



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:44 AM UTC

PDB ID : 1LTK / pdb_00001ltk
Title : CRYSTAL STRUCTURE OF PHOSPHOGLYCERATE KINASE FROM PLASMODIUM FALCIPARUM, IN THE OPEN CONFORMATION
Authors : Chattopadhyay, D.; Pal, B.; Smith, C.D.
Deposited on : 2002-05-20
Resolution : 3.00 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

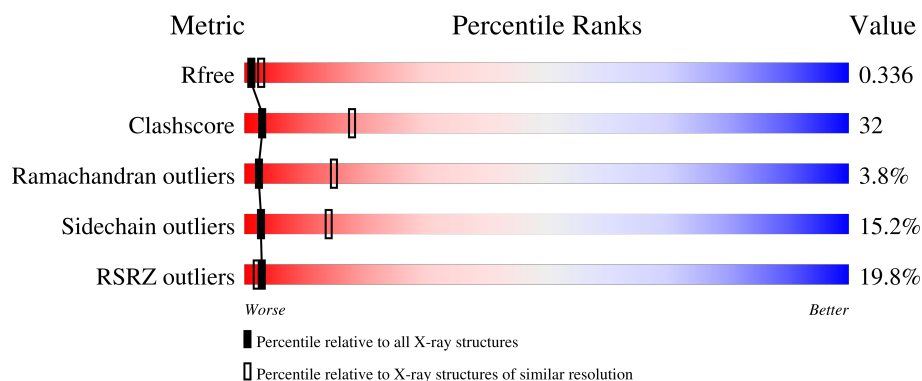
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	425	5% 47% 42% 9% .
1	B	425	12% 37% 44% 14% ..
1	C	425	40% 44% 41% 13% .

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
4	GOL	A	614	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9805 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 PHOSPHOGLYCERATE KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	Se	0	0	0
			3193	2024	546	612	3	8			
1	B	415	Total	C	N	O	S	Se	0	0	0
			3183	2018	544	610	3	8			
1	C	424	Total	C	N	O	S	Se	0	0	0
			3267	2068	566	621	3	9			

There are 30 discrepancies between the modelled and reference sequences:

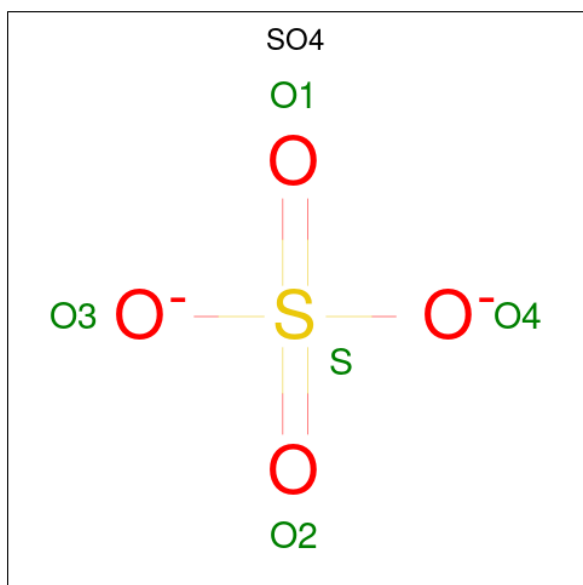
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP P27362
A	-7	HIS	-	expression tag	UNP P27362
A	-6	SER	-	expression tag	UNP P27362
A	-5	MSE	-	expression tag	UNP P27362
A	-4	HIS	-	expression tag	UNP P27362
A	-3	HIS	-	expression tag	UNP P27362
A	-2	HIS	-	expression tag	UNP P27362
A	-1	HIS	-	expression tag	UNP P27362
A	0	HIS	-	expression tag	UNP P27362
A	1	HIS	-	expression tag	UNP P27362
B	-8	GLY	-	expression tag	UNP P27362
B	-7	HIS	-	expression tag	UNP P27362
B	-6	SER	-	expression tag	UNP P27362
B	-5	MSE	-	expression tag	UNP P27362
B	-4	HIS	-	expression tag	UNP P27362
B	-3	HIS	-	expression tag	UNP P27362
B	-2	HIS	-	expression tag	UNP P27362
B	-1	HIS	-	expression tag	UNP P27362
B	0	HIS	-	expression tag	UNP P27362
B	1	HIS	-	expression tag	UNP P27362
C	-8	GLY	-	expression tag	UNP P27362
C	-7	HIS	-	expression tag	UNP P27362
C	-6	SER	-	expression tag	UNP P27362

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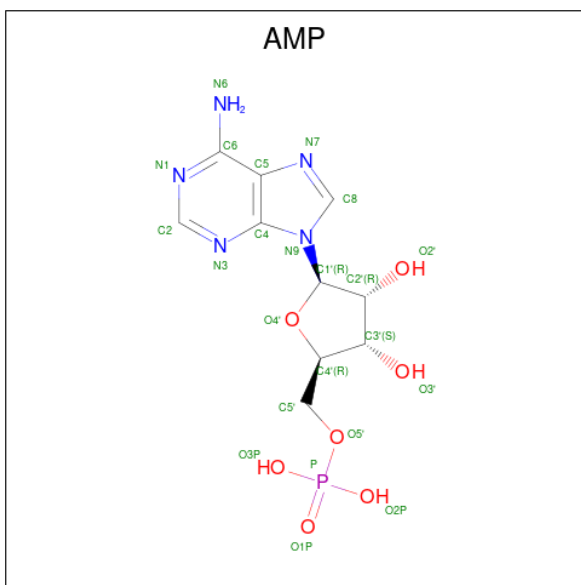
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	MSE	-	expression tag	UNP P27362
C	-4	HIS	-	expression tag	UNP P27362
C	-3	HIS	-	expression tag	UNP P27362
C	-2	HIS	-	expression tag	UNP P27362
C	-1	HIS	-	expression tag	UNP P27362
C	0	HIS	-	expression tag	UNP P27362
C	1	HIS	-	expression tag	UNP P27362

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



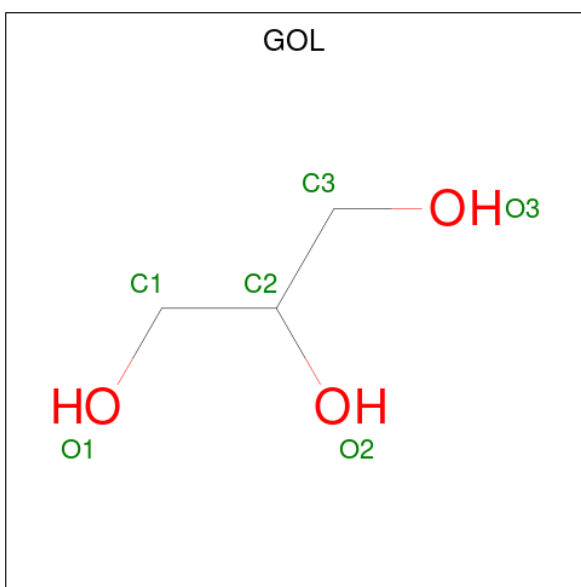
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

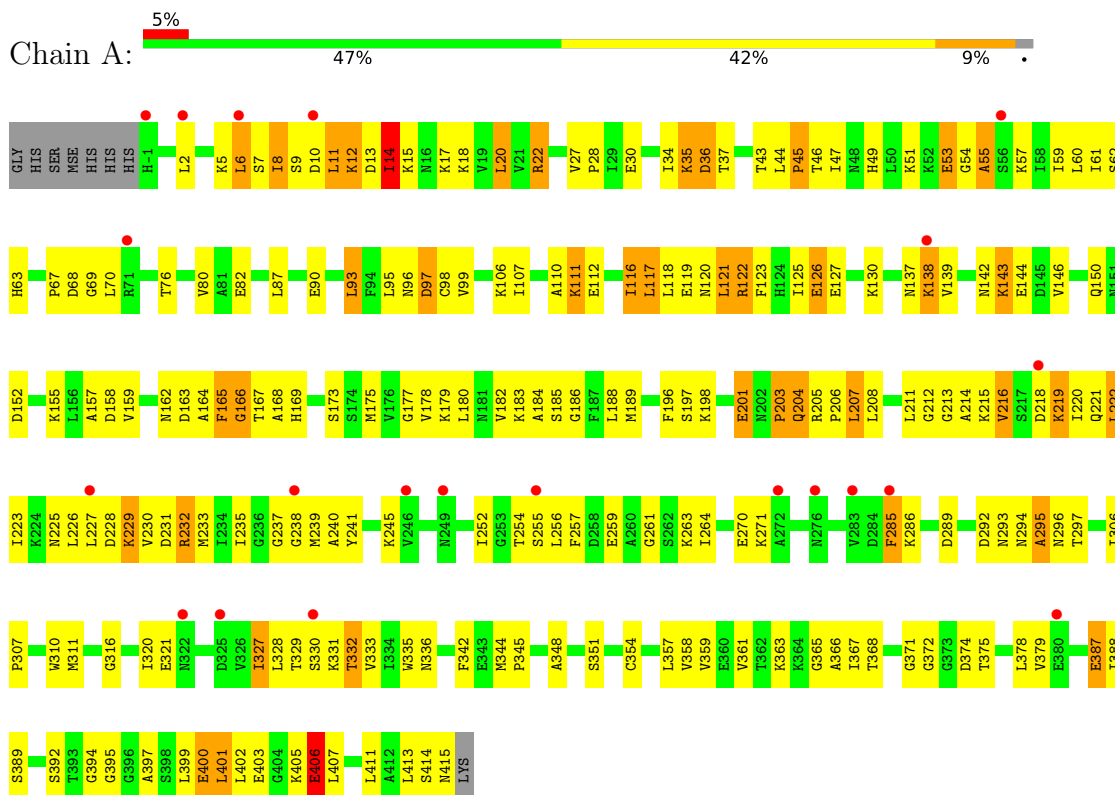
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	29	Total 29	O 29	0	0
5	B	21	Total 21	O 21	0	0
5	C	22	Total 22	O 22	0	0

