



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:09 PM UTC

PDB ID : 3AVT / pdb_00003avt
Title : Structure of viral RNA polymerase complex 1
Authors : Takeshita, D.; Tomita, K.
Deposited on : 2011-03-08
Resolution : 2.61 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

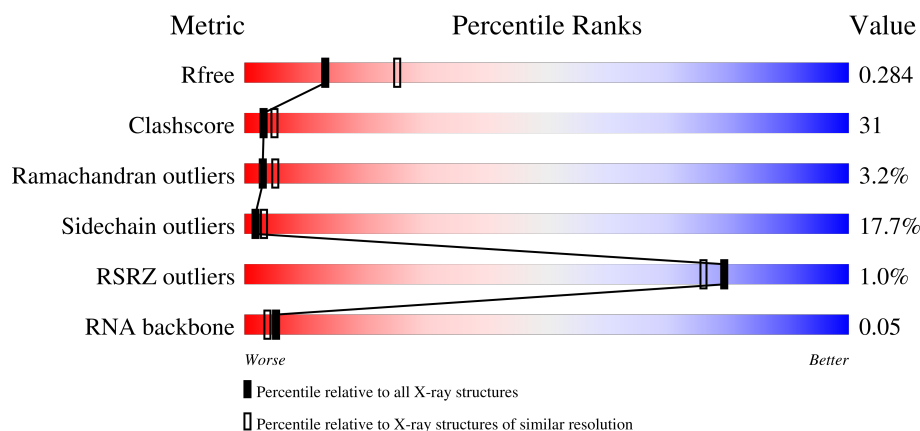
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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	1289	
2	T	7	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9495 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1203	Total	C	N	O	S	0	0	0
			9287	5865	1605	1772	45			

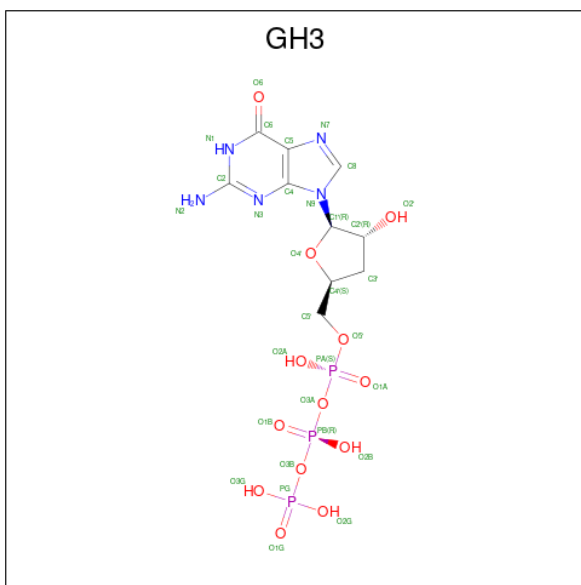
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	HIS	-	linker	UNP P0A6P3
A	1284	HIS	-	expression tag	UNP Q8LTE0
A	1285	HIS	-	expression tag	UNP Q8LTE0
A	1286	HIS	-	expression tag	UNP Q8LTE0
A	1287	HIS	-	expression tag	UNP Q8LTE0
A	1288	HIS	-	expression tag	UNP Q8LTE0
A	1289	HIS	-	expression tag	UNP Q8LTE0

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*UP*CP*GP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	4	Total	C	N	O	P	0	0	0
			85	38	16	27	4			

- Molecule 3 is 3'-DEOXY-GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GH3) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	T	1	Total 31	C 10	N 5	O 13	P 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0

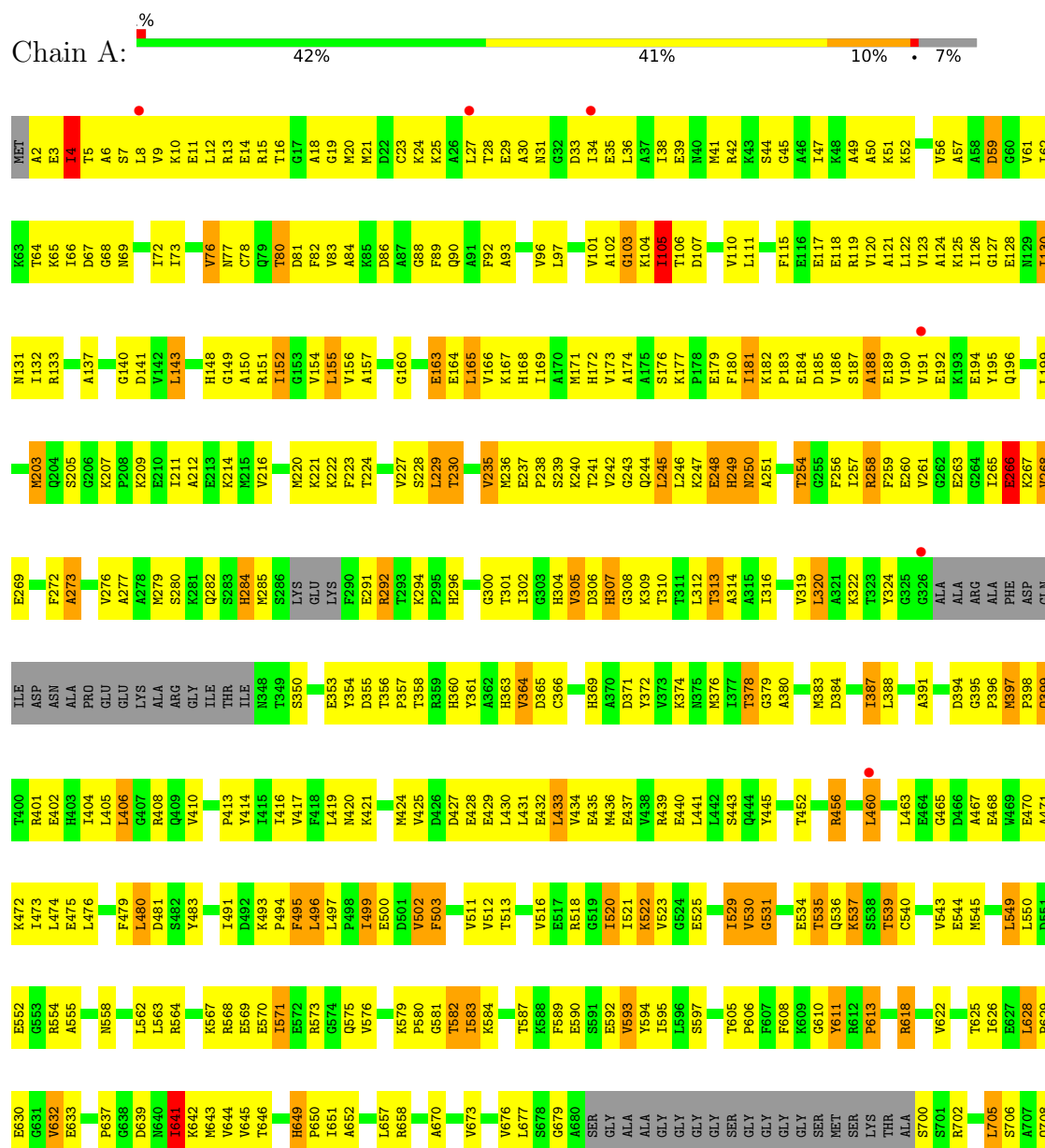
- Molecule 5 is water.

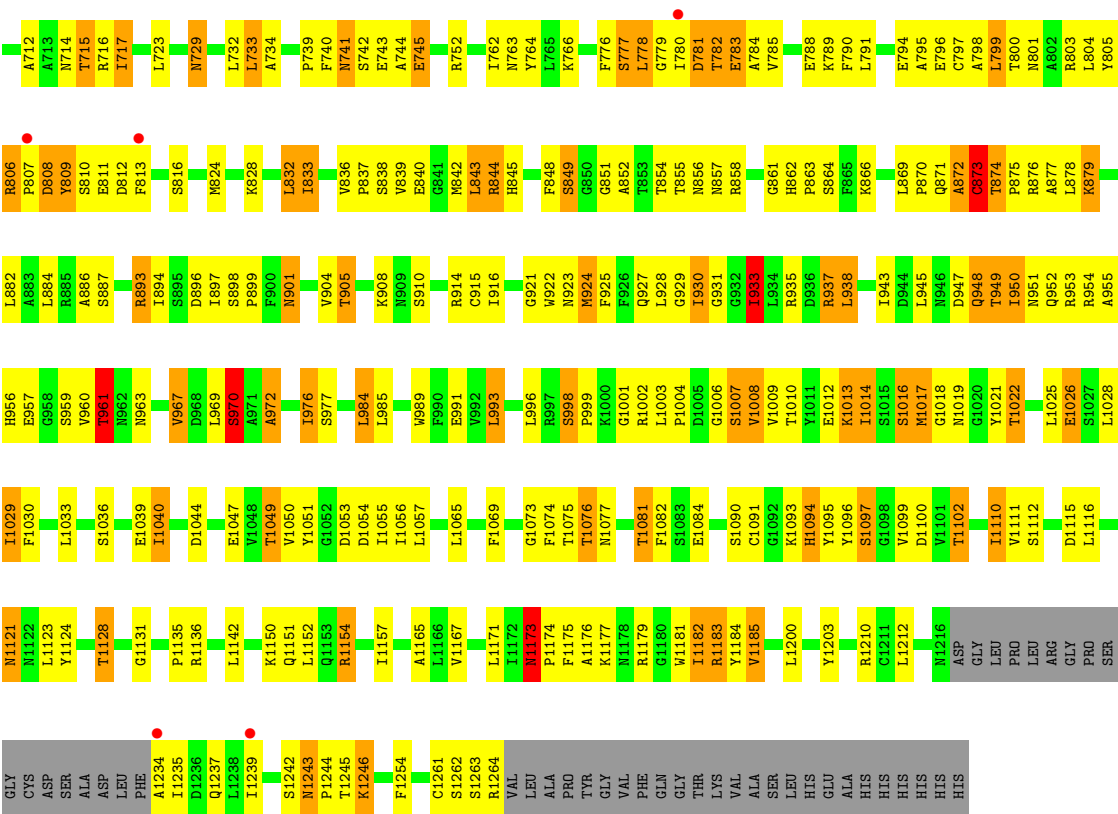
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	56	Total O 56 56	0	0
5	T	3	Total O 3 3	0	0

3 Residue-property plots

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

- Molecule 1: Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	139.12Å 255.99Å 101.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.61 19.99 – 2.61	Depositor EDS
% Data completeness (in resolution range)	91.8 (19.99-2.61) 98.8 (19.99-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.225 , 0.288 0.220 , 0.284	Depositor DCC
R_{free} test set	2786 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9495	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: GH3, CA

