



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:01 PM UTC

PDB ID : 1N1H / pdb_00001n1h
Title : Initiation complex of polymerase lambda3 from reovirus
Authors : Tao, Y.; Farsetta, D.L.; Nibert, M.L.; Harrison, S.C.
Deposited on : 2002-10-17
Resolution : 2.80 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

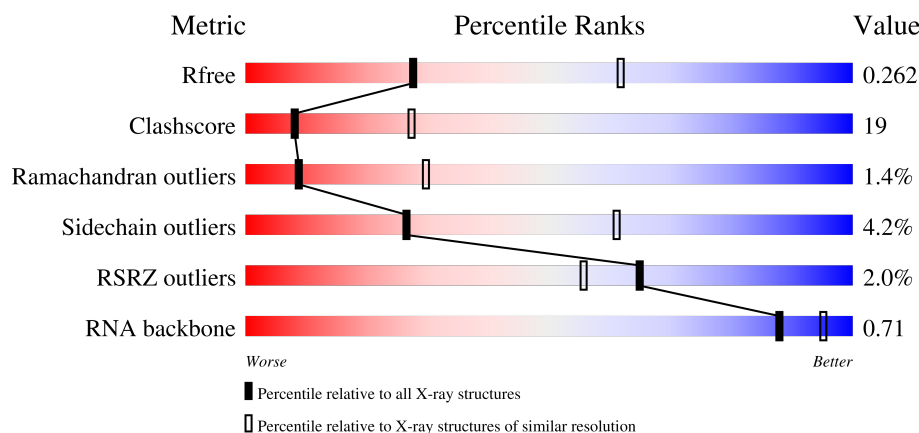
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

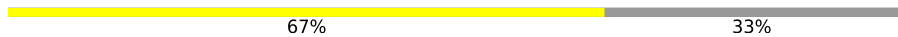
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	B	6	 67% 33%
2	A	1267	 2% 63% 34% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10367 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 5'-R(*AP*UP*UP*AP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			

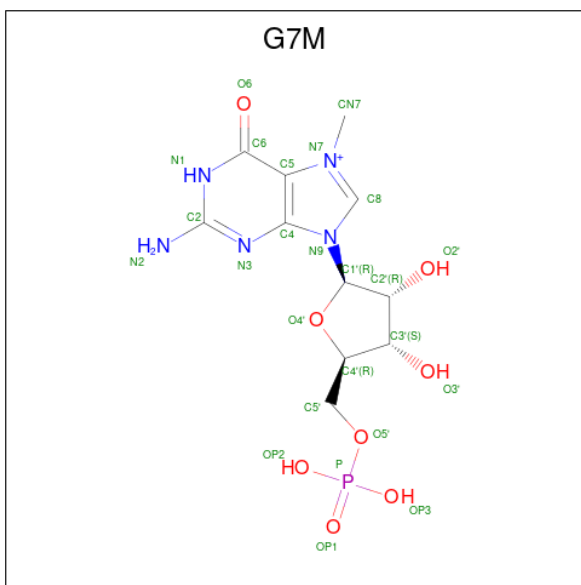
- Molecule 2 is a protein called Minor core protein lambda 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1264	Total	C	N	O	S	0	0	0
			9986	6369	1712	1841	64			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

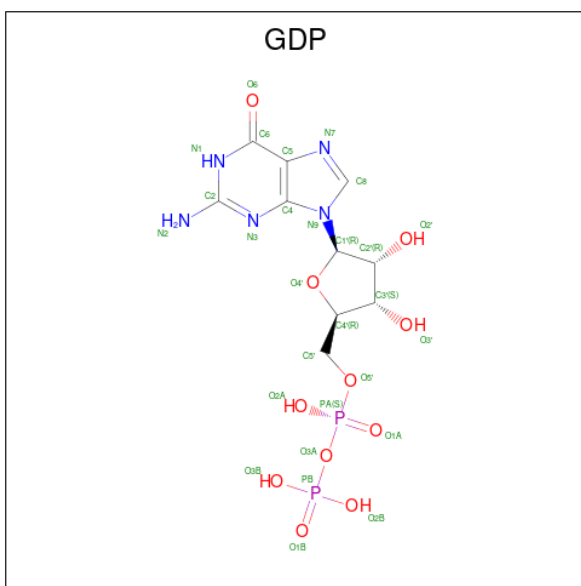
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is N7-METHYL-GUANOSINE-5'-MONOPHOSPHATE (CCD ID: G7M) (formula: C₁₁H₁₇N₅O₈P).



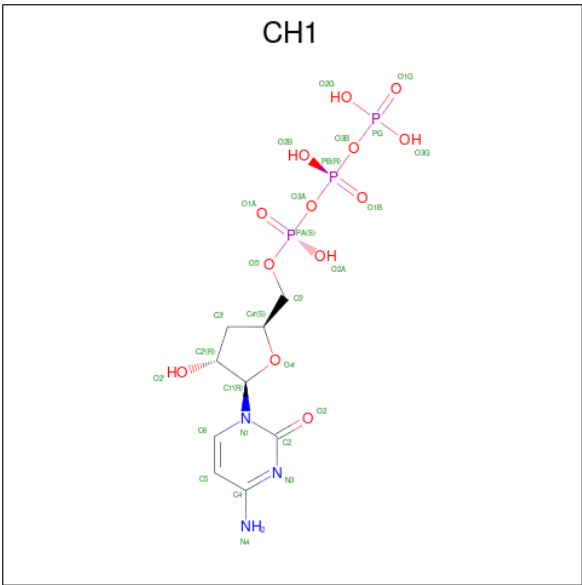
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	11	5	8	1		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CH1) (formula: $C_9H_{16}N_3O_{13}P_3$).

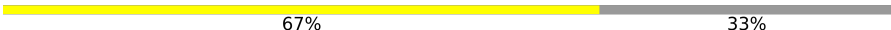


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	5	Total 5	O 5	0	0
8	A	178	Total 178	O 178	0	0

3 Residue-property plots [i](#)

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

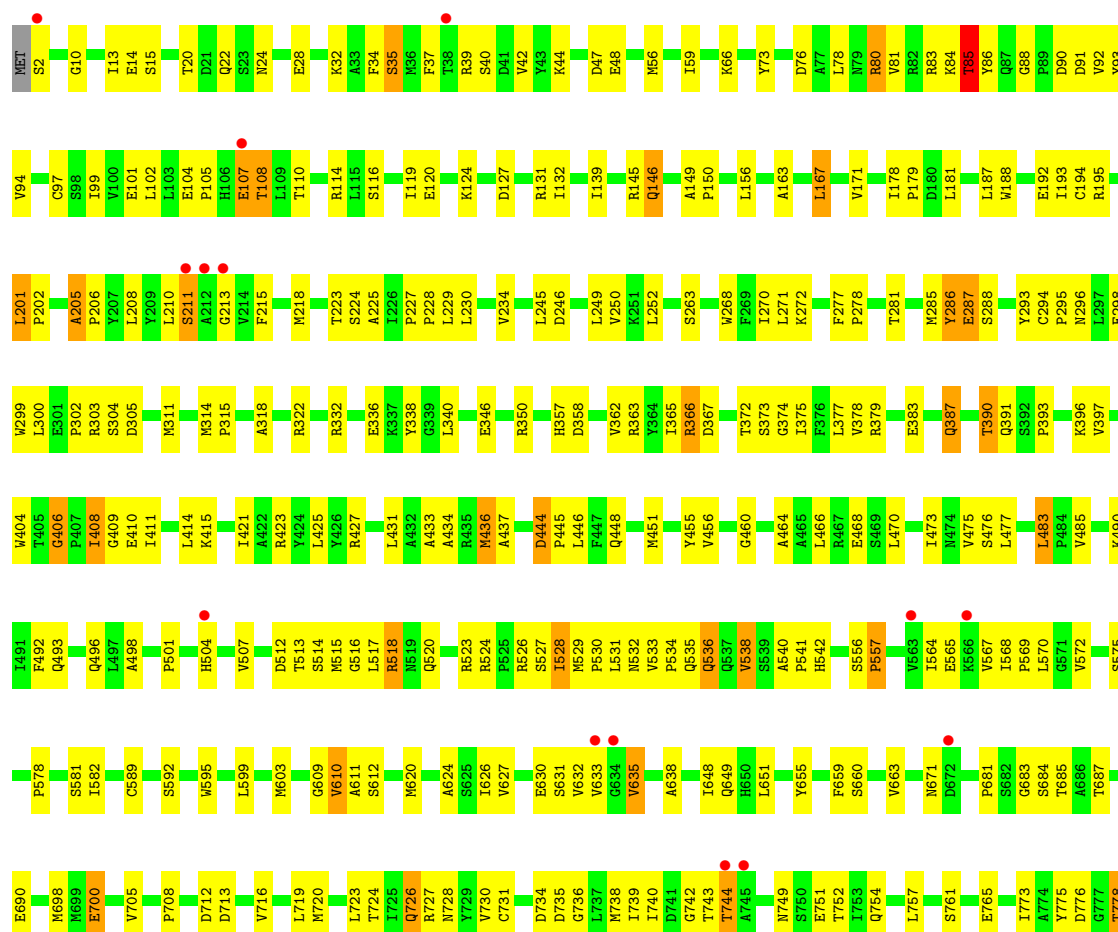
- Molecule 1: 5'-R(*AP*UP*UP*AP*GP*C)-3'

