



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:22 PM EDT

PDB ID : 6HRC / pdb_00006hrc
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 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

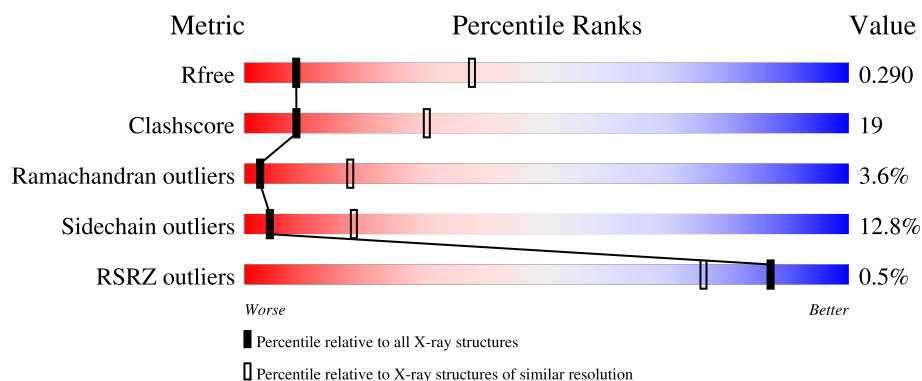
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	564	57% 37% 6%
1	B	564	55% 36% 9%
1	C	564	53% 37% 9%
1	D	564	55% 37% 7%

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 criteria:

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.

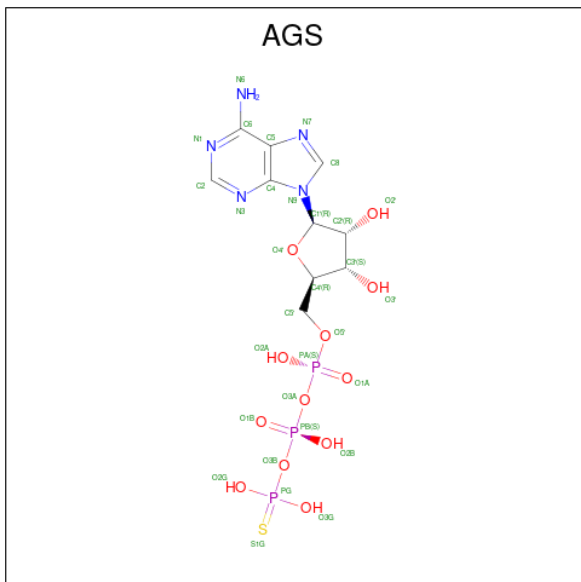
- Molecule 1 is a protein called WlaB protein.

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 (CCD ID: 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 (CCD ID: 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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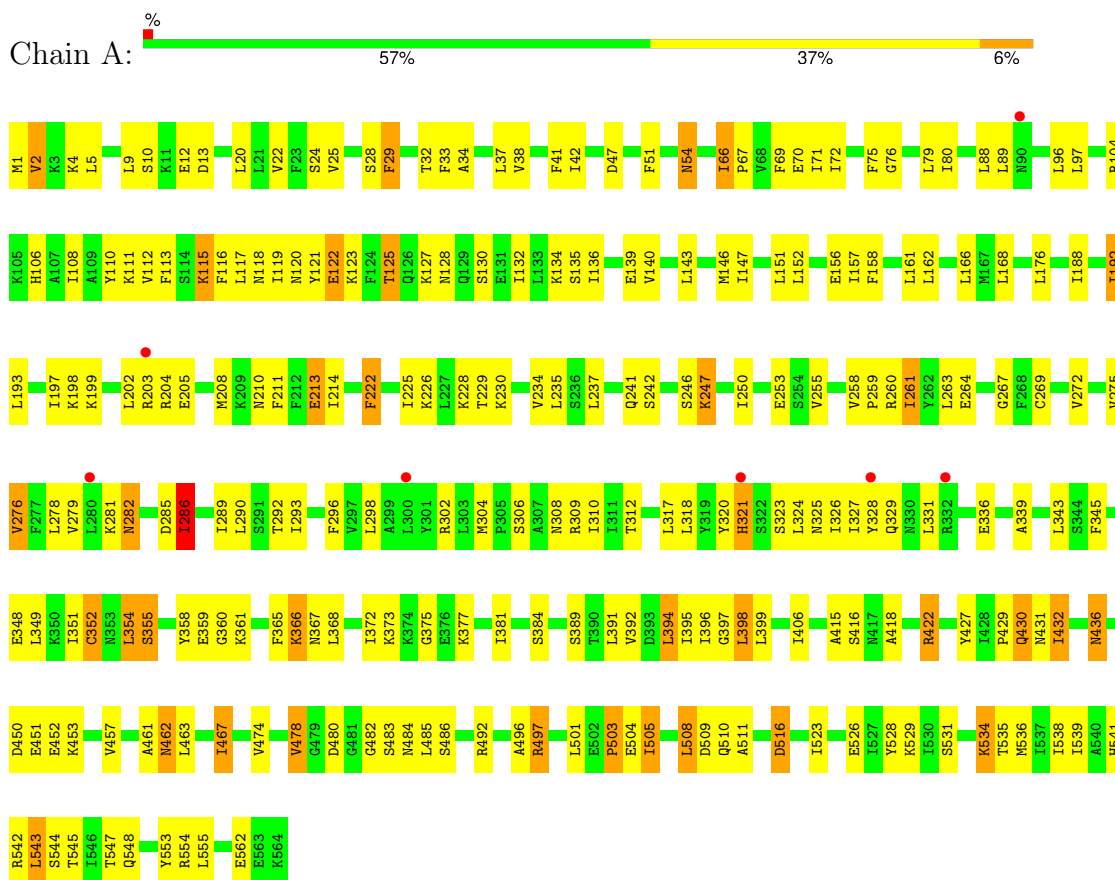
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	37	Total	O	0	0
			37	37		
4	D	31	Total	O	0	0
			31	31		

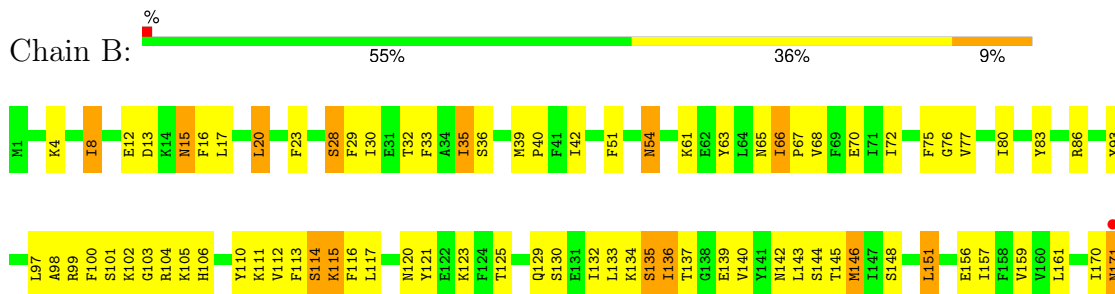
3 Residue-property plots

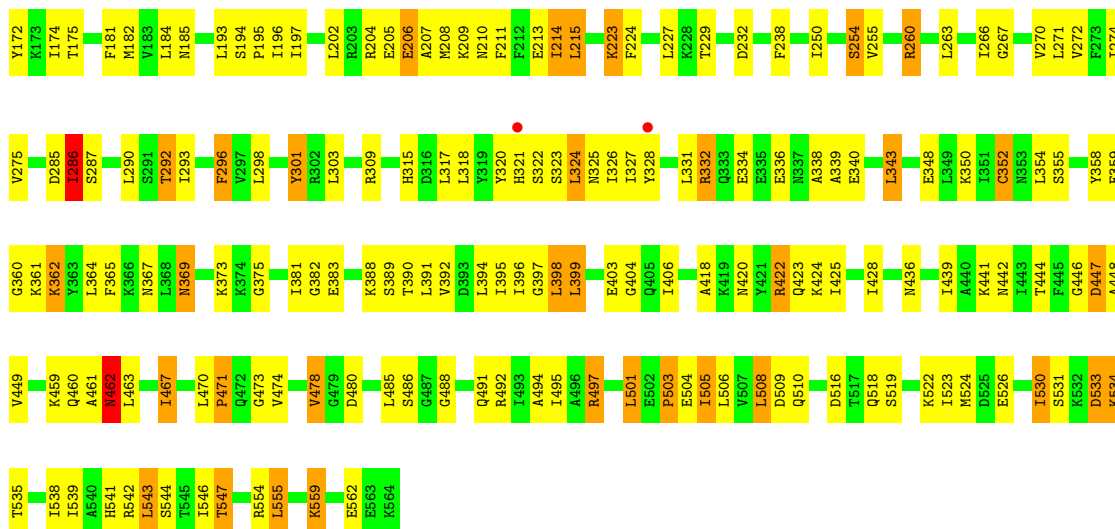
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