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	0.65	0/9456	0.99	26/12787 (0.2%)
2	T	0.60	0/94	0.57	0/144
All	All	0.65	0/9550	0.98	26/12931 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	961	THR	N-CA-C	8.56	120.23	111.07
1	A	1243	ASN	N-CA-C	8.33	121.52	110.36
1	A	976	ILE	CB-CA-C	-7.31	104.05	111.80
1	A	1243	ASN	CA-C-N	7.13	127.13	119.78
1	A	1243	ASN	C-N-CA	7.13	127.13	119.78
1	A	776	PHE	N-CA-C	-7.13	99.73	110.28
1	A	1018	GLY	N-CA-C	-7.09	105.99	113.58
1	A	777	SER	N-CA-C	-6.90	104.99	113.41
1	A	783	GLU	N-CA-C	-6.88	103.29	113.61
1	A	284	HIS	N-CA-C	-6.41	105.59	113.41
1	A	1173	ASN	CA-C-N	6.25	125.94	119.82
1	A	1173	ASN	C-N-CA	6.25	125.94	119.82
1	A	207	LYS	CA-C-N	5.95	127.27	119.84
1	A	207	LYS	C-N-CA	5.95	127.27	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1029	ILE	CB-CA-C	-5.57	104.84	111.97
1	A	743	GLU	N-CA-C	-5.39	105.51	111.71
1	A	649	HIS	N-CA-C	5.39	112.98	108.13
1	A	1026	GLU	N-CA-C	-5.38	106.22	112.89
1	A	998	SER	CA-C-N	5.32	124.65	118.85
1	A	998	SER	C-N-CA	5.32	124.65	118.85
1	A	886	ALA	N-CA-C	-5.25	106.13	112.54
1	A	933	ILE	N-CA-CB	5.17	116.59	110.55
1	A	105	ILE	CB-CA-C	-5.08	106.01	111.59
1	A	639	ASP	N-CA-C	5.07	117.75	109.59
1	A	729	ASN	N-CA-C	5.01	116.83	111.36
1	A	1121	ASN	N-CA-C	5.01	116.82	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	849	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9287	0	9273	580	0
2	T	85	0	45	9	0
3	A	31	0	12	2	0
3	T	31	0	12	0	0
4	A	2	0	0	0	0
5	A	56	0	0	2	0
5	T	3	0	0	0	0
All	All	9495	0	9342	584	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 31.

