



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2021 – 12:10 AM EDT

PDB ID : 3E3N
Title : The Glycogen phosphorylase b R state- AMP complex
Authors : Leonidas, D.D.; Zographos, S.E.; Oikonomakos, N.G.
Deposited on : 2008-08-07
Resolution : 2.70 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 : 2.23.1
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) : 2.23.1

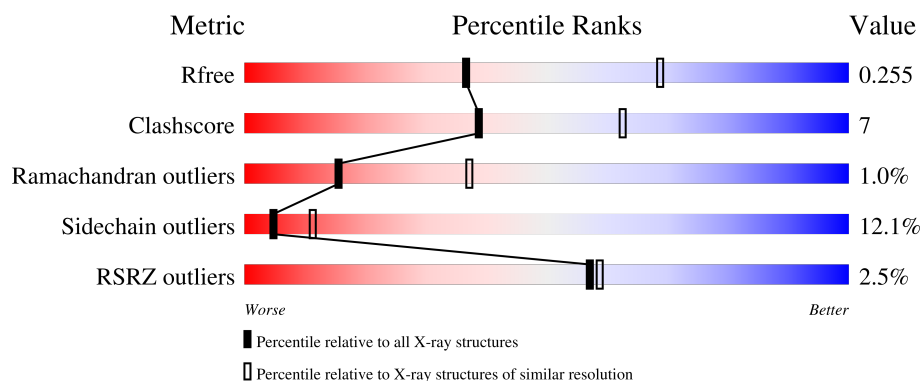
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	842	<div> <div>2%</div> <div>72% 20% 5% .</div> </div>
1	B	842	<div> <div>4%</div> <div>71% 21% 5% .</div> </div>
1	C	842	<div> <div>2%</div> <div>76% 15% 5% 5%</div> </div>
1	D	842	<div> <div>%</div> <div>76% 18% . .</div> </div>
1	E	842	<div> <div>2%</div> <div>73% 19% . 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	842	
1	G	842	
1	H	842	

2 Entry composition

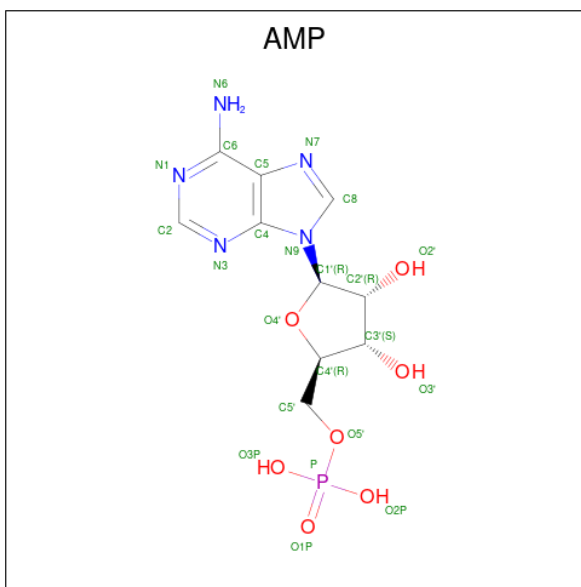
There are 4 unique types of molecules in this entry. The entry contains 53512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen phosphorylase, muscle form.

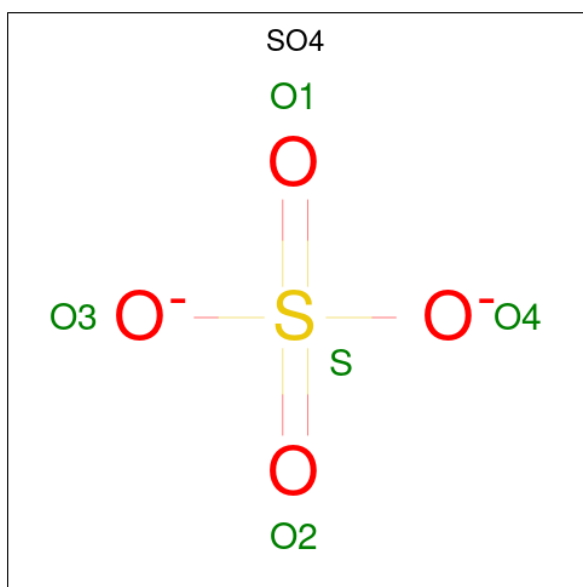
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	814	Total	C	N	O	P	S	0	0	0
			6635	4225	1175	1204	1	30			
1	B	815	Total	C	N	O	P	S	0	0	0
			6642	4230	1176	1205	1	30			
1	C	802	Total	C	N	O	P	S	0	0	0
			6536	4165	1155	1186	1	29			
1	D	815	Total	C	N	O	P	S	0	0	0
			6643	4229	1176	1207	1	30			
1	E	803	Total	C	N	O	P	S	0	0	0
			6545	4170	1156	1189	1	29			
1	F	813	Total	C	N	O	P	S	0	0	0
			6626	4220	1173	1202	1	30			
1	G	814	Total	C	N	O	P	S	0	0	0
			6635	4225	1175	1204	1	30			
1	H	814	Total	C	N	O	P	S	0	0	0
			6636	4224	1175	1206	1	30			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total	O	0	0
			56	56		
4	B	32	Total	O	0	0
			32	32		
4	C	36	Total	O	0	0
			36	36		
4	D	62	Total	O	0	0
			62	62		
4	E	27	Total	O	0	0
			27	27		
4	F	38	Total	O	0	0
			38	38		
4	G	69	Total	O	0	0
			69	69		
4	H	30	Total	O	0	0
			30	30		

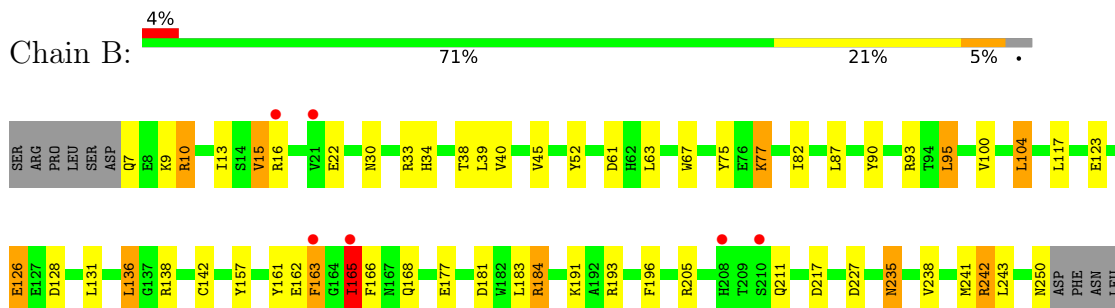
3 Residue-property plots

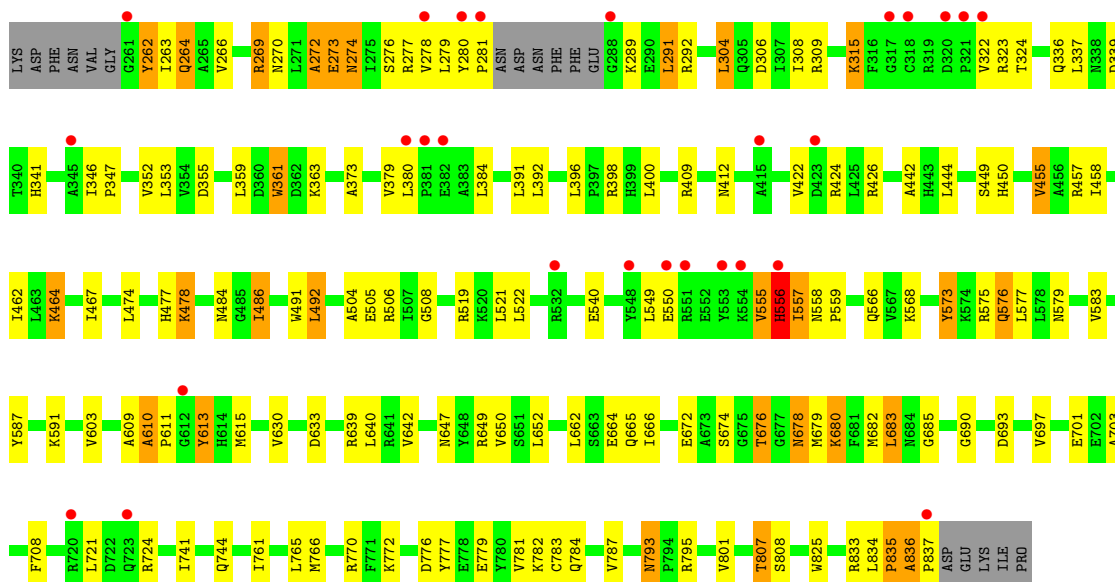
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

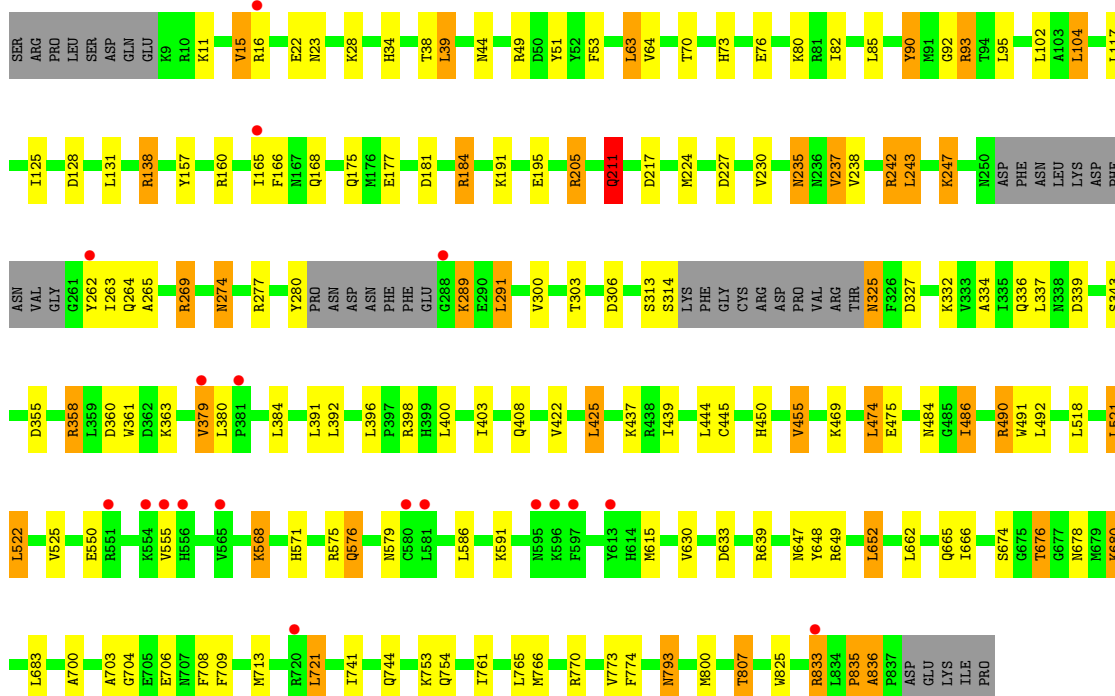
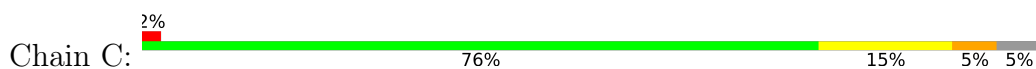


- Molecule 1: Glycogen phosphorylase, muscle form

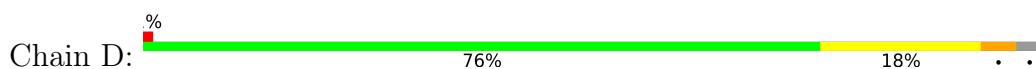


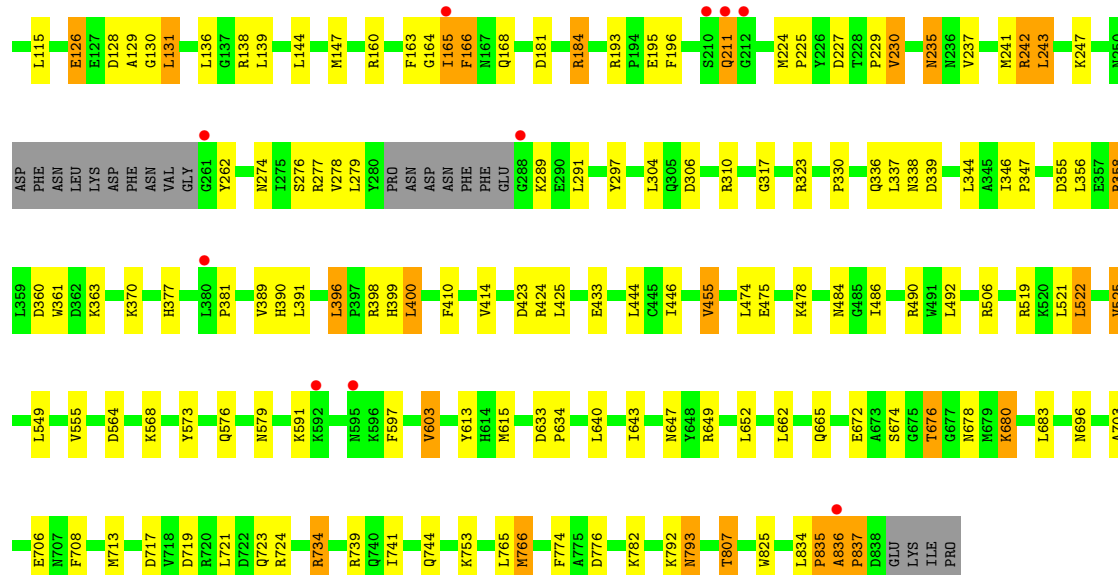


• Molecule 1: Glycogen phosphorylase, muscle form

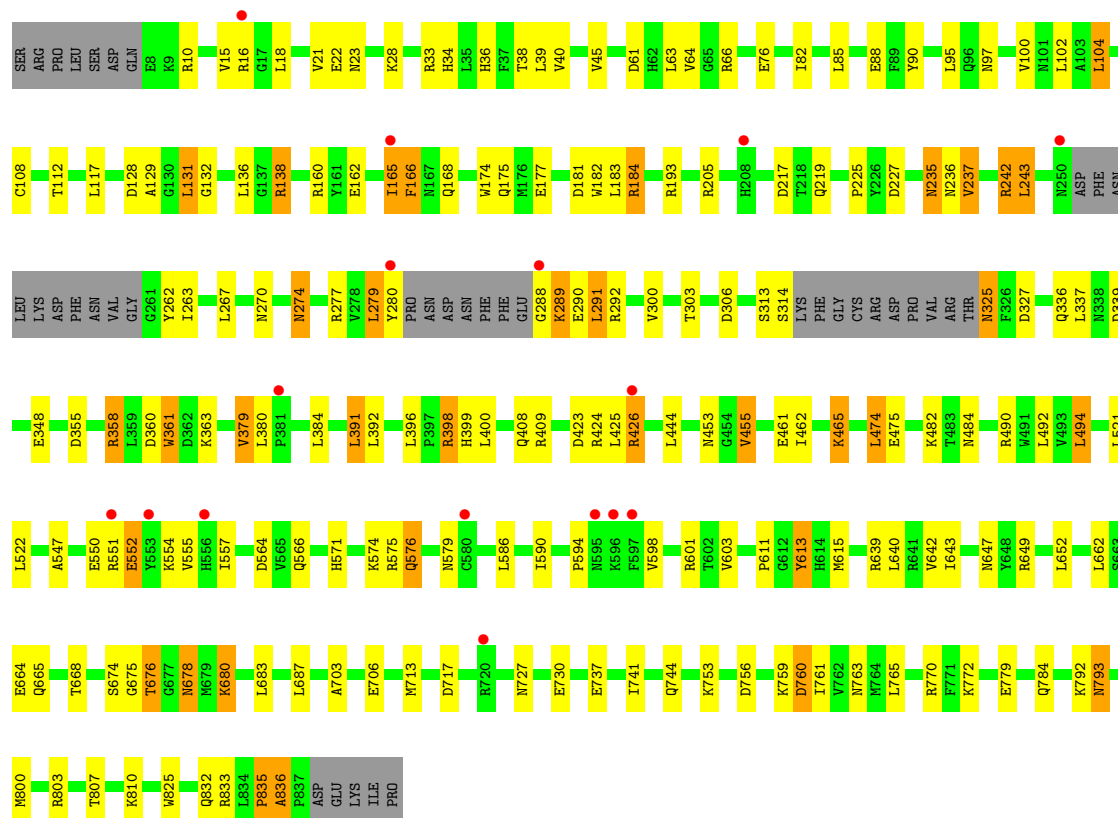


• Molecule 1: Glycogen phosphorylase, muscle form

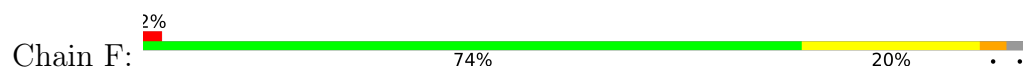


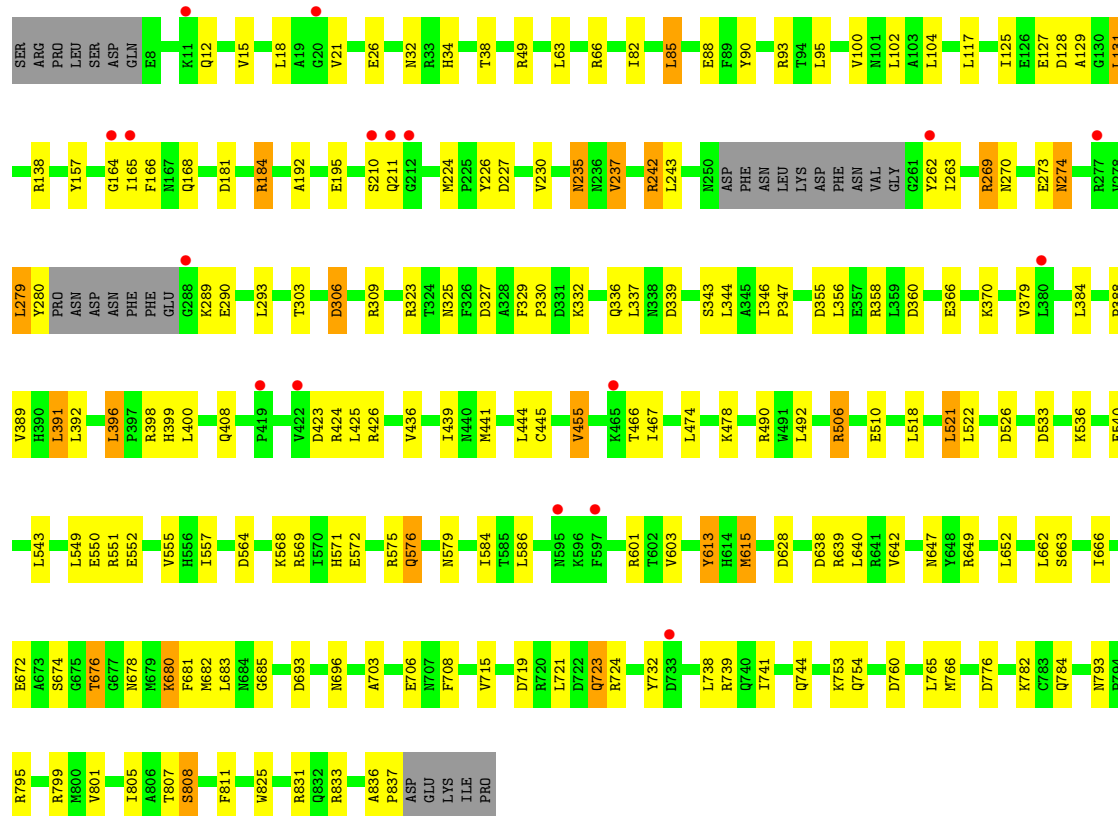


• Molecule 1: Glycogen phosphorylase, muscle form

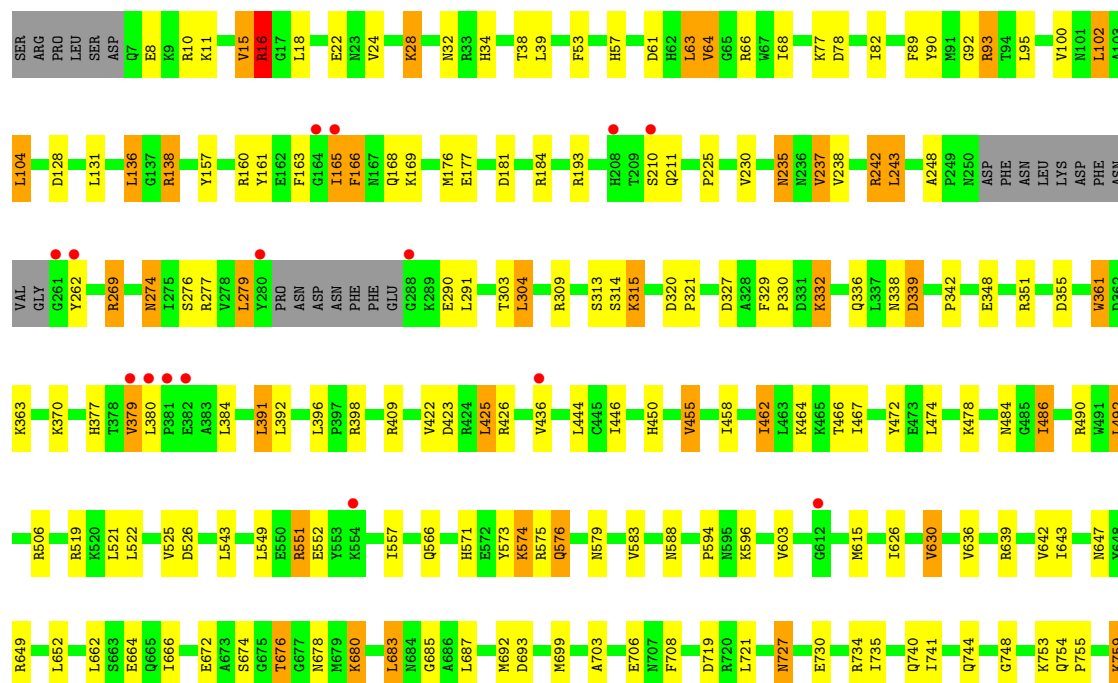
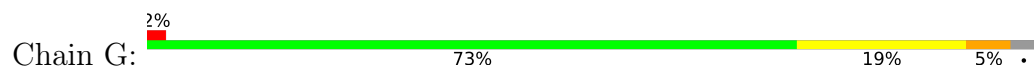


