



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:09 pm BST

PDB ID : 6HRC
Title : Outward-facing PglK with ATPgammaS bound
Authors : Perez, C.; Locher, K.P.
Deposited on : 2018-09-26
Resolution : 3.30 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

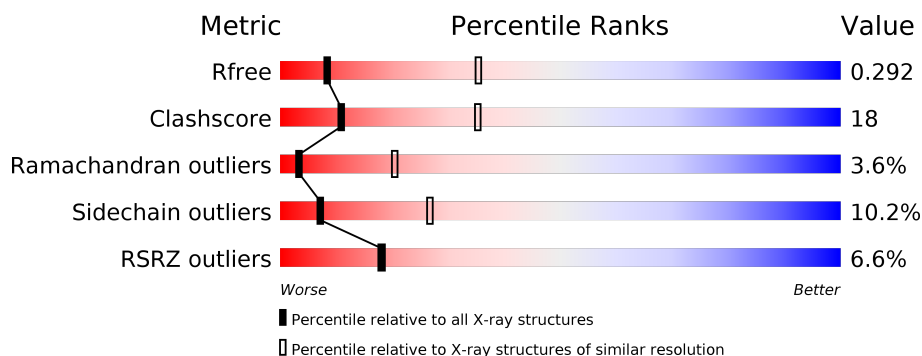
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	564	<div> <div>7%</div> <div> <div></div> <div>58%</div> <div>37%</div> <div>5%</div> </div> </div>
1	B	564	<div> <div>8%</div> <div> <div></div> <div>57%</div> <div>35%</div> <div>7%</div> </div> </div>
1	C	564	<div> <div>5%</div> <div> <div></div> <div>55%</div> <div>36%</div> <div>8%</div> </div> </div>
1	D	564	<div> <div>6%</div> <div> <div></div> <div>58%</div> <div>35%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AGS	B	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18482 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.

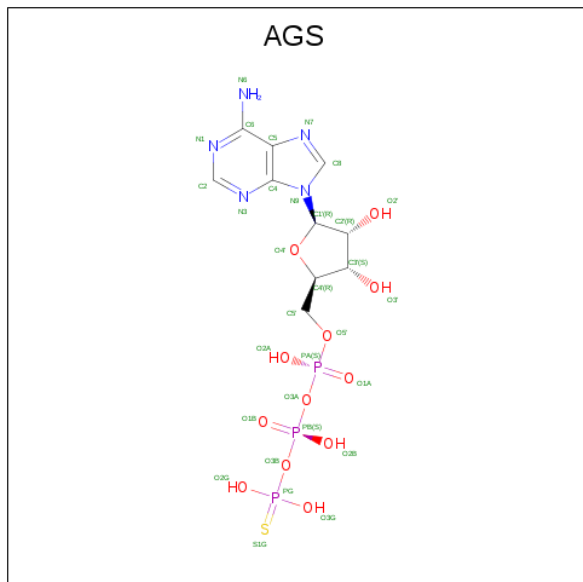
- Molecule 1 is a protein called WlaB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4555	2998	732	811	14			
1	B	564	Total	C	N	O	S	0	0	0
			4555	2998	732	811	14			
1	C	564	Total	C	N	O	S	0	0	0
			4555	2998	732	811	14			
1	D	564	Total	C	N	O	S	0	0	0
			4555	2998	732	811	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	conflict	UNP O86150
A	105	LYS	TYR	conflict	UNP O86150
A	338	ALA	LEU	conflict	UNP O86150
A	339	ALA	GLY	conflict	UNP O86150
A	510	GLN	GLU	engineered mutation	UNP O86150
B	2	VAL	LEU	conflict	UNP O86150
B	105	LYS	TYR	conflict	UNP O86150
B	338	ALA	LEU	conflict	UNP O86150
B	339	ALA	GLY	conflict	UNP O86150
B	510	GLN	GLU	engineered mutation	UNP O86150
C	2	VAL	LEU	conflict	UNP O86150
C	105	LYS	TYR	conflict	UNP O86150
C	338	ALA	LEU	conflict	UNP O86150
C	339	ALA	GLY	conflict	UNP O86150
C	510	GLN	GLU	engineered mutation	UNP O86150
D	2	VAL	LEU	conflict	UNP O86150
D	105	LYS	TYR	conflict	UNP O86150
D	338	ALA	LEU	conflict	UNP O86150
D	339	ALA	GLY	conflict	UNP O86150
D	510	GLN	GLU	engineered mutation	UNP O86150

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	36	Total	O	0	0
			36	36		

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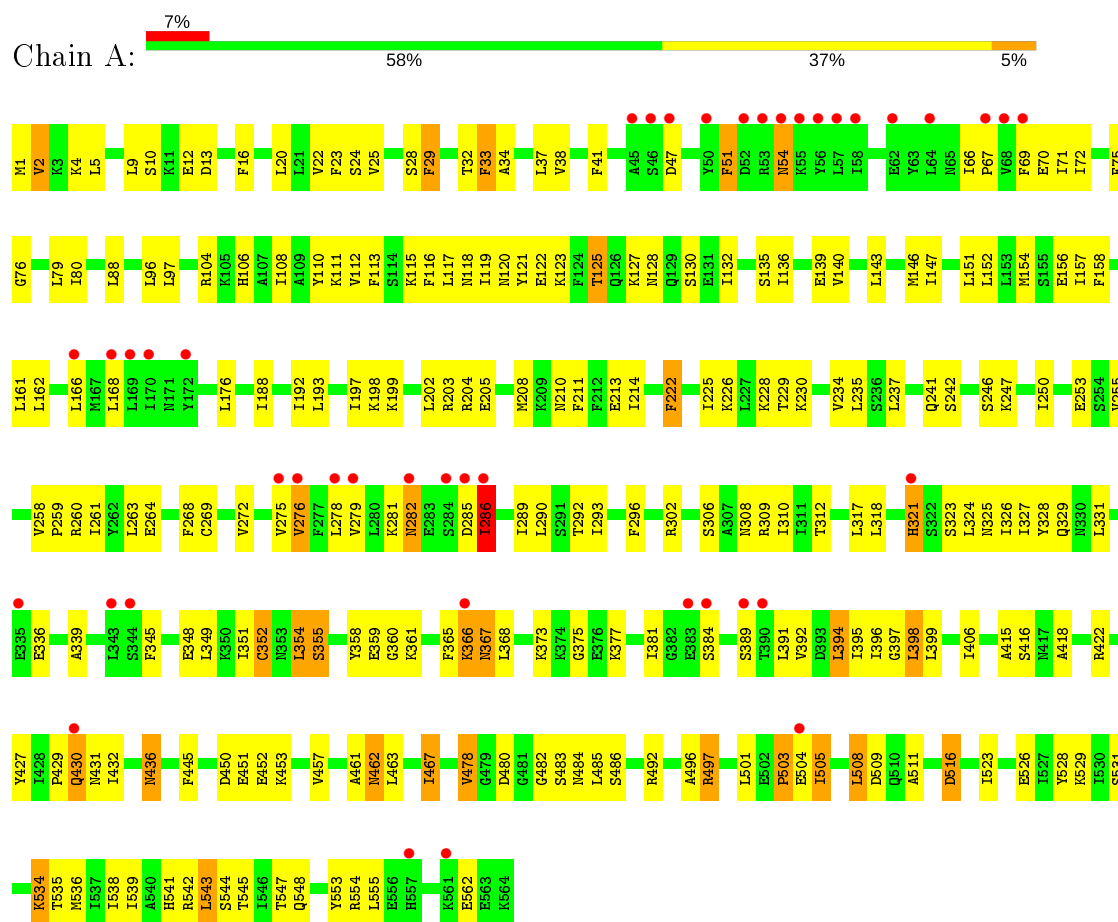
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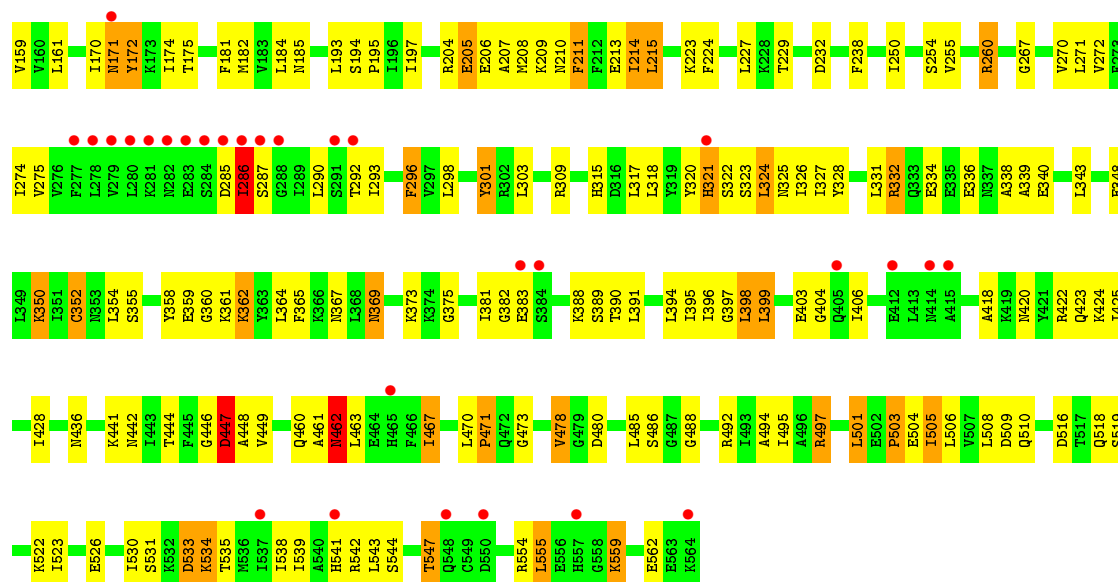
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	37	Total	O	0	0
			37	37		
4	D	31	Total	O	0	0
			31	31		

3 Residue-property plots

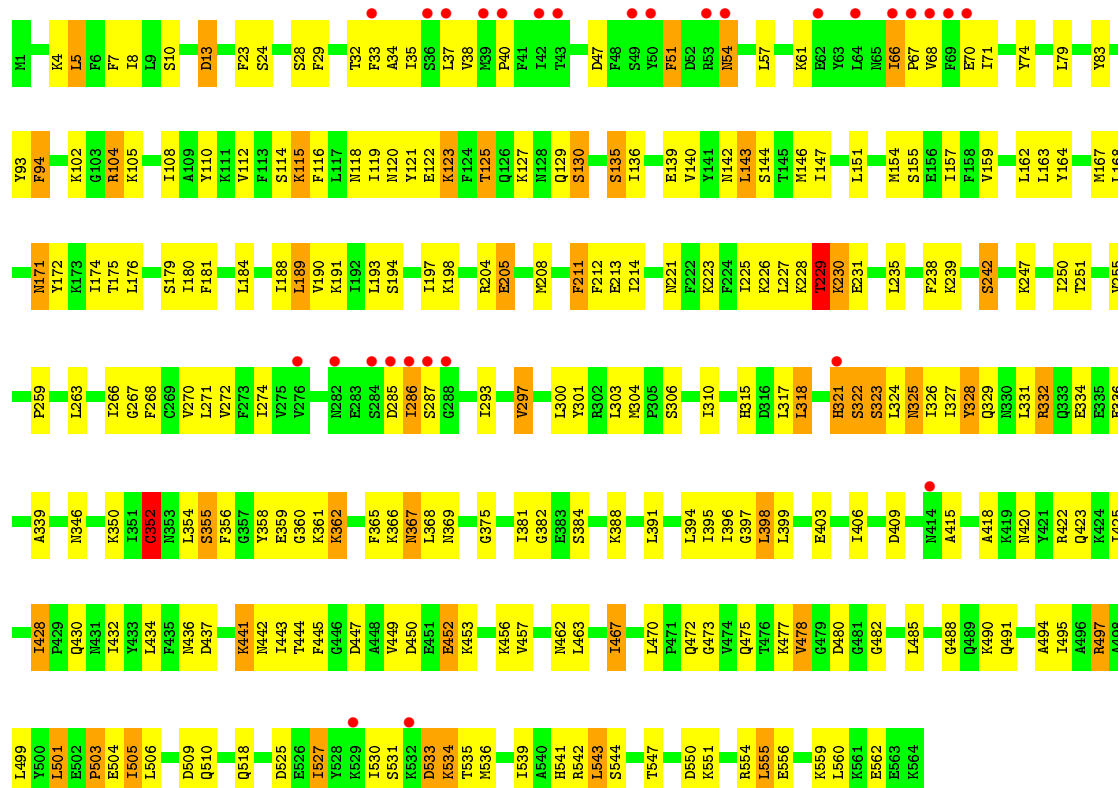
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: WlaB protein