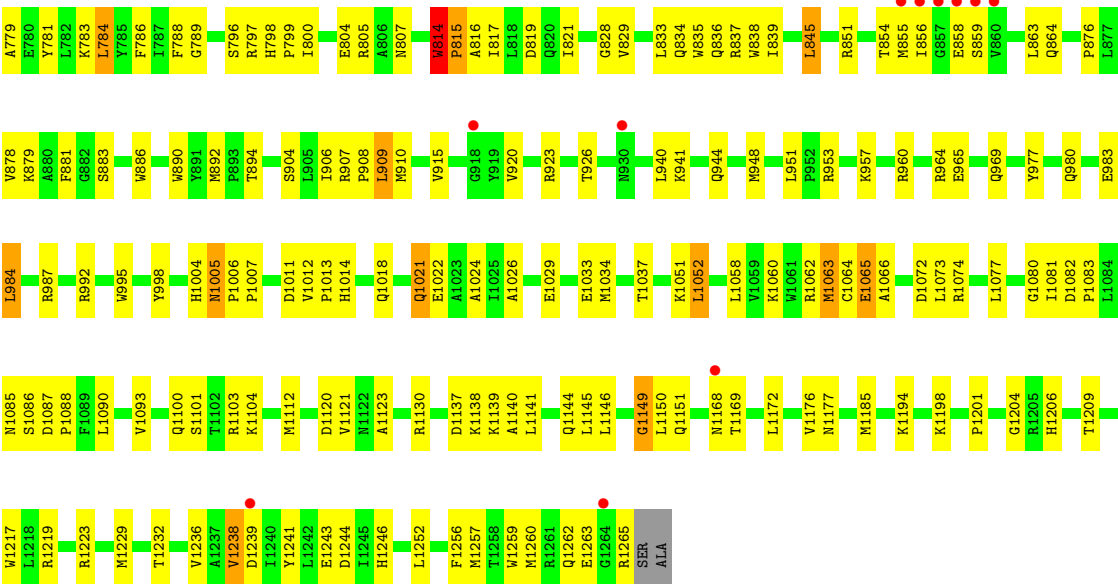
Chain B: 

A	U1283
U	A1284
	G1285
	C1286

- Molecule 2: Minor core protein lambda 3

Chain A: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.88Å 85.01Å 249.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 2.80 29.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	79.5 (29.71-2.80) 79.4 (29.71-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.268 0.206 , 0.262	Depositor DCC
R_{free} test set	2261 reflections (5.91%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10367	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: GH3, MN, CH1, GDP, G7M

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	B	0.54	0/94	0.60	0/144
2	A	0.47	0/10239	0.97	37/13905 (0.3%)
All	All	0.47	0/10333	0.97	37/14049 (0.3%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1194	LYS	N-CA-C	7.69	119.74	111.36
2	A	611	ALA	N-CA-C	7.30	119.93	111.02
2	A	211	SER	N-CA-C	-6.90	104.50	113.12
2	A	286	TYR	N-CA-C	6.75	120.86	111.74
2	A	287	GLU	N-CA-C	-6.70	104.21	112.38
2	A	85	THR	N-CA-C	6.52	119.93	110.28
2	A	1244	ASP	N-CA-C	6.36	118.81	108.76
2	A	612	SER	N-CA-C	6.34	119.17	111.82
2	A	406	GLY	N-CA-C	-6.26	104.41	112.10
2	A	181	LEU	N-CA-C	6.22	118.87	111.71
2	A	205	ALA	CA-C-N	6.16	125.78	119.56
2	A	205	ALA	C-N-CA	6.16	125.78	119.56
2	A	1149	GLY	N-CA-C	6.13	123.23	114.64
2	A	835	TRP	N-CA-C	5.96	118.29	111.02
2	A	408	ILE	N-CA-C	-5.93	97.00	109.34
2	A	59	ILE	CA-C-N	5.90	126.45	120.38
2	A	59	ILE	C-N-CA	5.90	126.45	120.38
2	A	201	LEU	CA-C-N	5.89	125.76	119.28
2	A	201	LEU	C-N-CA	5.89	125.76	119.28
2	A	1086	SER	N-CA-C	5.85	123.26	110.80
2	A	556	SER	N-CA-C	5.80	117.60	108.55
2	A	663	VAL	N-CA-C	5.65	115.74	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	814	TRP	N-CA-C	5.59	122.16	109.81
2	A	397	VAL	CA-C-N	5.52	125.83	119.92
2	A	397	VAL	C-N-CA	5.52	125.83	119.92
2	A	1080	GLY	N-CA-C	-5.52	107.34	113.79
2	A	624	ALA	N-CA-C	-5.43	103.52	110.53
2	A	784	LEU	N-CA-C	-5.39	100.39	109.07
2	A	88	GLY	CA-C-N	5.37	125.69	119.47
2	A	88	GLY	C-N-CA	5.37	125.69	119.47
2	A	444	ASP	CA-C-N	5.18	125.48	119.47
2	A	444	ASP	C-N-CA	5.18	125.48	119.47
2	A	483	LEU	CA-C-N	5.14	126.27	119.84
2	A	483	LEU	C-N-CA	5.14	126.27	119.84
2	A	739	ILE	N-CA-C	5.11	115.12	107.51
2	A	744	THR	N-CA-C	-5.04	105.88	112.23
2	A	1177	ASN	N-CA-C	5.03	118.67	112.24

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	B	85	0	44	7	0
2	A	9986	0	9903	391	0
3	A	2	0	0	0	0
4	A	25	0	14	0	0
5	A	27	0	12	2	0
6	A	28	0	12	0	0
7	A	31	0	12	0	0
8	A	178	0	0	27	0
8	B	5	0	0	3	0
All	All	10367	0	9997	393	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 19.

