA:O5'	2.15	0.47
1:B:475:ASP:OD1	1:B:475:ASP:N	2.44	0.47
1:B:696:ASP:OD1	1:B:762:TYR:HB3	2.14	0.47
1:B:501:ASN:OD1	1:B:502:PRO:HD2	2.15	0.47
1:A:450:VAL:HG21	1:A:472:PRO:HD2	1.96	0.47
1:B:889:LYS:HE3	1:B:1198:PHE:CD1	2.50	0.47
1:A:998:PRO:HG2	1:A:1001:LYS:HB2	1.98	0.46
1:B:476:VAL:HG13	1:B:492:VAL:HG22	1.96	0.46
1:A:799:LEU:HB2	1:A:800:PRO:HD3	1.96	0.46
1:A:1207:TYR:CD1	1:A:1207:TYR:C	2.93	0.46
1:B:1292:PHE:CD2	1:B:1293:LEU:HD13	2.50	0.46
1:A:522:GLN:HB3	1:A:678:LYS:HB3	1.97	0.46
1:A:922:MET:SD	1:A:1013:ALA:HB2	2.56	0.46
1:B:662:TRP:CE3	1:B:663:GLN:HG2	2.50	0.46
1:A:406:PRO:HB2	1:A:408:TRP:CD1	2.51	0.46
1:A:991:PHE:CG	1:A:999:LEU:HD23	2.50	0.46
1:B:655:LEU:HB2	1:B:657:LEU:HD21	1.98	0.46
1:B:1046:THR:HG22	1:B:1049:GLN:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1207:TYR:CD2	1:B:1311:LYS:HG2	2.51	0.46
1:B:923:ILE:HG22	1:B:924:ALA:N	2.31	0.46
1:B:712:GLY:O	1:B:746:TRP:HA	2.16	0.45
1:A:991:PHE:CD1	1:A:999:LEU:HD23	2.51	0.45
1:B:498:LEU:HD12	1:B:540:ILE:HD12	1.98	0.45
1:A:393:VAL:HG12	1:A:553:VAL:HG23	1.98	0.45
1:A:492:VAL:HA	1:A:519:MET:O	2.17	0.45
1:A:805:ARG:HD2	1:A:1028:ALA:HB2	1.98	0.45
1:B:585:ALA:HA	1:B:611:ARG:O	2.17	0.45
1:A:586:LYS:O	1:A:610:GLU:HG3	2.17	0.45
1:B:617:GLU:HA	1:B:645:PHE:O	2.16	0.45
1:B:1227:LEU:HD12	1:B:1268:ILE:HG21	1.98	0.45
1:A:1286:ARG:HD2	1:A:1286:ARG:HA	1.74	0.45
1:B:819:ARG:HH21	1:B:819:ARG:HG3	1.81	0.45
1:B:492:VAL:HA	1:B:519:MET:O	2.16	0.45
1:B:821:ILE:HG13	1:B:1170:ILE:HG23	1.98	0.45
1:B:473:PRO:HG2	1:B:476:VAL:CG2	2.47	0.45
1:B:493:VAL:HG21	1:B:521:GLU:HG3	1.99	0.45
1:B:922:MET:SD	1:B:1013:ALA:HB2	2.57	0.45
1:B:1039:TYR:CE1	1:B:1131:GLN:HG3	2.52	0.45
3:D:5:A:C2'	3:D:6:C:H5'	2.47	0.45
1:A:590:TYR:CE2	2:C:2:DA:H2''	2.52	0.44
1:A:523:GLY:HA3	8:A:1643:HOH:O	2.17	0.44
1:A:1370:LEU:HD23	1:A:1370:LEU:N	2.30	0.44
1:B:916:ARG:HB3	1:B:1017:TRP:CD1	2.52	0.44
1:B:714:MET:HB2	1:B:718:VAL:HG21	2.00	0.44
1:A:661:THR:HA	1:A:1047:PHE:HB3	1.99	0.44
1:B:696:ASP:OD1	1:B:763:PRO:HD2	2.17	0.44
1:A:496:ALA:HB3	1:A:538:ILE:HG22	1.99	0.44
1:A:721:ARG:HG3	1:A:725:VAL:HG23	2.00	0.44
1:A:1270:PRO:O	1:A:1271:GLU:C	2.60	0.44
1:B:495:SER:OG	1:B:516:LYS:HB2	2.18	0.44
1:B:1082:LEU:HD21	1:B:1115:VAL:HG12	2.00	0.44
1:A:419:GLU:HG3	1:A:450:VAL:HG11	1.99	0.44
1:A:1123:VAL:HA	8:A:1629:HOH:O	2.18	0.44
1:A:553:VAL:O	1:A:557:GLN:HG2	2.18	0.43
1:A:1120:GLN:HB2	1:A:1122:ILE:HD12	1.99	0.43
3:J:2:C:H2'	3:J:3:C:C6	2.53	0.43
1:A:815:ALA:HB1	1:A:1020:GLU:HG2	2.00	0.43
1:B:422:ARG:HD2	1:B:515:LEU:O	2.18	0.43
1:B:618:THR:HA	1:B:622:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:MET:HE3	1:A:812:MET:HB2	1.86	0.43
1:A:519:MET:HE2	1:A:519:MET:HB2	1.76	0.43
1:A:1179:LEU:HD23	1:A:1179:LEU:HA	1.87	0.43
1:B:1310:PHE:O	1:B:1314:TYR:HB3	2.19	0.43
1:B:590:TYR:HA	1:B:608:ILE:HA	2.01	0.43
2:I:7:DT:H2'	2:I:8:DG:C8	2.54	0.43
1:A:401:ILE:HD12	1:A:567:TRP:CH2	2.54	0.43