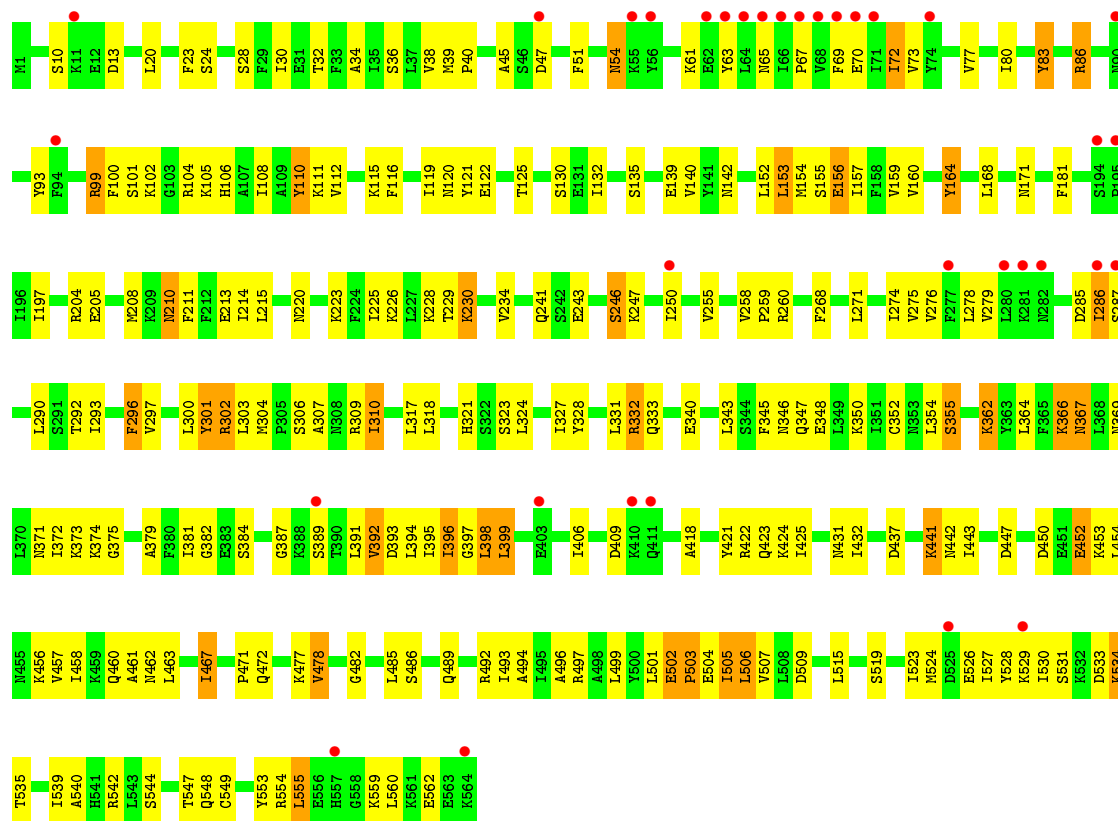


• Molecule 1: WlaB protein



• Molecule 1: WlaB protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.68 Å 145.98 Å 206.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 29.81 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.8 (20.00-3.30) 84.0 (29.81-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.18 Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.232 , 0.284 0.242 , 0.292	Depositor DCC
R_{free} test set	2695 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	106.1	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 86.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18482	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.32	0/4639	0.51	0/6244
1	B	0.37	0/4639	0.55	0/6244
1	C	0.35	0/4639	0.52	0/6244
1	D	0.33	0/4639	0.52	0/6244
All	All	0.34	0/18556	0.53	0/24976

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4555	0	4760	174	0
1	B	4555	0	4760	180	0
1	C	4555	0	4760	189	0
1	D	4555	0	4760	177	0
2	A	31	0	12	3	0
2	B	31	0	12	10	0
2	C	31	0	12	3	0
2	D	31	0	12	5	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	32	0	0	7	0
4	B	36	0	0	6	0
4	C	37	0	0	9	0
4	D	31	0	0	4	0
All	All	18482	0	19088	681	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 18.