All (584) 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:842:MET:HE1	1:A:930:ILE:HG22	1.26	1.16
1:A:1110:ILE:HD13	1:A:1110:ILE:O	1.49	1.11
1:A:723:LEU:HD23	1:A:1110:ILE:CD1	1.81	1.10
1:A:723:LEU:HD23	1:A:1110:ILE:HD11	1.30	1.09
1:A:961:THR:HG22	1:A:963:ASN:H	1.18	1.05
1:A:947:ASP:OD1	1:A:949:THR:HB	1.59	1.03
1:A:1154:ARG:HG3	1:A:1154:ARG:HH11	1.23	1.02
1:A:937:ARG:HH21	1:A:937:ARG:HG3	1.27	0.99
1:A:1019:ASN:HB3	1:A:1022:THR:CG2	1.93	0.98
1:A:930:ILE:HD11	1:A:1021:TYR:HB2	1.49	0.94
1:A:212:ALA:O	1:A:216:VAL:HG23	1.68	0.94
1:A:1017:MET:HB2	3:A:2502:GH3:HN22	1.32	0.93
1:A:15:ARG:HH21	1:A:38:ILE:HG21	1.32	0.93
1:A:1019:ASN:HB3	1:A:1022:THR:HG22	1.53	0.91
1:A:356:THR:HG21	1:A:481:ASP:OD1	1.72	0.90
1:A:949:THR:HG23	1:A:953:ARG:NH1	1.87	0.89
1:A:301:THR:HB	1:A:363:HIS:NE2	1.89	0.87
1:A:723:LEU:CD2	1:A:1110:ILE:HD11	2.04	0.87
1:A:1017:MET:HB2	3:A:2502:GH3:N2	1.89	0.87
1:A:7:SER:HB2	1:A:10:LYS:HB3	1.56	0.86
1:A:836:VAL:HG22	1:A:837:PRO:HD2	1.59	0.85
1:A:1100:ASP:OD1	1:A:1102:THR:HG22	1.77	0.84
1:A:1077:ASN:O	1:A:1081:THR:HG22	1.77	0.84
1:A:923:ASN:O	1:A:927:GLN:HG3	1.78	0.84
1:A:372:TYR:HE1	1:A:410:VAL:HG21	1.41	0.84
1:A:733:LEU:HD11	1:A:739:PRO:HD3	1.60	0.83
1:A:467:ALA:HA	1:A:470:GLU:HB2	1.58	0.83
1:A:752:ARG:H	1:A:763:ASN:HD21	1.24	0.82
1:A:806:ARG:H	1:A:807:PRO:HD3	1.42	0.82
1:A:126:ILE:HG23	1:A:399:GLN:HE22	1.45	0.82
1:A:93:ALA:HA	1:A:96:VAL:HG12	1.60	0.82
1:A:851:GLY:HA3	2:T:2105:C:H5'	1.61	0.82
1:A:854:THR:HG21	1:A:872:ALA:HB3	1.61	0.81
1:A:520:ILE:HD13	1:A:554:ARG:HG2	1.62	0.81
1:A:961:THR:CG2	1:A:963:ASN:H	1.94	0.80
1:A:884:LEU:O	1:A:887:SER:HB3	1.82	0.80
1:A:1173:ASN:ND2	1:A:1175:PHE:H	1.79	0.80
1:A:649:HIS:HB2	1:A:650:PRO:HD2	1.62	0.79
1:A:73:ILE:HB	1:A:155:LEU:HD22	1.61	0.79
1:A:1173:ASN:HD22	1:A:1175:PHE:H	1.30	0.79
1:A:930:ILE:C	1:A:930:ILE:HD12	2.07	0.79
1:A:950:ILE:HD12	1:A:950:ILE:C	2.08	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LEU:O	1:A:316:ILE:HG12	1.83	0.79
1:A:502:VAL:HG12	1:A:512:VAL:HG12	1.65	0.78
1:A:237:GLU:HG2	1:A:240:LYS:HZ1	1.47	0.78
1:A:1157:ILE:HG12	1:A:1165:ALA:HB3	1.65	0.78
1:A:764:TYR:OH	1:A:1094:HIS:HD2	1.66	0.77
1:A:183:PRO:HD3	1:A:230:THR:HB	1.67	0.77
1:A:237:GLU:HG2	1:A:240:LYS:NZ	1.99	0.77
1:A:80:THR:HG22	1:A:83:VAL:H	1.50	0.77
1:A:9:VAL:HG13	1:A:12:LEU:HB3	1.67	0.77
1:A:1173:ASN:HD22	1:A:1173:ASN:C	1.92	0.77
1:A:1110:ILE:HD13	1:A:1110:ILE:C	2.07	0.77
1:A:714:ASN:HD21	1:A:1254:PHE:H	1.34	0.76
1:A:502:VAL:HG11	1:A:571:ILE:HB	1.68	0.76
1:A:72:ILE:HG12	1:A:137:ALA:HB2	1.68	0.75
1:A:1154:ARG:HH11	1:A:1154:ARG:CG	1.97	0.75
1:A:435:GLU:HG2	1:A:436:MET:HE2	1.69	0.75
1:A:372:TYR:CE1	1:A:410:VAL:HG21	2.21	0.74
1:A:878:LEU:O	1:A:882:LEU:HG	1.87	0.74
1:A:935:ARG:HH22	2:T:2107:A:H4'	1.52	0.74
1:A:309:LYS:O	1:A:313:THR:HG22	1.87	0.73
1:A:1100:ASP:OD1	1:A:1102:THR:CG2	2.36	0.73
1:A:80:THR:CG2	1:A:83:VAL:H	2.00	0.73
1:A:1154:ARG:HG3	1:A:1154:ARG:NH1	1.98	0.73
1:A:180:PHE:CE2	1:A:186:VAL:HG12	2.23	0.73
1:A:163:GLU:HG2	1:A:164:GLU:H	1.53	0.73
1:A:20:MET:HE2	1:A:430:LEU:HG	1.71	0.72
1:A:38:ILE:HG13	1:A:39:GLU:N	2.04	0.72
1:A:432:GLU:HG2	1:A:456:ARG:HH22	1.54	0.72
1:A:165:LEU:O	1:A:169:ILE:HG12	1.90	0.72
1:A:806:ARG:O	1:A:806:ARG:HG2	1.90	0.71
1:A:950:ILE:HD12	1:A:950:ILE:O	1.91	0.71
1:A:307:HIS:CD2	1:A:391:ALA:H	2.09	0.71
1:A:854:THR:HG21	1:A:872:ALA:CB	2.20	0.70
1:A:356:THR:HG22	1:A:358:THR:H	1.55	0.70
1:A:1245:THR:O	1:A:1246:LYS:HE3	1.91	0.70
1:A:155:LEU:O	1:A:256:PHE:HA	1.92	0.70
1:A:491:ILE:HD13	1:A:555:ALA:HB3	1.73	0.69
1:A:302:ILE:O	1:A:388:LEU:HD12	1.92	0.69
1:A:305:VAL:HG13	1:A:306:ASP:H	1.57	0.69
1:A:15:ARG:NH2	1:A:38:ILE:HG21	2.05	0.69
1:A:626:ILE:HG22	1:A:645:VAL:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:SER:O	1:A:1022:THR:HG21	1.93	0.69
1:A:229:LEU:HG	1:A:242:VAL:HG11	1.74	0.68
1:A:111:LEU:HD23	1:A:111:LEU:H	1.59	0.68
1:A:187:SER:C	1:A:189:GLU:H	2.01	0.68
1:A:949:THR:HG23	1:A:953:ARG:HH12	1.58	0.68
1:A:800:THR:HG22	1:A:803:ARG:HH11	1.57	0.68
1:A:496:LEU:HD23	1:A:497:LEU:N	2.09	0.68
1:A:801:ASN:HD22	1:A:1012:GLU:HG3	1.59	0.68
1:A:752:ARG:H	1:A:763:ASN:ND2	1.91	0.68
1:A:80:THR:HG23	1:A:82:PHE:H	1.59	0.67
1:A:12:LEU:HD22	1:A:27:LEU:HD22	1.76	0.67
1:A:611:TYR:H	1:A:1181:TRP:HD1	1.40	0.67
1:A:836:VAL:CG2	1:A:837:PRO:HD2	2.24	0.67
1:A:723:LEU:HB3	1:A:1110:ILE:HD12	1.77	0.67
1:A:930:ILE:HD11	1:A:1021:TYR:CB	2.24	0.67
1:A:870:PRO:HG3	1:A:893:ARG:HG3	1.76	0.66
1:A:937:ARG:HG3	1:A:937:ARG:NH2	2.02	0.66
1:A:2:ALA:O	1:A:3:GLU:HG2	1.95	0.66
1:A:529:ILE:HD11	1:A:575:GLN:CD	2.21	0.66
1:A:874:THR:HG23	1:A:875:PRO:HD2	1.78	0.66
1:A:1057:LEU:HD23	1:A:1057:LEU:H	1.58	0.66
1:A:126:ILE:HG22	1:A:127:GLY:N	2.08	0.66
1:A:260:GLU:O	1:A:263:GLU:HG3	1.95	0.66
1:A:582:THR:HG22	1:A:583:ILE:HG12	1.76	0.66
1:A:783:GLU:OE1	1:A:905:THR:HG21	1.95	0.66
1:A:187:SER:O	1:A:190:VAL:HG12	1.96	0.66
1:A:1025:LEU:O	1:A:1029:ILE:HG12	1.96	0.65
1:A:1234:ALA:C	1:A:1235:ILE:HD12	2.21	0.65
1:A:244:GLN:O	1:A:248:GLU:HB3	1.96	0.65
1:A:611:TYR:HD1	1:A:1181:TRP:HB2	1.60	0.65
1:A:126:ILE:HG23	1:A:399:GLN:NE2	2.11	0.65
1:A:313:THR:HB	1:A:363:HIS:CE1	2.32	0.65
1:A:539:THR:HG23	1:A:564:ARG:HG2	1.77	0.65
1:A:779:GLY:C	1:A:781:ASP:H	2.04	0.65
1:A:949:THR:HG23	1:A:953:ARG:CZ	2.27	0.64
1:A:858:ARG:H	2:T:2104:G:P	2.20	0.64
1:A:901:ASN:C	1:A:901:ASN:HD22	2.06	0.64
1:A:180:PHE:CD2	1:A:186:VAL:HG12	2.32	0.64
1:A:39:GLU:HA	1:A:42:ARG:HB3	1.78	0.64
1:A:80:THR:HG23	1:A:82:PHE:N	2.12	0.64
1:A:534:GLU:O	1:A:536:GLN:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:HIS:HB3	1:A:152:ILE:HG23	1.80	0.64
1:A:280:SER:HB3	1:A:284:HIS:CE1	2.33	0.64
1:A:717:ILE:C	1:A:717:ILE:HD12	2.23	0.64
1:A:628:LEU:HB3	1:A:632:VAL:HG13	1.80	0.63
1:A:103:GLY:O	1:A:105:ILE:HG12	1.99	0.63
1:A:168:HIS:CD2	1:A:171:MET:HE2	2.33	0.63
1:A:59:ASP:O	1:A:77:ASN:HB2	1.98	0.63
1:A:152:ILE:HB	1:A:260:GLU:HG3	1.81	0.63
1:A:590:GLU:HB3	1:A:644:VAL:HG22	1.81	0.63
1:A:308:GLY:HA3	1:A:420:ASN:ND2	2.14	0.63
1:A:951:ASN:OD1	1:A:1049:THR:HG23	1.99	0.63
1:A:4:ILE:HB	1:A:8:LEU:HD22	1.81	0.62
1:A:57:ALA:HB1	1:A:78:CYS:O	1.98	0.62
1:A:562:LEU:H	1:A:562:LEU:HD12	1.64	0.62
1:A:948:GLN:O	1:A:952:GLN:HG3	1.98	0.62
1:A:985:LEU:HD13	1:A:993:LEU:HD13	1.82	0.62
1:A:471:ALA:HA	1:A:474:LEU:HD12	1.81	0.61
1:A:93:ALA:HA	1:A:96:VAL:CG1	2.30	0.61
1:A:828:LYS:NZ	1:A:1036:SER:HA	2.15	0.61
1:A:35:GLU:O	1:A:38:ILE:HG12	2.01	0.61
1:A:700:SER:O	1:A:1179:ARG:HD2	2.01	0.61
1:A:16:THR:HG22	1:A:18:ALA:H	1.66	0.60
1:A:296:HIS:CE1	1:A:360:HIS:HD2	2.19	0.60
1:A:1057:LEU:HD23	1:A:1057:LEU:N	2.14	0.60
1:A:83:VAL:HG21	1:A:128:GLU:CD	2.26	0.60
1:A:712:ALA:O	1:A:715:THR:HB	2.01	0.60
1:A:1049:THR:HG22	1:A:1056:ILE:HB	1.84	0.60
1:A:86:ASP:HA	1:A:402:GLU:OE1	2.01	0.60
1:A:894:ILE:HD12	1:A:894:ILE:H	1.67	0.60
1:A:157:ALA:O	1:A:254:THR:HG23	2.01	0.60
1:A:800:THR:HG21	1:A:1073:GLY:HA2	1.83	0.60
1:A:993:LEU:HD23	1:A:1021:TYR:CZ	2.36	0.60
1:A:181:ILE:HG23	1:A:185:ASP:OD1	2.02	0.59
1:A:976:ILE:O	1:A:1014:ILE:HG22	2.02	0.59
1:A:496:LEU:HD23	1:A:496:LEU:C	2.27	0.59
1:A:779:GLY:C	1:A:781:ASP:N	2.60	0.59
1:A:179:GLU:HB3	1:A:227:VAL:HG22	1.85	0.59
1:A:493:LYS:HB3	1:A:494:PRO:HD2	1.85	0.59
1:A:195:TYR:CD1	1:A:195:TYR:O	2.56	0.59
1:A:618:ARG:NH1	1:A:652:ALA:O	2.36	0.59
1:A:806:ARG:N	1:A:807:PRO:HD3	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:TYR:CD1	1:A:1021:TYR:C	2.80	0.59
1:A:806:ARG:H	1:A:807:PRO:CD	2.13	0.58
1:A:120:VAL:HA	1:A:123:VAL:HG12	1.85	0.58
1:A:65:LYS:HE3	1:A:101:VAL:HG21	1.85	0.58
1:A:41:MET:HA	1:A:44:SER:OG	2.02	0.58
1:A:356:THR:HG23	1:A:357:PRO:HD2	1.85	0.58
1:A:529:ILE:HG13	1:A:529:ILE:O	2.02	0.58
1:A:658:ARG:HG2	1:A:658:ARG:HH11	1.68	0.58
1:A:702:ARG:CB	1:A:705:LEU:HB2	2.34	0.58
1:A:190:VAL:HG13	1:A:191:VAL:HG23	1.83	0.58
1:A:956:HIS:O	1:A:959:SER:HB3	2.04	0.58
1:A:502:VAL:CG1	1:A:512:VAL:HG12	2.33	0.58
1:A:544:GLU:HB3	1:A:549:LEU:HG	1.86	0.58
1:A:30:ALA:HB1	1:A:36:LEU:HD23	1.85	0.57
1:A:611:TYR:N	1:A:1181:TRP:HD1	2.02	0.57
1:A:372:TYR:HE1	1:A:410:VAL:CG2	2.17	0.57
1:A:530:VAL:HG22	1:A:652:ALA:HB2	1.87	0.57
1:A:1121:ASN:HD21	1:A:1167:VAL:H	1.50	0.57
1:A:1182:ILE:HD12	1:A:1183:ARG:N	2.20	0.57
1:A:13:ARG:HD2	1:A:20:MET:SD	2.45	0.57
1:A:1176:ALA:O	1:A:1177:LYS:HD2	2.03	0.57
1:A:221:LYS:HD3	1:A:221:LYS:C	2.29	0.57
1:A:428:GLU:HG2	1:A:431:LEU:HD12	1.87	0.57
1:A:24:LYS:O	1:A:24:LYS:HG2	2.04	0.57
1:A:163:GLU:HG2	1:A:164:GLU:N	2.19	0.57
1:A:237:GLU:OE2	1:A:237:GLU:HA	2.04	0.57
1:A:128:GLU:O	1:A:130:ILE:HG22	2.05	0.57
1:A:214:LYS:HD3	1:A:1135:PRO:HG2	1.87	0.57
