



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 AM UTC

PDB ID : 3WRX / pdb_00003wrx
Title : Crystal structure of helicase complex 1
Authors : Matsumura, H.; Katoh, E.
Deposited on : 2014-02-27
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 ⓘ 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

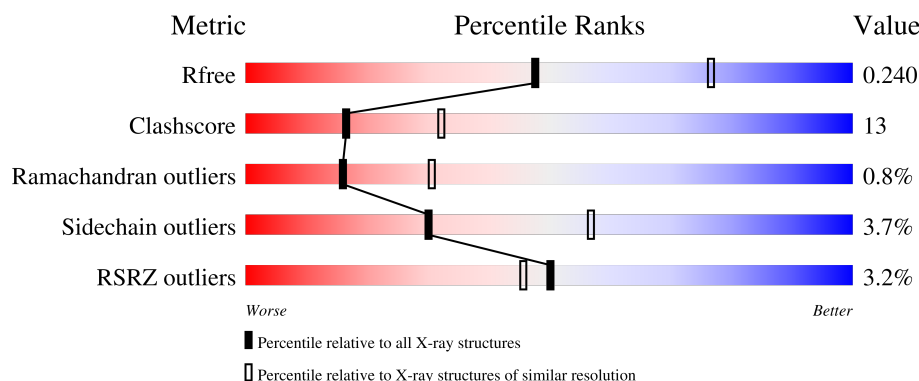
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	431	2% 70% 23% • •
1	B	431	2% 69% 26% • •
2	C	451	5% 68% 24% • •
2	D	451	3% 71% 22% • •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13971 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.

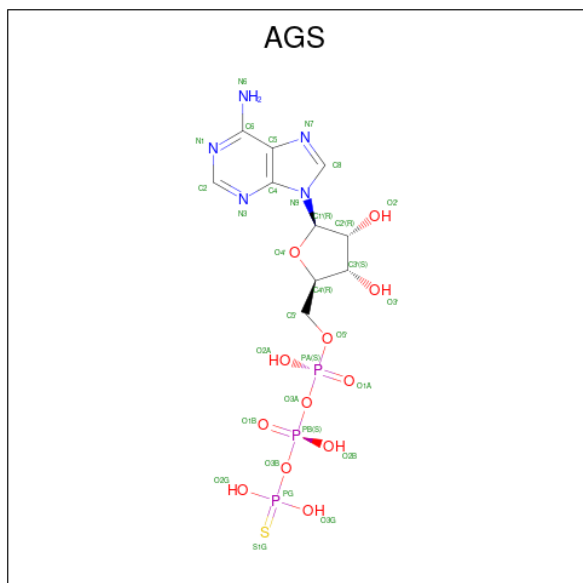
- Molecule 1 is a protein called Tm-1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3093	1956	515	603	19			
1	B	422	Total	C	N	O	S	0	0	0
			3165	1996	529	621	19			

- Molecule 2 is a protein called Replicase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	434	Total	C	N	O	S	0	0	0
			3406	2155	597	634	20			
2	D	431	Total	C	N	O	S	0	0	0
			3388	2146	598	624	20			

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg		
			1	1	0	0
4	C	1	Total	Mg		
			1	1	0	0
4	D	1	Total	Mg		
			1	1	0	0

- Molecule 5 is CESIUM ION (CCD ID: CS) (formula: Cs).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	Cs		
			5	5	0	0
5	B	5	Total	Cs		
			5	5	0	0
5	C	3	Total	Cs		
			3	3	0	0
5	D	5	Total	Cs		
			5	5	0	0

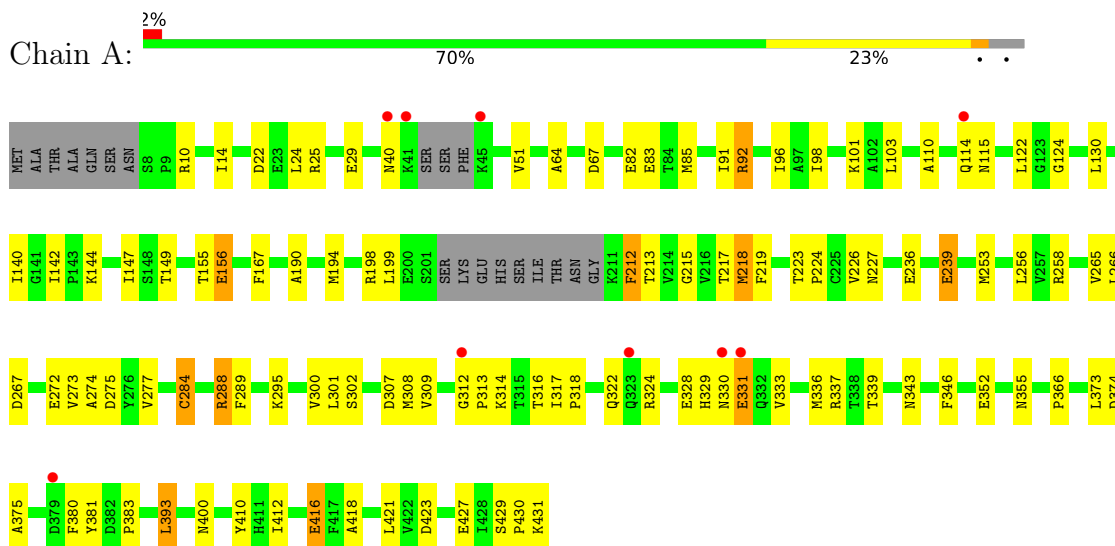
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	208	Total	O		
			208	208	0	0
6	B	161	Total	O		
			161	161	0	0
6	C	217	Total	O		
			217	217	0	0
6	D	188	Total	O		
			188	188	0	0

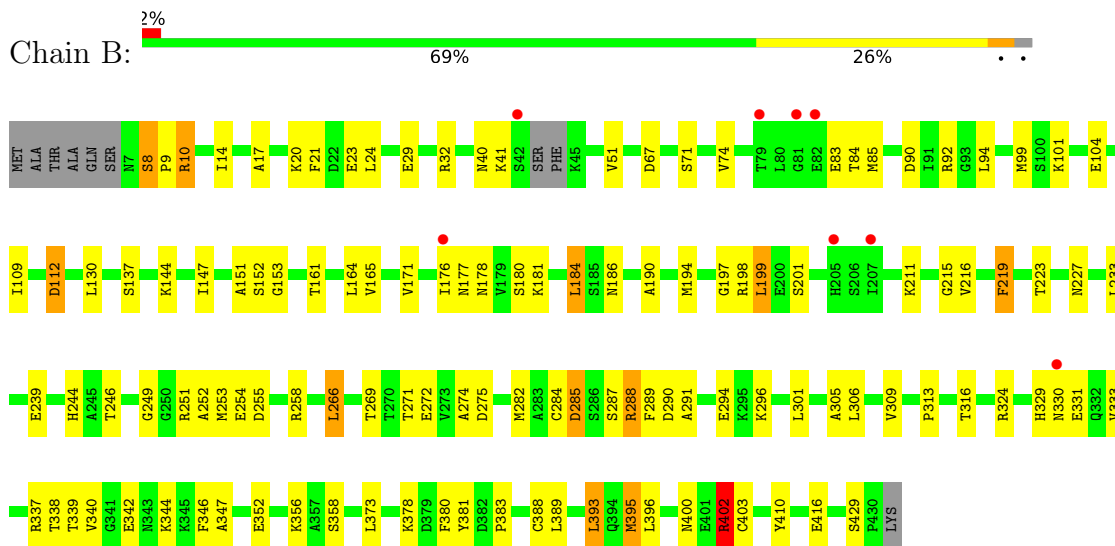
3 Residue-property plots [i](#)

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

- Molecule 1: Tm-1 protein

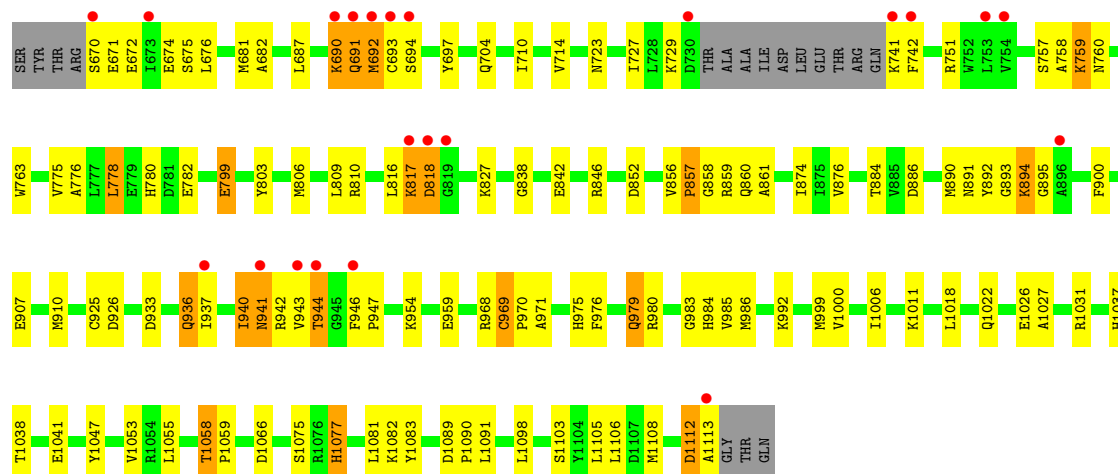


- Molecule 1: Tm-1 protein

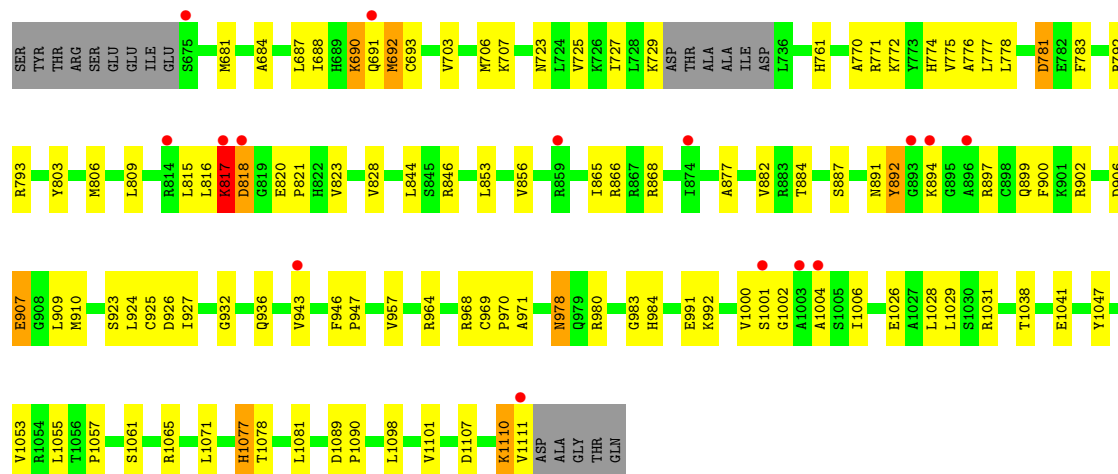
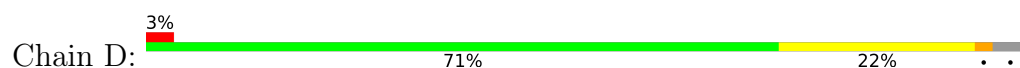