1:A:475:ASP:OD1	1:A:475:ASP:N	2.49	0.43
1:A:687:PRO:HD3	1:A:778:ARG:NH1	2.34	0.43
1:B:1094:TYR:OH	1:B:1164:ASP:OD2	2.24	0.43
1:B:1264:LYS:O	1:B:1267:ALA:HB3	2.19	0.43
1:A:524:CYS:SG	1:A:527:THR:HG23	2.59	0.43
1:B:394:VAL:HG22	1:B:553:VAL:HG12	2.01	0.43
1:A:615:PHE:HB3	1:A:647:VAL:HG22	2.01	0.43
1:A:1094:TYR:CE2	1:A:1146:PRO:HA	2.54	0.43
1:A:1107:LEU:O	1:A:1111:VAL:HG22	2.19	0.43
1:B:493:VAL:HG21	1:B:521:GLU:CG	2.49	0.43
1:B:660:ASN:HA	1:B:662:TRP:NE1	2.34	0.42
1:B:679:THR:HB	1:B:781:GLU:HB3	2.00	0.42
1:B:813:ARG:HB2	8:B:1615:HOH:O	2.19	0.42
1:A:585:ALA:HA	1:A:611:ARG:O	2.19	0.42
1:B:847:GLU:OE2	1:B:1360:LYS:NZ	2.37	0.42
1:B:1198:PHE:CE2	1:B:1318:PRO:HG3	2.54	0.42
1:A:664:PRO:HA	1:A:1046:THR:HA	2.01	0.42
1:A:1303:LEU:HD22	1:A:1332:ILE:HG13	2.02	0.42
1:B:745:MET:HE3	1:B:745:MET:HB3	1.77	0.42
1:B:846:TYR:CZ	1:B:1357:MET:HE2	2.53	0.42
1:B:816:ILE:HD11	1:B:1021:ILE:HG12	2.00	0.42
1:B:1110:LEU:O	1:B:1114:LEU:HG	2.20	0.42
1:A:719:ALA:HA	1:A:722:ILE:HD12	2.00	0.42
1:B:618:THR:OG1	1:B:619:GLY:N	2.53	0.42
1:B:481:MET:HE3	1:B:481:MET:HB3	1.83	0.42
1:A:540:ILE:CG1	1:A:541:PRO:HD2	2.44	0.41
1:A:579:GLN:HB2	1:A:618:THR:HG23	2.02	0.41
1:A:1106:ILE:HD11	1:A:1137:LEU:HD23	2.02	0.41
1:B:1310:PHE:HA	1:B:1321:VAL:HG11	2.02	0.41
1:A:440:TYR:O	1:A:442:PRO:HD3	2.20	0.41
1:A:940:SER:HA	1:A:986:LYS:HD3	2.03	0.41
1:A:952:LEU:HD12	1:A:952:LEU:C	2.46	0.41
1:A:1084:MET:HE2	1:A:1084:MET:HB3	1.93	0.41
1:A:1133:ARG:HA	1:A:1137:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:HG2	1:B:515:LEU:HB2	2.03	0.41
1:B:1308:THR:O	1:B:1312:LEU:HG	2.21	0.41
1:B:439:LYS:HE3	1:B:439:LYS:HB2	1.73	0.41
1:A:772:PHE:O	1:A:778:ARG:HD3	2.20	0.41
1:B:639:VAL:CG2	1:B:640:GLU:N	2.84	0.41
1:A:541:PRO:HB3	1:A:607:ILE:HD12	2.03	0.41
1:A:809:LYS:H	1:A:809:LYS:HG2	1.65	0.41
1:A:1106:ILE:HD11	1:A:1137:LEU:HD21	2.02	0.41
1:B:819:ARG:HG3	1:B:819:ARG:NH2	2.35	0.41
1:B:1207:TYR:CE2	1:B:1311:LYS:HG2	2.56	0.41
1:B:492:VAL:HG22	1:B:520:PHE:CE1	2.56	0.40
1:B:719:ALA:HA	1:B:722:ILE:HD12	2.03	0.40
1:B:1036:LEU:HB2	1:B:1040:LEU:HD12	2.03	0.40
1:B:1094:TYR:CE2	1:B:1146:PRO:HA	2.56	0.40
1:A:790:LYS:HB3	1:A:790:LYS:HE2	1.71	0.40
1:A:1095:ILE:HD11	1:A:1144:PRO:HD2	2.03	0.40
1:B:711:VAL:HG21	1:B:923:ILE:HG23	2.01	0.40
1:B:1081:PHE:CD1	1:B:1084:MET:HE2	2.56	0.40
1:B:1339:ARG:HB3	1:B:1342:GLU:HG3	2.04	0.40
1:A:1228:LYS:HG2	1:A:1312:LEU:HD11	2.04	0.40
1:B:737:GLY:HA3	1:B:781:GLU:O	2.21	0.40
1:A:1094:TYR:HD1	1:A:1161:HIS:CD2	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	923/1026 (90%)	901 (98%)	22 (2%)	0	100	100
1	B	904/1026 (88%)	884 (98%)	20 (2%)	0	100	100
All	All	1827/2052 (89%)	1785 (98%)	42 (2%)	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	
1	A	772/894 (86%)	743 (96%)	29 (4%)	29	58
1	B	760/894 (85%)	732 (96%)	28 (4%)	30	59
All	All	1532/1788 (86%)	1475 (96%)	57 (4%)	30	59