1:A:861:GLY:O	1:A:866:LYS:HE3	2.04	0.57
1:A:723:LEU:CD2	1:A:1110:ILE:CD1	2.70	0.56
1:A:384:ASP:O	1:A:413:PRO:HG2	2.04	0.56
1:A:387:ILE:HD12	1:A:476:LEU:HD21	1.85	0.56
1:A:862:HIS:HD2	1:A:864:SER:OG	1.89	0.56
1:A:957:GLU:C	1:A:959:SER:H	2.13	0.56
1:A:105:ILE:HG21	1:A:111:LEU:HD22	1.86	0.56
1:A:229:LEU:O	1:A:242:VAL:HB	2.06	0.56
1:A:388:LEU:HB3	1:A:417:VAL:HG22	1.86	0.56
2:T:2106:C:C2'	2:T:2107:A:H5'	2.35	0.56
1:A:105:ILE:CG2	1:A:110:VAL:HB	2.35	0.56
1:A:1093:LYS:HB3	1:A:1095:TYR:CE1	2.40	0.56
1:A:21:MET:HG3	1:A:424:MET:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ILE:O	1:A:320:LEU:HD23	2.06	0.56
1:A:1121:ASN:ND2	1:A:1167:VAL:H	2.03	0.56
2:T:2106:C:H2'	2:T:2107:A:H5'	1.88	0.56
1:A:9:VAL:HB	1:A:20:MET:HE3	1.86	0.55
1:A:369:HIS:NE2	1:A:406:LEU:HD23	2.21	0.55
1:A:188:ALA:O	1:A:192:GLU:HB2	2.07	0.55
1:A:641:ILE:HD13	1:A:642:LYS:O	2.07	0.55
1:A:168:HIS:HD2	1:A:171:MET:HE2	1.71	0.55
1:A:304:HIS:CE1	1:A:305:VAL:HG12	2.42	0.55
1:A:741:ASN:HD21	1:A:745:GLU:HB2	1.70	0.55
1:A:810:SER:O	1:A:811:GLU:HG2	2.06	0.55
1:A:579:LYS:O	1:A:582:THR:HB	2.06	0.55
1:A:430:LEU:HA	1:A:433:LEU:HB2	1.89	0.55
1:A:611:TYR:H	1:A:1181:TRP:CD1	2.23	0.55
1:A:809:TYR:HD1	1:A:811:GLU:HB2	1.72	0.55
1:A:970:SER:HB2	1:A:1075:THR:HG23	1.89	0.55
1:A:130:ILE:HG12	1:A:131:ASN:N	2.22	0.54
1:A:502:VAL:HG12	1:A:512:VAL:CG1	2.36	0.54
1:A:849:SER:HA	1:A:863:PRO:HG3	1.89	0.54
1:A:169:ILE:O	1:A:173:VAL:HG23	2.08	0.54
1:A:949:THR:HG22	1:A:950:ILE:N	2.21	0.54
1:A:78:CYS:HB3	1:A:89:PHE:CE2	2.41	0.54
1:A:605:THR:HG22	1:A:606:PRO:O	2.08	0.54
1:A:854:THR:HG23	1:A:855:THR:HG23	1.90	0.54
1:A:874:THR:HG22	1:A:877:ALA:H	1.72	0.54
1:A:73:ILE:HG23	1:A:259:PHE:CE1	2.43	0.54
1:A:812:ASP:O	1:A:813:PHE:C	2.50	0.54
1:A:132:ILE:N	1:A:132:ILE:HD12	2.23	0.54
1:A:25:LYS:O	1:A:28:THR:HG22	2.07	0.54
1:A:581:GLY:HA2	1:A:584:LYS:NZ	2.23	0.54
1:A:957:GLU:C	1:A:959:SER:N	2.64	0.54
1:A:120:VAL:HA	1:A:123:VAL:CG1	2.38	0.54
1:A:824:MET:HE1	1:A:1040:ILE:CD1	2.37	0.54
1:A:154:VAL:HG12	1:A:258:ARG:HB2	1.89	0.54
1:A:832:LEU:HD21	1:A:937:ARG:O	2.08	0.54
1:A:924:MET:HE1	1:A:928:LEU:HD21	1.90	0.54
1:A:151:ARG:O	1:A:261:VAL:HG23	2.08	0.53
1:A:629:PRO:HG2	1:A:632:VAL:HG11	1.89	0.53
1:A:105:ILE:HG23	1:A:110:VAL:HB	1.91	0.53
1:A:729:ASN:HD21	1:A:740:PHE:H	1.55	0.53
1:A:1150:LYS:HD2	1:A:1150:LYS:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:CD	1:A:1210:ARG:HH12	2.16	0.53
1:A:658:ARG:HG2	1:A:658:ARG:NH1	2.23	0.53
1:A:558:ASN:HB3	1:A:1210:ARG:HD3	1.90	0.53
1:A:740:PHE:HD2	1:A:745:GLU:HG2	1.74	0.53
1:A:1182:ILE:HG13	1:A:1184:TYR:CE2	2.44	0.53
1:A:107:ASP:HB3	1:A:110:VAL:HG23	1.91	0.53
1:A:1150:LYS:HD2	1:A:1150:LYS:N	2.23	0.53
1:A:851:GLY:HA3	2:T:2105:C:C5'	2.36	0.53
1:A:723:LEU:HD23	1:A:1110:ILE:HD12	1.86	0.52
1:A:949:THR:CG2	1:A:953:ARG:HH12	2.20	0.52
1:A:62:ILE:HD13	1:A:259:PHE:HB3	1.90	0.52
1:A:844:ARG:HH11	1:A:844:ARG:HB3	1.74	0.52
1:A:44:SER:O	1:A:47:ILE:HG22	2.09	0.52
1:A:130:ILE:CG1	1:A:131:ASN:N	2.71	0.52
1:A:33:ASP:OD1	1:A:36:LEU:HB2	2.09	0.52
1:A:65:LYS:HB2	1:A:97:LEU:HD11	1.91	0.52
1:A:794:GLU:HA	1:A:794:GLU:OE1	2.10	0.52
1:A:105:ILE:HD12	1:A:110:VAL:CG1	2.39	0.52
1:A:499:ILE:HD13	1:A:512:VAL:HG11	1.91	0.52
1:A:1243:ASN:HB2	1:A:1244:PRO:HD2	1.92	0.52
1:A:174:ALA:O	1:A:258:ARG:NH1	2.42	0.52
1:A:140:GLY:HA3	1:A:157:ALA:HB1	1.91	0.52
1:A:374:LYS:HE3	1:A:594:TYR:CZ	2.45	0.52
1:A:363:HIS:HD2	1:A:364:VAL:N	2.08	0.51
1:A:479:PHE:C	1:A:481:ASP:N	2.66	0.51
2:T:2104:G:H5''	2:T:2105:C:OP1	2.09	0.51
1:A:7:SER:CB	1:A:10:LYS:HB3	2.36	0.51
1:A:122:LEU:O	1:A:123:VAL:C	2.54	0.51
1:A:401:ARG:NH1	1:A:445:TYR:OH	2.42	0.51
1:A:562:LEU:HD12	1:A:562:LEU:N	2.25	0.51
1:A:143:LEU:C	1:A:143:LEU:HD12	2.36	0.51
1:A:187:SER:C	1:A:189:GLU:N	2.68	0.51
1:A:294:LYS:HE3	1:A:358:THR:O	2.11	0.51
1:A:440:GLU:HA	1:A:440:GLU:OE1	2.11	0.51
1:A:764:TYR:OH	1:A:1094:HIS:CD2	2.57	0.51
1:A:191:VAL:HA	1:A:194:GLU:HB3	1.92	0.51
1:A:806:ARG:N	1:A:807:PRO:CD	2.73	0.51
1:A:558:ASN:HD22	1:A:1210:ARG:HH21	1.59	0.51
1:A:808:ASP:C	1:A:810:SER:H	2.19	0.51
1:A:947:ASP:C	1:A:949:THR:H	2.18	0.50
1:A:66:ILE:HG13	1:A:66:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:SER:OG	1:A:744:ALA:HB3	2.11	0.50
1:A:894:ILE:HD12	1:A:894:ILE:N	2.25	0.50
1:A:4:ILE:HD12	1:A:5:THR:H	1.77	0.50
1:A:183:PRO:HD3	1:A:230:THR:CB	2.39	0.50
1:A:1100:ASP:OD1	1:A:1100:ASP:C	2.55	0.50
1:A:33:ASP:HB3	1:A:36:LEU:HB3	1.92	0.50
1:A:182:LYS:HB2	1:A:185:ASP:OD2	2.11	0.50
1:A:276:VAL:CG1	1:A:277:ALA:N	2.74	0.50
1:A:495:PHE:CD2	1:A:521:ILE:HB	2.46	0.50
1:A:608:PHE:HD1	1:A:633:GLU:O	1.94	0.50
1:A:954:ARG:NH2	1:A:1047:GLU:O	2.44	0.50
1:A:3:GLU:HB2	1:A:24:LYS:NZ	2.27	0.50
1:A:19:GLY:HA2	1:A:394:ASP:HA	1.93	0.50
1:A:610:GLY:O	1:A:611:TYR:C	2.55	0.50
1:A:249:HIS:O	1:A:250:ASN:CB	2.60	0.50
1:A:324:TYR:CG	1:A:357:PRO:HD3	2.47	0.50
1:A:511:VAL:HG23	1:A:562:LEU:HG	1.94	0.50
1:A:955:ALA:HB2	1:A:1090:SER:HB3	1.94	0.49
1:A:1057:LEU:N	1:A:1057:LEU:CD2	2.75	0.49
1:A:301:THR:HG23	1:A:309:LYS:HD2	1.93	0.49
1:A:324:TYR:CD1	1:A:357:PRO:HD3	2.47	0.49
1:A:1054:ASP:OD1	1:A:1091:CYS:N	2.43	0.49
1:A:408:ARG:O	1:A:408:ARG:HD3	2.11	0.49
1:A:833:ILE:HG23	1:A:989:TRP:NE1	2.26	0.49
1:A:901:ASN:C	1:A:901:ASN:ND2	2.71	0.49
1:A:950:ILE:C	1:A:950:ILE:CD1	2.78	0.49
1:A:67:ASP:O	1:A:69:ASN:N	2.46	0.49
1:A:133:ARG:HD2	1:A:133:ARG:O	2.12	0.49
1:A:319:VAL:HB	1:A:473:ILE:HG21	1.94	0.49
1:A:797:CYS:HB2	1:A:1012:GLU:HB3	1.93	0.49
1:A:1019:ASN:HB3	1:A:1022:THR:HG21	1.88	0.49
1:A:9:VAL:HG13	1:A:23:CYS:HB3	1.94	0.49
1:A:50:ALA:C	1:A:52:LYS:H	2.21	0.49
1:A:73:ILE:HG21	1:A:257:ILE:HG21	1.95	0.49
1:A:304:HIS:HB3	1:A:307:HIS:CG	2.47	0.49
1:A:300:GLY:HA3	1:A:383:MET:SD	2.53	0.49
1:A:432:GLU:HG2	1:A:456:ARG:NH2	2.23	0.49
1:A:741:ASN:ND2	1:A:745:GLU:HB2	2.27	0.49
1:A:1243:ASN:CB	1:A:1244:PRO:HD2	2.42	0.49
1:A:28:THR:HG23	1:A:29:GLU:HG3	1.94	0.49
1:A:806:ARG:O	1:A:806:ARG:CG	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:TYR:C	1:A:1021:TYR:HD1	2.18	0.49
1:A:172:HIS:C	1:A:172:HIS:CD2	2.90	0.49
1:A:1111:VAL:HG22	1:A:1115:ASP:OD2	2.13	0.49
1:A:9:VAL:CG1	1:A:12:LEU:HB3	2.41	0.48
1:A:93:ALA:CA	1:A:96:VAL:HG12	2.38	0.48
1:A:567:LYS:O	1:A:570:GLU:HG2	2.12	0.48
1:A:73:ILE:HB	1:A:155:LEU:CD2	2.38	0.48
1:A:378:THR:HG23	1:A:380:ALA:H	1.78	0.48
1:A:122:LEU:O	1:A:125:LYS:N	2.46	0.48
1:A:1150:LYS:H	1:A:1150:LYS:CD	2.27	0.48
1:A:801:ASN:ND2	1:A:1012:GLU:HG3	2.28	0.48
1:A:752:ARG:N	1:A:763:ASN:HD21	2.03	0.48
1:A:828:LYS:HZ3	1:A:1039:GLU:CD	2.21	0.48
1:A:1124:TYR:O	1:A:1128:THR:HB	2.14	0.48
1:A:4:ILE:CB	1:A:8:LEU:HD22	2.42	0.48
1:A:4:ILE:HD13	1:A:8:LEU:HB3	1.96	0.48
1:A:235:VAL:HG13	1:A:606:PRO:HG2	1.95	0.48
1:A:267:LYS:O	1:A:268:VAL:C	2.57	0.48
1:A:924:MET:CE	1:A:928:LEU:HG	2.44	0.48
1:A:576:VAL:HG21	1:A:583:ILE:HD12	1.96	0.48
1:A:597:SER:HA	1:A:637:PRO:HB3	1.96	0.48
1:A:848:PHE:O	1:A:849:SER:HB2	2.13	0.48
1:A:369:HIS:CD2	1:A:406:LEU:HD23	2.48	0.47
1:A:839:VAL:O	1:A:843:LEU:HB2	2.14	0.47
1:A:930:ILE:HA	1:A:933:ILE:HG23	1.96	0.47
1:A:777:SER:OG	1:A:778:LEU:HD13	2.14	0.47
1:A:21:MET:HE1	1:A:430:LEU:CD2	2.43	0.47
1:A:76:VAL:O	1:A:76:VAL:HG22	2.12	0.47
1:A:376:MET:HG3	1:A:410:VAL:CG2	2.44	0.47
1:A:734:ALA:HB1	1:A:1136:ARG:O	2.14	0.47
1:A:842:MET:HE1	1:A:930:ILE:CG2	2.20	0.47
1:A:930:ILE:CD1	1:A:1021:TYR:HB2	2.34	0.47
1:A:1074:PHE:N	1:A:1074:PHE:CD2	2.77	0.47
1:A:227:VAL:HG22	1:A:227:VAL:O	2.14	0.47
1:A:296:HIS:CE1	1:A:360:HIS:CD2	3.01	0.47
1:A:363:HIS:C	1:A:363:HIS:CD2	2.92	0.47
1:A:833:ILE:HD12	1:A:937:ARG:HG2	1.97	0.47
1:A:838:SER:HB2	1:A:840:GLU:CD	2.39	0.47
1:A:862:HIS:CD2	1:A:864:SER:OG	2.68	0.47
1:A:871:GLN:HE21	1:A:921:GLY:HA3	1.79	0.47
1:A:878:LEU:HD13	1:A:897:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:GLU:O	1:A:439:ARG:HG3	2.14	0.47
1:A:545:MET:HE2	1:A:550:LEU:HD11	1.97	0.47
1:A:388:LEU:HD22	1:A:404:ILE:HD11	1.96	0.47
1:A:521:ILE:HG23	1:A:521:ILE:O	2.14	0.47
1:A:784:ALA:O	1:A:788:GLU:HG3	2.14	0.47
1:A:862:HIS:CD2	1:A:864:SER:H	2.33	0.47
1:A:1003:LEU:HD12	1:A:1003:LEU:N	2.29	0.47
1:A:1185:VAL:CG1	1:A:1261:CYS:SG	3.03	0.47
1:A:49:ALA:HB2	1:A:123:VAL:HG11	1.97	0.47
1:A:410:VAL:HG22	1:A:410:VAL:O	2.15	0.47
1:A:733:LEU:CD1	1:A:739:PRO:HD3	2.39	0.47
1:A:898:SER:OG	1:A:899:PRO:HD2	2.14	0.47
1:A:967:VAL:HA	1:A:1081:THR:HB	1.96	0.47
1:A:714:ASN:ND2	1:A:1254:PHE:H	2.05	0.47
1:A:790:PHE:C	1:A:790:PHE:CD1	2.93	0.47
1:A:862:HIS:HD2	1:A:864:SER:H	1.63	0.47
1:A:977:SER:HA	1:A:1013:LYS:HA	1.97	0.47
1:A:245:LEU:HA	1:A:248:GLU:OE2	2.15	0.47
1:A:301:THR:HB	1:A:363:HIS:CE1	2.49	0.46
1:A:529:ILE:HD11	1:A:575:GLN:OE1	2.15	0.46