All (393) 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)
2:A:743:THR:HG22	2:A:744:THR:H	1.17	1.04
2:A:223:THR:HG22	2:A:225:ALA:H	1.21	1.01
2:A:1005:ASN:HD21	2:A:1263:GLU:HB3	1.23	1.00
2:A:410:GLU:H	2:A:649:GLN:NE2	1.61	0.98
2:A:724:THR:HG22	2:A:726:GLN:H	1.26	0.95
2:A:22:GLN:NE2	2:A:878:VAL:H	1.64	0.93
2:A:1085:ASN:HB2	8:A:1590:HOH:O	1.66	0.93
2:A:542:HIS:NE2	2:A:690:GLU:HG3	1.87	0.89
8:B:1454:HOH:O	2:A:514:SER:HB2	1.72	0.88
2:A:856:ILE:HB	2:A:859:SER:HB2	1.56	0.87
2:A:907:ARG:HB3	2:A:908:PRO:HD3	1.57	0.86
2:A:776:ASP:OD1	2:A:778:THR:HB	1.75	0.86
2:A:1112:MET:HE1	2:A:1150:LEU:HD11	1.57	0.84
2:A:104:GLU:HG3	2:A:116:SER:HA	1.60	0.84
2:A:81:VAL:H	2:A:671:ASN:HD21	1.26	0.83
2:A:78:LEU:HD12	2:A:80:ARG:NH2	1.92	0.83
2:A:743:THR:HG22	2:A:744:THR:N	1.94	0.82
2:A:855:MET:HE1	2:A:858:GLU:H	1.44	0.81
2:A:410:GLU:H	2:A:649:GLN:HE22	1.29	0.80
2:A:779:ALA:HB3	2:A:786:PHE:HB2	1.65	0.78
2:A:425:LEU:HD13	2:A:698:MET:HE3	1.66	0.78
2:A:736:GLY:HA2	8:A:1564:HOH:O	1.84	0.77
2:A:146:GLN:HE22	2:A:805:ARG:H	1.33	0.76
2:A:749:ASN:HD21	2:A:751:GLU:HB3	1.50	0.76
2:A:451:MET:HE2	2:A:451:MET:HA	1.65	0.75
2:A:520:GLN:NE2	2:A:523:ARG:HD3	2.03	0.72
2:A:1145:LEU:HB3	2:A:1150:LEU:HD22	1.72	0.72
2:A:1004:HIS:C	2:A:1006:PRO:HD3	2.15	0.72
2:A:603:MET:HE1	2:A:651:LEU:HD23	1.71	0.71
2:A:743:THR:CG2	2:A:744:THR:H	1.99	0.71
2:A:716:VAL:HG12	2:A:720:MET:HE3	1.72	0.71
2:A:957:LYS:HE3	2:A:1026:ALA:HB2	1.73	0.71
2:A:39:ARG:HH11	2:A:39:ARG:HG2	1.55	0.70
2:A:724:THR:HG22	2:A:726:GLN:N	2.05	0.70
2:A:944:GLN:HB3	2:A:948:MET:HE2	1.72	0.70
2:A:1090:LEU:HB2	8:A:1545:HOH:O	1.91	0.70
2:A:532:ASN:OD1	2:A:535:GLN:HG3	1.92	0.69
2:A:781:TYR:CE1	8:A:1564:HOH:O	2.46	0.69
2:A:105:PRO:HG3	2:A:218:MET:HE2	1.74	0.68
2:A:520:GLN:NE2	2:A:526:ARG:NH1	2.41	0.68
2:A:851:ARG:HH11	2:A:864:GLN:HE21	1.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:536:GLN:HE22	2:A:685:THR:H	1.41	0.68
2:A:298:GLU:HB2	2:A:311:MET:HE2	1.74	0.67
2:A:1058:LEU:HD13	8:A:1434:HOH:O	1.93	0.67
2:A:821:ILE:HD12	2:A:845:LEU:HD13	1.77	0.67
2:A:39:ARG:HE	2:A:208:LEU:HD22	1.60	0.67
2:A:829:VAL:HG13	2:A:890:TRP:CE2	2.29	0.67
2:A:92:VAL:CG1	2:A:383:GLU:HB3	2.24	0.67
2:A:227:PRO:HB2	2:A:228:PRO:HD3	1.77	0.67
2:A:1087:ASP:HA	8:A:1545:HOH:O	1.93	0.67
2:A:193:ILE:HD13	2:A:229:LEU:HD21	1.77	0.66
2:A:536:GLN:HA	2:A:536:GLN:HE21	1.60	0.66
2:A:783:LYS:HG3	2:A:797:ARG:NH1	2.11	0.66
2:A:363:ARG:NH2	8:A:1590:HOH:O	2.24	0.66
2:A:66:LYS:HB3	2:A:97:CYS:HA	1.78	0.65
2:A:411:ILE:C	2:A:411:ILE:HD12	2.21	0.65
2:A:410:GLU:N	2:A:649:GLN:NE2	2.41	0.65
2:A:314:MET:HE3	2:A:315:PRO:HD2	1.79	0.65
2:A:90:ASP:HB3	8:A:1569:HOH:O	1.95	0.65
2:A:1262:GLN:HG2	2:A:1265:ARG:NH1	2.12	0.65
2:A:171:VAL:HG11	2:A:1090:LEU:HD11	1.79	0.65
2:A:296:ASN:ND2	2:A:311:MET:HB2	2.12	0.65
2:A:298:GLU:HB2	2:A:311:MET:CE	2.26	0.64
2:A:436:MET:HE2	2:A:437:ALA:HA	1.79	0.64
2:A:406:GLY:HA3	2:A:630:GLU:O	1.99	0.63
2:A:532:ASN:OD1	2:A:534:PRO:HD2	1.98	0.63
2:A:246:ASP:O	2:A:250:VAL:HG23	1.98	0.63
2:A:285:MET:HG3	2:A:365:ILE:HD11	1.79	0.63
2:A:90:ASP:O	2:A:92:VAL:N	2.32	0.63
2:A:814:TRP:O	2:A:815:PRO:C	2.41	0.63
2:A:957:LYS:HE2	2:A:1024:ALA:O	1.99	0.63
2:A:393:PRO:HG3	2:A:592:SER:HA	1.79	0.63
2:A:540:ALA:HB3	2:A:541:PRO:HD3	1.81	0.63
2:A:22:GLN:HE22	2:A:878:VAL:H	1.41	0.62
2:A:396:LYS:HD2	2:A:765:GLU:HB3	1.79	0.62
2:A:408:ILE:HB	2:A:411:ILE:HD11	1.81	0.62
2:A:1219:ARG:O	2:A:1223:ARG:HG3	1.99	0.62
2:A:731:CYS:HA	8:A:1564:HOH:O	1.99	0.62
2:A:22:GLN:HE21	2:A:878:VAL:H	1.44	0.61
2:A:564:ILE:HG13	2:A:565:GLU:HG2	1.81	0.61
2:A:194:CYS:SG	2:A:206:PRO:HG2	2.40	0.61
2:A:1007:PRO:HD2	2:A:1144:GLN:NE2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1005:ASN:N	2:A:1006:PRO:HD3	2.16	0.61
2:A:101:GLU:HG2	2:A:102:LEU:HG	1.82	0.60
2:A:1065:GLU:H	2:A:1065:GLU:CD	2.08	0.60
2:A:965:GLU:O	2:A:969:GLN:HG3	2.02	0.60
2:A:944:GLN:HB3	2:A:948:MET:CE	2.31	0.60
2:A:1005:ASN:HB2	2:A:1130:ARG:HH22	1.67	0.60
2:A:716:VAL:HG12	2:A:720:MET:CE	2.32	0.59
2:A:293:TYR:CZ	2:A:1074:ARG:NH2	2.70	0.59
2:A:1206:HIS:HB2	2:A:1209:THR:OG1	2.03	0.59
2:A:1112:MET:CE	2:A:1150:LEU:HD11	2.29	0.59
2:A:995:TRP:CZ2	2:A:1006:PRO:HG3	2.38	0.59
2:A:76:ASP:OD2	2:A:80:ARG:HG3	2.03	0.59
2:A:926:THR:HG21	2:A:1246:HIS:CG	2.38	0.59
2:A:223:THR:HG21	8:A:1582:HOH:O	2.02	0.58
2:A:572:VAL:HG13	2:A:789:GLY:O	2.03	0.58
2:A:819:ASP:OD1	2:A:953:ARG:NH1	2.36	0.58
2:A:81:VAL:N	2:A:671:ASN:HD21	1.97	0.58
2:A:754:GLN:HE21	2:A:775:TYR:HD2	1.51	0.57
2:A:582:ILE:HG21	2:A:757:LEU:CD2	2.34	0.57
2:A:957:LYS:HD2	2:A:957:LYS:N	2.19	0.57
2:A:1005:ASN:ND2	2:A:1263:GLU:HB3	2.07	0.57
2:A:84:LYS:HD2	2:A:86:TYR:CZ	2.40	0.57
2:A:1201:PRO:HB2	2:A:1204:GLY:O	2.05	0.57
2:A:1246:HIS:HB3	8:A:1434:HOH:O	2.05	0.56
2:A:107:GLU:O	2:A:108:THR:CB	2.53	0.56
2:A:814:TRP:HB3	2:A:815:PRO:HD3	1.88	0.56
2:A:1120:ASP:HB3	2:A:1123:ALA:HB2	1.87	0.56
2:A:114:ARG:HG3	2:A:114:ARG:HH11	1.71	0.56
2:A:541:PRO:HB2	2:A:648:ILE:HD11	1.87	0.56
2:A:56:MET:HG2	2:A:188:TRP:CE2	2.41	0.55
2:A:92:VAL:HG11	2:A:383:GLU:HB3	1.88	0.55
2:A:854:THR:HG21	2:A:863:LEU:HG	1.87	0.55
2:A:80:ARG:HA	2:A:671:ASN:ND2	2.20	0.55
2:A:363:ARG:HH22	2:A:834:GLN:HE22	1.53	0.55
2:A:926:THR:CG2	2:A:1246:HIS:CG	2.89	0.55
2:A:1029:GLU:N	2:A:1029:GLU:OE1	2.37	0.55
2:A:433:ALA:HB1	2:A:610:VAL:HG23	1.88	0.55
2:A:1007:PRO:HD2	2:A:1144:GLN:CD	2.32	0.55
2:A:523:ARG:HG2	2:A:523:ARG:HH11	1.70	0.55
2:A:1085:ASN:O	2:A:1088:PRO:HD2	2.07	0.55
2:A:188:TRP:CZ2	2:A:192:GLU:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:907:ARG:HH12	2:A:1060:LYS:HE3	1.72	0.54
2:A:1072:ASP:OD1	2:A:1074:ARG:HD3	2.07	0.54
2:A:477:LEU:HB3	2:A:496:GLN:HB3	1.88	0.54
2:A:520:GLN:CD	2:A:526:ARG:HH12	2.15	0.54
2:A:408:ILE:HB	2:A:411:ILE:CD1	2.38	0.54
2:A:94:VAL:HG22	2:A:139:ILE:HG23	1.90	0.54
2:A:446:LEU:HD13	2:A:1149:GLY:HA3	1.90	0.54