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	411	GLU
1	A	431	LEU
1	A	446	THR
1	A	450	VAL
1	A	470	GLU
1	A	481	MET
1	A	484	ASN
1	A	520	PHE
1	A	545	SER
1	A	607	ILE
1	A	608	ILE
1	A	618	THR
1	A	743	LYS
1	A	809	LYS
1	A	810	VAL
1	A	811	LYS
1	A	812	MET
1	A	813	ARG
1	A	826	ARG
1	A	848	SER
1	A	854	THR
1	A	1058	SER
1	A	1177	LYS
1	A	1180	GLU
1	A	1212	GLU

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Mol	Chain	Res	Type
1	A	1217	SER
1	A	1220	SER
1	A	1305	ARG
1	A	1327	ARG
1	B	393	VAL
1	B	420	VAL
1	B	435	SER
1	B	439	LYS
1	B	446	THR
1	B	505	SER
1	B	514	LYS
1	B	621	THR
1	B	678	LYS
1	B	720	LYS
1	B	721	ARG
1	B	783	ARG
1	B	810	VAL
1	B	831	GLN
1	B	851	SER
1	B	852	ARG
1	B	899	GLN
1	B	901	ARG
1	B	911	ASN
1	B	1029	GLU
1	B	1102	LYS
1	B	1119	LYS
1	B	1120	GLN
1	B	1224	PHE
1	B	1237	GLU
1	B	1242	VAL
1	B	1284	VAL
1	B	1305	ARG