- Molecule 2: Replicase large subunit





• Molecule 2: Replicase large subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.22Å 133.71Å 195.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.31 – 2.50 46.31 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (46.31-2.50) 96.4 (46.31-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.196 , 0.240 0.196 , 0.240	Depositor DCC
R_{free} test set	3928 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13971	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: CS, AGS, MG

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	0.41	0/3141	0.95	9/4251 (0.2%)
1	B	0.41	0/3215	0.92	8/4353 (0.2%)
2	C	0.39	0/3468	0.93	11/4692 (0.2%)
2	D	0.39	0/3450	0.91	11/4667 (0.2%)
All	All	0.40	0/13274	0.93	39/17963 (0.2%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	969	CYS	N-CA-C	8.56	120.52	109.64
1	A	67	ASP	N-CA-C	-7.92	98.30	110.10
1	A	40	ASN	N-CA-C	-7.39	103.40	114.64
1	B	331	GLU	N-CA-C	-6.88	104.91	113.38
1	B	67	ASP	N-CA-C	-6.73	100.07	110.10
2	C	778	LEU	N-CA-C	6.53	120.51	110.20
2	D	969	CYS	N-CA-C	6.47	118.83	109.84
2	D	781	ASP	N-CA-C	-6.16	100.05	109.65
2	D	926	ASP	N-CA-C	-6.13	105.93	113.41
2	D	1053	VAL	N-CA-C	6.12	116.68	108.11
1	A	331	GLU	N-CA-C	-6.01	105.44	112.89
2	C	1077	HIS	N-CA-C	5.83	119.59	110.32
2	D	1077	HIS	N-CA-C	5.76	119.48	110.32
2	C	926	ASP	N-CA-C	-5.75	106.39	113.41
2	D	1061	SER	N-CA-C	5.68	117.15	111.07
1	B	402	ARG	N-CA-C	-5.67	106.24	114.12
1	A	284	CYS	N-CA-C	-5.66	102.09	110.46
1	A	239	GLU	N-CA-C	-5.64	100.51	109.59
2	C	682	ALA	N-CA-C	-5.60	102.61	110.50
2	D	1110	LYS	N-CA-C	5.53	118.37	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	LYS	CB-CA-C	-5.52	110.19	116.54
2	D	783	PHE	N-CA-C	5.49	120.09	113.17
1	A	64	ALA	CB-CA-C	-5.48	110.27	116.63
2	C	857	PRO	N-CA-C	5.47	121.29	113.47
2	C	884	THR	N-CA-C	-5.38	103.28	110.55
1	B	239	GLU	N-CA-C	-5.34	101.28	109.76
1	A	218	MET	N-CA-C	5.30	117.24	109.24
1	A	147	ILE	N-CA-C	-5.29	99.99	107.98
2	C	1053	VAL	N-CA-C	5.28	116.33	108.46
1	A	265	VAL	N-CA-C	5.23	115.65	108.12
1	B	147	ILE	N-CA-C	-5.21	100.26	108.23
2	C	876	VAL	N-CA-C	-5.20	107.76	112.96
2	D	910	MET	N-CA-C	-5.14	107.01	113.28
2	C	936	GLN	N-CA-C	-5.10	103.95	110.53
2	D	778	LEU	N-CA-C	5.07	117.98	110.48
1	B	8	SER	CA-C-N	5.04	124.95	119.76
1	B	8	SER	C-N-CA	5.04	124.95	119.76
2	C	852	ASP	N-CA-C	5.03	117.90	110.46
2	D	971	ALA	N-CA-C	5.02	117.40	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3093	0	3112	81	0
1	B	3165	0	3174	96	0
2	C	3406	0	3463	103	0
2	D	3388	0	3461	86	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	3	0	0	0	0
5	D	5	0	0	0	0
6	A	208	0	0	3	0
6	B	161	0	0	7	0
6	C	217	0	0	4	0
6	D	188	0	0	2	0
All	All	13971	0	13258	341	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 13.