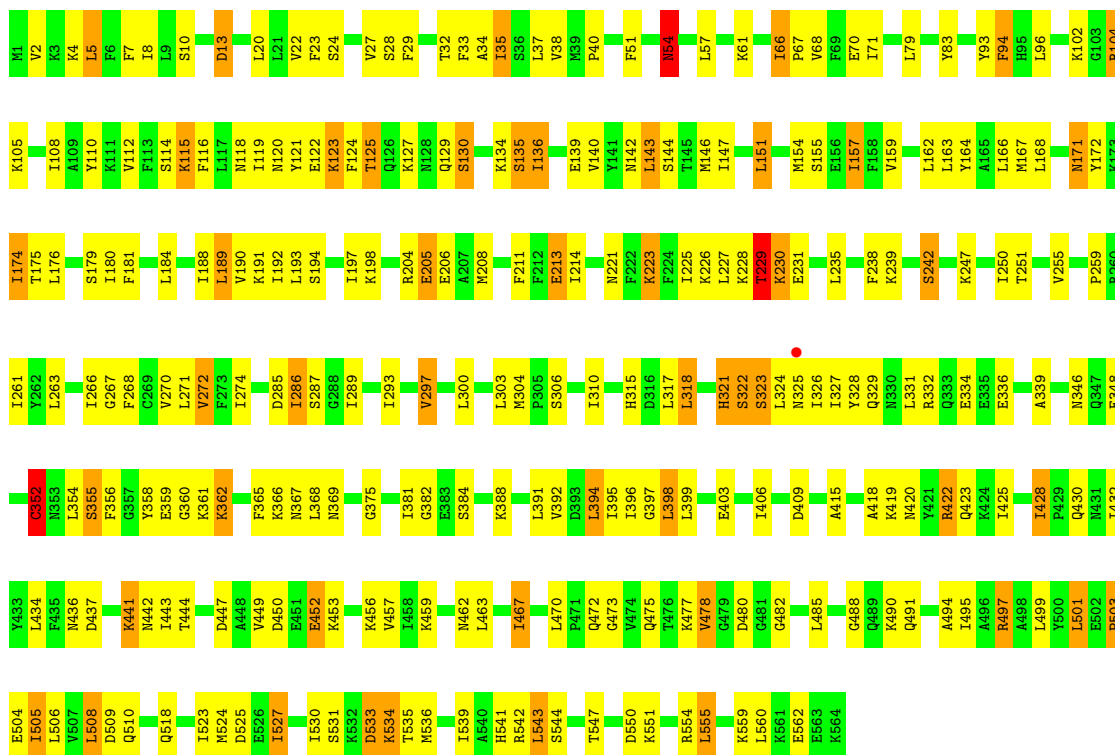
• Molecule 1: WlaB protein





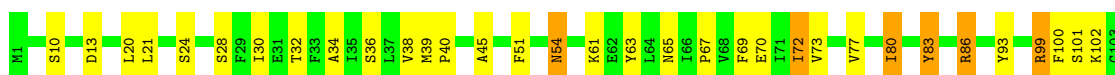
• Molecule 1: WlaB protein

Chain C: 53% 37% 9%



• Molecule 1: WlaB protein

Chain D: 55% 37% 7%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.68Å 145.98Å 206.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.8 (20.00-3.30) 90.3 (20.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.232 , 0.284 0.244 , 0.290	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 , 99.3	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	0.92	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: 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	0.23	0/4639	0.49	0/6244
1	B	0.31	0/4639	0.55	0/6244
1	C	0.27	0/4639	0.54	2/6244 (0.0%)
1	D	0.25	0/4639	0.53	2/6244 (0.0%)
All	All	0.27	0/18556	0.53	4/24976 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	ILE	CA-C-N	-5.79	115.55	122.44
1	C	136	ILE	C-N-CA	-5.79	115.55	122.44
1	D	136	ILE	CA-C-N	-5.38	116.03	122.44
1	D	136	ILE	C-N-CA	-5.38	116.03	122.44