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

Mol	Chain	Res	Type
1	A	400	ASN
1	A	474	ASN
1	A	484	ASN
1	A	522	GLN
1	A	613	HIS
1	A	814	GLN

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Mol	Chain	Res	Type
1	A	827	GLN
1	A	843	GLN
1	A	888	GLN
1	A	899	GLN
1	A	1161	HIS
1	A	1183	HIS
1	A	1260	GLN
1	B	504	ASN
1	B	579	GLN
1	B	613	HIS
1	B	673	GLN
1	B	777	GLN
1	B	833	HIS
1	B	858	HIS
1	B	911	ASN
1	B	1113	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	6/7 (85%)	0	0
3	J	5/7 (71%)	1 (20%)	0
All	All	11/14 (78%)	1 (9%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	J	5	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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$
6	PEG	B	1501	-	6,6,6	0.39	0	5,5,5	0.62	0
5	ZAN	A	1504	4	32,33,33	1.70	9 (28%)	46,52,52	2.00	14 (30%)
5	ZAN	B	1504	4	32,33,33	1.00	4 (12%)	46,52,52	1.10	3 (6%)

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
6	PEG	B	1501	-	-	2/4/4/4	-
5	ZAN	A	1504	4	-	4/19/38/38	0/3/3/3
5	ZAN	B	1504	4	-	6/19/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1504	ZAN	C5-C4	4.66	1.47	1.39
5	A	1504	ZAN	PB-O2B	3.65	1.51	1.46
5	A	1504	ZAN	PA-O2A	3.47	1.51	1.46
5	B	1504	ZAN	PB-O2B	2.82	1.50	1.46
5	A	1504	ZAN	C5-C6	2.78	1.48	1.41
5	B	1504	ZAN	PA-O2A	2.66	1.50	1.46
5	B	1504	ZAN	PA-O1A	-2.42	1.50	1.56
5	B	1504	ZAN	PB-O1B	-2.39	1.50	1.56
5	A	1504	ZAN	PB-O3B	2.27	1.61	1.59
5	A	1504	ZAN	C8-N7	2.21	1.35	1.31
5	A	1504	ZAN	C5-N7	-2.14	1.35	1.39
5	A	1504	ZAN	PA-O1A	-2.07	1.51	1.56
5	A	1504	ZAN	C4-N9	-2.06	1.33	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1504	ZAN	C5-C4-N3	-5.50	119.14	126.72
5	A	1504	ZAN	O1A-PA-O2A	4.56	119.65	109.87
5	A	1504	ZAN	N3-C4-N9	4.53	134.87	127.17
5	A	1504	ZAN	O1B-PB-O2B	4.09	118.63	109.87
5	B	1504	ZAN	O1B-PB-O2B	4.08	118.61	109.87
5	B	1504	ZAN	O1A-PA-O2A	4.02	118.49	109.87
5	A	1504	ZAN	C2-N3-C4	3.52	120.44	111.83
5	B	1504	ZAN	O5'-PA-O2A	-3.39	104.21	114.27
5	A	1504	ZAN	C4-C5-N7	-3.38	106.72	110.58
5	A	1504	ZAN	N3-C2-N1	-3.17	123.78	128.58
5	A	1504	ZAN	C4-N9-C8	3.11	109.00	105.74
5	A	1504	ZAN	O5'-PA-O2A	-2.49	106.89	114.27
5	A	1504	ZAN	C5-N7-C8	2.44	107.29	103.45
5	A	1504	ZAN	C2'-C1'-N9	-2.22	107.78	113.30
5	A	1504	ZAN	O2G-PG-O1G	2.15	115.84	107.80
5	A	1504	ZAN	C6-C5-N7	2.08	136.10	132.09
5	A	1504	ZAN	N9-C8-N7	-2.06	111.01	113.94

There are no chirality outliers.