All (341) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:899:GLN:HG3	2:D:924:LEU:HB3	1.51	0.91
2:C:691:GLN:HE21	2:C:694:SER:H	1.18	0.89
1:A:82:GLU:HA	1:A:85:MET:HE3	1.54	0.89
2:C:690:LYS:HD3	2:C:690:LYS:H	1.37	0.89
2:D:777:LEU:HD21	2:D:806:MET:HE1	1.56	0.87
2:C:940:ILE:HD13	2:C:940:ILE:H	1.37	0.85
1:A:155:THR:HG22	1:B:153:GLY:H	1.42	0.85
2:D:690:LYS:O	2:D:691:GLN:HG2	1.77	0.84
1:A:110:ALA:O	1:A:114:GLN:HB3	1.78	0.83
2:D:706:MET:HE1	2:D:823:VAL:HG22	1.61	0.83
2:C:968:ARG:HB2	3:C:1201:AGS:H3'	1.60	0.82
1:A:213:THR:HG22	1:A:239:GLU:HB3	1.61	0.81
2:D:894:LYS:H	2:D:894:LYS:HD2	1.47	0.80
2:C:759:LYS:HD3	2:C:759:LYS:N	2.01	0.75
1:B:10:ARG:HB2	1:B:10:ARG:HH11	1.53	0.73
1:B:344:LYS:HG2	1:B:388:CYS:SG	2.29	0.73
2:D:1110:LYS:HG3	2:D:1111:VAL:HG23	1.72	0.71
1:B:306:LEU:HD23	1:B:389:LEU:HD21	1.72	0.71
1:A:355:ASN:HA	1:A:400:ASN:ND2	2.05	0.71
2:C:1105:LEU:HA	2:C:1108:MET:HE2	1.72	0.71
1:B:329:HIS:HB3	1:B:333:VAL:HG13	1.72	0.71
1:B:84:THR:HG23	2:D:984:HIS:HE2	1.56	0.70
2:D:691:GLN:HG2	2:D:692:MET:H	1.56	0.70
2:C:723:ASN:HB3	2:C:742:PHE:HZ	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:THR:HG21	1:B:252:ALA:HB2	1.73	0.70
1:A:313:PRO:HB3	1:A:331:GLU:O	1.93	0.69
1:B:109:ILE:O	1:B:112:ASP:HB2	1.93	0.69
1:B:90:ASP:HB3	2:D:1065:ARG:NH1	2.08	0.68
1:A:223:THR:HG22	1:A:227:ASN:ND2	2.09	0.68
2:D:1098:LEU:O	2:D:1101:VAL:HG12	1.93	0.68
1:B:177:ASN:O	1:B:181:LYS:HG3	1.94	0.68
2:C:697:TYR:HB3	2:C:704:GLN:HG2	1.76	0.68
2:C:763:TRP:CD1	2:C:806:MET:HE1	2.29	0.68
1:B:400:ASN:ND2	1:B:403:CYS:HB3	2.09	0.67
2:C:741:LYS:N	2:C:757:SER:HG	1.92	0.67
1:B:313:PRO:HG2	1:B:316:THR:HG23	1.77	0.67
1:A:329:HIS:HB3	1:A:333:VAL:HG13	1.76	0.67
1:B:410:TYR:CE1	1:B:416:GLU:HG3	2.30	0.67
1:B:83:GLU:OE1	1:B:101:LYS:HD2	1.96	0.65
1:A:324:ARG:NH2	1:A:339:THR:HG23	2.12	0.65
2:D:1026:GLU:HA	2:D:1029:LEU:HD12	1.78	0.65
2:C:1105:LEU:HG	2:C:1108:MET:CE	2.26	0.65
2:C:687:LEU:HD12	2:C:775:VAL:HG21	1.79	0.64
1:A:98:ILE:HG21	2:C:1108:MET:HE1	1.80	0.64
1:A:85:MET:HB2	2:C:983:GLY:HA2	1.80	0.63
2:C:763:TRP:HA	2:C:778:LEU:HG	1.81	0.63
2:C:1112:ASP:O	2:C:1113:ALA:HB2	1.99	0.63
2:C:681:MET:CE	2:C:776:ALA:HB2	2.29	0.62
1:B:20:LYS:HE2	6:B:619:HOH:O	1.99	0.62
1:B:254:GLU:HG2	1:B:291:ALA:HB3	1.82	0.61
1:B:330:ASN:HB2	1:B:333:VAL:HG12	1.82	0.61
1:B:400:ASN:HD22	1:B:403:CYS:HB3	1.64	0.61
2:C:782:GLU:CD	2:C:782:GLU:H	2.07	0.61
1:B:85:MET:HE3	2:D:983:GLY:HA2	1.83	0.61
2:C:727:ILE:HG13	2:C:742:PHE:CD1	2.36	0.61
1:A:155:THR:HG21	1:B:151:ALA:O	2.01	0.60
2:C:1081:LEU:C	2:C:1081:LEU:HD23	2.26	0.60
2:C:1000:VAL:HG21	2:C:1006:ILE:HD11	1.82	0.60
1:B:90:ASP:HB3	2:D:1065:ARG:HH11	1.66	0.60
2:D:856:VAL:HG11	2:D:865:ILE:HD12	1.83	0.60
1:A:82:GLU:CA	1:A:85:MET:HE3	2.30	0.60
1:A:155:THR:CG2	1:B:153:GLY:H	2.14	0.60
1:B:85:MET:HB2	2:D:983:GLY:HA2	1.83	0.59
2:C:1058:THR:HG23	2:C:1059:PRO:HD2	1.84	0.59
2:C:886:ASP:HB3	2:C:890:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TYR:CE1	1:A:416:GLU:HG3	2.38	0.58
1:A:266:LEU:HD23	1:A:300:VAL:HB	1.86	0.57
2:D:706:MET:CE	2:D:823:VAL:HG22	2.30	0.57
1:A:10:ARG:HD2	1:A:114:GLN:NE2	2.20	0.57
2:C:976:PHE:O	2:C:979:GLN:HG3	2.05	0.57
1:A:82:GLU:O	1:A:85:MET:HG2	2.05	0.57
2:C:758:ALA:C	2:C:759:LYS:HD3	2.28	0.57
2:D:691:GLN:C	2:D:693:CYS:H	2.11	0.57
1:A:213:THR:HG23	6:A:739:HOH:O	2.04	0.57
2:C:1011:LYS:O	2:C:1011:LYS:HG3	2.04	0.56
1:B:84:THR:HG23	2:D:984:HIS:NE2	2.19	0.56
2:C:671:GLU:HA	2:C:674:GLU:OE2	2.05	0.56
2:C:940:ILE:HD13	2:C:940:ILE:N	2.13	0.56
2:C:1022:GLN:O	2:C:1026:GLU:HG2	2.05	0.56
2:C:859:ARG:HG3	2:C:859:ARG:HH11	1.70	0.56
1:A:337:ARG:HG2	1:A:380:PHE:CD2	2.40	0.56
2:D:777:LEU:CD2	2:D:806:MET:HE1	2.33	0.56
1:B:144:LYS:HG3	1:B:164:LEU:HA	1.87	0.55
1:B:275:ASP:OD2	1:B:309:VAL:HG13	2.06	0.55
1:A:22:ASP:OD1	1:A:25:ARG:NH1	2.39	0.55
1:B:40:ASN:O	1:B:41:LYS:C	2.49	0.55
2:D:816:LEU:O	2:D:817:LYS:HG2	2.06	0.55
1:A:284:CYS:HB2	1:A:288:ARG:HG2	1.89	0.55
2:D:691:GLN:CG	2:D:692:MET:N	2.69	0.55
1:B:271:THR:HB	1:B:305:ALA:HB3	1.89	0.55
1:B:324:ARG:NH2	1:B:339:THR:HG23	2.21	0.55
2:D:866:ARG:HG2	2:D:877:ALA:HB1	1.88	0.55
2:D:894:LYS:H	2:D:894:LYS:CD	2.16	0.55
1:A:274:ALA:HA	1:A:346:PHE:CE1	2.42	0.54
1:A:83:GLU:HB3	1:A:101:LYS:HE3	1.89	0.54
1:A:115:ASN:ND2	6:A:808:HOH:O	2.40	0.54
1:A:375:ALA:O	1:A:381:TYR:HB2	2.07	0.54
2:C:810:ARG:NH2	2:C:890:MET:O	2.40	0.54
2:C:891:ASN:HB3	2:C:894:LYS:HD3	1.89	0.54
2:C:1047:TYR:O	2:C:1077:HIS:HA	2.08	0.54
1:A:155:THR:HG22	1:B:153:GLY:O	2.08	0.54
2:D:1081:LEU:C	2:D:1081:LEU:HD23	2.33	0.54
1:B:219:PHE:HB2	1:B:269:THR:HG21	1.90	0.54
1:B:223:THR:HG22	1:B:227:ASN:ND2	2.22	0.54
2:C:860:GLN:HG3	6:C:1329:HOH:O	2.08	0.54
1:A:330:ASN:HB2	1:A:333:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:691:GLN:CG	2:D:692:MET:H	2.20	0.53
1:B:83:GLU:CD	1:B:101:LYS:HD2	2.32	0.53
2:D:703:VAL:HA	2:D:706:MET:HE3	1.90	0.53
2:C:691:GLN:NE2	2:C:694:SER:H	1.96	0.53
2:D:1000:VAL:HG21	2:D:1006:ILE:HD11	1.89	0.53
1:A:312:GLY:HA3	1:A:333:VAL:HA	1.91	0.53
2:D:1031:ARG:HH11	2:D:1031:ARG:HG2	1.74	0.53
2:D:725:VAL:HG12	2:D:729:LYS:HE2	1.91	0.53
2:D:770:ALA:O	2:D:771:ARG:HB2	2.08	0.53
1:A:215:GLY:C	1:A:253:MET:HE2	2.35	0.52
1:A:337:ARG:HG2	1:A:380:PHE:CG	2.45	0.52
2:C:1105:LEU:HG	2:C:1108:MET:HE2	1.90	0.52
1:B:215:GLY:C	1:B:253:MET:HE2	2.34	0.52
2:C:723:ASN:HB3	2:C:742:PHE:CZ	2.42	0.52
2:D:1000:VAL:HG11	2:D:1006:ILE:HD11	1.91	0.52
2:D:1038:THR:OG1	2:D:1041:GLU:HG3	2.10	0.52
1:B:197:GLY:O	1:B:201:SER:HB3	2.09	0.52
2:D:817:LYS:HG3	2:D:818:ASP:OD1	2.09	0.52
2:D:1089:ASP:HB2	2:D:1090:PRO:CD	2.38	0.52
1:A:194:MET:HG3	1:B:190:ALA:HB2	1.91	0.52
2:D:868:ARG:HG2	3:D:1201:AGS:N6	2.25	0.52
2:D:772:LYS:HD2	2:D:774:HIS:NE2	2.25	0.52
2:C:900:PHE:O	2:C:925:CYS:HA	2.10	0.52
2:C:691:GLN:CD	2:C:692:MET:N	2.68	0.52
2:C:984:HIS:HB3	2:C:986:MET:HE3	1.89	0.52
2:D:866:ARG:NH1	2:D:882:VAL:O	2.42	0.52
2:C:946:PHE:CD1	2:C:947:PRO:HD2	2.46	0.51
1:A:190:ALA:HB2	1:B:194:MET:CG	2.40	0.51
1:A:288:ARG:O	1:A:289:PHE:HB2	2.09	0.51
2:D:907:GLU:OE1	2:D:907:GLU:HA	2.10	0.51
1:A:194:MET:HE3	1:B:186:ASN:HB3	1.93	0.51
1:B:274:ALA:HA	1:B:346:PHE:CE1	2.46	0.51
2:C:727:ILE:HG13	2:C:742:PHE:CG	2.45	0.51
2:C:1112:ASP:O	2:C:1113:ALA:CB	2.58	0.51
2:C:827:LYS:HE3	2:C:959:GLU:OE2	2.11	0.51
2:C:942:ARG:O	2:C:942:ARG:HG2	2.10	0.51
2:C:690:LYS:H	2:C:690:LYS:CD	2.14	0.51
2:D:1028:LEU:CD2	2:D:1055:LEU:HD11	2.41	0.51
2:C:971:ALA:HB3	2:C:992:LYS:HA	1.93	0.50
1:B:83:GLU:HB3	1:B:101:LYS:HE3	1.93	0.50
2:C:893:GLY:O	2:C:895:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:964:ARG:HB3	2:D:984:HIS:O	2.11	0.50
2:C:817:LYS:O	2:C:818:ASP:HB2	2.11	0.50
1:A:373:LEU:HB3	1:A:380:PHE:HB2	1.94	0.50
1:B:373:LEU:O	1:B:378:LYS:HB2	2.10	0.50
2:D:946:PHE:CD1	2:D:947:PRO:HD2	2.46	0.50
2:C:1058:THR:HG23	2:C:1059:PRO:CD	2.42	0.50
2:D:1047:TYR:O	2:D:1077:HIS:HA	2.11	0.50
1:A:194:MET:CG	1:B:190:ALA:HB2	2.41	0.49
1:A:423:ASP:O	1:A:427:GLU:HG2	2.12	0.49
1:B:288:ARG:O	1:B:289:PHE:HB2	2.12	0.49
1:B:216:VAL:N	1:B:253:MET:HE2	2.28	0.49
1:A:198:ARG:NH1	6:A:634:HOH:O	2.37	0.49
1:A:98:ILE:CG2	2:C:1108:MET:HE1	2.42	0.49
2:D:1089:ASP:HB2	2:D:1090:PRO:HD2	1.95	0.49
2:D:691:GLN:O	2:D:693:CYS:N	2.46	0.49
2:D:761:HIS:HD2	6:D:1411:HOH:O	1.96	0.49
2:D:681:MET:CE	2:D:776:ALA:HB2	2.43	0.49
1:A:130:LEU:C	1:A:130:LEU:HD23	2.38	0.48
1:A:301:LEU:C	1:A:301:LEU:HD23	2.37	0.48
1:B:251:ARG:HD3	1:B:285:ASP:OD1	2.13	0.48
2:D:923:SER:O	2:D:924:LEU:HB2	2.12	0.48
1:B:395:MET:HE1	1:B:396:LEU:HD23	1.95	0.48
2:D:992:LYS:HE3	2:D:1107:ASP:OD1	2.13	0.48
1:B:90:ASP:CB	2:D:1065:ARG:NH1	2.77	0.48
2:C:691:GLN:HE21	2:C:693:CYS:H	1.61	0.48
1:A:272:GLU:HB3	1:A:284:CYS:HB3	1.93	0.48