8:B:1454:HOH:O	2:A:530:PRO:HB2	2.08	0.54
2:A:727:ARG:HD3	8:A:1562:HOH:O	2.07	0.54
2:A:814:TRP:O	2:A:816:ALA:N	2.41	0.54
2:A:409:GLY:HA3	2:A:649:GLN:NE2	2.23	0.54
2:A:998:TYR:CE2	2:A:1139:LYS:HD3	2.42	0.53
2:A:724:THR:H	2:A:728:ASN:HD22	1.56	0.53
2:A:83:ARG:HG3	2:A:83:ARG:HH11	1.73	0.53
2:A:564:ILE:HG13	2:A:565:GLU:CG	2.38	0.53
2:A:104:GLU:CG	2:A:116:SER:HA	2.34	0.53
2:A:393:PRO:CG	2:A:592:SER:HA	2.38	0.53
2:A:836:GLN:HG2	2:A:886:TRP:CE3	2.44	0.53
2:A:127:ASP:O	2:A:131:ARG:HG3	2.09	0.52
2:A:47:ASP:OD1	2:A:195:ARG:NH2	2.34	0.52
2:A:24:ASN:O	2:A:28:GLU:HG3	2.09	0.52
2:A:167:LEU:HD23	2:A:837:ARG:HD2	1.90	0.52
2:A:299:TRP:CD2	2:A:303:ARG:HG2	2.45	0.52
2:A:473:ILE:HG21	2:A:507:VAL:HG11	1.90	0.52
2:A:599:LEU:O	2:A:603:MET:HG2	2.09	0.52
1:B:1285:G:O6	2:A:518:ARG:HD2	2.09	0.52
2:A:578:PRO:HB2	2:A:742:GLY:HA3	1.92	0.52
2:A:907:ARG:CB	2:A:908:PRO:HD3	2.37	0.52
2:A:42:VAL:HG22	2:A:156:LEU:HD13	1.92	0.52
2:A:76:ASP:OD2	2:A:80:ARG:NH1	2.43	0.52
2:A:295:PRO:HD2	2:A:789:GLY:HA3	1.91	0.52
2:A:1172:LEU:HD21	2:A:1217:TRP:HA	1.91	0.52
2:A:1012:VAL:HB	2:A:1013:PRO:HD3	1.90	0.52
2:A:35:SER:HB3	5:A:1425:GDP:N7	2.25	0.52
2:A:736:GLY:CA	8:A:1564:HOH:O	2.53	0.51
2:A:149:ALA:HB1	2:A:150:PRO:CD	2.41	0.51
2:A:536:GLN:NE2	2:A:685:THR:HG23	2.25	0.51
2:A:926:THR:HG23	2:A:1246:HIS:CD2	2.45	0.51
2:A:271:LEU:HD23	8:A:1569:HOH:O	2.09	0.51
2:A:1120:ASP:HB3	2:A:1123:ALA:CB	2.41	0.51
2:A:314:MET:CE	2:A:315:PRO:HD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:338:TYR:O	2:A:340:LEU:HG	2.11	0.51
2:A:374:GLY:O	2:A:799:PRO:HG2	2.10	0.51
2:A:423:ARG:O	2:A:427:ARG:HG3	2.10	0.51
2:A:1100:GLN:HG3	2:A:1101:SER:N	2.25	0.50
2:A:1201:PRO:HG3	2:A:1209:THR:HG21	1.93	0.50
2:A:13:ILE:HD13	2:A:163:ALA:HB3	1.93	0.50
2:A:304:SER:O	2:A:1104:LYS:HE3	2.10	0.50
2:A:659:PHE:CZ	2:A:681:PRO:CG	2.93	0.50
2:A:749:ASN:ND2	2:A:752:THR:H	2.10	0.50
2:A:32:LYS:HG3	5:A:1425:GDP:O6	2.12	0.50
2:A:409:GLY:HA3	2:A:627:VAL:HG21	1.93	0.50
2:A:520:GLN:HE22	2:A:523:ARG:HD3	1.76	0.50
2:A:632:VAL:HB	2:A:635:VAL:HB	1.93	0.50
2:A:107:GLU:O	2:A:108:THR:HB	2.11	0.50
2:A:892:MET:HB2	2:A:1232:THR:HG23	1.93	0.50
2:A:411:ILE:HD12	2:A:411:ILE:O	2.12	0.50
2:A:513:THR:HG21	2:A:529:MET:HG2	1.94	0.50
2:A:757:LEU:HD22	2:A:773:ILE:HG21	1.94	0.50
2:A:1081:ILE:HD12	2:A:1088:PRO:CB	2.41	0.50
2:A:358:ASP:O	2:A:362:VAL:HG22	2.11	0.49
1:B:1286:C:H6	1:B:1286:C:O5'	1.95	0.49
2:A:208:LEU:CB	2:A:210:LEU:HD21	2.42	0.49
2:A:410:GLU:H	2:A:649:GLN:HE21	1.50	0.49
2:A:828:GLY:HA3	2:A:838:TRP:NE1	2.27	0.49
1:B:1285:G:H5''	2:A:460:GLY:N	2.28	0.49
2:A:83:ARG:HG2	2:A:92:VAL:HA	1.93	0.49
2:A:294:CYS:SG	2:A:314:MET:HB3	2.53	0.49
2:A:448:GLN:NE2	2:A:620:MET:H	2.11	0.49
2:A:839:ILE:HD13	2:A:876:PRO:HG2	1.95	0.49
2:A:904:SER:HB3	2:A:1229:MET:SD	2.53	0.49
2:A:436:MET:HE2	2:A:436:MET:C	2.38	0.49
2:A:538:VAL:HG13	2:A:651:LEU:HB2	1.94	0.49
2:A:582:ILE:HG21	2:A:757:LEU:HD21	1.94	0.49
2:A:1005:ASN:HD21	2:A:1263:GLU:CB	2.11	0.49
2:A:299:TRP:CE2	2:A:303:ARG:HG2	2.48	0.49
2:A:446:LEU:HD22	2:A:1149:GLY:C	2.38	0.49
2:A:797:ARG:C	2:A:799:PRO:HD3	2.38	0.49
2:A:114:ARG:HB2	2:A:215:PHE:CE1	2.48	0.49
2:A:581:SER:HA	2:A:738:MET:O	2.11	0.49
2:A:1052:LEU:HD22	2:A:1259:TRP:CE2	2.48	0.48
2:A:523:ARG:HG2	2:A:523:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:856:ILE:O	2:A:856:ILE:HG22	2.13	0.48
2:A:1082:ASP:HB2	2:A:1083:PRO:HD2	1.95	0.48
2:A:377:LEU:N	2:A:377:LEU:HD12	2.28	0.48
2:A:740:ILE:HD12	2:A:740:ILE:N	2.29	0.48
2:A:568:ILE:N	2:A:569:PRO:CD	2.76	0.48
2:A:800:ILE:HG13	8:A:1519:HOH:O	2.13	0.48
2:A:1064:CYS:HB3	2:A:1065:GLU:OE2	2.14	0.48
8:B:1563:HOH:O	2:A:515:MET:HB3	2.14	0.48
2:A:501:PRO:HD2	2:A:504:HIS:HD2	1.77	0.48
2:A:603:MET:HE3	2:A:648:ILE:HG23	1.96	0.48
2:A:39:ARG:HG2	2:A:39:ARG:NH1	2.27	0.48
2:A:314:MET:HE3	2:A:315:PRO:CD	2.44	0.48
2:A:455:TYR:O	2:A:490:LYS:HE2	2.13	0.48
2:A:1169:THR:HB	8:A:1594:HOH:O	2.12	0.48
2:A:915:VAL:HG13	2:A:920:VAL:HG22	1.96	0.48
2:A:208:LEU:HB3	2:A:210:LEU:HD21	1.94	0.47
2:A:436:MET:HE2	2:A:437:ALA:CA	2.43	0.47
2:A:1073:LEU:HG	2:A:1093:VAL:HG11	1.96	0.47
2:A:1052:LEU:HD11	2:A:1176:VAL:HG23	1.97	0.47
2:A:517:LEU:HD23	2:A:527:SER:HA	1.96	0.47
2:A:940:LEU:O	2:A:941:LYS:HB2	2.14	0.47
2:A:1082:ASP:HB2	2:A:1083:PRO:CD	2.44	0.47
2:A:93:TYR:HE2	8:A:1569:HOH:O	1.97	0.47
2:A:223:THR:HG22	2:A:225:ALA:N	2.06	0.47
2:A:473:ILE:HG13	2:A:475:VAL:HG23	1.95	0.47
2:A:523:ARG:HG2	2:A:524:ARG:N	2.29	0.47
2:A:1198:LYS:HG2	2:A:1241:TYR:CE1	2.50	0.47
2:A:271:LEU:HD13	2:A:377:LEU:CD2	2.43	0.47
2:A:277:PHE:HB2	2:A:278:PRO:HD3	1.95	0.47
2:A:659:PHE:CZ	2:A:681:PRO:HG3	2.48	0.47
2:A:1051:LYS:NZ	2:A:1262:GLN:OE1	2.48	0.47
2:A:146:GLN:NE2	2:A:805:ARG:H	2.08	0.47
2:A:881:PHE:O	2:A:909:LEU:HD12	2.15	0.47
2:A:957:LYS:HD3	2:A:1022:GLU:HA	1.96	0.47
2:A:1014:HIS:O	2:A:1018:GLN:HG3	2.16	0.47
2:A:1257:MET:HA	2:A:1260:MET:HE3	1.97	0.47
2:A:434:ALA:HA	2:A:609:GLY:O	2.15	0.46
2:A:286:TYR:C	2:A:288:SER:N	2.68	0.46
2:A:366:ARG:NH1	2:A:367:ASP:OD1	2.45	0.46
2:A:425:LEU:HD13	2:A:698:MET:CE	2.41	0.46
2:A:1066:ALA:HB1	2:A:1236:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1081:ILE:HD12	2:A:1088:PRO:HB2	1.97	0.46
2:A:39:ARG:NE	2:A:208:LEU:HD22	2.29	0.46
2:A:582:ILE:HG21	2:A:757:LEU:HD22	1.96	0.46
2:A:211:SER:C	2:A:213:GLY:H	2.23	0.46
2:A:314:MET:HE3	2:A:314:MET:HA	1.98	0.46
2:A:520:GLN:NE2	2:A:526:ARG:HH12	2.14	0.46
2:A:114:ARG:HG3	2:A:114:ARG:NH1	2.30	0.46
2:A:520:GLN:CD	2:A:526:ARG:NH1	2.74	0.46
2:A:73:TYR:HB2	2:A:132:ILE:HG23	1.98	0.46
2:A:295:PRO:HD3	8:A:1432:HOH:O	2.16	0.46
2:A:531:LEU:HD11	2:A:684:SER:HB2	1.97	0.46
2:A:1198:LYS:N	2:A:1198:LYS:HD2	2.31	0.46
2:A:1263:GLU:HA	2:A:1263:GLU:OE2	2.16	0.46
2:A:73:TYR:HB3	2:A:132:ILE:HD12	1.97	0.45
2:A:856:ILE:HB	2:A:859:SER:CB	2.38	0.45
2:A:281:THR:O	2:A:285:MET:HG2	2.16	0.45