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	176	0
1	B	4555	0	4760	187	0
1	C	4555	0	4760	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4555	0	4760	186	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
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	707	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (707) 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:O5'	2:B:601:AGS:H8	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:194:SER:HB2	1:C:318:LEU:HD22	1.71	0.72
1:B:115:LYS:NZ	1:B:332:ARG:O	2.23	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:C:503:PRO:HB3	1:C:534:LYS:HZ3	1.54	0.71
1:A:198:LYS:HG3	1:A:318:LEU:HD22	1.71	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: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:146:MET:HB2	1:B:321:HIS:HE1	1.60	0.67
1:B:156:GLU:HA	1:B:159:VAL:HG12	1.77	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:HE2	1:B:559:LYS:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:135:SER:C	1:B:136:ILE:HG12	2.25	0.61
1:D:30:ILE:HG22	1:D:86:ARG:HG3	1.82	0.61
1:D:350:LYS:HG3	1:D:371:ASN:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O5'	2:C:601:AGS:H8	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:4:LYS:NZ	1:B:326:ILE:HG12	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:228:LYS:C	1:C:230:LYS:H	2.12	0.57
1:D:99:ARG:HH11	1:D:99:ARG:HB3	1.69	0.57
1:D:247:LYS:O	1:D:250:ILE:HG13	2.05	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:460:GLN:HA	1:B:526:GLU:HG2	1.88	0.56
1:B:461:ALA:O	1:B:463:LEU:N	2.38	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:5:LEU:HG	1:A:321:HIS:HE1	1.71	0.56
1:A:47:ASP:HB3	4:A:729:HOH:O	2.05	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:B:63:TYR:CD1	1:B:65:ASN:HB2	2.41	0.56
1:A:1:MET:HE3	1:A:2:VAL:HG13	1.87	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:A:427:TYR:HE2	1:B:223:LYS:HZ3	1.53	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:355:SER:HB2	1:C:403:GLU:HB2	1.86	0.55
1:C:381:ILE:O	1:C:554:ARG:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:263:LEU:HB3	1:D:304:MET:HE3	1.89	0.55
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:O	1:C:367:ASN:ND2	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:A:253:GLU:HB3	1:B:98:ALA:HB1	1.89	0.54
1:B:76:GLY:O	1:B:80:ILE:HG23	2.08	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:116:PHE:HE2	1:A:331:LEU:HD13	1.73	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: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:A:267:GLY:HA3	1:A:304:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:210:ASN:HB3	1:D:241:GLN:HG3	1.90	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
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:72:ILE:HG23	4:A:712:HOH:O	2.08	0.52
1:A:543:LEU:O	1:A:545:THR:N	2.40	0.52
1:C:146:MET:SD	1:C:321:HIS:HA	2.49	0.52
1:D:120:ASN:OD1	1:D:121:TYR:N	2.43	0.52
1:C:32:THR:HG21	1:C:162:LEU:HD21	1.91	0.52
1:C:123:LYS:HD3	4:C:713:HOH:O	2.09	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:506:LEU:HG	1:D:534:LYS:HZ1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:292:THR:O	1:D:296:PHE:HB2	2.11	0.51
1:A:389:SER:HB2	2:A:601:AGS:O1B	2.11	0.50
1:A:392:VAL:HG21	1:A:539:ILE:HD11	1.93	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:HB2	1:B:332:ARG:CZ	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:37:LEU:HD11	1:C:79:LEU:CD1	2.41	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: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:D:348:GLU:OE2	1:D:410:LYS:NZ	2.29	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:39:MET:HB3	1:D:40:PRO:HD3	1.94	0.50
1:D:392:VAL:O	1:D:396:ILE:HG13	2.12	0.50
1:A:508:LEU:HD22	1:A:538:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:MET:HE3	1:D:298:LEU:HD22	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:5:LEU:HD21	1:C:147:ILE:CD1	2.43	0.49
1:C:223:LYS:HD3	1:D:121:TYR:CZ	2.47	0.49
1:C:543:LEU:O	1:C:544:SER:OG	2.29	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
1:B:362:LYS:H	1:B:362:LYS:HD3	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:D:450:ASP:H	1:D:500:TYR:HH	1.60	0.49
1:A:116:PHE:CE1	1:A:132:ILE:HG12	2.47	0.49
1:A:121:TYR:CE2	1:B:223:LYS:HD3	2.47	0.49
1:B:105:LYS:HG2	1:B:140:VAL:HG12	1.94	0.49
1:C:37:LEU:HD13	1:C:37:LEU:C	2.38	0.49
1:C:66:ILE:HG13	1:C:71:ILE:HG13	1.94	0.49
1:C:193:LEU:HD22	1:C:255:VAL:HG13	1.95	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:285:ASP:C	1:C:287:SER:H	2.22	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:142:ASN:CB	1:C:324:LEU:HD22	2.42	0.47
1:C:229:THR:O	1:C:231:GLU:N	2.47	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
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:41:PHE:HE1	1:A:76:GLY:HA2	1.80	0.47
1:A:355:SER:OG	1:A:367:ASN:N	2.33	0.47
1:B:142:ASN:HB3	1:B:324:LEU:CD2	2.44	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:139:GLU:O	1:A:324:LEU:HD21	2.14	0.47
1:A:272:VAL:HB	4:B:703:HOH:O	2.14	0.47
1:A:345:PHE:HE1	1:A:349:LEU:HB2	1.79	0.47
1:B:292:THR:O	1:B:296:PHE:HB3	2.14	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:HD12	1:B:170:ILE:H	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:12:GLU:O	1:B:15:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LYS:HD2	1:B:334:GLU:HB2	1.96	0.47
1:C:66:ILE:HB	1:C:70:GLU:HB2	1.97	0.47
1:C:550:ASP:OD1	1:C:551:LYS:N	2.47	0.47
1:D:271:LEU:O	1:D:274:ILE:HG13	2.15	0.47
1:A:41:PHE:CE1	1:A:76:GLY:HA2	2.50	0.46
1:A:351:ILE:HG23	1:A:354:LEU:HD13	1.96	0.46
1:B:543:LEU:O	1:B:544:SER:OG	2.28	0.46
1:C:322:SER:O	1:C:323:SER:C	2.58	0.46
1:D:285:ASP:C	1:D:287:SER:H	2.23	0.46
1:D:354:LEU:HD21	1:D:394:LEU:HD13	1.97	0.46
1:D:453:LYS:HB2	1:D:453:LYS:HE3	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:105:LYS:HZ3	1:D:140:VAL:HG11	1.80	0.46
1:D:208:MET:HA	1:D:211:PHE:CE2	2.50	0.46
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:B:142:ASN:HA	1:B:146:MET:HE2	1.97	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:ND2	1:D:367:ASN:O	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:B:461:ALA:C	1:B:463:LEU:H	2.23	0.45
1:D:467:ILE:H	1:D:467:ILE:HG12	1.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:GLU:N	1:D:243:GLU:OE1	2.49	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:268:PHE:HB3	1:D:83:TYR:CD2	2.51	0.45
1:C:434:LEU:HB3	1:C:478:VAL:HG11	1.97	0.45
1:D:302:ARG:HA	1:D:302:ARG:NE	2.30	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:4:LYS:NZ	1:A:326:ILE:HG12	2.32	0.45
1:A:135:SER:O	1:A:328:TYR:OH	2.34	0.45
1:A:317:LEU:O	1:A:321:HIS:HB3	2.16	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:66:ILE:HB	1:A:70:GLU:HB2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:37:LEU:HD22	1:C:37:LEU:C	2.43	0.44
1:D:501:LEU:HD12	1:D:501:LEU:HA	1.80	0.44
1:A:289:ILE:HG13	1:A:290:LEU:N	2.33	0.44
1:B:4:LYS:HZ1	1:B:326:ILE:HG12	1.82	0.44
1:B:285:ASP:C	1:B:287:SER:H	2.25	0.44
1:B:508:LEU:HD21	1:B:524:MET:HE1	2.00	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:H	1:B:467:ILE:HG12	1.54	0.44
1:D:20:LEU:HD23	1:D:20:LEU:HA	1.86	0.44
1:D:422:ARG:C	1:D:424:LYS:H	2.25	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
1:C:434:LEU:HD12	1:C:490:LYS:HG3	1.99	0.44
1:A:228:LYS:HD2	1:B:501:LEU:HD11	2.00	0.44
1:B:436:ASN:HB2	1:B:480:ASP:HA	2.00	0.44
1:C:54:ASN:HB3	1:C:57:LEU:HD23	2.00	0.44
1:C:306:SER:O	1:C:310:ILE:HG13	2.18	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:HD23	1:B:555:LEU:HA	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:A:20:LEU:O	1:A:24:SER:OG	2.26	0.43
1:B:510:GLN:N	1:B:539:ILE:O	2.50	0.43
1:C:191:LYS:HA	1:C:191:LYS:HD3	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:C:523:ILE:HG22	1:C:524:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:TYR:OH	1:D:390:THR:OG1	2.25	0.43
1:A:136:ILE:HD12	1:A:136:ILE:H	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:HD23	1:B:97:LEU:HA	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:503:PRO:HB2	1:A:534:LYS:HG3	2.00	0.43
1:C:129:GLN:HE22	1:D:220:ASN:HA	1.84	0.43
1:C:151:LEU:HD13	1:C:151:LEU:HA	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: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
1:B:66:ILE:HD12	1:B:70:GLU:O	2.19	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:SER:O	1:D:40:PRO:HD3	2.19	0.42
1:D:302:ARG:HA	1:D:302:ARG:HE	1.84	0.42
1:A:503:PRO:HB3	1:A:534:LYS:HZ3	1.84	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:C:228:LYS:C	1:C:230:LYS:N	2.77	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:38:VAL:HG22	1:C:83:TYR:HH	1.80	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:A:483:SER:O	2:B:601:AGS:N6	2.52	0.42
1:B:447:ASP:N	1:B:447:ASP:OD1	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
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:HD12	1:B:530:ILE:HA	1.75	0.42
1:B:534:LYS:HZ3	1:B:534:LYS:HG3	1.70	0.42
1:C:467:ILE:H	1:C:467:ILE:HG12	1.52	0.42
1:C:467:ILE:HG22	1:C:473:GLY:C	2.44	0.42
2:A:601:AGS:O3B	1:B:486:SER:HB2	2.20	0.42
1:B:461:ALA:C	1:B:463:LEU:N	2.78	0.42
1:C:423:GLN:HG2	1:D:229:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:157:ILE:HG22	1:A:310:ILE:HD12	2.01	0.42
1:A:272:VAL:CG2	1:B:80:ILE:HG22	2.50	0.42
1:B:171:ASN:O	1:B:175:THR:OG1	2.35	0.42
1:B:227:LEU:HD12	1:B:227:LEU:HA	1.85	0.42
1:C:94:PHE:HD1	1:C:94:PHE:HA	1.78	0.42
1:C:104:ARG:HD3	1:C:104:ARG:HA	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: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:222:PHE:HE1	1:B:117:LEU:HA	1.85	0.41
1:A:528:TYR:CE2	1:A:548:GLN:HB2	2.55	0.41
1:A:534:LYS:H	1:A:534:LYS:HD3	1.84	0.41
1:B:77:VAL:HA	1:B:80:ILE:HG12	2.02	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:339:ALA:CB	1:A:416:SER:HA	2.50	0.41
1:A:396:ILE:HG13	1:A:398:LEU:HD22	2.03	0.41
1:A:531:SER:HA	1:A:534:LYS:CE	2.50	0.41
1:B:72:ILE:H	1:B:72:ILE:HG13	1.72	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: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:HD12	1:D:530:ILE:HA	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:113:PHE:CE1	1:B:215:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:GLU:O	1:A:505:ILE:HB	2.21	0.41
1:B:61:LYS:HG3	4:B:706:HOH:O	2.19	0.41
1:B:214:ILE:H	1:B:214:ILE:HG12	1.42	0.41
1:D:343:LEU:HD12	1:D:343:LEU:HA	1.98	0.41
1:A:320:TYR:O	1:A:321:HIS:C	2.63	0.41
1:B:303:LEU:HD23	1:B:303:LEU:HA	1.89	0.41
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.89	0.41
1:B:343:LEU:HA	1:B:343:LEU:HD12	1.73	0.41
1:B:467:ILE:HG22	1:B:473:GLY:C	2.45	0.41
1:C:105:LYS:HB3	1:D:246:SER:OG	2.20	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:D:414:ASN:C	1:D:416:SER:H	2.29	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:5:LEU:HD23	1:A:5:LEU:HA	1.87	0.41
1:A:116:PHE:O	1:A:119:ILE:HG12	2.21	0.41
1:A:214:ILE:HD13	1:A:214:ILE:HG21	1.72	0.41
1:A:391:LEU:O	1:A:395:ILE:HG13	2.21	0.41
1:B:15:ASN:OD1	1:B:16:PHE:N	2.54	0.41
1:B:321:HIS:O	1:B:325:ASN:HB3	2.21	0.41
1:C:83:TYR:CD2	1:D:268:PHE:HB3	2.55	0.41
1:C:123:LYS:O	1:C:127:LYS:HG2	2.21	0.41
1:C:154:MET:O	1:C:157:ILE:HG13	2.21	0.41
1:C:221:ASN:O	1:C:225: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:D:276:VAL:HA	1:D:279:VAL:HG22	2.02	0.41
1:A:28:SER:HB2	1:A:162:LEU:HD12	2.02	0.41
1:A:106:HIS:O	1:A:110:TYR:HD2	2.04	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:C:508:LEU:HD21	1:C:524:MET:HE1	2.03	0.41
1:D:108:ILE:HA	1:D:111:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:ASP:O	1:D:399:LEU:HB2	2.21	0.41
1:D:534:LYS:HZ2	1:D:534:LYS:HG3	1.74	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:HE	1:B:260:ARG:HB2	1.74	0.40
1:B:396:ILE:HG22	1:B:425:ILE:HD12	2.03	0.40
1:B:424:LYS:HE3	1:B:504:GLU:OE1	2.20	0.40
1:B:444:THR:HG21	1:B:449:VAL:HG22	2.03	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:23:PHE:CE2	1:C:93:TYR:HB2	2.56	0.40
1:C:114:SER:O	1:C:118:ASN:ND2	2.52	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:124:PHE:CD1	1:C:124:PHE:C	2.98	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:72:ILE:HG13	1:D:73:VAL:N	2.36	0.40
1:D:332:ARG:HD3	1:D:332:ARG:HA	1.95	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%)	4	21
1	B	562/564 (100%)	484 (86%)	57 (10%)	21 (4%)	2	17
1	C	562/564 (100%)	490 (87%)	50 (9%)	22 (4%)	2	16
1	D	562/564 (100%)	486 (86%)	55 (10%)	21 (4%)	2	17
All	All	2248/2256 (100%)	1959 (87%)	209 (9%)	80 (4%)	2	17