All (681) 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:B:125:THR:HG21	2:B:601:AGS:HN62	1.27	1.00
1:C:509:ASP:HA	1:C:539:ILE:HB	1.54	0.90
1:C:38:VAL:HG22	1:C:83:TYR:OH	1.70	0.89
1:A:397:GLY:HA3	1:A:422:ARG:HD2	1.58	0.86
1:D:142:ASN:HB2	1:D:324:LEU:HD22	1.59	0.84
1:D:375:GLY:H	1:D:535:THR:HB	1.42	0.83
1:B:509:ASP:HA	1:B:539:ILE:HB	1.61	0.83
2:B:601:AGS:H8	2:B:601:AGS:O5'	1.79	0.82
1:C:204:ARG:HH12	1:C:324:LEU:HD11	1.44	0.81
1:B:207:ALA:O	1:B:211:PHE:HB3	1.81	0.81
1:D:160:VAL:O	1:D:164:TYR:HB2	1.80	0.81
1:C:323:SER:HB2	1:C:324:LEU:HD12	1.63	0.81
4:A:702:HOH:O	2:B:601:AGS:H3'	1.82	0.80
1:D:297:VAL:O	1:D:301:TYR:HB2	1.79	0.80
1:A:375:GLY:H	1:A:535:THR:HB	1.47	0.78
1:C:397:GLY:HA3	1:C:422:ARG:HD2	1.66	0.78
1:B:317:LEU:O	1:B:321:HIS:HB2	1.85	0.77
1:A:509:ASP:HA	1:A:539:ILE:HB	1.66	0.77
1:D:211:PHE:HA	1:D:214:ILE:HG22	1.66	0.76
1:C:503:PRO:HA	4:C:721:HOH:O	1.85	0.76
1:B:146:MET:HB2	1:B:321:HIS:CE1	2.20	0.76
1:C:142:ASN:HB2	1:C:324:LEU:HD22	1.67	0.76
1:C:501:LEU:HD11	1:D:228:LYS:HD2	1.68	0.75
1:D:139:GLU:HA	1:D:324:LEU:HD23	1.68	0.74
1:C:354:LEU:HD21	1:C:394:LEU:HD13	1.69	0.74
1:C:235:LEU:HD11	1:D:110:TYR:HD1	1.52	0.74
1:D:478:VAL:HG22	1:D:485:LEU:HD11	1.69	0.73
1:A:193:LEU:HD13	1:A:255:VAL:HG13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:SER:HB2	1:C:318:LEU:HD22	1.71	0.72
1:C:37:LEU:HD22	1:C:37:LEU:O	1.89	0.72
1:A:152:LEU:HD21	1:A:309:ARG:HG2	1.69	0.72
1:A:198:LYS:HG3	1:A:318:LEU:HD22	1.71	0.71
1:B:115:LYS:NZ	1:B:332:ARG:O	2.23	0.71
1:B:193:LEU:HD22	1:B:255:VAL:HG13	1.72	0.71
1:B:97:LEU:HD21	1:B:151:LEU:HG	1.73	0.70
1:A:242:SER:OG	1:B:106:HIS:ND1	2.24	0.70
1:D:300:LEU:O	1:D:304:MET:HG2	1.91	0.70
1:B:8:ILE:HG23	1:B:332:ARG:HH22	1.56	0.70
1:C:227:LEU:HD21	1:D:396:ILE:HD13	1.74	0.70
1:A:492:ARG:NH2	4:A:701:HOH:O	2.25	0.70
1:C:324:LEU:HB2	4:C:731:HOH:O	1.91	0.70
1:C:503:PRO:HB3	1:C:534:LYS:HZ3	1.57	0.69
1:A:118:ASN:HB3	1:A:336:GLU:HG3	1.73	0.69
1:B:503:PRO:HB3	1:B:534:LYS:HZ3	1.58	0.69
1:C:163:LEU:HD22	1:C:303:LEU:HD13	1.75	0.68
1:D:531:SER:HA	1:D:534:LYS:HE3	1.75	0.68
1:B:156:GLU:HA	1:B:159:VAL:HG12	1.77	0.67
1:B:146:MET:HB2	1:B:321:HIS:HE1	1.60	0.67
1:D:509:ASP:HA	1:D:539:ILE:HB	1.77	0.67
2:A:601:AGS:O5'	2:A:601:AGS:H8	1.95	0.66
1:A:158:PHE:HB2	4:A:721:HOH:O	1.96	0.66
1:C:37:LEU:HD11	1:C:79:LEU:CG	2.26	0.66
1:D:555:LEU:HD23	1:D:560:LEU:HB3	1.77	0.66
1:A:306:SER:O	1:A:310:ILE:HG12	1.94	0.66
1:C:321:HIS:O	1:C:325:ASN:HB2	1.95	0.66
1:C:450:ASP:HB3	1:C:453:LYS:HB3	1.76	0.66
1:C:115:LYS:HE3	1:C:336:GLU:HG3	1.77	0.66
1:C:102:LYS:HB2	1:D:250:ILE:HG22	1.77	0.66
1:B:420:ASN:HA	1:B:423:GLN:HG3	1.77	0.66
1:C:37:LEU:HD11	1:C:79:LEU:HG	1.76	0.66
1:D:327:ILE:O	1:D:331:LEU:HG	1.96	0.65
1:D:34:ALA:O	1:D:38:VAL:HG23	1.96	0.65
1:B:559:LYS:H	1:B:559:LYS:HE2	1.61	0.65
1:C:13:ASP:OD1	1:C:13:ASP:N	2.29	0.65
1:D:362:LYS:H	1:D:362:LYS:HD3	1.61	0.65
1:A:202:LEU:HD12	1:A:323:SER:HB3	1.79	0.65
1:B:197:ILE:HD11	1:B:255:VAL:HG11	1.78	0.65
1:B:533:ASP:OD2	1:B:533:ASP:N	2.30	0.65
1:C:34:ALA:O	1:C:38:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ILE:HG22	1:B:272:VAL:HG21	1.78	0.65
1:C:115:LYS:NZ	1:C:332:ARG:O	2.29	0.65
1:B:23:PHE:HD2	1:B:93:TYR:HD2	1.45	0.64
1:C:355:SER:OG	1:C:367:ASN:N	2.30	0.64
1:C:478:VAL:HG22	1:C:485:LEU:HD11	1.78	0.64
1:C:4:LYS:O	1:C:8:ILE:HG12	1.96	0.64
1:C:120:ASN:OD1	1:C:121:TYR:N	2.30	0.64
1:D:389:SER:HB2	2:D:601:AGS:O2B	1.98	0.64
1:A:358:TYR:O	1:A:360:GLY:N	2.31	0.64
1:D:205:GLU:HG3	1:D:323:SER:HB3	1.79	0.63
1:C:420:ASN:HA	1:C:423:GLN:HG3	1.80	0.63
1:D:225:ILE:HD13	1:D:234:VAL:HG21	1.81	0.63
1:A:427:TYR:HE2	1:B:223:LYS:HZ3	1.47	0.63
1:A:302:ARG:NH1	1:B:301:TYR:OH	2.23	0.63
1:B:205:GLU:HB2	1:B:323:SER:HB3	1.80	0.63
1:B:397:GLY:HA3	1:B:422:ARG:HG3	1.80	0.63
1:B:145:THR:HB	1:B:146:MET:SD	2.39	0.63
1:C:193:LEU:HD13	4:C:708:HOH:O	1.99	0.62
1:A:450:ASP:HB3	1:A:453:LYS:HB3	1.81	0.62
1:B:208:MET:HA	1:B:211:PHE:HD2	1.64	0.62
1:A:13:ASP:OD2	1:A:104:ARG:NH1	2.33	0.62
1:A:526:GLU:HA	1:A:529:LYS:HE3	1.81	0.62
1:C:418:ALA:O	1:C:422:ARG:HD3	2.00	0.62
1:C:37:LEU:O	1:C:40:PRO:HD2	1.98	0.62
1:D:350:LYS:HG3	1:D:371:ASN:HB3	1.82	0.61
1:D:30:ILE:HG22	1:D:86:ARG:HG3	1.82	0.61
1:C:197:ILE:HD11	1:C:255:VAL:HG11	1.82	0.61
1:B:115:LYS:HE3	1:B:336:GLU:HG3	1.82	0.61
1:B:35:ILE:HD11	1:B:298:LEU:HD21	1.83	0.61
1:B:136:ILE:HG22	1:B:136:ILE:O	2.01	0.61
1:A:97:LEU:HD22	1:A:151:LEU:HD21	1.81	0.61
1:A:348:GLU:HA	1:A:373:LYS:HA	1.83	0.61
1:B:424:LYS:HB3	1:B:504:GLU:HB3	1.81	0.61
1:C:115:LYS:HD2	1:C:334:GLU:HB2	1.82	0.61
1:D:443:ILE:HD12	1:D:496:ALA:HB3	1.82	0.61
1:D:347:GLN:O	1:D:374:LYS:N	2.26	0.61
1:B:324:LEU:HA	1:B:327:ILE:HG12	1.83	0.60
1:D:348:GLU:N	1:D:409:ASP:OD2	2.30	0.60
1:A:260:ARG:O	1:A:264:GLU:HG2	2.00	0.60
1:A:553:TYR:CE1	1:A:562:GLU:HG3	2.37	0.60
1:D:255:VAL:O	1:D:259:PRO:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:TYR:CE2	1:A:429:PRO:HB3	2.37	0.60
1:C:8:ILE:HG22	1:C:108:ILE:HD12	1.83	0.60
1:C:214:ILE:HD11	1:C:238:PHE:HA	1.84	0.60
1:A:9:LEU:HB3	1:A:13:ASP:HB2	1.84	0.60
1:B:389:SER:N	2:B:601:AGS:O1B	2.29	0.59
1:A:285:ASP:HA	1:A:289:ILE:HG23	1.84	0.59
1:A:358:TYR:HB2	1:A:361:LYS:HD2	1.84	0.59
2:C:601:AGS:H8	2:C:601:AGS:O5'	2.02	0.59
1:B:130:SER:OG	1:B:213:GLU:HG2	2.01	0.59
1:C:463:LEU:HB3	1:C:467:ILE:HD11	1.82	0.59
1:B:113:PHE:CZ	1:B:117:LEU:HD11	2.37	0.59
1:B:463:LEU:HB3	1:B:467:ILE:HD11	1.85	0.59
1:B:4:LYS:NZ	1:B:326:ILE:HG12	2.17	0.59
1:B:290:LEU:HA	1:B:293:ILE:HG22	1.84	0.59
1:C:317:LEU:O	1:C:321:HIS:HB2	2.03	0.59
1:D:142:ASN:HB2	1:D:324:LEU:CD2	2.31	0.59
1:B:39:MET:O	1:B:42:ILE:HG13	2.03	0.59
1:D:397:GLY:HA3	1:D:422:ARG:HG3	1.84	0.59
1:C:263:LEU:HA	1:C:266:ILE:HG22	1.85	0.59
1:C:555:LEU:HD23	1:C:560:LEU:HB3	1.85	0.59
1:B:146:MET:SD	1:B:146:MET:N	2.75	0.58
1:B:13:ASP:HB2	1:B:100:PHE:HE1	1.67	0.58
1:C:346:ASN:N	1:C:409:ASP:OD1	2.25	0.58
1:A:397:GLY:O	1:A:422:ARG:NH1	2.37	0.58
1:B:206:GLU:OE2	1:B:210:ASN:ND2	2.31	0.58
1:B:13:ASP:OD2	1:B:104:ARG:NH1	2.37	0.58
1:D:130:SER:OG	1:D:213:GLU:HG2	2.04	0.58
1:D:421:TYR:HA	1:D:424:LYS:HD2	1.86	0.58
1:B:508:LEU:HD22	1:B:538:ILE:HD12	1.86	0.57
1:C:323:SER:O	1:C:327:ILE:HG12	2.04	0.57
1:C:108:ILE:O	1:C:112:VAL:HG23	2.04	0.57
1:C:322:SER:O	1:C:326:ILE:HG12	2.04	0.57
1:A:429:PRO:O	1:A:431:ASN:N	2.37	0.57
1:D:122:GLU:O	1:D:125:THR:HG22	2.05	0.57
1:D:443:ILE:HD11	1:D:493:ILE:HG23	1.87	0.57
1:D:524:MET:HA	1:D:527:ILE:HG22	1.87	0.57
1:A:225:ILE:HD13	1:A:234:VAL:HG21	1.86	0.57
1:B:135:SER:C	1:B:136:ILE:HG12	2.25	0.57
2:C:601:AGS:O3B	1:D:486:SER:HB2	2.04	0.57
1:B:4:LYS:O	1:B:8:ILE:HG12	2.05	0.57
1:D:247:LYS:O	1:D:250:ILE:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ARG:HH11	1:D:99:ARG:HB3	1.69	0.57
1:B:358:TYR:HB2	1:B:361:LYS:HD2	1.87	0.56
1:B:171:ASN:HB3	1:B:174:ILE:HD11	1.86	0.56
1:B:197:ILE:HD12	1:B:315:HIS:CD2	2.40	0.56
1:B:461:ALA:O	1:B:463:LEU:N	2.38	0.56
1:B:460:GLN:HA	1:B:526:GLU:HG2	1.88	0.56
1:D:122:GLU:HA	1:D:125:THR:HG22	1.85	0.56
1:C:362:LYS:H	1:C:362:LYS:HD3	1.70	0.56
1:D:116:PHE:HE2	1:D:331:LEU:HD13	1.71	0.56
2:D:601:AGS:O5'	2:D:601:AGS:H8	2.06	0.56
1:C:208:MET:HA	1:C:211:PHE:CE2	2.40	0.56
1:D:505:ILE:HA	1:D:535:THR:O	2.06	0.56
1:C:204:ARG:NH1	1:C:324:LEU:HD11	2.19	0.56
1:D:346:ASN:N	1:D:409:ASP:OD1	2.33	0.56
1:A:367:ASN:O	1:A:367:ASN:ND2	2.38	0.56
1:A:427:TYR:HB2	1:B:227:LEU:HD23	1.86	0.56
1:A:47:ASP:HB3	4:A:729:HOH:O	2.05	0.56
1:A:5:LEU:HG	1:A:321:HIS:HE1	1.71	0.56
1:B:63:TYR:CD1	1:B:65:ASN:HB2	2.41	0.56
1:B:132:ILE:O	1:B:136:ILE:HG12	2.06	0.56
1:D:348:GLU:HA	1:D:373:LYS:HA	1.87	0.56
1:D:77:VAL:HA	1:D:80:ILE:HG22	1.88	0.55
1:A:365:PHE:HB3	1:A:368:LEU:HD23	1.87	0.55
1:B:142:ASN:HB3	1:B:324:LEU:HD22	1.88	0.55
1:C:441:LYS:O	1:C:443:ILE:N	2.38	0.55
1:A:211:PHE:HA	1:A:214:ILE:HG22	1.89	0.55
1:A:531:SER:HA	1:A:534:LYS:HE3	1.87	0.55
1:C:358:TYR:O	1:C:360:GLY:N	2.39	0.55
1:C:164:TYR:HE1	1:C:179:SER:HB2	1.70	0.55
1:A:541:HIS:HB3	1:B:516:ASP:HA	1.88	0.55
1:B:367:ASN:ND2	1:B:367:ASN:O	2.39	0.55
1:C:381:ILE:O	1:C:554:ARG:HA	2.07	0.55
1:C:355:SER:HB2	1:C:403:GLU:HB2	1.86	0.55
1:A:122:GLU:O	1:A:125:THR:HG22	2.07	0.55
1:B:132:ILE:O	1:B:136:ILE:CG1	2.54	0.55
1:C:172:TYR:HD2	4:C:712:HOH:O	1.88	0.55
1:C:272:VAL:HG21	1:D:80:ILE:HB	1.87	0.55
1:D:397:GLY:HA3	1:D:422:ARG:HD2	1.87	0.55
1:D:460:GLN:HA	1:D:526:GLU:HG2	1.89	0.55
1:A:528:TYR:CZ	1:A:548:GLN:HB2	2.41	0.55
1:C:396:ILE:HG13	1:C:398:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:519:SER:O	1:D:523:ILE:HG12	2.07	0.55
1:A:260:ARG:HG3	1:A:261:ILE:HD12	1.89	0.55
1:A:226:LYS:HE3	1:B:422:ARG:HH21	1.72	0.55
1:B:140:VAL:HG23	1:B:328:TYR:OH	2.07	0.55
1:C:367:ASN:ND2	1:C:367:ASN:O	2.38	0.55
1:C:436:ASN:HB2	1:C:480:ASP:HA	1.90	0.55
1:D:296:PHE:O	1:D:300:LEU:HB3	2.06	0.55
1:D:108:ILE:O	1:D:112:VAL:HG23	2.07	0.54
1:B:323:SER:HA	4:B:727:HOH:O	2.06	0.54
1:A:140:VAL:HB	1:A:328:TYR:OH	2.08	0.54
1:D:255:VAL:O	1:D:258:VAL:HG12	2.07	0.54
1:B:76:GLY:O	1:B:80:ILE:HG23	2.08	0.54
1:A:253:GLU:HB3	1:B:98:ALA:HB1	1.89	0.54
1:D:116:PHE:HZ	1:D:331:LEU:HD22	1.71	0.54
1:A:461:ALA:O	1:A:492:ARG:HD2	2.08	0.54
1:B:355:SER:HB2	1:B:403:GLU:HB2	1.88	0.54
1:C:171:ASN:HB3	1:C:174:ILE:HD11	1.88	0.54
1:C:544:SER:HA	1:C:547:THR:HG23	1.90	0.54
1:A:130:SER:OG	1:A:213:GLU:HG2	2.08	0.54
1:A:246:SER:OG	1:B:103:GLY:HA2	2.08	0.54
1:A:116:PHE:HE2	1:A:331:LEU:HD13	1.73	0.54
1:D:323:SER:O	1:D:327:ILE:HG12	2.07	0.54
1:A:429:PRO:HD2	1:A:432:ILE:HG22	1.89	0.54
1:A:484:ASN:HA	2:B:601:AGS:C6	2.38	0.54
1:B:16:PHE:CE2	1:B:100:PHE:HB2	2.43	0.54
1:B:36:SER:O	1:B:40:PRO:HD2	2.08	0.54
1:B:492:ARG:HA	1:B:495:ILE:HD12	1.88	0.54
1:D:461:ALA:O	1:D:463:LEU:N	2.41	0.54
1:D:381:ILE:O	1:D:554:ARG:HA	2.08	0.54
1:A:430:GLN:HG2	1:A:431:ASN:N	2.22	0.53
1:A:516:ASP:HA	1:B:541:HIS:HB3	1.89	0.53
1:D:454:LEU:O	1:D:458:ILE:HG12	2.08	0.53
1:B:32:THR:HG21	4:B:723:HOH:O	2.07	0.53
1:C:189:LEU:O	1:C:193:LEU:HB2	2.08	0.53
1:D:116:PHE:CZ	1:D:331:LEU:HD22	2.44	0.53
1:D:210:ASN:HB3	1:D:241:GLN:HG3	1.90	0.53
1:C:136:ILE:HG21	1:D:215:LEU:HD21	1.90	0.53
1:D:63:TYR:CD1	1:D:65:ASN:HB2	2.43	0.53
1:A:497:ARG:HD2	1:B:224:PHE:CZ	2.44	0.53
1:B:250:ILE:O	1:B:254:SER:OG	2.23	0.53
1:B:16:PHE:HE2	1:B:100:PHE:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:PRO:HB3	1:C:534:LYS:NZ	2.24	0.53
1:A:272:VAL:HG21	1:B:80:ILE:HG22	1.90	0.52
1:D:36:SER:O	1:D:39:MET:N	2.42	0.52
1:A:79:LEU:HD12	1:B:272:VAL:HG11	1.91	0.52
1:D:139:GLU:HB2	1:D:328:TYR:CE2	2.44	0.52
1:D:457:VAL:HG12	1:D:496:ALA:HB1	1.91	0.52
1:B:113:PHE:CE2	1:B:117:LEU:HD11	2.44	0.52
1:D:502:GLU:HB3	1:D:503:PRO:HD2	1.92	0.52
1:B:142:ASN:O	1:B:146:MET:HG2	2.09	0.52
1:A:543:LEU:O	1:A:545:THR:N	2.40	0.52
1:A:72:ILE:HG23	4:A:712:HOH:O	2.08	0.52
1:C:146:MET:SD	1:C:321:HIS:HA	2.49	0.52
1:C:228:LYS:C	1:C:230:LYS:H	2.12	0.52
1:D:120:ASN:OD1	1:D:121:TYR:N	2.43	0.52
1:C:123:LYS:HD3	4:C:713:HOH:O	2.09	0.52
1:C:32:THR:HG21	1:C:162:LEU:HD21	1.91	0.52
1:C:135:SER:OG	1:C:331:LEU:HD11	2.10	0.52
1:A:29:PHE:CD1	1:A:162:LEU:HD13	2.44	0.52
1:A:457:VAL:HG12	1:A:496:ALA:HB1	1.90	0.52
1:C:432:ILE:HD11	1:C:491:GLN:HG2	1.91	0.52
1:A:51:PHE:CZ	1:A:71:ILE:HG21	2.45	0.51
1:C:130:SER:OG	1:C:213:GLU:HG2	2.10	0.51
1:D:381:ILE:HD13	1:D:540:ALA:O	2.09	0.51
1:A:34:ALA:O	1:A:38:VAL:HG23	2.09	0.51
1:C:37:LEU:HD11	1:C:79:LEU:HD11	1.93	0.51
1:D:285:ASP:O	1:D:287:SER:N	2.36	0.51
1:A:136:ILE:HG21	1:B:215:LEU:HD11	1.91	0.51
1:A:285:ASP:O	1:A:286:ILE:HG13	2.11	0.51
1:D:307:ALA:HA	1:D:310:ILE:HG13	1.92	0.51
1:B:181:PHE:O	1:B:185:ASN:ND2	2.41	0.51
1:C:51:PHE:HD1	1:C:61:LYS:HB2	1.74	0.51
1:D:24:SER:HB3	1:D:93:TYR:OH	2.09	0.51
1:A:486:SER:HA	2:B:601:AGS:O2A	2.10	0.51
1:B:209:LYS:HG3	4:B:704:HOH:O	2.10	0.51
1:D:160:VAL:HG13	1:D:303:LEU:HD11	1.93	0.51
1:D:211:PHE:HB3	1:D:241:GLN:HB2	1.92	0.51
1:A:69:PHE:O	1:A:72:ILE:HG12	2.11	0.51
1:A:115:LYS:O	1:A:119:ILE:HG23	2.11	0.51
1:C:142:ASN:HB2	1:C:324:LEU:CD2	2.40	0.51
1:D:452:GLU:HG3	1:D:453:LYS:N	2.25	0.51
1:C:501:LEU:HD21	1:D:228:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:THR:O	1:D:296:PHE:HB2	2.11	0.51
1:A:392:VAL:HG21	1:A:539:ILE:HD11	1.93	0.50
1:A:389:SER:HB2	2:A:601:AGS:O1B	2.11	0.50
1:B:317:LEU:HG	1:B:321:HIS:CD2	2.46	0.50
1:D:13:ASP:OD2	1:D:104:ARG:NH1	2.44	0.50
1:D:63:TYR:HD1	1:D:65:ASN:HB2	1.76	0.50
1:A:247:LYS:O	1:A:250:ILE:HG13	2.10	0.50
1:B:332:ARG:CZ	1:B:332:ARG:HB2	2.40	0.50
1:B:348:GLU:OE1	1:B:350:LYS:NZ	2.45	0.50
1:C:247:LYS:O	1:C:251:THR:HG23	2.11	0.50
1:C:255:VAL:O	1:C:259:PRO:HD3	2.11	0.50
1:D:290:LEU:HA	1:D:293:ILE:HG22	1.93	0.50
1:C:327:ILE:O	1:C:331:LEU:HG	2.10	0.50
1:C:339:ALA:HB3	1:C:415:ALA:O	2.11	0.50
1:C:37:LEU:HD11	1:C:79:LEU:CD1	2.41	0.50
1:D:424:LYS:HB3	1:D:504:GLU:HB3	1.92	0.50
1:B:358:TYR:O	1:B:360:GLY:N	2.45	0.50
1:B:478:VAL:HG22	1:B:485:LEU:HD11	1.93	0.50
1:B:446:GLY:O	1:B:448:ALA:N	2.42	0.50
1:B:112:VAL:HG12	1:B:136:ILE:HD11	1.94	0.50
1:B:139:GLU:HA	1:B:142:ASN:HB2	1.94	0.50
1:C:10:SER:OG	1:C:13:ASP:OD1	2.21	0.50
1:C:155:SER:O	1:C:159:VAL:HG23	2.11	0.50
1:D:125:THR:HG21	2:D:601:AGS:HN62	1.76	0.50
1:D:155:SER:O	1:D:159:VAL:HG23	2.12	0.50
1:D:432:ILE:HG21	1:D:494:ALA:HB2	1.94	0.50
1:C:382:GLY:N	1:C:388:LYS:HD3	2.27	0.50
1:D:392:VAL:O	1:D:396:ILE:HG13	2.12	0.50
1:D:39:MET:HB3	1:D:40:PRO:HD3	1.94	0.50
1:A:508:LEU:HD22	1:A:538:ILE:HG23	1.94	0.49
1:A:199:LYS:O	1:A:203:ARG:HG3	2.11	0.49
1:B:503:PRO:HB3	1:B:534:LYS:NZ	2.26	0.49
1:D:418:ALA:O	1:D:422:ARG:HD3	2.12	0.49
1:A:354:LEU:HD21	1:A:394:LEU:HD13	1.94	0.49
1:C:223:LYS:HD3	1:D:121:TYR:CZ	2.47	0.49
1:C:5:LEU:HD21	1:C:147:ILE:CD1	2.43	0.49
1:C:116:PHE:HE2	1:C:331:LEU:HD13	1.76	0.49
1:C:122:GLU:O	1:C:125:THR:HG22	2.13	0.49
1:D:69:PHE:HD1	4:D:713:HOH:O	1.96	0.49
1:A:508:LEU:HD22	1:A:538:ILE:HD12	1.94	0.49
1:C:223:LYS:HD2	1:D:398:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LYS:HD3	1:B:362:LYS:H	1.76	0.49
1:D:140:VAL:HB	1:D:328:TYR:OH	2.13	0.49
1:A:282:ASN:O	1:A:282:ASN:ND2	2.39	0.49
1:A:354:LEU:HD11	1:A:394:LEU:HD22	1.94	0.49
1:D:274:ILE:O	1:D:278:LEU:HB2	2.12	0.49
1:A:121:TYR:CE2	1:B:223:LYS:HD3	2.47	0.49
1:A:116:PHE:CE1	1:A:132:ILE:HG12	2.47	0.49
1:B:105:LYS:HG2	1:B:140:VAL:HG12	1.94	0.49
1:C:193:LEU:HD22	1:C:255:VAL:HG13	1.95	0.49
1:C:66:ILE:HG13	1:C:71:ILE:HG13	1.94	0.49
1:B:494:ALA:O	1:B:497:ARG:HB2	2.13	0.48
1:C:104:ARG:O	1:C:108:ILE:HG12	2.13	0.48
1:C:38:VAL:HG22	1:C:83:TYR:HH	1.74	0.48
1:D:506:LEU:HG	1:D:534:LYS:HZ2	1.77	0.48
1:A:478:VAL:HG13	1:A:482:GLY:HA2	1.96	0.48
1:A:453:LYS:O	1:A:457:VAL:HG23	2.13	0.48
1:C:139:GLU:HA	1:C:324:LEU:HD23	1.96	0.48
1:A:28:SER:O	1:A:32:THR:HG23	2.13	0.48
1:A:120:ASN:OD1	1:A:121:TYR:N	2.47	0.48
1:A:467:ILE:H	1:A:467:ILE:HG12	1.37	0.48
1:A:503:PRO:HB3	1:A:534:LYS:HZ3	1.78	0.48
1:B:63:TYR:HD1	1:B:65:ASN:HB2	1.78	0.48
1:C:250:ILE:CG1	1:D:102:LYS:HB2	2.44	0.48
1:D:164:TYR:CZ	1:D:303:LEU:HD21	2.48	0.48
1:A:128:ASN:O	1:A:132:ILE:HG13	2.13	0.48
1:A:136:ILE:CG2	1:B:215:LEU:HD11	2.44	0.48
1:B:348:GLU:HA	1:B:373:LYS:HA	1.95	0.48
1:B:544:SER:HA	1:B:547:THR:HG23	1.95	0.48