2:A:39:ARG:HH11	2:A:39:ARG:CG	2.27	0.45
2:A:425:LEU:HB2	2:A:698:MET:HE1	1.97	0.45
1:B:1285:G:C5	2:A:528:ILE:HG12	2.51	0.45
2:A:83:ARG:HG3	2:A:83:ARG:NH1	2.31	0.45
2:A:245:LEU:HA	2:A:367:ASP:OD2	2.15	0.45
2:A:379:ARG:HH12	2:A:387:GLN:NE2	2.13	0.45
2:A:542:HIS:NE2	2:A:690:GLU:CG	2.69	0.45
2:A:659:PHE:CZ	2:A:681:PRO:HG2	2.52	0.45
2:A:80:ARG:HA	2:A:671:ASN:HD21	1.82	0.45
2:A:700:GLU:OE2	2:A:700:GLU:C	2.60	0.45
2:A:1150:LEU:CD1	2:A:1150:LEU:N	2.79	0.45
2:A:373:SER:OG	2:A:375:ILE:HG12	2.17	0.45
2:A:146:GLN:NE2	2:A:804:GLU:HA	2.31	0.45
2:A:167:LEU:CD2	2:A:837:ARG:HD2	2.47	0.45
2:A:1052:LEU:HD11	2:A:1176:VAL:CG2	2.47	0.45
2:A:14:GLU:C	2:A:20:THR:HG22	2.42	0.44
2:A:451:MET:HA	2:A:451:MET:CE	2.40	0.44
2:A:536:GLN:HA	2:A:536:GLN:NE2	2.31	0.44
2:A:270:ILE:HD12	2:A:373:SER:CB	2.48	0.44
2:A:589:CYS:SG	2:A:734:ASP:HB3	2.58	0.44
2:A:730:VAL:O	8:A:1564:HOH:O	2.21	0.44
2:A:1005:ASN:N	2:A:1006:PRO:CD	2.79	0.44
2:A:595:TRP:HA	2:A:599:LEU:HB2	2.00	0.44
2:A:781:TYR:HE1	8:A:1564:HOH:O	1.89	0.44
1:B:1285:G:N3	2:A:683:GLY:HA2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:210:LEU:HB3	2:A:211:SER:H	1.62	0.44
2:A:270:ILE:HD12	2:A:373:SER:HB2	1.99	0.44
2:A:719:LEU:O	2:A:723:LEU:HG	2.17	0.44
2:A:851:ARG:HB2	2:A:864:GLN:HE22	1.81	0.44
2:A:957:LYS:O	2:A:960:ARG:HG3	2.18	0.44
2:A:557:PRO:HD2	2:A:731:CYS:O	2.17	0.44
2:A:1168:ASN:ND2	2:A:1169:THR:H	2.16	0.44
2:A:245:LEU:HD22	2:A:367:ASP:HA	1.99	0.43
2:A:817:ILE:O	2:A:821:ILE:HG12	2.18	0.43
2:A:223:THR:CG2	2:A:224:SER:N	2.81	0.43
2:A:302:PRO:HG2	2:A:305:ASP:OD1	2.18	0.43
2:A:357:HIS:CE1	2:A:788:PHE:HB2	2.53	0.43
2:A:114:ARG:HB2	2:A:215:PHE:HE1	1.82	0.43
2:A:456:VAL:HG21	2:A:977:TYR:CE2	2.52	0.43
2:A:1150:LEU:N	2:A:1150:LEU:HD12	2.32	0.43
2:A:84:LYS:HD2	2:A:86:TYR:CE2	2.54	0.43
2:A:626:ILE:CG2	2:A:638:ALA:HB1	2.49	0.43
2:A:375:ILE:O	2:A:375:ILE:HG13	2.18	0.43
2:A:423:ARG:HE	2:A:427:ARG:NH2	2.17	0.43
2:A:464:ALA:O	2:A:468:GLU:HG2	2.19	0.43
2:A:512:ASP:OD1	2:A:660:SER:CB	2.67	0.43
2:A:557:PRO:CD	2:A:731:CYS:O	2.67	0.43
2:A:223:THR:HG22	2:A:224:SER:N	2.34	0.43
2:A:713:ASP:CG	2:A:716:VAL:HG23	2.44	0.43
2:A:1137:ASP:O	2:A:1138:LYS:C	2.62	0.43
2:A:40:SER:O	2:A:44:LYS:HG3	2.18	0.43
2:A:178:ILE:HA	2:A:179:PRO:HD3	1.94	0.43
2:A:318:ALA:HB2	8:A:1588:HOH:O	2.19	0.43
2:A:815:PRO:HB2	2:A:953:ARG:O	2.19	0.43
2:A:984:LEU:O	2:A:987:ARG:HB2	2.19	0.43
2:A:201:LEU:HA	2:A:202:PRO:HD3	1.78	0.42
2:A:230:LEU:O	2:A:234:VAL:HG23	2.19	0.42
2:A:1238:VAL:CG1	2:A:1239:ASP:N	2.81	0.42
2:A:116:SER:HB3	2:A:119:ILE:HG13	2.01	0.42
2:A:145:ARG:O	2:A:805:ARG:HD2	2.20	0.42
2:A:455:TYR:CE1	2:A:533:VAL:HG13	2.54	0.42
2:A:120:GLU:O	2:A:124:LYS:HG3	2.17	0.42
2:A:303:ARG:HG3	2:A:303:ARG:HH11	1.85	0.42
2:A:490:LYS:HA	2:A:493:GLN:HB2	2.00	0.42
2:A:523:ARG:NH1	2:A:524:ARG:O	2.52	0.42
2:A:575:SER:HB2	8:A:1540:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:205:ALA:HA	2:A:206:PRO:HD3	1.77	0.42
2:A:468:GLU:HG2	2:A:468:GLU:H	1.73	0.42
2:A:1060:LYS:HE3	8:A:1586:HOH:O	2.20	0.42
2:A:834:GLN:HB3	8:A:1456:HOH:O	2.19	0.42
2:A:863:LEU:HD23	2:A:863:LEU:HA	1.85	0.42
2:A:879:LYS:NZ	2:A:883:SER:O	2.44	0.42
2:A:1029:GLU:O	2:A:1033:GLU:HG3	2.20	0.42
2:A:268:TRP:NE1	2:A:272:LYS:HD2	2.35	0.42
2:A:632:VAL:HG12	2:A:633:VAL:N	2.35	0.42
2:A:410:GLU:N	2:A:649:GLN:HE21	2.14	0.42
2:A:851:ARG:HA	2:A:863:LEU:O	2.20	0.42
2:A:906:ILE:O	2:A:910:MET:HG3	2.20	0.42
2:A:1062:ARG:HD2	2:A:1243:GLU:OE2	2.19	0.42
2:A:287:GLU:HA	2:A:322:ARG:HB3	2.01	0.42
2:A:2:SER:N	2:A:48:GLU:OE1	2.54	0.41
2:A:188:TRP:CE2	2:A:192:GLU:HG3	2.55	0.41
2:A:485:VAL:HG12	2:A:1021:GLN:HG3	2.02	0.41
2:A:815:PRO:HG2	2:A:1034:MET:CE	2.49	0.41
2:A:15:SER:N	2:A:20:THR:HG22	2.34	0.41
2:A:39:ARG:NH1	2:A:39:ARG:CG	2.84	0.41
2:A:833:LEU:HD12	2:A:838:TRP:CD2	2.55	0.41
2:A:1011:ASP:O	2:A:1014:HIS:N	2.54	0.41
2:A:1252:LEU:HG	2:A:1256:PHE:CE2	2.54	0.41
2:A:570:LEU:HD21	2:A:730:VAL:HG21	2.01	0.41
2:A:651:LEU:HG	2:A:655:TYR:CE2	2.55	0.41
2:A:845:LEU:HD23	2:A:845:LEU:HA	1.91	0.41
2:A:944:GLN:H	2:A:944:GLN:CD	2.28	0.41
2:A:73:TYR:CB	2:A:132:ILE:HG23	2.51	0.41
2:A:516:GLY:O	2:A:517:LEU:HD23	2.19	0.41
2:A:814:TRP:CG	2:A:815:PRO:N	2.88	0.41
2:A:1081:ILE:HD12	2:A:1088:PRO:HB3	2.02	0.41
2:A:1146:LEU:HD23	2:A:1150:LEU:O	2.20	0.41
2:A:778:THR:CG2	2:A:779:ALA:N	2.84	0.41
2:A:346:GLU:O	2:A:350:ARG:HG3	2.20	0.41
2:A:783:LYS:HG3	2:A:797:ARG:HH12	1.83	0.41
2:A:1063:MET:HE3	2:A:1063:MET:HB2	1.82	0.41
2:A:332:ARG:O	2:A:336:GLU:HG2	2.20	0.41
2:A:520:GLN:CD	2:A:523:ARG:HD3	2.45	0.41
2:A:983:GLU:O	2:A:987:ARG:HG3	2.21	0.41
1:B:1284:A:C2	2:A:807:ASN:ND2	2.89	0.41
2:A:22:GLN:HE21	2:A:878:VAL:N	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:34:PHE:HD1	2:A:156:LEU:HD23	1.86	0.41
2:A:249:LEU:HD23	2:A:252:LEU:HD12	2.03	0.41
2:A:421:ILE:HD12	2:A:421:ILE:HA	1.87	0.41
2:A:436:MET:HE2	2:A:437:ALA:N	2.36	0.41
2:A:705:VAL:O	2:A:708:PRO:HD2	2.21	0.41
2:A:798:HIS:N	2:A:799:PRO:HD3	2.36	0.41
2:A:834:GLN:NE2	8:A:1590:HOH:O	2.29	0.41
1:B:1283:U:H5''	8:A:1596:HOH:O	2.21	0.41
2:A:821:ILE:HD12	2:A:845:LEU:CD1	2.49	0.41
2:A:992:ARG:O	2:A:995:TRP:N	2.54	0.41
2:A:390:THR:HG22	2:A:391:GLN:N	2.35	0.40
2:A:1137:ASP:O	2:A:1140:ALA:HB3	2.21	0.40
2:A:1138:LYS:O	2:A:1141:LEU:N	2.54	0.40
2:A:372:THR:O	2:A:796:SER:HB2	2.21	0.40
2:A:92:VAL:HG13	2:A:383:GLU:HB3	2.03	0.40
2:A:332:ARG:NH1	2:A:332:ARG:HG2	2.37	0.40
2:A:444:ASP:HA	2:A:445:PRO:HD3	1.95	0.40
2:A:483:LEU:HD23	2:A:483:LEU:HA	1.94	0.40
2:A:1005:ASN:O	2:A:1006:PRO:C	2.65	0.40
2:A:85:THR:HG22	8:A:1487:HOH:O	2.22	0.40
2:A:404:TRP:O	2:A:415:LYS:HE3	2.22	0.40
2:A:448:GLN:HE21	2:A:448:GLN:HB3	1.68	0.40
2:A:492:PHE:O	2:A:496:GLN:HG3	2.21	0.40
2:A:951:LEU:HD13	2:A:1037:THR:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	1262/1267 (100%)	1174 (93%)	70 (6%)	18 (1%)	9	30