All (12) torsion outliers are listed below:

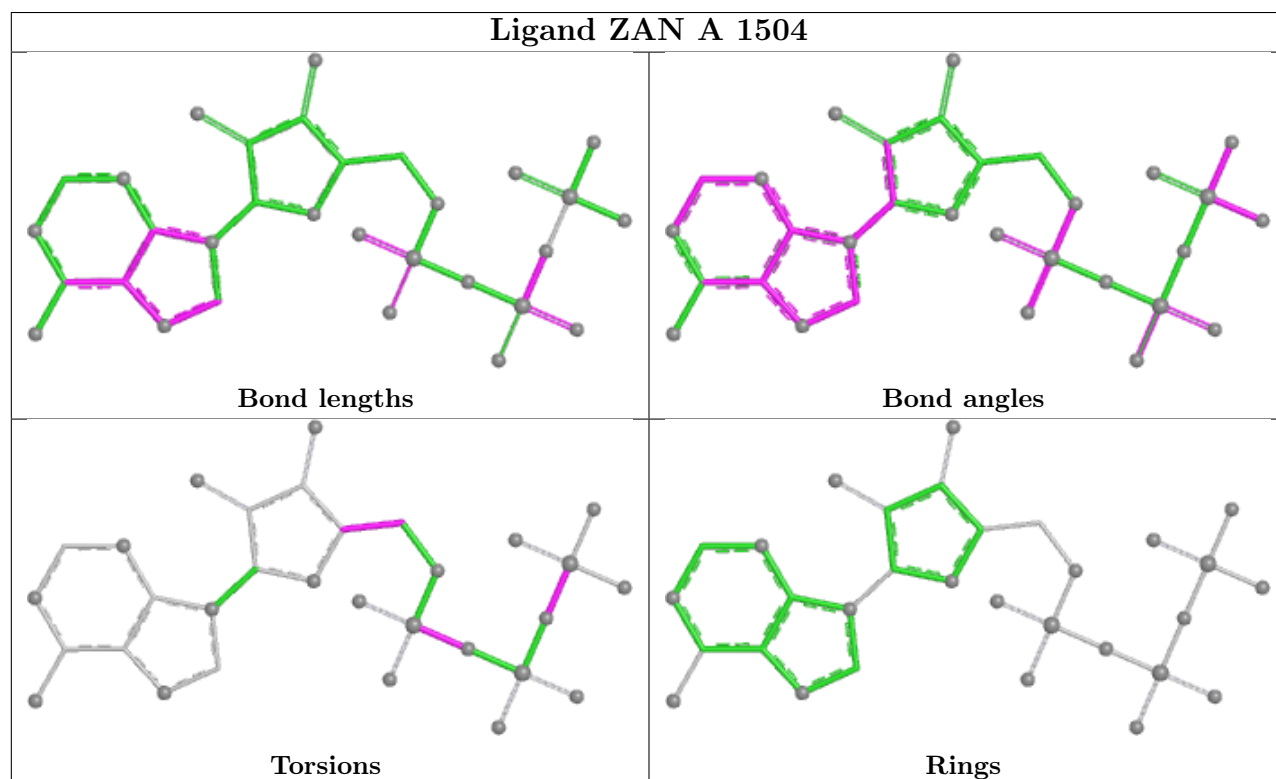
Mol	Chain	Res	Type	Atoms
5	A	1504	ZAN	PB-N3A-PA-O2A
5	B	1504	ZAN	PB-N3A-PA-O5'
5	B	1504	ZAN	PB-O3B-PG-O2G
5	A	1504	ZAN	C3'-C4'-C5'-O5'
5	B	1504	ZAN	C3'-C4'-C5'-O5'
5	A	1504	ZAN	O4'-C4'-C5'-O5'
5	B	1504	ZAN	O4'-C4'-C5'-O5'
6	B	1501	PEG	O1-C1-C2-O2
5	B	1504	ZAN	PB-O3B-PG-O1G
5	B	1504	ZAN	PB-O3B-PG-O3G
6	B	1501	PEG	C1-C2-O2-C3
5	A	1504	ZAN	PB-O3B-PG-O2G