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	453 (90%)	51 (10%)	7	26
1	B	504/504 (100%)	426 (84%)	78 (16%)	2	12
1	C	504/504 (100%)	433 (86%)	71 (14%)	3	14
1	D	504/504 (100%)	445 (88%)	59 (12%)	5	20
All	All	2016/2016 (100%)	1757 (87%)	259 (13%)	4	18

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	12	GLU
1	A	29	PHE
1	A	42	ILE
1	A	54	ASN
1	A	66	ILE
1	A	75	PHE
1	A	88	LEU
1	A	89	LEU
1	A	115	LYS
1	A	122	GLU
1	A	125	THR
1	A	134	LYS
1	A	166	LEU
1	A	168	LEU
1	A	176	LEU

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Mol	Chain	Res	Type
1	A	192	ILE
1	A	213	GLU
1	A	229	THR
1	A	230	LYS
1	A	247	LYS
1	A	258	VAL
1	A	261	ILE
1	A	269	CYS
1	A	276	VAL
1	A	282	ASN
1	A	286	ILE
1	A	298	LEU
1	A	308	ASN
1	A	312	THR
1	A	343	LEU
1	A	352	CYS
1	A	372	ILE
1	A	394	LEU
1	A	398	LEU
1	A	422	ARG
1	A	430	GLN
1	A	432	ILE
1	A	452	GLU
1	A	462	ASN
1	A	467	ILE
1	A	474	VAL
1	A	478	VAL
1	A	497	ARG
1	A	501	LEU
1	A	508	LEU
1	A	510	GLN
1	A	516	ASP
1	A	534	LYS
1	A	542	ARG
1	A	555	LEU
1	B	8	ILE
1	B	15	ASN
1	B	17	LEU
1	B	20	LEU
1	B	28	SER
1	B	29	PHE
1	B	33	PHE

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Mol	Chain	Res	Type
1	B	35	ILE
1	B	54	ASN
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	111	LYS
1	B	114	SER
1	B	115	LYS
1	B	123	LYS
1	B	129	GLN
1	B	133	LEU
1	B	134	LYS
1	B	135	SER
1	B	143	LEU
1	B	144	SER
1	B	146	MET
1	B	148	SER
1	B	151	LEU
1	B	182	MET
1	B	184	LEU
1	B	196	ILE
1	B	202	LEU
1	B	206	GLU
1	B	214	ILE
1	B	215	LEU
1	B	223	LYS
1	B	229	THR
1	B	232	ASP
1	B	254	SER
1	B	260	ARG
1	B	263	LEU
1	B	266	ILE
1	B	286	ILE
1	B	292	THR
1	B	296	PHE
1	B	301	TYR
1	B	309	ARG
1	B	322	SER
1	B	324	LEU

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Mol	Chain	Res	Type
1	B	332	ARG
1	B	343	LEU
1	B	362	LYS
1	B	369	ASN
1	B	383	GLU
1	B	392	VAL
1	B	398	LEU
1	B	422	ARG
1	B	439	ILE
1	B	459	LYS
1	B	462	ASN
1	B	467	ILE
1	B	474	VAL
1	B	478	VAL
1	B	491	GLN
1	B	497	ARG
1	B	501	LEU
1	B	506	LEU
1	B	508	LEU
1	B	518	GLN
1	B	530	ILE
1	B	533	ASP
1	B	534	LYS
1	B	542	ARG
1	B	546	ILE
1	B	547	THR
1	B	555	LEU
1	B	559	LYS
1	B	562	GLU
1	C	2	VAL
1	C	5	LEU
1	C	13	ASP
1	C	20	LEU
1	C	22	VAL
1	C	27	VAL
1	C	29	PHE
1	C	33	PHE
1	C	35	ILE
1	C	54	ASN
1	C	66	ILE
1	C	94	PHE
1	C	96	LEU

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Mol	Chain	Res	Type
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	134	LYS
1	C	143	LEU
1	C	144	SER
1	C	151	LEU
1	C	157	ILE
1	C	166	LEU
1	C	174	ILE
1	C	184	LEU
1	C	189	LEU
1	C	192	ILE
1	C	205	GLU
1	C	206	GLU
1	C	213	GLU
1	C	223	LYS
1	C	226	LYS
1	C	229	THR
1	C	242	SER
1	C	261	ILE
1	C	272	VAL
1	C	286	ILE
1	C	289	ILE
1	C	297	VAL
1	C	318	LEU
1	C	323	SER
1	C	348	GLU
1	C	352	CYS
1	C	362	LYS
1	C	384	SER
1	C	392	VAL
1	C	394	LEU
1	C	398	LEU
1	C	419	LYS
1	C	422	ARG
1	C	452	GLU
1	C	459	LYS
1	C	462	ASN

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Mol	Chain	Res	Type
1	C	467	ILE
1	C	478	VAL
1	C	497	ARG
1	C	501	LEU
1	C	506	LEU
1	C	508	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	559	LYS
1	C	562	GLU
1	D	10	SER
1	D	21	LEU
1	D	54	ASN
1	D	72	ILE
1	D	80	ILE
1	D	83	TYR
1	D	86	ARG
1	D	99	ARG
1	D	101	SER
1	D	110	TYR
1	D	123	LYS
1	D	131	GLU
1	D	134	LYS
1	D	151	LEU
1	D	152	LEU
1	D	153	LEU
1	D	156	GLU
1	D	161	LEU
1	D	164	TYR
1	D	168	LEU
1	D	181	PHE
1	D	199	LYS
1	D	204	ARG
1	D	210	ASN
1	D	213	GLU
1	D	226	LYS

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Mol	Chain	Res	Type
1	D	230	LYS
1	D	246	SER
1	D	260	ARG
1	D	293	ILE
1	D	301	TYR
1	D	302	ARG
1	D	310	ILE
1	D	318	LEU
1	D	350	LYS
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	422	ARG
1	D	431	ASN
1	D	447	ASP
1	D	452	GLU
1	D	467	ILE
1	D	472	GLN
1	D	474	VAL
1	D	478	VAL
1	D	497	ARG
1	D	506	LEU
1	D	507	VAL
1	D	530	ILE
1	D	533	ASP
1	D	534	LYS
1	D	542	ARG
1	D	555	LEU
1	D	559	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	325	ASN
1	A	430	GLN
1	A	455	ASN
1	A	489	GLN