• Molecule 1: Glycogen phosphorylase, muscle form



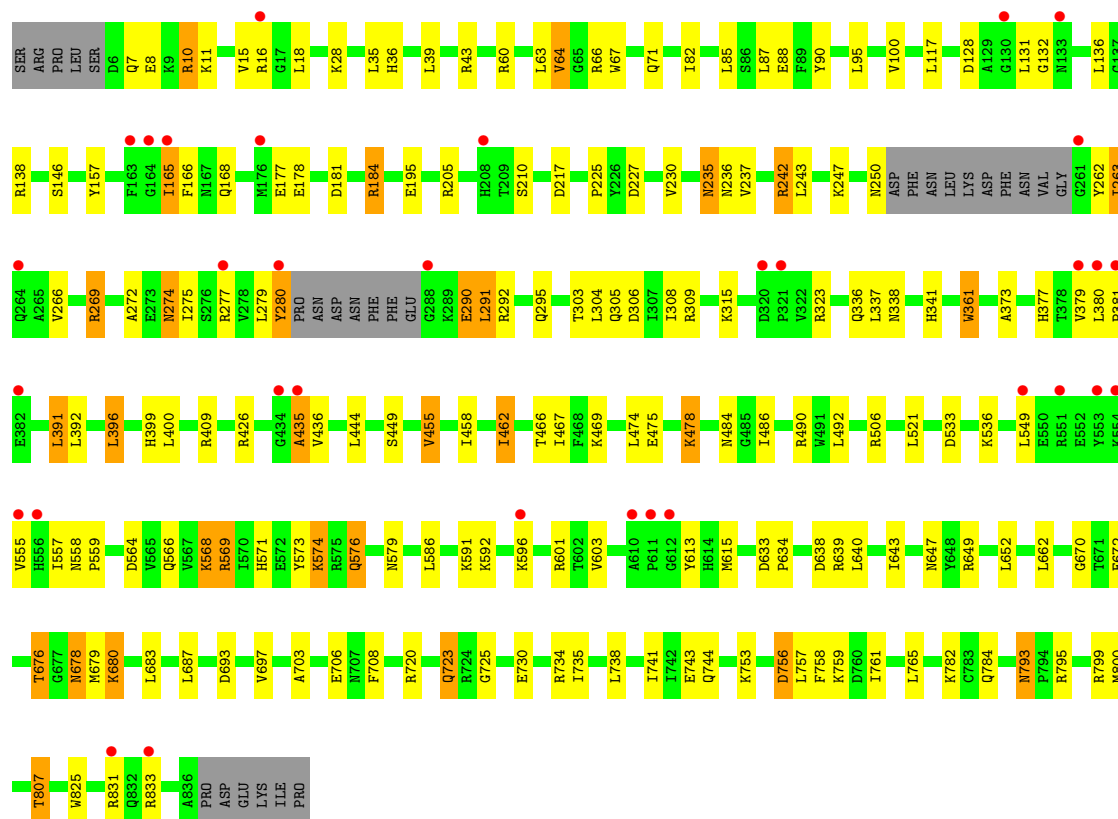
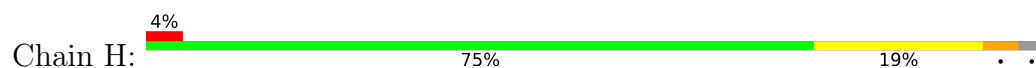


• Molecule 1: Glycogen phosphorylase, muscle form





- Molecule 1: Glycogen phosphorylase, muscle form



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.02Å 188.08Å 175.91Å 90.00° 108.92° 90.00°	Depositor
Resolution (Å)	29.79 – 2.70 29.79 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.79-2.70) 94.2 (29.79-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.256 0.193 , 0.255	Depositor DCC
R_{free} test set	9450 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53512	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 74.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5777e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, LLP, AMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/6756	0.65	2/9137 (0.0%)
1	B	0.44	0/6764	0.62	2/9149 (0.0%)
1	C	0.44	0/6654	0.61	0/8999
1	D	0.46	0/6764	0.64	3/9148 (0.0%)
1	E	0.44	0/6663	0.61	1/9011 (0.0%)
1	F	0.46	0/6747	0.63	0/9125
1	G	0.47	0/6756	0.66	1/9137 (0.0%)
1	H	0.44	0/6756	0.61	0/9136
All	All	0.45	0/53860	0.63	9/72842 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	LEU	CA-CB-CG	6.06	129.23	115.30
1	G	136	LEU	CA-CB-CG	5.78	128.58	115.30
1	A	136	LEU	CA-CB-CG	5.67	128.34	115.30
1	D	400	LEU	CA-CB-CG	5.53	128.02	115.30
1	B	556	HIS	CB-CA-C	5.50	121.39	110.40
1	D	136	LEU	CA-CB-CG	5.39	127.70	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	136	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	392	LEU	CA-CB-CG	5.14	127.12	115.30
1	D	85	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	454	GLY	Peptide
1	H	7	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6635	0	6598	107	0
1	B	6642	0	6605	125	0
1	C	6536	0	6500	88	0
1	D	6643	0	6602	81	0
1	E	6545	0	6506	102	0
1	F	6626	0	6590	90	0
1	G	6635	0	6598	120	0
1	H	6636	0	6595	103	0
2	A	23	0	12	1	0
2	B	23	0	12	2	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
2	E	23	0	12	0	0
2	F	23	0	12	0	0
2	G	23	0	12	1	0
2	H	23	0	12	1	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	10	0	0	1	0
3	H	10	0	0	0	0
4	A	56	0	0	1	0
4	B	32	0	0	1	0
4	C	36	0	0	3	0
4	D	62	0	0	1	0
4	E	27	0	0	2	0
4	F	38	0	0	0	0
4	G	69	0	0	1	0
4	H	30	0	0	3	0
All	All	53512	0	52690	793	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 7.

