Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 07:58 PM EST

PDB ID	:	1MWH
Title	:	REOVIRUS POLYMERASE LAMBDA3 BOUND TO MRNA CAP ANALOG
Authors	:	Tao, Y.; Farsetta, D.L.; Nibert, M.L.; Harrison, S.C.
Deposited on	:	2002-09-29
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

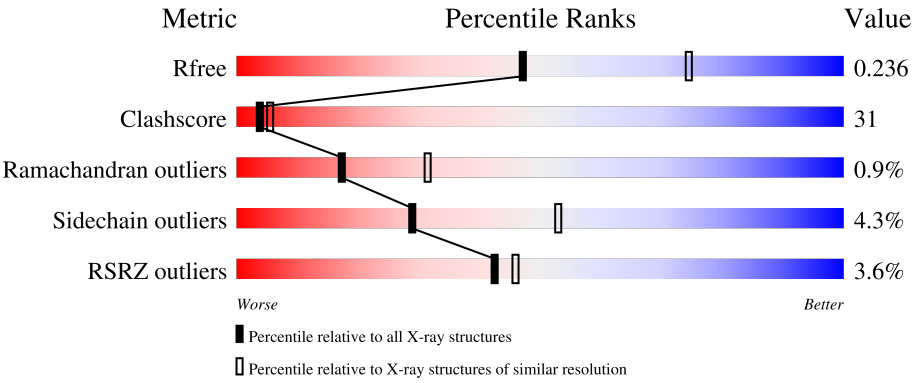
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1267	4% 60% 36%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10653 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.

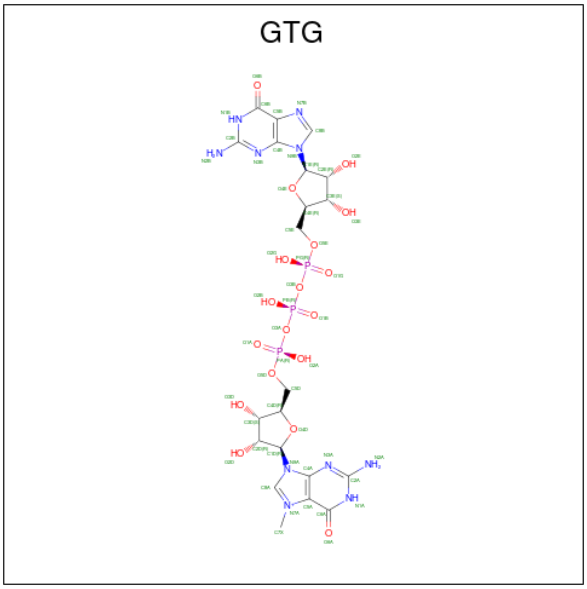
- Molecule 1 is a protein called MINOR CORE PROTEIN LAMBDA 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1256	9929	6337	1697	1831	64	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	1	1	1	0	0

- Molecule 3 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-GUANOSINE (three-letter code: GTG) (formula: $C_{21}H_{30}N_{10}O_{18}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	52	21	10	18	3	0	0

- Molecule 4 is water.

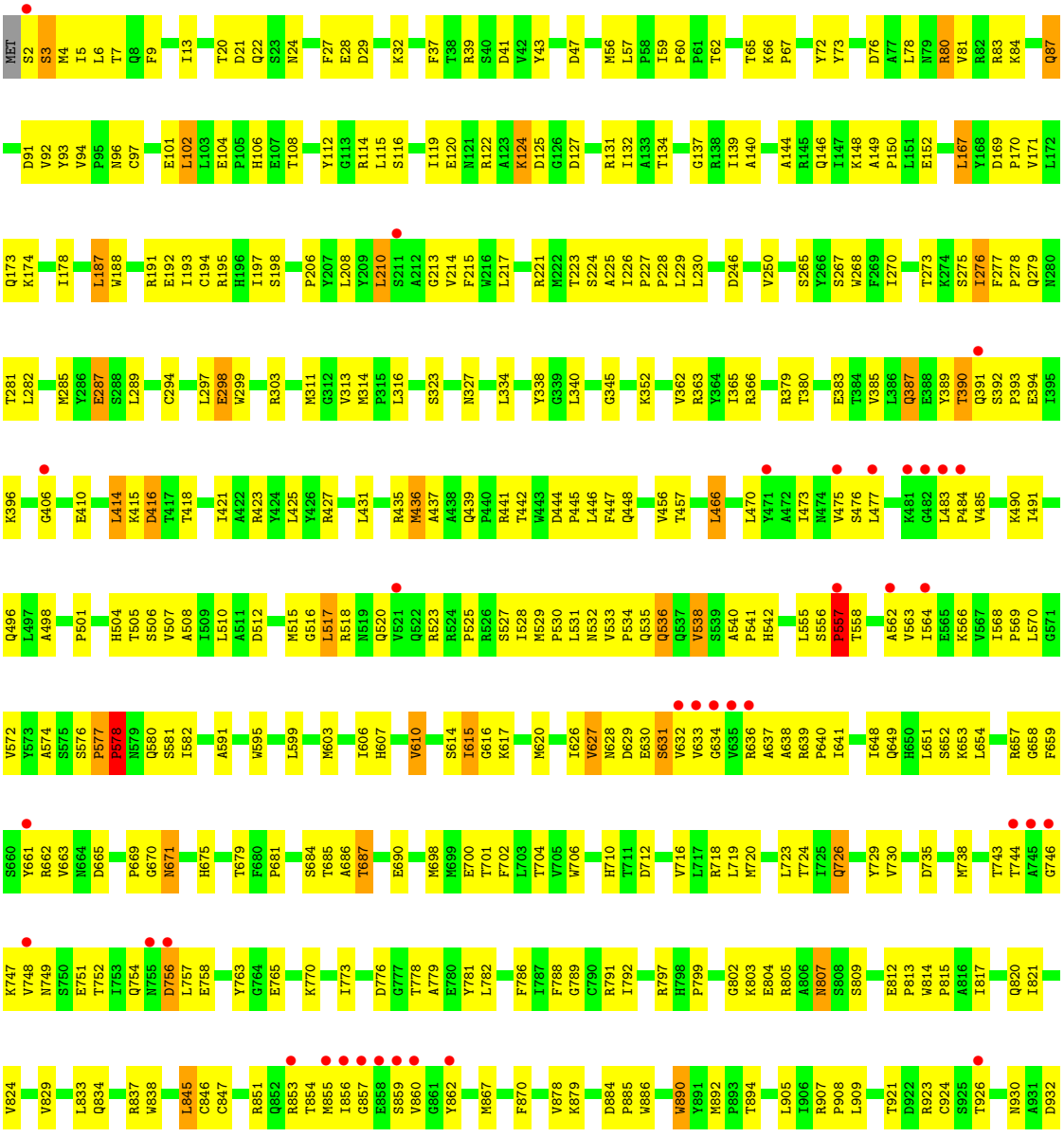
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	671	Total	O	0	0
			671	671		

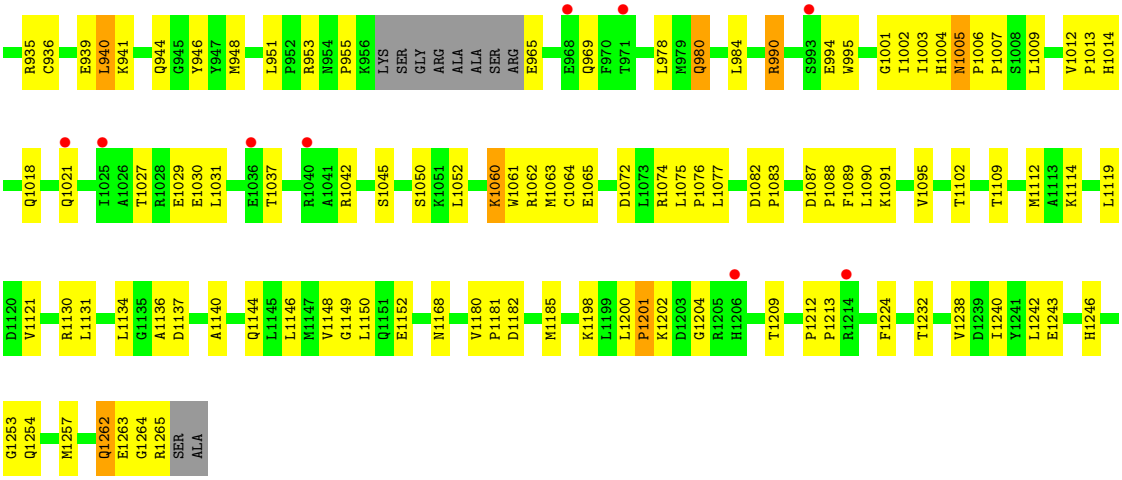
3 Residue-property plots (i)

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: MINOR CORE PROTEIN LAMBDA 3

Chain A:




B935 C936 E939 L940 K941 Q944 G945 Y946 Y947 M948 L951 P952 R953 N954 P955 K956 LYS SER GLY ARG ALA ALA SER ARG E965 E968 Q969 F970 T971 L978 H979 Q980 L984 R990 S993 E994 W995 G1001 I1002 I1003 H1004 N1005 P1006 P1007 S1008 L1009 V1012 P1013 H1014
Q1018 Q1021 I1025 A1026 T1027 R1028 E1029 E1030 L1031 E1036 T1037 R1040 A1041 R1042 S1045 S1050 K1051 L1052 K1060 W1061 R1062 M1063 C1064 E1065 D1072 L1073 R1074 L1075 P1076 L1077 D1082 P1083 D1087 P1088 F1089 L1090 K1091 V1095 T1102 T1109 M1112 A1113 K1114 L1119
D1120 V1121 R1130 L1131 L1134 G1135 A1136 D1137 A1140 Q1144 L1145 L1146 M1147 V1148 G1149 L1150 Q1151 E1152 N1168 V1180 P1181 D1182 M1185 K1198 L1199 L1200 P1201 K1202 D1203 G1204 R1205 H1206 T1209 P1212 P1213 K1214 F1224 T1232 V1238 D1239 I1240 Y1241 L1242 E1243 H1246
G1253 Q1254 M1257 Q1262 E1263 G1264 R1265 SER ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.89Å 84.94Å 249.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 2.50 49.88 – 2.49	Depositor EDS
% Data completeness (in resolution range)	93.1 (49.88-2.50) 93.1 (49.88-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.245 0.199 , 0.236	Depositor DCC
R_{free} test set	2636 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10653	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GTG, MN

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	0.46	2/10181 (0.0%)	0.67	7/13828 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	LYS	C-O	7.75	1.38	1.23
1	A	969	GLN	CG-CD	5.00	1.62	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	577	PRO	C-N-CD	-19.99	76.63	120.60
1	A	577	PRO	C-N-CA	13.73	179.66	122.00
1	A	557	PRO	CA-N-CD	-7.58	100.88	111.50
1	A	578	PRO	CA-N-CD	-6.01	103.09	111.50
1	A	1264	GLY	C-N-CA	-5.48	108.00	121.70
1	A	556	SER	C-N-CD	-5.46	108.59	120.60
1	A	1264	GLY	N-CA-C	-5.34	99.76	113.10

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	A	9929	0	9840	607	0
2	A	1	0	0	0	0
3	A	52	0	25	5	0
4	A	671	0	0	302	1
All	All	10653	0	9865	612	1