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Mol	Chain	Res	Type
1	B	129	GLN
1	B	171	ASN
1	B	321	HIS
1	C	118	ASN
1	C	218	ASN
1	C	241	GLN
1	C	315	HIS
1	C	337	ASN
1	C	405	GLN
1	C	436	ASN
1	D	126	GLN
1	D	128	ASN
1	D	185	ASN
1	D	455	ASN
1	D	484	ASN

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 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	A	601	-	32,33,33	2.04	6 (18%)	45,52,52	1.89	10 (22%)
2	AGS	C	601	3	32,33,33	2.03	6 (18%)	45,52,52	1.89	10 (22%)
2	AGS	B	601	3	32,33,33	2.04	6 (18%)	45,52,52	1.89	10 (22%)
2	AGS	D	601	-	32,33,33	2.04	6 (18%)	45,52,52	1.90	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
2	AGS	A	601	-	-	2/21/38/38	0/3/3/3
2	AGS	C	601	3	-	5/21/38/38	0/3/3/3
2	AGS	B	601	3	-	6/21/38/38	0/3/3/3
2	AGS	D	601	-	-	1/21/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	AGS	PG-S1G	7.99	2.08	1.90
2	A	601	AGS	PG-S1G	7.96	2.07	1.90
2	B	601	AGS	PG-S1G	7.95	2.07	1.90
2	C	601	AGS	PG-S1G	7.94	2.07	1.90
2	A	601	AGS	C5-C4	4.74	1.47	1.39
2	B	601	AGS	C5-C4	4.74	1.47	1.39
2	D	601	AGS	C5-C4	4.74	1.47	1.39
2	C	601	AGS	C5-C4	4.72	1.47	1.39
2	B	601	AGS	C5-C6	2.78	1.48	1.41
2	D	601	AGS	C5-C6	2.76	1.48	1.41
2	A	601	AGS	C5-C6	2.75	1.48	1.41
2	C	601	AGS	C5-C6	2.74	1.48	1.41
2	A	601	AGS	C8-N7	2.40	1.36	1.31
2	B	601	AGS	C8-N7	2.36	1.36	1.31
2	D	601	AGS	C8-N7	2.35	1.36	1.31
2	C	601	AGS	C8-N7	2.33	1.36	1.31
2	B	601	AGS	C5-N7	-2.25	1.35	1.39
2	A	601	AGS	C5-N7	-2.24	1.35	1.39
2	D	601	AGS	C5-N7	-2.21	1.35	1.39
2	C	601	AGS	C5-N7	-2.19	1.35	1.39
2	A	601	AGS	PG-O2G	2.09	1.61	1.54
2	C	601	AGS	PG-O2G	2.08	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	AGS	PG-O2G	2.07	1.61	1.54
2	D	601	AGS	PG-O2G	2.07	1.61	1.54

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	AGS	C5-C4-N3	-5.87	118.63	126.72
2	C	601	AGS	C5-C4-N3	-5.86	118.65	126.72
2	D	601	AGS	C5-C4-N3	-5.85	118.66	126.72
2	A	601	AGS	C5-C4-N3	-5.85	118.67	126.72
2	B	601	AGS	N3-C4-N9	4.62	135.02	127.17
2	A	601	AGS	N3-C4-N9	4.60	134.99	127.17
2	C	601	AGS	N3-C4-N9	4.60	134.99	127.17
2	D	601	AGS	N3-C4-N9	4.58	134.95	127.17
2	B	601	AGS	C2-N3-C4	3.72	120.92	111.83
2	C	601	AGS	C2-N3-C4	3.70	120.87	111.83
2	D	601	AGS	C2-N3-C4	3.69	120.84	111.83
2	A	601	AGS	C2-N3-C4	3.69	120.84	111.83
2	D	601	AGS	C4-C5-N7	-3.54	106.53	110.58
2	C	601	AGS	C4-C5-N7	-3.52	106.56	110.58
2	A	601	AGS	C4-C5-N7	-3.50	106.58	110.58
2	B	601	AGS	C4-C5-N7	-3.48	106.60	110.58
2	A	601	AGS	PB-O3B-PG	-3.47	120.47	133.17
2	D	601	AGS	PB-O3B-PG	-3.46	120.50	133.17
2	C	601	AGS	PB-O3B-PG	-3.46	120.51	133.17
2	B	601	AGS	PB-O3B-PG	-3.46	120.53	133.17
2	B	601	AGS	N3-C2-N1	-3.23	123.69	128.58
2	D	601	AGS	N3-C2-N1	-3.20	123.73	128.58
2	C	601	AGS	N3-C2-N1	-3.20	123.74	128.58
2	A	601	AGS	N3-C2-N1	-3.19	123.75	128.58
2	A	601	AGS	C4-N9-C8	2.60	108.47	105.74
2	D	601	AGS	C5-N7-C8	2.58	107.51	103.45
2	D	601	AGS	C4-N9-C8	2.58	108.44	105.74
2	A	601	AGS	C3'-C2'-C1'	2.57	106.33	101.46
2	C	601	AGS	C4-N9-C8	2.56	108.43	105.74
2	B	601	AGS	C3'-C2'-C1'	2.56	106.31	101.46
2	B	601	AGS	C4-N9-C8	2.56	108.42	105.74
2	D	601	AGS	C3'-C2'-C1'	2.55	106.29	101.46
2	A	601	AGS	C5-N7-C8	2.55	107.45	103.45
2	C	601	AGS	C3'-C2'-C1'	2.55	106.28	101.46
2	B	601	AGS	C5-N7-C8	2.54	107.44	103.45
2	C	601	AGS	C5-N7-C8	2.53	107.43	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	AGS	C6-C5-N7	2.11	136.16	132.09
2	A	601	AGS	C6-C5-N7	2.08	136.11	132.09
2	C	601	AGS	C6-C5-N7	2.08	136.11	132.09
2	B	601	AGS	C6-C5-N7	2.08	136.09	132.09

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	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	C5'-O5'-PA-O3A
2	C	601	AGS	C5'-O5'-PA-O1A
2	B	601	AGS	PG-O3B-PB-O2B
2	A	601	AGS	PA-O3A-PB-O1B
2	C	601	AGS	PA-O3A-PB-O1B
2	A	601	AGS	PA-O3A-PB-O2B
2	C	601	AGS	PA-O3A-PB-O2B
2	D	601	AGS	PA-O3A-PB-O1B