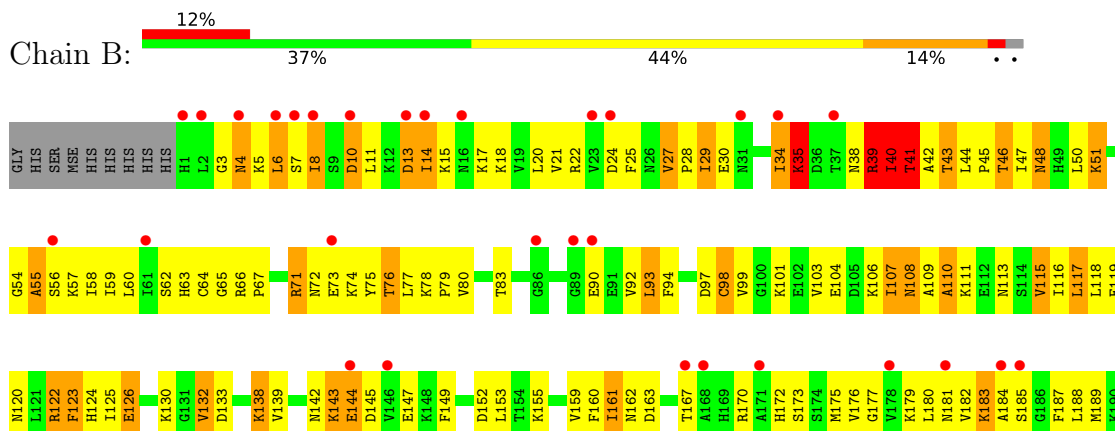
3 Residue-property plots

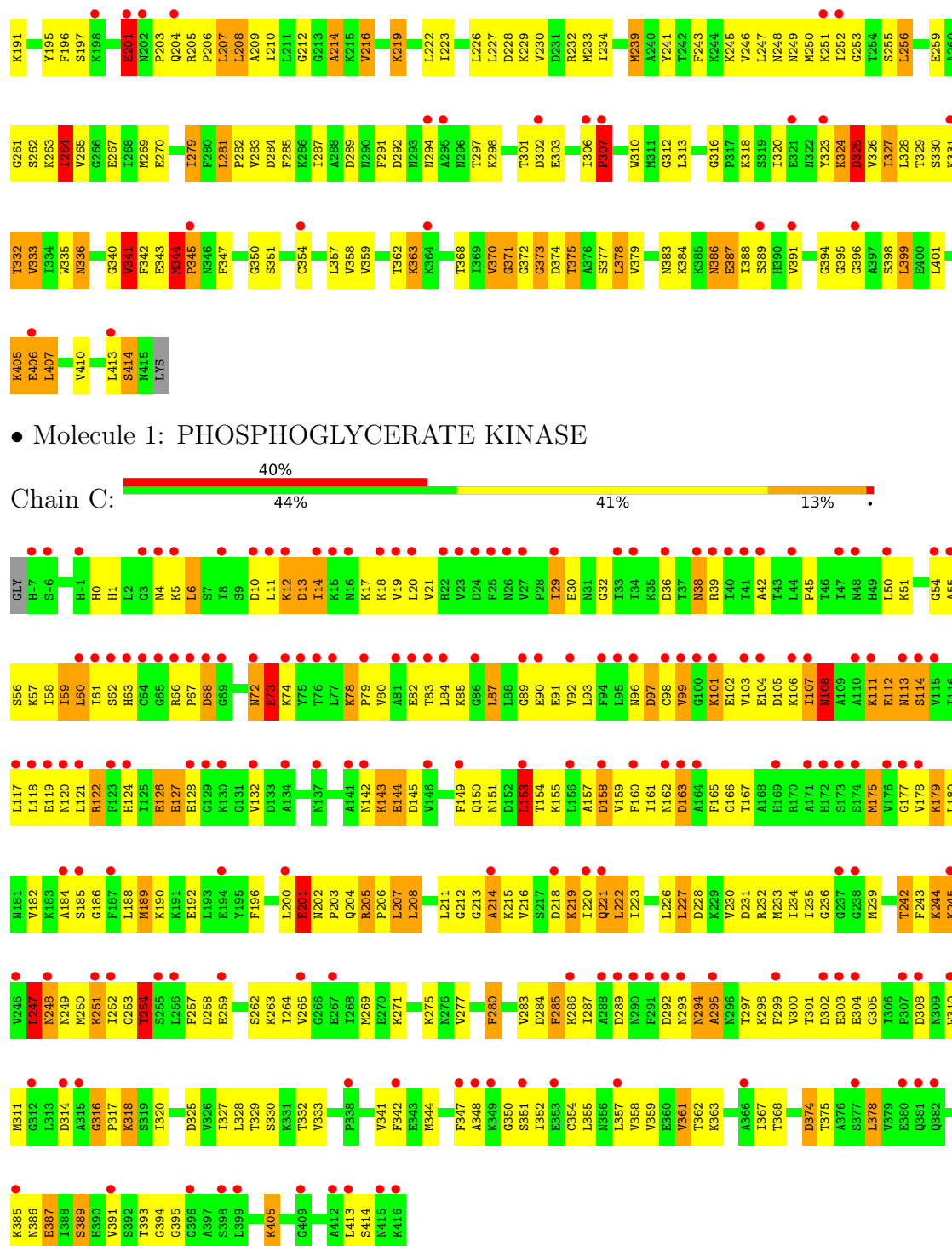
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: PHOSPHOGLYCERATE KINASE





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.03Å 147.61Å 206.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 3.00 19.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (19.93-3.00) 94.4 (19.93-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.54 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.258 0.305 , 0.336	Depositor DCC
R_{free} test set	3455 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9805	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.01	0/3227	1.25	19/4329 (0.4%)
1	B	0.99	2/3217 (0.1%)	1.29	28/4315 (0.6%)
1	C	0.99	0/3306	1.21	20/4431 (0.5%)
All	All	1.00	2/9750 (0.0%)	1.25	67/13075 (0.5%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	183	LYS	CA-C	-5.13	1.47	1.53
1	B	40	ILE	CA-CB	5.09	1.61	1.54

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	THR	N-CA-C	-10.31	99.46	113.18
1	B	39	ARG	N-CA-C	-9.83	96.79	110.35
1	B	279	ILE	N-CA-C	9.49	120.69	111.67
1	A	406	GLU	N-CA-C	8.99	124.68	112.90
1	B	123	PHE	N-CA-C	-8.91	102.18	113.23
1	A	201	GLU	CA-C-N	-8.24	115.03	122.28
1	A	201	GLU	C-N-CA	-8.24	115.03	122.28
1	A	14	ILE	N-CA-C	-8.23	105.47	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ILE	N-CA-C	-8.07	103.33	111.88
1	C	354	CYS	N-CA-C	-7.95	102.56	111.14
1	B	107	ILE	N-CA-C	-7.83	103.17	110.53
1	B	267	GLU	N-CA-C	-7.50	103.05	111.07
1	C	214	ALA	N-CA-C	7.46	119.19	111.14
1	A	216	VAL	N-CA-C	-7.45	104.71	113.42
1	B	324	LYS	N-CA-C	-7.30	103.48	113.18
1	A	374	ASP	N-CA-C	-7.28	103.34	111.71
1	C	316	GLY	CA-C-N	6.98	126.23	118.97
1	C	316	GLY	C-N-CA	6.98	126.23	118.97
1	B	333	VAL	N-CA-C	6.91	118.76	108.46
1	A	327	ILE	N-CA-C	6.80	116.92	110.53
1	B	76	THR	CB-CA-C	-6.73	99.13	109.89
1	C	153	LEU	N-CA-C	-6.69	103.91	111.14
1	A	37	THR	N-CA-C	6.69	120.42	112.93
1	B	327	ILE	N-CA-C	6.53	116.56	110.42
1	B	216	VAL	N-CA-C	-6.51	105.80	113.42
1	A	333	VAL	N-CA-C	6.42	117.54	108.17
1	A	286	LYS	N-CA-C	-6.41	99.57	109.76
1	A	321	GLU	N-CA-C	-6.38	104.54	112.90
1	C	327	ILE	N-CA-C	6.34	116.97	110.82
1	A	354	CYS	N-CA-C	-6.20	104.44	111.14
1	B	264	ILE	N-CA-C	6.18	118.04	112.17
1	B	110	ALA	N-CA-C	-6.17	99.69	109.07
1	B	325	ASP	N-CA-C	-6.17	105.25	112.89
1	A	401	LEU	N-CA-C	-6.08	104.73	111.36
1	A	123	PHE	N-CA-C	-6.06	105.88	113.28
1	C	231	ASP	N-CA-C	-6.02	106.07	113.41
1	C	387	GLU	N-CA-C	-6.00	105.91	113.72
1	C	362	THR	N-CA-C	-5.96	104.87	111.36
1	B	214	ALA	N-CA-C	5.94	117.42	111.07
1	B	387	GLU	N-CA-C	-5.92	106.39	113.97
1	A	8	ILE	N-CA-C	-5.90	104.10	110.23
1	C	389	SER	N-CA-C	5.87	118.16	111.11
1	A	237	GLY	N-CA-C	5.87	127.09	113.18
1	C	14	ILE	N-CA-C	-5.86	106.77	111.81
1	B	35	LYS	N-CA-C	5.81	119.19	111.75
1	C	96	ASN	N-CA-C	5.78	118.52	111.82
1	B	239	MSE	N-CA-C	-5.71	106.16	113.01
1	C	280	PHE	N-CA-C	5.67	118.78	107.62
1	A	306	ILE	N-CA-C	5.62	113.44	107.76
1	B	115	VAL	N-CA-C	5.59	116.53	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	213	GLY	N-CA-C	5.56	117.23	111.95
1	C	333	VAL	N-CA-C	5.46	115.75	108.11
1	A	295	ALA	N-CA-C	-5.45	100.79	109.23
1	C	227	LEU	CA-C-N	-5.42	113.83	122.66
1	C	227	LEU	C-N-CA	-5.42	113.83	122.66
1	B	344	MSE	CA-C-N	5.39	126.58	119.84
1	B	344	MSE	C-N-CA	5.39	126.58	119.84
1	A	53	GLU	N-CA-C	-5.38	106.59	114.39
1	C	108	ASN	N-CA-C	5.35	119.30	112.34
1	B	101	LYS	N-CA-C	-5.32	105.93	112.90
1	B	219	LYS	N-CA-C	-5.26	105.18	113.02
1	B	80	VAL	N-CA-C	-5.22	104.99	112.35
1	C	127	GLU	N-CA-C	-5.15	103.06	111.04
1	B	196	PHE	N-CA-C	-5.14	105.37	111.69
1	C	5	LYS	N-CA-C	5.06	116.98	108.73
1	B	27	VAL	CA-C-N	5.01	126.11	119.84
1	B	27	VAL	C-N-CA	5.01	126.11	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	195	TYR	Sidechain

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	3193	0	3296	203	0
1	B	3183	0	3292	238	2
1	C	3267	0	3361	204	2
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	23	0	12	1	0
3	B	23	0	12	2	0
3	C	23	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	6	0	4	0	0
5	A	29	0	0	0	0
5	B	21	0	0	2	0
5	C	22	0	0	2	0
All	All	9805	0	9989	637	2

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 32.