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 (612) 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:926:THR:HG21	1:A:1246:HIS:CG	1.61	1.36
1:A:277:PHE:HB2	4:A:2545:HOH:O	1.17	1.32
1:A:1146:LEU:HD22	4:A:2486:HOH:O	1.19	1.28
1:A:558:THR:HB	4:A:2600:HOH:O	1.14	1.27
1:A:197:ILE:HG12	4:A:2593:HOH:O	1.33	1.26
1:A:279:GLN:HB3	4:A:2648:HOH:O	1.28	1.23
1:A:1181:PRO:HD3	4:A:2611:HOH:O	1.30	1.23
1:A:1005:ASN:HB2	4:A:2454:HOH:O	1.39	1.22
1:A:529:MET:HG2	4:A:2531:HOH:O	1.39	1.20
1:A:718:ARG:HD2	4:A:2490:HOH:O	1.36	1.20
1:A:617:LYS:HE2	4:A:2414:HOH:O	1.43	1.19
1:A:1077:LEU:HD13	4:A:2652:HOH:O	1.37	1.19
1:A:637:ALA:HB3	4:A:2461:HOH:O	1.43	1.18
1:A:926:THR:CG2	1:A:1246:HIS:CD2	2.26	1.17
3:A:1425:GTG:O1G	4:A:2450:HOH:O	1.61	1.17
1:A:334:LEU:HD22	4:A:2597:HOH:O	1.46	1.14
1:A:1114:LYS:HE2	4:A:2580:HOH:O	1.49	1.11
1:A:93:TYR:HA	4:A:2501:HOH:O	1.49	1.11
1:A:447:PHE:CD2	4:A:2634:HOH:O	2.03	1.10
1:A:39:ARG:HB3	4:A:2613:HOH:O	1.52	1.07
1:A:860:VAL:HA	4:A:2578:HOH:O	1.53	1.06
1:A:879:LYS:HG3	4:A:2650:HOH:O	1.54	1.06
1:A:746:GLY:HA2	4:A:2474:HOH:O	1.54	1.06
1:A:719:LEU:HD12	4:A:2471:HOH:O	1.54	1.05
1:A:1262:GLN:HA	1:A:1265:ARG:HH11	1.16	1.05
1:A:93:TYR:HB2	4:A:2606:HOH:O	1.54	1.05
1:A:837:ARG:CD	4:A:2408:HOH:O	2.05	1.05
1:A:926:THR:HG21	1:A:1246:HIS:CD2	1.89	1.04
1:A:856:ILE:HB	4:A:2434:HOH:O	1.54	1.04
1:A:223:THR:HG22	1:A:225:ALA:H	1.24	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:SER:HB2	4:A:2463:HOH:O	1.57	1.02
1:A:1148:VAL:CG2	4:A:2667:HOH:O	2.07	1.02
1:A:1060:LYS:HE3	4:A:2555:HOH:O	1.60	1.02
1:A:926:THR:HG23	1:A:1246:HIS:CD2	1.91	1.02
1:A:1257:MET:SD	4:A:2547:HOH:O	2.19	1.01
1:A:505:THR:HA	4:A:2491:HOH:O	1.60	1.01
1:A:749:ASN:HD21	1:A:751:GLU:HB3	1.24	1.00
1:A:475:VAL:HA	4:A:2524:HOH:O	1.60	1.00
1:A:62:THR:HG23	4:A:2428:HOH:O	1.60	0.99
1:A:743:THR:HG22	1:A:744:THR:H	1.24	0.98
1:A:926:THR:CG2	1:A:1246:HIS:CG	2.45	0.98
1:A:323:SER:HB3	4:A:2645:HOH:O	1.64	0.98
1:A:669:PRO:HA	4:A:2493:HOH:O	1.64	0.97
1:A:278:PRO:HD3	4:A:2545:HOH:O	1.65	0.96
1:A:748:VAL:HG22	4:A:2443:HOH:O	1.65	0.96
1:A:1119:LEU:HD11	4:A:2563:HOH:O	1.65	0.96
1:A:557:PRO:HG2	1:A:781:TYR:OH	1.64	0.96
1:A:837:ARG:HD3	4:A:2408:HOH:O	1.63	0.95
1:A:362:VAL:HA	4:A:2488:HOH:O	1.66	0.95
1:A:747:LYS:HE3	4:A:2645:HOH:O	1.66	0.95
1:A:909:LEU:HD13	4:A:2643:HOH:O	1.65	0.94
1:A:1148:VAL:HG21	4:A:2667:HOH:O	1.66	0.94
1:A:743:THR:HG22	1:A:744:THR:N	1.81	0.92
1:A:807:ASN:CG	4:A:2577:HOH:O	2.07	0.91
1:A:724:THR:HG22	1:A:726:GLN:H	1.34	0.91
1:A:47:ASP:HA	4:A:2629:HOH:O	1.69	0.90
1:A:178:ILE:HD12	4:A:2408:HOH:O	1.70	0.90
1:A:770:LYS:HE2	4:A:2436:HOH:O	1.69	0.90
1:A:22:GLN:NE2	1:A:878:VAL:H	1.70	0.90
1:A:80:ARG:NE	4:A:2508:HOH:O	2.02	0.89
1:A:192:GLU:HG2	4:A:2644:HOH:O	1.72	0.89
1:A:1012:VAL:HG23	4:A:2563:HOH:O	1.72	0.89
1:A:735:ASP:CG	4:A:2423:HOH:O	2.11	0.88
1:A:1140:ALA:HA	4:A:2655:HOH:O	1.73	0.87
1:A:475:VAL:CA	4:A:2524:HOH:O	2.18	0.87
1:A:1061:TRP:CE3	4:A:2543:HOH:O	2.26	0.87
1:A:303:ARG:NE	4:A:2588:HOH:O	2.01	0.87
1:A:747:LYS:CE	4:A:2645:HOH:O	2.20	0.86
1:A:791:ARG:NH1	4:A:2390:HOH:O	2.07	0.86
1:A:119:ILE:HG12	4:A:2550:HOH:O	1.76	0.86
1:A:749:ASN:HD22	1:A:752:THR:H	1.20	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:PHE:HA	4:A:2669:HOH:O	1.74	0.86
1:A:1074:ARG:CZ	4:A:2558:HOH:O	2.22	0.86
1:A:221:ARG:NE	4:A:2411:HOH:O	2.03	0.85
1:A:1102:THR:HG21	4:A:2660:HOH:O	1.74	0.85
1:A:81:VAL:H	1:A:671:ASN:HD21	1.24	0.84
1:A:303:ARG:NH2	4:A:2588:HOH:O	2.10	0.84
1:A:965:GLU:N	4:A:2393:HOH:O	2.08	0.84
1:A:510:LEU:HD11	4:A:2646:HOH:O	1.78	0.84
1:A:1004:HIS:CD2	4:A:2487:HOH:O	2.30	0.84
1:A:859:SER:CB	4:A:2463:HOH:O	2.17	0.84
1:A:20:THR:HG21	4:A:2415:HOH:O	1.76	0.84
1:A:470:LEU:HD11	4:A:2491:HOH:O	1.77	0.83
1:A:749:ASN:ND2	1:A:751:GLU:HB3	1.94	0.83
1:A:758:GLU:HB3	4:A:2642:HOH:O	1.78	0.83
1:A:1119:LEU:HD21	4:A:2563:HOH:O	1.79	0.83
1:A:1074:ARG:NH2	4:A:2558:HOH:O	2.12	0.83
1:A:415:LYS:NZ	4:A:2499:HOH:O	2.11	0.82
1:A:447:PHE:HD2	4:A:2634:HOH:O	1.45	0.82
1:A:1254:GLN:NE2	4:A:2547:HOH:O	2.12	0.81
1:A:924:CYS:HA	4:A:2395:HOH:O	1.81	0.81
1:A:1089:PHE:HB2	4:A:2476:HOH:O	1.78	0.81
1:A:1262:GLN:HA	1:A:1265:ARG:NH1	1.94	0.81
1:A:1004:HIS:C	1:A:1006:PRO:HD3	2.01	0.81
1:A:93:TYR:CB	4:A:2606:HOH:O	2.19	0.81
1:A:122:ARG:NH1	4:A:2550:HOH:O	2.07	0.81
1:A:743:THR:CG2	1:A:744:THR:H	1.93	0.81
1:A:735:ASP:CB	4:A:2423:HOH:O	2.29	0.80
1:A:807:ASN:HB2	4:A:2577:HOH:O	1.80	0.80
1:A:847:CYS:SG	4:A:2537:HOH:O	2.38	0.80
1:A:641:ILE:HG12	4:A:2424:HOH:O	1.81	0.80
1:A:93:TYR:CA	4:A:2501:HOH:O	2.16	0.80
1:A:936:CYS:SG	1:A:940:LEU:HD11	2.22	0.79
1:A:807:ASN:CB	4:A:2577:HOH:O	2.28	0.79
1:A:173:GLN:OE1	4:A:2627:HOH:O	2.01	0.79
1:A:718:ARG:NH1	4:A:2490:HOH:O	2.07	0.79
1:A:653:LYS:HE2	4:A:2646:HOH:O	1.81	0.78
1:A:1001:GLY:O	4:A:2487:HOH:O	2.01	0.78
1:A:632:VAL:HA	4:A:2598:HOH:O	1.81	0.78
1:A:101:GLU:HG2	1:A:102:LEU:HD13	1.65	0.78
1:A:345:GLY:O	4:A:2417:HOH:O	2.02	0.77
1:A:505:THR:C	4:A:2521:HOH:O	2.23	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:LYS:CD	4:A:2442:HOH:O	2.31	0.77
1:A:628:ASN:OD1	4:A:2526:HOH:O	2.03	0.76
1:A:1137:ASP:HB3	4:A:2511:HOH:O	1.84	0.76
1:A:221:ARG:NH2	4:A:2411:HOH:O	2.18	0.76
1:A:1152:GLU:OE1	4:A:2664:HOH:O	2.02	0.76
1:A:770:LYS:CE	4:A:2436:HOH:O	2.32	0.76
1:A:885:PRO:N	4:A:2650:HOH:O	2.19	0.76
1:A:267:SER:HB3	4:A:2606:HOH:O	1.87	0.75
1:A:447:PHE:CE2	4:A:2634:HOH:O	2.34	0.75
1:A:704:THR:HB	4:A:2610:HOH:O	1.85	0.74
1:A:941:LYS:HE2	4:A:2438:HOH:O	1.85	0.74
1:A:303:ARG:CZ	4:A:2588:HOH:O	2.33	0.74
1:A:792:ILE:HD12	4:A:2488:HOH:O	1.87	0.74
1:A:562:ALA:HB1	4:A:2618:HOH:O	1.87	0.74
1:A:515:MET:HE2	1:A:527:SER:HB3	1.69	0.74
1:A:626:ILE:HA	4:A:2424:HOH:O	1.87	0.74
1:A:29:ASP:OD1	4:A:2435:HOH:O	2.05	0.74
1:A:747:LYS:HD3	4:A:2442:HOH:O	1.86	0.74
1:A:1072:ASP:OD1	1:A:1074:ARG:HD3	1.88	0.74
1:A:476:SER:N	4:A:2524:HOH:O	2.20	0.74
1:A:637:ALA:CB	4:A:2461:HOH:O	2.15	0.74
1:A:654:LEU:CD1	4:A:2669:HOH:O	2.35	0.74
1:A:294:CYS:SG	1:A:577:PRO:HD2	2.28	0.73
1:A:56:MET:HG2	1:A:188:TRP:CE2	2.23	0.73
1:A:924:CYS:CA	4:A:2395:HOH:O	2.33	0.73
1:A:926:THR:HG21	1:A:1246:HIS:CB	2.18	0.73
1:A:144:ALA:O	4:A:2386:HOH:O	2.07	0.73
1:A:536:GLN:HA	1:A:536:GLN:HE21	1.53	0.73
1:A:114:ARG:HB2	1:A:215:PHE:HE1	1.52	0.73
1:A:114:ARG:HB2	1:A:215:PHE:CE1	2.23	0.73
1:A:855:MET:HE3	4:A:2633:HOH:O	1.86	0.73
1:A:152:GLU:HG2	4:A:2613:HOH:O	1.88	0.72
1:A:379:ARG:HH12	1:A:387:GLN:NE2	1.86	0.72
1:A:626:ILE:CA	4:A:2424:HOH:O	2.37	0.72
1:A:146:GLN:HE22	1:A:805:ARG:H	1.38	0.72
1:A:1062:ARG:NH1	4:A:2651:HOH:O	2.22	0.72
1:A:886:TRP:HA	4:A:2439:HOH:O	1.90	0.72
1:A:654:LEU:HD11	4:A:2669:HOH:O	1.88	0.72
1:A:855:MET:HB3	4:A:2633:HOH:O	1.88	0.71
1:A:1082:ASP:N	4:A:2476:HOH:O	2.22	0.71