All (793) 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:C:274:ASN:HA	1:C:277:ARG:HG3	1.34	1.09
1:G:274:ASN:HA	1:G:277:ARG:HG3	1.42	1.01
1:D:336:GLN:HE21	1:D:825:TRP:HE1	0.99	0.98
1:H:336:GLN:HE21	1:H:825:TRP:HE1	1.08	0.94
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.48	0.92
1:G:168:GLN:HE21	1:G:647:ASN:H	1.17	0.92
1:E:336:GLN:HE21	1:E:825:TRP:HE1	1.17	0.92
1:A:274:ASN:HA	1:A:277:ARG:HG3	1.53	0.91
1:B:336:GLN:NE2	1:B:825:TRP:HE1	1.70	0.89
1:C:168:GLN:HE21	1:C:647:ASN:H	1.19	0.89
1:F:168:GLN:HE21	1:F:647:ASN:H	1.21	0.89
1:B:168:GLN:HE21	1:B:647:ASN:H	1.20	0.88
1:F:336:GLN:HE21	1:F:825:TRP:HE1	1.17	0.88
1:B:165:ILE:HG23	1:B:166:PHE:H	1.40	0.86
1:H:336:GLN:NE2	1:H:825:TRP:HE1	1.73	0.86
1:B:278:VAL:HG22	1:B:279:LEU:O	1.77	0.85
1:D:336:GLN:NE2	1:D:825:TRP:HE1	1.72	0.85
1:C:703:ALA:HA	1:C:807:THR:HG21	1.58	0.85
1:B:280:TYR:OH	1:B:291:LEU:HD12	1.78	0.84
1:A:615:MET:CE	1:A:761:ILE:HG12	2.08	0.84
1:F:336:GLN:NE2	1:F:825:TRP:HE1	1.76	0.83
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.44	0.82
1:D:21:VAL:HB	1:D:26:GLU:HG3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:703:ALA:HA	1:F:807:THR:HG21	1.61	0.82
1:C:22:GLU:OE1	1:C:104:LEU:HD11	1.78	0.81
1:C:336:GLN:HE21	1:C:825:TRP:HE1	1.27	0.81
1:F:455:VAL:HG13	1:F:674:SER:HB2	1.61	0.81
1:B:703:ALA:HA	1:B:807:THR:HG21	1.61	0.80
1:H:85:LEU:HD21	1:H:303:THR:HG21	1.64	0.80
1:F:672:GLU:HB2	1:F:693:ASP:OD2	1.82	0.79
1:C:92:GLY:O	1:C:93:ARG:HB2	1.81	0.79
1:G:336:GLN:HE21	1:G:825:TRP:HE1	1.29	0.79
1:D:168:GLN:HE21	1:D:647:ASN:H	1.31	0.79
1:A:336:GLN:HE21	1:A:825:TRP:HE1	1.30	0.78
1:H:676:THR:HG22	1:H:680:LLP:H5'1	1.63	0.78
1:G:615:MET:CE	1:G:761:ILE:HG12	2.14	0.78
1:C:676:THR:HG22	1:C:680:LLP:H5'1	1.65	0.77
1:E:336:GLN:NE2	1:E:825:TRP:HE1	1.81	0.77
1:F:168:GLN:NE2	1:F:647:ASN:H	1.81	0.77
1:G:168:GLN:NE2	1:G:647:ASN:H	1.81	0.77
1:H:615:MET:CE	1:H:761:ILE:HG12	2.14	0.76
1:B:87:LEU:HD12	1:B:341:HIS:HB3	1.66	0.75
1:C:568:LYS:HD2	1:C:680:LLP:OP2	1.87	0.75
1:H:165:ILE:CG2	1:H:166:PHE:H	1.99	0.75
1:H:676:THR:HG21	4:H:909:HOH:O	1.87	0.74
1:C:336:GLN:NE2	1:C:825:TRP:HE1	1.85	0.74
1:B:250:ASN:HD21	1:B:269:ARG:HH21	1.36	0.74
1:H:615:MET:HE2	1:H:761:ILE:HG12	1.67	0.74
1:D:455:VAL:HG13	1:D:674:SER:HB2	1.69	0.74
1:G:269:ARG:HG2	1:G:269:ARG:HH11	1.53	0.73
1:D:522:LEU:O	1:D:525:VAL:HG23	1.88	0.73
1:H:168:GLN:HE21	1:H:647:ASN:H	1.37	0.73
1:C:455:VAL:HG13	1:C:674:SER:HB2	1.69	0.72
1:H:703:ALA:HA	1:H:807:THR:HG21	1.71	0.72
1:B:336:GLN:HE21	1:B:825:TRP:HE1	1.35	0.72
1:A:455:VAL:HG13	1:A:674:SER:HB2	1.71	0.71
1:C:450:HIS:HE1	4:C:879:HOH:O	1.71	0.71
1:A:85:LEU:HD21	1:A:303:THR:HG21	1.71	0.71
1:A:336:GLN:NE2	1:A:825:TRP:HE1	1.89	0.71
1:A:455:VAL:HG22	1:A:484:ASN:OD1	1.91	0.71
1:E:66:ARG:HD3	1:E:236:ASN:OD1	1.90	0.71
1:E:174:TRP:CD2	1:H:435:ALA:HB2	2.26	0.70
1:G:309:ARG:NH2	2:G:843:AMP:O1P	2.24	0.70
1:B:165:ILE:HG23	1:B:166:PHE:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ILE:O	1:B:266:VAL:HG23	1.91	0.70
1:E:703:ALA:HA	1:E:807:THR:HG21	1.73	0.70
1:E:274:ASN:HA	1:E:277:ARG:HG3	1.73	0.70
1:H:280:TYR:OH	1:H:291:LEU:HD13	1.91	0.70
1:G:355:ASP:OD2	1:G:398:ARG:HD3	1.92	0.69
1:A:93:ARG:O	1:A:490:ARG:NH2	2.23	0.69
1:H:138:ARG:HG3	4:H:909:HOH:O	1.93	0.69
1:G:703:ALA:HA	1:G:807:THR:HG21	1.74	0.69
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.57	0.69
1:A:677:GLY:N	1:A:680:LLP:OP1	2.27	0.68
1:D:555:VAL:HG21	1:D:643:ILE:HD11	1.75	0.68
1:A:676:THR:HG22	1:A:680:LLP:H5'1	1.75	0.68
1:D:66:ARG:CG	1:D:66:ARG:HH11	2.06	0.68
1:C:168:GLN:NE2	1:C:647:ASN:H	1.91	0.68
1:G:15:VAL:HA	1:G:18:LEU:HD12	1.74	0.68
1:H:181:ASP:O	1:H:184:ARG:HD2	1.94	0.68
1:G:269:ARG:HG2	1:G:269:ARG:NH1	2.08	0.68
1:B:262:TYR:HB3	1:B:264:GLN:HG2	1.76	0.68
1:D:66:ARG:HH11	1:D:66:ARG:HG2	1.57	0.67
1:D:235:ASN:HD22	1:D:235:ASN:H	1.41	0.67
1:E:227:ASP:OD1	1:E:242:ARG:HD2	1.93	0.67
1:F:355:ASP:OD2	1:F:398:ARG:HD3	1.92	0.67
1:E:557:ILE:HD11	1:E:643:ILE:HD11	1.76	0.67
1:A:168:GLN:HE21	1:A:647:ASN:H	1.41	0.67
1:H:678:ASN:HD22	1:H:679:MET:H	1.41	0.67
1:H:227:ASP:OD1	1:H:242:ARG:HD3	1.93	0.67
1:A:703:ALA:HA	1:A:807:THR:HG21	1.75	0.66
1:G:557:ILE:HD11	1:G:643:ILE:CD1	2.25	0.66
1:H:263:ILE:O	1:H:266:VAL:HG23	1.95	0.66
1:B:181:ASP:O	1:B:184:ARG:HD2	1.95	0.66
1:E:676:THR:HG22	1:E:680:LLP:H5'2	1.76	0.66
1:G:526:ASP:OD1	1:G:799:ARG:NH1	2.28	0.66
1:H:678:ASN:HD22	1:H:679:MET:N	1.94	0.66
1:G:336:GLN:NE2	1:G:825:TRP:HE1	1.94	0.66
1:F:21:VAL:HB	1:F:26:GLU:HG3	1.78	0.66
1:G:615:MET:HE1	1:G:761:ILE:HG12	1.76	0.66
1:B:168:GLN:NE2	1:B:647:ASN:H	1.93	0.66
1:A:138:ARG:O	1:A:138:ARG:HG3	1.96	0.65
1:E:97:ASN:HA	1:E:494:LEU:HD11	1.78	0.65
1:E:675:GLY:O	1:E:678:ASN:ND2	2.26	0.65
1:C:34:HIS:HD2	1:C:38:THR:OG1	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLU:HG2	1:A:391:LEU:HD21	1.77	0.65
1:B:361:TRP:CZ3	1:B:409:ARG:HD2	2.32	0.65
1:G:450:HIS:HE1	4:G:879:HOH:O	1.78	0.65
1:G:235:ASN:HD22	1:G:237:VAL:H	1.42	0.65
1:A:568:LYS:HE2	1:A:665:GLN:OE1	1.96	0.65
1:F:235:ASN:HD22	1:F:235:ASN:H	1.43	0.65
1:G:93:ARG:O	1:G:490:ARG:NH2	2.29	0.65
1:A:227:ASP:OD1	1:A:242:ARG:HD3	1.96	0.65
1:E:193:ARG:HB2	1:E:225:PRO:HG2	1.78	0.65
1:E:455:VAL:HG13	1:E:674:SER:HB2	1.79	0.64
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.80	0.64
1:C:615:MET:HE1	1:C:761:ILE:HG12	1.80	0.64
1:E:551:ARG:O	1:E:552:GLU:HG2	1.98	0.64
1:F:227:ASP:OD1	1:F:242:ARG:HD3	1.98	0.63
1:G:615:MET:HE2	1:G:761:ILE:HG12	1.80	0.63
1:B:306:ASP:OD1	1:B:309:ARG:NH1	2.32	0.63
1:G:676:THR:HG22	1:G:680:LLP:H5'1	1.80	0.63
1:H:564:ASP:HB3	1:H:603:VAL:HA	1.80	0.63
1:E:280:TYR:OH	1:E:291:LEU:HD13	1.99	0.63
1:H:205:ARG:NH1	1:H:217:ASP:OD2	2.32	0.63
1:A:526:ASP:OD1	1:A:799:ARG:NH1	2.31	0.63
1:E:325:ASN:HD22	1:E:327:ASP:H	1.45	0.63
1:G:361:TRP:CZ3	1:G:409:ARG:HD2	2.33	0.63
1:B:9:LYS:HA	4:B:856:HOH:O	1.98	0.63
1:B:676:THR:HG22	1:B:680:LLP:H5'1	1.80	0.62
1:E:676:THR:HG22	1:E:680:LLP:C5'	2.29	0.62
1:B:235:ASN:HA	1:B:833:ARG:HG2	1.80	0.62
1:G:792:LYS:O	1:G:794:PRO:HD3	1.99	0.62
1:H:165:ILE:HG23	1:H:166:PHE:H	1.62	0.62
1:H:568:LYS:HG3	1:H:574:LYS:HG2	1.81	0.62
1:E:28:LYS:NZ	1:F:12:GLN:HE22	1.97	0.62
1:E:129:ALA:HB1	1:E:131:LEU:HD22	1.81	0.62
1:F:343:SER:HB3	1:F:445:CYS:SG	2.39	0.62
1:G:557:ILE:HD11	1:G:643:ILE:HD11	1.81	0.62
1:E:160:ARG:HB2	1:E:243:LEU:HB3	1.79	0.62
1:H:305:GLN:HG3	4:H:927:HOH:O	1.99	0.62
1:F:615:MET:HA	1:F:615:MET:CE	2.30	0.62
1:E:21:VAL:HB	1:E:23:ASN:HD22	1.64	0.62
1:E:34:HIS:HD2	1:E:38:THR:OG1	1.83	0.62
1:F:21:VAL:HB	1:F:26:GLU:CG	2.29	0.61
1:B:281:PRO:HB3	1:B:611:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASP:O	1:A:184:ARG:HD2	2.01	0.61
1:A:168:GLN:NE2	1:A:647:ASN:H	1.98	0.61
1:G:138:ARG:O	1:G:138:ARG:HD3	2.01	0.61
1:H:756:ASP:O	1:H:758:PHE:N	2.34	0.61
1:F:235:ASN:HA	1:F:833:ARG:HG2	1.83	0.61
1:F:550:GLU:C	1:F:552:GLU:H	2.04	0.61
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.83	0.60
1:D:344:LEU:O	1:D:347:PRO:HD2	2.01	0.60
1:A:325:ASN:HD21	1:A:327:ASP:HB2	1.65	0.60
1:C:85:LEU:HD21	1:C:303:THR:HG21	1.81	0.60
1:E:615:MET:HE3	1:E:761:ILE:HG12	1.83	0.60
1:G:594:PRO:O	1:G:639:ARG:NH2	2.27	0.60
1:G:34:HIS:HD2	1:G:38:THR:OG1	1.83	0.60
1:G:161:TYR:HA	1:G:276:SER:O	2.02	0.60
1:G:741:ILE:HA	1:G:744:GLN:HE21	1.65	0.60
1:F:571:HIS:H	1:F:576:GLN:NE2	2.00	0.60
1:H:165:ILE:HG23	1:H:166:PHE:N	2.16	0.60
1:E:88:GLU:HG2	1:E:132:GLY:HA2	1.83	0.60
1:E:102:LEU:HB3	1:E:104:LEU:HD22	1.83	0.60
1:D:713:MET:HB3	1:D:717:ASP:HB2	1.83	0.60
1:B:355:ASP:OD2	1:B:398:ARG:HD3	2.02	0.59
1:F:506:ARG:NH2	1:F:533:ASP:OD2	2.34	0.59
1:B:161:TYR:HA	1:B:276:SER:O	2.01	0.59
1:B:549:LEU:HD23	1:B:557:ILE:HG13	1.84	0.59
1:C:93:ARG:O	1:C:490:ARG:NH2	2.34	0.59
1:C:265:ALA:O	1:C:269:ARG:HB3	2.03	0.59
1:F:518:LEU:O	1:F:521:LEU:HB2	2.02	0.59
1:C:235:ASN:H	1:C:235:ASN:HD22	1.50	0.59
1:G:269:ARG:HH11	1:G:269:ARG:CG	2.16	0.59
1:H:165:ILE:CG2	1:H:166:PHE:N	2.64	0.59
1:A:36:HIS:CD2	1:B:15:VAL:HG22	2.38	0.59
1:G:466:THR:OG1	1:G:467:ILE:HD12	2.03	0.59
1:H:227:ASP:OD1	1:H:242:ARG:CD	2.51	0.59
1:D:741:ILE:HA	1:D:744:GLN:HE21	1.68	0.58
1:E:174:TRP:CG	1:H:435:ALA:HB2	2.37	0.58
1:G:15:VAL:HG13	1:H:36:HIS:CD2	2.37	0.58
1:B:672:GLU:HB2	1:B:693:ASP:OD2	2.03	0.58
1:B:235:ASN:H	1:B:235:ASN:HD22	1.51	0.58
1:G:64:VAL:O	1:G:68:ILE:HG12	2.04	0.58
1:G:748:GLY:HA3	1:G:755:PRO:HA	1.86	0.58
1:H:467:ILE:HD12	1:H:467:ILE:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:ILE:HB	1:F:347:PRO:HD3	1.85	0.58
1:B:346:ILE:HB	1:B:347:PRO:HD3	1.85	0.58
1:E:279:LEU:HD22	1:E:280:TYR:H	1.67	0.58
1:F:738:LEU:HD12	1:F:741:ILE:HD11	1.85	0.58
1:C:211:GLN:HG2	1:C:358:ARG:NH1	2.19	0.57
1:G:676:THR:CG2	1:G:680:LLP:H4'1	2.33	0.57
1:D:64:VAL:O	1:D:68:ILE:HG12	2.04	0.57
1:H:250:ASN:HD21	1:H:269:ARG:HH21	1.50	0.57
1:D:34:HIS:HD2	1:D:38:THR:OG1	1.87	0.57
1:B:834:LEU:HG	1:B:835:PRO:HD2	1.87	0.57
1:D:739:ARG:HH11	1:D:739:ARG:HG3	1.69	0.57
1:H:455:VAL:HG13	1:H:484:ASN:ND2	2.20	0.57
1:H:703:ALA:CA	1:H:807:THR:HG21	2.34	0.57
1:A:730:GLU:HB3	1:A:734:ARG:HH12	1.68	0.57
1:G:235:ASN:ND2	1:G:237:VAL:H	2.02	0.57
1:H:8:GLU:O	1:H:11:LYS:HG2	2.05	0.57
1:E:181:ASP:OD2	1:E:184:ARG:HB3	2.05	0.57
1:E:355:ASP:OD2	1:E:398:ARG:HD3	2.05	0.57
1:G:34:HIS:HE1	1:G:61:ASP:OD2	1.87	0.57
1:A:793:ASN:C	1:A:793:ASN:HD22	2.09	0.56
1:F:741:ILE:HA	1:F:744:GLN:HE21	1.70	0.56
1:B:615:MET:CE	1:B:761:ILE:HG12	2.35	0.56
1:C:474:LEU:HD13	1:C:475:GLU:HG3	1.87	0.56
1:H:458:ILE:O	1:H:462:ILE:HG23	2.05	0.56
1:A:157:TYR:CE2	1:A:242:ARG:HG2	2.41	0.56
1:A:557:ILE:HD11	1:A:643:ILE:HD11	1.87	0.56
1:F:85:LEU:HD21	1:F:303:THR:HG21	1.87	0.56
1:H:361:TRP:CZ3	1:H:409:ARG:HD2	2.40	0.56
1:B:241:MET:HG2	1:B:243:LEU:HD13	1.87	0.56
1:G:269:ARG:HH22	1:H:277:ARG:CZ	2.18	0.56
1:G:793:ASN:C	1:G:793:ASN:HD22	2.09	0.56
1:D:52:TYR:CZ	1:D:126:GLU:HB3	2.41	0.56
1:H:615:MET:HE1	1:H:761:ILE:HG12	1.87	0.56
1:D:102:LEU:HB3	1:D:104:LEU:HD22	1.87	0.55
1:D:703:ALA:HA	1:D:807:THR:HG21	1.88	0.55
1:F:564:ASP:HB3	1:F:603:VAL:HA	1.88	0.55
1:A:680:LLP:NZ	1:A:680:LLP:O3	2.37	0.55
1:D:241:MET:HG2	1:D:243:LEU:HD13	1.86	0.55
1:B:87:LEU:HD12	1:B:341:HIS:CB	2.36	0.55
1:G:446:ILE:O	1:G:478:LYS:HE3	2.07	0.55
1:G:455:VAL:HG22	1:G:484:ASN:OD1	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:HH11	1:A:16:ARG:CG	2.14	0.55
1:B:379:VAL:HG13	1:B:380:LEU:HG	1.88	0.55
1:C:224:MET:SD	1:C:247:LYS:NZ	2.79	0.55
1:B:227:ASP:OD1	1:B:242:ARG:HD3	2.07	0.55
1:E:33:ARG:HG3	1:F:18:LEU:HD22	1.88	0.55
1:F:723:GLN:O	1:F:723:GLN:HG2	2.06	0.55
1:G:34:HIS:CD2	1:G:38:THR:OG1	2.59	0.55
1:G:338:ASN:OD1	1:G:377:HIS:NE2	2.37	0.55
1:G:730:GLU:HB3	1:G:734:ARG:HH22	1.71	0.55
1:D:355:ASP:OD2	1:D:398:ARG:HD3	2.06	0.55
1:E:423:ASP:O	1:E:426:ARG:HD3	2.07	0.55
1:H:338:ASN:ND2	1:H:377:HIS:NE2	2.55	0.55
1:C:235:ASN:CG	1:C:237:VAL:HG13	2.27	0.55
1:A:525:VAL:O	1:A:799:ARG:HD2	2.07	0.55
1:C:227:ASP:OD1	1:C:242:ARG:CD	2.55	0.55
1:E:274:ASN:C	1:E:274:ASN:HD22	2.10	0.54
1:F:682:MET:HE1	1:F:811:PHE:CD2	2.42	0.54
1:H:138:ARG:O	1:H:138:ARG:HD3	2.08	0.54
1:H:290:GLU:HG2	1:H:391:LEU:HD21	1.88	0.54
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.90	0.54
1:D:224:MET:SD	1:D:247:LYS:NZ	2.77	0.54
1:H:569:ARG:NH2	1:H:571:HIS:HD2	2.05	0.54
1:A:557:ILE:HD11	1:A:643:ILE:CD1	2.38	0.54
1:B:93:ARG:HG2	1:B:126:GLU:HG3	1.88	0.54
1:C:591:LYS:HE3	1:C:633:ASP:OD2	2.07	0.54
1:H:672:GLU:HB2	1:H:693:ASP:OD2	2.07	0.54
1:B:609:ALA:O	1:B:610:ALA:HB3	2.07	0.54
1:C:227:ASP:OD1	1:C:242:ARG:HD2	2.07	0.54
1:D:344:LEU:C	1:D:347:PRO:HD2	2.28	0.54
1:A:703:ALA:CA	1:A:807:THR:HG21	2.37	0.54
1:E:168:GLN:HE21	1:E:647:ASN:H	1.55	0.54
1:F:676:THR:HG22	1:F:680:LLP:H5'1	1.90	0.54
1:E:615:MET:HE1	1:E:761:ILE:HA	1.89	0.54
1:E:97:ASN:CA	1:E:494:LEU:HD11	2.38	0.54
1:D:676:THR:HG22	1:D:680:LLP:H5'1	1.89	0.54
1:C:343:SER:HB2	1:C:445:CYS:SG	2.48	0.54
1:G:795:ARG:O	1:G:799:ARG:HG3	2.08	0.54
1:H:250:ASN:ND2	1:H:269:ARG:HH21	2.06	0.54
1:A:227:ASP:OD1	1:A:242:ARG:CD	2.55	0.54
1:A:280:TYR:OH	1:A:291:LEU:CD1	2.56	0.53
1:C:235:ASN:HA	1:C:833:ARG:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:836:ALA:HB1	1:D:837:PRO:HD2	1.89	0.53
1:E:235:ASN:CG	1:E:237:VAL:HG13	2.27	0.53
1:G:248:ALA:CB	1:G:269:ARG:HG3	2.38	0.53
1:H:557:ILE:HD11	1:H:643:ILE:HD12	1.90	0.53
1:A:355:ASP:OD2	1:A:398:ARG:HD3	2.09	0.53
1:B:835:PRO:O	1:B:836:ALA:HB2	2.07	0.53
1:C:741:ILE:HA	1:C:744:GLN:HE21	1.74	0.53
1:D:399:HIS:HD2	4:D:851:HOH:O	1.90	0.53
1:E:348:GLU:OE1	1:E:399:HIS:HE1	1.91	0.53
1:F:157:TYR:CE2	1:F:242:ARG:HG2	2.43	0.53
1:G:730:GLU:HB3	1:G:734:ARG:NH2	2.22	0.53
1:C:205:ARG:NH1	1:C:217:ASP:OD2	2.40	0.53
1:D:193:ARG:HB3	1:D:196:PHE:HD2	1.74	0.53
1:E:235:ASN:HA	1:E:833:ARG:HG2	1.90	0.53
1:E:235:ASN:H	1:E:235:ASN:HD22	1.55	0.53
1:E:803:ARG:O	1:E:807:THR:HG22	2.08	0.53
1:B:384:LEU:HD23	1:B:442:ALA:HB2	1.90	0.53
1:E:687:LEU:HD22	1:E:800:MET:HE2	1.89	0.53
1:H:157:TYR:CE2	1:H:242:ARG:HG2	2.44	0.53
1:C:615:MET:HE3	1:C:615:MET:HA	1.91	0.53
1:F:549:LEU:HB3	1:F:557:ILE:HG13	1.91	0.53
3:G:844:SO4:O4	1:H:43:ARG:NH1	2.39	0.53
1:G:549:LEU:HD23	1:G:557:ILE:HG13	1.91	0.53
1:B:315:LYS:CE	1:B:322:VAL:HG11	2.39	0.52
1:B:583:VAL:HG11	1:B:642:VAL:HG21	1.91	0.52
1:C:90:TYR:CE2	1:C:680:LLP:H2'3	2.44	0.52
1:G:455:VAL:HG13	1:G:674:SER:HB2	1.91	0.52
1:G:703:ALA:CA	1:G:807:THR:HG21	2.38	0.52
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.91	0.52
1:B:87:LEU:CD1	1:B:341:HIS:HB3	2.35	0.52
1:D:793:ASN:C	1:D:793:ASN:HD22	2.13	0.52
1:F:306:ASP:OD1	1:F:309:ARG:NH1	2.42	0.52
1:G:467:ILE:HD12	1:G:467:ILE:H	1.73	0.52
1:A:727:ASN:ND2	1:A:729:GLN:H	2.05	0.52
1:B:138:ARG:HH11	1:B:491:TRP:HE1	1.57	0.52
1:B:315:LYS:HE2	1:B:322:VAL:HG11	1.91	0.52
1:B:504:ALA:HA	1:B:508:GLY:O	2.10	0.52
1:C:518:LEU:O	1:C:521:LEU:HB2	2.10	0.52
1:E:760:ASP:HA	1:E:763:ASN:HB2	1.92	0.52
1:H:741:ILE:HA	1:H:744:GLN:HE21	1.74	0.52
1:B:455:VAL:HG12	1:B:674:SER:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.92	0.52
1:C:835:PRO:O	1:C:836:ALA:HB2	2.10	0.52
1:D:168:GLN:NE2	1:D:647:ASN:H	2.02	0.52
1:G:379:VAL:HG13	1:G:380:LEU:HG	1.92	0.52
1:B:373:ALA:HA	1:B:449:SER:HB3	1.92	0.51
1:C:648:TYR:HA	1:C:652:LEU:HD12	1.92	0.51
1:D:410:PHE:O	1:D:414:VAL:HG23	2.09	0.51
1:D:446:ILE:O	1:D:478:LYS:HE3	2.09	0.51
1:G:685:GLY:HA2	1:G:801:VAL:HG13	1.92	0.51
1:H:466:THR:OG1	1:H:467:ILE:HD12	2.09	0.51
1:D:836:ALA:HB1	1:D:837:PRO:CD	2.41	0.51
1:F:575:ARG:HD3	1:F:666:ILE:O	2.10	0.51
1:B:273:GLU:HB3	1:B:277:ARG:NH2	2.26	0.51
1:B:309:ARG:NH2	2:B:843:AMP:OI1P	2.43	0.51
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.91	0.51
1:B:575:ARG:HH22	1:B:776:ASP:HB2	1.74	0.51
1:G:290:GLU:HG2	1:G:391:LEU:HD21	1.93	0.51
1:A:193:ARG:HB3	1:A:196:PHE:HD2	1.75	0.51
1:A:403:ILE:HG21	1:A:439:ILE:HD13	1.93	0.51
1:B:450:HIS:O	1:B:478:LYS:HG2	2.11	0.51
1:G:687:LEU:HD13	1:G:800:MET:HE1	1.92	0.51
1:H:591:LYS:HE3	1:H:633:ASP:OD2	2.11	0.51
1:B:272:ALA:O	1:B:274:ASN:N	2.44	0.51
1:E:168:GLN:HG3	1:E:175:GLN:HG3	1.92	0.51
1:G:583:VAL:HG11	1:G:642:VAL:HG21	1.91	0.51
1:G:721:LEU:HD23	1:G:772:LYS:HD3	1.93	0.51
1:H:235:ASN:H	1:H:235:ASN:HD22	1.58	0.51
1:C:263:ILE:HG13	1:C:263:ILE:O	2.11	0.51
1:A:289:LYS:HD3	1:A:289:LYS:N	2.25	0.51
1:G:766:MET:CE	1:G:774:PHE:HE2	2.24	0.51
1:F:88:GLU:HG2	1:F:279:LEU:HD11	1.93	0.50
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.92	0.50
1:C:15:VAL:HG13	1:D:36:HIS:CD2	2.46	0.50
1:E:575:ARG:HD2	1:E:668:THR:OG1	2.11	0.50
1:G:32:ASN:HB3	1:H:18:LEU:HD11	1.93	0.50
1:E:21:VAL:HB	1:E:23:ASN:ND2	2.26	0.50
1:A:575:ARG:HD3	1:A:666:ILE:O	2.10	0.50
1:A:727:ASN:C	1:A:727:ASN:HD22	2.14	0.50
1:B:165:ILE:CG2	1:B:166:PHE:N	2.74	0.50
1:C:211:GLN:HE21	1:C:211:GLN:HA	1.76	0.50
1:H:306:ASP:OD1	1:H:309:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:458:ILE:HG13	1:H:697:VAL:HG21	1.92	0.50
1:B:591:LYS:HE3	1:B:633:ASP:OD2	2.11	0.50
1:C:181:ASP:O	1:C:184:ARG:HD2	2.11	0.50
1:E:603:VAL:HG22	1:E:642:VAL:HG22	1.94	0.50
1:C:138:ARG:HH11	1:C:491:TRP:HE1	1.60	0.50
1:G:313:SER:O	1:G:315:LYS:N	2.45	0.50
1:H:738:LEU:HD12	1:H:741:ILE:HD11	1.93	0.50
1:A:308:ILE:HD13	1:A:352:VAL:HG11	1.94	0.50
1:D:338:ASN:OD1	1:D:377:HIS:NE2	2.45	0.50
1:G:458:ILE:O	1:G:462:ILE:HG23	2.12	0.50
1:G:160:ARG:HB2	1:G:243:LEU:HB3	1.94	0.49
1:G:467:ILE:HD12	1:G:467:ILE:N	2.27	0.49
1:G:552:GLU:HA	1:G:552:GLU:OE1	2.11	0.49
1:G:8:GLU:OE1	1:G:8:GLU:HA	2.11	0.49
1:H:247:LYS:NZ	1:H:247:LYS:HB3	2.27	0.49
1:C:168:GLN:HG3	1:C:175:GLN:HG3	1.94	0.49
1:C:325:ASN:HD22	1:C:327:ASP:H	1.59	0.49
1:A:15:VAL:O	1:A:16:ARG:C	2.51	0.49
1:A:835:PRO:O	1:A:836:ALA:HB2	2.13	0.49
1:E:138:ARG:HG3	1:E:138:ARG:O	2.13	0.49
1:E:270:ASN:HD21	1:F:269:ARG:HH12	1.59	0.49
1:H:274:ASN:HB3	1:H:277:ARG:HD2	1.95	0.49
1:H:379:VAL:HG13	1:H:380:LEU:HG	1.94	0.49
1:B:613:TYR:CE1	1:B:615:MET:HB3	2.47	0.49
1:B:665:GLN:O	1:B:690:GLY:HA2	2.12	0.49
1:B:777:TYR:O	1:B:781:VAL:HG12	2.12	0.49
1:F:805:ILE:O	1:F:808:SER:HB2	2.12	0.49
1:H:379:VAL:HG21	1:H:670:GLY:O	2.12	0.49
1:H:558:ASN:HD22	1:H:638:ASP:HB2	1.76	0.49
1:H:743:GLU:HA	1:H:743:GLU:OE2	2.12	0.49
1:A:21:VAL:HG22	4:A:890:HOH:O	2.13	0.49
1:B:682:MET:HE3	1:B:808:SER:HA	1.93	0.49
1:A:235:ASN:ND2	1:A:237:VAL:H	2.11	0.49
1:A:396:LEU:HB3	1:A:399:HIS:HB2	1.95	0.49
1:D:66:ARG:CG	1:D:66:ARG:NH1	2.71	0.49
1:E:97:ASN:HA	1:E:494:LEU:CD1	2.43	0.49
1:F:550:GLU:HG2	1:F:555:VAL:O	2.13	0.49
1:H:166:PHE:HB2	1:H:178:GLU:O	2.13	0.49
1:B:273:GLU:HB3	1:B:277:ARG:HH22	1.78	0.49
1:C:280:TYR:OH	1:C:291:LEU:HD12	2.13	0.48
1:E:741:ILE:HA	1:E:744:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:615:MET:HA	1:F:615:MET:HE2	1.93	0.48
1:H:66:ARG:HD3	1:H:236:ASN:OD1	2.12	0.48
1:A:41:LYS:HE3	1:A:50:ASP:OD1	2.13	0.48
1:E:34:HIS:HE1	1:E:61:ASP:OD2	1.96	0.48
1:E:205:ARG:NH1	1:E:217:ASP:OD2	2.46	0.48
1:G:39:LEU:HD21	1:G:53:PHE:HB2	1.95	0.48
1:C:44:ASN:HD22	1:D:317:GLY:HA2	1.79	0.48