All (637) 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:250:MSE:HE2	1:C:252:ILE:HG22	1.41	1.02
1:B:42:ALA:HB1	1:B:188:LEU:HD21	1.40	1.02
1:A:93:LEU:HB3	1:A:116:ILE:HG23	1.43	0.98
1:B:264:ILE:HD13	1:B:264:ILE:H	1.28	0.96
1:A:331:LYS:HA	1:A:331:LYS:HE2	1.49	0.93
1:A:12:LYS:HD3	1:A:12:LYS:H	1.34	0.92
1:B:56:SER:O	1:B:57:LYS:HD2	1.68	0.92
1:A:14:ILE:HD12	1:A:14:ILE:H	1.33	0.92
1:B:46:THR:HG21	1:B:163:ASP:OD2	1.70	0.92
1:B:316:GLY:O	1:B:320:ILE:HG12	1.70	0.91
1:A:233:MSE:HE3	1:A:235:ILE:HD11	1.52	0.90
1:A:204:GLN:HE21	1:A:204:GLN:H	1.16	0.90
1:B:76:THR:HG23	1:B:119:GLU:OE1	1.73	0.87
1:B:336:ASN:HB2	1:B:371:GLY:HA3	1.57	0.86
1:A:2:LEU:HD21	1:A:401:LEU:HD21	1.60	0.84
1:C:342:PHE:HA	1:C:348:ALA:HB2	1.63	0.81
1:A:328:LEU:HD23	1:A:361:VAL:HG22	1.63	0.81
1:B:206:PRO:HG2	1:B:330:SER:HA	1.59	0.81
1:C:163:ASP:OD1	1:C:188:LEU:HB2	1.82	0.80
1:A:204:GLN:H	1:A:204:GLN:NE2	1.79	0.79
1:C:244:LYS:HE2	1:C:248:ASN:OD1	1.82	0.79
1:A:185:SER:HB2	1:A:189:MSE:HG2	1.64	0.79
1:B:359:VAL:HG13	1:B:387:GLU:HB3	1.62	0.79
1:C:21:VAL:HG12	1:C:161:ILE:HB	1.64	0.79
1:A:61:ILE:HB	1:A:121:LEU:HD11	1.64	0.79
1:A:327:ILE:HG22	1:A:361:VAL:HG21	1.64	0.79
1:A:204:GLN:O	1:A:332:THR:HG22	1.82	0.78
1:A:130:LYS:HB2	1:A:138:LYS:HE2	1.65	0.78
1:A:197:SER:HB2	1:A:201:GLU:OE1	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LEU:H	1:B:256:LEU:HD23	1.48	0.78
1:B:333:VAL:HB	1:B:368:THR:HG22	1.66	0.77
1:B:373:GLY:O	1:B:375:THR:N	2.18	0.77
1:A:252:ILE:HG12	1:A:255:SER:HB2	1.66	0.76
1:B:39:ARG:O	1:B:40:ILE:HG12	1.85	0.76
1:C:207:LEU:CD2	1:C:230:VAL:HA	2.16	0.75
1:B:252:ILE:HG23	1:B:255:SER:HB2	1.69	0.75
1:B:264:ILE:HD13	1:B:264:ILE:N	2.01	0.75
1:B:6:LEU:HD23	1:B:7:SER:H	1.51	0.75
1:B:107:ILE:HG13	1:B:108:ASN:N	2.02	0.75
1:B:8:ILE:HA	1:B:11:LEU:HD13	1.68	0.74
1:A:203:PRO:HB2	1:A:332:THR:HG21	1.69	0.74
1:A:6:LEU:HD13	1:A:184:ALA:HB2	1.70	0.74
1:A:220:ILE:HG23	1:A:264:ILE:HG21	1.69	0.74
1:B:344:MSE:HE3	1:B:347:PHE:CE1	2.22	0.74
1:C:142:ASN:HB2	1:C:145:ASP:OD2	1.89	0.73
1:C:59:ILE:HD11	1:C:118:LEU:HD11	1.69	0.73
1:A:254:THR:HG21	1:A:311:MSE:HE2	1.69	0.73
1:C:348:ALA:O	1:C:352:ILE:HG13	1.88	0.73
1:A:60:LEU:HB2	1:A:117:LEU:HD23	1.70	0.73
1:A:99:VAL:HB	1:A:152:ASP:HB3	1.70	0.72
1:A:214:ALA:H	3:A:501:AMP:H5'1	1.52	0.72
1:C:72:ASN:N	1:C:72:ASN:HD22	1.86	0.72
1:B:313:LEU:HD13	1:B:344:MSE:CE	2.19	0.72
1:C:243:PHE:HE1	1:C:269:MSE:HE3	1.54	0.72
1:C:162:ASN:ND2	1:C:175:MSE:HE2	2.04	0.72
1:C:204:GLN:O	1:C:332:THR:HG22	1.91	0.71
1:B:232:ARG:HH12	1:B:329:THR:HB	1.54	0.71
1:A:18:LYS:O	1:A:157:ALA:HB1	1.90	0.71
1:A:230:VAL:HG12	1:A:231:ASP:N	2.06	0.71
1:B:204:GLN:HB2	1:B:331:LYS:HE3	1.73	0.70
1:C:142:ASN:HB3	1:C:144:GLU:OE2	1.91	0.70
1:A:221:GLN:HG3	1:A:403:GLU:HG2	1.74	0.70
1:C:300:VAL:HG13	1:C:304:GLU:HB2	1.73	0.70
1:A:126:GLU:H	1:A:126:GLU:CD	2.00	0.70
1:B:92:VAL:HG22	1:B:115:VAL:CG2	2.21	0.69
1:B:30:GLU:OE1	1:B:35:LYS:HD2	1.92	0.69
1:C:73:GLU:CD	1:C:73:GLU:H	1.99	0.69
1:C:215:LYS:HG3	1:C:218:ASP:OD1	1.91	0.69
1:C:223:ILE:HD11	1:C:239:MSE:HE1	1.74	0.69
1:C:228:ASP:HB3	1:C:275:LYS:HE3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ASP:OD2	1:C:186:GLY:HA3	1.93	0.69
1:C:121:LEU:HB3	1:C:127:GLU:HG3	1.75	0.69
1:A:328:LEU:HD23	1:A:361:VAL:CG2	2.23	0.68
1:C:368:THR:O	1:C:389:SER:HB2	1.93	0.68
1:C:329:THR:O	1:C:329:THR:HG22	1.92	0.68
1:B:197:SER:O	1:B:201:GLU:HB2	1.94	0.68
1:B:130:LYS:HD2	1:B:138:LYS:HE3	1.74	0.68
1:A:8:ILE:O	1:A:11:LEU:HB2	1.94	0.68
1:B:185:SER:HB2	1:B:189:MSE:HG2	1.76	0.68
1:A:6:LEU:HD22	1:A:7:SER:N	2.09	0.67
1:A:328:LEU:HA	1:A:361:VAL:HG22	1.76	0.67
1:C:242:THR:HG21	1:C:258:ASP:H	1.58	0.67
1:A:27:VAL:HG23	1:A:28:PRO:HD2	1.75	0.67
1:B:160:PHE:HB2	1:B:180:LEU:HD12	1.75	0.67
1:C:245:LYS:O	1:C:249:ASN:HA	1.95	0.66
1:C:207:LEU:HD23	1:C:230:VAL:HA	1.78	0.66
1:C:235:ILE:HG23	1:C:239:MSE:HE2	1.78	0.66
1:C:72:ASN:HD22	1:C:72:ASN:H	1.42	0.65
1:B:375:THR:O	1:B:379:VAL:HG23	1.96	0.65
1:C:214:ALA:H	3:C:503:AMP:C5'	2.09	0.65
1:C:162:ASN:CG	1:C:189:MSE:HE2	2.22	0.65
1:C:251:LYS:NZ	1:C:252:ILE:H	1.94	0.65
1:A:189:MSE:HE3	1:A:413:LEU:HD11	1.79	0.64
1:C:12:LYS:HE2	1:C:12:LYS:HA	1.79	0.64
1:A:57:LYS:HE2	1:A:110:ALA:O	1.97	0.64
1:A:95:LEU:HD22	1:A:106:LYS:HE2	1.78	0.64
1:C:328:LEU:HA	1:C:361:VAL:HG13	1.78	0.64
1:C:300:VAL:HG11	1:C:305:GLY:O	1.98	0.63
1:C:342:PHE:CD1	1:C:378:LEU:HD23	2.33	0.63
1:A:221:GLN:HE21	1:B:405:LYS:NZ	1.96	0.63
1:C:6:LEU:CD2	1:C:10:ASP:HB2	2.28	0.63
1:C:85:LYS:HE3	1:C:91:GLU:OE2	1.99	0.63
1:C:90:GLU:O	1:C:91:GLU:HB3	1.99	0.62
1:A:219:LYS:HZ1	1:A:239:MSE:HE2	1.65	0.62
1:C:29:ILE:HG13	1:C:30:GLU:N	2.14	0.62
1:A:218:ASP:O	1:A:219:LYS:HD3	2.00	0.62
1:C:82:GLU:O	1:C:85:LYS:HB2	2.00	0.62
1:C:18:LYS:O	1:C:157:ALA:HB1	1.99	0.62
1:A:143:LYS:CD	1:A:143:LYS:H	2.09	0.62
1:A:185:SER:HB2	1:A:189:MSE:CG	2.29	0.62
1:B:51:LYS:NZ	1:B:90:GLU:OE2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HD11	1:B:83:THR:HG21	1.82	0.61
1:A:207:LEU:HA	1:A:332:THR:HG23	1.81	0.61
1:A:264:ILE:HG22	1:A:264:ILE:O	1.99	0.61
1:A:256:LEU:HD21	1:B:147:GLU:OE1	2.01	0.61
1:A:142:ASN:HA	1:A:143:LYS:HE3	1.83	0.61
1:C:207:LEU:HD21	1:C:230:VAL:HG22	1.83	0.61
1:B:65:GLY:HA3	1:B:75:TYR:CD2	2.37	0.60
1:B:132:VAL:HG23	1:B:133:ASP:O	2.00	0.60
1:C:189:MSE:HE3	1:C:413:LEU:HD11	1.83	0.60
1:C:342:PHE:HA	1:C:348:ALA:CB	2.30	0.60
1:B:204:GLN:HG3	1:B:332:THR:HG22	1.81	0.60
1:A:97:ASP:O	1:A:118:LEU:HB3	2.02	0.60
1:B:44:LEU:N	1:B:45:PRO:HD2	2.15	0.60
1:B:28:PRO:HB2	1:B:35:LYS:HB2	1.83	0.60
1:C:99:VAL:HG11	1:C:153:LEU:HD12	1.83	0.60
1:C:250:MSE:HG2	1:C:251:LYS:N	2.16	0.60
1:C:55:ALA:HB3	1:C:58:ILE:HD11	1.84	0.60
1:A:220:ILE:HD13	1:A:264:ILE:HG12	1.83	0.59
1:B:22:ARG:HH22	1:B:63:HIS:CD2	2.20	0.59
1:C:254:THR:HB	1:C:311:MSE:HB3	1.83	0.59
1:C:359:VAL:O	1:C:363:LYS:HD3	2.03	0.59
1:B:67:PRO:HG2	1:B:122:ARG:O	2.02	0.59
1:B:152:ASP:O	1:B:153:LEU:C	2.45	0.59
1:C:101:LYS:H	1:C:101:LYS:HD2	1.66	0.59
1:A:61:ILE:HG22	1:A:118:LEU:HD12	1.83	0.59
1:A:6:LEU:HD22	1:A:7:SER:H	1.67	0.58
1:A:214:ALA:HB1	1:A:256:LEU:HD13	1.86	0.58
1:C:214:ALA:H	3:C:503:AMP:H5'1	1.67	0.58
1:A:12:LYS:HD3	1:A:12:LYS:N	2.13	0.58
1:A:13:ASP:O	1:A:17:LYS:HD2	2.03	0.58
1:B:283:VAL:HG11	1:B:318:LYS:HG2	1.85	0.58
1:A:2:LEU:HD22	1:A:401:LEU:HD11	1.85	0.58
1:C:344:MSE:HE3	1:C:347:PHE:CD1	2.38	0.58
1:C:78:LYS:HB3	1:C:79:PRO:HD3	1.85	0.58
1:B:167:THR:HG22	1:B:167:THR:O	2.03	0.58
1:A:361:VAL:HG12	1:A:366:ALA:HB3	1.85	0.58
1:A:8:ILE:CD1	1:A:46:THR:HG23	2.34	0.58
1:A:62:SER:OG	1:A:63:HIS:N	2.34	0.58
1:C:301:THR:OG1	1:C:304:GLU:HG3	2.03	0.57
1:C:259:GLU:O	1:C:262:SER:OG	2.21	0.57
1:A:163:ASP:CG	1:A:186:GLY:HA3	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLY:O	1:A:239:MSE:HG3	2.05	0.57
1:A:223:ILE:HG23	1:A:233:MSE:HE1	1.86	0.57
1:C:207:LEU:HA	1:C:332:THR:HG23	1.87	0.57
1:A:107:ILE:HG12	1:A:116:ILE:HD13	1.85	0.57
1:B:56:SER:O	1:B:57:LYS:CD	2.49	0.57
1:B:117:LEU:C	1:B:117:LEU:HD23	2.29	0.57