1:A:1121:ASN:ND2	5:A:3503:HOH:O	2.48	0.46
1:A:657:LEU:H	1:A:673:VAL:CG2	2.28	0.46
1:A:9:VAL:HB	1:A:20:MET:CE	2.45	0.46
1:A:1212:LEU:HD23	1:A:1212:LEU:HA	1.68	0.46
1:A:809:TYR:CD1	1:A:811:GLU:HB2	2.51	0.46
1:A:496:LEU:C	1:A:496:LEU:CD2	2.88	0.46
2:T:2106:C:O2'	2:T:2107:A:H5'	2.16	0.46
1:A:64:THR:HG23	1:A:64:THR:O	2.15	0.46
1:A:857:ASN:H	1:A:857:ASN:ND2	2.13	0.46
1:A:376:MET:HE2	1:A:410:VAL:HG23	1.98	0.46
1:A:947:ASP:C	1:A:949:THR:N	2.74	0.46
1:A:117:GLU:O	1:A:120:VAL:HG22	2.16	0.46
1:A:123:VAL:HG13	1:A:124:ALA:N	2.31	0.46
1:A:133:ARG:HD2	1:A:133:ARG:C	2.41	0.46
1:A:272:PHE:HZ	1:A:313:THR:HG21	1.81	0.46
1:A:630:GLU:HA	1:A:630:GLU:OE1	2.16	0.46
1:A:969:LEU:HD23	1:A:1076:THR:HA	1.98	0.46
1:A:970:SER:O	1:A:972:ALA:N	2.41	0.46
1:A:534:GLU:O	1:A:535:THR:C	2.59	0.45
1:A:589:PHE:CZ	1:A:645:VAL:HB	2.52	0.45
1:A:795:ALA:O	1:A:798:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:LEU:O	1:A:1051:TYR:HE1	1.98	0.45
1:A:1047:GLU:OE2	1:A:1047:GLU:HA	2.16	0.45
1:A:143:LEU:HB2	1:A:156:VAL:O	2.17	0.45
1:A:414:TYR:HB3	1:A:483:TYR:CE2	2.52	0.45
1:A:160:GLY:C	1:A:251:ALA:HB2	2.41	0.45
1:A:476:LEU:O	1:A:479:PHE:HB2	2.16	0.45
1:A:20:MET:HG3	1:A:430:LEU:HD23	1.98	0.45
1:A:92:PHE:CE1	1:A:132:ILE:HD11	2.51	0.45
1:A:794:GLU:OE1	1:A:1013:LYS:NZ	2.43	0.45
1:A:222:LYS:C	1:A:224:THR:N	2.74	0.45
1:A:273:ALA:O	1:A:276:VAL:HG12	2.16	0.45
1:A:715:THR:CG2	1:A:716:ARG:N	2.77	0.45
1:A:951:ASN:OD1	1:A:1049:THR:CG2	2.64	0.45
1:A:167:LYS:O	1:A:171:MET:HG3	2.17	0.45
1:A:824:MET:HE1	1:A:1040:ILE:HD11	1.99	0.45
1:A:322:LYS:HD3	1:A:470:GLU:OE2	2.17	0.45
1:A:1093:LYS:HB3	1:A:1095:TYR:HE1	1.81	0.45
1:A:405:LEU:HD13	1:A:445:TYR:CE2	2.52	0.44
1:A:872:ALA:O	1:A:873:CYS:CB	2.61	0.44
1:A:301:THR:HG22	1:A:365:ASP:HA	1.99	0.44
1:A:21:MET:HG2	1:A:425:VAL:HG22	1.99	0.44
1:A:187:SER:O	1:A:189:GLU:N	2.50	0.44
1:A:249:HIS:O	1:A:250:ASN:HB3	2.16	0.44
1:A:12:LEU:HD23	1:A:23:CYS:HB3	1.98	0.44
1:A:118:GLU:O	1:A:121:ALA:HB3	2.18	0.44
1:A:194:GLU:HG3	1:A:220:MET:SD	2.57	0.44
1:A:388:LEU:HD22	1:A:404:ILE:CD1	2.47	0.44
1:A:593:VAL:HB	1:A:670:ALA:O	2.17	0.44
1:A:985:LEU:CD1	1:A:993:LEU:HD13	2.46	0.44
1:A:1050:VAL:HG22	1:A:1055:ILE:HG12	1.98	0.44
1:A:408:ARG:HD3	1:A:408:ARG:C	2.42	0.44
1:A:543:VAL:O	1:A:549:LEU:HD23	2.18	0.44
1:A:949:THR:CG2	1:A:950:ILE:N	2.80	0.44
1:A:1004:PRO:C	1:A:1006:GLY:H	2.26	0.44
1:A:276:VAL:HG13	1:A:277:ALA:N	2.32	0.44
1:A:361:TYR:CZ	1:A:480:LEU:HB3	2.52	0.44
1:A:276:VAL:CG2	1:A:314:ALA:HA	2.48	0.44
1:A:984:LEU:HD23	1:A:1029:ILE:HD12	2.00	0.44
1:A:41:MET:O	1:A:45:GLY:N	2.51	0.43
1:A:401:ARG:CZ	1:A:401:ARG:HB3	2.49	0.43
1:A:356:THR:HG22	1:A:358:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:MET:HE1	1:A:1040:ILE:HG13	1.99	0.43
1:A:871:GLN:HB2	1:A:922:TRP:CD1	2.53	0.43
1:A:1110:ILE:CD1	1:A:1110:ILE:C	2.75	0.43
1:A:130:ILE:O	1:A:131:ASN:HB3	2.18	0.43
1:A:521:ILE:HD12	1:A:525:GLU:OE2	2.18	0.43
1:A:857:ASN:H	1:A:857:ASN:HD22	1.66	0.43
1:A:1128:THR:HG23	1:A:1131:GLY:H	1.82	0.43
1:A:61:VAL:CG1	1:A:84:ALA:HB1	2.48	0.43
1:A:154:VAL:HG12	1:A:258:ARG:CB	2.48	0.43
1:A:238:PRO:HB2	1:A:1171:LEU:HD22	2.01	0.43
1:A:308:GLY:HA3	1:A:420:ASN:HD22	1.83	0.43
1:A:879:LYS:HG2	5:A:3512:HOH:O	2.17	0.43
1:A:522:LYS:HG3	1:A:552:GLU:HB3	2.00	0.43
1:A:1111:VAL:HG23	1:A:1112:SER:N	2.34	0.43
1:A:876:ARG:HE	1:A:876:ARG:HB3	1.59	0.43
1:A:969:LEU:HD21	1:A:1069:PHE:CD2	2.54	0.43
1:A:111:LEU:H	1:A:111:LEU:CD2	2.27	0.43
1:A:521:ILE:O	1:A:552:GLU:HA	2.18	0.43
1:A:723:LEU:HD23	1:A:1110:ILE:CG1	2.43	0.43
1:A:729:ASN:ND2	1:A:732:LEU:HD12	2.34	0.43
1:A:828:LYS:HZ2	1:A:1036:SER:HA	1.82	0.43
1:A:12:LEU:HD23	1:A:23:CYS:O	2.18	0.43
1:A:316:ILE:HG21	1:A:354:TYR:CZ	2.54	0.43
1:A:1077:ASN:O	1:A:1081:THR:CG2	2.56	0.43
1:A:222:LYS:O	1:A:224:THR:N	2.51	0.43
1:A:924:MET:O	1:A:925:PHE:C	2.62	0.43
1:A:176:SER:O	1:A:177:LYS:C	2.61	0.42
1:A:177:LYS:HG2	1:A:258:ARG:CZ	2.49	0.42
1:A:265:ILE:O	1:A:266:GLU:HG2	2.18	0.42
1:A:1094:HIS:N	1:A:1094:HIS:ND1	2.66	0.42
1:A:1173:ASN:HA	1:A:1174:PRO:HD2	1.80	0.42
1:A:611:TYR:HB3	1:A:626:ILE:HD11	2.00	0.42
1:A:379:GLY:HA2	1:A:658:ARG:NH2	2.35	0.42
1:A:732:LEU:HD22	1:A:766:LYS:HD2	2.01	0.42
1:A:12:LEU:HG	1:A:12:LEU:O	2.20	0.42
1:A:228:SER:O	1:A:229:LEU:C	2.62	0.42
1:A:611:TYR:CE2	1:A:613:PRO:HG3	2.54	0.42
1:A:111:LEU:O	1:A:115:PHE:HD1	2.03	0.42
1:A:396:PRO:HD2	1:A:434:VAL:HG13	2.02	0.42
1:A:523:VAL:HA	1:A:540:CYS:SG	2.60	0.42
1:A:531:GLY:HA3	1:A:575:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:MET:CG	1:A:425:VAL:HG22	2.49	0.42
1:A:184:GLU:CD	1:A:184:GLU:H	2.28	0.42
1:A:199:LEU:HD23	1:A:199:LEU:O	2.18	0.42
1:A:220:MET:O	1:A:224:THR:HG23	2.19	0.42
1:A:579:LYS:HA	1:A:580:PRO:HD3	1.89	0.42
1:A:805:TYR:O	1:A:806:ARG:HB2	2.19	0.42
1:A:938:LEU:HD13	1:A:938:LEU:HA	1.68	0.42
1:A:157:ALA:C	1:A:254:THR:HG23	2.43	0.42
1:A:537:LYS:HE2	1:A:537:LYS:HB3	1.87	0.42
1:A:857:ASN:O	1:A:858:ARG:C	2.62	0.42
1:A:1003:LEU:N	1:A:1003:LEU:CD1	2.82	0.42
1:A:1057:LEU:CD1	1:A:1065:LEU:HD22	2.50	0.42
1:A:291:GLU:O	1:A:291:GLU:HG2	2.18	0.42
1:A:629:PRO:HD3	1:A:642:LYS:O	2.20	0.42
1:A:852:ALA:HB2	2:T:2104:G:H5'	2.02	0.42
1:A:13:ARG:CD	1:A:20:MET:SD	3.08	0.42
1:A:80:THR:HG22	1:A:83:VAL:HB	2.01	0.42
1:A:265:ILE:O	1:A:266:GLU:CB	2.68	0.42
1:A:421:LYS:HG3	1:A:460:LEU:HD23	2.01	0.42
1:A:833:ILE:HD12	1:A:833:ILE:HA	1.51	0.42
1:A:908:LYS:HD2	1:A:914:ARG:HB2	2.01	0.42
1:A:845:HIS:C	1:A:929:GLY:HA2	2.45	0.41
1:A:1044:ASP:HB3	1:A:1047:GLU:HG2	2.00	0.41
1:A:1157:ILE:HG22	1:A:1185:VAL:HG11	2.01	0.41
1:A:89:PHE:CD1	1:A:89:PHE:O	2.73	0.41
1:A:356:THR:O	1:A:357:PRO:C	2.63	0.41
1:A:397:MET:O	1:A:398:PRO:C	2.63	0.41
1:A:503:PHE:HE1	1:A:513:THR:HG23	1.85	0.41
1:A:558:ASN:HB3	1:A:1210:ARG:HB3	2.01	0.41
1:A:558:ASN:CB	1:A:1210:ARG:HB3	2.50	0.41
1:A:88:GLY:C	1:A:90:GLN:N	2.77	0.41
1:A:236:MET:HG2	1:A:608:PHE:CZ	2.55	0.41
1:A:472:LYS:O	1:A:475:GLU:HB3	2.20	0.41
1:A:629:PRO:HD2	1:A:632:VAL:HG11	2.02	0.41
1:A:930:ILE:HD12	1:A:931:GLY:N	2.34	0.41
1:A:957:GLU:O	1:A:961:THR:HB	2.19	0.41
1:A:34:ILE:O	1:A:38:ILE:HG23	2.21	0.41
1:A:495:PHE:HA	1:A:518:ARG:O	2.19	0.41
1:A:957:GLU:O	1:A:959:SER:N	2.53	0.41
1:A:4:ILE:HD13	1:A:8:LEU:CB	2.50	0.41
1:A:279:MET:HA	1:A:282:GLN:HE21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ARG:HA	1:A:292:ARG:HD3	1.82	0.41
1:A:729:ASN:ND2	1:A:740:PHE:H	2.18	0.41
1:A:924:MET:HE1	1:A:928:LEU:CD2	2.51	0.41
1:A:1007:SER:O	1:A:1008:VAL:HG13	2.20	0.41
1:A:76:VAL:HG11	1:A:93:ALA:CB	2.50	0.41
1:A:1026:GLU:O	1:A:1030:PHE:CD1	2.73	0.41
1:A:782:THR:OG1	1:A:783:GLU:N	2.52	0.41
1:A:799:LEU:HD12	1:A:799:LEU:HA	1.78	0.41
1:A:897:ILE:O	1:A:897:ILE:HG23	2.21	0.41
1:A:242:VAL:O	1:A:243:GLY:C	2.63	0.41
1:A:366:CYS:SG	1:A:383:MET:HE1	2.60	0.41
1:A:597:SER:HA	1:A:637:PRO:CB	2.49	0.41
1:A:657:LEU:H	1:A:673:VAL:HG22	1.85	0.41
1:A:954:ARG:NH1	1:A:1049:THR:HB	2.36	0.41
1:A:1185:VAL:HG11	1:A:1261:CYS:SG	2.61	0.41
1:A:143:LEU:C	1:A:143:LEU:CD1	2.93	0.41
1:A:151:ARG:HB3	1:A:152:ILE:HG22	2.02	0.41
1:A:441:LEU:HD23	1:A:441:LEU:HA	1.96	0.41
1:A:495:PHE:CE2	1:A:521:ILE:HB	2.56	0.41
1:A:708:GLN:HB3	1:A:1151:GLN:HE21	1.85	0.41
1:A:1001:GLY:HA3	1:A:1009:VAL:CG2	2.51	0.41
1:A:1014:ILE:O	1:A:1014:ILE:HG13	2.21	0.41
1:A:1082:PHE:CD1	1:A:1082:PHE:N	2.89	0.41
1:A:1142:LEU:HD23	1:A:1142:LEU:HA	1.79	0.41
1:A:222:LYS:C	1:A:224:THR:H	2.29	0.41
1:A:395:GLY:O	1:A:396:PRO:C	2.63	0.41
1:A:840:GLU:CD	1:A:840:GLU:H	2.29	0.41
1:A:105:ILE:HG22	1:A:106:THR:N	2.36	0.40
1:A:503:PHE:CD2	1:A:1203:TYR:HB2	2.56	0.40
1:A:677:LEU:HD23	1:A:677:LEU:HA	1.86	0.40
1:A:993:LEU:HD23	1:A:1021:TYR:CE1	2.56	0.40
1:A:1026:GLU:HG3	1:A:1030:PHE:CE1	2.56	0.40
1:A:143:LEU:HD12	1:A:143:LEU:O	2.20	0.40
1:A:181:ILE:HG13	1:A:182:LYS:HG3	2.04	0.40
1:A:203:MET:HE3	1:A:209:LYS:HA	2.03	0.40
1:A:397:MET:HE2	1:A:397:MET:HA	2.03	0.40
1:A:839:VAL:HG12	1:A:843:LEU:HD23	2.03	0.40
1:A:1096:TYR:O	1:A:1097:SER:C	2.63	0.40
1:A:11:GLU:HA	1:A:14:GLU:HB2	2.02	0.40
1:A:427:ASP:C	1:A:429:GLU:H	2.29	0.40
1:A:463:LEU:C	1:A:465:GLY:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:SER:HA	1:A:999:PRO:HD3	1.81	0.40
1:A:1262:SER:O	1:A:1264:ARG:N	2.55	0.40
1:A:20:MET:C	1:A:21:MET:HE2	2.46	0.40
1:A:626:ILE:HG21	1:A:643:MET:SD	2.61	0.40
1:A:629:PRO:HG2	1:A:632:VAL:CG1	2.50	0.40
1:A:1100:ASP:CG	1:A:1102:THR:HG22	2.43	0.40
1:A:62:ILE:HD13	1:A:259:PHE:CB	2.51	0.40
1:A:220:MET:HE2	1:A:220:MET:HA	2.02	0.40
1:A:305:VAL:HG13	1:A:306:ASP:N	2.30	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	1193/1289 (93%)	1030 (86%)	125 (10%)	38 (3%)	3 5