1:B:180:SER:O	1:B:184:LEU:HB2	2.14	0.48
1:B:429:SER:HB3	6:B:685:HOH:O	2.12	0.48
2:D:681:MET:HE2	2:D:776:ALA:HB2	1.94	0.48
1:A:91:ILE:HD13	2:C:1098:LEU:HG	1.95	0.48
2:C:691:GLN:CD	2:C:692:MET:H	2.21	0.48
2:D:690:LYS:HD2	2:D:691:GLN:NE2	2.28	0.48
1:B:74:VAL:HG21	1:B:99:MET:SD	2.54	0.48
2:D:902:ARG:HG2	2:D:927:ILE:HG22	1.96	0.48
2:C:940:ILE:H	2:C:940:ILE:CD1	2.19	0.48
1:B:246:THR:HA	1:B:282:MET:HB3	1.94	0.47
2:C:1038:THR:OG1	2:C:1041:GLU:HG3	2.14	0.47
1:A:91:ILE:HG23	2:C:975:HIS:CD2	2.49	0.47
1:A:343:ASN:HA	1:A:346:PHE:CD2	2.49	0.47
1:B:333:VAL:HG23	6:B:661:HOH:O	2.14	0.47
1:A:142:ILE:O	1:A:144:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLU:O	1:A:431:LYS:HE2	2.14	0.47
1:B:340:VAL:O	1:B:344:LYS:HG3	2.14	0.47
2:C:691:GLN:HE21	2:C:694:SER:N	2.00	0.47
1:A:301:LEU:HD23	1:A:302:SER:N	2.30	0.47
2:D:853:LEU:HD22	2:D:900:PHE:CE2	2.49	0.47
2:C:681:MET:HA	2:C:681:MET:HE2	1.95	0.47
2:C:933:ASP:HB3	2:C:936:GLN:HG2	1.96	0.47
2:D:897:ARG:HD2	2:D:924:LEU:HD21	1.97	0.47
1:B:301:LEU:C	1:B:301:LEU:HD23	2.40	0.46
2:C:892:TYR:C	2:C:894:LYS:H	2.22	0.46
2:C:1089:ASP:HB2	2:C:1090:PRO:CD	2.44	0.46
2:D:846:ARG:HD3	6:D:1420:HOH:O	2.15	0.46
1:A:130:LEU:HD23	1:A:130:LEU:O	2.14	0.46
1:B:74:VAL:CG2	1:B:99:MET:SD	3.04	0.46
2:C:681:MET:N	2:C:775:VAL:O	2.49	0.46
1:A:217:THR:HG21	1:A:267:ASP:OD2	2.16	0.46
1:A:167:PHE:CE2	1:B:165:VAL:HG21	2.51	0.46
2:C:690:LYS:O	2:C:691:GLN:HB2	2.14	0.46
2:D:687:LEU:HD12	2:D:775:VAL:HG21	1.97	0.46
1:A:275:ASP:OD2	1:A:309:VAL:HG13	2.16	0.46
1:B:23:GLU:HA	1:B:176:ILE:HD11	1.97	0.46
1:B:85:MET:HE3	2:D:983:GLY:CA	2.45	0.46
2:D:816:LEU:HD22	2:D:821:PRO:HA	1.96	0.46
2:C:910:MET:HG2	2:C:937:ILE:O	2.16	0.46
1:B:198:ARG:NE	6:B:662:HOH:O	2.41	0.46
1:B:347:ALA:HB1	1:B:393:LEU:HD13	1.98	0.46
2:D:691:GLN:C	2:D:693:CYS:N	2.74	0.46
1:A:313:PRO:O	1:A:316:THR:HB	2.16	0.45
1:A:213:THR:HG22	1:A:239:GLU:CB	2.40	0.45
1:A:218:MET:SD	1:A:218:MET:C	3.00	0.45
1:B:337:ARG:HD3	1:B:338:THR:N	2.32	0.45
1:B:395:MET:HE2	1:B:396:LEU:HA	1.99	0.45
2:D:992:LYS:NZ	2:D:1107:ASP:OD1	2.49	0.45
1:A:429:SER:N	1:A:430:PRO:HD3	2.31	0.45
2:C:856:VAL:HG21	2:C:861:ALA:HB1	1.98	0.45
2:D:970:PRO:HB3	2:D:991:GLU:HB2	1.99	0.45
1:A:92:ARG:HD3	1:A:96:ILE:HD12	1.98	0.45
2:D:844:LEU:HD21	2:D:865:ILE:HG23	1.99	0.45
1:A:122:LEU:N	1:A:122:LEU:HD23	2.31	0.45
2:C:943:VAL:O	2:C:944:THR:C	2.60	0.45
2:C:763:TRP:CG	2:C:806:MET:HE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:891:ASN:O	2:D:892:TYR:C	2.60	0.44
1:A:329:HIS:O	1:A:330:ASN:ND2	2.48	0.44
1:A:381:TYR:CZ	1:A:383:PRO:HD3	2.53	0.44
1:B:272:GLU:HB3	1:B:284:CYS:HB3	1.98	0.44
1:B:296:LYS:HE2	1:B:358:SER:OG	2.18	0.44
2:C:980:ARG:NH1	2:C:980:ARG:HB3	2.32	0.44
2:D:968:ARG:HG3	2:D:1078:THR:HG22	1.99	0.44
1:B:17:ALA:O	1:B:21:PHE:HB2	2.18	0.44
1:B:313:PRO:HG2	1:B:316:THR:CG2	2.46	0.44
1:B:244:HIS:O	1:B:249:GLY:HA3	2.17	0.44
2:C:838:GLY:O	2:C:842:GLU:HG3	2.18	0.44
2:C:1027:ALA:HB1	2:C:1031:ARG:HH12	1.81	0.44
1:A:223:THR:N	1:A:224:PRO:CD	2.81	0.43
1:B:284:CYS:HB2	1:B:288:ARG:HG2	2.00	0.43
1:B:339:THR:OG1	1:B:342:GLU:HG3	2.18	0.43
1:B:352:GLU:OE2	1:B:356:LYS:HE3	2.17	0.43
2:D:900:PHE:O	2:D:925:CYS:HA	2.18	0.43
2:D:902:ARG:HG2	2:D:927:ILE:CG2	2.48	0.43
1:A:218:MET:HB2	1:A:226:VAL:HG21	1.99	0.43
2:C:893:GLY:C	2:C:895:GLY:N	2.76	0.43
2:C:692:MET:HE1	2:C:714:VAL:HB	2.01	0.43
2:D:781:ASP:OD1	2:D:781:ASP:C	2.61	0.43
2:D:816:LEU:C	2:D:818:ASP:H	2.26	0.43
2:D:894:LYS:HD2	2:D:894:LYS:N	2.25	0.43
1:A:14:ILE:HG12	1:A:51:VAL:HB	2.01	0.43
1:A:275:ASP:OD2	1:A:309:VAL:HA	2.19	0.43
1:A:308:MET:HA	1:A:336:MET:O	2.17	0.43
1:B:29:GLU:OE2	1:B:32:ARG:NH2	2.51	0.43
1:B:393:LEU:HD12	1:B:393:LEU:HA	1.86	0.43
2:D:691:GLN:HG2	2:D:692:MET:N	2.26	0.43
1:A:122:LEU:HD23	1:A:122:LEU:H	1.84	0.43
1:A:124:GLY:HA2	1:A:149:THR:OG1	2.19	0.43
2:D:723:ASN:O	2:D:727:ILE:HG13	2.18	0.43
1:A:314:LYS:HD3	1:A:328:GLU:CD	2.44	0.43
2:C:940:ILE:N	2:C:940:ILE:CD1	2.80	0.43
2:C:933:ASP:CG	2:C:936:GLN:HG2	2.44	0.43
2:D:684:ALA:O	2:D:688:ILE:HG13	2.18	0.43
2:D:817:LYS:HB2	2:D:817:LYS:NZ	2.34	0.43
2:C:941:ASN:HD21	2:C:946:PHE:HB3	1.84	0.43
1:B:14:ILE:HG12	1:B:51:VAL:HB	2.01	0.42
2:C:894:LYS:O	2:C:894:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:985:VAL:O	2:C:986:MET:HE2	2.19	0.42
1:A:223:THR:HG22	1:A:227:ASN:HD21	1.83	0.42
2:C:933:ASP:HB3	2:C:936:GLN:CG	2.49	0.42
2:D:1055:LEU:O	2:D:1057:PRO:HD3	2.20	0.42
1:A:258:ARG:HA	1:A:295:LYS:HE3	2.02	0.42
1:B:178:ASN:HB2	6:B:669:HOH:O	2.19	0.42
1:B:373:LEU:HB3	1:B:380:PHE:HB2	2.01	0.42
1:A:212:PHE:C	1:A:212:PHE:CD2	2.98	0.42
1:A:418:ALA:O	1:A:421:LEU:HB2	2.20	0.42
1:B:94:LEU:HD21	2:D:978:ASN:HB3	2.01	0.42
1:B:255:ASP:OD1	1:B:258:ARG:NH1	2.50	0.42
2:C:856:VAL:HG22	2:C:857:PRO:HD2	2.02	0.42
2:C:999:MET:HE3	2:C:999:MET:HB3	1.91	0.42
2:D:906:ASP:O	2:D:907:GLU:HB2	2.18	0.42
1:B:275:ASP:OD2	1:B:309:VAL:HA	2.19	0.42
1:A:155:THR:HG23	1:B:152:SER:HA	2.02	0.42
1:B:199:LEU:HD12	1:B:199:LEU:HA	1.91	0.42
2:C:979:GLN:HE21	2:C:979:GLN:HB2	1.52	0.42
1:B:176:ILE:HG22	1:B:181:LYS:HE2	2.02	0.42
2:C:969:CYS:HA	2:C:970:PRO:HD3	1.83	0.42
2:D:792:ARG:HG2	2:D:793:ARG:HG3	2.00	0.42
1:A:156:GLU:CD	1:A:156:GLU:C	2.87	0.42
1:B:104:GLU:HG3	1:B:137:SER:OG	2.19	0.42
2:C:729:LYS:HB3	2:C:729:LYS:HE2	1.87	0.42
1:B:101:LYS:HG3	6:B:755:HOH:O	2.19	0.42
2:C:858:GLY:HA3	6:C:1329:HOH:O	2.19	0.42
2:C:1000:VAL:HG23	2:C:1000:VAL:O	2.19	0.42
1:A:190:ALA:HB2	1:B:194:MET:HG3	2.02	0.41
1:B:8:SER:HA	1:B:9:PRO:HD2	1.91	0.41
2:D:1065:ARG:HG3	2:D:1065:ARG:NH2	2.34	0.41
1:B:337:ARG:HG2	1:B:380:PHE:CG	2.55	0.41
2:C:691:GLN:NE2	2:C:693:CYS:H	2.19	0.41
2:C:1083:TYR:CZ	2:C:1091:LEU:HD23	2.55	0.41
2:C:1089:ASP:HB2	2:C:1090:PRO:HD2	2.01	0.41
1:B:389:LEU:O	1:B:393:LEU:HB2	2.21	0.41
2:C:1075:SER:HA	6:C:1317:HOH:O	2.19	0.41
2:C:760:ASN:HA	2:C:780:HIS:CE1	2.54	0.41
2:C:1006:ILE:HD12	2:C:1055:LEU:CD2	2.51	0.41
2:C:670:SER:N	6:C:1487:HOH:O	2.52	0.41
2:C:985:VAL:C	2:C:986:MET:HE2	2.44	0.41
2:C:1066:ASP:OD1	2:C:1066:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:706:MET:HE1	2:D:823:VAL:CG2	2.42	0.41
1:B:233:LEU:HD11	1:B:266:LEU:HD13	2.02	0.41
2:D:856:VAL:O	2:D:884:THR:HA	2.20	0.41
1:A:393:LEU:HD13	1:A:393:LEU:HA	1.93	0.41
2:D:1002:GLY:C	2:D:1004:ALA:N	2.77	0.41
1:A:273:VAL:O	1:A:277:VAL:HG23	2.21	0.41
1:B:402:ARG:HG3	1:B:402:ARG:HH11	1.84	0.41
2:C:799:GLU:N	2:C:799:GLU:CD	2.79	0.41
1:A:366:PRO:HG3	1:A:412:ILE:HB	2.03	0.41
1:B:71:SER:O	1:B:74:VAL:HG22	2.20	0.41
1:B:101:LYS:HD3	1:B:101:LYS:HA	1.91	0.41
1:B:223:THR:CG2	1:B:227:ASN:ND2	2.84	0.41
2:C:672:GLU:O	2:C:675:SER:OG	2.39	0.41
2:D:816:LEU:O	2:D:818:ASP:N	2.47	0.41
2:D:909:LEU:HG	2:D:932:GLY:HA3	2.03	0.41
1:A:317:ILE:O	1:A:318:PRO:C	2.63	0.41
2:C:676:LEU:HD23	2:C:810:ARG:HD3	2.02	0.41
2:C:1018:LEU:HA	2:C:1037:HIS:O	2.21	0.41
2:D:707:LYS:NZ	2:D:820:GLU:OE1	2.50	0.41
1:A:307:ASP:OD1	1:A:374:ASP:HB2	2.21	0.40
2:C:891:ASN:O	2:C:894:LYS:HB3	2.20	0.40
2:C:710:ILE:HD13	2:C:816:LEU:HD11	2.02	0.40
2:D:887:SER:O	2:D:891:ASN:HB2	2.21	0.40
1:B:130:LEU:HD23	1:B:130:LEU:C	2.46	0.40
1:B:287:SER:O	1:B:290:ASP:HB2	2.20	0.40
2:C:980:ARG:HB3	2:C:980:ARG:HH11	1.87	0.40
1:B:381:TYR:CZ	1:B:383:PRO:HG3	2.56	0.40
2:D:828:VAL:CG1	2:D:957:VAL:HG12	2.52	0.40
1:B:171:VAL:HB	6:B:722:HOH:O	2.21	0.40
2:C:1081:LEU:HD23	2:C:1082:LYS:N	2.37	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	406/431 (94%)	380 (94%)	26 (6%)	0	100	100
1	B	418/431 (97%)	391 (94%)	27 (6%)	0	100	100
2	C	430/451 (95%)	407 (95%)	16 (4%)	7 (2%)	7	14
2	D	427/451 (95%)	401 (94%)	20 (5%)	6 (1%)	9	17
All	All	1681/1764 (95%)	1579 (94%)	89 (5%)	13 (1%)	16	31