1:C:207:LEU:HD22	1:C:230:VAL:HA	1.84	0.57
1:C:242:THR:HG22	1:C:257:PHE:HA	1.86	0.57
1:B:210:ILE:HD11	1:B:327:ILE:HD11	1.87	0.57
1:C:11:LEU:HD21	1:C:184:ALA:HB2	1.86	0.57
1:C:232:ARG:HH22	1:C:329:THR:CG2	2.18	0.57
1:C:251:LYS:HZ2	1:C:252:ILE:H	1.52	0.57
1:B:189:MSE:HE3	1:B:413:LEU:HD11	1.86	0.57
1:A:254:THR:HG22	1:A:254:THR:O	2.05	0.56
1:B:163:ASP:OD1	1:B:188:LEU:HB2	2.05	0.56
1:B:261:GLY:HA2	1:B:264:ILE:HD11	1.87	0.56
1:C:207:LEU:CD2	1:C:230:VAL:HG22	2.34	0.56
1:A:44:LEU:HD11	1:A:87:LEU:HD13	1.87	0.56
1:A:219:LYS:NZ	1:A:239:MSE:HE2	2.19	0.56
1:A:254:THR:O	1:A:254:THR:CG2	2.53	0.56
1:A:295:ALA:O	1:A:297:THR:HG23	2.04	0.56
1:C:160:PHE:HB2	1:C:180:LEU:HD12	1.87	0.56
1:C:189:MSE:O	1:C:190:LYS:C	2.49	0.56
1:C:234:ILE:HG12	1:C:280:PHE:HB2	1.87	0.56
1:C:329:THR:O	1:C:329:THR:CG2	2.53	0.56
1:B:44:LEU:O	1:B:48:ASN:HB2	2.05	0.56
1:B:214:ALA:H	3:B:502:AMP:H5'1	1.70	0.56
1:B:256:LEU:HD23	1:B:256:LEU:N	2.19	0.56
1:C:63:HIS:CG	1:C:122:ARG:HD2	2.41	0.56
1:C:101:LYS:H	1:C:101:LYS:CD	2.18	0.56
1:A:13:ASP:HB3	1:A:17:LYS:NZ	2.21	0.56
1:A:59:ILE:HG12	1:A:107:ILE:HD13	1.87	0.56
1:A:2:LEU:HD21	1:A:401:LEU:CD2	2.34	0.56
1:A:165:PHE:O	1:A:167:THR:N	2.39	0.56
1:A:169:HIS:HA	1:A:407:LEU:HD23	1.88	0.56
1:A:406:GLU:CG	1:A:411:LEU:HD11	2.36	0.56
1:A:119:GLU:HG3	1:A:120:ASN:N	2.19	0.55
1:A:27:VAL:CG2	1:A:28:PRO:HD2	2.35	0.55
1:A:185:SER:CB	1:A:189:MSE:HG2	2.36	0.55
1:B:15:LYS:HA	1:B:54:GLY:HA3	1.88	0.55
1:B:329:THR:HG22	1:B:329:THR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:HG12	1:A:231:ASP:H	1.71	0.55
1:C:143:LYS:CD	1:C:143:LYS:H	2.18	0.55
1:A:54:GLY:O	1:A:55:ALA:O	2.23	0.55
1:A:220:ILE:CG2	1:A:264:ILE:HG21	2.36	0.55
1:C:359:VAL:HG13	1:C:387:GLU:HB3	1.88	0.55
1:A:336:ASN:OD1	1:A:372:GLY:HA2	2.07	0.55
1:C:220:ILE:HD13	1:C:264:ILE:HG13	1.89	0.55
1:A:359:VAL:HG13	1:A:387:GLU:HB3	1.89	0.55
1:C:299:PHE:CD2	1:C:317:PRO:HD3	2.42	0.55
1:B:107:ILE:HG13	1:B:108:ASN:H	1.72	0.54
1:B:126:GLU:CD	1:B:126:GLU:H	2.15	0.54
1:C:300:VAL:CG1	1:C:304:GLU:HB2	2.37	0.54
1:A:406:GLU:HG3	1:A:411:LEU:HD11	1.89	0.54
1:C:192:GLU:OE2	1:C:393:THR:HG22	2.07	0.54
1:C:202:ASN:CG	1:C:202:ASN:O	2.49	0.54
1:C:219:LYS:O	1:C:223:ILE:HG13	2.07	0.54
1:B:328:LEU:HD21	1:B:357:LEU:HD23	1.89	0.54
1:B:265:VAL:O	1:B:269:MSE:HG2	2.08	0.54
1:C:215:LYS:O	1:C:219:LYS:NZ	2.40	0.54
1:B:395:GLY:HA2	1:B:398:SER:OG	2.08	0.54
1:A:14:ILE:HD12	1:A:14:ILE:N	2.13	0.54
1:A:137:ASN:O	1:A:139:VAL:HG23	2.08	0.54
1:A:400:GLU:HB3	1:A:405:LYS:HB2	1.88	0.54
1:B:204:GLN:H	1:B:332:THR:HG21	1.73	0.54
1:B:14:ILE:HD12	1:B:14:ILE:O	2.07	0.54
1:B:51:LYS:HD3	1:B:113:ASN:ND2	2.23	0.54
1:A:216:VAL:HG13	1:A:261:GLY:HA3	1.88	0.54
1:B:59:ILE:H	1:B:59:ILE:HD12	1.72	0.54
1:A:8:ILE:HD13	1:A:46:THR:HG23	1.90	0.53
1:A:238:GLY:HA2	1:A:241:TYR:HD2	1.73	0.53
1:C:357:LEU:O	1:C:361:VAL:HG22	2.09	0.53
1:A:166:GLY:HA2	1:A:397:ALA:HB3	1.90	0.53
1:B:46:THR:HG22	1:B:187:PHE:HB2	1.90	0.53
1:B:302:ASP:N	1:B:302:ASP:OD1	2.40	0.53
1:B:289:ASP:HB3	1:B:310:TRP:CZ2	2.43	0.53
1:C:177:GLY:O	1:C:179:LYS:HG2	2.08	0.53
1:B:368:THR:O	1:B:389:SER:HB2	2.08	0.53
1:C:284:ASP:OD2	1:C:318:LYS:HB2	2.09	0.53
1:B:269:MSE:HE1	1:B:279:ILE:HG13	1.89	0.53
1:A:264:ILE:O	1:A:264:ILE:CG2	2.56	0.53
1:B:335:TRP:CD1	1:B:335:TRP:C	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLY:O	1:B:342:PHE:N	2.40	0.53
1:C:207:LEU:HD23	1:C:230:VAL:HG13	1.91	0.53
1:A:110:ALA:O	1:A:111:LYS:C	2.50	0.53
1:A:164:ALA:C	1:A:165:PHE:O	2.50	0.53
1:B:14:ILE:HA	1:B:17:LYS:HE2	1.91	0.53
1:A:22:ARG:NH2	1:A:63:HIS:ND1	2.51	0.53
1:B:29:ILE:HG13	1:B:30:GLU:N	2.24	0.53
1:B:6:LEU:CD2	1:B:7:SER:H	2.21	0.52
1:B:406:GLU:O	1:B:407:LEU:CB	2.56	0.52
1:C:211:LEU:HD13	1:C:223:ILE:HG12	1.89	0.52
1:A:205:ARG:HD2	1:A:231:ASP:OD2	2.10	0.52
1:B:107:ILE:CG1	1:B:108:ASN:N	2.71	0.52
1:A:344:MSE:CE	1:B:144:GLU:HG2	2.40	0.52
1:B:241:TYR:OH	1:B:312:GLY:HA3	2.09	0.52
1:C:82:GLU:HA	1:C:85:LYS:HD2	1.90	0.52
1:A:15:LYS:HA	1:A:54:GLY:HA3	1.91	0.52
1:A:254:THR:CG2	1:A:311:MSE:HE2	2.39	0.52
1:A:232:ARG:NH2	1:A:329:THR:HB	2.25	0.52
1:B:38:ASN:O	1:B:41:THR:HB	2.10	0.52
1:B:399:LEU:HD12	5:B:627:HOH:O	2.09	0.52
1:A:13:ASP:HB3	1:A:17:LYS:HZ1	1.74	0.52
1:B:359:VAL:CG1	1:B:387:GLU:HB3	2.36	0.52
1:A:204:GLN:HE21	1:A:204:GLN:N	1.96	0.52
1:B:216:VAL:HG13	1:B:261:GLY:HA3	1.92	0.52
1:A:14:ILE:N	1:A:14:ILE:CD1	2.72	0.52
1:A:289:ASP:HB3	1:A:310:TRP:CZ2	2.45	0.52
1:A:357:LEU:O	1:A:361:VAL:HG23	2.09	0.52
1:B:227:LEU:HG	1:B:233:MSE:HE1	1.92	0.52
1:C:6:LEU:HD21	1:C:10:ASP:HB2	1.92	0.52
1:C:144:GLU:CD	1:C:144:GLU:H	2.18	0.52
1:A:8:ILE:HD11	1:A:186:GLY:HA2	1.92	0.52
1:B:320:ILE:HD12	1:B:350:GLY:HA2	1.91	0.51
1:B:204:GLN:O	1:B:332:THR:HG22	2.10	0.51
1:C:132:VAL:HG23	1:C:132:VAL:O	2.10	0.51
1:C:85:LYS:HG2	1:C:91:GLU:HA	1.92	0.51
1:C:259:GLU:OE1	1:C:259:GLU:HA	2.10	0.51
1:C:97:ASP:OD1	1:C:97:ASP:N	2.43	0.51
1:B:406:GLU:O	1:B:407:LEU:HB2	2.10	0.51
1:C:208:LEU:HD23	1:C:233:MSE:HA	1.93	0.51
1:C:301:THR:O	1:C:302:ASP:C	2.51	0.51
1:B:126:GLU:HG3	1:B:149:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:HA	1:B:206:PRO:C	2.35	0.51
1:C:243:PHE:CE1	1:C:269:MSE:HE3	2.40	0.51
1:C:314:ASP:OD2	1:C:350:GLY:HA3	2.11	0.51
1:B:206:PRO:HG3	1:B:232:ARG:NH2	2.26	0.51
1:C:72:ASN:O	1:C:74:LYS:N	2.44	0.51
1:C:99:VAL:CG1	1:C:153:LEU:HD12	2.41	0.51
1:C:242:THR:CG2	1:C:258:ASP:H	2.22	0.51
1:A:35:LYS:O	1:A:36:ASP:HB2	2.10	0.51
1:A:67:PRO:O	1:A:68:ASP:HB2	2.11	0.51
1:A:331:LYS:O	1:A:366:ALA:HB1	2.11	0.51
1:B:64:CYS:HB2	1:B:77:LEU:HD21	1.93	0.51
1:B:170:ARG:HB3	1:B:172:HIS:CD2	2.45	0.51
1:C:63:HIS:HB2	1:C:122:ARG:HD2	1.91	0.51
1:C:385:LYS:HE3	1:C:391:VAL:HB	1.93	0.51
1:B:117:LEU:HD23	1:B:118:LEU:N	2.26	0.51
1:C:163:ASP:CG	1:C:186:GLY:HA3	2.36	0.51
1:B:6:LEU:HD23	1:B:7:SER:N	2.21	0.50
1:B:261:GLY:O	1:B:262:SER:C	2.53	0.50
1:B:5:LYS:HE3	1:B:410:VAL:O	2.11	0.50
1:B:103:VAL:HG23	1:B:104:GLU:N	2.26	0.50
1:A:331:LYS:HA	1:A:331:LYS:CE	2.32	0.50
1:B:143:LYS:CD	1:B:143:LYS:H	2.24	0.50
1:B:143:LYS:CD	1:B:143:LYS:N	2.75	0.50
1:B:185:SER:HB2	1:B:189:MSE:CG	2.41	0.50
1:B:287:ILE:HD12	1:B:307:PRO:HD2	1.92	0.50
1:C:6:LEU:HD23	1:C:10:ASP:HB2	1.94	0.50
1:C:264:ILE:HG22	1:C:264:ILE:O	2.11	0.50
1:A:230:VAL:CG1	1:A:231:ASP:N	2.75	0.50
1:A:316:GLY:O	1:A:320:ILE:HG13	2.11	0.50
1:B:170:ARG:HB3	1:B:172:HIS:NE2	2.27	0.50
1:A:2:LEU:CD2	1:A:401:LEU:HD11	2.42	0.50
1:A:221:GLN:HE21	1:B:405:LYS:HZ3	1.58	0.50
1:C:185:SER:HB2	1:C:189:MSE:CB	2.42	0.50
1:C:121:LEU:HB3	1:C:127:GLU:CG	2.41	0.50
1:B:39:ARG:C	1:B:40:ILE:HG23	2.37	0.50
1:C:159:VAL:HG22	1:C:182:VAL:HB	1.94	0.50
1:C:285:PHE:CD1	1:C:285:PHE:N	2.80	0.50
1:B:256:LEU:H	1:B:256:LEU:CD2	2.14	0.50
1:C:204:GLN:O	1:C:332:THR:CG2	2.58	0.50
1:C:247:LEU:HD11	1:C:265:VAL:HG12	1.93	0.50
1:A:164:ALA:O	1:A:175:MSE:HE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LEU:HD12	1:B:347:PHE:CZ	2.47	0.49
1:C:358:VAL:O	1:C:361:VAL:HG23	2.11	0.49
1:B:160:PHE:HB3	1:B:183:LYS:HG2	1.94	0.49
1:C:228:ASP:HB3	1:C:275:LYS:CE	2.39	0.49