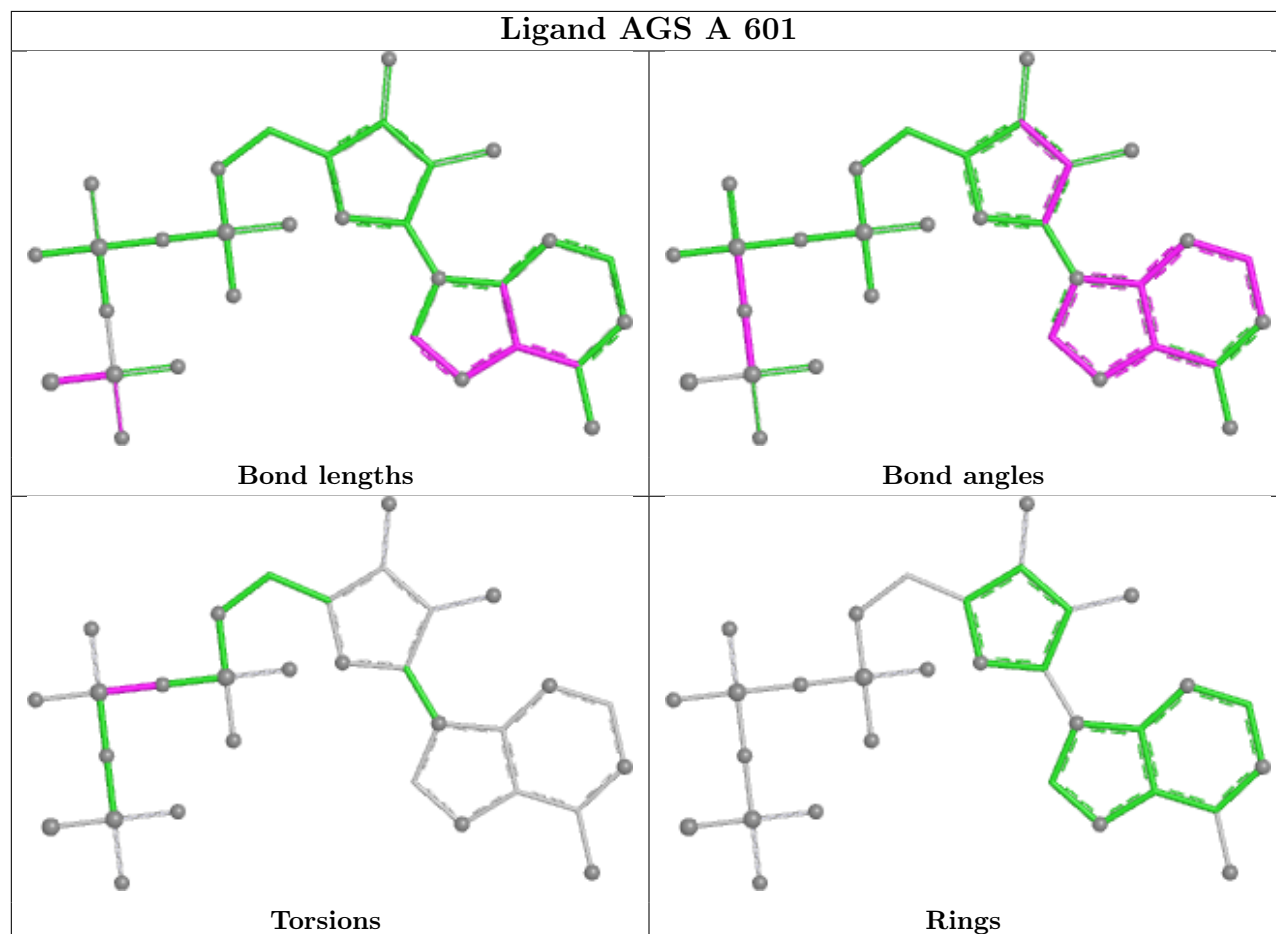
There are no ring outliers.

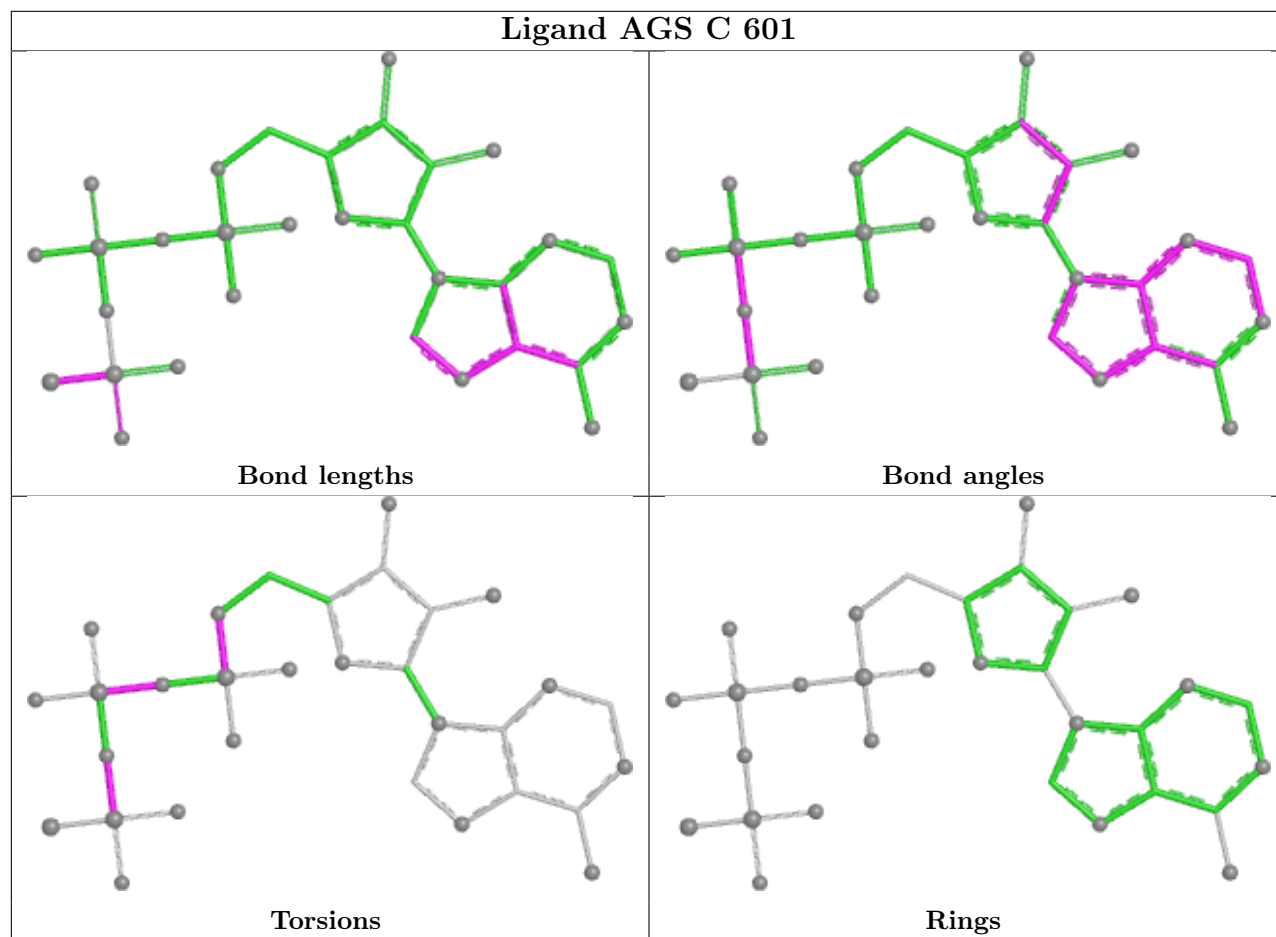
4 monomers are involved in 21 short contacts:

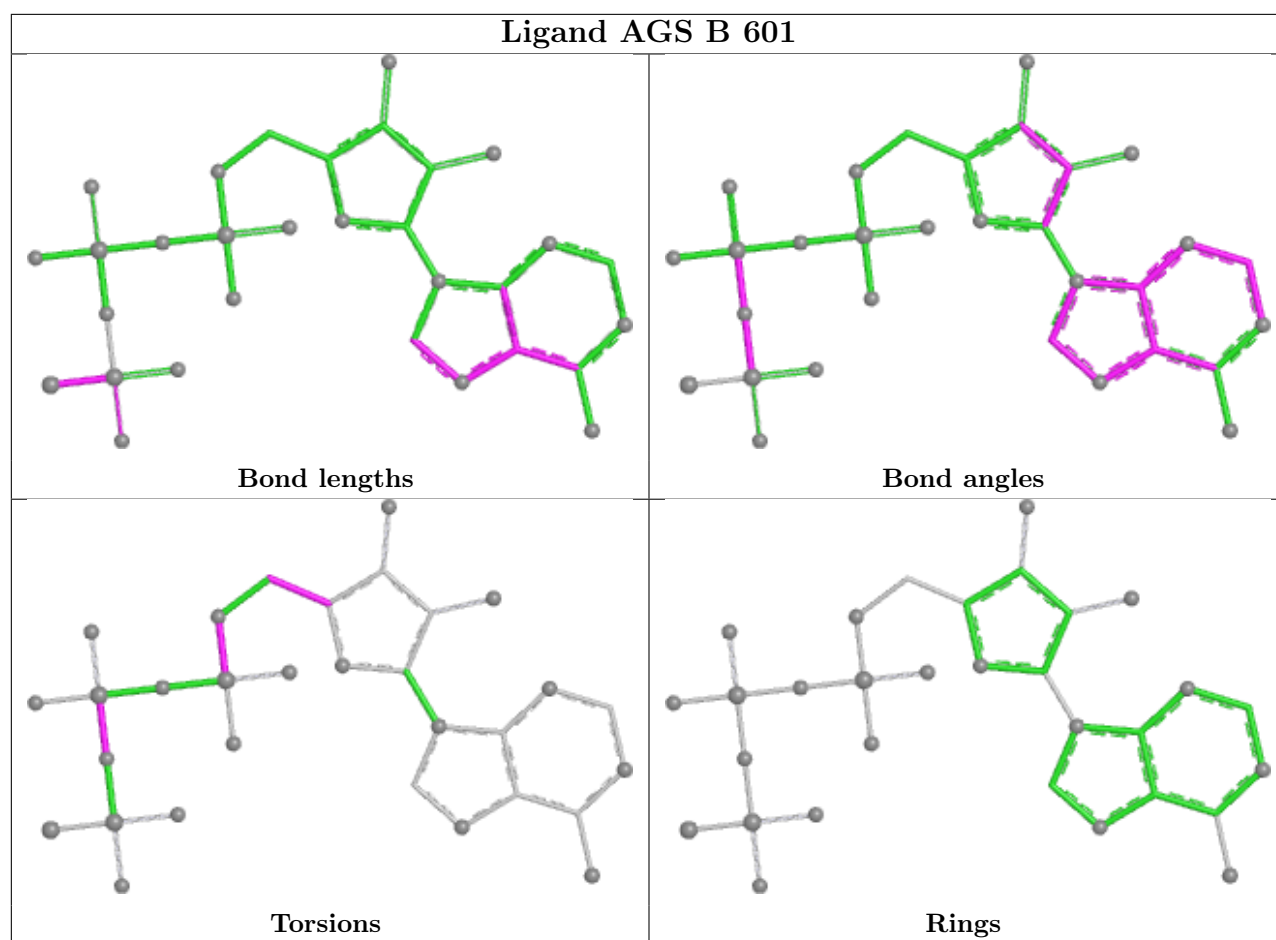
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	AGS	3	0
2	C	601	AGS	3	0
2	B	601	AGS	10	0
2	D	601	AGS	5	0