1:C:28:SER:HB2	1:C:159:VAL:HG22	1.96	0.48
1:A:345:PHE:CE1	1:A:349:LEU:HB2	2.49	0.48
1:B:470:LEU:HD12	1:B:471:PRO:HD2	1.95	0.48
1:C:38:VAL:CG2	1:C:83:TYR:OH	2.53	0.48
1:D:246:SER:O	1:D:250:ILE:HG23	2.14	0.48
1:D:553:TYR:CE1	1:D:562:GLU:HG3	2.49	0.48
1:A:113:PHE:CE2	1:A:117:LEU:HD11	2.48	0.47
1:C:229:THR:O	1:C:231:GLU:N	2.47	0.47
1:C:142:ASN:CB	1:C:324:LEU:HD22	2.42	0.47
1:D:396:ILE:HG21	1:D:425:ILE:HG21	1.96	0.47
1:B:390:THR:OG1	2:B:601:AGS:O1A	2.32	0.47
1:C:531:SER:HA	1:C:534:LYS:HE3	1.96	0.47
1:D:366:LYS:O	1:D:367:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:PRO:HG2	1:D:70:GLU:HG3	1.96	0.47
1:A:116:PHE:CE2	1:A:331:LEU:HD13	2.49	0.47
1:C:398:LEU:HD22	1:C:398:LEU:H	1.79	0.47
1:C:7:PHE:HD2	1:C:329:GLN:HG3	1.79	0.47
1:D:153:LEU:HG	4:D:708:HOH:O	2.14	0.47
1:D:531:SER:HA	1:D:534:LYS:CE	2.44	0.47
1:D:544:SER:HA	1:D:547:THR:HG23	1.96	0.47
1:A:355:SER:OG	1:A:367:ASN:N	2.33	0.47
1:A:41:PHE:HE1	1:A:76:GLY:HA2	1.80	0.47
1:B:142:ASN:HB3	1:B:324:LEU:CD2	2.44	0.47
1:D:105:LYS:HZ3	1:D:140:VAL:HG11	1.80	0.47
1:D:396:ILE:HD13	1:D:398:LEU:HD22	1.97	0.47
1:D:526:GLU:HA	1:D:529:LYS:HE3	1.97	0.47
1:A:272:VAL:HB	4:B:703:HOH:O	2.14	0.47
1:B:292:THR:O	1:B:296:PHE:HB3	2.14	0.47
1:A:139:GLU:O	1:A:324:LEU:HD21	2.14	0.47
1:A:345:PHE:HE1	1:A:349:LEU:HB2	1.79	0.47
1:C:488:GLY:HA3	1:D:384:SER:OG	2.14	0.47
1:D:51:PHE:HD1	1:D:61:LYS:HB2	1.80	0.47
1:A:4:LYS:HE2	1:A:329:GLN:HG2	1.96	0.47
1:A:250:ILE:HG22	1:B:102:LYS:HB2	1.96	0.47
1:B:170:ILE:H	1:B:170:ILE:HD12	1.79	0.47
1:D:461:ALA:O	1:D:492:ARG:HD2	2.14	0.47
1:A:436:ASN:HB2	1:A:480:ASP:HA	1.97	0.47
1:C:285:ASP:O	1:C:287:SER:N	2.43	0.47
1:C:497:ARG:NH1	4:C:704:HOH:O	2.47	0.47
1:D:461:ALA:HA	1:D:523:ILE:HD12	1.97	0.47
1:A:276:VAL:O	1:A:279:VAL:HG22	2.15	0.47
1:B:115:LYS:HD2	1:B:334:GLU:HB2	1.96	0.47
1:B:12:GLU:O	1:B:15:ASN:N	2.48	0.47
1:C:550:ASP:OD1	1:C:551:LYS:N	2.47	0.47
1:C:66:ILE:HB	1:C:70:GLU:HB2	1.97	0.47
1:D:271:LEU:O	1:D:274:ILE:HG13	2.15	0.47
1:A:351:ILE:HG23	1:A:354:LEU:HD13	1.96	0.46
1:A:41:PHE:CE1	1:A:76:GLY:HA2	2.50	0.46
1:D:354:LEU:HD21	1:D:394:LEU:HD13	1.97	0.46
1:D:453:LYS:HE3	1:D:453:LYS:HB2	1.69	0.46
1:A:355:SER:HA	1:A:366:LYS:H	1.81	0.46
1:B:112:VAL:HG12	1:B:136:ILE:CD1	2.46	0.46
1:C:190:VAL:HG22	1:C:315:HIS:CE1	2.50	0.46
1:D:208:MET:HA	1:D:211:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:VAL:HG11	1:D:507:VAL:HG11	1.98	0.46
1:A:462:ASN:OD1	1:A:523:ILE:HD11	2.14	0.46
1:B:30:ILE:HG22	1:B:86:ARG:HG3	1.97	0.46
1:B:116:PHE:CZ	1:B:331:LEU:HD22	2.50	0.46
1:D:285:ASP:O	1:D:286:ILE:HG12	2.15	0.46
1:D:364:LEU:HD21	2:D:601:AGS:H5'1	1.98	0.46
1:A:108:ILE:O	1:A:112:VAL:HG23	2.15	0.46
1:A:289:ILE:O	1:A:293:ILE:HG22	2.15	0.46
1:C:322:SER:HB2	4:C:716:HOH:O	2.15	0.46
1:C:472:GLN:HB3	1:C:475:GLN:HB3	1.98	0.46
1:A:197:ILE:HD12	1:A:197:ILE:H	1.81	0.46
1:A:210:ASN:HB3	1:A:241:GLN:HG3	1.98	0.46
1:B:20:LEU:HD22	1:B:151:LEU:HD11	1.98	0.46
1:B:146:MET:CB	1:B:321:HIS:CE1	2.97	0.46
1:C:5:LEU:HD21	1:C:147:ILE:HD11	1.98	0.46
1:D:367:ASN:O	1:D:367:ASN:ND2	2.40	0.46
1:A:292:THR:O	1:A:296:PHE:HB2	2.16	0.46
1:C:428:ILE:HD13	1:C:495:ILE:HG12	1.96	0.46
2:D:601:AGS:O2B	2:D:601:AGS:S1G	2.74	0.46
1:B:398:LEU:HD13	1:B:398:LEU:H	1.81	0.46
1:C:365:PHE:HB3	1:C:368:LEU:HD23	1.97	0.46
1:B:157:ILE:O	1:B:161:LEU:HG	2.17	0.45
1:D:467:ILE:HG12	1:D:467:ILE:H	1.34	0.45
1:B:375:GLY:H	1:B:535:THR:HB	1.81	0.45
1:C:239:LYS:HG2	1:D:106:HIS:HE1	1.80	0.45
1:C:434:LEU:HB3	1:C:478:VAL:HG11	1.97	0.45
1:A:451:GLU:N	1:D:243:GLU:OE1	2.49	0.45
1:D:302:ARG:NE	1:D:302:ARG:HA	2.30	0.45
1:C:268:PHE:HB3	1:D:83:TYR:CD2	2.51	0.45
1:A:214:ILE:HD11	1:A:237:LEU:HB2	1.98	0.45
1:A:544:SER:HA	1:A:547:THR:HG23	1.97	0.45
1:A:71:ILE:HB	4:A:712:HOH:O	2.16	0.45
1:C:250:ILE:HG13	1:D:102:LYS:HB2	1.98	0.45
1:D:156:GLU:HG3	1:D:306:SER:OG	2.15	0.45
1:D:492:ARG:HG3	1:D:515:LEU:HD21	1.98	0.45
1:C:228:LYS:O	1:C:230:LYS:N	2.47	0.45
1:C:266:ILE:O	1:C:270:VAL:HG13	2.16	0.45
1:C:271:LEU:O	1:C:274:ILE:HG12	2.17	0.45
1:D:396:ILE:CD1	1:D:398:LEU:HD22	2.47	0.45
1:C:121:TYR:CE2	1:D:223:LYS:HD3	2.51	0.45
1:A:135:SER:O	1:A:328:TYR:OH	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:O	1:A:321:HIS:HB3	2.16	0.45
1:A:4:LYS:NZ	1:A:326:ILE:HG12	2.32	0.45
1:B:382:GLY:N	1:B:388:LYS:HD3	2.32	0.45
1:B:418:ALA:O	1:B:422:ARG:HD3	2.17	0.45
1:B:503:PRO:HB2	1:B:504:GLU:H	1.46	0.45
1:C:430:GLN:NE2	2:C:601:AGS:S1G	2.86	0.45
1:D:450:ASP:HB3	1:D:453:LYS:HB3	1.99	0.45
1:A:197:ILE:HD11	1:A:255:VAL:HG11	1.99	0.45
1:B:352:CYS:HA	1:B:369:ASN:OD1	2.16	0.45
1:B:197:ILE:HD11	1:B:255:VAL:CG1	2.45	0.45
1:B:381:ILE:O	1:B:554:ARG:HA	2.17	0.45
1:C:24:SER:OG	1:C:155:SER:HB2	2.17	0.45
1:D:152:LEU:HD11	1:D:309:ARG:HB3	1.98	0.45
1:A:111:LYS:HB2	1:A:111:LYS:HE3	1.64	0.44
1:D:197:ILE:HD11	1:D:255:VAL:HG11	1.99	0.44
1:A:143:LEU:O	1:A:147:ILE:HG12	2.17	0.44
1:A:208:MET:HA	1:A:211:PHE:CE2	2.52	0.44
1:A:66:ILE:HB	1:A:70:GLU:HB2	1.99	0.44
1:C:470:LEU:HD12	4:D:707:HOH:O	2.16	0.44
1:D:230:LYS:HB3	1:D:230:LYS:HE2	1.81	0.44
1:D:317:LEU:O	1:D:321:HIS:CB	2.65	0.44
1:A:478:VAL:HG22	1:A:485:LEU:HD11	1.99	0.44
1:B:285:ASP:O	1:B:287:SER:N	2.43	0.44
1:C:470:LEU:HB3	1:C:473:GLY:HA2	2.00	0.44
1:C:533:ASP:OD2	1:C:533:ASP:N	2.50	0.44
1:A:327:ILE:O	1:A:331:LEU:HG	2.17	0.44
1:A:418:ALA:O	1:A:422:ARG:HD3	2.17	0.44
1:A:508:LEU:HB2	1:A:538:ILE:HA	1.98	0.44
1:B:146:MET:HG3	1:B:320:TYR:HB2	2.00	0.44
1:D:501:LEU:HA	1:D:501:LEU:HD12	1.80	0.44
1:A:289:ILE:HG13	1:A:290:LEU:N	2.33	0.44
1:C:300:LEU:HD22	1:C:304:MET:HG3	1.99	0.44
1:D:100:PHE:O	1:D:104:ARG:HG2	2.17	0.44
1:B:467:ILE:HG12	1:B:467:ILE:H	1.54	0.44
1:C:37:LEU:HD13	1:C:37:LEU:C	2.38	0.44
1:D:20:LEU:HA	1:D:20:LEU:HD23	1.86	0.44
1:D:503:PRO:HB3	1:D:534:LYS:HD2	1.98	0.44
1:A:389:SER:OG	1:A:509:ASP:OD2	2.36	0.44
1:C:223:LYS:HD3	1:D:121:TYR:CE2	2.53	0.44
1:A:204:ARG:HG3	1:A:205:GLU:N	2.32	0.44
1:B:365:PHE:HE1	1:B:394:LEU:HD12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:LEU:HD12	1:C:490:LYS:HG3	1.99	0.44
1:B:436:ASN:HB2	1:B:480:ASP:HA	2.00	0.44
1:A:228:LYS:HD2	1:B:501:LEU:HD11	2.00	0.44
1:C:306:SER:O	1:C:310:ILE:HG13	2.18	0.44
1:C:54:ASN:HB3	1:C:57:LEU:HD23	2.00	0.44
1:A:20:LEU:HD21	1:A:96:LEU:HB3	1.99	0.43
1:B:140:VAL:N	1:B:328:TYR:OH	2.50	0.43
1:B:555:LEU:HA	1:B:555:LEU:HD23	1.73	0.43
1:A:553:TYR:HE1	1:A:562:GLU:HG3	1.83	0.43
1:C:167:MET:O	1:C:175:THR:OG1	2.32	0.43
1:C:228:LYS:O	1:C:229:THR:HG22	2.19	0.43
1:B:510:GLN:N	1:B:539:ILE:O	2.50	0.43
1:C:191:LYS:HD3	1:C:191:LYS:HA	1.60	0.43
1:C:375:GLY:H	1:C:535:THR:HB	1.84	0.43
1:D:441:LYS:O	1:D:443:ILE:N	2.51	0.43
1:D:489:GLN:O	1:D:493:ILE:HG13	2.18	0.43
1:B:470:LEU:HB3	1:B:473:GLY:HA2	1.99	0.43
1:A:136:ILE:H	1:A:136:ILE:HD12	1.83	0.43
1:A:211:PHE:HB3	1:A:241:GLN:HB2	2.01	0.43
1:A:377:LYS:HA	1:A:536:MET:O	2.18	0.43
1:A:384:SER:OG	1:B:488:GLY:HA3	2.18	0.43
1:B:531:SER:HA	1:B:534:LYS:HE3	2.00	0.43
1:C:452:GLU:O	1:C:456:LYS:HG2	2.18	0.43
1:D:340:GLU:O	1:D:340:GLU:HG3	2.19	0.43
1:D:457:VAL:HG13	1:D:499:LEU:HB2	2.01	0.43
1:A:156:GLU:HB3	1:A:310:ILE:HD13	1.99	0.43
1:A:199:LYS:HB2	1:A:199:LYS:HE3	1.87	0.43
1:A:235:LEU:HD22	1:B:114:SER:HB2	2.00	0.43
1:B:97:LEU:HA	1:B:97:LEU:HD23	1.67	0.43
1:C:527:ILE:O	1:C:530:ILE:HG22	2.18	0.43
1:D:345:PHE:HE2	4:D:702:HOH:O	2.02	0.43
1:D:503:PRO:HB2	1:D:504:GLU:H	1.38	0.43
1:A:20:LEU:O	1:A:24:SER:OG	2.26	0.43
1:A:503:PRO:HB2	1:A:534:LYS:HG3	2.00	0.43
1:C:151:LEU:HA	1:C:151:LEU:HD13	1.89	0.43
1:C:267:GLY:HA2	1:C:270:VAL:HG22	1.99	0.43
1:C:391:LEU:O	1:C:395:ILE:HG13	2.18	0.43
1:C:129:GLN:HE22	1:D:220:ASN:HA	1.84	0.43
1:D:379:ALA:HB2	1:D:549:CYS:SG	2.58	0.43
1:D:443:ILE:CD1	1:D:493:ILE:HG23	2.48	0.43
1:A:275:VAL:O	1:A:279:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LYS:HE2	1:B:334:GLU:O	2.19	0.43
1:B:120:ASN:OD1	1:B:121:TYR:N	2.52	0.43
1:B:66:ILE:HD12	1:B:70:GLU:O	2.19	0.43
1:C:432:ILE:CD1	1:C:491:GLN:HG2	2.48	0.43
1:D:28:SER:O	1:D:32:THR:HG22	2.18	0.43
1:D:397:GLY:HA3	1:D:422:ARG:CG	2.49	0.43
1:B:215:LEU:HD21	1:B:238:PHE:CD1	2.54	0.43
1:C:115:LYS:O	1:C:119:ILE:HG23	2.19	0.43
1:C:317:LEU:O	1:C:321:HIS:CB	2.66	0.43
1:C:437:ASP:O	1:C:477:LYS:HA	2.19	0.43
1:D:396:ILE:HG22	1:D:425:ILE:HG12	2.00	0.43
1:D:478:VAL:HG13	1:D:482:GLY:HA2	2.00	0.43
1:B:12:GLU:N	1:B:12:GLU:OE1	2.52	0.43
1:B:354:LEU:HA	1:B:404:GLY:HA3	2.01	0.43
1:B:391:LEU:O	1:B:395:ILE:HG13	2.19	0.43
1:B:462:ASN:HB3	1:B:522:LYS:HD2	2.01	0.43
1:C:143:LEU:HD12	1:C:328:TYR:HD1	1.84	0.43
1:C:181:PHE:HZ	1:C:266:ILE:HG13	1.83	0.43
1:C:297:VAL:HG13	4:C:722:HOH:O	2.19	0.43
1:A:122:GLU:HA	1:A:125:THR:HB	2.00	0.42
1:A:157:ILE:O	1:A:161:LEU:HG	2.19	0.42
1:B:267:GLY:O	1:B:270:VAL:HG12	2.18	0.42
1:C:396:ILE:HB	1:C:425:ILE:HG13	2.01	0.42
1:D:302:ARG:HE	1:D:302:ARG:HA	1.84	0.42
1:D:36:SER:O	1:D:40:PRO:HD3	2.19	0.42
1:B:271:LEU:O	1:B:274:ILE:HG22	2.19	0.42
1:B:441:LYS:O	1:B:442:ASN:HB2	2.19	0.42
1:B:504:GLU:O	1:B:505:ILE:HB	2.19	0.42
1:D:154:MET:O	1:D:157:ILE:HG13	2.19	0.42
1:A:10:SER:N	1:A:13:ASP:OD1	2.45	0.42
1:A:188:ILE:O	1:A:192:ILE:HB	2.20	0.42
1:B:28:SER:HB2	1:B:159:VAL:HB	2.01	0.42
1:C:352:CYS:HA	1:C:369:ASN:ND2	2.35	0.42
1:B:207:ALA:O	1:B:211:PHE:CB	2.62	0.42
1:C:164:TYR:CE2	1:C:168:LEU:HD11	2.55	0.42
1:D:116:PHE:CE2	1:D:331:LEU:HD13	2.52	0.42
1:A:339:ALA:HB3	1:A:415:ALA:O	2.20	0.42
1:B:447:ASP:N	1:B:447:ASP:OD1	2.52	0.42
1:A:483:SER:O	2:B:601:AGS:N6	2.52	0.42
1:C:176:LEU:O	1:C:180:ILE:HG12	2.19	0.42
1:C:211:PHE:HD1	1:C:238:PHE:CE1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:PHE:CG	1:C:394:LEU:HD11	2.54	0.42
1:C:441:LYS:HA	4:C:711:HOH:O	2.18	0.42
1:A:259:PRO:O	1:A:263:LEU:HG	2.20	0.42
1:C:457:VAL:HG13	1:C:499:LEU:HB2	2.01	0.42
1:C:503:PRO:HB2	1:C:504:GLU:H	1.52	0.42
1:A:158:PHE:CB	4:A:721:HOH:O	2.63	0.42
1:B:51:PHE:HD1	1:B:61:LYS:HB2	1.84	0.42
1:B:530:ILE:HA	1:B:530:ILE:HD12	1.75	0.42
1:B:534:LYS:HG3	1:B:534:LYS:HZ3	1.70	0.42
1:C:467:ILE:H	1:C:467:ILE:HG12	1.52	0.42
2:A:601:AGS:O3B	1:B:486:SER:HB2	2.20	0.42
1:C:423:GLN:HG2	1:D:229:THR:OG1	2.20	0.42
1:D:317:LEU:O	1:D:321:HIS:HB3	2.19	0.42
1:A:321:HIS:O	1:A:325:ASN:N	2.48	0.42
1:B:172:TYR:O	1:B:175:THR:HB	2.20	0.42
1:B:461:ALA:C	1:B:463:LEU:H	2.23	0.42
1:A:157:ILE:HG22	1:A:310:ILE:HD12	2.01	0.42
1:B:171:ASN:O	1:B:175:THR:OG1	2.35	0.42
1:B:227:LEU:HA	1:B:227:LEU:HD12	1.85	0.42
1:A:272:VAL:CG2	1:B:80:ILE:HG22	2.50	0.42
1:C:104:ARG:HA	1:C:104:ARG:HD3	1.78	0.42
1:C:188:ILE:HG13	1:C:189:LEU:N	2.35	0.42
1:C:358:TYR:O	1:C:361:LYS:N	2.37	0.42
1:C:94:PHE:HA	1:C:94:PHE:HD1	1.78	0.42
1:D:115:LYS:O	1:D:119:ILE:HG23	2.20	0.42
1:B:399:LEU:HD23	1:B:399:LEU:HA	1.86	0.41
1:C:238:PHE:O	1:C:242:SER:HB3	2.19	0.41
1:A:146:MET:SD	1:A:321:HIS:HB2	2.60	0.41
1:A:534:LYS:H	1:A:534:LYS:HD3	1.84	0.41
1:A:528:TYR:CE2	1:A:548:GLN:HB2	2.55	0.41
1:A:222:PHE:HE1	1:B:117:LEU:HA	1.85	0.41
1:B:77:VAL:HA	1:B:80:ILE:HG12	2.02	0.41
1:C:322:SER:O	1:C:323:SER:C	2.58	0.41
1:D:350:LYS:HG3	1:D:371:ASN:CB	2.49	0.41
1:D:452:GLU:O	1:D:456:LYS:HG2	2.20	0.41
1:A:289:ILE:HA	1:A:292:THR:HG22	2.01	0.41
1:C:437:ASP:HA	1:C:477:LYS:HD3	2.02	0.41
1:D:116:PHE:CE1	1:D:132:ILE:HG12	2.56	0.41
1:A:1:MET:HE3	1:A:2:VAL:HG13	2.02	0.41
1:A:396:ILE:HG13	1:A:398:LEU:HD22	2.03	0.41
1:A:339:ALA:CB	1:A:416:SER:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:SER:HA	1:A:534:LYS:CE	2.50	0.41
1:B:358:TYR:CE2	2:B:601:AGS:C4	3.03	0.41
1:B:364:LEU:HD21	2:B:601:AGS:O4'	2.21	0.41
1:B:72:ILE:H	1:B:72:ILE:HG13	1.72	0.41
1:C:205:GLU:HG3	1:C:323:SER:HB3	2.02	0.41
1:C:444:THR:HG21	1:C:449:VAL:HG22	2.02	0.41
1:C:505:ILE:HG12	1:C:535:THR:CG2	2.51	0.41
1:D:528:TYR:CE2	1:D:548:GLN:HB2	2.55	0.41
1:D:530:ILE:HA	1:D:530:ILE:HD12	1.80	0.41
1:A:278:LEU:HA	1:A:281:LYS:O	2.21	0.41
1:B:204:ARG:HH21	1:B:204:ARG:HB3	1.85	0.41
1:B:354:LEU:HD12	1:B:404:GLY:HA3	2.02	0.41
1:C:108:ILE:HB	1:C:140:VAL:HG23	2.01	0.41
1:D:391:LEU:O	1:D:395:ILE:HG13	2.20	0.41
1:A:504:GLU:O	1:A:505:ILE:HB	2.21	0.41
1:B:214:ILE:H	1:B:214:ILE:HG12	1.42	0.41
1:A:113:PHE:CE1	1:B:215:LEU:HD22	2.56	0.41
1:B:61:LYS:HG3	4:B:706:HOH:O	2.19	0.41
1:D:343:LEU:HA	1:D:343:LEU:HD12	1.98	0.41
1:B:303:LEU:HD23	1:B:303:LEU:HA	1.89	0.41
1:B:318:LEU:HA	1:B:318:LEU:HD23	1.89	0.41
1:B:343:LEU:HA	1:B:343:LEU:HD12	1.73	0.41
1:C:453:LYS:O	1:C:457:VAL:HG23	2.20	0.41
1:C:494:ALA:O	1:C:497:ARG:HB2	2.21	0.41
1:C:543:LEU:HB3	1:C:544:SER:H	1.73	0.41
1:D:197:ILE:CG1	1:D:255:VAL:HG11	2.51	0.41
1:C:105:LYS:HB3	1:D:246:SER:OG	2.20	0.41
1:D:437:ASP:O	1:D:477:LYS:HA	2.20	0.41
1:A:123:LYS:O	1:A:127:LYS:HG2	2.21	0.41
1:A:381:ILE:O	1:A:554:ARG:HA	2.20	0.41
1:B:285:ASP:O	1:B:286:ILE:HG12	2.21	0.41
1:D:503:PRO:HB3	1:D:534:LYS:CD	2.51	0.41
1:A:391:LEU:O	1:A:395:ILE:HG13	2.21	0.41
1:B:321:HIS:O	1:B:325:ASN:HB3	2.21	0.41
1:C:154:MET:O	1:C:157:ILE:HG13	2.21	0.41
1:C:293:ILE:O	1:C:297:VAL:HB	2.21	0.41
1:C:447:ASP:OD1	1:D:230:LYS:HE3	2.20	0.41
1:C:478:VAL:HG13	1:C:482:GLY:HA2	2.03	0.41
1:C:83:TYR:CD2	1:D:268:PHE:HB3	2.55	0.41
1:A:116:PHE:O	1:A:119:ILE:HG12	2.21	0.41
1:A:214:ILE:HG21	1:A:214:ILE:HD13	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:HD23	1:A:5:LEU:HA	1.87	0.41
1:B:15:ASN:OD1	1:B:16:PHE:N	2.54	0.41
1:C:123:LYS:O	1:C:127:LYS:HG2	2.21	0.41
1:C:221:ASN:O	1:C:225:ILE:HG13	2.21	0.41
1:D:276:VAL:HA	1:D:279:VAL:HG22	2.02	0.41
1:A:106:HIS:O	1:A:110:TYR:HD2	2.04	0.41
1:A:28:SER:HB2	1:A:162:LEU:HD12	2.02	0.41
1:A:463:LEU:HB3	1:A:467:ILE:HD11	2.03	0.41
1:C:174:ILE:H	1:C:174:ILE:HG13	1.52	0.41
1:C:198:LYS:HB2	1:C:318:LEU:HD23	2.03	0.41
1:D:108:ILE:HA	1:D:111:LYS:HE3	2.03	0.41
1:D:393:ASP:O	1:D:399:LEU:HB2	2.21	0.41
1:A:22:VAL:O	1:A:25:VAL:HG12	2.21	0.40
1:A:503:PRO:O	1:A:504:GLU:HB2	2.21	0.40
1:A:508:LEU:HG	1:A:511:ALA:HB3	2.01	0.40
1:B:194:SER:N	1:B:195:PRO:HD2	2.36	0.40
1:B:260:ARG:HB2	1:B:260:ARG:HE	1.74	0.40
1:B:396:ILE:HG22	1:B:425:ILE:HD12	2.03	0.40
1:B:444:THR:HG21	1:B:449:VAL:HG22	2.03	0.40
1:B:424:LYS:HE3	1:B:504:GLU:OE1	2.20	0.40
1:C:112:VAL:HB	1:C:136:ILE:HD13	2.03	0.40
1:C:143:LEU:HD23	1:C:143:LEU:HA	1.75	0.40
1:D:555:LEU:HD23	1:D:555:LEU:HA	1.87	0.40
1:C:114:SER:O	1:C:118:ASN:ND2	2.52	0.40
1:C:23:PHE:CE2	1:C:93:TYR:HB2	2.56	0.40
1:D:228:LYS:HE2	1:D:228:LYS:HB3	1.91	0.40
1:D:271:LEU:O	1:D:275:VAL:HG13	2.21	0.40
1:B:519:SER:O	1:B:523:ILE:HG12	2.21	0.40
1:C:208:MET:HA	1:C:211:PHE:HE2	1.85	0.40
1:C:510:GLN:OE1	1:C:541:HIS:ND1	2.54	0.40
1:D:381:ILE:HD12	1:D:382:GLY:H	1.86	0.40
1:D:531:SER:HA	1:D:534:LYS:HD3	2.03	0.40
1:B:272:VAL:HA	1:B:275:VAL:HG22	2.03	0.40
1:B:362:LYS:HE3	4:B:733:HOH:O	2.22	0.40
1:C:35:ILE:HD12	1:C:35:ILE:HA	1.92	0.40
1:A:33:PHE:O	1:A:37:LEU:HG	2.21	0.40
1:D:332:ARG:HA	1:D:332:ARG:HD3	1.95	0.40
1:D:72:ILE:HG13	1:D:73:VAL:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	562/564 (100%)	499 (89%)	47 (8%)	16 (3%)	5	25
1	B	562/564 (100%)	484 (86%)	57 (10%)	21 (4%)	3	20
1	C	562/564 (100%)	490 (87%)	50 (9%)	22 (4%)	3	18
1	D	562/564 (100%)	486 (86%)	55 (10%)	21 (4%)	3	20
All	All	2248/2256 (100%)	1959 (87%)	209 (9%)	80 (4%)	3	20