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ALA
1	A	250	ASN
1	A	266	GLU
1	A	268	VAL
1	A	305	VAL
1	A	806	ARG
1	A	970	SER
1	A	4	ILE
1	A	68	GLY
1	A	102	ALA
1	A	188	ALA
1	A	223	PHE

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Mol	Chain	Res	Type
1	A	611	TYR
1	A	780	ILE
1	A	872	ALA
1	A	1007	SER
1	A	1263	SER
1	A	31	ASN
1	A	104	LYS
1	A	150	ALA
1	A	247	LYS
1	A	495	PHE
1	A	51	LYS
1	A	149	GLY
1	A	229	LEU
1	A	269	GLU
1	A	350	SER
1	A	873	CYS
1	A	972	ALA
1	A	1097	SER
1	A	103	GLY
1	A	273	ALA
1	A	141	ASP
1	A	531	GLY
1	A	679	GLY
1	A	613	PRO
1	A	904	VAL
1	A	641	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
1	A	995/1060 (94%)	819 (82%)	176 (18%)	2 3

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	56	VAL
1	A	59	ASP
1	A	76	VAL
1	A	80	THR
1	A	81	ASP
1	A	105	ILE
1	A	119	ARG
1	A	130	ILE
1	A	143	LEU
1	A	152	ILE
1	A	155	LEU
1	A	163	GLU
1	A	165	LEU
1	A	166	VAL
1	A	181	ILE
1	A	196	GLN
1	A	203	MET
1	A	205	SER
1	A	211	ILE
1	A	230	THR
1	A	235	VAL
1	A	239	SER
1	A	241	THR
1	A	245	LEU
1	A	246	LEU
1	A	248	GLU
1	A	249	HIS
1	A	254	THR
1	A	258	ARG
1	A	266	GLU
1	A	285	MET
1	A	292	ARG
1	A	307	HIS
1	A	310	THR
1	A	313	THR
1	A	320	LEU
1	A	353	GLU
1	A	355	ASP
1	A	364	VAL
1	A	371	ASP
1	A	378	THR
1	A	387	ILE

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Mol	Chain	Res	Type
1	A	397	MET
1	A	399	GLN
1	A	406	LEU
1	A	416	ILE
1	A	419	LEU
1	A	433	LEU
1	A	437	GLU
1	A	443	SER
1	A	452	THR
1	A	456	ARG
1	A	460	LEU
1	A	468	GLU
1	A	480	LEU
1	A	496	LEU
1	A	499	ILE
1	A	502	VAL
1	A	503	PHE
1	A	516	VAL
1	A	520	ILE
1	A	522	LYS
1	A	529	ILE
1	A	530	VAL
1	A	535	THR
1	A	537	LYS
1	A	539	THR
1	A	549	LEU
1	A	563	LEU
1	A	568	ARG
1	A	569	GLU
1	A	571	ILE
1	A	573	ARG
1	A	582	THR
1	A	583	ILE
1	A	587	THR
1	A	592	GLU
1	A	593	VAL
1	A	595	ILE
1	A	618	ARG
1	A	622	VAL
1	A	625	THR
1	A	628	LEU
1	A	632	VAL