1:D:235:ASN:HD22	1:D:235:ASN:N	2.05	0.48
1:F:93:ARG:O	1:F:490:ARG:NH2	2.46	0.48
1:A:515:LEU:HD23	1:A:809:GLY:HA2	1.95	0.48
1:B:166:PHE:CD2	1:B:177:GLU:HB3	2.47	0.48
1:B:263:ILE:O	1:B:266:VAL:N	2.45	0.48
1:B:609:ALA:O	1:B:610:ALA:CB	2.60	0.48
1:D:163:PHE:HE2	1:D:277:ARG:HD3	1.78	0.48
1:F:235:ASN:OD1	1:F:237:VAL:HG13	2.13	0.48
1:F:703:ALA:CA	1:F:807:THR:HG21	2.39	0.48
1:G:102:LEU:HB3	1:G:104:LEU:HD22	1.94	0.48
1:A:579:ASN:C	1:A:579:ASN:HD22	2.17	0.48
1:C:49:ARG:HA	1:C:125:ILE:HG21	1.94	0.48
1:C:680:LLP:O3	1:C:680:LLP:NZ	2.47	0.48
1:E:162:GLU:HA	1:E:183:LEU:HD12	1.95	0.48
1:E:474:LEU:HD13	1:E:475:GLU:HG3	1.95	0.48
1:G:680:LLP:O3	1:G:680:LLP:NZ	2.46	0.48
1:G:734:ARG:HG3	1:G:735:ILE:HG13	1.96	0.48
1:H:165:ILE:HD12	1:H:166:PHE:CD1	2.49	0.48
1:B:67:TRP:HD1	1:B:238:VAL:HG12	1.79	0.48
1:E:28:LYS:HZ1	1:F:12:GLN:HE22	1.61	0.48
1:F:270:ASN:O	1:F:274:ASN:ND2	2.44	0.48
1:G:687:LEU:HD13	1:G:800:MET:CE	2.43	0.48
1:B:457:ARG:NH2	1:B:701:GLU:OE2	2.46	0.48
1:B:721:LEU:HD12	1:B:724:ARG:HE	1.79	0.48
1:C:615:MET:CE	1:C:761:ILE:HG12	2.43	0.48
1:D:713:MET:HG3	1:D:776:ASP:OD1	2.14	0.48
1:H:60:ARG:O	1:H:64:VAL:HG13	2.13	0.48
1:B:292:ARG:NH2	1:B:341:HIS:CD2	2.82	0.48
1:D:336:GLN:NE2	1:D:825:TRP:NE1	2.53	0.48
1:E:290:GLU:HG3	1:E:391:LEU:HD21	1.96	0.48
1:H:687:LEU:HD13	1:H:800:MET:HE2	1.95	0.48
1:A:475:GLU:OE1	1:A:478:LYS:HE2	2.13	0.48
1:B:157:TYR:CE2	1:B:242:ARG:HG2	2.48	0.48
1:D:235:ASN:H	1:D:235:ASN:ND2	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:626:ILE:O	1:G:630:VAL:HG13	2.14	0.48
1:H:379:VAL:HG13	1:H:380:LEU:N	2.28	0.48
1:A:518:LEU:O	1:A:521:LEU:HB2	2.14	0.47
1:G:672:GLU:HB2	1:G:693:ASP:OD2	2.14	0.47
1:H:475:GLU:OE1	1:H:478:LYS:HE2	2.13	0.47
1:B:455:VAL:HG13	1:B:484:ASN:ND2	2.29	0.47
1:F:192:ALA:HB2	1:F:226:TYR:CE2	2.49	0.47
1:A:280:TYR:OH	1:A:291:LEU:HD12	2.14	0.47
1:B:783:CYS:O	1:B:787:VAL:HG23	2.15	0.47
1:F:693:ASP:O	1:F:696:ASN:HB2	2.13	0.47
1:A:727:ASN:HD21	1:A:729:GLN:HB3	1.78	0.47
1:E:713:MET:HG2	1:E:717:ASP:HB3	1.95	0.47
1:F:34:HIS:HD2	1:F:38:THR:OG1	1.96	0.47
1:B:250:ASN:HD21	1:B:269:ARG:NH2	2.08	0.47
1:B:477:HIS:HB3	1:E:358:ARG:CZ	2.45	0.47
1:B:573:TYR:HE2	1:B:672:GLU:HG2	1.78	0.47
1:G:583:VAL:HG11	1:G:642:VAL:CG2	2.45	0.47
1:G:676:THR:HG23	1:G:680:LLP:H4'1	1.97	0.47
1:A:741:ILE:HA	1:A:744:GLN:NE2	2.29	0.47
1:C:235:ASN:H	1:C:235:ASN:ND2	2.12	0.47
1:D:34:HIS:CD2	1:D:38:THR:OG1	2.67	0.47
1:E:165:ILE:O	1:E:166:PHE:O	2.32	0.47
1:F:66:ARG:HH12	1:F:837:PRO:HG3	1.80	0.47
1:F:569:ARG:NH1	3:F:845:SO4:O4	2.48	0.47
1:G:330:PRO:HB3	1:G:370:LYS:HB3	1.96	0.47
1:B:95:LEU:HD12	1:B:123:GLU:HG2	1.95	0.47
1:F:388:PRO:HG2	1:F:391:LEU:HB2	1.97	0.47
1:A:522:LEU:O	1:A:525:VAL:HG22	2.15	0.47
1:E:737:GLU:HB2	4:E:852:HOH:O	2.15	0.47
1:G:22:GLU:OE2	1:G:66:ARG:NH2	2.47	0.47
1:G:422:VAL:HA	1:G:425:LEU:HD23	1.97	0.47
1:E:379:VAL:HG22	1:E:462:ILE:HD11	1.97	0.47
1:F:680:LLP:O3	1:F:680:LLP:NZ	2.47	0.47
1:A:309:ARG:NH2	2:A:843:AMP:O1P	2.48	0.46
1:B:227:ASP:OD1	1:B:242:ARG:CD	2.63	0.46
1:F:293:LEU:HD21	1:F:392:LEU:HD13	1.97	0.46
1:F:575:ARG:HH22	1:F:776:ASP:HB2	1.80	0.46
1:F:613:TYR:CE1	1:F:615:MET:HB3	2.50	0.46
1:D:455:VAL:CG1	1:D:674:SER:HB2	2.44	0.46
1:D:475:GLU:OE1	1:D:478:LYS:HE2	2.16	0.46
1:G:835:PRO:O	1:G:836:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:594:PRO:O	1:E:639:ARG:NH2	2.49	0.46
1:G:486:ILE:HG12	1:G:680:LLP:HG3	1.97	0.46
1:A:157:TYR:CG	1:A:303:THR:HG23	2.50	0.46
1:B:165:ILE:HD12	1:B:166:PHE:CD1	2.51	0.46
1:E:379:VAL:HG12	1:E:380:LEU:HG	1.96	0.46
1:G:16:ARG:HG2	1:G:16:ARG:HH11	1.80	0.46
1:H:165:ILE:HG22	1:H:166:PHE:H	1.79	0.46
1:H:506:ARG:NH2	1:H:533:ASP:OD2	2.40	0.46
1:A:424:ARG:HA	1:A:427:ARG:HB2	1.97	0.46
1:F:455:VAL:CG1	1:F:674:SER:HB2	2.39	0.46
1:B:566:GLN:HB2	1:B:664:GLU:HB2	1.97	0.46
1:D:144:LEU:HD23	1:D:147:MET:HE3	1.98	0.46
1:D:211:GLN:HG3	1:D:358:ARG:HH22	1.79	0.46
1:D:227:ASP:OD1	1:D:242:ARG:HD3	2.16	0.46
1:E:571:HIS:H	1:E:576:GLN:NE2	2.13	0.46
1:C:486:ILE:HD11	1:C:680:LLP:HE2	1.98	0.46
1:C:766:MET:HE1	1:C:774:PHE:HE2	1.81	0.46
1:D:63:LEU:HD13	1:D:229:PRO:HB2	1.97	0.46
1:G:361:TRP:CZ3	1:G:409:ARG:CD	2.97	0.46
1:G:727:ASN:C	1:G:727:ASN:HD22	2.18	0.46
1:B:205:ARG:NH1	1:B:217:ASP:OD2	2.49	0.46
1:B:270:ASN:O	1:B:274:ASN:ND2	2.49	0.46
1:C:80:LYS:HE2	1:C:334:ALA:HB2	1.96	0.46
1:E:455:VAL:HG22	1:E:484:ASN:OD1	2.15	0.46
1:F:211:GLN:NE2	1:F:211:GLN:HA	2.31	0.46
1:H:793:ASN:C	1:H:793:ASN:HD22	2.19	0.46
1:B:7:GLN:C	1:B:9:LYS:H	2.19	0.46
1:H:88:GLU:HG2	1:H:132:GLY:HA2	1.98	0.46
1:H:304:LEU:O	1:H:308:ILE:HD12	2.16	0.46
1:A:528:GLU:OE2	1:A:795:ARG:NH1	2.49	0.46
1:B:550:GLU:HA	1:B:555:VAL:CG2	2.45	0.46
1:B:793:ASN:C	1:B:793:ASN:HD22	2.19	0.46
1:D:129:ALA:HB1	1:D:131:LEU:HD22	1.97	0.46
1:E:108:CYS:O	1:E:112:THR:HG23	2.15	0.46
1:H:573:TYR:HE2	1:H:672:GLU:HG2	1.81	0.46
1:D:766:MET:HE3	1:D:774:PHE:HE2	1.81	0.45
1:D:564:ASP:HB3	1:D:603:VAL:HA	1.98	0.45
1:D:573:TYR:HE2	1:D:672:GLU:OE1	1.99	0.45
1:E:687:LEU:HD13	1:E:800:MET:HE1	1.97	0.45
1:G:34:HIS:CD2	1:G:57:HIS:HB3	2.51	0.45
1:G:163:PHE:CE1	1:G:181:ASP:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:464:LYS:HD2	1:G:472:TYR:CE1	2.51	0.45
1:H:720:ARG:HG3	1:H:723:GLN:HE22	1.82	0.45
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.98	0.45
1:A:583:VAL:HG11	1:A:642:VAL:HG21	1.98	0.45
1:A:665:GLN:HB2	1:A:696:ASN:HD21	1.81	0.45
1:C:85:LEU:CD2	1:C:303:THR:HG21	2.44	0.45
1:E:361:TRP:CZ3	1:E:409:ARG:HD2	2.51	0.45
1:G:78:ASP:OD2	1:G:332:LYS:HE3	2.16	0.45
1:C:571:HIS:H	1:C:576:GLN:NE2	2.14	0.45
1:E:793:ASN:C	1:E:793:ASN:HD22	2.20	0.45
1:F:584:ILE:HG22	1:F:741:ILE:HG22	1.98	0.45
1:H:309:ARG:NH2	2:H:843:AMP:O1P	2.49	0.45
1:H:680:LLP:NZ	1:H:680:LLP:O3	2.47	0.45
1:B:353:LEU:HB3	1:B:359:LEU:HD12	1.97	0.45
1:B:685:GLY:HA2	1:B:801:VAL:HG13	1.98	0.45
1:D:597:PHE:HE2	1:D:792:LYS:HD2	1.81	0.45
1:E:280:TYR:HD2	1:E:292:ARG:HH11	1.64	0.45
1:F:682:MET:HE1	1:F:811:PHE:HD2	1.81	0.45
1:A:463:LEU:HD23	1:A:467:ILE:HD13	1.99	0.45
1:E:547:ALA:O	1:E:551:ARG:HG2	2.17	0.45
1:F:343:SER:CB	1:F:445:CYS:SG	3.05	0.45
1:H:549:LEU:HD23	1:H:557:ILE:HG13	1.98	0.45
1:B:34:HIS:HD2	1:B:38:THR:OG1	2.00	0.45
1:E:613:TYR:CE1	1:E:615:MET:HB3	2.51	0.45
1:G:24:VAL:O	1:G:28:LYS:HG2	2.16	0.45
1:G:766:MET:HE3	1:G:766:MET:HA	1.98	0.45
1:H:458:ILE:HD11	1:H:697:VAL:HG11	1.98	0.45
1:F:129:ALA:HB1	1:F:131:LEU:HD22	1.97	0.45
1:F:279:LEU:HD22	1:F:280:TYR:H	1.82	0.45
1:A:66:ARG:HD3	1:A:236:ASN:OD1	2.17	0.45
1:D:835:PRO:O	1:D:836:ALA:O	2.35	0.45
1:G:274:ASN:C	1:G:274:ASN:HD22	2.20	0.45
1:C:28:LYS:NZ	1:D:12:GLN:HE22	2.14	0.44
1:C:280:TYR:OH	1:C:291:LEU:CD1	2.65	0.44
1:F:719:ASP:C	1:F:721:LEU:H	2.19	0.44
1:G:89:PHE:O	1:G:131:LEU:HB3	2.17	0.44
1:H:373:ALA:HA	1:H:449:SER:HB3	1.99	0.44
1:H:601:ARG:NH2	1:H:784:GLN:OE1	2.50	0.44
1:A:269:ARG:HH22	1:B:277:ARG:CZ	2.29	0.44
1:A:685:GLY:HA2	1:A:801:VAL:HG13	2.00	0.44
1:B:615:MET:HE3	1:B:761:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:VAL:HG22	1:C:484:ASN:ND2	2.33	0.44
1:D:665:GLN:HB2	1:D:696:ASN:HD21	1.83	0.44
1:E:289:LYS:HB2	1:E:289:LYS:NZ	2.33	0.44
1:E:550:GLU:HG2	1:E:555:VAL:O	2.17	0.44
1:F:344:LEU:C	1:F:347:PRO:HD2	2.38	0.44
1:A:60:ARG:O	1:A:64:VAL:HG13	2.17	0.44
1:A:280:TYR:OH	1:A:291:LEU:HD13	2.16	0.44
1:B:650:VAL:HA	1:B:680:LLP:H2'1	2.00	0.44
1:E:235:ASN:HD22	1:E:235:ASN:N	2.13	0.44
1:A:101:ASN:O	1:A:234:ARG:HG2	2.18	0.44
1:B:308:ILE:HD13	1:B:352:VAL:HG11	1.99	0.44
1:C:73:HIS:O	1:C:76:GLU:HG3	2.18	0.44
1:D:703:ALA:CA	1:D:807:THR:HG21	2.48	0.44
1:E:235:ASN:H	1:E:235:ASN:ND2	2.14	0.44
1:E:615:MET:CE	1:E:761:ILE:HG12	2.45	0.44
1:H:720:ARG:HG3	1:H:723:GLN:NE2	2.32	0.44
1:H:756:ASP:O	1:H:759:LYS:HG2	2.18	0.44
1:A:89:PHE:O	1:A:131:LEU:HB3	2.18	0.44
1:C:160:ARG:HB2	1:C:243:LEU:HB3	1.99	0.44
1:G:351:ARG:O	1:G:355:ASP:HB2	2.18	0.44
1:G:588:ASN:HD21	1:G:744:GLN:HE22	1.64	0.44
1:A:161:TYR:HA	1:A:276:SER:O	2.17	0.44
1:C:355:ASP:OD2	1:C:398:ARG:HD3	2.17	0.44
1:D:193:ARG:HB2	1:D:225:PRO:HG2	1.99	0.44
1:G:248:ALA:HB3	1:G:269:ARG:HG3	1.99	0.44
1:A:33:ARG:HE	1:B:33:ARG:HH21	1.64	0.44
1:B:492:LEU:HG	1:B:683:LEU:HD22	1.99	0.44
1:G:525:VAL:HG12	1:G:799:ARG:NH1	2.32	0.44
1:H:557:ILE:HD11	1:H:643:ILE:CD1	2.48	0.44
1:A:16:ARG:CG	1:A:16:ARG:NH1	2.77	0.44
1:B:587:TYR:CD1	1:B:630:VAL:HG12	2.53	0.44
1:C:51:TYR:CD2	1:C:117:LEU:HD11	2.53	0.44
1:C:403:ILE:HG21	1:C:439:ILE:HD13	2.00	0.44
1:G:165:ILE:HD13	1:G:165:ILE:HA	1.80	0.44
1:D:160:ARG:HB2	1:D:243:LEU:HB3	2.00	0.43
1:D:455:VAL:HG22	1:D:484:ASN:OD1	2.18	0.43
1:E:713:MET:HE1	1:E:772:LYS:HD3	2.00	0.43
1:G:575:ARG:HD3	1:G:666:ILE:O	2.17	0.43
1:H:396:LEU:HB3	1:H:399:HIS:HB2	1.99	0.43
1:A:15:VAL:HA	1:A:18:LEU:HD12	1.99	0.43
1:E:461:GLU:O	1:E:465:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:ARG:HA	1:F:125:ILE:HG21	2.00	0.43
1:B:575:ARG:NH2	1:B:776:ASP:HB2	2.33	0.43
1:D:346:ILE:HB	1:D:347:PRO:HD3	2.00	0.43
1:F:575:ARG:NH2	1:F:776:ASP:HB2	2.32	0.43
1:F:732:TYR:CZ	1:F:739:ARG:HG2	2.53	0.43
1:F:836:ALA:HB1	1:F:837:PRO:HD2	2.00	0.43
1:G:566:GLN:HB2	1:G:664:GLU:HB2	1.99	0.43
1:B:678:ASN:HD22	1:B:679:MET:HG3	1.83	0.43
1:B:836:ALA:HB1	1:B:837:PRO:HD2	1.99	0.43
1:C:227:ASP:OD1	1:C:242:ARG:HD3	2.17	0.43
1:D:165:ILE:HD12	1:D:166:PHE:CD1	2.53	0.43
1:A:351:ARG:O	1:A:355:ASP:HB2	2.19	0.43
1:A:792:LYS:O	1:A:794:PRO:HD3	2.18	0.43
1:F:466:THR:OG1	1:F:467:ILE:N	2.52	0.43
1:G:63:LEU:HD22	1:G:238:VAL:HG11	1.99	0.43
1:G:573:TYR:CE2	1:G:574:LYS:HD2	2.53	0.43
1:G:759:LYS:HE3	1:G:759:LYS:HB3	1.85	0.43
1:B:10:ARG:HB3	1:B:13:ILE:HD12	2.00	0.43
1:B:138:ARG:NH1	1:B:142:CYS:SG	2.91	0.43
1:C:92:GLY:O	1:C:93:ARG:CB	2.60	0.43
1:E:270:ASN:HD21	1:F:269:ARG:NH1	2.17	0.43
1:E:564:ASP:HB3	1:E:603:VAL:HA	2.00	0.43
1:E:590:ILE:HG12	1:E:598:VAL:HG21	2.01	0.43
1:F:66:ARG:NH1	1:F:837:PRO:HG3	2.33	0.43
1:A:807:THR:O	1:A:807:THR:HG23	2.19	0.43
1:E:453:ASN:ND2	1:E:482:LYS:HB2	2.32	0.43
1:F:325:ASN:HD21	1:F:327:ASP:HB2	1.84	0.43
1:F:601:ARG:NH2	1:F:784:GLN:OE1	2.50	0.43
1:F:676:THR:CG2	1:F:680:LLP:H4'1	2.48	0.43
1:H:275:ILE:HG23	1:H:295:GLN:HA	2.00	0.43
1:A:200:VAL:HG11	1:A:298:PHE:HA	2.01	0.43
1:C:455:VAL:HG22	1:C:484:ASN:OD1	2.18	0.43
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.83	0.43
1:B:577:LEU:HD23	1:B:577:LEU:HA	1.89	0.43
1:C:709:PHE:CE2	1:C:800:MET:HE1	2.53	0.43
4:C:875:HOH:O	1:D:45:VAL:HG11	2.18	0.43
1:E:727:ASN:O	1:E:730:GLU:HB2	2.19	0.43
1:F:127:GLU:OE2	1:F:184:ARG:NH1	2.52	0.43
1:H:573:TYR:CZ	1:H:574:LYS:HD2	2.54	0.43
1:A:30:ASN:HB3	1:A:58:THR:HG23	2.01	0.42
1:A:455:VAL:CG1	1:A:674:SER:HB2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LYS:H	1:B:464:LYS:HG2	1.65	0.42
1:D:130:GLY:O	1:D:164:GLY:HA2	2.19	0.42
1:H:292:ARG:HH21	1:H:341:HIS:CD2	2.35	0.42
1:D:67:TRP:O	1:D:71:GLN:HG2	2.19	0.42
1:E:379:VAL:CG1	1:E:380:LEU:HG	2.49	0.42
1:F:795:ARG:O	1:F:799:ARG:HG3	2.19	0.42
1:G:636:VAL:O	1:G:639:ARG:HD3	2.18	0.42
1:A:353:LEU:HA	1:A:357:GLU:HB2	2.00	0.42
1:B:77:LYS:HA	1:B:77:LYS:HD2	1.84	0.42
1:C:568:LYS:HE2	1:C:665:GLN:OE1	2.18	0.42
1:E:279:LEU:CD2	1:E:280:TYR:H	2.32	0.42
1:C:235:ASN:OD1	1:C:237:VAL:HG13	2.19	0.42
1:C:313:SER:O	1:C:314:SER:C	2.57	0.42
1:D:297:TYR:CD2	1:D:396:LEU:HD11	2.54	0.42
1:E:665:GLN:HG3	1:E:678:ASN:HB3	2.00	0.42
1:F:663:SER:HB2	1:F:681:PHE:CG	2.55	0.42
1:G:22:GLU:CD	1:G:66:ARG:HH22	2.22	0.42
1:A:33:ARG:HH12	1:B:30:ASN:HD21	1.66	0.42
1:B:163:PHE:HB3	1:B:277:ARG:O	2.19	0.42
1:C:571:HIS:O	1:C:576:GLN:NE2	2.52	0.42
1:D:396:LEU:HB3	1:D:399:HIS:HB2	2.02	0.42
1:F:366:GLU:HG3	1:F:370:LYS:HE3	2.02	0.42
1:G:161:TYR:CZ	1:G:279:LEU:HG	2.55	0.42
1:A:446:ILE:O	1:A:478:LYS:HE3	2.19	0.42
1:A:692:MET:HB3	1:A:714:ARG:HD2	2.01	0.42
1:B:304:LEU:HD12	1:B:304:LEU:HA	1.90	0.42
1:C:102:LEU:HB3	1:C:104:LEU:HD22	2.02	0.42
1:C:211:GLN:HG2	1:C:358:ARG:HH11	1.85	0.42
1:C:713:MET:HE3	1:C:721:LEU:HD13	2.00	0.42
1:D:330:PRO:HB3	1:D:370:LYS:HB3	2.01	0.42
1:E:676:THR:HG22	1:E:680:LLP:H5'1	2.01	0.42
1:H:263:ILE:O	1:H:266:VAL:N	2.53	0.42
1:A:428:MET:SD	1:A:470:ASP:HB3	2.60	0.42
1:B:486:ILE:HG12	1:B:680:LLP:HG3	2.02	0.42
1:C:34:HIS:CD2	1:C:38:THR:OG1	2.67	0.42
1:A:379:VAL:HG13	1:A:380:LEU:HG	2.02	0.42
1:A:630:VAL:HG21	1:A:642:VAL:HG23	2.02	0.42
1:B:575:ARG:HD3	1:B:666:ILE:O	2.20	0.42
1:B:741:ILE:HA	1:B:744:GLN:HE21	1.84	0.42
1:A:97:ASN:HD22	1:A:494:LEU:HD12	1.85	0.42
1:A:754:GLN:HG2	1:D:433:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ILE:HG13	1:B:697:VAL:HG21	2.01	0.42
1:E:727:ASN:HD21	1:H:725:GLY:HA3	1.85	0.42
1:F:181:ASP:O	1:F:184:ARG:HD3	2.20	0.42
1:G:157:TYR:CE2	1:G:242:ARG:HG2	2.55	0.42
1:G:157:TYR:CD2	1:G:303:THR:HG23	2.55	0.42
1:A:381:PRO:HA	1:A:384:LEU:HD22	2.00	0.42
1:E:177:GLU:OE2	1:E:611:PRO:HB3	2.20	0.42
1:E:835:PRO:O	1:E:836:ALA:HB2	2.20	0.42
1:A:732:TYR:O	1:A:739:ARG:HG3	2.20	0.41
1:B:138:ARG:NH1	1:B:491:TRP:HE1	2.18	0.41
1:B:784:GLN:O	1:B:787:VAL:HB	2.20	0.41
1:C:575:ARG:HG2	1:C:773:VAL:HG22	2.02	0.41
1:D:28:LYS:HB2	1:D:115:LEU:HD11	2.02	0.41
1:D:93:ARG:HG2	1:D:126:GLU:HG3	2.00	0.41
1:D:230:VAL:O	1:D:230:VAL:CG2	2.67	0.41
1:E:227:ASP:OD1	1:E:242:ARG:CD	2.64	0.41
1:G:304:LEU:HD22	1:G:348:GLU:HG3	2.02	0.41
1:G:339:ASP:O	1:G:342:PRO:HD2	2.20	0.41
1:G:766:MET:HE1	1:G:774:PHE:HE2	1.84	0.41
1:C:575:ARG:HD3	1:C:666:ILE:O	2.20	0.41
1:E:18:LEU:HD11	1:F:32:ASN:HB3	2.02	0.41
1:F:227:ASP:OD1	1:F:242:ARG:CD	2.67	0.41
1:G:551:ARG:HE	1:G:551:ARG:HB3	1.62	0.41
1:H:734:ARG:HG3	1:H:735:ILE:HG13	2.01	0.41
1:H:795:ARG:O	1:H:799:ARG:HG3	2.20	0.41
1:A:445:CYS:O	1:A:449:SER:OG	2.38	0.41
1:A:727:ASN:ND2	1:A:729:GLN:HB3	2.35	0.41
1:B:22:GLU:HB3	1:B:104:LEU:HD11	2.01	0.41
1:B:555:VAL:HB	1:B:556:HIS:H	1.59	0.41
1:C:138:ARG:O	1:C:138:ARG:HG3	2.20	0.41
1:D:734:ARG:H	1:D:734:ARG:HG2	1.57	0.41
1:C:450:HIS:CE1	4:C:879:HOH:O	2.58	0.41
1:C:703:ALA:CA	1:C:807:THR:HG21	2.40	0.41
1:D:139:LEU:HD23	1:D:377:HIS:HE1	1.85	0.41
1:E:85:LEU:HD21	1:E:303:THR:HG21	2.02	0.41
1:E:182:TRP:CE2	1:E:183:LEU:HG	2.55	0.41
1:G:571:HIS:H	1:G:576:GLN:HE21	1.67	0.41
1:H:10:ARG:H	1:H:10:ARG:HG2	1.59	0.41
1:B:721:LEU:HD23	1:B:772:LYS:HD3	2.02	0.41
1:C:793:ASN:C	1:C:793:ASN:HD22	2.24	0.41
1:D:165:ILE:O	1:D:166:PHE:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:GLU:HG3	1:F:391:LEU:HD21	2.03	0.41
1:F:536:LYS:HD3	1:F:536:LYS:HA	1.88	0.41
1:H:225:PRO:HB2	1:H:242:ARG:HD2	2.02	0.41
1:H:558:ASN:HA	1:H:559:PRO:HD3	1.93	0.41
1:H:566:GLN:HE22	1:H:576:GLN:HA	1.85	0.41
1:A:22:GLU:CD	1:A:66:ARG:HH22	2.22	0.41
1:B:162:GLU:HA	1:B:183:LEU:HD12	2.03	0.41
1:D:633:ASP:HA	1:D:634:PRO:HD3	1.91	0.41
1:D:719:ASP:C	1:D:721:LEU:H	2.23	0.41
1:E:455:VAL:HG22	1:E:484:ASN:CG	2.41	0.41
1:G:492:LEU:HB2	1:G:683:LEU:HD13	2.02	0.41
1:H:87:LEU:HD13	1:H:341:HIS:CB	2.51	0.41
1:C:550:GLU:HG2	1:C:555:VAL:O	2.21	0.41
1:D:181:ASP:O	1:D:184:ARG:HD2	2.20	0.41
1:E:601:ARG:NH2	1:E:784:GLN:OE1	2.45	0.41
1:G:486:ILE:HD11	1:G:680:LLP:HE3	2.03	0.41
1:H:730:GLU:HB3	1:H:734:ARG:HH12	1.85	0.41
1:B:52:TYR:CZ	1:B:126:GLU:HB3	2.56	0.41
1:B:558:ASN:HA	1:B:559:PRO:HD3	1.94	0.41
1:C:70:THR:O	1:C:73:HIS:HB3	2.21	0.41
1:E:288:GLY:HA2	4:E:862:HOH:O	2.20	0.41
1:G:166:PHE:CD2	1:G:177:GLU:HB3	2.56	0.41
1:G:320:ASP:HA	1:G:321:PRO:HD3	1.86	0.41
1:H:676:THR:N	1:H:680:LLP:OP1	2.53	0.41
1:B:193:ARG:HB3	1:B:196:PHE:HD2	1.86	0.41
1:B:455:VAL:CG1	1:B:674:SER:HB2	2.51	0.41
1:C:379:VAL:CG1	1:C:380:LEU:HG	2.51	0.41
1:F:192:ALA:HB1	1:F:224:MET:CE	2.51	0.41
1:A:49:ARG:HG2	1:A:53:PHE:CE2	2.56	0.41
1:B:75:TYR:CE1	2:B:843:AMP:C8	3.09	0.41
1:B:138:ARG:HD3	1:B:491:TRP:HZ2	1.86	0.41
1:B:665:GLN:HG3	1:B:678:ASN:HB3	2.02	0.41
1:C:39:LEU:HD11	1:C:53:PHE:HB3	2.03	0.41
1:C:157:TYR:CE2	1:C:242:ARG:HG2	2.56	0.41
1:C:235:ASN:HD22	1:C:235:ASN:N	2.12	0.41
1:D:47:THR:HB	1:D:48:PRO:HD2	2.03	0.41
1:D:144:LEU:HD23	1:D:147:MET:CE	2.51	0.41
1:E:566:GLN:HB2	1:E:664:GLU:HB2	2.03	0.41
1:E:680:LLP:H5'1	1:E:680:LLP:H4'1	1.90	0.41
1:F:396:LEU:HB3	1:F:399:HIS:HB2	2.03	0.41
1:F:603:VAL:HG23	1:F:642:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:ARG:O	1:G:225:PRO:HD2	2.21	0.41
1:G:329:PHE:HB3	1:G:330:PRO:HD3	2.03	0.41
1:H:87:LEU:HD13	1:H:341:HIS:HB3	2.03	0.41
1:H:195:GLU:CD	1:H:195:GLU:H	2.24	0.41
1:H:633:ASP:HA	1:H:634:PRO:HD3	1.86	0.41
1:C:422:VAL:O	1:C:425:LEU:HB2	2.21	0.40
1:C:700:ALA:O	1:C:704:GLY:N	2.48	0.40
1:F:329:PHE:HB3	1:F:330:PRO:HD3	2.03	0.40
1:F:439:ILE:HG22	1:F:441:MET:SD	2.61	0.40
1:G:822:ARG:HD3	1:G:828:GLU:OE2	2.20	0.40
1:B:280:TYR:HH	1:B:291:LEU:HD12	1.79	0.40
1:E:313:SER:O	1:E:314:SER:C	2.59	0.40
1:F:564:ASP:HB3	1:F:603:VAL:HG12	2.02	0.40
1:A:601:ARG:NH2	1:A:784:GLN:OE1	2.51	0.40
1:B:412:ASN:HD22	1:B:412:ASN:HA	1.63	0.40
1:C:63:LEU:HD22	1:C:238:VAL:HG11	2.04	0.40
1:C:455:VAL:HG22	1:C:484:ASN:CG	2.41	0.40
1:F:571:HIS:ND1	1:F:572:GLU:N	2.69	0.40
1:G:77:LYS:HD3	1:G:77:LYS:HA	1.74	0.40
1:G:699:MET:HA	1:G:811:PHE:CZ	2.56	0.40
1:A:24:VAL:O	1:A:28:LYS:HG2	2.21	0.40
1:A:33:ARG:HE	1:B:33:ARG:NH2	2.20	0.40
1:A:193:ARG:HH22	1:B:40:VAL:HG12	1.87	0.40
1:A:400:LEU:HD23	1:A:400:LEU:HA	1.90	0.40
1:E:36:HIS:O	1:E:40:VAL:HA	2.22	0.40
1:B:10:ARG:H	1:B:10:ARG:HG2	1.55	0.40
1:D:597:PHE:CE2	1:D:792:LYS:HD2	2.54	0.40
1:F:21:VAL:HB	1:F:26:GLU:HG2	2.03	0.40
1:F:685:GLY:HA2	1:F:801:VAL:HG13	2.04	0.40
1:G:138:ARG:HD3	1:G:138:ARG:C	2.42	0.40
1:G:165:ILE:HD12	1:G:166:PHE:CD1	2.57	0.40
1:H:67:TRP:O	1:H:71:GLN:HG2	2.21	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	807/842 (96%)	771 (96%)	27 (3%)	9 (1%)	14	34
1	B	808/842 (96%)	757 (94%)	39 (5%)	12 (2%)	10	26
1	C	793/842 (94%)	745 (94%)	40 (5%)	8 (1%)	15	37
1	D	808/842 (96%)	763 (94%)	38 (5%)	7 (1%)	17	40
1	E	794/842 (94%)	752 (95%)	36 (4%)	6 (1%)	19	43
1	F	806/842 (96%)	759 (94%)	42 (5%)	5 (1%)	25	50
1	G	807/842 (96%)	763 (94%)	34 (4%)	10 (1%)	13	32
1	H	807/842 (96%)	756 (94%)	44 (6%)	7 (1%)	17	40
All	All	6430/6736 (96%)	6066 (94%)	300 (5%)	64 (1%)	15	37