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	503	PRO
1	B	68	VAL
1	B	338	ALA
1	B	462	ASN
1	B	503	PRO
1	B	505	ILE
1	C	321	HIS
1	C	322	SER
1	C	359	GLU
1	D	462	ASN
1	D	503	PRO
1	A	67	PRO
1	A	359	GLU
1	A	543	LEU
1	B	359	GLU
1	B	447	ASP
1	C	67	PRO
1	C	230	LYS
1	C	286	ILE
1	C	503	PRO
1	D	135	SER
1	D	286	ILE

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Mol	Chain	Res	Type
1	D	355	SER
1	D	505	ILE
1	A	54	ASN
1	A	286	ILE
1	A	354	LEU
1	A	355	SER
1	A	505	ILE
1	B	54	ASN
1	B	286	ILE
1	B	340	GLU
1	B	399	LEU
1	C	54	ASN
1	C	135	SER
1	C	355	SER
1	C	399	LEU
1	C	543	LEU
1	D	54	ASN
1	D	352	CYS
1	D	406	ILE
1	A	399	LEU
1	A	406	ILE
1	B	171	ASN
1	B	339	ALA
1	B	352	CYS
1	B	428	ILE
1	C	229	THR
1	C	366	LYS
1	C	406	ILE
1	C	428	ILE
1	C	441	LYS
1	C	442	ASN
1	D	171	ASN
1	D	366	LYS
1	D	396	ILE
1	D	399	LEU
1	A	222	PHE
1	A	321	HIS
1	A	366	LYS
1	A	436	ASN
1	B	67	PRO
1	B	136	ILE
1	B	137	THR