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	691	GLN
2	C	1112	ASP
2	C	894	LYS
2	D	692	MET
2	D	817	LYS
2	D	818	ASP
2	D	1001	SER
2	C	818	ASP
2	D	892	TYR
2	C	692	MET
2	C	944	THR
2	C	941	ASN
2	D	943	VAL

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	347/363 (96%)	332 (96%)	15 (4%)	26	51
1	B	356/363 (98%)	342 (96%)	14 (4%)	28	55
2	C	383/397 (96%)	367 (96%)	16 (4%)	26	52
2	D	381/397 (96%)	371 (97%)	10 (3%)	40	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1467/1520 (96%)	1412 (96%)	55 (4%)	30 57

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	29	GLU
1	A	92	ARG
1	A	103	LEU
1	A	140	ILE
1	A	156	GLU
1	A	199	LEU
1	A	212	PHE
1	A	219	PHE
1	A	256	LEU
1	A	288	ARG
1	A	322	GLN
1	A	352	GLU
1	A	393	LEU
1	A	416	GLU
1	B	10	ARG
1	B	24	LEU
1	B	92	ARG
1	B	112	ASP
1	B	184	LEU
1	B	199	LEU
1	B	219	PHE
1	B	266	LEU
1	B	285	ASP
1	B	288	ARG
1	B	294	GLU
1	B	393	LEU
1	B	395	MET
1	B	402	ARG
2	C	690	LYS
2	C	751	ARG
2	C	759	LYS
2	C	799	GLU
2	C	803	TYR
2	C	809	LEU
2	C	817	LYS
2	C	846	ARG

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Mol	Chain	Res	Type
2	C	874	ILE
2	C	907	GLU
2	C	940	ILE
2	C	954	LYS
2	C	979	GLN
2	C	1058	THR
2	C	1103	SER
2	C	1106	LEU
2	D	690	LYS
2	D	803	TYR
2	D	809	LEU
2	D	815	LEU
2	D	817	LYS
2	D	907	GLU
2	D	936	GLN
2	D	978	ASN
2	D	980	ARG
2	D	1071	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	114	GLN
1	A	115	ASN
1	A	227	ASN
1	A	330	ASN
1	B	61	ASN
1	B	209	ASN
1	B	227	ASN
1	B	330	ASN
1	B	400	ASN
1	B	404	GLN
2	C	691	GLN
2	C	704	GLN
2	C	760	ASN
2	C	891	ASN
2	C	979	GLN
2	C	997	GLN
2	C	1040	HIS
2	D	689	HIS
2	D	691	GLN

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Mol	Chain	Res	Type
2	D	704	GLN
2	D	761	HIS
2	D	780	HIS
2	D	891	ASN
2	D	936	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 25 ligands modelled in this entry, 21 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AGS	A	501	-	32,33,33	1.67	7 (21%)	45,52,52	2.01	11 (24%)
3	AGS	C	1201	4	32,33,33	1.42	6 (18%)	45,52,52	1.99	9 (20%)
3	AGS	B	501	-	32,33,33	1.62	7 (21%)	45,52,52	2.02	10 (22%)
3	AGS	D	1201	4	32,33,33	1.49	3 (9%)	45,52,52	1.99	10 (22%)

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	AGS	A	501	-	-	2/21/38/38	0/3/3/3
3	AGS	C	1201	4	-	2/21/38/38	0/3/3/3
3	AGS	B	501	-	-	2/21/38/38	0/3/3/3
3	AGS	D	1201	4	-	4/21/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	AGS	PA-O3A	4.75	1.64	1.59
3	A	501	AGS	PB-O3A	4.38	1.64	1.59
3	D	1201	AGS	PB-O3A	4.31	1.64	1.59
3	D	1201	AGS	PA-O3A	4.11	1.63	1.59
3	B	501	AGS	PB-O3A	3.63	1.63	1.59
3	A	501	AGS	PA-O3A	3.52	1.63	1.59
3	C	1201	AGS	PB-O3B	3.07	1.62	1.59
3	A	501	AGS	PB-O3B	2.92	1.62	1.59
3	C	1201	AGS	PB-O3A	2.91	1.62	1.59
3	A	501	AGS	PB-O1B	2.90	1.60	1.50
3	B	501	AGS	PA-O1A	2.87	1.60	1.50
3	C	1201	AGS	PA-O1A	2.78	1.60	1.50
3	A	501	AGS	PA-O1A	2.75	1.60	1.50
3	C	1201	AGS	PA-O3A	2.74	1.62	1.59
3	D	1201	AGS	C5-C4	2.36	1.43	1.39
3	C	1201	AGS	C5-C4	2.27	1.43	1.39
3	B	501	AGS	PG-O3G	2.25	1.62	1.54
3	A	501	AGS	PG-O2G	2.18	1.61	1.54
3	B	501	AGS	PG-O2G	2.17	1.61	1.54
3	A	501	AGS	PG-O3G	2.14	1.61	1.54
3	C	1201	AGS	C6-N6	2.10	1.39	1.34
3	B	501	AGS	C5-C4	2.08	1.42	1.39
3	B	501	AGS	C5-N7	-2.01	1.35	1.39

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	AGS	PB-O3B-PG	-5.65	112.49	133.17
3	A	501	AGS	PB-O3B-PG	-5.51	113.02	133.17
3	D	1201	AGS	PB-O3B-PG	-5.45	113.23	133.17
3	C	1201	AGS	C5-C4-N3	-5.35	119.35	126.72
3	D	1201	AGS	C5-C4-N3	-5.30	119.42	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1201	AGS	PB-O3B-PG	-5.21	114.12	133.17
3	B	501	AGS	C5-C4-N3	-5.04	119.78	126.72
3	A	501	AGS	C5-C4-N3	-4.94	119.91	126.72
3	A	501	AGS	N3-C2-N1	-4.82	121.28	128.58
3	B	501	AGS	N3-C2-N1	-4.74	121.40	128.58
3	D	1201	AGS	N3-C2-N1	-4.66	121.53	128.58
3	C	1201	AGS	N3-C2-N1	-4.62	121.58	128.58
3	C	1201	AGS	N3-C4-N9	4.56	134.92	127.17
3	D	1201	AGS	N3-C4-N9	4.49	134.79	127.17
3	B	501	AGS	N3-C4-N9	4.25	134.39	127.17
3	A	501	AGS	N3-C4-N9	4.21	134.33	127.17
3	C	1201	AGS	C5-N7-C8	3.94	109.64	103.45
3	C	1201	AGS	C2-N3-C4	3.83	121.19	111.83
3	D	1201	AGS	C5-N7-C8	3.76	109.36	103.45
3	B	501	AGS	C2-N3-C4	3.76	121.01	111.83
3	D	1201	AGS	C2-N3-C4	3.75	121.00	111.83
3	A	501	AGS	C2-N3-C4	3.71	120.89	111.83
3	A	501	AGS	C5-N7-C8	3.65	109.19	103.45
3	B	501	AGS	C5-N7-C8	3.61	109.12	103.45
3	C	1201	AGS	C4-C5-N7	-3.14	106.99	110.58
3	A	501	AGS	C4-C5-N7	-2.92	107.25	110.58
3	B	501	AGS	C4-C5-N7	-2.87	107.30	110.58
3	D	1201	AGS	C4-C5-N7	-2.78	107.41	110.58
3	A	501	AGS	N9-C8-N7	-2.72	110.08	113.94
3	C	1201	AGS	N9-C8-N7	-2.61	110.24	113.94
3	A	501	AGS	O3G-PG-O3B	2.58	113.24	104.64
3	B	501	AGS	N9-C8-N7	-2.55	110.33	113.94
3	D	1201	AGS	N9-C8-N7	-2.37	110.58	113.94
3	A	501	AGS	PA-O5'-C5'	-2.31	108.12	121.35
3	B	501	AGS	O3G-PG-O3B	2.30	112.30	104.64
3	C	1201	AGS	PA-O5'-C5'	-2.22	108.61	121.35
3	B	501	AGS	PA-O5'-C5'	-2.19	108.80	121.35
3	D	1201	AGS	PA-O5'-C5'	-2.13	109.14	121.35
3	D	1201	AGS	O2G-PG-O3B	2.11	111.69	104.64
3	A	501	AGS	O2A-PA-O3A	2.06	112.84	107.27