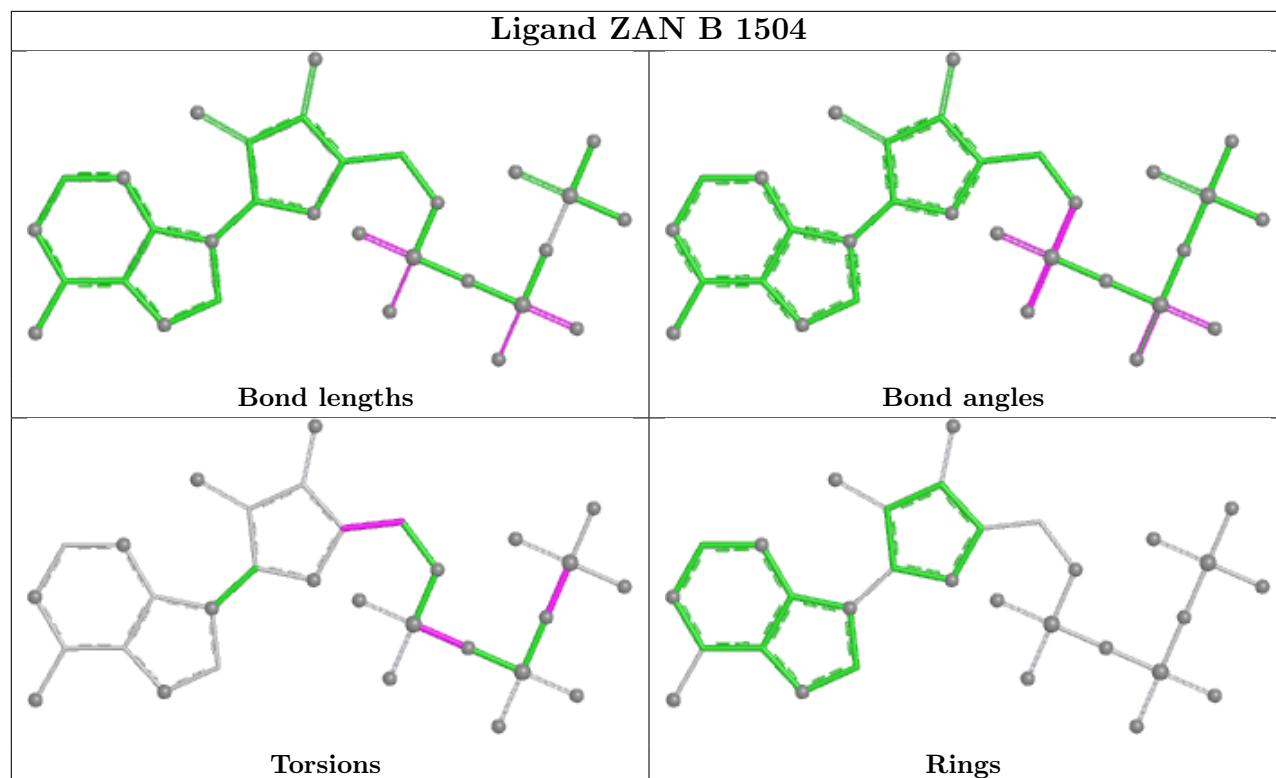
There are no ring outliers.

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	A	937/1026 (91%)	-0.03	7 (0%) 84 83	40, 74, 119, 177	0
1	B	920/1026 (89%)	-0.03	15 (1%) 70 68	39, 72, 118, 159	0
2	C	10/14 (71%)	-0.43	0 100 100	55, 64, 116, 147	0
2	I	14/14 (100%)	0.24	0 100 100	53, 75, 158, 167	2 (14%)
3	D	7/7 (100%)	-0.13	0 100 100	50, 72, 128, 148	0
3	J	6/7 (85%)	0.00	0 100 100	52, 79, 119, 153	0
All	All	1894/2094 (90%)	-0.03	22 (1%) 76 75	39, 73, 119, 177	2 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1315	HIS	3.5
1	B	849	TYR	3.3
1	B	460	LEU	3.1
1	A	1138	GLY	3.0
1	B	1181	ALA	2.9
1	A	1318	PRO	2.8
1	B	436	LEU	2.8
1	B	1252	ASP	2.7
1	A	1139	GLY	2.7
1	B	543	PRO	2.5
1	B	1370	LEU	2.5
1	A	1140	ALA	2.5
1	B	1244	ASN	2.4
1	B	871	GLN	2.4
1	A	390	HIS	2.3
1	B	1210	PHE	2.3
1	B	410	HIS	2.2
1	B	391	ALA	2.1
1	B	1363	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	910	LEU	2.1
1	B	605	LYS	2.0
1	A	1182	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