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	166	PHE
1	A	835	PRO
1	B	16	ARG
1	B	273	GLU
1	B	835	PRO
1	C	16	ARG
1	C	835	PRO
1	D	166	PHE
1	D	836	ALA
1	E	166	PHE
1	E	835	PRO
1	G	314	SER
1	G	835	PRO
1	H	16	ARG
1	H	757	LEU
1	A	211	GLN
1	A	556	HIS
1	B	211	GLN
1	B	272	ALA
1	B	555	VAL
1	C	211	GLN
1	D	20	GLY

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Mol	Chain	Res	Type
1	F	210	SER
1	G	92	GLY
1	G	166	PHE
1	G	210	SER
1	G	211	GLN
1	A	836	ALA
1	B	556	HIS
1	B	610	ALA
1	C	93	ARG
1	C	166	PHE
1	C	289	LYS
1	E	16	ARG
1	G	16	ARG
1	H	435	ALA
1	A	436	VAL
1	B	264	GLN
1	B	836	ALA
1	C	522	LEU
1	C	836	ALA
1	D	381	PRO
1	D	837	PRO
1	E	552	GLU
1	F	166	PHE
1	F	551	ARG
1	A	263	ILE
1	B	165	ILE
1	G	93	ARG
1	G	436	VAL
1	G	836	ALA
1	H	272	ALA
1	H	436	VAL
1	A	555	VAL
1	B	557	ILE
1	D	211	GLN
1	E	836	ALA
1	E	263	ILE
1	F	164	GLY
1	F	263	ILE
1	H	555	VAL
1	H	381	PRO
1	D	835	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	703/730 (96%)	613 (87%)	90 (13%)	4	10
1	B	704/730 (96%)	624 (89%)	80 (11%)	5	13
1	C	692/730 (95%)	609 (88%)	83 (12%)	5	11
1	D	704/730 (96%)	616 (88%)	88 (12%)	4	10
1	E	693/730 (95%)	609 (88%)	84 (12%)	5	11
1	F	702/730 (96%)	613 (87%)	89 (13%)	4	10
1	G	703/730 (96%)	618 (88%)	85 (12%)	5	11
1	H	703/730 (96%)	622 (88%)	81 (12%)	5	13
All	All	5604/5840 (96%)	4924 (88%)	680 (12%)	5	11

All (680) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	11	LYS
1	A	15	VAL
1	A	16	ARG
1	A	28	LYS
1	A	30	ASN
1	A	39	LEU
1	A	63	LEU
1	A	64	VAL
1	A	82	ILE
1	A	90	TYR
1	A	95	LEU
1	A	100	VAL
1	A	102	LEU
1	A	128	ASP
1	A	131	LEU
1	A	136	LEU
1	A	138	ARG
1	A	165	ILE

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Mol	Chain	Res	Type
1	A	184	ARG
1	A	205	ARG
1	A	235	ASN
1	A	237	VAL
1	A	242	ARG
1	A	243	LEU
1	A	262	TYR
1	A	269	ARG
1	A	274	ASN
1	A	289	LYS
1	A	291	LEU
1	A	306	ASP
1	A	322	VAL
1	A	337	LEU
1	A	339	ASP
1	A	358	ARG
1	A	360	ASP
1	A	361	TRP
1	A	363	LYS
1	A	384	LEU
1	A	391	LEU
1	A	392	LEU
1	A	395	LEU
1	A	396	LEU
1	A	400	LEU
1	A	424	ARG
1	A	426	ARG
1	A	444	LEU
1	A	449	SER
1	A	455	VAL
1	A	474	LEU
1	A	477	HIS
1	A	478	LYS
1	A	486	ILE
1	A	490	ARG
1	A	492	LEU
1	A	521	LEU
1	A	522	LEU
1	A	525	VAL
1	A	540	GLU
1	A	543	LEU
1	A	555	VAL

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Mol	Chain	Res	Type
1	A	568	LYS
1	A	574	LYS
1	A	576	GLN
1	A	579	ASN
1	A	586	LEU
1	A	596	LYS
1	A	603	VAL
1	A	640	LEU
1	A	649	ARG
1	A	652	LEU
1	A	662	LEU
1	A	676	THR
1	A	678	ASN
1	A	683	LEU
1	A	692	MET
1	A	706	GLU
1	A	708	PHE
1	A	723	GLN
1	A	727	ASN
1	A	754	GLN
1	A	756	ASP
1	A	765	LEU
1	A	766	MET
1	A	778	GLU
1	A	782	LYS
1	A	793	ASN
1	A	796	GLU
1	A	807	THR
1	A	834	LEU
1	B	10	ARG
1	B	15	VAL
1	B	39	LEU
1	B	45	VAL
1	B	63	LEU
1	B	77	LYS
1	B	82	ILE
1	B	90	TYR
1	B	95	LEU
1	B	100	VAL
1	B	104	LEU
1	B	117	LEU
1	B	126	GLU

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Mol	Chain	Res	Type
1	B	128	ASP
1	B	131	LEU
1	B	136	LEU
1	B	163	PHE
1	B	165	ILE
1	B	184	ARG
1	B	191	LYS
1	B	235	ASN
1	B	242	ARG
1	B	262	TYR
1	B	269	ARG
1	B	274	ASN
1	B	289	LYS
1	B	291	LEU
1	B	304	LEU
1	B	315	LYS
1	B	323	ARG
1	B	324	THR
1	B	337	LEU
1	B	339	ASP
1	B	361	TRP
1	B	363	LYS
1	B	391	LEU
1	B	392	LEU
1	B	396	LEU
1	B	400	LEU
1	B	422	VAL
1	B	424	ARG
1	B	426	ARG
1	B	444	LEU
1	B	455	VAL
1	B	462	ILE
1	B	464	LYS
1	B	467	ILE
1	B	474	LEU
1	B	478	LYS
1	B	486	ILE
1	B	492	LEU
1	B	505	GLU
1	B	506	ARG
1	B	519	ARG
1	B	521	LEU

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Mol	Chain	Res	Type
1	B	522	LEU
1	B	540	GLU
1	B	568	LYS
1	B	573	TYR
1	B	576	GLN
1	B	579	ASN
1	B	603	VAL
1	B	613	TYR
1	B	639	ARG
1	B	640	LEU
1	B	649	ARG
1	B	652	LEU
1	B	662	LEU
1	B	676	THR
1	B	678	ASN
1	B	683	LEU
1	B	708	PHE
1	B	765	LEU
1	B	766	MET
1	B	770	ARG
1	B	779	GLU
1	B	782	LYS
1	B	793	ASN
1	B	795	ARG
1	B	807	THR
1	C	11	LYS
1	C	15	VAL
1	C	23	ASN
1	C	39	LEU
1	C	63	LEU
1	C	64	VAL
1	C	82	ILE
1	C	90	TYR
1	C	95	LEU
1	C	104	LEU
1	C	128	ASP
1	C	131	LEU
1	C	138	ARG
1	C	165	ILE
1	C	177	GLU
1	C	184	ARG
1	C	191	LYS

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Mol	Chain	Res	Type
1	C	195	GLU
1	C	205	ARG
1	C	211	GLN
1	C	230	VAL
1	C	235	ASN
1	C	237	VAL
1	C	242	ARG
1	C	243	LEU
1	C	247	LYS
1	C	262	TYR
1	C	264	GLN
1	C	269	ARG
1	C	274	ASN
1	C	289	LYS
1	C	291	LEU
1	C	300	VAL
1	C	306	ASP
1	C	325	ASN
1	C	332	LYS
1	C	337	LEU
1	C	339	ASP
1	C	358	ARG
1	C	360	ASP
1	C	361	TRP
1	C	363	LYS
1	C	379	VAL
1	C	384	LEU
1	C	391	LEU
1	C	392	LEU
1	C	396	LEU
1	C	400	LEU
1	C	408	GLN
1	C	425	LEU
1	C	437	LYS
1	C	444	LEU
1	C	455	VAL
1	C	469	LYS
1	C	474	LEU
1	C	486	ILE
1	C	490	ARG
1	C	492	LEU
1	C	521	LEU

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Mol	Chain	Res	Type
1	C	522	LEU
1	C	525	VAL
1	C	568	LYS
1	C	576	GLN
1	C	579	ASN
1	C	586	LEU
1	C	630	VAL
1	C	639	ARG
1	C	649	ARG
1	C	652	LEU
1	C	662	LEU
1	C	676	THR
1	C	678	ASN
1	C	683	LEU
1	C	706	GLU
1	C	708	PHE
1	C	721	LEU
1	C	753	LYS
1	C	754	GLN
1	C	765	LEU
1	C	770	ARG
1	C	793	ASN
1	C	807	THR
1	C	833	ARG
1	D	8	GLU
1	D	10	ARG
1	D	15	VAL
1	D	21	VAL
1	D	39	LEU
1	D	63	LEU
1	D	82	ILE
1	D	85	LEU
1	D	90	TYR
1	D	95	LEU
1	D	100	VAL
1	D	104	LEU
1	D	126	GLU
1	D	128	ASP
1	D	131	LEU
1	D	138	ARG
1	D	165	ILE
1	D	184	ARG

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Mol	Chain	Res	Type
1	D	195	GLU
1	D	230	VAL
1	D	235	ASN
1	D	237	VAL
1	D	242	ARG
1	D	243	LEU
1	D	262	TYR
1	D	274	ASN
1	D	276	SER
1	D	278	VAL
1	D	279	LEU
1	D	289	LYS
1	D	291	LEU
1	D	304	LEU
1	D	306	ASP
1	D	310	ARG
1	D	323	ARG
1	D	337	LEU
1	D	339	ASP
1	D	356	LEU
1	D	358	ARG
1	D	360	ASP
1	D	361	TRP
1	D	363	LYS
1	D	389	VAL
1	D	390	HIS
1	D	391	LEU
1	D	396	LEU
1	D	400	LEU
1	D	423	ASP
1	D	424	ARG
1	D	425	LEU
1	D	444	LEU
1	D	455	VAL
1	D	474	LEU
1	D	486	ILE
1	D	490	ARG
1	D	492	LEU
1	D	506	ARG
1	D	519	ARG
1	D	521	LEU
1	D	522	LEU

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Mol	Chain	Res	Type
1	D	525	VAL
1	D	549	LEU
1	D	568	LYS
1	D	576	GLN
1	D	579	ASN
1	D	591	LYS
1	D	603	VAL
1	D	613	TYR
1	D	615	MET
1	D	640	LEU
1	D	649	ARG
1	D	652	LEU
1	D	662	LEU
1	D	676	THR
1	D	678	ASN
1	D	683	LEU
1	D	706	GLU
1	D	708	PHE
1	D	723	GLN
1	D	724	ARG
1	D	734	ARG
1	D	753	LYS
1	D	765	LEU
1	D	766	MET
1	D	782	LYS
1	D	793	ASN
1	D	807	THR
1	D	834	LEU
1	E	10	ARG
1	E	15	VAL
1	E	22	GLU
1	E	39	LEU
1	E	45	VAL
1	E	63	LEU
1	E	64	VAL
1	E	76	GLU
1	E	82	ILE
1	E	90	TYR
1	E	95	LEU
1	E	100	VAL
1	E	104	LEU
1	E	117	LEU

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Mol	Chain	Res	Type
1	E	128	ASP
1	E	131	LEU
1	E	138	ARG
1	E	165	ILE
1	E	184	ARG
1	E	219	GLN
1	E	235	ASN
1	E	237	VAL
1	E	242	ARG
1	E	243	LEU
1	E	262	TYR
1	E	267	LEU
1	E	274	ASN
1	E	279	LEU
1	E	289	LYS
1	E	291	LEU
1	E	300	VAL
1	E	306	ASP
1	E	325	ASN
1	E	337	LEU
1	E	339	ASP
1	E	358	ARG
1	E	360	ASP
1	E	361	TRP
1	E	363	LYS
1	E	379	VAL
1	E	384	LEU
1	E	391	LEU
1	E	392	LEU
1	E	396	LEU
1	E	398	ARG
1	E	400	LEU
1	E	408	GLN
1	E	424	ARG
1	E	425	LEU
1	E	426	ARG
1	E	444	LEU
1	E	455	VAL
1	E	465	LYS
1	E	474	LEU
1	E	490	ARG
1	E	492	LEU

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Mol	Chain	Res	Type
1	E	494	LEU
1	E	521	LEU
1	E	522	LEU
1	E	554	LYS
1	E	574	LYS
1	E	576	GLN
1	E	579	ASN
1	E	586	LEU
1	E	613	TYR
1	E	640	LEU
1	E	649	ARG
1	E	652	LEU
1	E	662	LEU
1	E	676	THR
1	E	678	ASN
1	E	683	LEU
1	E	706	GLU
1	E	753	LYS
1	E	756	ASP
1	E	759	LYS
1	E	760	ASP
1	E	765	LEU
1	E	770	ARG
1	E	779	GLU
1	E	792	LYS
1	E	793	ASN
1	E	810	LYS
1	E	832	GLN
1	F	15	VAL
1	F	63	LEU
1	F	82	ILE
1	F	85	LEU
1	F	90	TYR
1	F	95	LEU
1	F	100	VAL
1	F	102	LEU
1	F	104	LEU
1	F	117	LEU
1	F	128	ASP
1	F	131	LEU
1	F	138	ARG
1	F	165	ILE

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Mol	Chain	Res	Type
1	F	184	ARG
1	F	195	GLU
1	F	230	VAL
1	F	235	ASN
1	F	237	VAL
1	F	242	ARG
1	F	243	LEU
1	F	262	TYR
1	F	269	ARG
1	F	273	GLU
1	F	274	ASN
1	F	279	LEU
1	F	289	LYS
1	F	306	ASP
1	F	323	ARG
1	F	332	LYS
1	F	337	LEU
1	F	339	ASP
1	F	356	LEU
1	F	358	ARG
1	F	360	ASP
1	F	379	VAL
1	F	384	LEU
1	F	389	VAL
1	F	391	LEU
1	F	396	LEU
1	F	400	LEU
1	F	408	GLN
1	F	423	ASP
1	F	424	ARG
1	F	425	LEU
1	F	426	ARG
1	F	436	VAL
1	F	444	LEU
1	F	455	VAL
1	F	474	LEU
1	F	478	LYS
1	F	492	LEU
1	F	506	ARG
1	F	510	GLU
1	F	521	LEU
1	F	522	LEU