1:A:1074:ARG:NH1	4:A:2558:HOH:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:CYS:N	4:A:2395:HOH:O	2.23	0.71
1:A:32:LYS:HD2	4:A:2435:HOH:O	1.91	0.71
1:A:797:ARG:HD2	4:A:2624:HOH:O	1.89	0.71
1:A:1082:ASP:O	4:A:2476:HOH:O	2.09	0.71
1:A:191:ARG:NH1	4:A:2629:HOH:O	2.24	0.71
1:A:92:VAL:C	4:A:2501:HOH:O	2.30	0.71
1:A:365:ILE:HB	4:A:2488:HOH:O	1.90	0.71
1:A:506:SER:N	4:A:2521:HOH:O	2.24	0.71
1:A:1202:LYS:HB3	4:A:2651:HOH:O	1.90	0.71
1:A:1060:LYS:HG2	4:A:2459:HOH:O	1.91	0.70
1:A:197:ILE:O	1:A:221:ARG:NH1	2.20	0.70
1:A:93:TYR:N	4:A:2501:HOH:O	2.25	0.70
1:A:1061:TRP:CZ3	4:A:2543:HOH:O	2.42	0.70
1:A:470:LEU:CG	4:A:2491:HOH:O	2.38	0.70
1:A:1185:MET:HB3	4:A:2660:HOH:O	1.92	0.70
1:A:884:ASP:C	4:A:2650:HOH:O	2.29	0.70
1:A:615:ILE:HG23	1:A:616:GLY:H	1.55	0.70
1:A:630:GLU:OE1	4:A:2526:HOH:O	2.08	0.70
1:A:41:ASP:OD2	4:A:2420:HOH:O	2.07	0.69
1:A:221:ARG:NH1	1:A:221:ARG:HB2	2.08	0.69
1:A:637:ALA:N	4:A:2461:HOH:O	2.25	0.69
1:A:718:ARG:NH2	4:A:2620:HOH:O	2.25	0.69
1:A:568:ILE:HG13	4:A:2614:HOH:O	1.90	0.69
1:A:80:ARG:NH2	4:A:2508:HOH:O	2.25	0.69
1:A:441:ARG:HD2	4:A:2427:HOH:O	1.92	0.69
1:A:754:GLN:O	1:A:758:GLU:HG3	1.93	0.69
1:A:821:ILE:HG23	1:A:845:LEU:HD13	1.75	0.69
1:A:941:LYS:CE	4:A:2438:HOH:O	2.39	0.69
1:A:39:ARG:CB	4:A:2613:HOH:O	2.24	0.69
1:A:1005:ASN:HB2	1:A:1130:ARG:HH22	1.57	0.69
1:A:675:HIS:HD2	4:A:2412:HOH:O	1.77	0.68
1:A:978:LEU:O	4:A:2626:HOH:O	2.10	0.68
1:A:80:ARG:CZ	4:A:2508:HOH:O	2.39	0.68
1:A:470:LEU:CD1	4:A:2491:HOH:O	2.34	0.68
1:A:807:ASN:HD22	1:A:807:ASN:H	1.41	0.68
1:A:847:CYS:HA	4:A:2537:HOH:O	1.92	0.68
1:A:457:THR:N	4:A:2592:HOH:O	2.26	0.68
1:A:83:ARG:HG2	1:A:92:VAL:HA	1.75	0.68
1:A:614:SER:O	4:A:2414:HOH:O	2.12	0.67
1:A:921:THR:HG23	1:A:932:ASP:HB2	1.74	0.67
1:A:470:LEU:HG	4:A:2491:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:VAL:HG13	4:A:2602:HOH:O	1.92	0.67
1:A:1263:GLU:OE1	4:A:2589:HOH:O	2.12	0.67
1:A:445:PRO:HD2	4:A:2467:HOH:O	1.93	0.67
1:A:536:GLN:HE22	1:A:685:THR:H	1.42	0.67
1:A:221:ARG:HB2	1:A:221:ARG:HH11	1.59	0.67
1:A:281:THR:O	1:A:285:MET:HG2	1.94	0.67
1:A:1005:ASN:N	1:A:1006:PRO:HD3	2.10	0.67
1:A:510:LEU:CD1	4:A:2646:HOH:O	2.35	0.67
1:A:747:LYS:NZ	4:A:2645:HOH:O	2.27	0.66
1:A:712:ASP:OD1	4:A:2513:HOH:O	2.12	0.66
1:A:528:ILE:O	1:A:530:PRO:HD3	1.95	0.66
1:A:1137:ASP:CA	4:A:2511:HOH:O	2.44	0.66
1:A:1077:LEU:CD1	4:A:2652:HOH:O	2.14	0.66
1:A:658:GLY:O	4:A:2669:HOH:O	2.13	0.65
1:A:1137:ASP:N	4:A:2511:HOH:O	2.29	0.65
1:A:718:ARG:CZ	4:A:2620:HOH:O	2.44	0.65
1:A:807:ASN:H	1:A:807:ASN:ND2	1.95	0.65
1:A:1005:ASN:HD21	1:A:1263:GLU:HB3	1.61	0.65
1:A:615:ILE:HG23	1:A:616:GLY:N	2.11	0.65
1:A:1140:ALA:HB2	4:A:2511:HOH:O	1.95	0.65
1:A:892:MET:HB2	1:A:1232:THR:HG23	1.78	0.65
1:A:1062:ARG:HD2	1:A:1243:GLU:OE2	1.97	0.65
1:A:1005:ASN:ND2	1:A:1263:GLU:HB3	2.12	0.65
1:A:507:VAL:N	4:A:2521:HOH:O	2.13	0.64
1:A:1140:ALA:CA	4:A:2655:HOH:O	2.34	0.64
1:A:637:ALA:CA	4:A:2461:HOH:O	2.44	0.64
1:A:1130:ARG:NH1	4:A:2454:HOH:O	2.03	0.64
1:A:856:ILE:HD13	4:A:2434:HOH:O	1.96	0.64
3:A:1425:GTG:H5B1	4:A:2615:HOH:O	1.96	0.64
1:A:313:VAL:HG21	4:A:2558:HOH:O	1.97	0.64
1:A:475:VAL:C	4:A:2524:HOH:O	2.33	0.64
1:A:995:TRP:CZ2	1:A:1006:PRO:HG3	2.33	0.64
1:A:20:THR:HG22	1:A:21:ASP:O	1.98	0.64
1:A:582:ILE:HG21	1:A:757:LEU:HD21	1.79	0.64
1:A:558:THR:HG22	1:A:558:THR:O	1.98	0.63
1:A:65:THR:HG23	4:A:2451:HOH:O	1.97	0.63
1:A:22:GLN:HE21	1:A:878:VAL:H	1.44	0.63
1:A:393:PRO:HD3	1:A:591:ALA:O	1.99	0.63
1:A:352:LYS:HG2	4:A:2661:HOH:O	1.98	0.63
1:A:1112:MET:HE1	4:A:2667:HOH:O	1.99	0.63
1:A:365:ILE:HD12	4:A:2488:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:PRO:HG3	1:A:1031:LEU:HA	1.81	0.62
1:A:227:PRO:HB2	1:A:228:PRO:HD3	1.82	0.62
1:A:632:VAL:HG13	4:A:2552:HOH:O	1.98	0.62
1:A:1087:ASP:HB3	1:A:1088:PRO:HD3	1.81	0.62
1:A:617:LYS:CE	4:A:2414:HOH:O	2.17	0.62
1:A:1082:ASP:HB2	1:A:1083:PRO:CD	2.29	0.62
1:A:444:ASP:CG	4:A:2467:HOH:O	2.37	0.62
1:A:542:HIS:NE2	1:A:690:GLU:HG3	2.15	0.62
1:A:817:ILE:O	1:A:821:ILE:HG12	2.00	0.62
1:A:1201:PRO:HB2	1:A:1204:GLY:O	2.00	0.62
1:A:221:ARG:CZ	4:A:2411:HOH:O	2.38	0.62
1:A:909:LEU:HB3	4:A:2643:HOH:O	1.99	0.62
1:A:1075:LEU:HG	4:A:2652:HOH:O	2.00	0.62
1:A:837:ARG:HG3	4:A:2408:HOH:O	2.00	0.62
1:A:416:ASP:CA	4:A:2557:HOH:O	2.47	0.61
1:A:776:ASP:OD1	1:A:778:THR:HB	2.00	0.61
1:A:572:VAL:HG13	1:A:789:GLY:O	2.00	0.61
1:A:653:LYS:NZ	4:A:2453:HOH:O	2.32	0.61
1:A:78:LEU:HD12	1:A:80:ARG:NH2	2.16	0.61
1:A:423:ARG:HE	1:A:427:ARG:NH2	1.98	0.61
1:A:362:VAL:CA	4:A:2488:HOH:O	2.38	0.60
1:A:994:GLU:OE1	4:A:2448:HOH:O	2.16	0.60
1:A:716:VAL:HG13	1:A:756:ASP:HB2	1.84	0.60
1:A:923:ARG:C	4:A:2395:HOH:O	2.39	0.60
1:A:1061:TRP:HE3	4:A:2543:HOH:O	1.71	0.60
1:A:2:SER:N	1:A:6:LEU:HB2	2.17	0.60
1:A:2:SER:O	1:A:5:ILE:N	2.34	0.60
1:A:210:LEU:HB2	1:A:213:GLY:O	2.02	0.60
1:A:614:SER:HA	4:A:2414:HOH:O	2.01	0.60
1:A:425:LEU:HB2	1:A:698:MET:HE1	1.82	0.60
1:A:1112:MET:CE	1:A:1150:LEU:HD11	2.32	0.60
1:A:1238:VAL:O	4:A:2401:HOH:O	2.16	0.59
1:A:807:ASN:HD22	1:A:807:ASN:N	1.98	0.59
1:A:576:SER:O	1:A:577:PRO:C	2.40	0.59
1:A:926:THR:HG23	1:A:1246:HIS:HD2	1.58	0.59
1:A:437:ALA:HB2	1:A:610:VAL:HG22	1.84	0.59
1:A:221:ARG:HB3	4:A:2593:HOH:O	2.02	0.59
1:A:446:LEU:HD13	1:A:1149:GLY:HA3	1.83	0.59
3:A:1425:GTG:H4'	4:A:2591:HOH:O	2.03	0.59
1:A:146:GLN:NE2	1:A:805:ARG:H	2.01	0.59
1:A:1060:LYS:CE	4:A:2555:HOH:O	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:O	4:A:2593:HOH:O	2.16	0.58
1:A:1029:GLU:CD	1:A:1029:GLU:H	2.05	0.58
1:A:1082:ASP:HB2	1:A:1083:PRO:HD2	1.84	0.58
1:A:137:GLY:HA2	4:A:2639:HOH:O	2.03	0.58
1:A:749:ASN:HD22	1:A:752:THR:N	1.98	0.58
1:A:879:LYS:HE2	4:A:2650:HOH:O	2.01	0.58
1:A:1014:HIS:O	1:A:1018:GLN:HG3	2.03	0.58
1:A:491:ILE:N	4:A:2592:HOH:O	2.36	0.58
1:A:632:VAL:CA	4:A:2598:HOH:O	2.46	0.58
1:A:1224:PHE:HE2	4:A:2611:HOH:O	1.86	0.58
1:A:837:ARG:CG	4:A:2408:HOH:O	2.41	0.58
1:A:582:ILE:HG21	1:A:757:LEU:CD2	2.34	0.57
1:A:76:ASP:OD2	1:A:80:ARG:NH1	2.37	0.57
1:A:542:HIS:NE2	1:A:690:GLU:CG	2.66	0.57
1:A:557:PRO:HG2	1:A:781:TYR:HH	1.66	0.57
1:A:595:TRP:HA	1:A:599:LEU:HB2	1.86	0.57
1:A:627:VAL:N	4:A:2424:HOH:O	2.37	0.57
1:A:338:TYR:O	1:A:340:LEU:HG	2.04	0.57
1:A:557:PRO:HG2	1:A:781:TYR:CZ	2.39	0.57
1:A:137:GLY:O	4:A:2639:HOH:O	2.18	0.57
1:A:414:LEU:HD11	1:A:418:THR:HG21	1.86	0.57
1:A:542:HIS:HE2	1:A:690:GLU:CG	2.17	0.57
1:A:1262:GLN:HG3	1:A:1265:ARG:NH1	2.19	0.57
1:A:907:ARG:HB3	1:A:908:PRO:HD3	1.86	0.56
1:A:948:MET:HE1	1:A:1042:ARG:HG3	1.87	0.56
1:A:416:ASP:N	4:A:2557:HOH:O	2.39	0.56
1:A:944:GLN:HB3	1:A:948:MET:HE2	1.86	0.56
1:A:1007:PRO:HD2	1:A:1144:GLN:NE2	2.20	0.56
1:A:743:THR:CG2	1:A:744:THR:N	2.51	0.56
1:A:1137:ASP:O	4:A:2511:HOH:O	2.18	0.56
1:A:414:LEU:CD1	1:A:418:THR:HG21	2.35	0.56