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	AGS	PB-O3B-PG-O2G
3	A	501	AGS	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
3	D	1201	AGS	C2'-C1'-N9-C8
3	D	1201	AGS	PB-O3A-PA-O1A
3	D	1201	AGS	PB-O3A-PA-O2A
3	B	501	AGS	PB-O3B-PG-O2G
3	B	501	AGS	PB-O3B-PG-O3G
3	D	1201	AGS	O4'-C1'-N9-C8
3	C	1201	AGS	PB-O3A-PA-O1A
3	C	1201	AGS	PB-O3A-PA-O2A

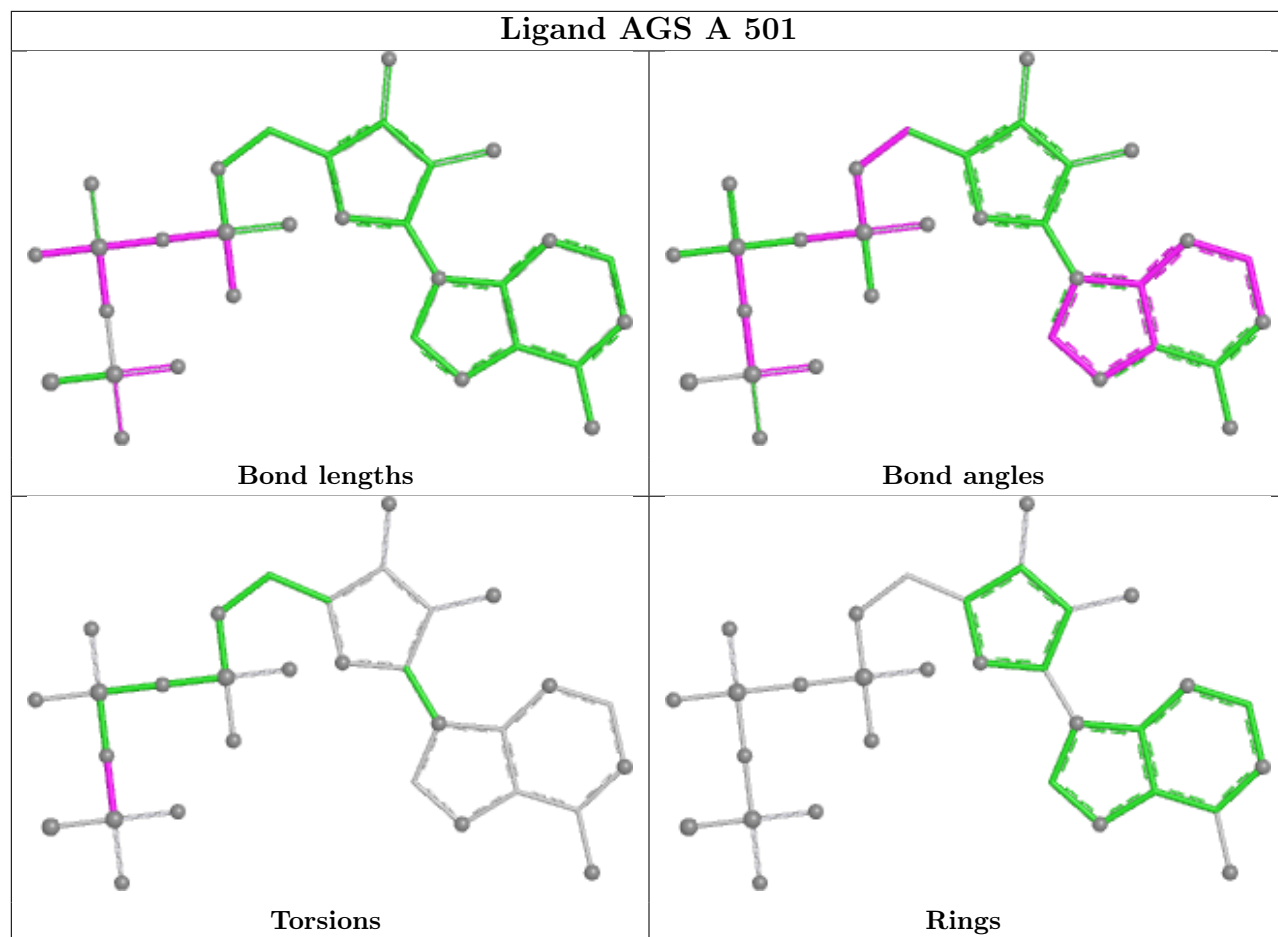
There are no ring outliers.

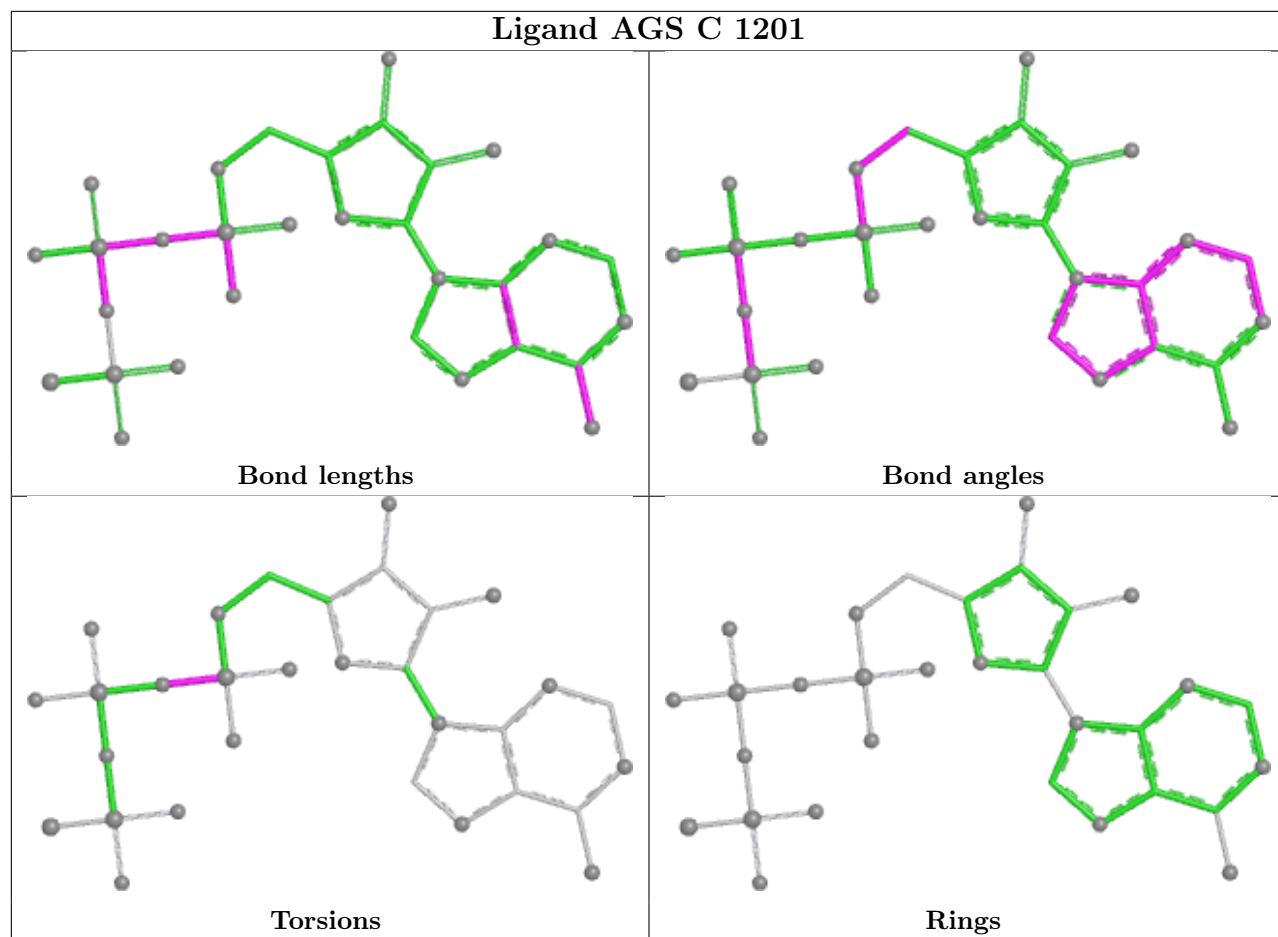
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1201	AGS	1	0
3	D	1201	AGS	1	0