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Mol	Chain	Res	Type
1	F	526	ASP
1	F	540	GLU
1	F	543	LEU
1	F	568	LYS
1	F	576	GLN
1	F	579	ASN
1	F	586	LEU
1	F	613	TYR
1	F	615	MET
1	F	628	ASP
1	F	638	ASP
1	F	639	ARG
1	F	640	LEU
1	F	649	ARG
1	F	652	LEU
1	F	662	LEU
1	F	676	THR
1	F	678	ASN
1	F	683	LEU
1	F	706	GLU
1	F	708	PHE
1	F	715	VAL
1	F	723	GLN
1	F	724	ARG
1	F	753	LYS
1	F	754	GLN
1	F	760	ASP
1	F	765	LEU
1	F	766	MET
1	F	782	LYS
1	F	793	ASN
1	F	808	SER
1	F	831	ARG
1	G	10	ARG
1	G	11	LYS
1	G	15	VAL
1	G	16	ARG
1	G	28	LYS
1	G	63	LEU
1	G	64	VAL
1	G	82	ILE
1	G	90	TYR

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Mol	Chain	Res	Type
1	G	95	LEU
1	G	100	VAL
1	G	102	LEU
1	G	104	LEU
1	G	128	ASP
1	G	136	LEU
1	G	138	ARG
1	G	165	ILE
1	G	169	LYS
1	G	176	MET
1	G	184	ARG
1	G	230	VAL
1	G	235	ASN
1	G	237	VAL
1	G	242	ARG
1	G	243	LEU
1	G	262	TYR
1	G	269	ARG
1	G	274	ASN
1	G	279	LEU
1	G	291	LEU
1	G	304	LEU
1	G	315	LYS
1	G	327	ASP
1	G	332	LYS
1	G	339	ASP
1	G	361	TRP
1	G	363	LYS
1	G	379	VAL
1	G	384	LEU
1	G	391	LEU
1	G	392	LEU
1	G	396	LEU
1	G	423	ASP
1	G	425	LEU
1	G	426	ARG
1	G	444	LEU
1	G	455	VAL
1	G	462	ILE
1	G	474	LEU
1	G	486	ILE
1	G	492	LEU

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Mol	Chain	Res	Type
1	G	506	ARG
1	G	519	ARG
1	G	521	LEU
1	G	522	LEU
1	G	543	LEU
1	G	551	ARG
1	G	574	LYS
1	G	576	GLN
1	G	579	ASN
1	G	596	LYS
1	G	603	VAL
1	G	630	VAL
1	G	649	ARG
1	G	652	LEU
1	G	662	LEU
1	G	676	THR
1	G	678	ASN
1	G	683	LEU
1	G	692	MET
1	G	706	GLU
1	G	708	PHE
1	G	719	ASP
1	G	727	ASN
1	G	740	GLN
1	G	753	LYS
1	G	754	GLN
1	G	759	LYS
1	G	765	LEU
1	G	766	MET
1	G	770	ARG
1	G	778	GLU
1	G	792	LYS
1	G	793	ASN
1	G	807	THR
1	H	10	ARG
1	H	15	VAL
1	H	28	LYS
1	H	35	LEU
1	H	39	LEU
1	H	63	LEU
1	H	64	VAL
1	H	82	ILE

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Mol	Chain	Res	Type
1	H	90	TYR
1	H	95	LEU
1	H	100	VAL
1	H	117	LEU
1	H	128	ASP
1	H	131	LEU
1	H	136	LEU
1	H	146	SER
1	H	165	ILE
1	H	177	GLU
1	H	184	ARG
1	H	210	SER
1	H	230	VAL
1	H	235	ASN
1	H	237	VAL
1	H	242	ARG
1	H	243	LEU
1	H	262	TYR
1	H	263	ILE
1	H	269	ARG
1	H	274	ASN
1	H	279	LEU
1	H	280	TYR
1	H	290	GLU
1	H	291	LEU
1	H	315	LYS
1	H	323	ARG
1	H	337	LEU
1	H	361	TRP
1	H	391	LEU
1	H	392	LEU
1	H	396	LEU
1	H	400	LEU
1	H	426	ARG
1	H	444	LEU
1	H	455	VAL
1	H	462	ILE
1	H	469	LYS
1	H	474	LEU
1	H	478	LYS
1	H	486	ILE
1	H	490	ARG

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Mol	Chain	Res	Type
1	H	492	LEU
1	H	521	LEU
1	H	536	LYS
1	H	568	LYS
1	H	569	ARG
1	H	574	LYS
1	H	576	GLN
1	H	579	ASN
1	H	586	LEU
1	H	592	LYS
1	H	596	LYS
1	H	613	TYR
1	H	639	ARG
1	H	640	LEU
1	H	649	ARG
1	H	652	LEU
1	H	662	LEU
1	H	676	THR
1	H	678	ASN
1	H	683	LEU
1	H	706	GLU
1	H	708	PHE
1	H	723	GLN
1	H	753	LYS
1	H	756	ASP
1	H	765	LEU
1	H	782	LYS
1	H	793	ASN
1	H	807	THR
1	H	831	ARG
1	H	833	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (182) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	34	HIS
1	A	97	ASN
1	A	168	GLN
1	A	235	ASN
1	A	274	ASN
1	A	325	ASN

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Mol	Chain	Res	Type
1	A	336	GLN
1	A	399	HIS
1	A	408	GLN
1	A	450	HIS
1	A	481	ASN
1	A	541	ASN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	696	ASN
1	A	723	GLN
1	A	727	ASN
1	A	744	GLN
1	A	768	HIS
1	A	793	ASN
1	B	12	GLN
1	B	30	ASN
1	B	34	HIS
1	B	44	ASN
1	B	73	HIS
1	B	168	GLN
1	B	235	ASN
1	B	250	ASN
1	B	274	ASN
1	B	325	ASN
1	B	336	GLN
1	B	412	ASN
1	B	453	ASN
1	B	481	ASN
1	B	539	GLN
1	B	541	ASN
1	B	560	ASN
1	B	566	GLN
1	B	576	GLN
1	B	579	ASN
1	B	614	HIS
1	B	678	ASN
1	B	727	ASN
1	B	744	GLN
1	B	793	ASN
1	C	12	GLN
1	C	23	ASN

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Mol	Chain	Res	Type
1	C	30	ASN
1	C	34	HIS
1	C	44	ASN
1	C	97	ASN
1	C	168	GLN
1	C	235	ASN
1	C	264	GLN
1	C	274	ASN
1	C	325	ASN
1	C	336	GLN
1	C	399	HIS
1	C	412	ASN
1	C	450	HIS
1	C	453	ASN
1	C	481	ASN
1	C	541	ASN
1	C	560	ASN
1	C	566	GLN
1	C	576	GLN
1	C	579	ASN
1	C	727	ASN
1	C	744	GLN
1	C	793	ASN
1	D	12	GLN
1	D	30	ASN
1	D	34	HIS
1	D	97	ASN
1	D	168	GLN
1	D	235	ASN
1	D	274	ASN
1	D	336	GLN
1	D	399	HIS
1	D	412	ASN
1	D	481	ASN
1	D	541	ASN
1	D	560	ASN
1	D	566	GLN
1	D	576	GLN
1	D	579	ASN
1	D	678	ASN
1	D	696	ASN
1	D	723	GLN

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Mol	Chain	Res	Type
1	D	727	ASN
1	D	744	GLN
1	D	793	ASN
1	E	12	GLN
1	E	23	ASN
1	E	34	HIS
1	E	168	GLN
1	E	211	GLN
1	E	235	ASN
1	E	270	ASN
1	E	274	ASN
1	E	336	GLN
1	E	399	HIS
1	E	412	ASN
1	E	481	ASN
1	E	541	ASN
1	E	566	GLN
1	E	576	GLN
1	E	579	ASN
1	E	727	ASN
1	E	744	GLN
1	E	793	ASN
1	F	12	GLN
1	F	30	ASN
1	F	34	HIS
1	F	97	ASN
1	F	168	GLN
1	F	211	GLN
1	F	235	ASN
1	F	325	ASN
1	F	336	GLN
1	F	390	HIS
1	F	399	HIS
1	F	412	ASN
1	F	453	ASN
1	F	477	HIS
1	F	481	ASN
1	F	541	ASN
1	F	560	ASN
1	F	566	GLN
1	F	576	GLN
1	F	579	ASN

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Mol	Chain	Res	Type
1	F	723	GLN
1	F	727	ASN
1	F	744	GLN
1	F	767	HIS
1	F	793	ASN
1	G	12	GLN
1	G	34	HIS
1	G	62	HIS
1	G	73	HIS
1	G	97	ASN
1	G	168	GLN
1	G	235	ASN
1	G	274	ASN
1	G	325	ASN
1	G	336	GLN
1	G	450	HIS
1	G	481	ASN
1	G	541	ASN
1	G	566	GLN
1	G	579	ASN
1	G	678	ASN
1	G	723	GLN
1	G	727	ASN
1	G	744	GLN
1	G	754	GLN
1	G	793	ASN
1	H	34	HIS
1	H	168	GLN
1	H	235	ASN
1	H	250	ASN
1	H	264	GLN
1	H	274	ASN
1	H	325	ASN
1	H	336	GLN
1	H	338	ASN
1	H	341	HIS
1	H	376	ASN
1	H	399	HIS
1	H	412	ASN
1	H	481	ASN
1	H	541	ASN
1	H	566	GLN

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Mol	Chain	Res	Type
1	H	579	ASN
1	H	678	ASN
1	H	723	GLN
1	H	727	ASN
1	H	744	GLN
1	H	793	ASN
1	H	832	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	LLP	E	680	1	23,24,25	1.67	3 (13%)	25,32,34	1.58	6 (24%)
1	LLP	G	680	1	23,24,25	1.58	3 (13%)	25,32,34	1.53	5 (20%)
1	LLP	D	680	1	23,24,25	1.74	4 (17%)	25,32,34	1.45	6 (24%)
1	LLP	F	680	1	23,24,25	1.60	3 (13%)	25,32,34	1.43	4 (16%)
1	LLP	H	680	1	23,24,25	1.72	4 (17%)	25,32,34	1.29	5 (20%)
1	LLP	C	680	1	23,24,25	1.67	3 (13%)	25,32,34	1.39	4 (16%)
1	LLP	A	680	1	23,24,25	1.84	4 (17%)	25,32,34	1.43	5 (20%)
1	LLP	B	680	1	23,24,25	1.75	5 (21%)	25,32,34	1.40	5 (20%)

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
1	LLP	E	680	1	-	1/16/17/19	0/1/1/1
1	LLP	G	680	1	-	0/16/17/19	0/1/1/1
1	LLP	D	680	1	-	4/16/17/19	0/1/1/1
1	LLP	F	680	1	-	2/16/17/19	0/1/1/1
1	LLP	H	680	1	-	3/16/17/19	0/1/1/1
1	LLP	C	680	1	-	3/16/17/19	0/1/1/1
1	LLP	A	680	1	-	2/16/17/19	0/1/1/1
1	LLP	B	680	1	-	3/16/17/19	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	O3-C3	-6.24	1.22	1.37
1	C	680	LLP	O3-C3	-5.77	1.23	1.37
1	B	680	LLP	O3-C3	-5.77	1.23	1.37
1	H	680	LLP	O3-C3	-5.73	1.23	1.37
1	E	680	LLP	O3-C3	-5.61	1.23	1.37
1	D	680	LLP	O3-C3	-5.50	1.24	1.37
1	F	680	LLP	O3-C3	-5.47	1.24	1.37
1	G	680	LLP	O3-C3	-5.34	1.24	1.37
1	A	680	LLP	C2-N1	2.81	1.39	1.33
1	H	680	LLP	C4-C4'	2.73	1.51	1.46
1	G	680	LLP	C2-N1	2.70	1.38	1.33
1	B	680	LLP	C4-C4'	2.63	1.51	1.46
1	H	680	LLP	C2-N1	2.62	1.38	1.33
1	C	680	LLP	C4-C4'	2.61	1.51	1.46
1	E	680	LLP	C4-C4'	2.59	1.51	1.46
1	D	680	LLP	C4-C5	-2.54	1.38	1.42
1	B	680	LLP	C2-N1	2.51	1.38	1.33
1	F	680	LLP	C2-N1	2.45	1.38	1.33
1	E	680	LLP	C2-N1	2.45	1.38	1.33
1	C	680	LLP	C2-N1	2.38	1.38	1.33
1	A	680	LLP	C4-C5	-2.33	1.39	1.42
1	G	680	LLP	C4-C4'	2.31	1.51	1.46
1	D	680	LLP	C2-N1	2.28	1.38	1.33
1	D	680	LLP	C4-C4'	2.25	1.50	1.46
1	F	680	LLP	C4-C4'	2.23	1.50	1.46
1	H	680	LLP	C4'-NZ	2.16	1.34	1.27
1	A	680	LLP	C4-C4'	2.08	1.50	1.46
1	B	680	LLP	C4'-NZ	2.03	1.34	1.27
1	B	680	LLP	C6-N1	2.02	1.38	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	680	LLP	OP4-C5'-C5	3.63	116.27	109.35
1	B	680	LLP	OP4-C5'-C5	3.35	115.74	109.35
1	G	680	LLP	CE-NZ-C4'	-3.35	108.61	118.90
1	A	680	LLP	CE-NZ-C4'	-3.13	109.28	118.90
1	B	680	LLP	CE-NZ-C4'	-3.12	109.32	118.90
1	E	680	LLP	CE-NZ-C4'	-2.96	109.82	118.90
1	C	680	LLP	C5-C6-N1	-2.94	118.93	123.82
1	G	680	LLP	C5-C6-N1	-2.91	118.98	123.82
1	A	680	LLP	C5-C6-N1	-2.85	119.08	123.82
1	F	680	LLP	C5-C6-N1	-2.74	119.26	123.82
1	A	680	LLP	C4-C4'-NZ	-2.73	111.78	124.31
1	C	680	LLP	C4-C4'-NZ	-2.66	112.09	124.31
1	D	680	LLP	CE-NZ-C4'	-2.64	110.78	118.90
1	G	680	LLP	C4-C4'-NZ	-2.62	112.26	124.31
1	F	680	LLP	C4-C4'-NZ	-2.60	112.35	124.31
1	E	680	LLP	C5-C6-N1	-2.60	119.48	123.82
1	G	680	LLP	C4-C3-C2	-2.54	118.62	120.19
1	C	680	LLP	CE-NZ-C4'	-2.48	111.27	118.90
1	F	680	LLP	CE-NZ-C4'	-2.48	111.29	118.90
1	A	680	LLP	OP3-P-OP4	-2.45	100.22	106.73
1	H	680	LLP	CE-NZ-C4'	-2.44	111.41	118.90
1	D	680	LLP	C4-C4'-NZ	-2.41	113.22	124.31
1	H	680	LLP	C4-C4'-NZ	-2.39	113.33	124.31
1	H	680	LLP	C5-C6-N1	-2.37	119.86	123.82
1	D	680	LLP	C5-C4-C4'	-2.31	117.77	121.56
1	H	680	LLP	OP3-P-OP4	-2.28	100.66	106.73
1	A	680	LLP	OP3-P-OP2	2.27	116.29	107.64
1	B	680	LLP	C4-C4'-NZ	-2.26	113.94	124.31
1	E	680	LLP	C4-C4'-NZ	-2.25	113.97	124.31
1	G	680	LLP	OP3-P-OP2	2.24	116.18	107.64
1	D	680	LLP	C5-C6-N1	-2.20	120.16	123.82
1	B	680	LLP	C5-C6-N1	-2.18	120.19	123.82
1	F	680	LLP	OP3-P-OP2	2.17	115.93	107.64
1	D	680	LLP	OP3-P-OP2	2.15	115.83	107.64
1	H	680	LLP	OP3-P-OP2	2.12	115.76	107.64
1	E	680	LLP	OP3-P-OP2	2.12	115.75	107.64
1	C	680	LLP	OP3-P-OP2	2.12	115.73	107.64
1	D	680	LLP	OP2-P-OP4	-2.09	101.17	106.73
1	B	680	LLP	OP3-P-OP2	2.06	115.51	107.64
1	E	680	LLP	C5-C4-C4'	-2.03	118.22	121.56

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	680	LLP	C5'-OP4-P-OP2
1	A	680	LLP	C5'-OP4-P-OP3
1	B	680	LLP	C5'-OP4-P-OP1
1	B	680	LLP	C5'-OP4-P-OP2
1	B	680	LLP	C5'-OP4-P-OP3
1	C	680	LLP	C5'-OP4-P-OP1
1	C	680	LLP	C5'-OP4-P-OP2
1	C	680	LLP	C5'-OP4-P-OP3
1	D	680	LLP	C5'-OP4-P-OP2
1	D	680	LLP	C5'-OP4-P-OP3
1	H	680	LLP	C5'-OP4-P-OP1
1	H	680	LLP	C5'-OP4-P-OP2
1	H	680	LLP	C5'-OP4-P-OP3
1	F	680	LLP	C4-C5-C5'-OP4
1	D	680	LLP	CE-CD-CG-CB
1	F	680	LLP	C6-C5-C5'-OP4
1	E	680	LLP	CD-CE-NZ-C4'
1	D	680	LLP	C5'-OP4-P-OP1

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	680	LLP	4	0
1	G	680	LLP	6	0
1	D	680	LLP	1	0
1	F	680	LLP	3	0
1	H	680	LLP	3	0
1	C	680	LLP	5	0
1	A	680	LLP	3	0
1	B	680	LLP	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SO4	E	844	-	4,4,4	0.12	0	6,6,6	0.24	0
3	SO4	G	845	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	C	844	-	4,4,4	0.15	0	6,6,6	0.21	0
2	AMP	F	843	-	22,25,25	1.04	2 (9%)	25,38,38	1.46	4 (16%)
2	AMP	C	843	-	22,25,25	1.07	2 (9%)	25,38,38	1.31	4 (16%)
2	AMP	G	843	-	22,25,25	0.96	1 (4%)	25,38,38	1.47	3 (12%)
3	SO4	A	844	-	4,4,4	0.12	0	6,6,6	0.20	0
3	SO4	C	845	-	4,4,4	0.15	0	6,6,6	0.21	0
3	SO4	F	845	-	4,4,4	0.12	0	6,6,6	0.18	0
2	AMP	A	843	-	22,25,25	1.10	3 (13%)	25,38,38	1.39	4 (16%)
2	AMP	D	843	-	22,25,25	1.09	3 (13%)	25,38,38	1.49	4 (16%)
2	AMP	E	843	-	22,25,25	1.05	2 (9%)	25,38,38	1.32	4 (16%)
3	SO4	D	845	-	4,4,4	0.11	0	6,6,6	0.17	0
3	SO4	B	844	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	E	845	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	H	899	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	A	845	-	4,4,4	0.13	0	6,6,6	0.15	0
2	AMP	H	843	-	22,25,25	1.00	2 (9%)	25,38,38	1.42	4 (16%)
3	SO4	F	844	-	4,4,4	0.15	0	6,6,6	0.22	0
3	SO4	H	844	-	4,4,4	0.13	0	6,6,6	0.18	0
2	AMP	B	843	-	22,25,25	1.02	1 (4%)	25,38,38	1.29	2 (8%)
3	SO4	G	844	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	D	844	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	B	845	-	4,4,4	0.12	0	6,6,6	0.16	0

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	AMP	E	843	-	-	0/6/26/26	0/3/3/3
2	AMP	B	843	-	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	F	843	-	-	0/6/26/26	0/3/3/3
2	AMP	C	843	-	-	0/6/26/26	0/3/3/3
2	AMP	G	843	-	-	0/6/26/26	0/3/3/3
2	AMP	H	843	-	-	0/6/26/26	0/3/3/3
2	AMP	A	843	-	-	0/6/26/26	0/3/3/3
2	AMP	D	843	-	-	0/6/26/26	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	843	AMP	C5-C4	2.67	1.48	1.40
2	H	843	AMP	C5-C4	2.67	1.48	1.40
2	D	843	AMP	C5-C4	2.66	1.48	1.40
2	E	843	AMP	C5-C4	2.65	1.48	1.40
2	C	843	AMP	C5-C4	2.64	1.47	1.40
2	A	843	AMP	C5-C4	2.61	1.47	1.40
2	G	843	AMP	C5-C4	2.33	1.47	1.40
2	F	843	AMP	O4'-C1'	2.30	1.44	1.41
2	A	843	AMP	O4'-C1'	2.24	1.44	1.41
2	F	843	AMP	C5-C4	2.18	1.46	1.40
2	C	843	AMP	C2-N3	2.16	1.35	1.32
2	D	843	AMP	O4'-C1'	2.14	1.44	1.41
2	H	843	AMP	O4'-C1'	2.08	1.44	1.41
2	D	843	AMP	C2-N3	2.07	1.35	1.32
2	E	843	AMP	C2-N3	2.07	1.35	1.32
2	A	843	AMP	C2-N3	2.05	1.35	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	843	AMP	N3-C2-N1	-3.68	122.92	128.68
2	E	843	AMP	N3-C2-N1	-3.61	123.04	128.68
2	B	843	AMP	N3-C2-N1	-3.60	123.05	128.68
2	G	843	AMP	O5'-P-O1P	-3.53	96.57	106.47
2	D	843	AMP	N3-C2-N1	-3.47	123.26	128.68
2	C	843	AMP	N3-C2-N1	-3.45	123.28	128.68
2	H	843	AMP	N3-C2-N1	-3.37	123.41	128.68
2	G	843	AMP	N3-C2-N1	-3.35	123.44	128.68
2	D	843	AMP	C4-C5-N7	-3.32	105.94	109.40
2	A	843	AMP	N3-C2-N1	-3.16	123.73	128.68
2	F	843	AMP	C4-C5-N7	-3.05	106.22	109.40
2	D	843	AMP	P-O5'-C5'	2.78	125.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	843	AMP	O5'-P-O1P	-2.77	98.71	106.47
2	A	843	AMP	O5'-P-O1P	-2.64	99.08	106.47
2	D	843	AMP	O5'-P-O1P	-2.52	99.42	106.47
2	H	843	AMP	O5'-P-O1P	-2.43	99.65	106.47
2	G	843	AMP	C3'-C2'-C1'	2.42	104.63	100.98
2	A	843	AMP	C3'-C2'-C1'	2.40	104.60	100.98
2	H	843	AMP	C2-N1-C6	2.37	122.81	118.75
2	E	843	AMP	C3'-C2'-C1'	2.31	104.46	100.98
2	H	843	AMP	N6-C6-N1	2.22	123.18	118.57
2	C	843	AMP	C3'-C2'-C1'	2.21	104.30	100.98
2	C	843	AMP	C2-N1-C6	2.19	122.50	118.75
2	F	843	AMP	C3'-C2'-C1'	2.18	104.26	100.98
2	E	843	AMP	C4-C5-N7	-2.17	107.13	109.40
2	B	843	AMP	C2-N1-C6	2.16	122.44	118.75
2	E	843	AMP	C2-N1-C6	2.12	122.37	118.75
2	C	843	AMP	N6-C6-N1	2.07	122.88	118.57
2	A	843	AMP	P-O5'-C5'	2.01	123.82	118.30

There are no chirality outliers.