1:A:854:THR:OG1	1:A:856:ILE:HD11	2.05	0.56
1:A:944:GLN:HB3	1:A:948:MET:CE	2.35	0.56
1:A:1112:MET:HE3	1:A:1150:LEU:HD11	1.88	0.56
1:A:32:LYS:HG2	1:A:851:ARG:CZ	2.35	0.56
1:A:829:VAL:HG13	1:A:890:TRP:CE2	2.40	0.56
1:A:837:ARG:CZ	4:A:2408:HOH:O	2.52	0.56
1:A:936:CYS:O	1:A:940:LEU:HG	2.06	0.56
1:A:670:GLY:N	4:A:2493:HOH:O	2.26	0.56
1:A:1027:THR:HG22	1:A:1030:GLU:CG	2.36	0.56
1:A:299:TRP:CD2	1:A:303:ARG:HG2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:VAL:HB	1:A:534:PRO:HD3	1.87	0.56
1:A:716:VAL:O	1:A:720:MET:HG3	2.05	0.55
3:A:1425:GTG:C4E	4:A:2615:HOH:O	2.54	0.55
1:A:1198:LYS:NZ	4:A:2638:HOH:O	2.25	0.55
1:A:1002:ILE:HD13	1:A:1136:ALA:HB2	1.88	0.55
1:A:1005:ASN:CB	1:A:1130:ARG:HH22	2.20	0.55
1:A:363:ARG:HH22	1:A:834:GLN:HE22	1.54	0.55
1:A:837:ARG:NE	4:A:2408:HOH:O	2.27	0.55
1:A:797:ARG:HG2	1:A:797:ARG:HH11	1.72	0.55
1:A:582:ILE:HD12	1:A:757:LEU:HD11	1.89	0.55
1:A:140:ALA:HB3	4:A:2639:HOH:O	2.07	0.54
1:A:246:ASP:O	1:A:250:VAL:HG23	2.08	0.54
1:A:515:MET:HA	1:A:529:MET:HE3	1.90	0.54
1:A:125:ASP:HB2	4:A:2546:HOH:O	2.07	0.54
1:A:87:GLN:HG2	1:A:268:TRP:CH2	2.43	0.54
1:A:1027:THR:HG22	1:A:1030:GLU:HG3	1.88	0.54
1:A:188:TRP:CZ2	1:A:192:GLU:HG3	2.42	0.54
1:A:541:PRO:HB2	1:A:648:ILE:HD11	1.89	0.54
1:A:120:GLU:O	1:A:124:LYS:HG3	2.08	0.53
1:A:905:LEU:HD23	1:A:1063:MET:CE	2.39	0.53
1:A:1148:VAL:HG23	4:A:2667:HOH:O	1.90	0.53
1:A:385:VAL:HG22	1:A:515:MET:SD	2.48	0.53
1:A:529:MET:HE2	1:A:661:TYR:CD1	2.44	0.53
1:A:879:LYS:CG	4:A:2650:HOH:O	2.33	0.53
1:A:303:ARG:HG3	1:A:303:ARG:HH11	1.72	0.53
1:A:856:ILE:CD1	4:A:2434:HOH:O	2.55	0.53
1:A:907:ARG:NH2	4:A:2459:HOH:O	2.42	0.53
1:A:1119:LEU:CG	4:A:2563:HOH:O	2.55	0.53
1:A:859:SER:HB3	4:A:2434:HOH:O	2.09	0.53
1:A:43:TYR:HE2	4:A:2613:HOH:O	1.91	0.53
1:A:195:ARG:HD3	4:A:2666:HOH:O	2.09	0.53
1:A:441:ARG:CD	4:A:2427:HOH:O	2.51	0.53
1:A:529:MET:HE3	1:A:529:MET:HA	1.91	0.53
1:A:421:ILE:HD11	1:A:701:THR:HG22	1.91	0.52
1:A:2:SER:O	1:A:3:SER:C	2.48	0.52
1:A:477:LEU:HB3	1:A:496:GLN:HB3	1.91	0.52
1:A:614:SER:CA	4:A:2414:HOH:O	2.57	0.52
1:A:905:LEU:HD23	1:A:1063:MET:HE1	1.92	0.52
1:A:396:LYS:HD2	1:A:765:GLU:HB3	1.92	0.52
1:A:1009:LEU:HA	4:A:2563:HOH:O	2.08	0.52
1:A:115:LEU:HD21	1:A:134:THR:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:LEU:HG	4:A:2471:HOH:O	2.08	0.52
1:A:112:TYR:HB3	1:A:215:PHE:HB3	1.91	0.52
1:A:951:LEU:HD13	1:A:1037:THR:HG22	1.92	0.52
1:A:820:GLN:O	1:A:824:VAL:HG23	2.10	0.51
1:A:829:VAL:HG13	1:A:890:TRP:NE1	2.25	0.51
1:A:1119:LEU:CD2	4:A:2563:HOH:O	2.49	0.51
1:A:792:ILE:CD1	4:A:2488:HOH:O	2.52	0.51
1:A:770:LYS:HG2	4:A:2436:HOH:O	2.10	0.51
1:A:3:SER:O	1:A:7:THR:N	2.41	0.51
1:A:22:GLN:HE22	1:A:878:VAL:H	1.53	0.51
1:A:617:LYS:HB2	4:A:2414:HOH:O	2.09	0.51
1:A:748:VAL:HA	4:A:2059:HOH:O	2.10	0.51
1:A:582:ILE:HB	1:A:738:MET:HB3	1.92	0.51
1:A:595:TRP:HB3	4:A:2608:HOH:O	2.09	0.51
1:A:797:ARG:HG2	1:A:797:ARG:NH1	2.25	0.51
1:A:1004:HIS:NE2	4:A:2487:HOH:O	2.34	0.51
1:A:39:ARG:C	4:A:2613:HOH:O	2.48	0.51
1:A:1119:LEU:CD1	4:A:2563:HOH:O	2.39	0.51
1:A:39:ARG:CA	4:A:2613:HOH:O	2.52	0.50
1:A:289:LEU:HD21	1:A:316:LEU:HB3	1.92	0.50
1:A:542:HIS:HE2	1:A:690:GLU:HG2	1.77	0.50
1:A:171:VAL:HG11	1:A:1090:LEU:HD11	1.93	0.50
1:A:323:SER:CB	4:A:2645:HOH:O	2.41	0.50
1:A:298:GLU:HB2	1:A:311:MET:CE	2.42	0.50
1:A:436:MET:HE2	1:A:442:THR:OG1	2.12	0.50
1:A:846:CYS:SG	1:A:870:PHE:CD1	3.04	0.50
1:A:617:LYS:NZ	4:A:2414:HOH:O	2.42	0.50
1:A:926:THR:HG1	1:A:1246:HIS:CD2	2.29	0.50
1:A:1012:VAL:CG2	4:A:2563:HOH:O	2.43	0.50
1:A:193:ILE:HD13	1:A:229:LEU:HD21	1.94	0.50
1:A:634:GLY:N	4:A:2522:HOH:O	2.44	0.50
1:A:756:ASP:C	1:A:756:ASP:OD1	2.50	0.50
1:A:626:ILE:C	4:A:2424:HOH:O	2.49	0.49
1:A:797:ARG:HD3	4:A:2497:HOH:O	2.10	0.49
1:A:127:ASP:O	1:A:131:ARG:HG3	2.12	0.49
1:A:148:LYS:HG2	1:A:803:LYS:HB2	1.93	0.49
1:A:484:PRO:HB2	1:A:1021:GLN:HE21	1.77	0.49
1:A:704:THR:CB	4:A:2610:HOH:O	2.50	0.49
1:A:516:GLY:O	1:A:517:LEU:HD12	2.13	0.49
1:A:1007:PRO:HD2	1:A:1144:GLN:HE22	1.76	0.49
3:A:1425:GTG:C4D	4:A:2591:HOH:O	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TYR:CE1	1:A:379:ARG:HD3	2.48	0.49
1:A:223:THR:HG21	4:A:2200:HOH:O	2.10	0.49
1:A:837:ARG:HG2	4:A:2368:HOH:O	2.12	0.49
1:A:275:SER:O	1:A:278:PRO:HD2	2.12	0.49
1:A:744:THR:C	1:A:746:GLY:H	2.16	0.49
1:A:847:CYS:CA	4:A:2537:HOH:O	2.53	0.49
1:A:570:LEU:HD21	1:A:730:VAL:HG21	1.94	0.48
1:A:297:LEU:HB2	4:A:2621:HOH:O	2.13	0.48
1:A:532:ASN:OD1	1:A:535:GLN:HG3	2.13	0.48
1:A:1064:CYS:HB3	1:A:1065:GLU:OE2	2.13	0.48
1:A:1121:VAL:HG13	4:A:2566:HOH:O	2.12	0.48
1:A:106:HIS:CE1	1:A:108:THR:H	2.31	0.48
1:A:563:VAL:HG12	1:A:568:ILE:HD11	1.95	0.48
1:A:1005:ASN:N	1:A:1006:PRO:CD	2.77	0.48
1:A:92:VAL:HG11	1:A:383:GLU:HB3	1.94	0.48
1:A:490:LYS:C	4:A:2592:HOH:O	2.51	0.48
1:A:501:PRO:HB2	1:A:504:HIS:HD2	1.78	0.48
1:A:392:SER:HB3	1:A:393:PRO:HD2	1.95	0.48
1:A:1065:GLU:H	1:A:1065:GLU:CD	2.16	0.48
1:A:1130:ARG:NH2	4:A:2454:HOH:O	2.43	0.48
1:A:555:LEU:O	1:A:730:VAL:HA	2.13	0.48
1:A:379:ARG:CB	4:A:2501:HOH:O	2.62	0.48
1:A:735:ASP:OD2	4:A:2423:HOH:O	2.19	0.48
1:A:757:LEU:HD22	1:A:773:ILE:HG21	1.96	0.48
1:A:856:ILE:O	4:A:2463:HOH:O	2.20	0.48
1:A:67:PRO:O	1:A:97:CYS:HB3	2.14	0.48
1:A:706:TRP:O	1:A:710:HIS:HD2	1.95	0.48
1:A:24:ASN:ND2	1:A:28:GLU:OE2	2.42	0.47
1:A:394:GLU:OE2	4:A:2641:HOH:O	2.20	0.47
1:A:564:ILE:HG22	1:A:1185:MET:HB2	1.96	0.47
1:A:566:LYS:HD3	1:A:782:LEU:O	2.14	0.47
1:A:410:GLU:N	1:A:649:GLN:OE1	2.38	0.47
1:A:606:ILE:O	1:A:610:VAL:HB	2.14	0.47
1:A:1075:LEU:HA	1:A:1076:PRO:HD3	1.80	0.47
1:A:20:THR:CG2	4:A:2415:HOH:O	2.47	0.47
1:A:285:MET:HG3	1:A:365:ILE:HD11	1.96	0.47
1:A:294:CYS:SG	1:A:314:MET:HB3	2.54	0.47
1:A:389:TYR:HD1	1:A:679:THR:HB	1.79	0.47
1:A:821:ILE:HD12	1:A:845:LEU:HD13	1.97	0.47
1:A:167:LEU:HD22	1:A:837:ARG:HD2	1.95	0.47
1:A:385:VAL:HG21	1:A:663:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:ASP:C	4:A:2511:HOH:O	2.52	0.47
1:A:223:THR:HG22	1:A:224:SER:N	2.29	0.47
1:A:20:THR:CB	4:A:2415:HOH:O	2.63	0.47
1:A:92:VAL:CG1	1:A:383:GLU:HB3	2.44	0.47
1:A:149:ALA:HB1	1:A:150:PRO:CD	2.44	0.47
1:A:856:ILE:HD13	4:A:2176:HOH:O	2.14	0.47
1:A:746:GLY:CA	4:A:2474:HOH:O	2.35	0.47
1:A:747:LYS:NZ	4:A:2442:HOH:O	2.15	0.47
1:A:829:VAL:HG13	1:A:890:TRP:CD1	2.49	0.47
1:A:390:THR:CG2	1:A:391:GLN:HG3	2.45	0.47
1:A:632:VAL:N	4:A:2598:HOH:O	2.47	0.47
1:A:518:ARG:HA	1:A:804:GLU:OE2	2.15	0.47
1:A:194:CYS:SG	1:A:206:PRO:HG2	2.55	0.46
1:A:671:ASN:N	1:A:671:ASN:HD22	2.12	0.46
1:A:797:ARG:CZ	4:A:2497:HOH:O	2.63	0.46
1:A:1027:THR:HG23	1:A:1030:GLU:H	1.79	0.46
1:A:195:ARG:NH2	4:A:2629:HOH:O	2.48	0.46
1:A:990:ARG:HB3	4:A:2486:HOH:O	2.14	0.46
1:A:385:VAL:HG21	1:A:663:VAL:HG21	1.96	0.46
1:A:557:PRO:HG2	1:A:781:TYR:CE2	2.51	0.46
1:A:702:PHE:HB2	1:A:763:TYR:CE2	2.50	0.46