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	91	ASP
2	A	108	THR
2	A	814	TRP
2	A	146	GLN
2	A	687	THR
2	A	10	GLY
2	A	263	SER
2	A	964	ARG
2	A	110	THR
2	A	1185	MET
2	A	498	ALA
2	A	557	PRO
2	A	815	PRO
2	A	631	SER
2	A	567	VAL
2	A	635	VAL
2	A	1005	ASN
2	A	99	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	
2	A	1081/1083 (100%)	1036 (96%)	45 (4%)	26	61

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	35	SER
2	A	37	PHE
2	A	80	ARG
2	A	85	THR
2	A	107	GLU
2	A	167	LEU
2	A	187	LEU

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Mol	Chain	Res	Type
2	A	300	LEU
2	A	366	ARG
2	A	378	VAL
2	A	387	GLN
2	A	390	THR
2	A	414	LEU
2	A	431	LEU
2	A	436	MET
2	A	466	LEU
2	A	470	LEU
2	A	476	SER
2	A	518	ARG
2	A	528	ILE
2	A	536	GLN
2	A	538	VAL
2	A	610	VAL
2	A	700	GLU
2	A	712	ASP
2	A	726	GLN
2	A	735	ASP
2	A	761	SER
2	A	778	THR
2	A	784	LEU
2	A	845	LEU
2	A	894	THR
2	A	909	LEU
2	A	923	ARG
2	A	980	GLN
2	A	984	LEU
2	A	1021	GLN
2	A	1052	LEU
2	A	1063	MET
2	A	1065	GLU
2	A	1077	LEU
2	A	1103	ARG
2	A	1121	VAL
2	A	1151	GLN
2	A	1238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	8	GLN
2	A	22	GLN
2	A	121	ASN
2	A	146	GLN
2	A	283	HIS
2	A	296	ASN
2	A	387	GLN
2	A	448	GLN
2	A	496	GLN
2	A	499	ASN
2	A	504	HIS
2	A	520	GLN
2	A	536	GLN
2	A	537	GLN
2	A	580	GLN
2	A	646	ASN
2	A	649	GLN
2	A	671	ASN
2	A	710	HIS
2	A	728	ASN
2	A	749	ASN
2	A	754	GLN
2	A	820	GLN
2	A	834	GLN
2	A	852	GLN
2	A	864	GLN
2	A	917	ASN
2	A	980	GLN
2	A	1005	ASN
2	A	1021	GLN
2	A	1165	GLN
2	A	1168	ASN
2	A	1246	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	3/6 (50%)	0	0

There are no RNA backbone outliers to report.

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 [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	GDP	A	1425	4	25,29,30	1.97	10 (40%)	39,44,47	2.50	11 (28%)
7	GH3	A	1293	-	31,33,33	1.94	3 (9%)	44,52,52	1.49	8 (18%)
4	G7M	A	1424	5	27,27,27	2.11	9 (33%)	41,42,42	3.10	14 (34%)
6	CH1	A	1291	3	27,29,29	2.60	6 (22%)	37,45,45	2.59	14 (37%)

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	GDP	A	1425	4	-	4/13/31/32	0/3/3/3
7	GH3	A	1293	-	-	6/22/34/34	0/3/3/3
4	G7M	A	1424	5	-	5/10/26/26	0/3/3/3
6	CH1	A	1291	3	-	5/22/34/34	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1291	CH1	PA-O3A	8.46	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1293	GH3	PA-O3A	6.82	1.66	1.59
6	A	1291	CH1	PB-O3B	6.74	1.66	1.59
6	A	1291	CH1	PB-O3A	5.79	1.65	1.59
7	A	1293	GH3	PB-O3B	5.67	1.65	1.59
4	A	1424	G7M	P-O5'	-5.36	1.43	1.60
4	A	1424	G7M	C1'-N9	4.18	1.59	1.47
4	A	1424	G7M	C2'-C3'	-4.17	1.42	1.53
5	A	1425	GDP	C6-N1	3.59	1.45	1.38
5	A	1425	GDP	C2'-C3'	-3.49	1.43	1.53
5	A	1425	GDP	PA-O5'	3.35	1.72	1.59
5	A	1425	GDP	C4-N3	3.00	1.41	1.34
5	A	1425	GDP	O4'-C4'	-2.92	1.38	1.45
4	A	1424	G7M	C3'-C4'	-2.86	1.45	1.53
5	A	1425	GDP	C2-N1	2.73	1.44	1.37
4	A	1424	G7M	O3'-C3'	-2.52	1.36	1.43
4	A	1424	G7M	P-OP1	2.42	1.58	1.50
6	A	1291	CH1	C6-C5	2.38	1.40	1.35
7	A	1293	GH3	PB-O2B	-2.37	1.44	1.55
4	A	1424	G7M	C8-N7	-2.30	1.29	1.33
5	A	1425	GDP	C1'-N9	2.28	1.54	1.47
4	A	1424	G7M	O6-C6	-2.22	1.19	1.23
5	A	1425	GDP	PA-O1A	2.19	1.58	1.50
4	A	1424	G7M	O2'-C2'	-2.18	1.37	1.43
5	A	1425	GDP	C2-N3	2.08	1.38	1.33
6	A	1291	CH1	PG-O1G	2.07	1.56	1.50
6	A	1291	CH1	PB-O1B	2.03	1.57	1.50
5	A	1425	GDP	C8-N9	2.01	1.42	1.37

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1425	GDP	O2A-PA-O3A	-8.43	84.49	107.27
4	A	1424	G7M	OP2-P-O5'	-7.35	87.51	106.67
6	A	1291	CH1	O3G-PG-O1G	-7.32	82.32	110.83
4	A	1424	G7M	O4'-C4'-C5'	7.20	132.39	109.33
6	A	1291	CH1	O3G-PG-O3B	-7.00	81.15	104.64
5	A	1425	GDP	O5'-C5'-C4'	6.87	132.38	108.99
4	A	1424	G7M	OP3-P-O5'	6.52	123.68	106.67
4	A	1424	G7M	OP2-P-OP3	6.48	132.11	107.80
4	A	1424	G7M	O3'-C3'-C4'	6.11	128.63	111.08
6	A	1291	CH1	O3G-PG-O2G	-5.13	88.57	107.80
5	A	1425	GDP	O5'-PA-O1A	5.02	128.84	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1424	G7M	OP2-P-OP1	-4.81	92.09	110.83
4	A	1424	G7M	C5'-C4'-C3'	-4.81	97.91	115.21
4	A	1424	G7M	O4'-C4'-C3'	4.78	114.65	105.15
6	A	1291	CH1	O2-C2-N3	-4.69	114.94	122.33
7	A	1293	GH3	O4'-C4'-C5'	4.59	117.61	109.34
4	A	1424	G7M	C3'-C2'-C1'	4.31	109.61	101.46
5	A	1425	GDP	O3A-PA-O1A	-4.03	98.59	110.70
5	A	1425	GDP	O2A-PA-O5'	-3.74	90.61	107.57
4	A	1424	G7M	CN7-N7-C5	3.69	131.40	126.80
6	A	1291	CH1	O4'-C4'-C5'	3.47	115.59	109.34
6	A	1291	CH1	C3'-C4'-C5'	-3.41	106.28	113.30
4	A	1424	G7M	C8-N7-C5	-3.40	103.53	107.78
4	A	1424	G7M	C2'-C1'-N9	3.37	122.63	113.25
5	A	1425	GDP	O2A-PA-O1A	3.18	127.26	112.44
4	A	1424	G7M	C4-C5-N7	3.04	112.64	107.67
5	A	1425	GDP	C3'-C2'-C1'	3.02	107.17	101.46
7	A	1293	GH3	O2G-PG-O3B	3.01	114.73	104.64
6	A	1291	CH1	O2A-PA-O3A	2.76	114.74	107.27
7	A	1293	GH3	O4'-C1'-C2'	2.73	109.08	106.51
5	A	1425	GDP	PA-O5'-C5'	-2.68	105.99	121.35
6	A	1291	CH1	C6-N1-C2	-2.67	115.96	120.46
6	A	1291	CH1	O2G-PG-O3B	2.63	113.45	104.64
4	A	1424	G7M	C6-C5-N7	-2.59	128.93	132.17
6	A	1291	CH1	O3B-PG-O1G	2.55	124.46	111.04
6	A	1291	CH1	O4'-C1'-C2'	-2.55	104.11	106.51
6	A	1291	CH1	O2B-PB-O3B	2.54	114.15	107.27
5	A	1425	GDP	C4'-O4'-C1'	-2.32	104.34	109.47
7	A	1293	GH3	O3B-PB-O1B	-2.18	104.16	110.70
7	A	1293	GH3	O3A-PA-O1A	-2.14	104.27	110.70
6	A	1291	CH1	N1-C2-N3	2.10	122.45	118.80
7	A	1293	GH3	C1'-N9-C8	2.09	132.68	126.73
7	A	1293	GH3	N9-C8-N7	2.08	117.25	113.40
5	A	1425	GDP	C2-N3-C4	2.04	115.82	112.30
7	A	1293	GH3	O4'-C4'-C3'	2.03	107.64	105.07
6	A	1291	CH1	O2G-PG-O1G	2.02	118.70	110.83
5	A	1425	GDP	N9-C8-N7	2.01	117.14	113.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1424	G7M	C5'-O5'-P-OP2