There are no torsion outliers.

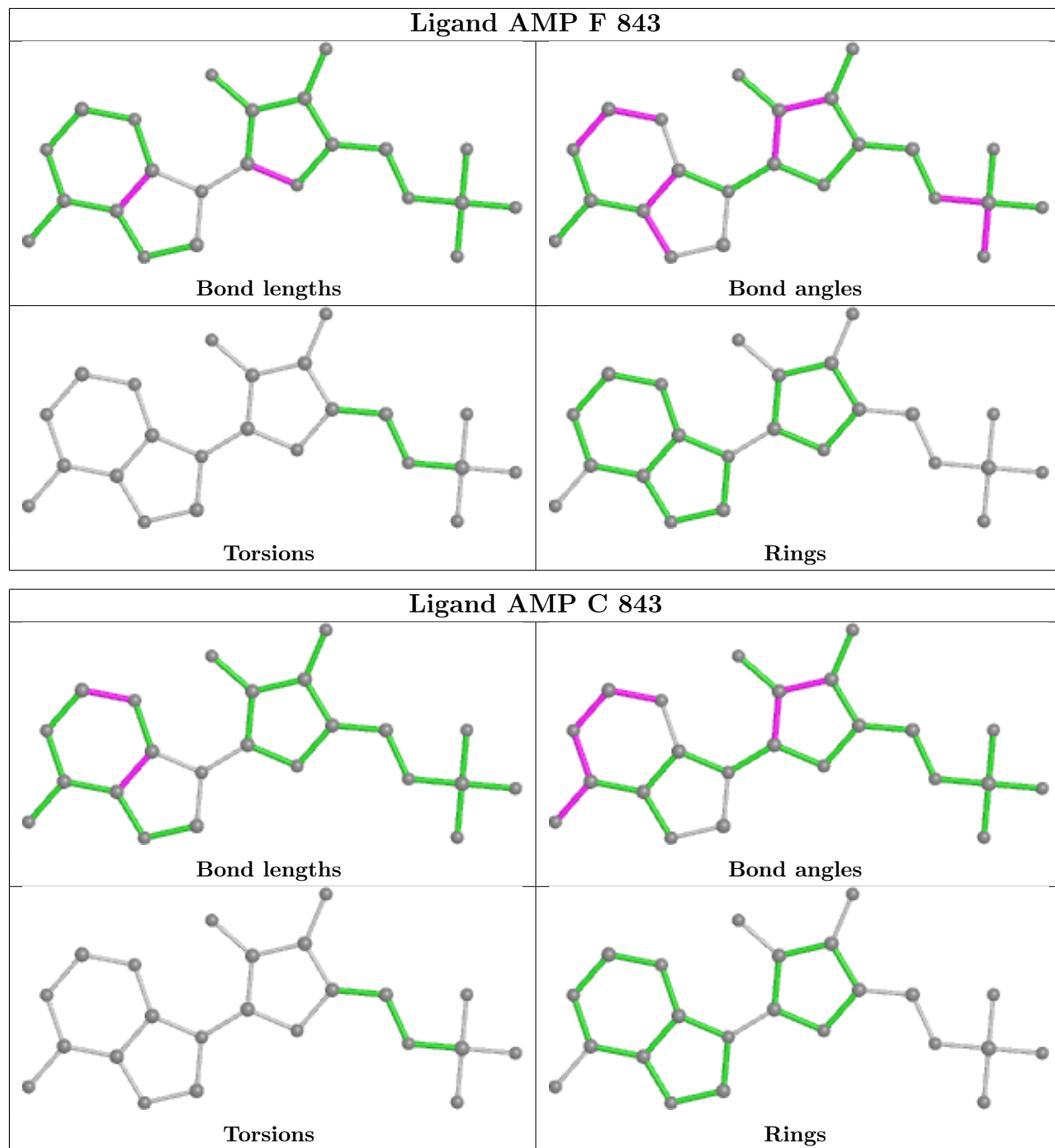
There are no ring outliers.

6 monomers are involved in 7 short contacts:

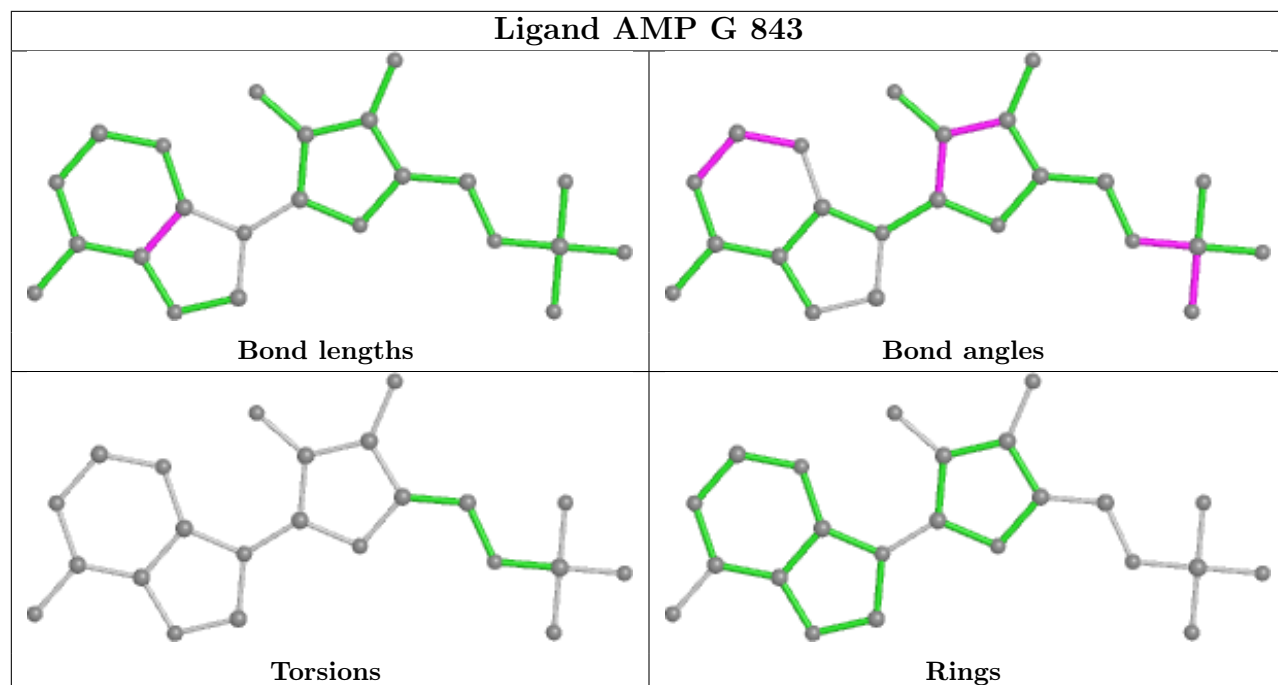
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	843	AMP	1	0
3	F	845	SO4	1	0
2	A	843	AMP	1	0
2	H	843	AMP	1	0
2	B	843	AMP	2	0
3	G	844	SO4	1	0

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

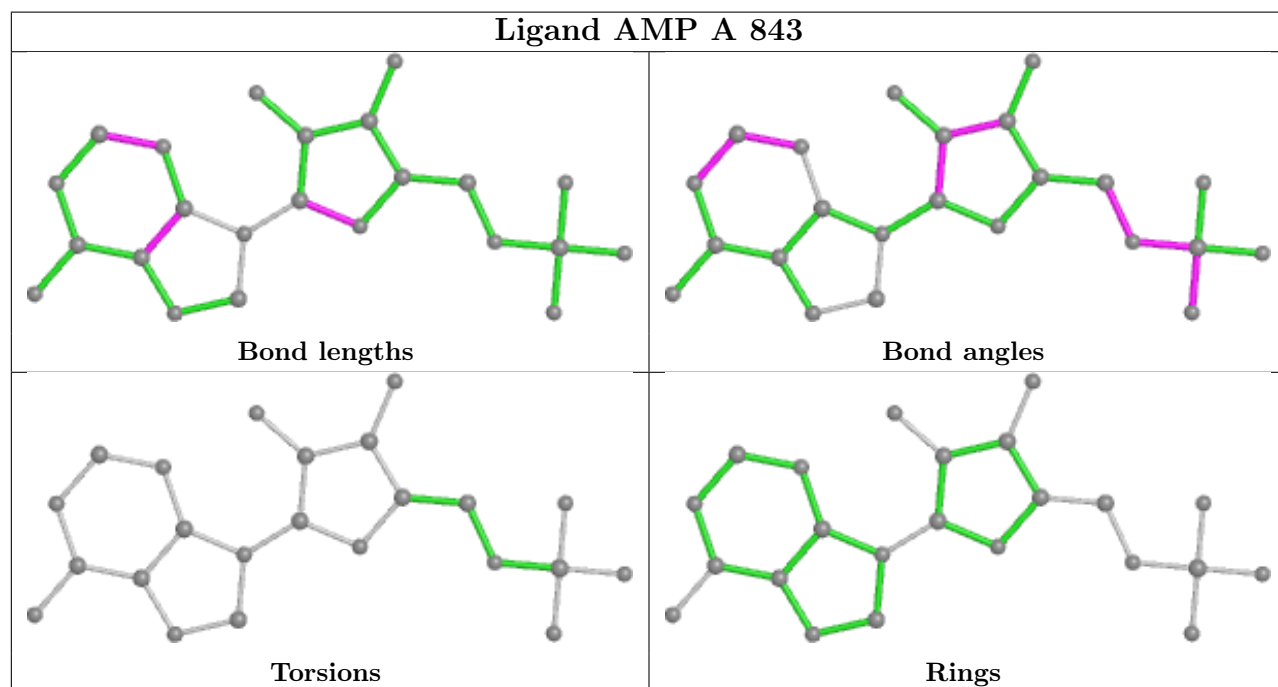
equivalents in the CSD to analyse the geometry.