1:C:230:VAL:HG12	1:C:232:ARG:H	1.76	0.49
1:A:34:ILE:HD11	1:A:80:VAL:HG22	1.95	0.49
1:A:125:ILE:HG13	1:A:130:LYS:O	2.12	0.49
1:B:354:CYS:O	1:B:358:VAL:HG23	2.12	0.49
1:A:44:LEU:HB2	1:A:45:PRO:HD3	1.94	0.49
1:A:212:GLY:C	1:A:239:MSE:HE3	2.38	0.49
1:A:327:ILE:HG22	1:A:361:VAL:CG2	2.39	0.49
1:B:223:ILE:HD11	1:B:239:MSE:HE1	1.93	0.49
1:B:388:ILE:HD12	1:B:388:ILE:H	1.77	0.49
1:C:67:PRO:O	1:C:68:ASP:C	2.55	0.49
1:A:368:THR:O	1:A:389:SER:HB2	2.13	0.49
1:B:99:VAL:HG12	1:B:153:LEU:HD23	1.94	0.49
1:C:316:GLY:O	1:C:320:ILE:HG13	2.13	0.49
1:B:388:ILE:HD12	1:B:388:ILE:N	2.28	0.49
1:B:22:ARG:NH1	1:B:62:SER:HA	2.28	0.48
1:B:251:LYS:HE3	1:B:253:GLY:H	1.77	0.48
1:C:212:GLY:HA2	1:C:236:GLY:O	2.13	0.48
1:B:378:LEU:O	1:B:378:LEU:HD22	2.13	0.48
1:B:54:GLY:O	1:B:55:ALA:HB3	2.14	0.48
1:B:92:VAL:HG22	1:B:115:VAL:HG23	1.92	0.48
1:B:208:LEU:HD22	1:B:209:ALA:N	2.28	0.48
1:B:406:GLU:HA	1:B:406:GLU:OE1	2.13	0.48
1:C:11:LEU:HD22	1:C:182:VAL:HG11	1.95	0.48
1:C:29:ILE:HD11	1:C:32:GLY:C	2.39	0.48
1:B:297:THR:HA	1:B:310:TRP:HZ3	1.78	0.48
1:C:292:ASP:OD2	1:C:293:ASN:N	2.46	0.48
1:C:54:GLY:O	1:C:55:ALA:C	2.56	0.48
1:A:289:ASP:OD2	1:A:296:ASN:HB2	2.14	0.48
1:B:301:THR:C	1:B:303:GLU:N	2.71	0.48
1:C:150:GLN:O	1:C:154:THR:OG1	2.26	0.48
1:C:185:SER:HB2	1:C:189:MSE:HB2	1.95	0.48
1:A:143:LYS:H	1:A:143:LYS:HE3	1.78	0.48
1:A:165:PHE:C	1:A:167:THR:H	2.22	0.48
1:B:51:LYS:HD3	1:B:113:ASN:HD21	1.79	0.48
1:B:104:GLU:O	1:B:108:ASN:HB2	2.13	0.48
1:B:11:LEU:HD12	1:B:11:LEU:N	2.28	0.48
1:B:14:ILE:HA	1:B:17:LYS:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:PRO:HB2	1:B:310:TRP:HB2	1.96	0.48
1:C:162:ASN:O	1:C:189:MSE:HG3	2.14	0.48
1:A:119:GLU:CG	1:A:120:ASN:N	2.76	0.48
1:A:143:LYS:H	1:A:143:LYS:CE	2.27	0.47
1:B:324:LYS:O	1:B:328:LEU:HG	2.14	0.47
1:C:227:LEU:HB3	1:C:271:LYS:HD3	1.96	0.47
1:A:119:GLU:CG	1:A:120:ASN:H	2.26	0.47
1:C:201:GLU:C	1:C:203:PRO:HD3	2.39	0.47
1:C:230:VAL:HG12	1:C:232:ARG:N	2.30	0.47
1:A:5:LYS:HD2	1:A:414:SER:O	2.14	0.47
1:B:138:LYS:HD2	1:B:139:VAL:H	1.79	0.47
1:B:368:THR:OG1	1:B:388:ILE:HG23	2.14	0.47
1:A:285:PHE:N	1:A:285:PHE:CD1	2.82	0.47
1:B:106:LYS:O	1:B:110:ALA:HB2	2.15	0.47
1:C:102:GLU:O	1:C:105:ASP:HB2	2.13	0.47
1:A:225:ASN:O	1:A:225:ASN:CG	2.58	0.47
1:C:60:LEU:HD12	1:C:117:LEU:HD13	1.97	0.47
1:C:289:ASP:HB3	1:C:310:TRP:CE2	2.50	0.47
1:A:61:ILE:CG2	1:A:118:LEU:HD12	2.45	0.47
1:A:163:ASP:OD2	1:A:188:LEU:HB2	2.15	0.47
1:B:384:LYS:HD3	1:B:387:GLU:HG3	1.95	0.47
1:C:101:LYS:HD2	1:C:101:LYS:N	2.28	0.47
1:A:144:GLU:HG3	1:B:291:PHE:CE2	2.49	0.47
1:C:56:SER:C	1:C:57:LYS:HG2	2.40	0.47
1:C:294:ASN:O	1:C:295:ALA:C	2.58	0.47
1:B:143:LYS:H	1:B:143:LYS:HE2	1.80	0.47
1:C:142:ASN:HA	1:C:143:LYS:HE3	1.97	0.47
1:A:137:ASN:OD1	1:B:28:PRO:HA	2.15	0.47
1:B:108:ASN:O	1:B:109:ALA:HB3	2.13	0.47
1:B:160:PHE:O	1:B:183:LYS:HA	2.15	0.47
1:A:43:THR:O	1:A:47:ILE:HG13	2.15	0.46
1:B:11:LEU:HD11	1:B:184:ALA:CB	2.45	0.46
1:B:78:LYS:N	1:B:79:PRO:HD2	2.31	0.46
1:B:119:GLU:HG3	1:B:120:ASN:N	2.29	0.46
1:C:151:ASN:O	1:C:155:LYS:HG3	2.16	0.46
1:A:392:SER:C	1:A:394:GLY:H	2.23	0.46
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.72	0.46
1:A:344:MSE:HE1	1:B:144:GLU:HG2	1.97	0.46
1:B:98:CYS:SG	1:B:124:HIS:ND1	2.87	0.46
1:B:177:GLY:O	1:B:179:LYS:HG2	2.15	0.46
1:C:214:ALA:H	3:C:503:AMP:H5'2	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LYS:HG3	1:B:94:PHE:CD2	2.51	0.46
1:C:355:LEU:O	1:C:359:VAL:HG23	2.15	0.46
1:A:30:GLU:HB2	1:A:35:LYS:NZ	2.29	0.46
1:B:13:ASP:O	1:B:17:LYS:NZ	2.40	0.46
1:B:93:LEU:HB3	1:B:116:ILE:HG23	1.96	0.46
1:B:159:VAL:HG13	1:B:182:VAL:HB	1.97	0.46
1:B:14:ILE:HA	1:B:17:LYS:NZ	2.31	0.46
1:B:18:LYS:NZ	1:B:108:ASN:ND2	2.64	0.46
1:B:261:GLY:C	1:B:263:LYS:N	2.72	0.46
1:A:130:LYS:CB	1:A:138:LYS:HE2	2.42	0.46
1:A:183:LYS:HE3	1:B:259:GLU:OE1	2.16	0.46
1:A:62:SER:O	1:A:121:LEU:HD13	2.16	0.46
1:A:238:GLY:HA2	1:A:241:TYR:CD2	2.51	0.46
1:B:243:PHE:O	1:B:247:LEU:HB2	2.16	0.46
1:C:108:ASN:HD22	1:C:108:ASN:HA	1.57	0.46
1:C:227:LEU:CD2	1:C:233:MSE:HE3	2.45	0.46
1:A:126:GLU:CD	1:A:126:GLU:N	2.73	0.46
1:B:176:VAL:HG12	1:B:176:VAL:O	2.16	0.46
1:C:14:ILE:O	1:C:17:LYS:HG3	2.15	0.46
1:A:119:GLU:HG3	1:A:120:ASN:H	1.81	0.46
1:A:205:ARG:HB3	1:A:206:PRO:HA	1.98	0.46
1:B:142:ASN:HB2	1:B:145:ASP:OD2	2.15	0.46
1:B:313:LEU:HB2	1:B:347:PHE:CD2	2.51	0.46
1:B:342:PHE:CE1	1:B:378:LEU:HB2	2.51	0.46
1:B:6:LEU:CD2	1:B:7:SER:N	2.79	0.45
1:B:395:GLY:O	1:B:396:GLY:C	2.59	0.45
1:C:206:PRO:HG2	1:C:330:SER:HA	1.97	0.45
1:A:177:GLY:O	1:A:179:LYS:N	2.50	0.45
1:B:58:ILE:HB	1:B:115:VAL:HG12	1.97	0.45
1:B:298:LYS:HE2	1:B:310:TRP:CH2	2.51	0.45
1:B:344:MSE:HE3	1:B:347:PHE:CD1	2.51	0.45
1:A:168:ALA:HA	1:A:175:MSE:HE2	1.98	0.45
1:A:252:ILE:CG1	1:A:255:SER:HB2	2.40	0.45
1:A:328:LEU:HA	1:A:361:VAL:CG2	2.44	0.45
1:C:68:ASP:HB2	1:C:132:VAL:HG22	1.98	0.45
1:C:103:VAL:C	1:C:105:ASP:N	2.74	0.45
1:C:126:GLU:HG3	1:C:149:PHE:HB2	1.99	0.45
1:C:178:VAL:HG12	1:C:178:VAL:O	2.17	0.45
1:A:293:ASN:O	1:A:294:ASN:HB3	2.16	0.45
1:B:313:LEU:HD13	1:B:344:MSE:HE1	1.95	0.45
1:C:302:ASP:OD1	1:C:303:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PRO:CG	1:A:122:ARG:HB3	2.46	0.45
1:A:159:VAL:HG13	1:A:182:VAL:HB	1.99	0.45
1:A:263:LYS:C	1:A:264:ILE:HD12	2.41	0.45
1:A:400:GLU:HA	1:A:403:GLU:HB2	1.98	0.45
1:C:62:SER:C	1:C:121:LEU:HD12	2.42	0.45
1:C:105:ASP:O	1:C:106:LYS:C	2.59	0.45
1:A:212:GLY:CA	1:A:239:MSE:HE3	2.46	0.45
1:B:247:LEU:HD11	1:B:269:MSE:HG3	1.99	0.45
1:B:407:LEU:HD23	1:B:410:VAL:HG21	1.98	0.45
1:C:112:GLU:C	1:C:114:SER:H	2.25	0.45
1:C:162:ASN:HD21	1:C:175:MSE:HE2	1.80	0.45
1:C:355:LEU:HD22	1:C:378:LEU:HD13	1.99	0.45
1:A:8:ILE:O	1:A:9:SER:C	2.59	0.45
1:B:22:ARG:HH12	1:B:63:HIS:HD2	1.64	0.45
1:C:142:ASN:HB3	1:C:144:GLU:CD	2.42	0.45
1:C:243:PHE:CD1	1:C:265:VAL:HG13	2.52	0.45
1:A:168:ALA:CA	1:A:175:MSE:HE2	2.46	0.44
1:B:47:ILE:HD11	1:B:60:LEU:HD11	1.99	0.44
1:B:72:ASN:O	1:B:74:LYS:N	2.50	0.44
1:C:42:ALA:O	1:C:45:PRO:HD2	2.15	0.44
1:C:57:LYS:NZ	1:C:107:ILE:O	2.44	0.44
1:C:61:ILE:HG22	1:C:118:LEU:HD12	1.99	0.44
1:C:287:ILE:HG13	1:C:310:TRP:HE3	1.83	0.44
1:B:261:GLY:O	1:B:264:ILE:HD13	2.18	0.44
1:B:285:PHE:CD1	1:B:285:PHE:N	2.85	0.44
1:B:344:MSE:CE	1:B:347:PHE:CD1	3.00	0.44
1:A:127:GLU:HA	1:A:173:SER:HB2	2.00	0.44
1:A:211:LEU:CD1	1:A:223:ILE:HG12	2.47	0.44
1:A:307:PRO:HG2	1:A:310:TRP:CG	2.52	0.44
1:B:11:LEU:N	1:B:11:LEU:CD1	2.79	0.44
1:B:125:ILE:HG23	1:B:126:GLU:N	2.32	0.44
1:C:90:GLU:O	1:C:91:GLU:CB	2.64	0.44
1:C:205:ARG:HA	1:C:206:PRO:C	2.42	0.44
1:A:59:ILE:HG12	1:A:107:ILE:CD1	2.48	0.44
1:B:8:ILE:C	1:B:10:ASP:H	2.24	0.44
1:C:162:ASN:OD1	1:C:189:MSE:HE2	2.18	0.44
1:A:8:ILE:HG13	1:A:185:SER:O	2.17	0.44
1:B:21:VAL:HA	1:B:161:ILE:O	2.17	0.44
1:B:117:LEU:C	1:B:117:LEU:CD2	2.90	0.44
1:B:207:LEU:HD13	1:B:230:VAL:HA	1.99	0.44
1:A:20:LEU:HD23	1:A:59:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:CG1	1:B:108:ASN:H	2.30	0.44
1:C:263:LYS:O	1:C:264:ILE:HD13	2.17	0.44