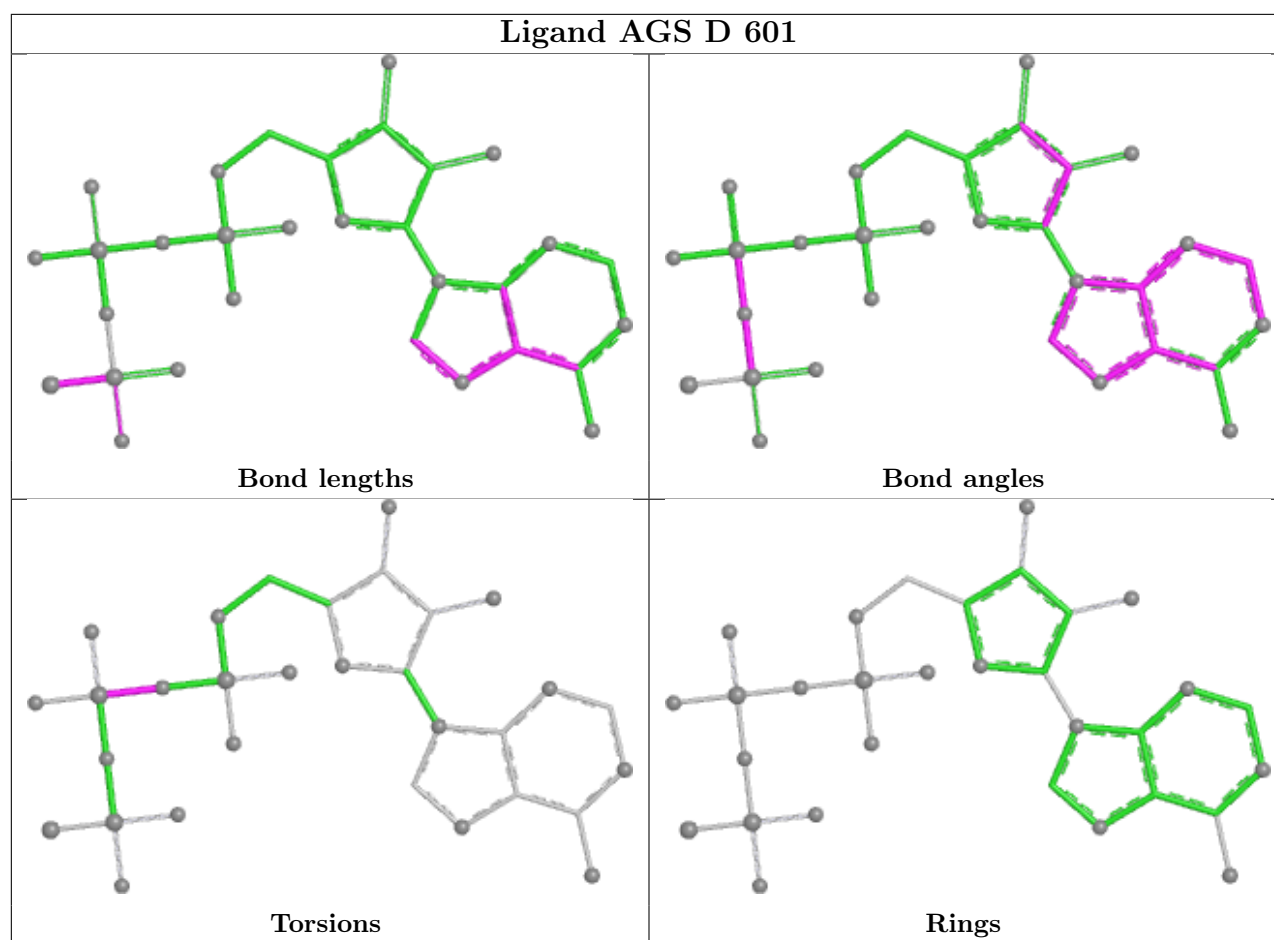
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	564/564 (100%)	-0.26	7 (1%) 76 58	64, 143, 291, 584	0
1	B	564/564 (100%)	-0.30	3 (0%) 87 76	44, 115, 261, 366	0
1	C	564/564 (100%)	-0.29	1 (0%) 91 86	58, 119, 275, 346	0
1	D	564/564 (100%)	-0.27	1 (0%) 91 86	60, 131, 288, 450	0
All	All	2256/2256 (100%)	-0.28	12 (0%) 87 76	44, 127, 280, 584	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	HIS	4.7
1	A	321	HIS	4.6
1	A	280	LEU	3.4
1	A	328	TYR	3.0
1	D	321	HIS	2.9
1	A	332	ARG	2.4
1	B	328	TYR	2.4
1	A	300	LEU	2.3
1	C	325	ASN	2.3
1	A	203	ARG	2.2
1	B	171	ASN	2.2
1	A	90	ASN	2.1

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](#)

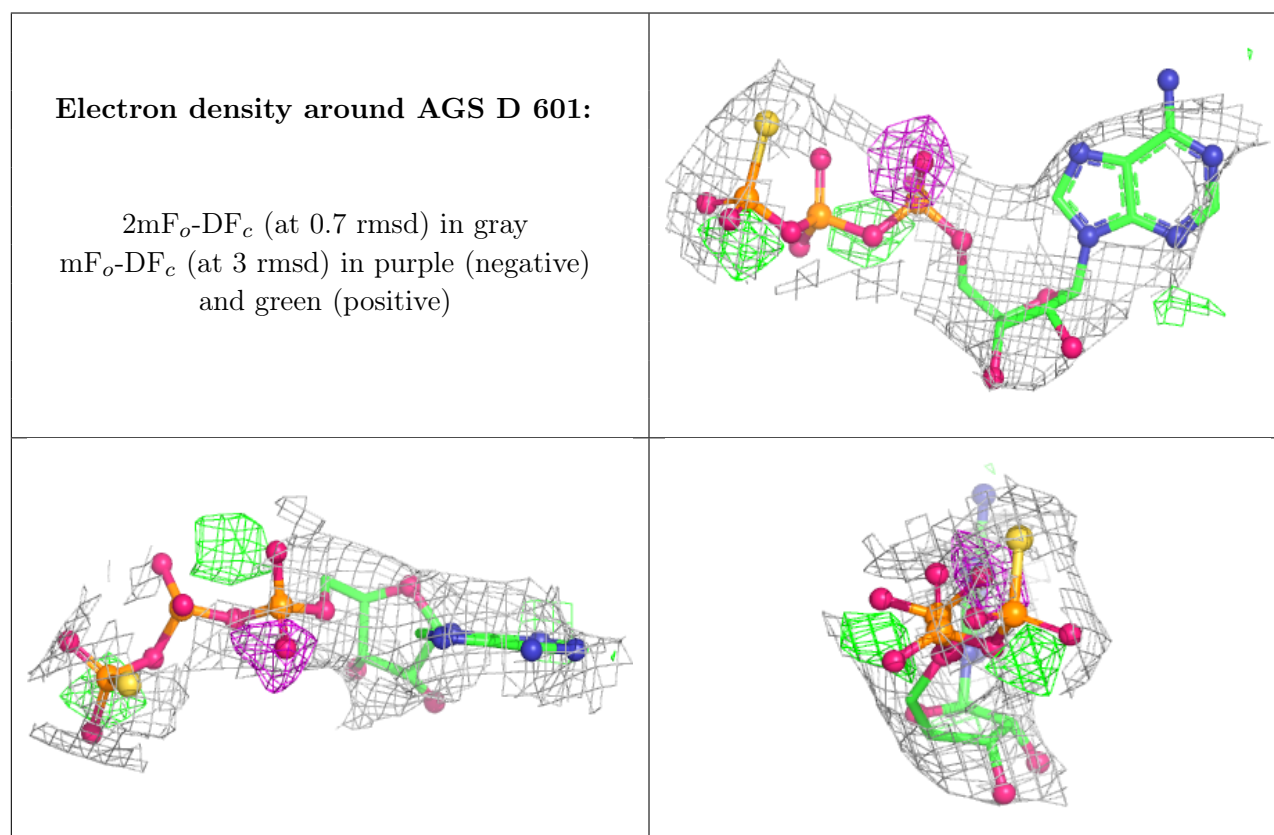
There are no oligosaccharides in this entry.