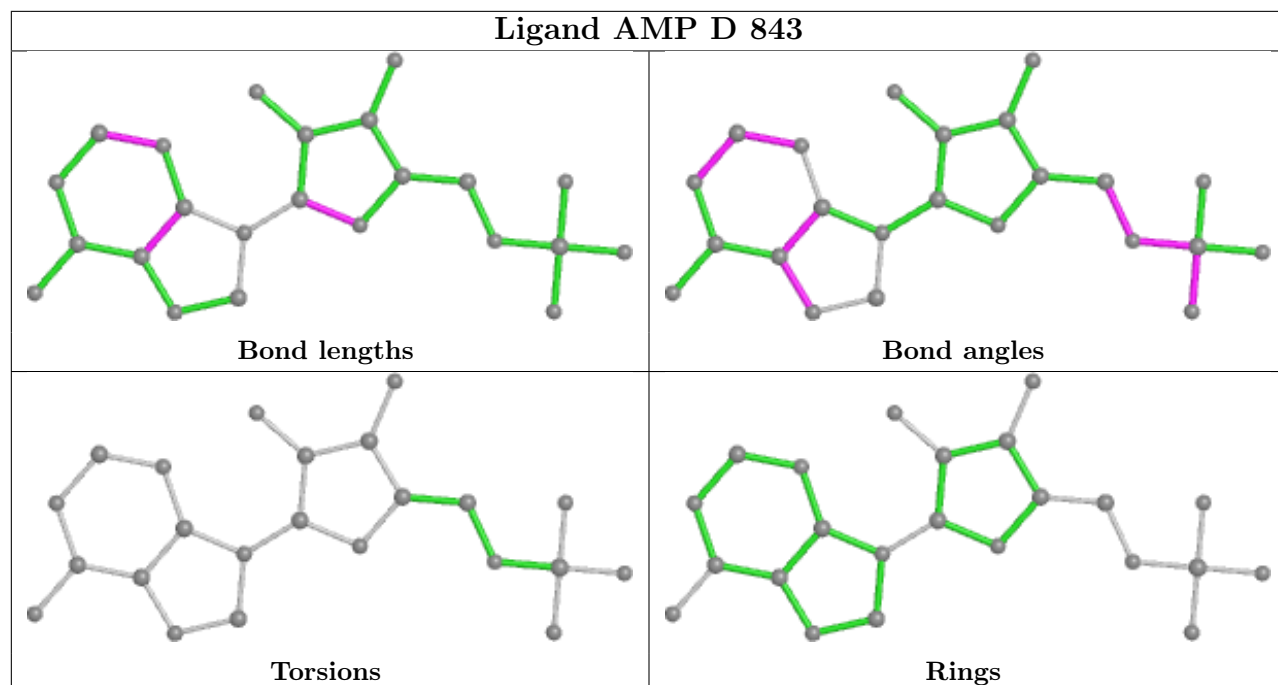
Ligand AMP G 843



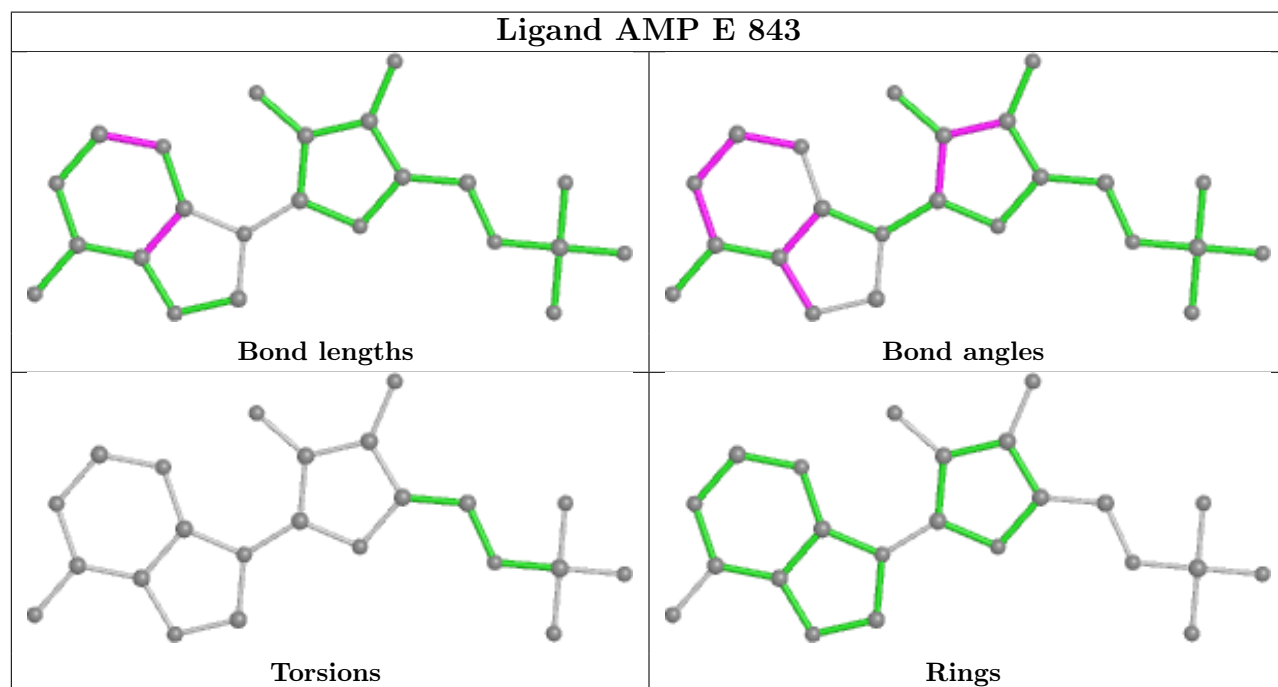
Ligand AMP A 843

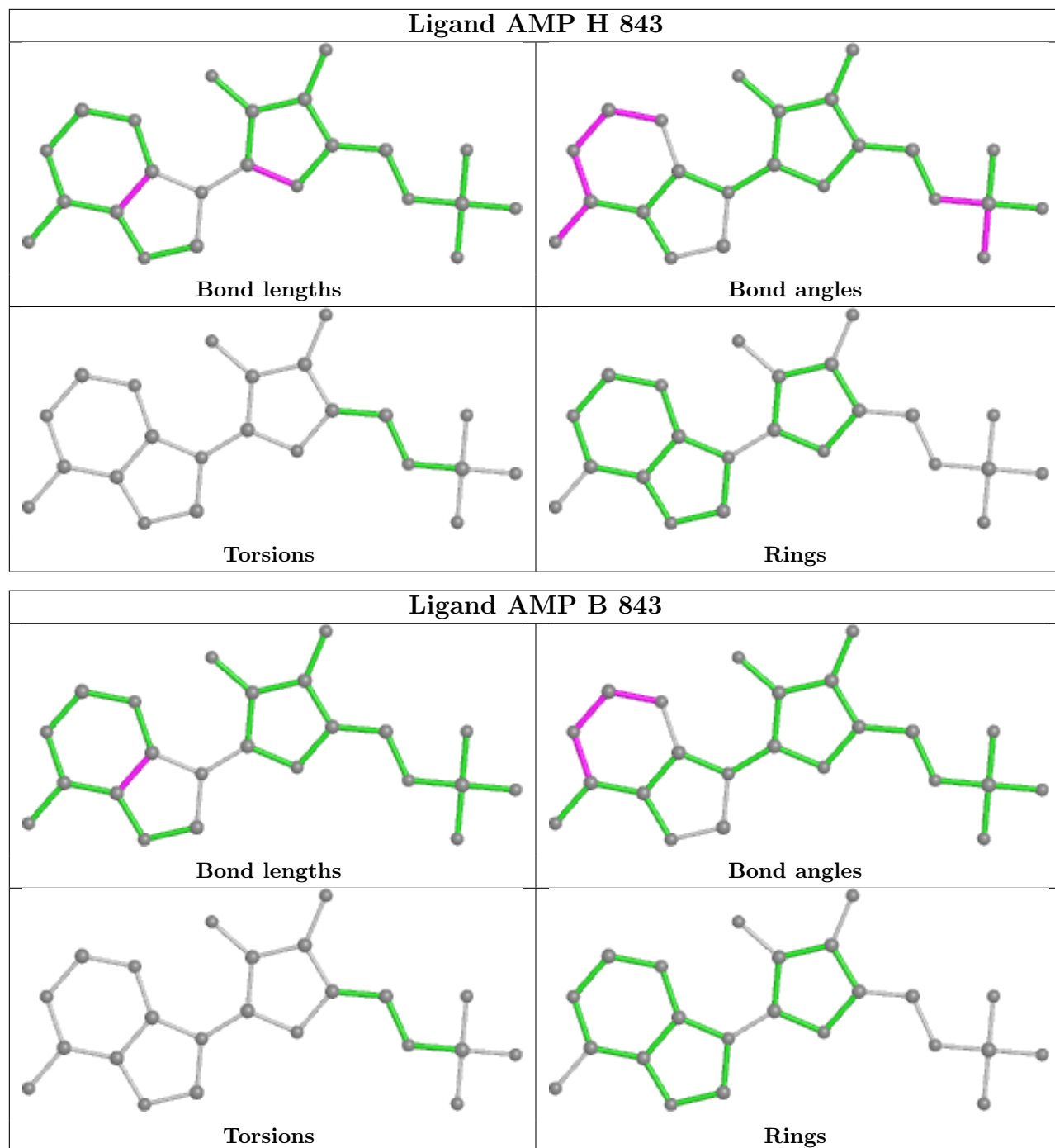


Ligand AMP D 843



Ligand AMP E 843





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	813/842 (96%)	-0.33	18 (2%) 62 63	7, 21, 42, 58	0
1	B	814/842 (96%)	-0.04	33 (4%) 37 36	4, 25, 50, 75	0
1	C	801/842 (95%)	-0.18	19 (2%) 59 60	3, 21, 41, 54	0
1	D	814/842 (96%)	-0.23	11 (1%) 75 77	6, 22, 38, 54	0
1	E	802/842 (95%)	-0.17	16 (1%) 65 67	5, 23, 43, 54	0
1	F	812/842 (96%)	-0.22	17 (2%) 63 65	3, 20, 38, 57	0
1	G	813/842 (96%)	-0.29	16 (1%) 65 67	7, 21, 41, 57	0
1	H	813/842 (96%)	-0.04	33 (4%) 37 36	8, 28, 54, 69	0
All	All	6482/6736 (96%)	-0.19	163 (2%) 57 59	3, 23, 44, 75	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	288	GLY	6.8
1	A	288	GLY	6.5
1	B	210	SER	6.3
1	C	288	GLY	6.3
1	H	380	LEU	5.8
1	B	281	PRO	5.7
1	E	288	GLY	5.6
1	G	288	GLY	5.3
1	C	165	ILE	5.0
1	B	163	PHE	4.6
1	H	288	GLY	4.5
1	F	288	GLY	4.3
1	B	380	LEU	4.3
1	H	165	ILE	4.2
1	B	320	ASP	4.2
1	H	320	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	261	GLY	3.8
1	F	165	ILE	3.7
1	C	551	ARG	3.7
1	H	555	VAL	3.7
1	G	165	ILE	3.6
1	B	317	GLY	3.6
1	B	208	HIS	3.5
1	F	380	LEU	3.5
1	B	280	TYR	3.5
1	H	381	PRO	3.5
1	D	7	GLN	3.5
1	H	163	PHE	3.4
1	A	835	PRO	3.4
1	H	556	HIS	3.4
1	H	382	GLU	3.4
1	B	381	PRO	3.3
1	B	837	PRO	3.3
1	F	20	GLY	3.3
1	A	210	SER	3.3
1	H	553	TYR	3.3
1	B	16	ARG	3.2
1	F	210	SER	3.2
1	C	554	LYS	3.1
1	C	580	CYS	3.1
1	G	380	LEU	3.1
1	B	554	LYS	3.1
1	C	556	HIS	3.1
1	B	321	PRO	3.1
1	C	597	PHE	3.1
1	H	130	GLY	3.1
1	H	261	GLY	3.0
1	B	165	ILE	3.0
1	F	211	GLN	3.0
1	A	165	ILE	3.0
1	B	723	GLN	3.0
1	B	553	TYR	2.9
1	D	212	GLY	2.9
1	E	16	ARG	2.9
1	D	211	GLN	2.9
1	E	556	HIS	2.9
1	B	551	ARG	2.9
1	H	321	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	554	LYS	2.8
1	G	382	GLU	2.8
1	G	554	LYS	2.8
1	G	262	TYR	2.8
1	F	597	PHE	2.8
1	G	379	VAL	2.8
1	H	610	ALA	2.8
1	A	551	ARG	2.8
1	F	164	GLY	2.8
1	A	836	ALA	2.8
1	A	380	LEU	2.8
1	B	288	GLY	2.8
1	E	551	ARG	2.8
1	H	208	HIS	2.7
1	B	382	GLU	2.7
1	D	595	ASN	2.7
1	B	556	HIS	2.6
1	G	208	HIS	2.6
1	G	381	PRO	2.6
1	C	595	ASN	2.6
1	G	612	GLY	2.6
1	H	434	GLY	2.6
1	C	833	ARG	2.6
1	E	595	ASN	2.5
1	A	208	HIS	2.5
1	H	612	GLY	2.5
1	F	11	LYS	2.5
1	A	382	GLU	2.5
1	H	611	PRO	2.5
1	E	720	ARG	2.5
1	H	831	ARG	2.5
1	A	211	GLN	2.4
1	H	280	TYR	2.4
1	F	262	TYR	2.4
1	D	380	LEU	2.4
1	H	176	MET	2.4
1	F	277	ARG	2.4
1	H	16	ARG	2.4
1	H	549	LEU	2.4
1	C	262	TYR	2.4
1	E	597	PHE	2.4
1	B	21	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	280	TYR	2.3
1	A	592	LYS	2.3
1	D	261	GLY	2.3
1	H	164	GLY	2.3
1	E	165	ILE	2.3
1	E	580	CYS	2.3
1	F	733	ASP	2.3
1	F	212	GLY	2.3
1	A	280	TYR	2.3
1	G	280	TYR	2.3
1	A	612	GLY	2.3
1	B	612	GLY	2.3
1	G	261	GLY	2.3
1	G	210	SER	2.3
1	A	163	PHE	2.3
1	H	833	ARG	2.3
1	C	555	VAL	2.3
1	G	164	GLY	2.2
1	D	210	SER	2.2
1	F	419	PRO	2.2
1	F	595	ASN	2.2
1	G	836	ALA	2.2
1	B	278	VAL	2.2
1	D	165	ILE	2.2
1	H	133	ASN	2.2
1	D	592	LYS	2.2
1	H	277	ARG	2.2
1	E	381	PRO	2.2
1	G	436	VAL	2.2
1	B	550	GLU	2.2
1	B	261	GLY	2.2
1	B	415	ALA	2.2
1	H	435	ALA	2.2
1	E	553	TYR	2.1
1	H	551	ARG	2.1
1	B	532	ARG	2.1
1	C	596	LYS	2.1
1	B	318	CYS	2.1
1	C	581	LEU	2.1
1	E	250	ASN	2.1
1	A	554	LYS	2.1
1	E	426	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	836	ALA	2.1
1	C	381	PRO	2.1
1	H	596	LYS	2.1
1	A	555	VAL	2.1
1	B	548	TYR	2.1
1	C	613	TYR	2.1
1	C	720	ARG	2.1
1	B	322	VAL	2.1
1	H	379	VAL	2.1
1	E	596	LYS	2.1
1	B	423	ASP	2.1
1	E	208	HIS	2.0
1	B	720	ARG	2.0
1	A	381	PRO	2.0
1	C	379	VAL	2.0
1	F	422	VAL	2.0
1	C	16	ARG	2.0
1	C	565	VAL	2.0
1	B	345	ALA	2.0
1	F	465	LYS	2.0
1	H	264	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	LLP	B	680	24/25	0.96	0.18	19,27,31,32	0
1	LLP	F	680	24/25	0.96	0.15	15,17,22,23	0
1	LLP	D	680	24/25	0.97	0.15	16,17,21,24	0
1	LLP	E	680	24/25	0.97	0.14	16,19,22,23	0
1	LLP	C	680	24/25	0.97	0.14	13,16,23,23	0
1	LLP	G	680	24/25	0.97	0.17	17,18,21,23	0
1	LLP	H	680	24/25	0.97	0.14	22,25,27,27	0
1	LLP	A	680	24/25	0.98	0.14	17,19,22,24	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

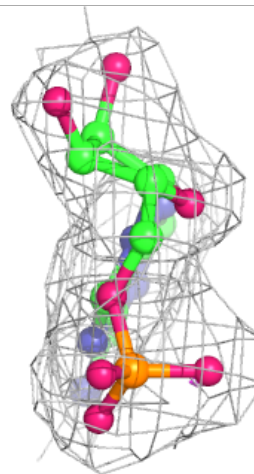
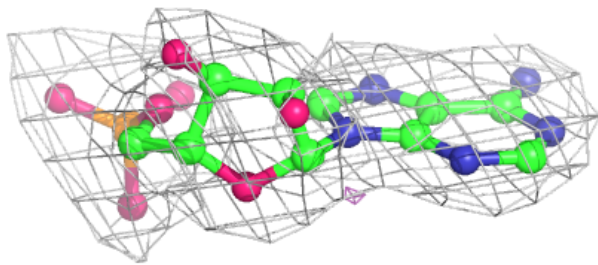
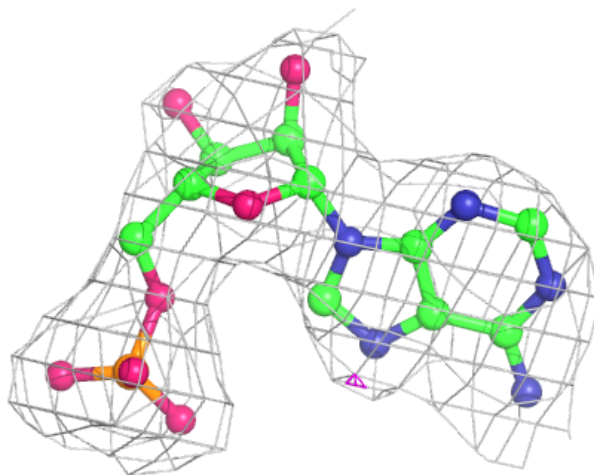
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	E	845	5/5	0.82	0.19	95,95,96,96	0
3	SO4	C	844	5/5	0.90	0.15	88,88,88,88	0
3	SO4	A	845	5/5	0.90	0.15	97,98,98,98	0
3	SO4	F	845	5/5	0.90	0.18	86,86,87,87	0
3	SO4	B	845	5/5	0.91	0.18	90,90,90,91	0
3	SO4	D	845	5/5	0.92	0.15	83,84,84,85	0
3	SO4	G	845	5/5	0.94	0.16	82,83,83,84	0
3	SO4	H	899	5/5	0.94	0.13	80,80,80,81	0
3	SO4	C	845	5/5	0.95	0.16	58,59,60,60	0
3	SO4	B	844	5/5	0.95	0.14	67,67,68,68	0
2	AMP	E	843	23/23	0.97	0.10	33,37,39,39	0
2	AMP	F	843	23/23	0.97	0.12	20,26,27,27	0
2	AMP	G	843	23/23	0.97	0.10	23,28,30,30	0
3	SO4	E	844	5/5	0.97	0.10	71,72,73,73	0
2	AMP	H	843	23/23	0.97	0.13	28,34,34,36	0
3	SO4	F	844	5/5	0.97	0.15	58,59,59,60	0
2	AMP	B	843	23/23	0.97	0.11	26,35,36,36	0
2	AMP	C	843	23/23	0.97	0.10	28,32,34,34	0
2	AMP	D	843	23/23	0.97	0.13	27,29,31,31	0
2	AMP	A	843	23/23	0.98	0.10	25,27,29,29	0
3	SO4	D	844	5/5	0.98	0.08	66,66,66,67	0
3	SO4	H	844	5/5	0.98	0.11	46,46,46,47	0
3	SO4	A	844	5/5	0.98	0.07	47,47,48,48	0
3	SO4	G	844	5/5	0.99	0.09	40,41,42,42	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.

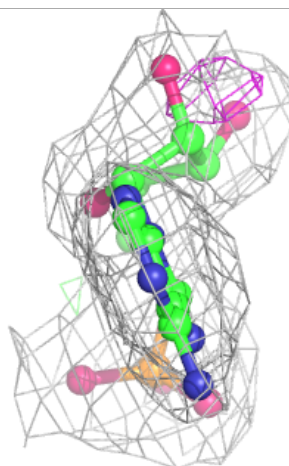
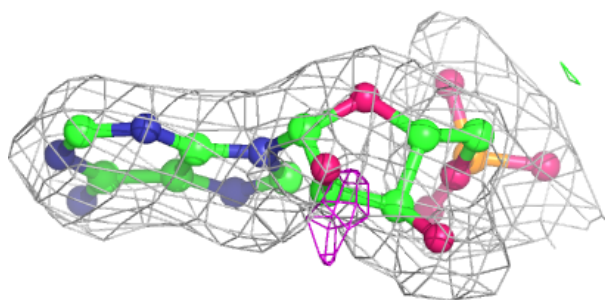
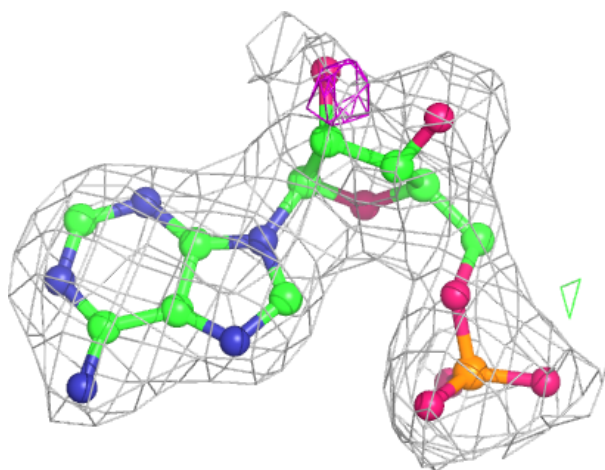
Electron density around AMP E 843:

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



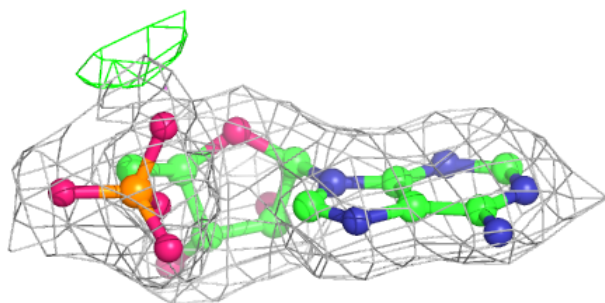
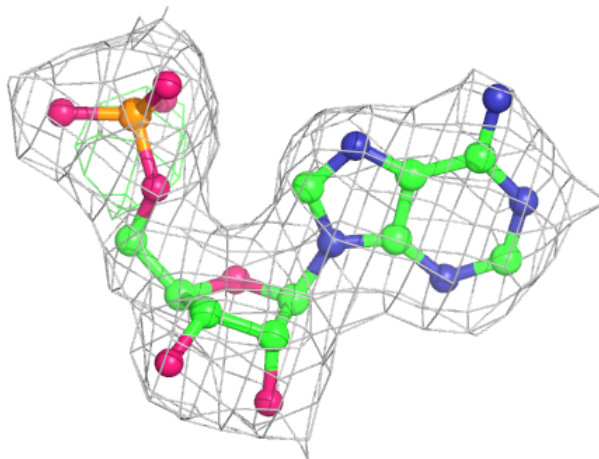
Electron density around AMP F 843:

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



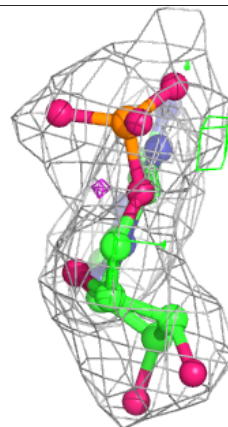
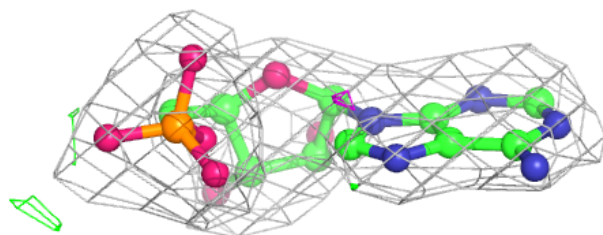
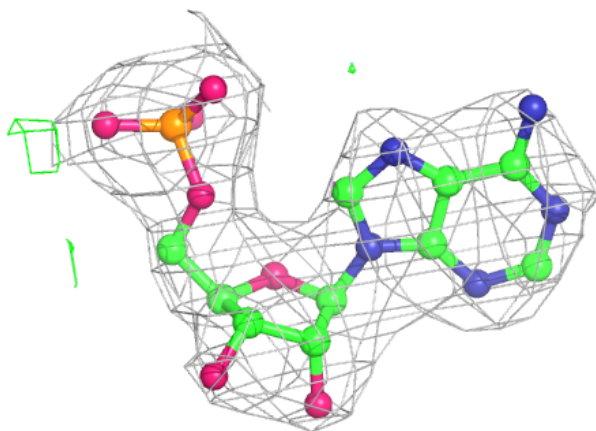
Electron density around AMP G 843:

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



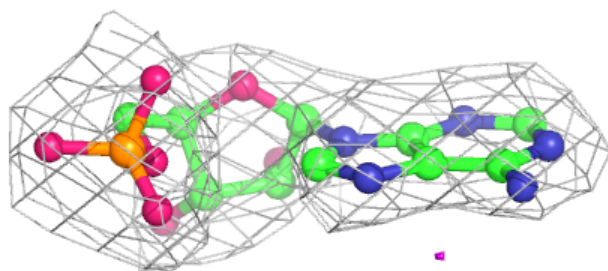
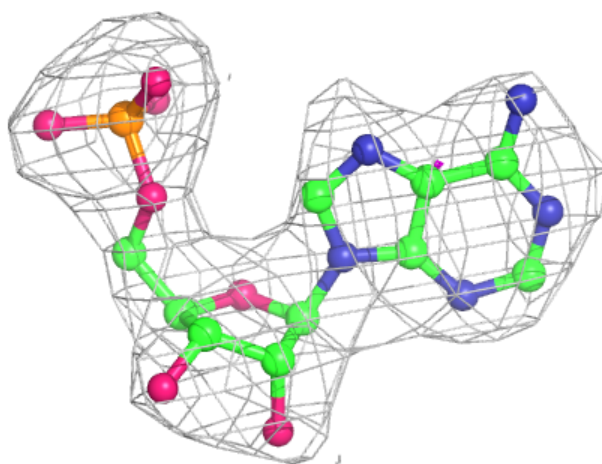
Electron density around AMP H 843:

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



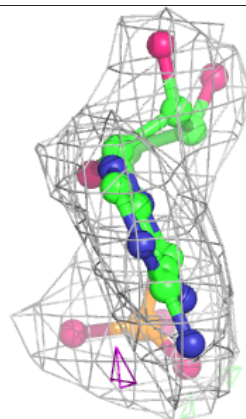
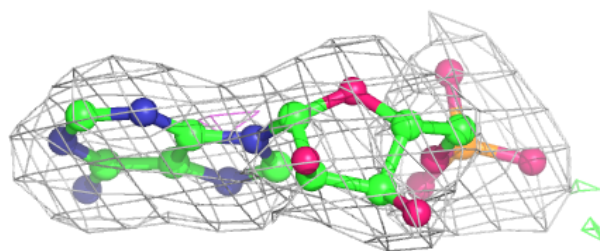
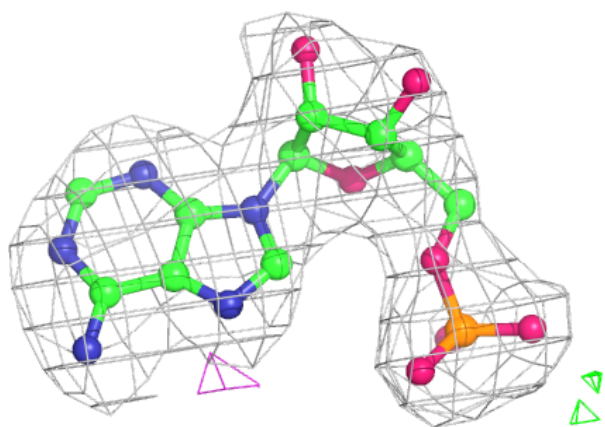
Electron density around AMP B 843:

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



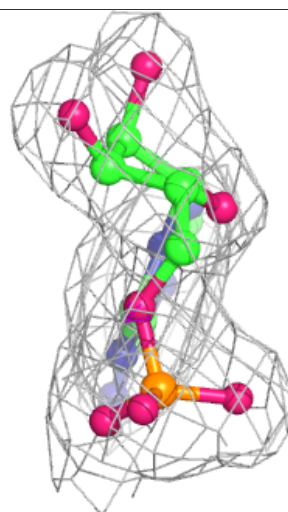
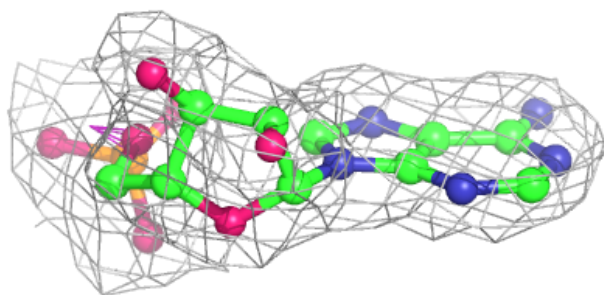
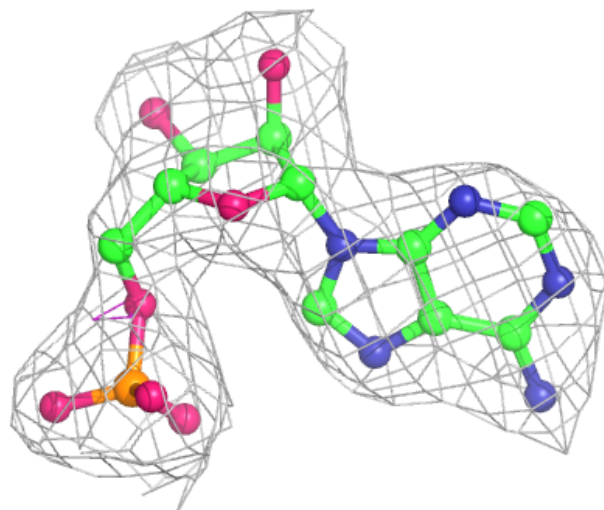
Electron density around AMP C 843:

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



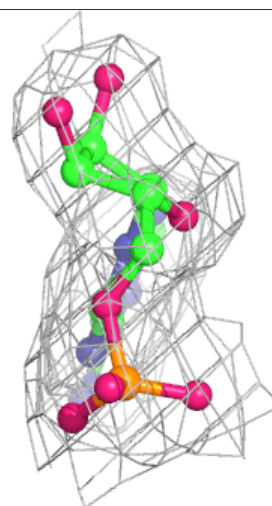
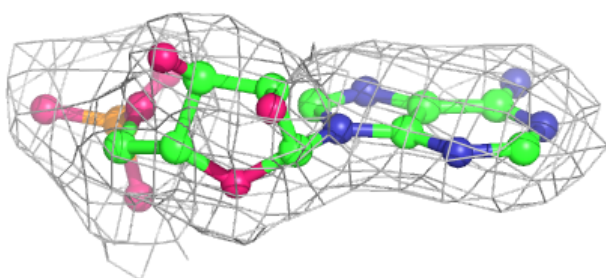
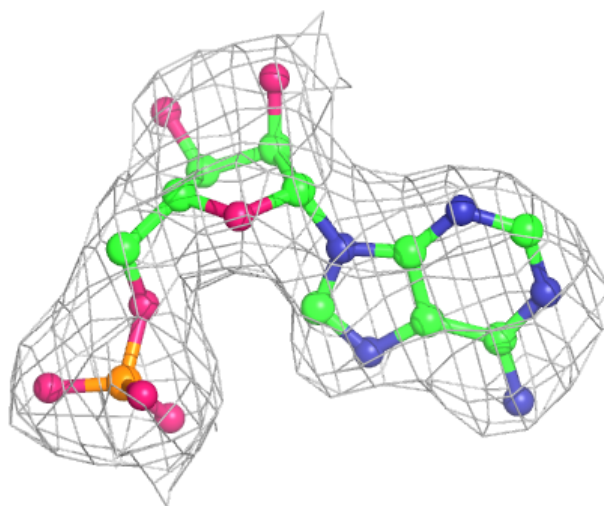
Electron density around AMP D 843:

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



Electron density around AMP A 843:

$2mF_o-DF_c$ (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.