1:C:287:ILE:HG13	1:C:310:TRP:CE3	2.53	0.44
1:A:162:ASN:HD21	1:A:175:MSE:HE3	1.83	0.44
1:A:261:GLY:C	1:A:263:LYS:N	2.72	0.44
1:B:24:ASP:OD1	1:B:24:ASP:C	2.60	0.44
1:C:36:ASP:OD2	1:C:36:ASP:C	2.61	0.44
1:C:286:LYS:HE2	1:C:297:THR:HB	2.00	0.44
1:B:4:ASN:O	1:B:4:ASN:CG	2.61	0.44
1:A:8:ILE:HD11	1:A:46:THR:HG23	2.00	0.43
1:B:249:ASN:O	1:B:250:MSE:C	2.61	0.43
1:B:359:VAL:O	1:B:362:THR:HB	2.18	0.43
1:B:248:ASN:O	1:B:249:ASN:HB3	2.16	0.43
1:B:284:ASP:HA	1:B:301:THR:HA	2.00	0.43
1:C:0:HIS:O	1:C:1:HIS:HB2	2.17	0.43
1:C:251:LYS:HZ1	1:C:253:GLY:H	1.66	0.43
1:C:201:GLU:O	1:C:203:PRO:HD3	2.17	0.43
1:A:49:HIS:O	1:A:53:GLU:HG2	2.18	0.43
1:A:146:VAL:O	1:A:150:GLN:HG3	2.19	0.43
1:B:378:LEU:C	1:B:378:LEU:HD13	2.43	0.43
1:C:36:ASP:OD2	1:C:38:ASN:HB2	2.19	0.43
1:C:299:PHE:CE2	1:C:317:PRO:HD3	2.53	0.43
1:B:72:ASN:OD1	1:B:72:ASN:C	2.61	0.43
1:B:370:VAL:HG21	1:B:379:VAL:HG21	2.00	0.43
1:A:165:PHE:CD2	1:A:166:GLY:N	2.83	0.43
1:B:98:CYS:SG	1:B:124:HIS:CE1	3.11	0.43
1:B:306:ILE:O	1:B:307:PRO:O	2.35	0.43
1:C:342:PHE:HD1	1:C:378:LEU:HD23	1.77	0.43
1:C:63:HIS:CB	1:C:122:ARG:HD2	2.49	0.43
1:C:66:ARG:O	1:C:68:ASP:N	2.50	0.43
1:A:14:ILE:H	1:A:14:ILE:CD1	2.08	0.43
1:A:162:ASN:HB3	1:A:189:MSE:HE2	2.01	0.43
1:C:232:ARG:HH22	1:C:329:THR:HG22	1.84	0.43
1:A:51:LYS:HE2	1:A:90:GLU:OE1	2.18	0.43
1:A:99:VAL:CB	1:A:152:ASP:HB3	2.44	0.43
1:B:59:ILE:HD12	1:B:59:ILE:N	2.33	0.43
1:C:300:VAL:HG12	1:C:301:THR:N	2.33	0.43
1:A:51:LYS:CE	1:A:90:GLU:OE1	2.67	0.43
1:A:158:ASP:C	1:A:180:LEU:HD13	2.44	0.43
1:A:169:HIS:CA	1:A:407:LEU:HD23	2.49	0.43
1:A:206:PRO:HG2	1:A:330:SER:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ASP:HB3	1:A:271:LYS:NZ	2.33	0.43
1:A:342:PHE:HA	1:A:348:ALA:HB2	2.01	0.43
1:B:71:ARG:HD2	1:B:123:PHE:CD2	2.54	0.43
1:B:108:ASN:HD22	1:B:108:ASN:HA	1.53	0.43
1:B:234:ILE:HD11	1:B:326:VAL:HG11	2.00	0.43
1:A:198:LYS:HD3	1:A:367:ILE:HD13	2.01	0.42
1:B:8:ILE:CA	1:B:11:LEU:HD13	2.44	0.42
1:B:116:ILE:HD12	1:B:116:ILE:N	2.34	0.42
1:C:66:ARG:C	1:C:68:ASP:H	2.27	0.42
1:A:169:HIS:HB3	1:A:407:LEU:CD2	2.48	0.42
1:A:222:LEU:HD23	1:A:402:LEU:O	2.19	0.42
1:A:379:VAL:HG11	1:A:388:ILE:HD12	2.00	0.42
1:B:284:ASP:CG	1:B:316:GLY:HA3	2.43	0.42
1:A:11:LEU:HD23	1:A:11:LEU:HA	1.86	0.42
1:C:63:HIS:CD2	1:C:63:HIS:C	2.97	0.42
1:C:166:GLY:HA2	1:C:394:GLY:HA2	2.01	0.42
1:A:54:GLY:O	1:A:55:ALA:C	2.61	0.42
1:A:239:MSE:O	1:A:240:ALA:C	2.61	0.42
1:B:264:ILE:N	1:B:264:ILE:CD1	2.73	0.42
1:C:132:VAL:O	1:C:132:VAL:CG2	2.66	0.42
1:B:39:ARG:C	1:B:41:THR:H	2.27	0.42
1:B:284:ASP:C	1:B:285:PHE:CD1	2.98	0.42
1:C:56:SER:O	1:C:57:LYS:HG2	2.19	0.42
1:C:61:ILE:O	1:C:61:ILE:HG13	2.19	0.42
1:C:80:VAL:O	1:C:84:LEU:HG	2.20	0.42
1:C:328:LEU:HD21	1:C:357:LEU:HD23	2.00	0.42
1:A:289:ASP:OD1	1:A:289:ASP:C	2.63	0.42
1:C:83:THR:O	1:C:87:LEU:HD22	2.20	0.42
1:C:221:GLN:OE1	1:C:405:LYS:HE2	2.18	0.42
1:A:69:GLY:O	1:A:70:LEU:HD23	2.19	0.42
1:B:167:THR:O	1:B:167:THR:CG2	2.68	0.42
1:B:226:LEU:C	1:B:228:ASP:H	2.27	0.42
1:C:72:ASN:C	1:C:74:LYS:N	2.77	0.42
1:C:294:ASN:O	1:C:295:ALA:O	2.37	0.42
1:A:9:SER:O	1:A:10:ASP:HB2	2.19	0.42
1:A:169:HIS:HB3	1:A:407:LEU:HD23	2.02	0.42
1:A:406:GLU:HG2	1:A:411:LEU:HD11	2.00	0.42
1:B:110:ALA:O	1:B:111:LYS:C	2.62	0.42
1:B:170:ARG:HH21	1:B:170:ARG:HG3	1.84	0.42
1:C:98:CYS:SG	1:C:124:HIS:CD2	3.13	0.42
1:C:112:GLU:O	1:C:114:SER:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:ASP:HB2	5:C:626:HOH:O	2.19	0.42
1:B:40:ILE:O	1:B:40:ILE:HG13	2.19	0.42
1:A:295:ALA:O	1:A:296:ASN:C	2.62	0.42
1:B:76:THR:HG22	1:B:78:LYS:H	1.84	0.42
1:B:152:ASP:O	1:B:155:LYS:HG2	2.20	0.42
1:A:130:LYS:HD3	1:A:138:LYS:HE3	2.02	0.41
1:A:164:ALA:O	1:A:165:PHE:O	2.38	0.41
1:A:215:LYS:HB3	1:A:218:ASP:OD1	2.20	0.41
1:A:375:THR:O	1:A:378:LEU:HB3	2.20	0.41
1:B:25:PHE:CD2	1:B:40:ILE:HG22	2.54	0.41
1:B:167:THR:HB	1:B:175:MSE:HE3	2.01	0.41
1:B:289:ASP:HB3	1:B:310:TRP:CE2	2.55	0.41
1:B:313:LEU:HD22	1:B:341:VAL:HG21	2.01	0.41
1:A:226:LEU:O	1:A:227:LEU:C	2.63	0.41
1:A:240:ALA:O	1:A:241:TYR:C	2.63	0.41
1:B:281:LEU:HD23	1:B:282:PRO:HD2	2.02	0.41
1:B:325:ASP:OD1	1:B:325:ASP:N	2.53	0.41
1:C:72:ASN:O	1:C:72:ASN:ND2	2.53	0.41
1:A:363:LYS:C	1:A:365:GLY:H	2.28	0.41
1:B:35:LYS:HE3	1:B:35:LYS:HA	2.03	0.41
1:B:298:LYS:HG2	1:B:310:TRP:CZ3	2.55	0.41
1:C:298:LYS:HB2	1:C:298:LYS:HE3	1.87	0.41
1:C:301:THR:O	1:C:304:GLU:N	2.53	0.41
1:A:197:SER:O	1:A:201:GLU:HB2	2.21	0.41
1:B:63:HIS:HB2	1:B:122:ARG:HD3	2.02	0.41
1:B:230:VAL:CG1	1:B:232:ARG:O	2.68	0.41
1:B:370:VAL:HB	1:B:391:VAL:HG22	2.02	0.41
1:C:19:VAL:HG21	1:C:50:LEU:CD2	2.51	0.41
1:C:128:GLU:HB2	5:C:618:HOH:O	2.20	0.41
1:B:162:ASN:O	1:B:189:MSE:HE2	2.20	0.41
1:A:44:LEU:N	1:A:45:PRO:CD	2.83	0.41
1:C:85:LYS:HE3	1:C:91:GLU:CD	2.45	0.41
1:C:119:GLU:CD	1:C:120:ASN:H	2.28	0.41
1:C:208:LEU:HD23	1:C:232:ARG:O	2.21	0.41
1:A:329:THR:HG22	1:A:329:THR:O	2.20	0.41
1:B:261:GLY:HA2	1:B:264:ILE:CD1	2.51	0.41
1:C:18:LYS:N	1:C:158:ASP:OD1	2.50	0.41
1:A:76:THR:HA	1:A:119:GLU:OE2	2.21	0.41
1:A:196:PHE:HB3	1:A:401:LEU:HD21	2.03	0.41
1:B:7:SER:O	1:B:10:ASP:HB3	2.20	0.41
1:B:65:GLY:HA3	1:B:75:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LYS:NZ	1:B:363:LYS:HB3	2.35	0.41
1:C:20:LEU:HD12	1:C:59:ILE:O	2.20	0.41
1:B:43:THR:C	1:B:45:PRO:HD2	2.46	0.41
1:B:204:GLN:O	1:B:331:LYS:HB2	2.21	0.41
1:C:121:LEU:CB	1:C:127:GLU:HG3	2.47	0.41
1:B:3:GLY:O	1:B:4:ASN:HB2	2.21	0.40
1:B:27:VAL:HA	1:B:28:PRO:HD3	1.87	0.40
1:B:39:ARG:C	1:B:41:THR:N	2.75	0.40
1:B:43:THR:HG23	1:B:47:ILE:HD12	2.03	0.40
1:B:384:LYS:O	1:B:388:ILE:HD12	2.21	0.40
1:C:63:HIS:CE1	1:C:122:ARG:NH1	2.89	0.40
1:C:98:CYS:SG	1:C:124:HIS:HD2	2.44	0.40
1:C:196:PHE:O	1:C:200:LEU:HG	2.21	0.40
1:C:222:LEU:CD2	1:C:226:LEU:HD11	2.51	0.40
1:A:127:GLU:OE2	1:A:173:SER:HB2	2.20	0.40
1:B:7:SER:O	1:B:8:ILE:C	2.64	0.40
1:B:301:THR:O	1:B:302:ASP:C	2.65	0.40
1:C:143:LYS:H	1:C:143:LYS:HE3	1.85	0.40
1:C:165:PHE:CD2	1:C:165:PHE:C	2.98	0.40
1:A:112:GLU:OE2	1:A:112:GLU:HA	2.21	0.40
1:A:335:TRP:CE3	1:A:358:VAL:HG21	2.56	0.40
1:B:99:VAL:CG1	1:B:153:LEU:HD23	2.51	0.40
1:B:269:MSE:HE3	5:B:607:HOH:O	2.21	0.40
1:A:245:LYS:HD3	1:A:257:PHE:CE1	2.56	0.40
1:B:17:LYS:O	1:B:55:ALA:HA	2.21	0.40
1:B:143:LYS:N	1:B:143:LYS:HD3	2.37	0.40
1:B:212:GLY:O	1:B:219:LYS:HE2	2.22	0.40
1:B:214:ALA:HB3	3:B:502:AMP:H5'2	2.03	0.40
1:B:232:ARG:HH22	1:B:329:THR:CG2	2.34	0.40
1:B:246:VAL:HG11	1:B:265:VAL:CG2	2.51	0.40
1:B:343:GLU:H	1:B:343:GLU:CD	2.30	0.40
1:B:362:THR:HG21	1:B:387:GLU:O	2.21	0.40
1:B:372:GLY:O	1:B:373:GLY:O	2.40	0.40
1:C:232:ARG:HA	1:C:277:VAL:HG13	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ASN:ND2	1:C:386:ASN:ND2[7_545]	1.43	0.77
1:B:345:PRO:O	1:C:89:GLY:CA[7_545]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/425 (98%)	373 (90%)	33 (8%)	9 (2%)	5	26
1	B	413/425 (97%)	342 (83%)	50 (12%)	21 (5%)	1	10
1	C	422/425 (99%)	357 (85%)	48 (11%)	17 (4%)	2	14
All	All	1250/1275 (98%)	1072 (86%)	131 (10%)	47 (4%)	2	15