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Mol	Chain	Res	Type
1	A	641	ILE
1	A	646	THR
1	A	651	ILE
1	A	676	VAL
1	A	705	LEU
1	A	706	SER
1	A	715	THR
1	A	717	ILE
1	A	733	LEU
1	A	741	ASN
1	A	745	GLU
1	A	762	ILE
1	A	778	LEU
1	A	781	ASP
1	A	782	THR
1	A	785	VAL
1	A	789	LYS
1	A	791	LEU
1	A	796	GLU
1	A	799	LEU
1	A	804	LEU
1	A	808	ASP
1	A	809	TYR
1	A	816	SER
1	A	832	LEU
1	A	833	ILE
1	A	843	LEU
1	A	844	ARG
1	A	856	ASN
1	A	869	LEU
1	A	873	CYS
1	A	874	THR
1	A	879	LYS
1	A	893	ARG
1	A	896	ASP
1	A	901	ASN
1	A	905	THR
1	A	910	SER
1	A	915	CYS
1	A	916	ILE
1	A	924	MET
1	A	930	ILE

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Mol	Chain	Res	Type
1	A	933	ILE
1	A	937	ARG
1	A	938	LEU
1	A	943	ILE
1	A	948	GLN
1	A	949	THR
1	A	950	ILE
1	A	960	VAL
1	A	961	THR
1	A	967	VAL
1	A	970	SER
1	A	984	LEU
1	A	991	GLU
1	A	993	LEU
1	A	996	LEU
1	A	1002	ARG
1	A	1008	VAL
1	A	1010	THR
1	A	1013	LYS
1	A	1014	ILE
1	A	1016	SER
1	A	1017	MET
1	A	1022	THR
1	A	1028	LEU
1	A	1033	LEU
1	A	1040	ILE
1	A	1049	THR
1	A	1053	ASP
1	A	1076	THR
1	A	1081	THR
1	A	1084	GLU
1	A	1094	HIS
1	A	1099	VAL
1	A	1102	THR
1	A	1110	ILE
1	A	1116	LEU
1	A	1123	LEU
1	A	1128	THR
1	A	1152	LEU
1	A	1154	ARG
1	A	1173	ASN
1	A	1182	ILE

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Mol	Chain	Res	Type
1	A	1183	ARG
1	A	1185	VAL
1	A	1200	LEU
1	A	1237	GLN
1	A	1239	ILE
1	A	1242	SER
1	A	1246	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	55	ASN
1	A	90	GLN
1	A	114	GLN
1	A	147	GLN
1	A	168	HIS
1	A	282	GLN
1	A	284	HIS
1	A	296	HIS
1	A	298	ASN
1	A	307	HIS
1	A	360	HIS
1	A	363	HIS
1	A	399	GLN
1	A	409	GLN
1	A	558	ASN
1	A	586	HIS
1	A	614	GLN
1	A	714	ASN
1	A	729	ASN
1	A	741	ASN
1	A	763	ASN
1	A	814	ASN
1	A	857	ASN
1	A	862	HIS
1	A	871	GLN
1	A	901	ASN
1	A	948	GLN
1	A	1077	ASN
1	A	1094	HIS
1	A	1121	ASN

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Mol	Chain	Res	Type
1	A	1122	ASN
1	A	1155	ASN
1	A	1173	ASN
1	A	1178	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	T	3/7 (42%)	1 (33%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	T	2105	C

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GH3	A	2502	4	31,33,33	2.42	10 (32%)	44,52,52	2.30	16 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GH3	T	2501	-	31,33,33	2.82	13 (41%)	44,52,52	2.40	15 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GH3	A	2502	4	-	1/22/34/34	0/3/3/3
3	GH3	T	2501	-	-	5/22/34/34	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	2501	GH3	O6-C6	8.21	1.39	1.23
3	A	2502	GH3	O6-C6	8.05	1.38	1.23
3	T	2501	GH3	C2-N2	6.46	1.49	1.34
3	T	2501	GH3	PA-O3A	6.33	1.66	1.59
3	A	2502	GH3	C2-N2	6.22	1.48	1.34
3	T	2501	GH3	PB-O3A	4.65	1.64	1.59
3	T	2501	GH3	C8-N9	-3.29	1.30	1.37
3	A	2502	GH3	C8-N9	-3.08	1.30	1.37
3	A	2502	GH3	C5-N7	-3.04	1.33	1.39
3	A	2502	GH3	C5-C4	2.95	1.46	1.38
3	T	2501	GH3	C5-C4	2.95	1.46	1.38
3	T	2501	GH3	C5-N7	-2.89	1.33	1.39
3	T	2501	GH3	C8-N7	-2.73	1.24	1.32
3	A	2502	GH3	C4-N9	2.62	1.44	1.38
3	A	2502	GH3	C8-N7	-2.61	1.25	1.32
3	A	2502	GH3	PA-O3A	2.59	1.62	1.59
3	A	2502	GH3	PB-O3B	-2.56	1.56	1.59
3	T	2501	GH3	C3'-C2'	-2.53	1.46	1.52
3	T	2501	GH3	C3'-C4'	-2.50	1.47	1.52
3	T	2501	GH3	C4-N9	2.39	1.44	1.38
3	T	2501	GH3	PA-O1A	2.18	1.58	1.50
3	T	2501	GH3	O2'-C2'	-2.10	1.38	1.43
3	A	2502	GH3	C3'-C4'	-2.02	1.48	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2502	GH3	N9-C4-N3	6.12	138.19	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	2501	GH3	N9-C4-N3	5.72	137.39	125.95
3	T	2501	GH3	C1'-N9-C4	-5.55	110.08	126.49
3	T	2501	GH3	C8-N7-C5	5.23	113.57	104.26
3	A	2502	GH3	C8-N7-C5	5.15	113.44	104.26
3	T	2501	GH3	C1'-N9-C8	4.86	140.55	126.73
3	A	2502	GH3	C5-C4-N3	-4.83	120.71	128.39
3	A	2502	GH3	C1'-N9-C4	-4.51	113.15	126.49
3	T	2501	GH3	C5-C4-N3	-4.16	121.77	128.39
3	A	2502	GH3	C1'-N9-C8	4.02	138.16	126.73
3	T	2501	GH3	C6-C5-N7	4.00	137.57	130.29
3	T	2501	GH3	C2-N3-C4	3.98	119.16	112.30
3	A	2502	GH3	C2-N3-C4	3.88	118.98	112.30
3	A	2502	GH3	C6-C5-N7	3.61	136.86	130.29
3	T	2501	GH3	O4'-C1'-N9	3.44	116.16	108.36
3	T	2501	GH3	C4-C5-N7	-3.30	105.44	110.67
3	A	2502	GH3	C4-C5-N7	-3.19	105.62	110.67
3	T	2501	GH3	O6-C6-C5	-2.78	119.19	126.53
3	T	2501	GH3	C5-C4-N9	-2.69	100.84	105.66
3	A	2502	GH3	C5-C4-N9	-2.54	101.10	105.66
3	T	2501	GH3	O4'-C4'-C5'	2.36	113.59	109.34
3	A	2502	GH3	O4'-C4'-C5'	2.36	113.59	109.34
3	A	2502	GH3	O6-C6-C5	-2.33	120.38	126.53
3	A	2502	GH3	C5-C6-N1	2.23	118.93	113.25
3	T	2501	GH3	N2-C2-N1	2.23	121.47	116.76
3	T	2501	GH3	C5-C6-N1	2.23	118.93	113.25
3	A	2502	GH3	C2'-C3'-C4'	2.23	106.99	102.97
3	A	2502	GH3	O2B-PB-O3A	2.15	113.08	107.27
3	T	2501	GH3	O2A-PA-O3A	2.12	113.00	107.27
3	A	2502	GH3	C4'-O4'-C1'	-2.10	106.75	109.69
3	A	2502	GH3	O4'-C1'-N9	2.05	113.02	108.36

There are no chirality outliers.

All (6) torsion outliers are listed below:

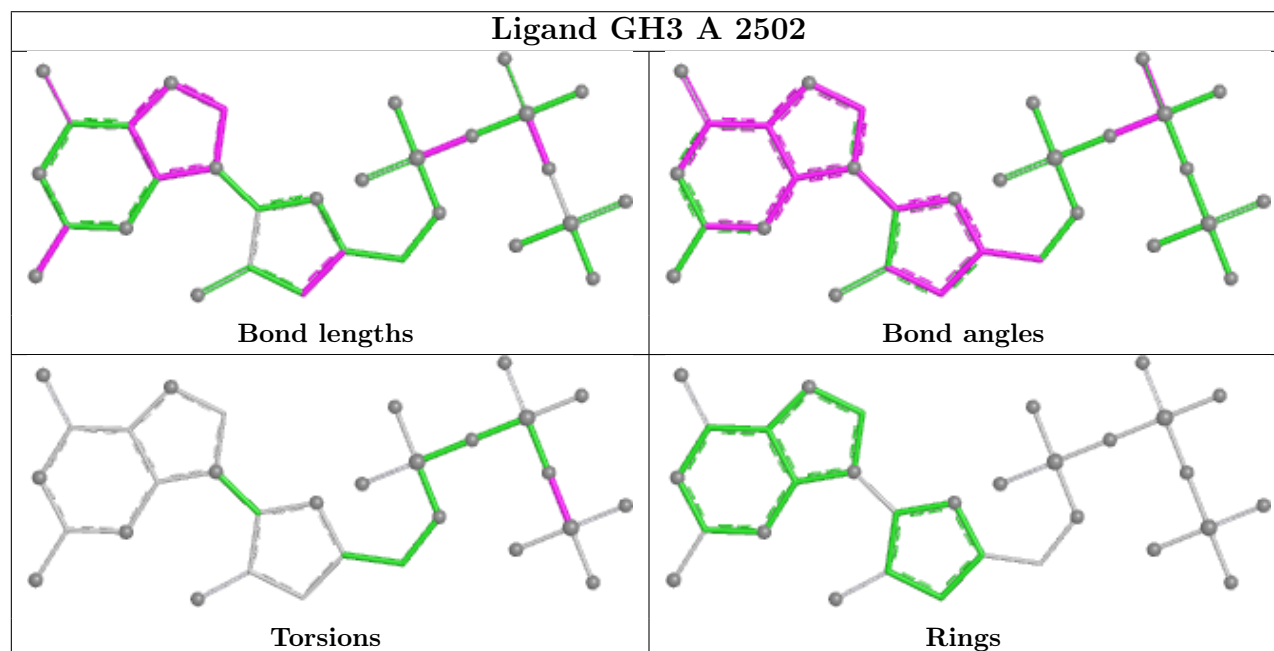
Mol	Chain	Res	Type	Atoms
3	A	2502	GH3	PB-O3B-PG-O3G
3	T	2501	GH3	PB-O3B-PG-O2G
3	T	2501	GH3	PB-O3A-PA-O5'
3	T	2501	GH3	PB-O3B-PG-O1G
3	T	2501	GH3	PG-O3B-PB-O2B
3	T	2501	GH3	PA-O3A-PB-O2B