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Mol	Chain	Res	Type
1	B	406	ILE
1	C	171	ASN
1	C	352	CYS
1	D	45	ALA
1	D	333	GLN
1	D	423	GLN
1	D	442	ASN
1	D	502	GLU
1	A	352	CYS
1	B	543	LEU
1	C	505	ILE
1	D	441	LYS
1	B	471	PRO
1	C	68	VAL
1	D	387	GLY
1	D	471	PRO

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	504/504 (100%)	462 (92%)	42 (8%)	11	36
1	B	504/504 (100%)	446 (88%)	58 (12%)	5	22
1	C	504/504 (100%)	446 (88%)	58 (12%)	5	22
1	D	504/504 (100%)	457 (91%)	47 (9%)	9	30
All	All	2016/2016 (100%)	1811 (90%)	205 (10%)	7	27

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	12	GLU
1	A	16	PHE
1	A	23	PHE
1	A	29	PHE

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Mol	Chain	Res	Type
1	A	33	PHE
1	A	51	PHE
1	A	54	ASN
1	A	75	PHE
1	A	88	LEU
1	A	125	THR
1	A	154	MET
1	A	166	LEU
1	A	168	LEU
1	A	176	LEU
1	A	229	THR
1	A	230	LYS
1	A	258	VAL
1	A	268	PHE
1	A	269	CYS
1	A	276	VAL
1	A	282	ASN
1	A	286	ILE
1	A	308	ASN
1	A	312	THR
1	A	352	CYS
1	A	367	ASN
1	A	394	LEU
1	A	398	LEU
1	A	430	GLN
1	A	445	PHE
1	A	452	GLU
1	A	462	ASN
1	A	467	ILE
1	A	478	VAL
1	A	497	ARG
1	A	501	LEU
1	A	508	LEU
1	A	516	ASP
1	A	534	LYS
1	A	542	ARG
1	A	555	LEU
1	B	15	ASN
1	B	17	LEU
1	B	20	LEU
1	B	28	SER
1	B	29	PHE

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Mol	Chain	Res	Type
1	B	33	PHE
1	B	51	PHE
1	B	66	ILE
1	B	75	PHE
1	B	83	TYR
1	B	99	ARG
1	B	101	SER
1	B	110	TYR
1	B	114	SER
1	B	123	LYS
1	B	134	LYS
1	B	135	SER
1	B	144	SER
1	B	148	SER
1	B	151	LEU
1	B	172	TYR
1	B	182	MET
1	B	184	LEU
1	B	205	GLU
1	B	211	PHE
1	B	214	ILE
1	B	215	LEU
1	B	229	THR
1	B	232	ASP
1	B	260	ARG
1	B	286	ILE
1	B	296	PHE
1	B	301	TYR
1	B	309	ARG
1	B	321	HIS
1	B	322	SER
1	B	324	LEU
1	B	332	ARG
1	B	350	LYS
1	B	362	LYS
1	B	369	ASN
1	B	383	GLU
1	B	398	LEU
1	B	447	ASP
1	B	462	ASN
1	B	467	ILE
1	B	478	VAL

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Mol	Chain	Res	Type
1	B	497	ARG
1	B	501	LEU
1	B	506	LEU
1	B	518	GLN
1	B	533	ASP
1	B	534	LYS
1	B	542	ARG
1	B	547	THR
1	B	555	LEU
1	B	559	LYS
1	B	562	GLU
1	C	5	LEU
1	C	13	ASP
1	C	29	PHE
1	C	33	PHE
1	C	47	ASP
1	C	51	PHE
1	C	66	ILE
1	C	74	TYR
1	C	94	PHE
1	C	104	ARG
1	C	110	TYR
1	C	115	LYS
1	C	123	LYS
1	C	125	THR
1	C	130	SER
1	C	143	LEU
1	C	144	SER
1	C	184	LEU
1	C	189	LEU
1	C	205	GLU
1	C	211	PHE
1	C	212	PHE
1	C	226	LYS
1	C	229	THR
1	C	242	SER
1	C	286	ILE
1	C	297	VAL
1	C	301	TYR
1	C	318	LEU
1	C	323	SER
1	C	325	ASN

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Mol	Chain	Res	Type
1	C	328	TYR
1	C	332	ARG
1	C	350	LYS
1	C	352	CYS
1	C	362	LYS
1	C	367	ASN
1	C	384	SER
1	C	398	LEU
1	C	445	PHE
1	C	452	GLU
1	C	462	ASN
1	C	467	ILE
1	C	478	VAL
1	C	497	ARG
1	C	501	LEU
1	C	506	LEU
1	C	518	GLN
1	C	525	ASP
1	C	527	ILE
1	C	533	ASP
1	C	534	LYS
1	C	536	MET
1	C	542	ARG
1	C	555	LEU
1	C	556	GLU
1	C	559	LYS
1	C	562	GLU
1	D	10	SER
1	D	23	PHE
1	D	47	ASP
1	D	54	ASN
1	D	72	ILE
1	D	83	TYR
1	D	86	ARG
1	D	99	ARG
1	D	101	SER
1	D	110	TYR
1	D	153	LEU
1	D	156	GLU
1	D	164	TYR
1	D	168	LEU
1	D	181	PHE

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Mol	Chain	Res	Type
1	D	204	ARG
1	D	210	ASN
1	D	226	LYS
1	D	230	LYS
1	D	246	SER
1	D	260	ARG
1	D	296	PHE
1	D	301	TYR
1	D	302	ARG
1	D	310	ILE
1	D	318	LEU
1	D	332	ARG
1	D	355	SER
1	D	362	LYS
1	D	367	ASN
1	D	369	ASN
1	D	372	ILE
1	D	392	VAL
1	D	398	LEU
1	D	431	ASN
1	D	447	ASP
1	D	452	GLU
1	D	467	ILE
1	D	472	GLN
1	D	478	VAL
1	D	497	ARG
1	D	506	LEU
1	D	533	ASP
1	D	534	LYS
1	D	542	ARG
1	D	555	LEU
1	D	559	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	129	GLN
1	B	321	HIS
1	C	337	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	AGS	D	601	-	26,33,33	1.89	3 (11%)	26,52,52	1.59	4 (15%)
2	AGS	C	601	3	26,33,33	1.88	4 (15%)	26,52,52	1.59	4 (15%)
2	AGS	B	601	3	26,33,33	1.89	3 (11%)	26,52,52	1.59	4 (15%)
2	AGS	A	601	-	26,33,33	1.89	3 (11%)	26,52,52	1.59	4 (15%)

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
2	AGS	D	601	-	-	1/17/38/38	0/3/3/3
2	AGS	C	601	3	-	5/17/38/38	0/3/3/3
2	AGS	B	601	3	-	6/17/38/38	0/3/3/3
2	AGS	A	601	-	-	2/17/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	AGS	PG-S1G	7.97	2.08	1.90
2	A	601	AGS	PG-S1G	7.95	2.07	1.90
2	B	601	AGS	PG-S1G	7.94	2.07	1.90
2	C	601	AGS	PG-S1G	7.92	2.07	1.90
2	A	601	AGS	C5-C4	2.50	1.47	1.40
2	B	601	AGS	C5-C4	2.50	1.47	1.40
2	D	601	AGS	C5-C4	2.50	1.47	1.40
2	C	601	AGS	C5-C4	2.49	1.47	1.40
2	A	601	AGS	PG-O2G	2.03	1.61	1.54
2	C	601	AGS	PG-O2G	2.02	1.61	1.54
2	C	601	AGS	PG-O3G	-2.01	1.48	1.54
2	B	601	AGS	PG-O2G	2.01	1.61	1.54
2	D	601	AGS	PG-O2G	2.01	1.61	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	AGS	PA-O3A-PB	-3.60	120.47	132.83
2	C	601	AGS	PA-O3A-PB	-3.60	120.48	132.83
2	B	601	AGS	PA-O3A-PB	-3.59	120.51	132.83
2	D	601	AGS	PA-O3A-PB	-3.59	120.51	132.83
2	A	601	AGS	C3'-C2'-C1'	3.55	106.33	100.98
2	B	601	AGS	C3'-C2'-C1'	3.54	106.31	100.98
2	D	601	AGS	C3'-C2'-C1'	3.53	106.29	100.98
2	C	601	AGS	C3'-C2'-C1'	3.52	106.28	100.98
2	B	601	AGS	N3-C2-N1	-3.19	123.69	128.68
2	D	601	AGS	N3-C2-N1	-3.17	123.73	128.68
2	C	601	AGS	N3-C2-N1	-3.16	123.74	128.68
2	A	601	AGS	N3-C2-N1	-3.15	123.75	128.68
2	D	601	AGS	C4-C5-N7	-2.75	106.53	109.40
2	C	601	AGS	C4-C5-N7	-2.72	106.56	109.40
2	A	601	AGS	C4-C5-N7	-2.71	106.58	109.40
2	B	601	AGS	C4-C5-N7	-2.69	106.60	109.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	AGS	PB-O3B-PG-O2G
2	C	601	AGS	PB-O3B-PG-O3G
2	B	601	AGS	C5'-O5'-PA-O3A