1:A:1134:LEU:HA	1:A:1257:MET:CE	2.46	0.46
1:A:1027:THR:CG2	1:A:1030:GLU:H	2.29	0.46
1:A:299:TRP:CE2	1:A:303:ARG:HG2	2.51	0.46
1:A:456:VAL:HA	4:A:2592:HOH:O	2.15	0.46
1:A:542:HIS:CE1	1:A:690:GLU:HG3	2.50	0.46
1:A:879:LYS:CE	4:A:2650:HOH:O	2.60	0.46
1:A:9:PHE:O	1:A:13:ILE:HG13	2.16	0.46
1:A:389:TYR:OH	1:A:527:SER:HB2	2.16	0.46
1:A:448:GLN:NE2	1:A:620:MET:H	2.14	0.46
1:A:633:VAL:HA	4:A:2244:HOH:O	2.16	0.46
1:A:930:ASN:ND2	4:A:2395:HOH:O	2.47	0.46
1:A:379:ARG:HB3	4:A:2501:HOH:O	2.16	0.46
1:A:512:ASP:HB3	1:A:662:ARG:HG3	1.98	0.46
1:A:833:LEU:HD12	1:A:838:TRP:CD2	2.51	0.46
1:A:223:THR:CG2	1:A:224:SER:N	2.79	0.45
1:A:779:ALA:HB3	1:A:786:PHE:HB2	1.96	0.45
1:A:935:ARG:O	1:A:939:GLU:HG3	2.16	0.45
1:A:909:LEU:HD22	4:A:2643:HOH:O	2.17	0.45
1:A:557:PRO:HD2	1:A:730:VAL:HG12	1.97	0.45
1:A:577:PRO:HD3	1:A:788:PHE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:THR:HG22	1:A:726:GLN:N	2.15	0.45
1:A:809:SER:CB	4:A:2577:HOH:O	2.63	0.45
1:A:20:THR:HG22	1:A:21:ASP:N	2.31	0.45
1:A:665:ASP:HB3	1:A:671:ASN:HB2	1.98	0.45
1:A:686:ALA:O	1:A:687:THR:C	2.55	0.45
1:A:833:LEU:HD12	1:A:838:TRP:CE3	2.52	0.45
1:A:1004:HIS:C	1:A:1006:PRO:CD	2.82	0.45
1:A:1140:ALA:CB	4:A:2655:HOH:O	2.62	0.45
1:A:281:THR:OG1	1:A:282:LEU:N	2.48	0.45
1:A:389:TYR:HE2	1:A:515:MET:CE	2.30	0.45
1:A:83:ARG:NH1	1:A:84:LYS:O	2.49	0.45
1:A:94:VAL:HG22	1:A:139:ILE:HG23	1.99	0.45
1:A:421:ILE:HD11	1:A:701:THR:CG2	2.47	0.44
1:A:529:MET:HA	1:A:529:MET:CE	2.46	0.44
1:A:538:VAL:HG13	1:A:651:LEU:HB2	1.98	0.44
1:A:748:VAL:HA	4:A:2443:HOH:O	2.16	0.44
1:A:940:LEU:HG	1:A:940:LEU:H	1.70	0.44
1:A:3:SER:O	1:A:7:THR:HB	2.17	0.44
1:A:221:ARG:HH11	1:A:221:ARG:CB	2.30	0.44
1:A:1140:ALA:CB	4:A:2511:HOH:O	2.59	0.44
1:A:198:SER:HA	1:A:217:LEU:HD21	1.98	0.44
1:A:287:GLU:HB2	4:A:2310:HOH:O	2.16	0.44
1:A:926:THR:HG22	1:A:926:THR:O	2.17	0.44
1:A:1002:ILE:HG21	1:A:1136:ALA:HB2	2.00	0.44
1:A:56:MET:HG2	1:A:188:TRP:CD2	2.53	0.44
1:A:273:THR:O	1:A:276:ILE:HG12	2.17	0.44
1:A:1200:LEU:C	1:A:1200:LEU:HD23	2.38	0.44
1:A:797:ARG:C	1:A:799:PRO:HD3	2.38	0.44
1:A:580:GLN:OE1	1:A:747:LYS:HB2	2.18	0.44
1:A:279:GLN:HG3	1:A:327:ASN:HD22	1.83	0.44
1:A:501:PRO:HD2	1:A:504:HIS:CD2	2.53	0.44
1:A:837:ARG:NH1	4:A:2408:HOH:O	2.51	0.44
1:A:946:TYR:OH	1:A:1050:SER:HB3	2.17	0.44
1:A:421:ILE:HD13	1:A:763:TYR:HE1	1.82	0.43
1:A:555:LEU:HB3	1:A:729:TYR:O	2.18	0.43
1:A:149:ALA:HB1	1:A:150:PRO:HD2	2.00	0.43
1:A:485:VAL:HG12	1:A:1021:GLN:CG	2.48	0.43
1:A:568:ILE:N	1:A:569:PRO:CD	2.80	0.43
1:A:659:PHE:CE2	1:A:681:PRO:HD3	2.52	0.43
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.84	0.43
1:A:87:GLN:HB3	1:A:268:TRP:CZ2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:ARG:CZ	4:A:2454:HOH:O	2.58	0.43
1:A:441:ARG:NH1	4:A:2580:HOH:O	2.39	0.43
1:A:470:LEU:HD23	1:A:477:LEU:HD21	2.00	0.43
1:A:614:SER:C	4:A:2414:HOH:O	2.52	0.43
1:A:1180:VAL:HA	4:A:2611:HOH:O	2.18	0.43
1:A:20:THR:CG2	1:A:21:ASP:N	2.81	0.43
1:A:814:TRP:CD2	1:A:815:PRO:HB3	2.53	0.43
1:A:1002:ILE:HD13	1:A:1136:ALA:CB	2.49	0.43
1:A:525:PRO:HD3	4:A:2001:HOH:O	2.19	0.43
1:A:473:ILE:HG13	1:A:475:VAL:HG23	2.01	0.43
1:A:603:MET:HE3	1:A:652:SER:OG	2.18	0.43
1:A:631:SER:C	4:A:2598:HOH:O	2.56	0.43
1:A:845:LEU:HD23	1:A:845:LEU:HA	1.90	0.43
1:A:169:ASP:HA	1:A:170:PRO:HD3	1.90	0.43
1:A:540:ALA:HB3	1:A:541:PRO:HD3	2.01	0.43
1:A:2:SER:O	1:A:4:MET:N	2.52	0.42
1:A:39:ARG:HE	1:A:208:LEU:HD22	1.84	0.42
1:A:47:ASP:CA	4:A:2629:HOH:O	2.47	0.42
1:A:379:ARG:HH12	1:A:387:GLN:HE22	1.61	0.42
1:A:406:GLY:HA3	1:A:630:GLU:O	2.19	0.42
1:A:639:ARG:HA	1:A:640:PRO:HD3	1.92	0.42
1:A:1109:THR:HG22	1:A:1168:ASN:HD21	1.83	0.42
1:A:32:LYS:CD	4:A:2435:HOH:O	2.59	0.42
1:A:379:ARG:NH2	4:A:2011:HOH:O	2.50	0.42
1:A:603:MET:HE1	1:A:651:LEU:HB3	2.00	0.42
1:A:859:SER:HB3	4:A:2463:HOH:O	2.02	0.42
1:A:515:MET:HA	1:A:529:MET:CE	2.49	0.42
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.87	0.42
1:A:287:GLU:N	4:A:2505:HOH:O	2.49	0.42
1:A:3:SER:O	1:A:7:THR:CB	2.67	0.42
1:A:270:ILE:HA	4:A:2235:HOH:O	2.20	0.42
1:A:435:ARG:O	1:A:439:GLN:HG3	2.19	0.42
1:A:456:VAL:C	4:A:2592:HOH:O	2.56	0.42
1:A:1029:GLU:CD	1:A:1029:GLU:N	2.72	0.42
1:A:855:MET:C	1:A:856:ILE:HD12	2.40	0.42
1:A:59:ILE:HA	1:A:60:PRO:HD3	1.93	0.42
1:A:1201:PRO:HA	1:A:1242:LEU:O	2.19	0.42
1:A:1240:ILE:C	4:A:2543:HOH:O	2.58	0.42
1:A:1253:GLY:O	1:A:1257:MET:HG3	2.20	0.42
1:A:27:PHE:CG	1:A:867:MET:HB3	2.54	0.42
1:A:72:TYR:O	1:A:83:ARG:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:CB	4:A:2546:HOH:O	2.66	0.42
1:A:380:THR:OG1	1:A:383:GLU:HG2	2.20	0.42
1:A:529:MET:CE	1:A:661:TYR:CD1	3.02	0.42
1:A:603:MET:CE	1:A:651:LEU:HB3	2.50	0.42
1:A:834:GLN:NE2	4:A:2003:HOH:O	2.50	0.42
1:A:1212:PRO:HA	1:A:1213:PRO:HD3	1.89	0.42
1:A:385:VAL:CG2	1:A:515:MET:SD	3.08	0.42
1:A:654:LEU:HD12	4:A:2669:HOH:O	2.09	0.42
1:A:268:TRP:N	4:A:2606:HOH:O	2.50	0.41
1:A:390:THR:HG23	1:A:391:GLN:HG3	2.02	0.41
1:A:529:MET:HG3	1:A:661:TYR:CZ	2.55	0.41
1:A:558:THR:CB	4:A:2600:HOH:O	2.03	0.41
1:A:39:ARG:HH11	1:A:39:ARG:CG	2.33	0.41
1:A:416:ASP:CB	4:A:2557:HOH:O	2.68	0.41
1:A:616:GLY:C	1:A:617:LYS:HG3	2.40	0.41
1:A:626:ILE:CG2	1:A:638:ALA:HB1	2.50	0.41
1:A:941:LYS:HE3	4:A:2438:HOH:O	2.15	0.41
1:A:1003:ILE:HG12	1:A:1131:LEU:HD21	2.02	0.41
1:A:603:MET:HE1	1:A:651:LEU:HD23	2.02	0.41
1:A:1012:VAL:HB	1:A:1013:PRO:HD3	2.01	0.41
1:A:96:ASN:OD1	1:A:265:SER:HA	2.20	0.41
1:A:193:ILE:O	1:A:197:ILE:HG13	2.20	0.41
1:A:66:LYS:HA	1:A:67:PRO:HD3	1.89	0.41
1:A:879:LYS:CD	4:A:2650:HOH:O	2.65	0.41
1:A:629:ASP:O	1:A:636:ARG:HA	2.20	0.41
1:A:980:GLN:HE21	1:A:980:GLN:HB3	1.69	0.41
1:A:1201:PRO:HG3	1:A:1209:THR:HG21	2.01	0.41
1:A:73:TYR:HB2	1:A:132:ILE:HG23	2.03	0.41
1:A:523:ARG:HD2	4:A:2548:HOH:O	2.21	0.41
1:A:531:LEU:HD11	1:A:684:SER:HB2	2.03	0.41
1:A:466:LEU:HD12	1:A:508:ALA:HB1	2.02	0.41
1:A:520:GLN:OE1	1:A:523:ARG:NH1	2.54	0.41
1:A:542:HIS:NE2	1:A:690:GLU:HG2	2.35	0.41
1:A:574:ALA:HB1	1:A:581:SER:HB3	2.03	0.41
1:A:188:TRP:CE2	1:A:192:GLU:HG3	2.55	0.41
1:A:1091:LYS:O	1:A:1095:VAL:HB	2.22	0.41
1:A:483:LEU:HA	1:A:483:LEU:HD23	1.81	0.40
1:A:812:GLU:HA	1:A:813:PRO:HD3	1.87	0.40
1:A:226:ILE:O	1:A:230:LEU:HG	2.21	0.40
1:A:444:ASP:HA	4:A:2467:HOH:O	2.20	0.40
1:A:532:ASN:OD1	1:A:534:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ARG:HA	1:A:862:TYR:CD1	2.56	0.40
1:A:1112:MET:HE1	1:A:1150:LEU:HD11	2.04	0.40
1:A:104:GLU:HG3	1:A:116:SER:HB2	2.03	0.40
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.92	0.40
1:A:456:VAL:CA	4:A:2592:HOH:O	2.70	0.40
1:A:501:PRO:HB2	1:A:504:HIS:CD2	2.57	0.40
1:A:607:HIS:HB2	1:A:648:ILE:HG21	2.04	0.40
1:A:799:PRO:HB2	1:A:802:GLY:HA3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2299:HOH:O	4:A:2582:HOH:O[4_475]	2.11	0.09