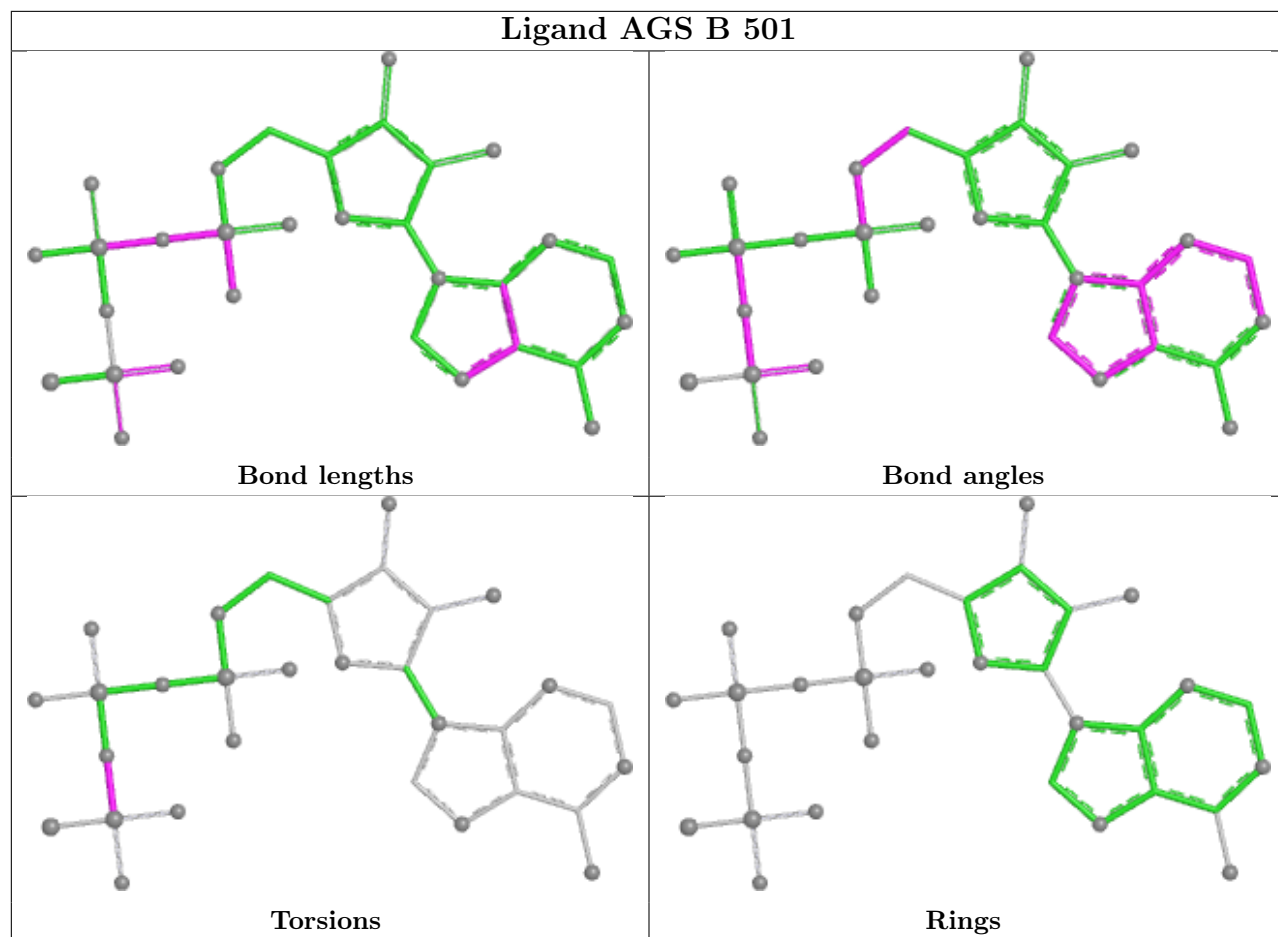
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

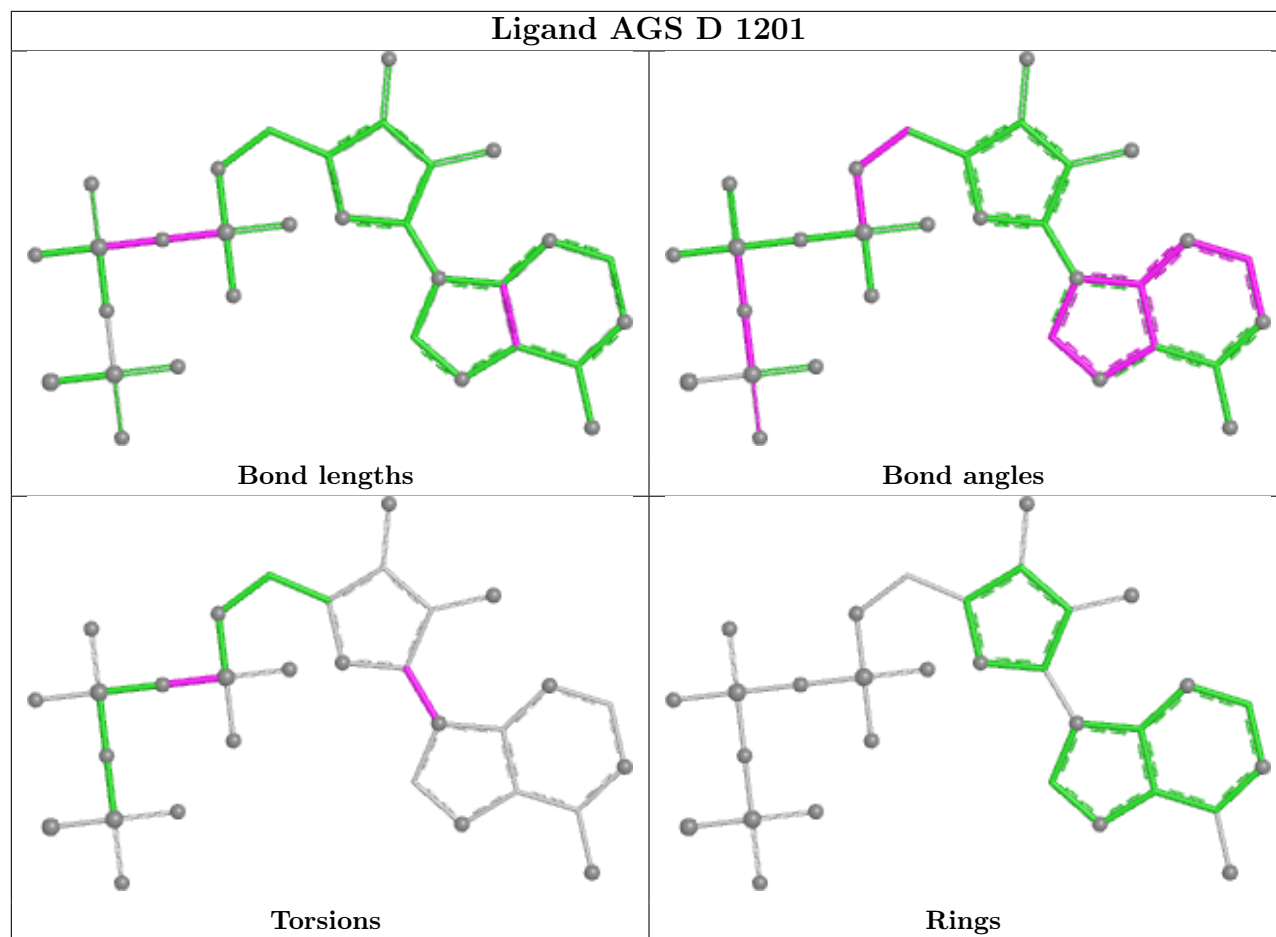
Ligand AGS A 501





Ligand AGS B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	412/431 (95%)	-0.16	9 (2%) 62 58	14, 27, 58, 76	0
1	B	422/431 (97%)	-0.07	8 (1%) 66 62	14, 30, 57, 81	0
2	C	434/451 (96%)	0.03	22 (5%) 33 29	14, 29, 61, 80	0
2	D	431/451 (95%)	0.05	15 (3%) 47 42	16, 32, 59, 72	0
All	All	1699/1764 (96%)	-0.03	54 (3%) 50 46	14, 30, 59, 81	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1113	ALA	5.3
2	C	670	SER	4.3
2	C	819	GLY	4.0
2	C	741	LYS	4.0
2	D	874	ILE	3.6
2	C	691	GLN	3.5
2	C	742	PHE	3.5
2	C	693	CYS	3.4
2	D	1111	VAL	3.4
2	C	818	ASP	3.2
1	A	41	LYS	3.2
2	C	896	ALA	3.1
2	C	692	MET	3.0
1	A	312	GLY	3.0
2	C	943	VAL	2.9
2	D	1001	SER	2.8
2	C	694	SER	2.8
1	B	81	GLY	2.8
2	C	937	ILE	2.8
1	A	330	ASN	2.7
2	D	1003	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	114	GLN	2.7
1	A	45	LYS	2.6
2	C	754	VAL	2.6
1	A	331	GLU	2.6
1	B	205	HIS	2.6
2	C	753	LEU	2.6
2	D	817	LYS	2.6
1	B	82	GLU	2.5
2	C	817	LYS	2.5
2	D	1004	ALA	2.5
2	C	944	THR	2.5
1	B	207	ILE	2.4
2	D	818	ASP	2.4
1	B	42	SER	2.3
2	D	675	SER	2.3
1	A	323	GLN	2.3
2	C	730	ASP	2.3
2	C	690	LYS	2.3
1	A	40	ASN	2.3
1	A	379	ASP	2.3
2	D	814	ARG	2.2
2	D	691	GLN	2.2
2	C	941	ASN	2.2
2	D	894	LYS	2.2
1	B	176	ILE	2.1
2	D	896	ALA	2.1
1	B	330	ASN	2.0
2	C	673	ILE	2.0
2	C	946	PHE	2.0
2	D	859	ARG	2.0
2	D	943	VAL	2.0
2	D	893	GLY	2.0
1	B	79	THR	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 ⓘ