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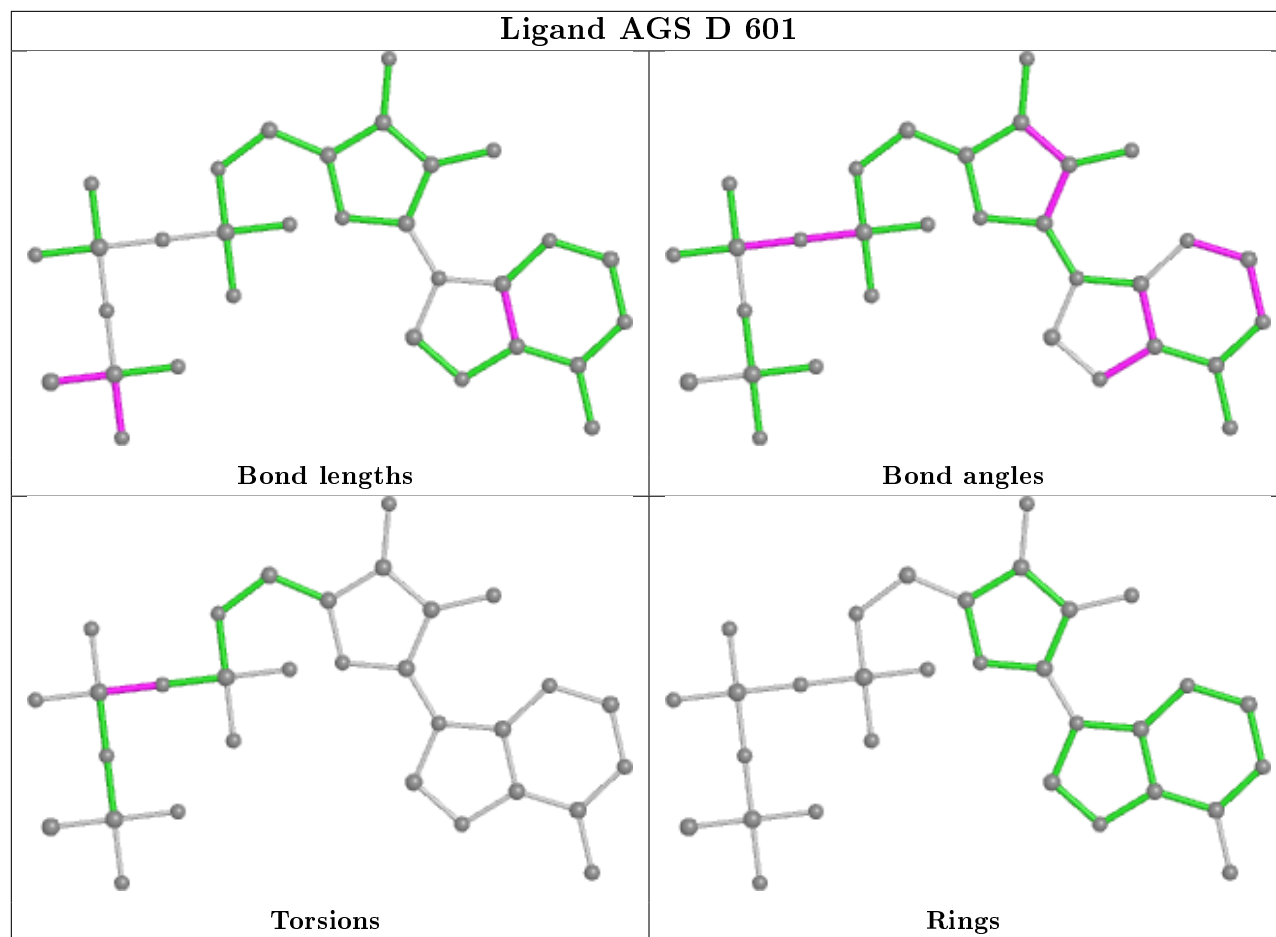
Mol	Chain	Res	Type	Atoms
2	B	601	AGS	O4'-C4'-C5'-O5'
2	B	601	AGS	C3'-C4'-C5'-O5'
2	B	601	AGS	C5'-O5'-PA-O1A
2	B	601	AGS	C5'-O5'-PA-O2A
2	B	601	AGS	PG-O3B-PB-O2B
2	C	601	AGS	PA-O3A-PB-O1B
2	A	601	AGS	PA-O3A-PB-O1B
2	D	601	AGS	PA-O3A-PB-O1B
2	C	601	AGS	PA-O3A-PB-O2B
2	A	601	AGS	PA-O3A-PB-O2B
2	C	601	AGS	C5'-O5'-PA-O1A

There are no ring outliers.

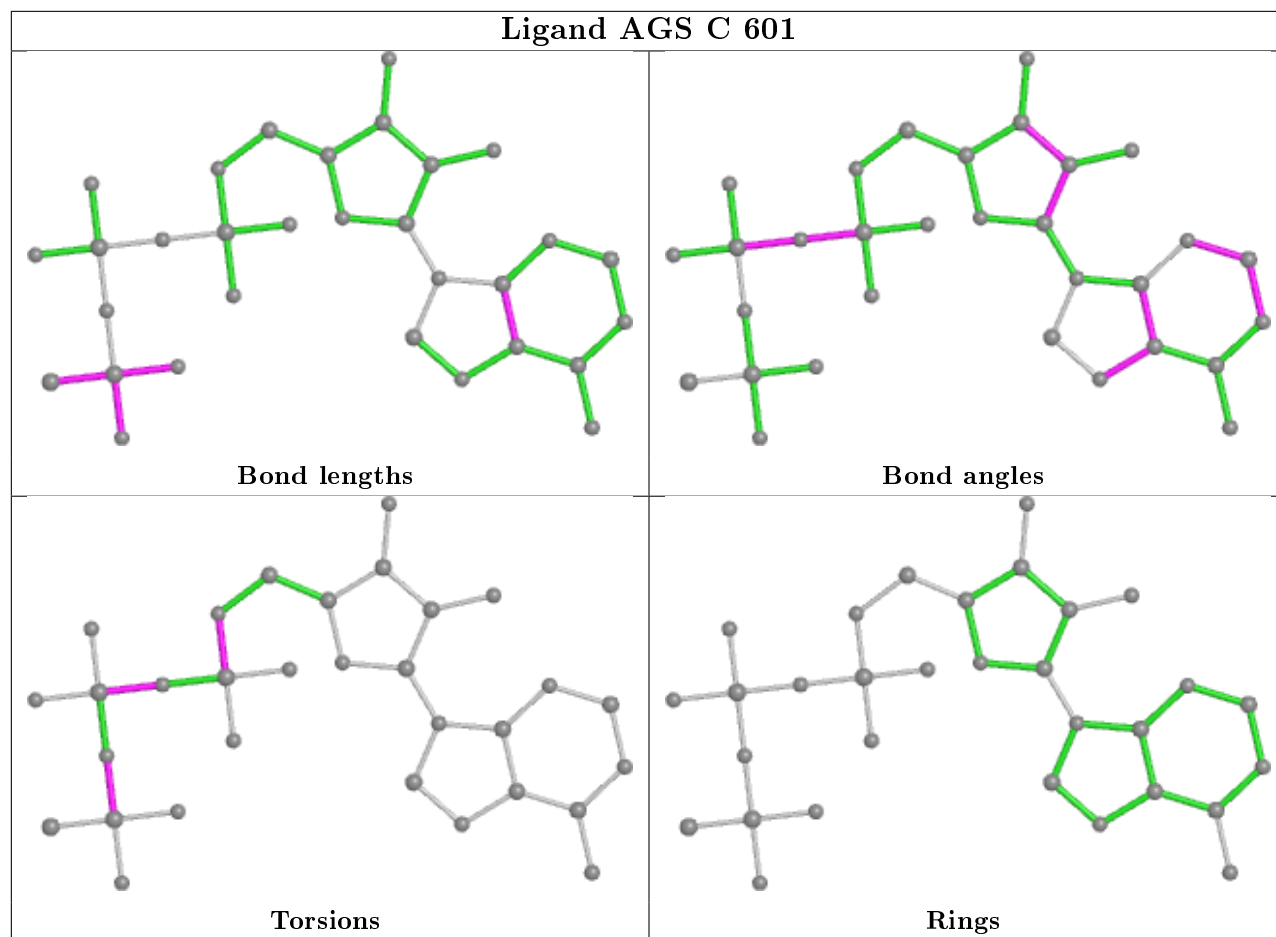
4 monomers are involved in 21 short contacts:

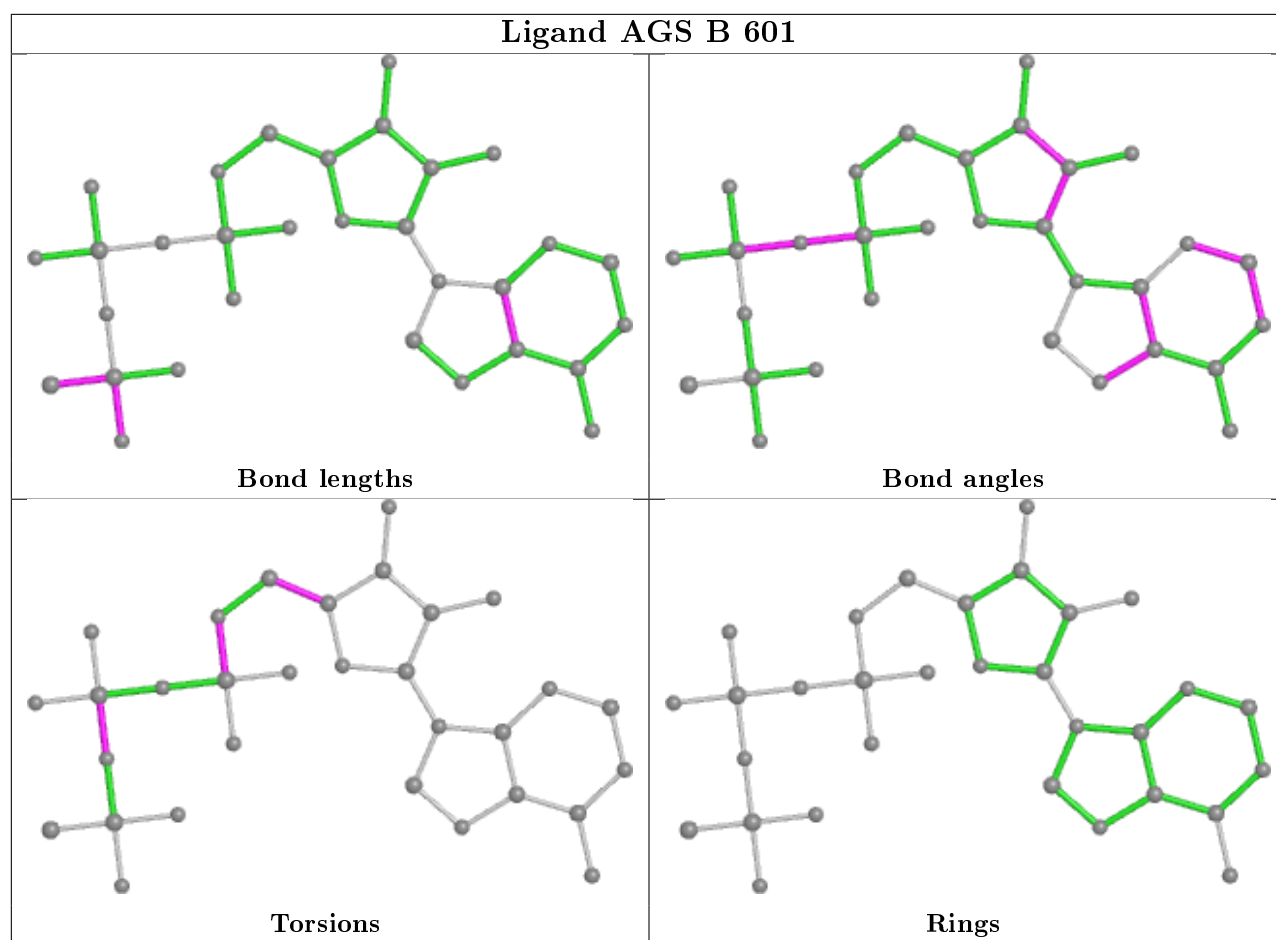
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	AGS	5	0
2	C	601	AGS	3	0
2	B	601	AGS	10	0
2	A	601	AGS	3	0

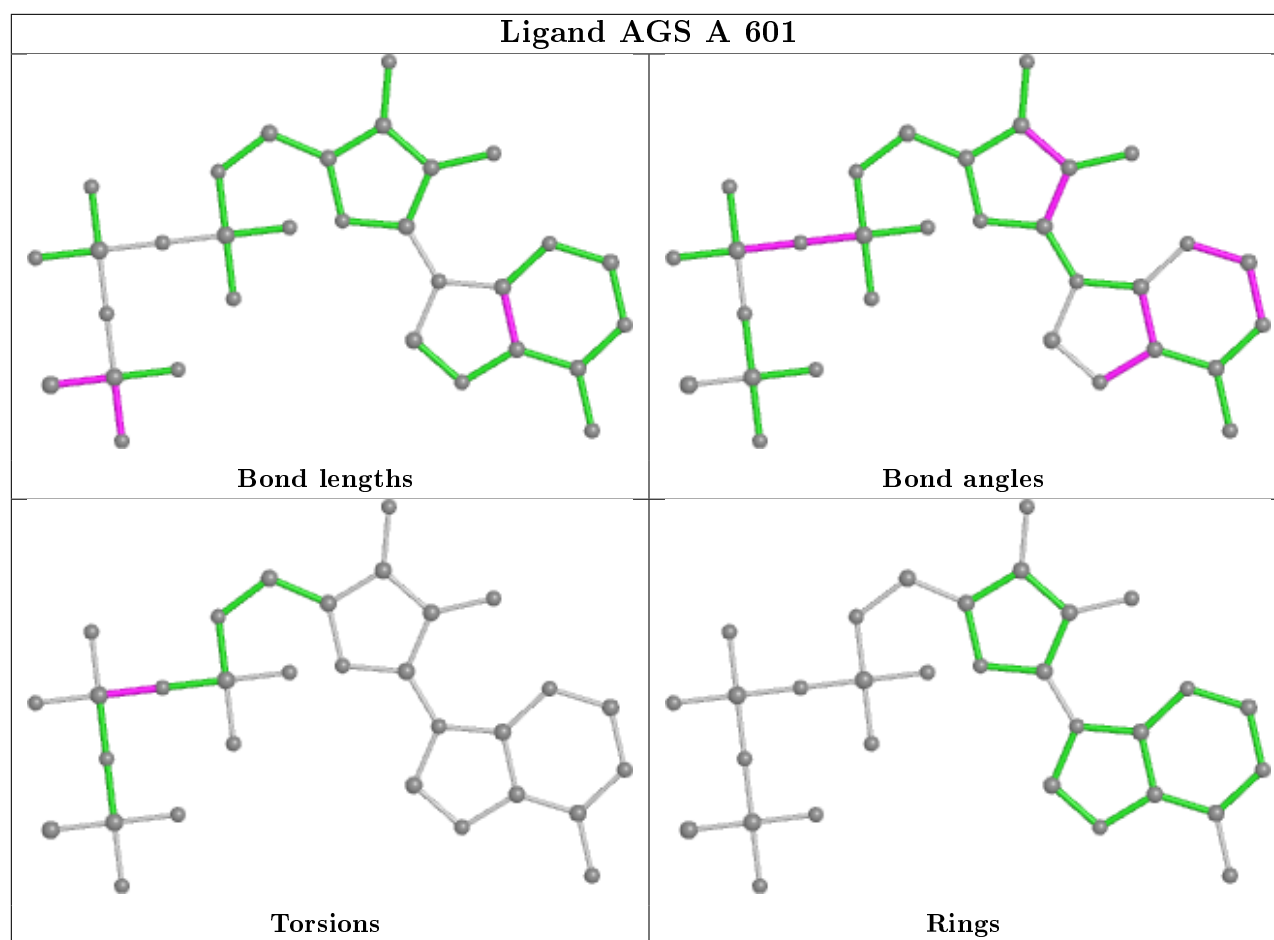
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 C 601