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	1252/1267 (99%)	1175 (94%)	66 (5%)	11 (1%)	17 31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	578	PRO
1	A	615	ILE
1	A	498	ALA
1	A	687	THR
1	A	1201	PRO
1	A	91	ASP
1	A	631	SER

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Mol	Chain	Res	Type
1	A	1005	ASN
1	A	276	ILE
1	A	857	GLY

5.3.2 Protein sidechains (i)

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	1076/1083 (99%)	1030 (96%)	46 (4%)	29 53

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	57	LEU
1	A	80	ARG
1	A	87	GLN
1	A	102	LEU
1	A	167	LEU
1	A	174	LYS
1	A	187	LEU
1	A	210	LEU
1	A	214	VAL
1	A	287	GLU
1	A	298	GLU
1	A	366	ARG
1	A	387	GLN
1	A	390	THR
1	A	414	LEU
1	A	416	ASP
1	A	431	LEU
1	A	436	MET
1	A	466	LEU
1	A	517	LEU
1	A	536	GLN
1	A	538	VAL

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Mol	Chain	Res	Type
1	A	557	PRO
1	A	578	PRO
1	A	610	VAL
1	A	627	VAL
1	A	657	ARG
1	A	671	ASN
1	A	700	GLU
1	A	726	GLN
1	A	756	ASP
1	A	807	ASN
1	A	845	LEU
1	A	890	TRP
1	A	894	THR
1	A	940	LEU
1	A	953	ARG
1	A	980	GLN
1	A	984	LEU
1	A	990	ARG
1	A	1045	SER
1	A	1052	LEU
1	A	1060	LYS
1	A	1182	ASP
1	A	1262	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	87	GLN
1	A	121	ASN
1	A	146	GLN
1	A	283	HIS
1	A	387	GLN
1	A	439	GLN
1	A	448	GLN
1	A	499	ASN
1	A	504	HIS
1	A	536	GLN
1	A	628	ASN
1	A	664	ASN
1	A	671	ASN
1	A	675	HIS

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Mol	Chain	Res	Type
1	A	710	HIS
1	A	728	ASN
1	A	749	ASN
1	A	755	ASN
1	A	807	ASN
1	A	834	GLN
1	A	930	ASN
1	A	980	GLN
1	A	1004	HIS
1	A	1005	ASN
1	A	1021	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GTG	A	1425	-	46,57,57	2.16	14 (30%)	47,90,90	3.08	17 (36%)