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Mol	Chain	Res	Type	Atoms
4	A	1424	G7M	O4'-C4'-C5'-O5'
5	A	1425	GDP	C5'-O5'-PA-O3A
5	A	1425	GDP	C5'-O5'-PA-O1A
6	A	1291	CH1	C3'-C4'-C5'-O5'
6	A	1291	CH1	O4'-C4'-C5'-O5'
6	A	1291	CH1	C5'-O5'-PA-O1A
7	A	1293	GH3	PB-O3B-PG-O2G
4	A	1424	G7M	C3'-C4'-C5'-O5'
7	A	1293	GH3	O4'-C4'-C5'-O5'
5	A	1425	GDP	C5'-O5'-PA-O2A
6	A	1291	CH1	C5'-O5'-PA-O3A
4	A	1424	G7M	C4'-C5'-O5'-P
7	A	1293	GH3	PB-O3A-PA-O1A
4	A	1424	G7M	C5'-O5'-P-OP3
7	A	1293	GH3	PB-O3B-PG-O3G
5	A	1425	GDP	PB-O3A-PA-O5'
6	A	1291	CH1	PB-O3A-PA-O2A
7	A	1293	GH3	PB-O3A-PA-O2A
7	A	1293	GH3	PB-O3B-PG-O1G

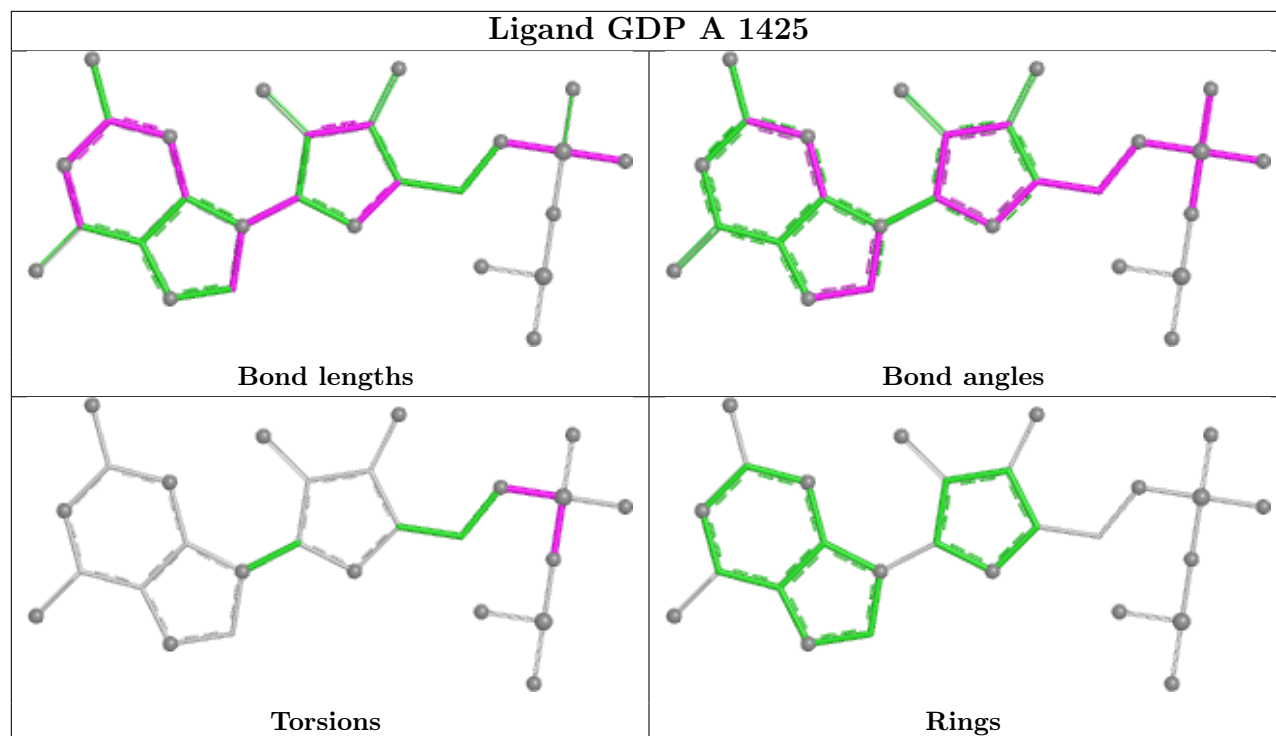
There are no ring outliers.

1 monomer is involved in 2 short contacts:

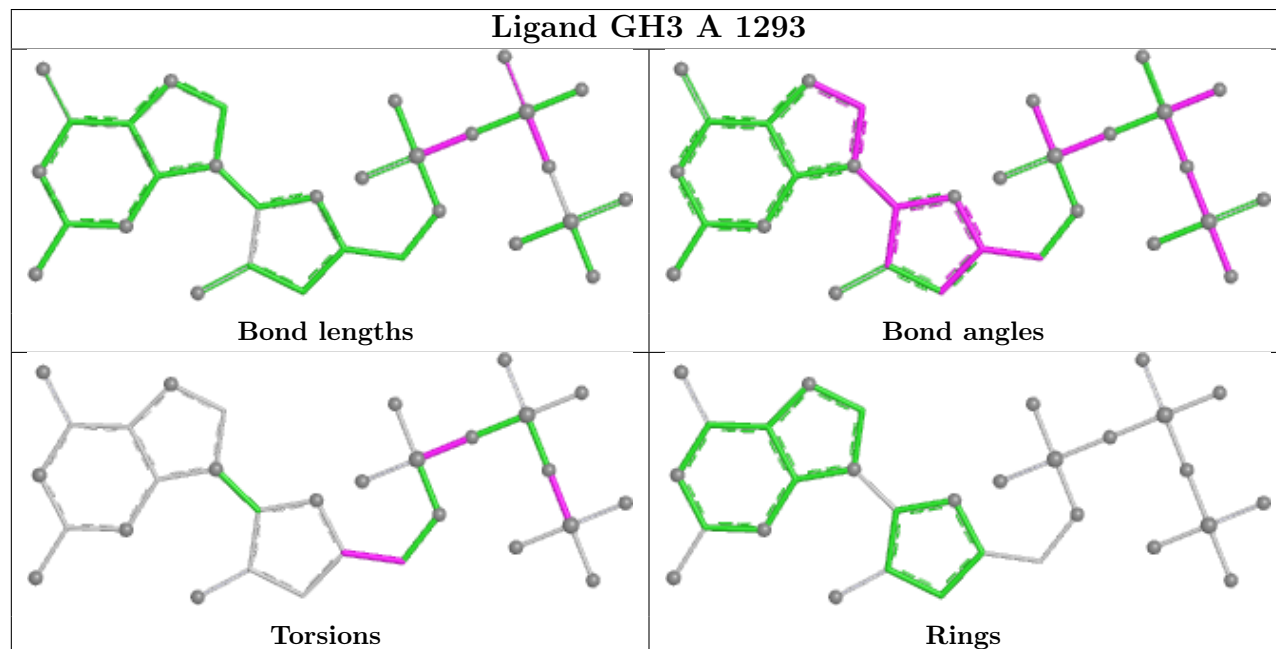
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1425	GDP	2	0

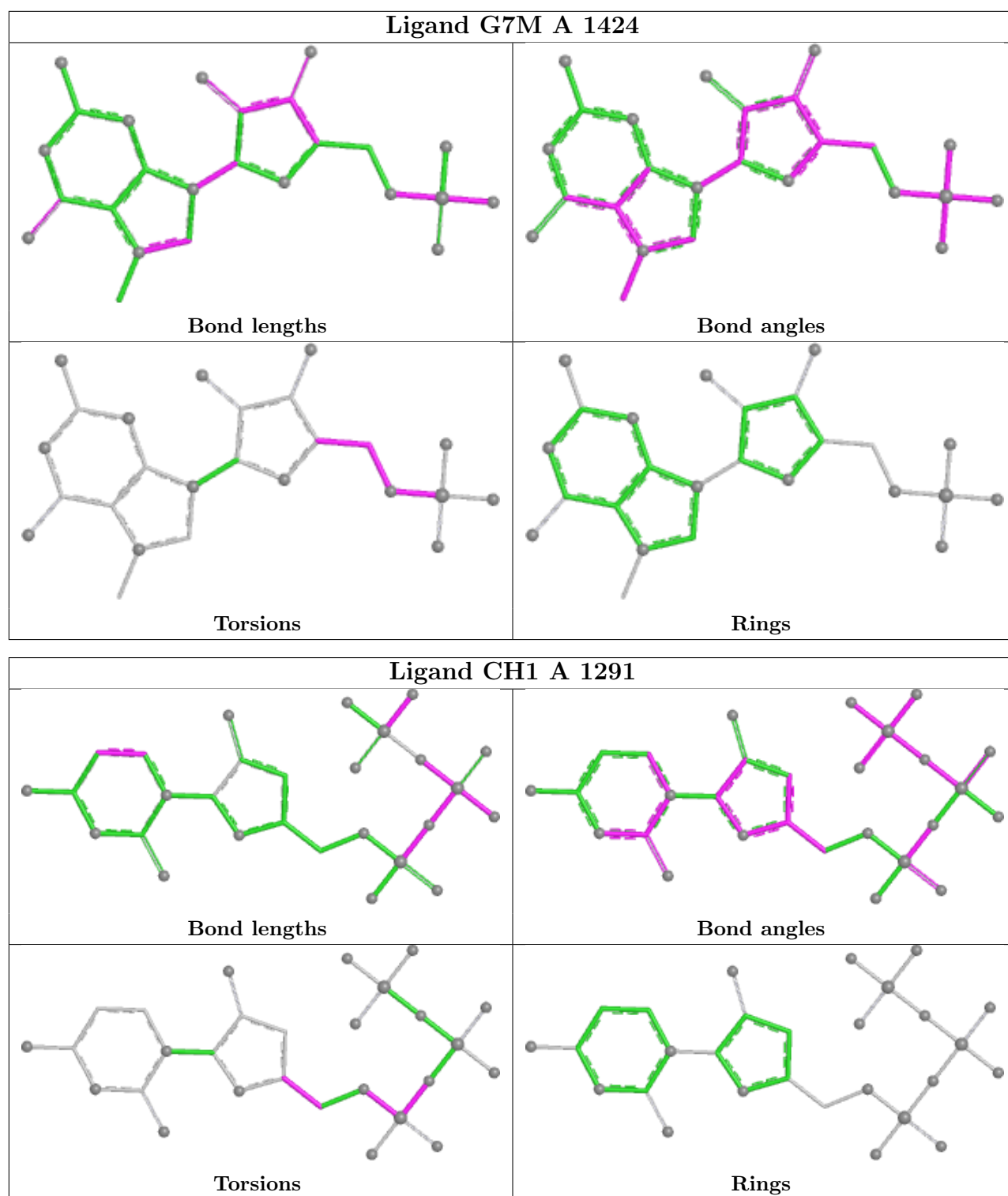
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 GDP A 1425