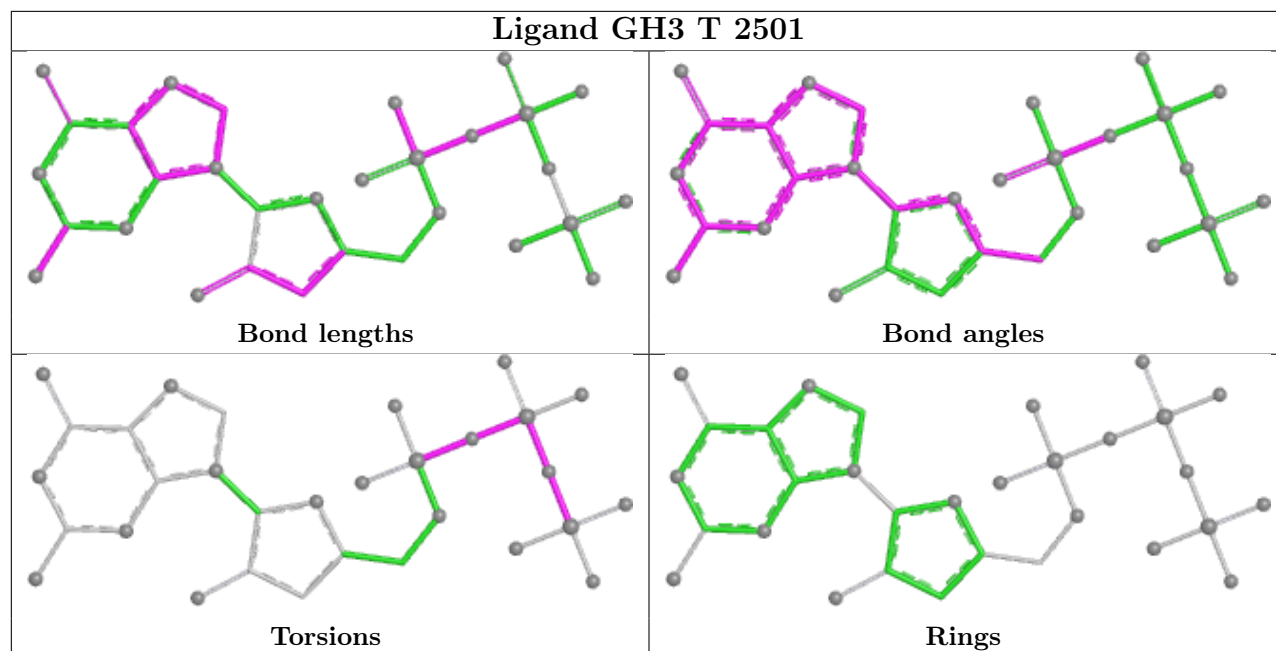
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2502	GH3	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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1203/1289 (93%)	-0.28	11 (0%) 81 78	18, 63, 117, 142	0
2	T	4/7 (57%)	1.83	1 (25%) 2 1	84, 91, 91, 98	0
All	All	1207/1296 (93%)	-0.28	12 (0%) 79 76	18, 63, 117, 142	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	807	PRO	4.0
1	A	1234	ALA	3.8
1	A	780	ILE	3.6
1	A	34	ILE	2.6
2	T	2106	C	2.6
1	A	191	VAL	2.5
1	A	326	GLY	2.4
1	A	1239	ILE	2.2
1	A	8	LEU	2.1
1	A	460	LEU	2.0
1	A	813	PHE	2.0
1	A	27	LEU	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](#)

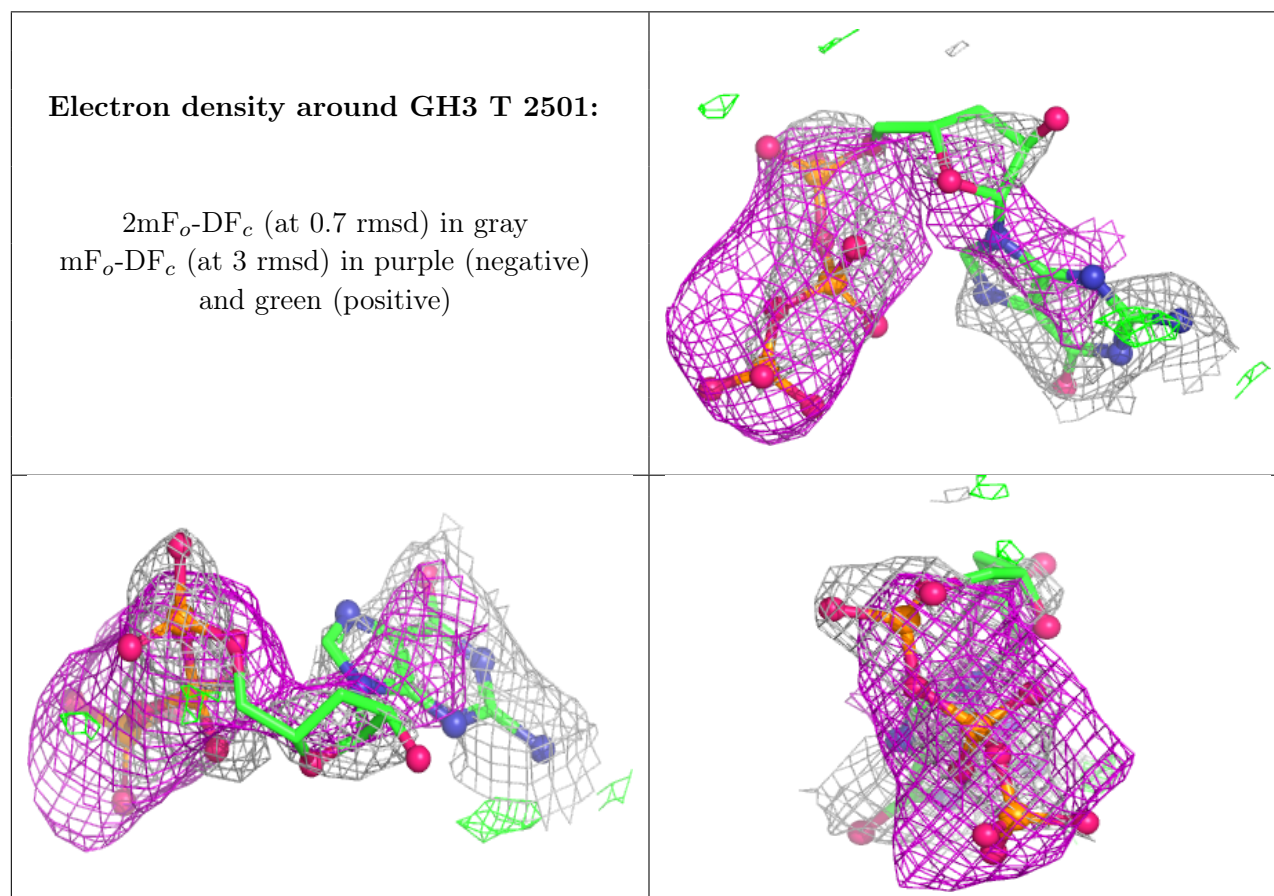
There are no oligosaccharides in this entry.

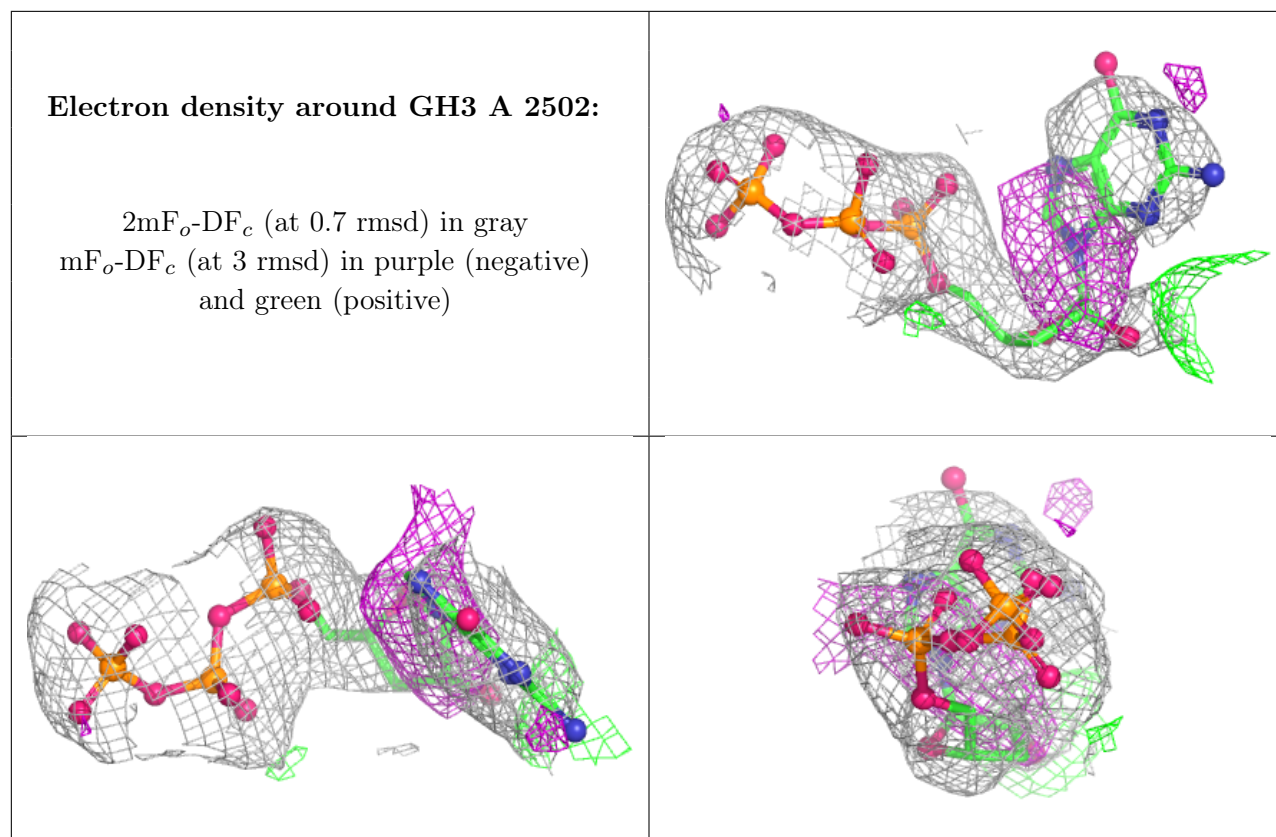
6.4 Ligands [i](#)

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
3	GH3	T	2501	31/31	0.52	0.16	65,92,109,128	0
3	GH3	A	2502	31/31	0.86	0.10	57,78,91,92	0
4	CA	A	3002	1/1	0.90	0.09	69,69,69,69	0
4	CA	A	3001	1/1	0.98	0.04	59,59,59,59	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.