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	GTG	A	1425	-	-	11/24/64/64	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1425	GTG	C2D-C3D	-5.44	1.38	1.53
3	A	1425	GTG	PA-O5D	-4.96	1.39	1.59
3	A	1425	GTG	C2D-C1D	4.17	1.60	1.53
3	A	1425	GTG	C6B-N1B	3.94	1.43	1.37
3	A	1425	GTG	C3D-C4D	-3.78	1.43	1.53
3	A	1425	GTG	PB-O1B	3.75	1.64	1.50
3	A	1425	GTG	O3D-C3D	-3.55	1.34	1.43
3	A	1425	GTG	C2E-C3E	-3.42	1.44	1.53
3	A	1425	GTG	O4E-C4E	-2.66	1.39	1.45
3	A	1425	GTG	C5D-C4D	-2.58	1.43	1.51
3	A	1425	GTG	C8A-N9A	2.48	1.37	1.33
3	A	1425	GTG	O4D-C1D	2.44	1.44	1.41
3	A	1425	GTG	PG-O5E	2.38	1.68	1.59
3	A	1425	GTG	C2B-N1B	2.37	1.43	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1425	GTG	O4D-C4D-C5D	7.69	134.67	109.37
3	A	1425	GTG	PA-O5D-C5D	6.67	160.77	121.68
3	A	1425	GTG	O5E-C5E-C4E	6.40	131.03	108.99
3	A	1425	GTG	O3D-C3D-C4D	6.37	129.47	111.05
3	A	1425	GTG	O2B-PB-O1B	-5.70	84.04	112.24
3	A	1425	GTG	C5D-C4D-C3D	-5.26	95.48	115.18
3	A	1425	GTG	O4D-C4D-C3D	5.19	115.39	105.11
3	A	1425	GTG	O5E-PG-O1G	5.13	129.13	109.07
3	A	1425	GTG	PB-O3A-PA	-5.10	115.32	132.83
3	A	1425	GTG	C3D-C2D-C1D	4.92	108.39	100.98
3	A	1425	GTG	C3E-C2E-C1E	4.29	107.44	100.98
3	A	1425	GTG	O5D-PA-O1A	3.81	123.94	109.07
3	A	1425	GTG	O2G-PG-O5E	-3.19	92.92	107.75
3	A	1425	GTG	O2G-PG-O1G	3.17	127.93	112.24
3	A	1425	GTG	PG-O5E-C5E	-3.13	103.32	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1425	GTG	PG-O3B-PB	-2.15	125.44	132.83
3	A	1425	GTG	O5D-C5D-C4D	-2.07	101.88	108.99

There are no chirality outliers.

All (11) torsion outliers are listed below:

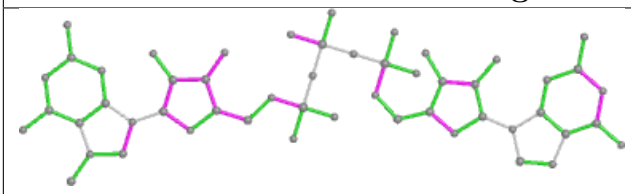
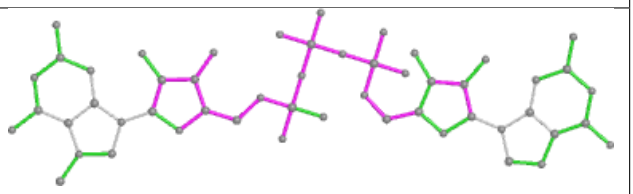
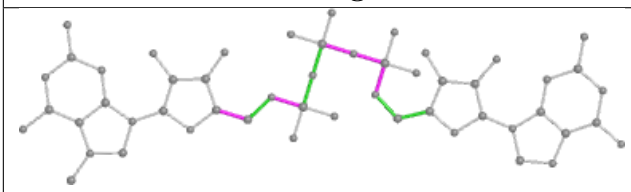
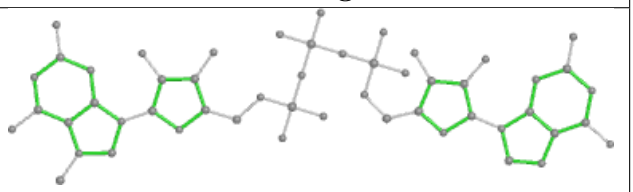
Mol	Chain	Res	Type	Atoms
3	A	1425	GTG	C5D-O5D-PA-O1A
3	A	1425	GTG	C5D-O5D-PA-O2A
3	A	1425	GTG	C5D-O5D-PA-O3A
3	A	1425	GTG	O4D-C4D-C5D-O5D
3	A	1425	GTG	C3D-C4D-C5D-O5D
3	A	1425	GTG	C5E-O5E-PG-O1G
3	A	1425	GTG	PB-O3B-PG-O5E
3	A	1425	GTG	C5E-O5E-PG-O3B
3	A	1425	GTG	PG-O3B-PB-O2B
3	A	1425	GTG	C5E-O5E-PG-O2G
3	A	1425	GTG	PB-O3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1425	GTG	5	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 then 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 GTG A 1425	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1256/1267 (99%)	0.21	45 (3%) 42 46	17, 31, 53, 83	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	855	MET	6.8
1	A	2	SER	6.7
1	A	857	GLY	6.6
1	A	860	VAL	6.5
1	A	859	SER	6.0
1	A	858	GLU	5.8
1	A	856	ILE	5.4
1	A	744	THR	5.2
1	A	634	GLY	5.1
1	A	484	PRO	4.6
1	A	632	VAL	4.5
1	A	483	LEU	4.3
1	A	633	VAL	4.2
1	A	471	TYR	3.4
1	A	1025	ILE	3.4
1	A	746	GLY	3.1
1	A	748	VAL	3.1
1	A	482	GLY	3.1
1	A	745	ALA	3.0
1	A	557	PRO	3.0
1	A	926	THR	2.9
1	A	635	VAL	2.9
1	A	391	GLN	2.8
1	A	853	ARG	2.7
1	A	1040	ARG	2.7
1	A	756	ASP	2.5
1	A	406	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	475	VAL	2.4
1	A	968	GLU	2.4
1	A	481	LYS	2.4
1	A	1021	GLN	2.4
1	A	993	SER	2.4
1	A	477	LEU	2.3
1	A	562	ALA	2.3
1	A	661	TYR	2.2
1	A	862	TYR	2.2
1	A	1214	ARG	2.2
1	A	211	SER	2.2
1	A	755	ASN	2.2
1	A	636	ARG	2.1
1	A	564	ILE	2.1
1	A	971	THR	2.1
1	A	1036	GLU	2.1
1	A	521	VAL	2.0
1	A	1206	HIS	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

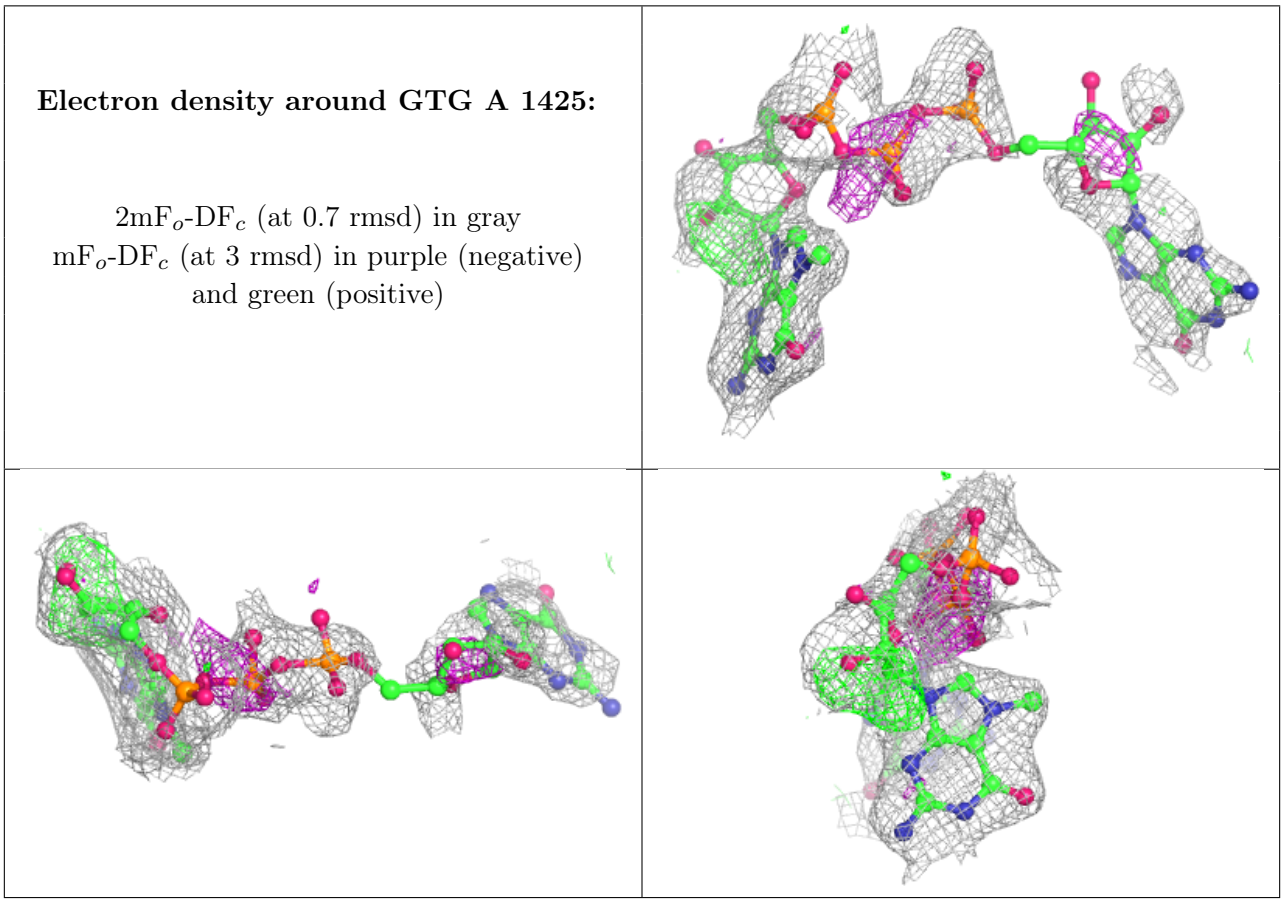
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GTG	A	1425	52/52	0.76	0.30	43,81,90,91	0
2	MN	A	1500	1/1	0.99	0.07	54,54,54,54	0

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 GTG 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)



6.5 Other polymers (i)

There are no such residues in this entry.