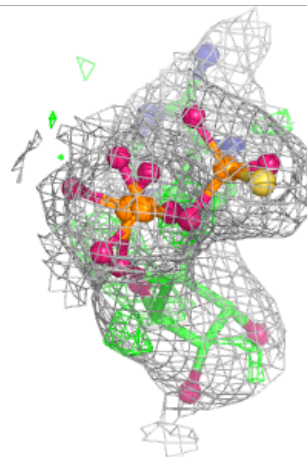
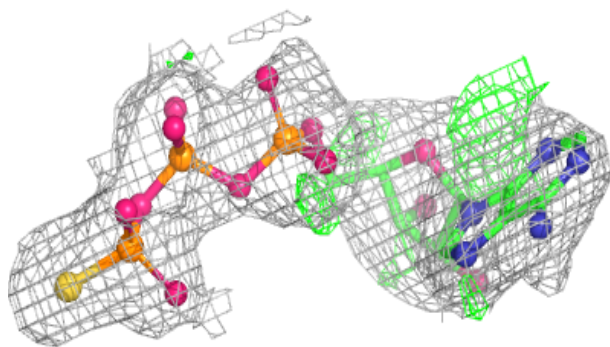
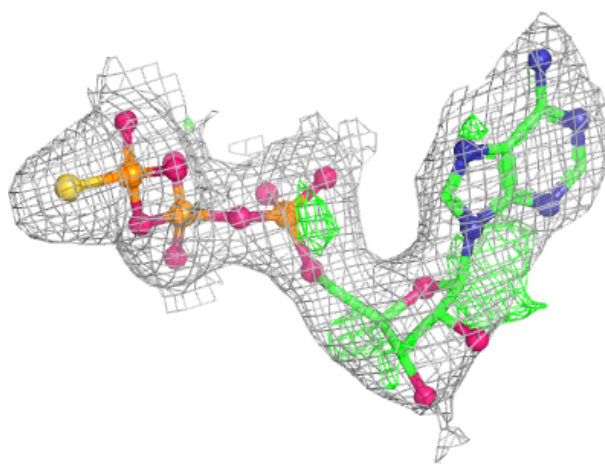
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CS	B	505	1/1	0.91	0.13	104,104,104,104	0
5	CS	C	1205	1/1	0.93	0.23	131,131,131,131	0
3	AGS	D	1201	31/31	0.96	0.10	14,48,63,63	0
5	CS	C	1204	1/1	0.96	0.14	103,103,103,103	0
5	CS	A	507	1/1	0.96	0.12	92,92,92,92	0
5	CS	D	1204	1/1	0.96	0.13	131,131,131,131	0
5	CS	D	1206	1/1	0.96	0.16	101,101,101,101	0
5	CS	D	1207	1/1	0.96	0.14	115,115,115,115	0
3	AGS	B	501	31/31	0.97	0.07	19,23,29,30	0
5	CS	B	503	1/1	0.97	0.04	59,59,59,59	0
3	AGS	C	1201	31/31	0.97	0.10	14,37,55,56	0
3	AGS	A	501	31/31	0.97	0.06	16,21,29,35	0
5	CS	D	1203	1/1	0.98	0.13	95,95,95,95	0
5	CS	A	504	1/1	0.98	0.04	52,52,52,52	0
5	CS	A	505	1/1	0.98	0.06	66,66,66,66	0
5	CS	B	504	1/1	0.98	0.09	83,83,83,83	0
4	MG	A	502	1/1	0.99	0.04	17,17,17,17	0
4	MG	C	1202	1/1	0.99	0.03	11,11,11,11	0
5	CS	A	506	1/1	0.99	0.02	32,32,32,32	0
5	CS	D	1205	1/1	0.99	0.10	85,85,85,85	0
5	CS	B	506	1/1	0.99	0.09	73,73,73,73	0
5	CS	A	503	1/1	0.99	0.04	56,56,56,56	0
5	CS	B	502	1/1	1.00	0.05	54,54,54,54	0
5	CS	C	1203	1/1	1.00	0.01	29,29,29,29	0
4	MG	D	1202	1/1	1.00	0.01	22,22,22,22	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.

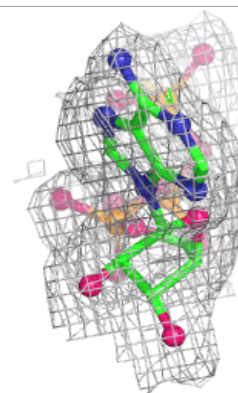
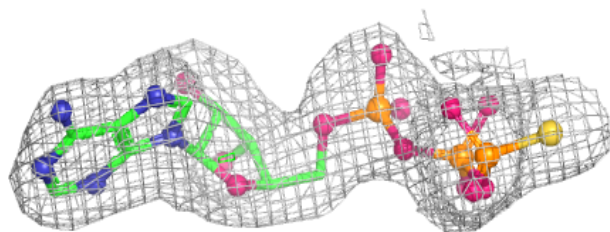
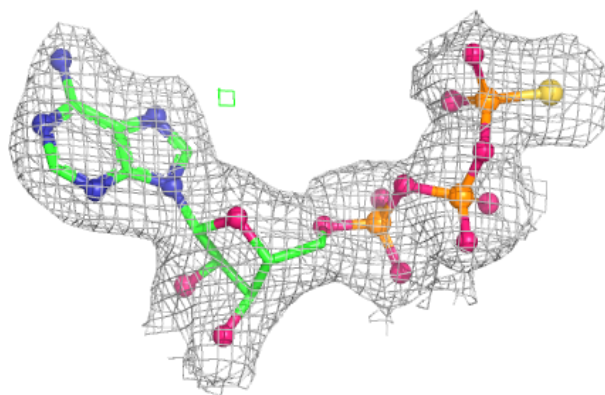
Electron density around AGS D 1201:

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

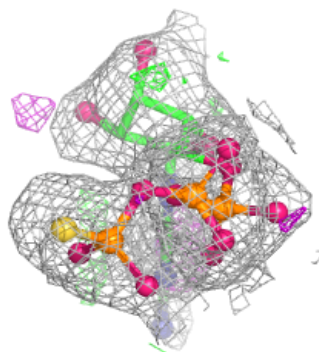
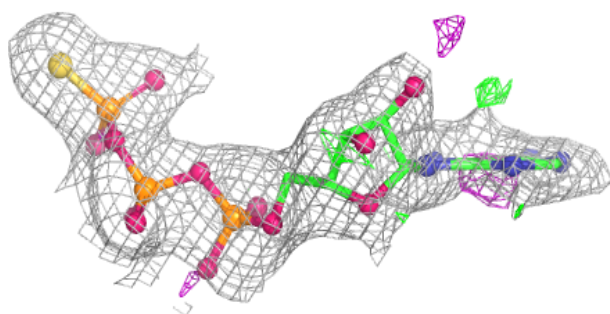
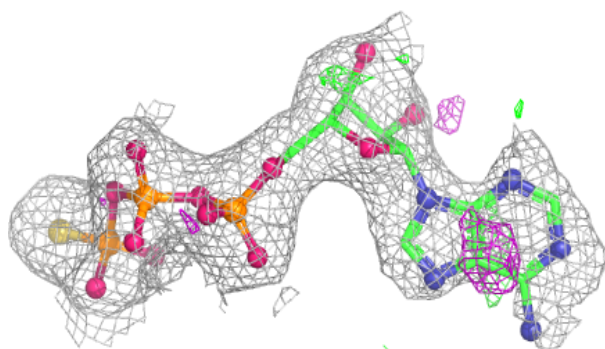


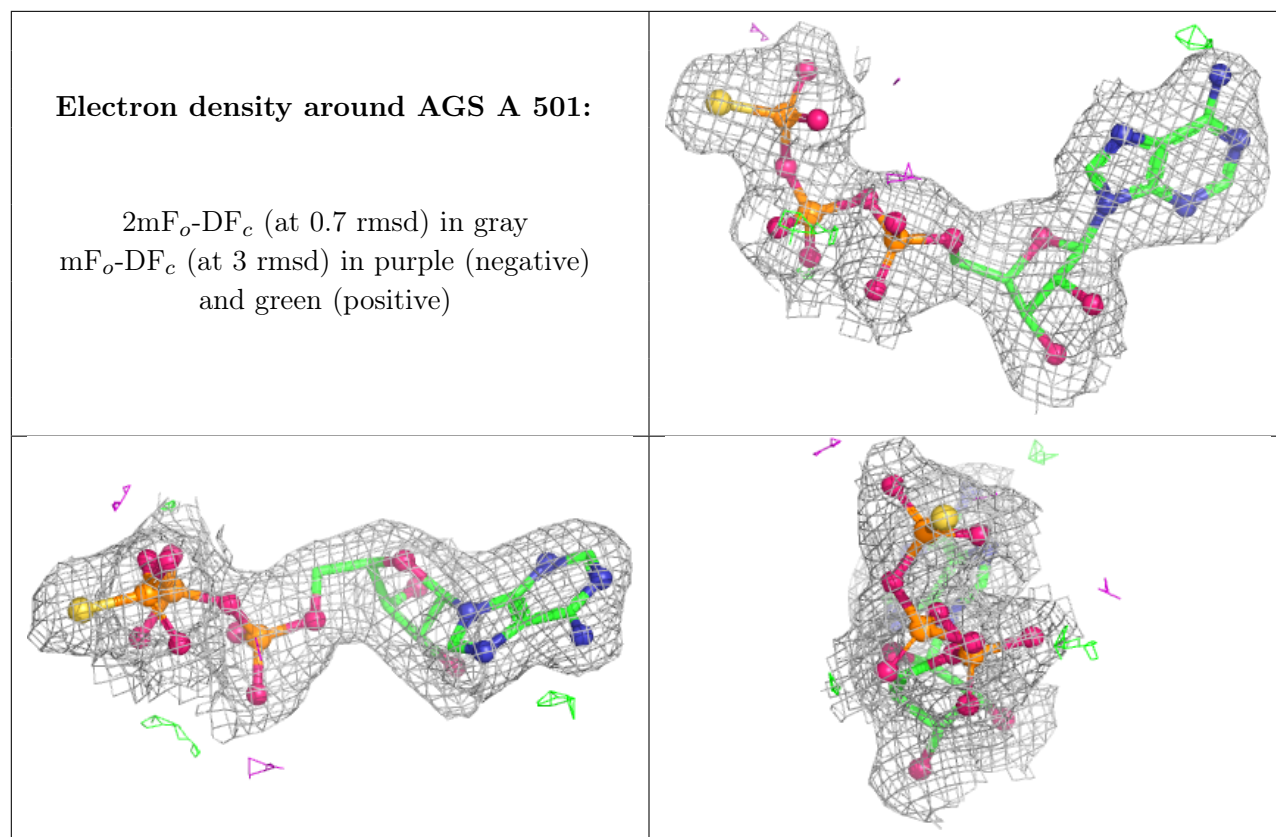
Electron density around AGS B 501:

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

**Electron density around AGS C 1201:**

$2mF_o-DF_c$ (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.