Ligand GH3 A 1293





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	4/6 (66%)	0.34	0 100 100	21, 25, 49, 65	0
2	A	1264/1267 (99%)	0.24	25 (1%) 65 56	6, 21, 43, 73	0
All	All	1268/1273 (99%)	0.24	25 (1%) 65 56	6, 21, 43, 73	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	859	SER	4.8
2	A	857	GLY	4.7
2	A	2	SER	4.2
2	A	745	ALA	3.9
2	A	744	THR	3.9
2	A	212	ALA	3.5
2	A	211	SER	3.3
2	A	633	VAL	3.3
2	A	213	GLY	3.1
2	A	858	GLU	2.9
2	A	856	ILE	2.9
2	A	855	MET	2.9
2	A	672	ASP	2.7
2	A	566	LYS	2.4
2	A	634	GLY	2.3
2	A	918	GLY	2.3
2	A	930	ASN	2.3
2	A	504	HIS	2.2
2	A	107	GLU	2.1
2	A	1239	ASP	2.1
2	A	860	VAL	2.1
2	A	1168	ASN	2.1
2	A	38	THR	2.0
2	A	563	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	A	1264	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

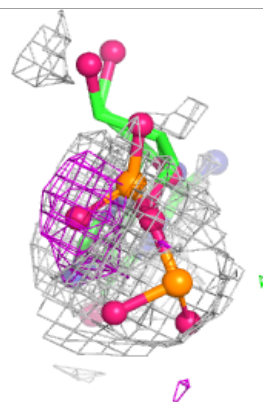
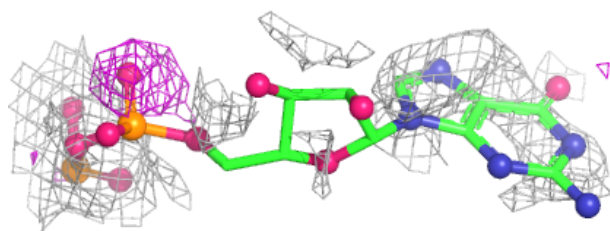
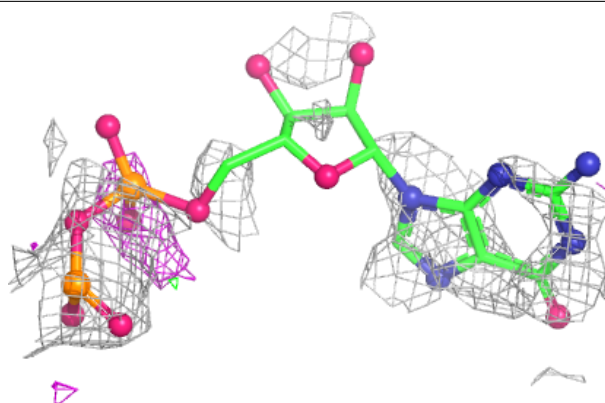
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GDP	A	1425	27/28	0.72	0.20	93,97,102,103	0
7	GH3	A	1293	31/31	0.77	0.20	77,83,90,91	0
4	G7M	A	1424	25/25	0.80	0.18	41,52,80,87	0
6	CH1	A	1291	28/28	0.86	0.17	62,66,69,69	0
3	MN	A	1301	1/1	0.96	0.05	32,32,32,32	0
3	MN	A	1302	1/1	0.99	0.06	35,35,35,35	0

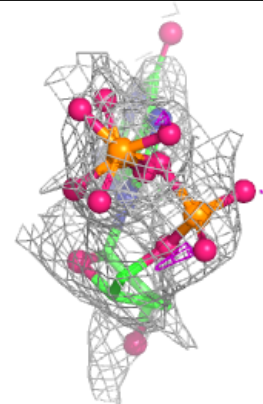
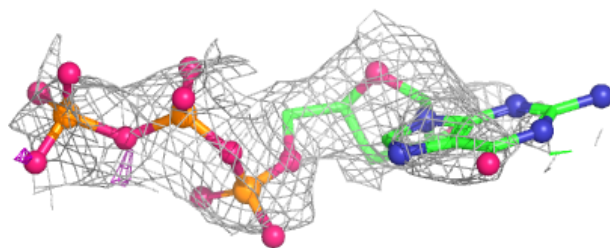
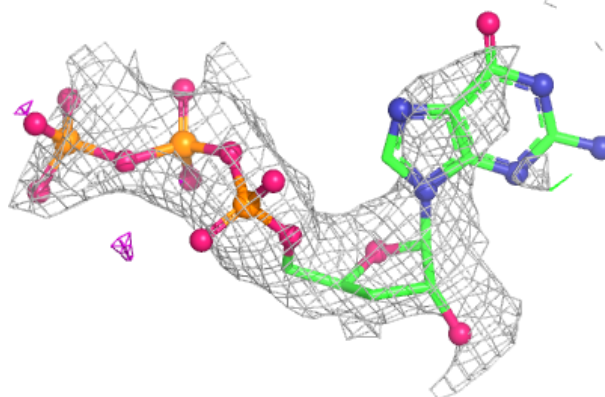
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP A 1425:

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

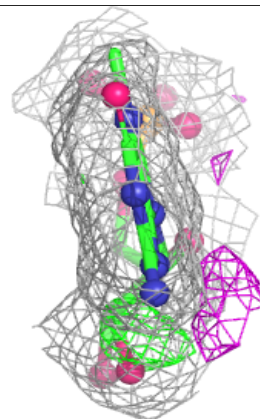
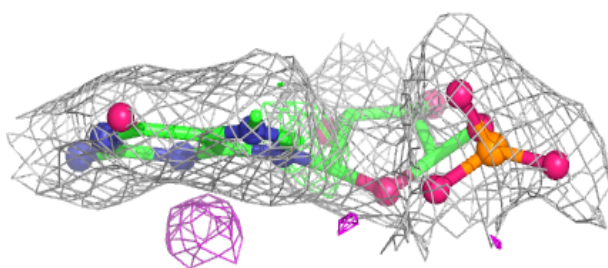
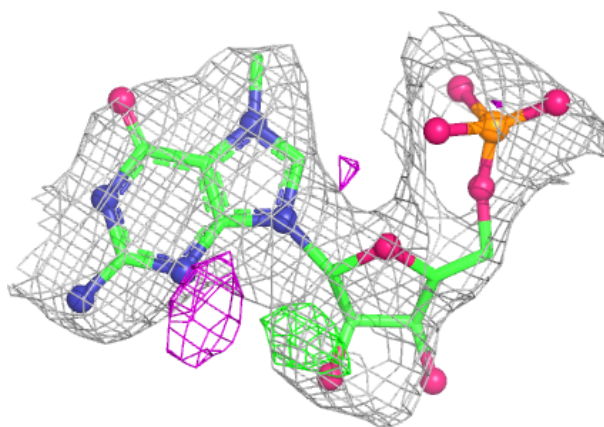
**Electron density around GH3 A 1293:**

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

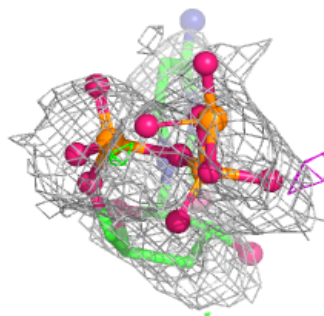
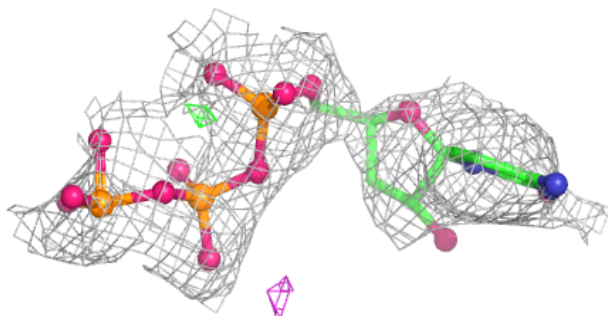
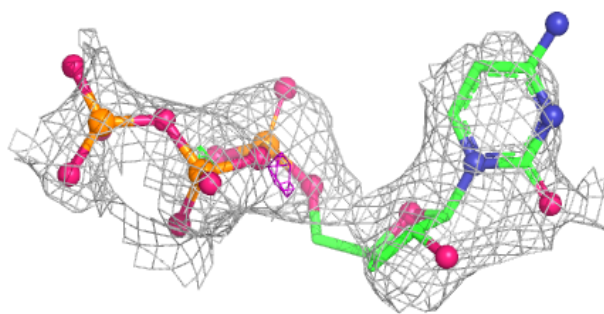


Electron density around G7M A 1424:

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

**Electron density around CH1 A 1291:**

$2mF_o-DF_c$ (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.