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	55	ALA
1	B	4	ASN
1	B	307	PRO
1	B	374	ASP
1	C	68	ASP
1	C	111	LYS
1	C	112	GLU
1	C	295	ALA
1	C	308	ASP
1	A	111	LYS
1	A	165	PHE
1	A	166	GLY
1	A	229	LYS
1	B	34	ILE
1	B	341	VAL
1	B	371	GLY
1	B	414	SER
1	C	4	ASN
1	C	13	ASP
1	C	73	GLU
1	C	113	ASN
1	C	201	GLU
1	C	395	GLY

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Mol	Chain	Res	Type
1	A	395	GLY
1	B	73	GLU
1	B	373	GLY
1	B	203	PRO
1	C	254	THR
1	A	178	VAL
1	B	10	ASP
1	B	40	ILE
1	B	201	GLU
1	B	336	ASN
1	B	405	LYS
1	C	12	LYS
1	C	122	ARG
1	C	179	LYS
1	C	247	LEU
1	B	8	ILE
1	B	13	ASP
1	B	55	ALA
1	B	138	LYS
1	B	345	PRO
1	A	371	GLY
1	B	394	GLY
1	C	107	ILE

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	351/351 (100%)	310 (88%)	41 (12%)	5	23
1	B	351/351 (100%)	291 (83%)	60 (17%)	2	11
1	C	360/351 (103%)	300 (83%)	60 (17%)	2	12
All	All	1062/1053 (101%)	901 (85%)	161 (15%)	3	14