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.

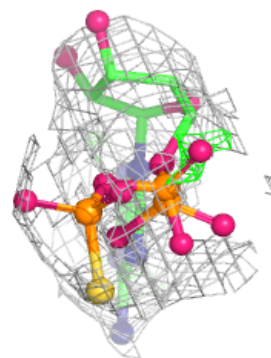
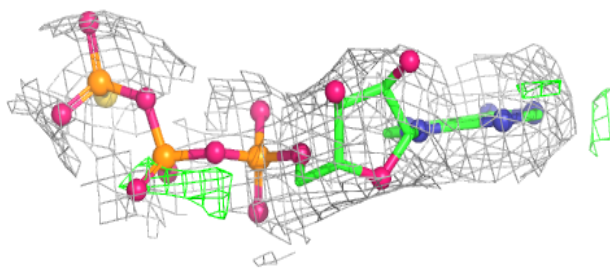
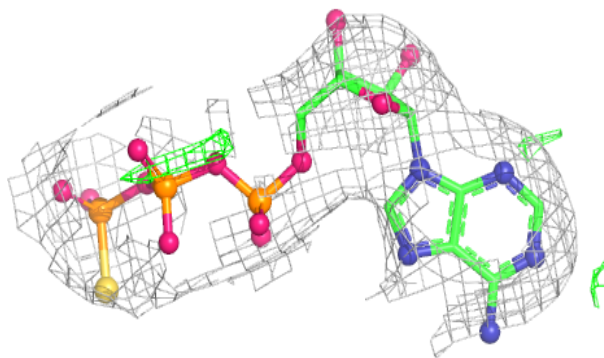
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	602	1/1	0.90	0.09	104,104,104,104	0
2	AGS	D	601	31/31	0.92	0.11	43,121,168,276	0
2	AGS	A	601	31/31	0.92	0.11	59,118,158,208	0
2	AGS	B	601	31/31	0.94	0.08	71,92,130,225	0
2	AGS	C	601	31/31	0.96	0.07	45,81,139,289	0
3	MG	C	602	1/1	0.99	0.05	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.

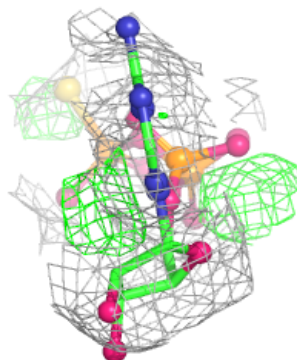
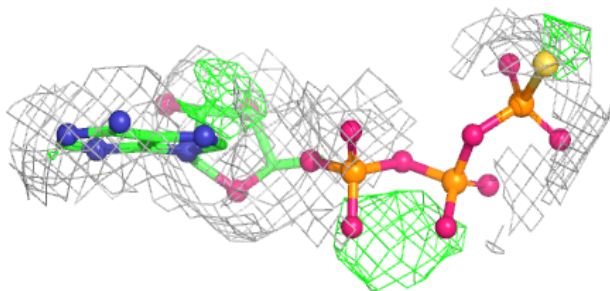
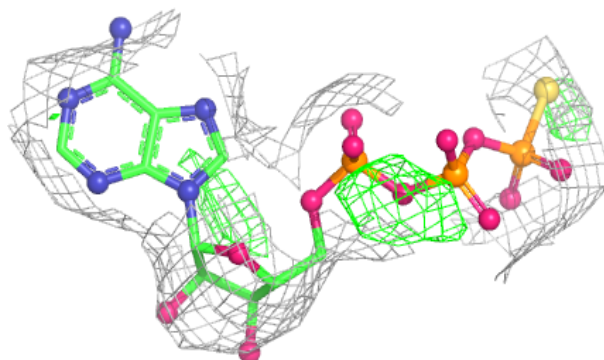


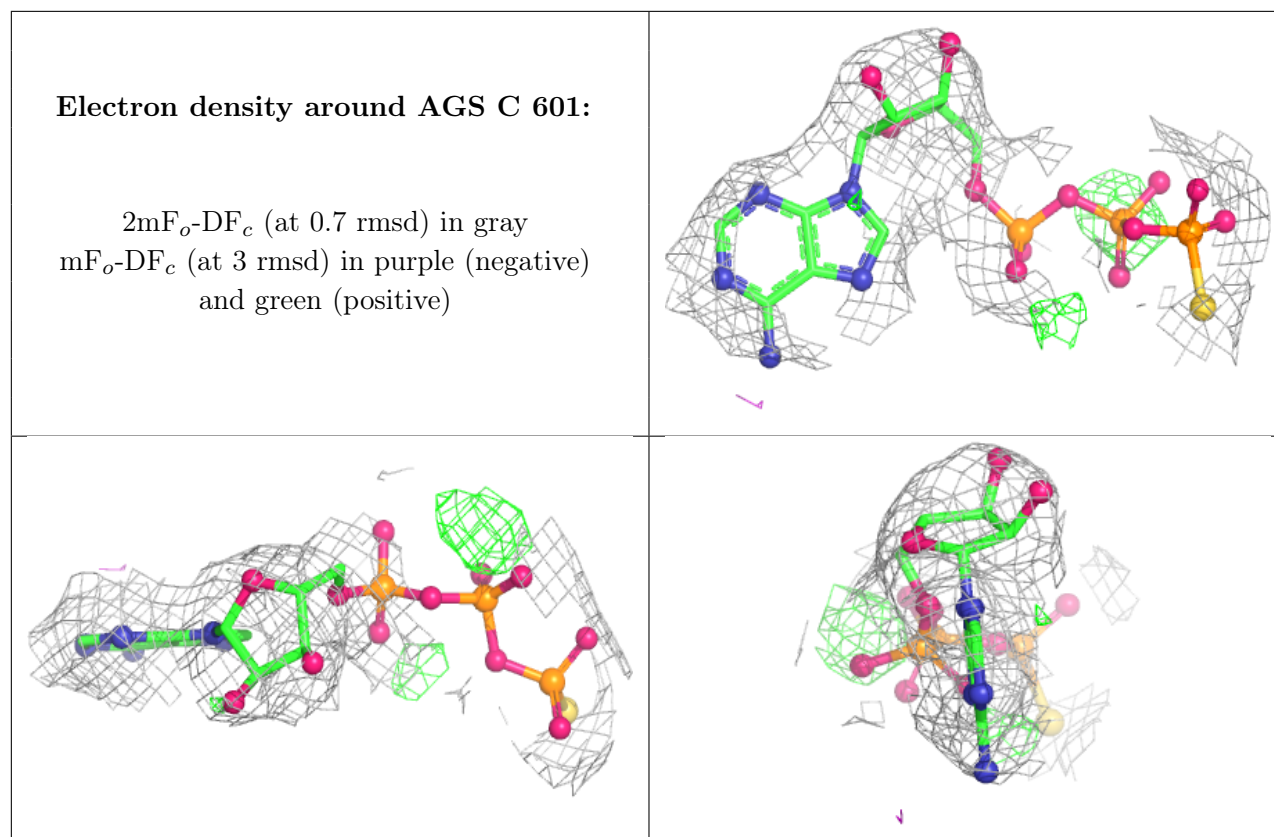
Electron density around AGS A 601:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.