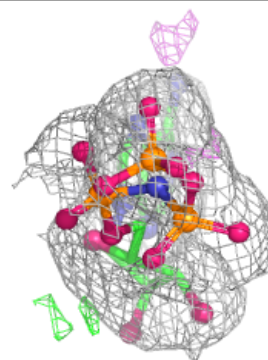
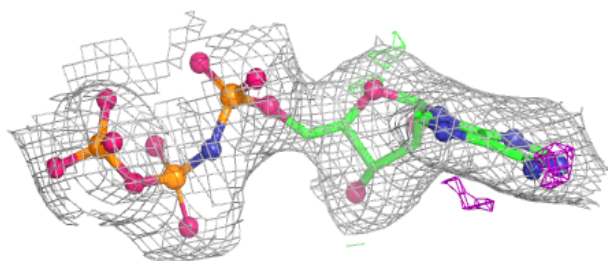
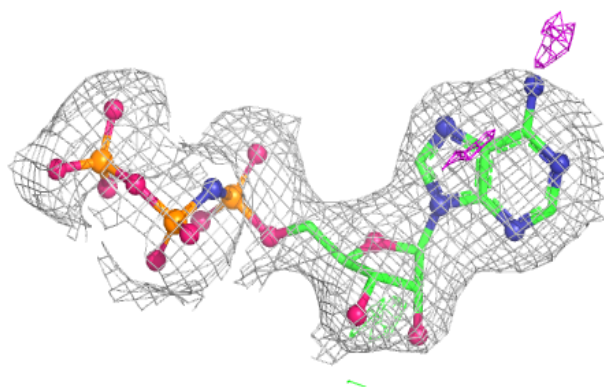
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	I	101	1/1	0.90	0.07	109,109,109,109	0
7	MG	B	1505	1/1	0.92	0.10	60,60,60,60	0
6	PEG	B	1501	7/7	0.94	0.10	75,90,102,102	0
4	CA	C	101	1/1	0.95	0.07	91,91,91,91	0
5	ZAN	B	1504	31/31	0.95	0.07	40,52,69,72	0
4	CA	A	1503	1/1	0.96	0.04	82,82,82,82	0
5	ZAN	A	1504	31/31	0.98	0.05	40,49,55,58	0
4	CA	A	1501	1/1	0.98	0.05	46,46,46,46	0
4	CA	B	1502	1/1	0.99	0.05	46,46,46,46	0
4	CA	B	1503	1/1	0.99	0.02	50,50,50,50	0
4	CA	A	1502	1/1	1.00	0.02	50,50,50,50	0

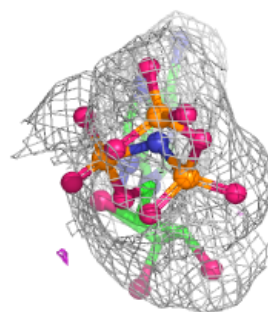
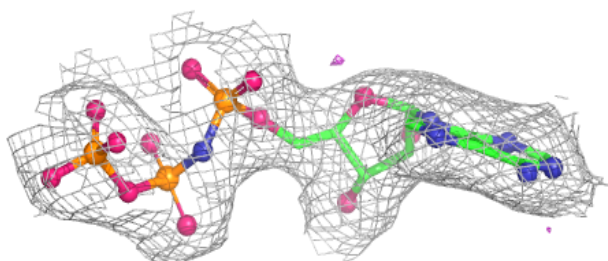
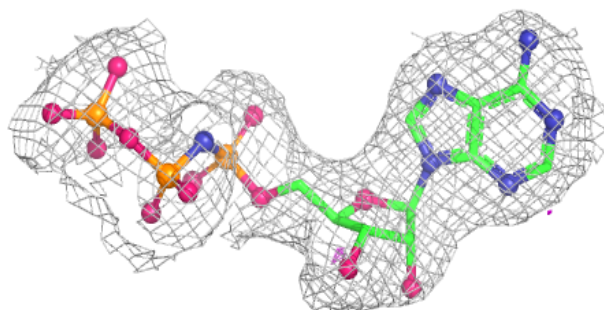
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZAN B 1504:

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

**Electron density around ZAN A 1504:**

$2mF_o-DF_c$ (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.