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	564/564 (100%)	0.07	42 (7%)	14 14	64, 143, 291, 584	0
1	B	564/564 (100%)	0.14	43 (7%)	13 13	44, 115, 261, 366	0
1	C	564/564 (100%)	0.06	29 (5%)	28 26	58, 119, 275, 346	0
1	D	564/564 (100%)	0.01	34 (6%)	21 21	60, 131, 288, 450	0
All	All	2256/2256 (100%)	0.07	148 (6%)	18 18	44, 127, 280, 584	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	SER	13.0
1	C	69	PHE	11.4
1	C	287	SER	11.3
1	C	286	ILE	9.5
1	C	285	ASP	9.2
1	D	65	ASN	8.7
1	A	62	GLU	8.1
1	C	62	GLU	8.0
1	A	53	ARG	7.7
1	A	282	ASN	7.3
1	B	564	LYS	7.2
1	B	280	LEU	7.1
1	D	277	PHE	6.9
1	D	63	TYR	6.8
1	A	285	ASP	6.8
1	B	283	GLU	6.8
1	D	64	LEU	6.7
1	A	557	HIS	6.6
1	C	70	GLU	6.5
1	A	46	SER	6.4
1	D	62	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	285	ASP	6.1
1	B	288	GLY	5.9
1	A	69	PHE	5.7
1	B	71	ILE	5.6
1	B	63	TYR	5.5
1	B	281	LYS	5.5
1	B	65	ASN	5.4
1	A	52	ASP	5.1
1	C	53	ARG	5.0
1	C	36	SER	5.0
1	B	287	SER	4.9
1	A	54	ASN	4.8
1	D	66	ILE	4.8
1	C	49	SER	4.6
1	C	64	LEU	4.6
1	D	74	TYR	4.6
1	C	50	TYR	4.6
1	D	280	LEU	4.5
1	B	282	ASN	4.4
1	C	67	PRO	4.4
1	A	383	GLU	4.3
1	A	57	LEU	4.2
1	D	410	LYS	4.2
1	A	64	LEU	4.1
1	C	532	LYS	4.1
1	B	292	THR	4.0
1	B	557	HIS	4.0
1	D	557	HIS	4.0
1	B	278	LEU	4.0
1	C	43	THR	3.9
1	C	284	SER	3.9
1	C	66	ILE	3.9
1	B	277	PHE	3.9
1	A	366	LYS	3.9
1	B	66	ILE	3.8
1	C	37	LEU	3.8
1	A	389	SER	3.8
1	C	39	MET	3.8
1	D	282	ASN	3.8
1	B	46	SER	3.7
1	B	286	ILE	3.7
1	D	56	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	169	LEU	3.6
1	B	72	ILE	3.6
1	D	11	LYS	3.5
1	B	73	VAL	3.5
1	A	168	LEU	3.5
1	D	55	LYS	3.5
1	C	42	ILE	3.4
1	C	282	ASN	3.4
1	C	288	GLY	3.4
1	B	62	GLU	3.4
1	A	284	SER	3.3
1	B	405	GLN	3.3
1	B	465	HIS	3.3
1	A	172	TYR	3.3
1	A	276	VAL	3.2
1	C	33	PHE	3.2
1	B	550	ASP	3.2
1	B	414	ASN	3.2
1	A	50	TYR	3.2
1	D	287	SER	3.2
1	D	71	ILE	3.1
1	D	281	LYS	3.1
1	D	286	ILE	3.0
1	D	194	SER	3.0
1	C	68	VAL	2.9
1	B	50	TYR	2.9
1	D	69	PHE	2.9
1	A	279	VAL	2.9
1	A	321	HIS	2.8
1	A	278	LEU	2.8
1	D	90	ASN	2.8
1	A	68	VAL	2.8
1	B	51	PHE	2.8
1	A	561	LYS	2.8
1	A	275	VAL	2.8
1	A	58	ILE	2.7
1	A	335	GLU	2.7
1	D	195	PRO	2.7
1	A	47	ASP	2.7
1	D	529	LYS	2.7
1	D	403	GLU	2.6
1	B	415	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	2.6
1	A	343	LEU	2.6
1	A	430	GLN	2.6
1	B	55	LYS	2.5
1	A	504	GLU	2.5
1	C	529	LYS	2.5
1	D	564	LYS	2.5
1	B	412	GLU	2.5
1	B	321	HIS	2.4
1	B	383	GLU	2.4
1	A	286	ILE	2.4
1	B	43	THR	2.4
1	C	276	VAL	2.4
1	A	166	LEU	2.4
1	D	67	PRO	2.4
1	A	56	TYR	2.4
1	A	55	LYS	2.3
1	C	54	ASN	2.3
1	D	47	ASP	2.3
1	D	94	PHE	2.3
1	D	70	GLU	2.3
1	B	541	HIS	2.3
1	B	548	GLN	2.3
1	B	49	SER	2.3
1	A	45	ALA	2.3
1	B	537	ILE	2.3
1	C	321	HIS	2.3
1	B	384	SER	2.3
1	A	170	ILE	2.2
1	A	384	SER	2.2
1	B	291	SER	2.2
1	A	67	PRO	2.2
1	B	64	LEU	2.2
1	C	414	ASN	2.2
1	A	344	SER	2.1
1	D	411	GLN	2.1
1	D	250	ILE	2.1
1	A	390	THR	2.1
1	D	525	ASP	2.1
1	C	40	PRO	2.0
1	D	68	VAL	2.0
1	B	171	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	389	SER	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 carbohydrates in this entry.

6.4 Ligands [i](#)

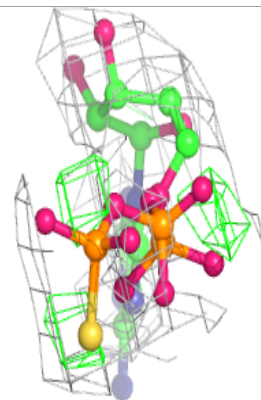
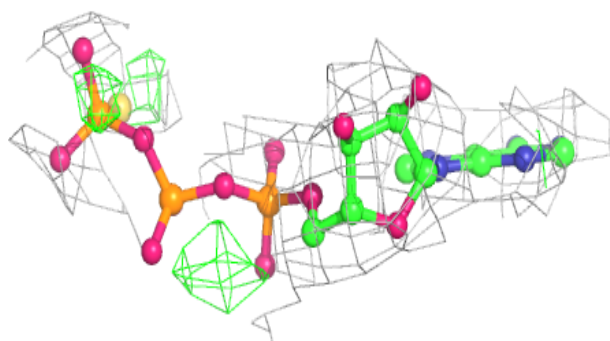
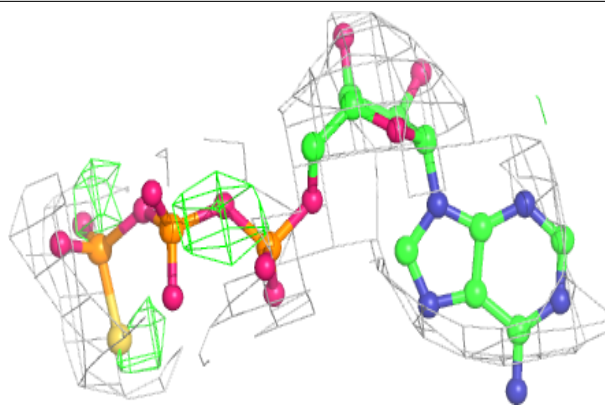
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AGS	D	601	31/31	0.91	0.24	43,121,168,276	0
2	AGS	A	601	31/31	0.95	0.27	59,118,158,208	0
2	AGS	B	601	31/31	0.96	0.20	71,92,130,225	0
2	AGS	C	601	31/31	0.96	0.16	45,81,139,289	0
3	MG	B	602	1/1	0.96	0.34	104,104,104,104	0
3	MG	C	602	1/1	0.98	0.10	112,112,112,112	0

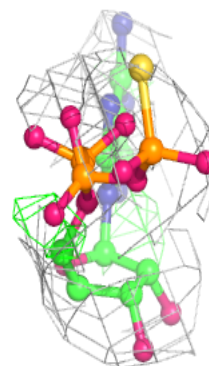
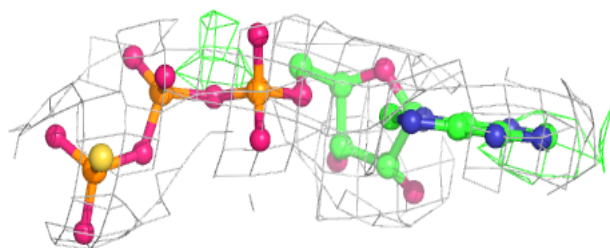
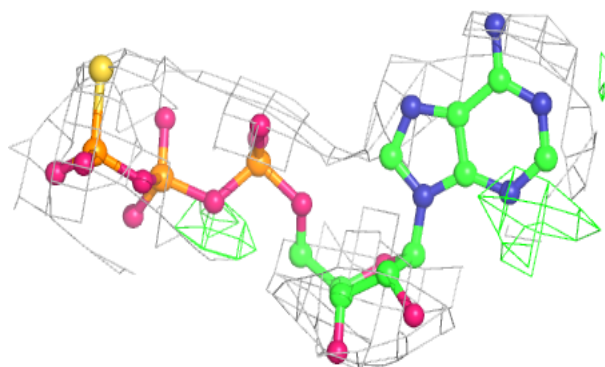
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS D 601:

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

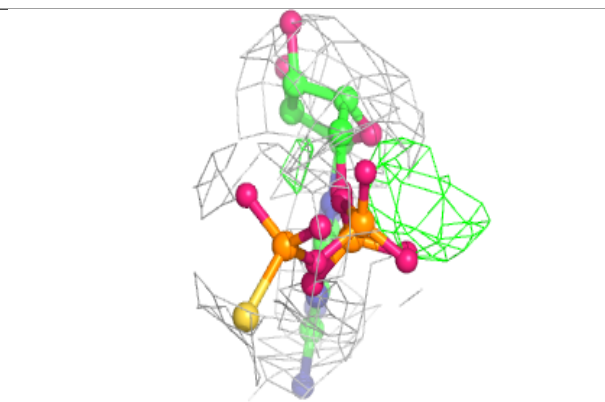
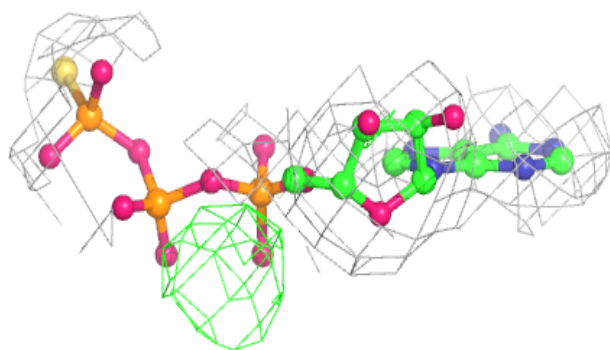
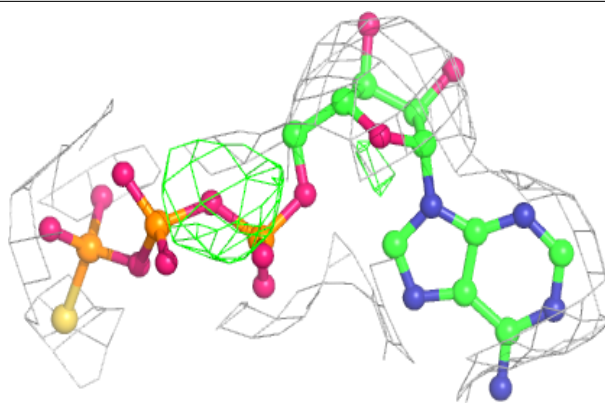
**Electron density around AGS A 601:**

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

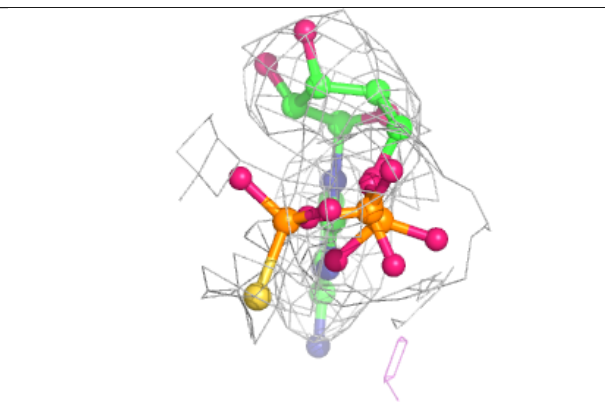
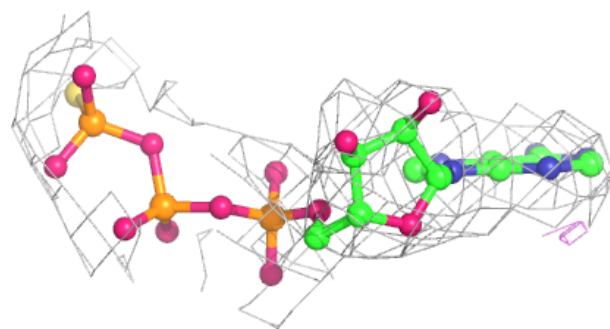
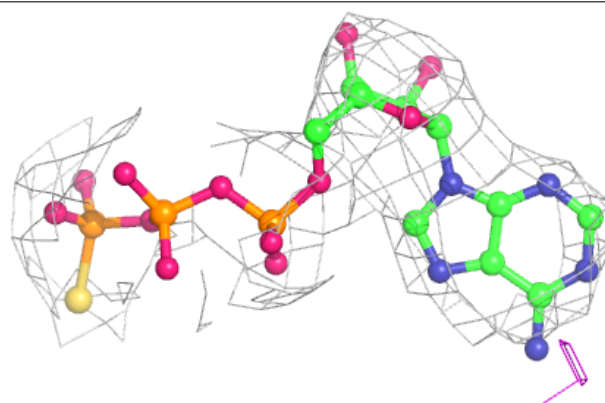


Electron density around AGS B 601:

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

**Electron density around AGS C 601:**

$2mF_o-DF_c$ (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.