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	11	LEU
1	A	12	LYS
1	A	14	ILE
1	A	20	LEU
1	A	22	ARG
1	A	35	LYS
1	A	45	PRO
1	A	82	GLU
1	A	93	LEU
1	A	96	ASN
1	A	97	ASP
1	A	98	CYS
1	A	116	ILE
1	A	117	LEU
1	A	121	LEU
1	A	122	ARG
1	A	126	GLU
1	A	138	LYS
1	A	143	LYS
1	A	155	LYS
1	A	203	PRO
1	A	204	GLN
1	A	207	LEU
1	A	208	LEU
1	A	219	LYS
1	A	222	LEU
1	A	229	LYS
1	A	232	ARG
1	A	259	GLU
1	A	270	GLU
1	A	285	PHE
1	A	292	ASP
1	A	332	THR
1	A	345	PRO
1	A	351	SER
1	A	387	GLU
1	A	399	LEU
1	A	400	GLU
1	A	406	GLU
1	A	415	ASN
1	B	6	LEU
1	B	20	LEU

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Mol	Chain	Res	Type
1	B	29	ILE
1	B	34	ILE
1	B	35	LYS
1	B	39	ARG
1	B	40	ILE
1	B	41	THR
1	B	43	THR
1	B	46	THR
1	B	48	ASN
1	B	50	LEU
1	B	51	LYS
1	B	66	ARG
1	B	71	ARG
1	B	93	LEU
1	B	97	ASP
1	B	98	CYS
1	B	108	ASN
1	B	117	LEU
1	B	122	ARG
1	B	126	GLU
1	B	132	VAL
1	B	143	LYS
1	B	144	GLU
1	B	161	ILE
1	B	173	SER
1	B	181	ASN
1	B	191	LYS
1	B	201	GLU
1	B	207	LEU
1	B	208	LEU
1	B	222	LEU
1	B	229	LYS
1	B	245	LYS
1	B	256	LEU
1	B	264	ILE
1	B	270	GLU
1	B	281	LEU
1	B	292	ASP
1	B	294	ASN
1	B	307	PRO
1	B	323	TYR
1	B	325	ASP

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Mol	Chain	Res	Type
1	B	332	THR
1	B	341	VAL
1	B	344	MSE
1	B	351	SER
1	B	363	LYS
1	B	370	VAL
1	B	375	THR
1	B	377	SER
1	B	378	LEU
1	B	383	ASN
1	B	386	ASN
1	B	399	LEU
1	B	401	LEU
1	B	406	GLU
1	B	407	LEU
1	B	414	SER
1	C	6	LEU
1	C	13	ASP
1	C	29	ILE
1	C	38	ASN
1	C	39	ARG
1	C	51	LYS
1	C	59	ILE
1	C	60	LEU
1	C	72	ASN
1	C	73	GLU
1	C	78	LYS
1	C	87	LEU
1	C	92	VAL
1	C	93	LEU
1	C	97	ASP
1	C	99	VAL
1	C	101	LYS
1	C	104	GLU
1	C	108	ASN
1	C	111	LYS
1	C	113	ASN
1	C	114	SER
1	C	126	GLU
1	C	143	LYS
1	C	144	GLU
1	C	153	LEU

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Mol	Chain	Res	Type
1	C	158	ASP
1	C	163	ASP
1	C	167	THR
1	C	175	MSE
1	C	189	MSE
1	C	201	GLU
1	C	205	ARG
1	C	207	LEU
1	C	208	LEU
1	C	216	VAL
1	C	219	LYS
1	C	221	GLN
1	C	222	LEU
1	C	242	THR
1	C	244	LYS
1	C	245	LYS
1	C	247	LEU
1	C	248	ASN
1	C	251	LYS
1	C	254	THR
1	C	283	VAL
1	C	285	PHE
1	C	294	ASN
1	C	318	LYS
1	C	325	ASP
1	C	341	VAL
1	C	351	SER
1	C	361	VAL
1	C	367	ILE
1	C	374	ASP
1	C	375	THR
1	C	378	LEU
1	C	405	LYS
1	C	414	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	49	HIS
1	A	108	ASN
1	A	113	ASN

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Mol	Chain	Res	Type
1	A	124	HIS
1	A	204	GLN
1	A	221	GLN
1	A	225	ASN
1	A	248	ASN
1	A	278	GLN
1	A	322	ASN
1	A	356	ASN
1	B	16	ASN
1	B	63	HIS
1	B	108	ASN
1	B	113	ASN
1	B	135	ASN
1	B	142	ASN
1	B	225	ASN
1	B	248	ASN
1	B	278	GLN
1	B	415	ASN
1	C	-3	HIS
1	C	-1	HIS
1	C	72	ASN
1	C	96	ASN
1	C	108	ASN
1	C	113	ASN
1	C	124	HIS
1	C	172	HIS
1	C	202	ASN
1	C	296	ASN
1	C	415	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 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
2	SO4	B	606	-	4,4,4	0.37	0	6,6,6	0.21	0
4	GOL	A	614	-	5,5,5	4.52	4 (80%)	5,5,5	6.07	3 (60%)
2	SO4	C	604	-	4,4,4	0.43	0	6,6,6	0.21	0
3	AMP	B	502	-	25,25,25	2.45	10 (40%)	37,38,38	1.42	7 (18%)
3	AMP	A	501	-	25,25,25	2.61	10 (40%)	37,38,38	1.43	6 (16%)
3	AMP	C	503	-	25,25,25	2.40	8 (32%)	37,38,38	1.43	9 (24%)
2	SO4	A	605	-	4,4,4	0.43	0	6,6,6	0.19	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
3	AMP	B	502	-	-	4/10/26/26	0/3/3/3
4	GOL	A	614	-	-	2/4/4/4	-
3	AMP	C	503	-	-	4/10/26/26	0/3/3/3
3	AMP	A	501	-	-	5/10/26/26	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	614	GOL	C3-C2	-7.90	1.21	1.51
3	A	501	AMP	C3'-C4'	6.95	1.70	1.53
3	C	503	AMP	C3'-C4'	6.70	1.70	1.53
3	B	502	AMP	C3'-C4'	6.55	1.69	1.53
3	B	502	AMP	O3'-C3'	4.72	1.54	1.43
3	A	501	AMP	O3'-C3'	4.58	1.54	1.43
3	C	503	AMP	C2'-C3'	4.44	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	AMP	O3'-C3'	4.38	1.53	1.43
4	A	614	GOL	O1-C1	4.18	1.60	1.42
3	B	502	AMP	C2'-C3'	3.93	1.64	1.53
3	A	501	AMP	C2'-C3'	3.92	1.64	1.53
4	A	614	GOL	O3-C3	3.55	1.57	1.42
3	A	501	AMP	C2'-C1'	3.53	1.64	1.53
3	A	501	AMP	C5-C4	3.36	1.45	1.39
3	C	503	AMP	C8-N9	2.98	1.42	1.37
3	A	501	AMP	C8-N9	2.88	1.42	1.37
4	A	614	GOL	O2-C2	-2.80	1.35	1.43
3	B	502	AMP	C2'-C1'	2.79	1.62	1.53
3	A	501	AMP	C8-N7	2.78	1.37	1.31
3	B	502	AMP	C5-C4	2.78	1.44	1.39
3	B	502	AMP	C8-N9	2.72	1.42	1.37
3	C	503	AMP	C2'-C1'	2.69	1.61	1.53
3	A	501	AMP	C1'-N9	2.65	1.53	1.46
3	A	501	AMP	O4'-C4'	2.62	1.50	1.45
3	C	503	AMP	C5-C4	2.44	1.43	1.39
3	B	502	AMP	O4'-C4'	2.40	1.50	1.45
3	B	502	AMP	C8-N7	2.40	1.36	1.31
3	C	503	AMP	C8-N7	2.39	1.36	1.31
3	C	503	AMP	C5'-C4'	2.16	1.58	1.51
3	B	502	AMP	O4'-C1'	2.13	1.46	1.42
3	B	502	AMP	C5'-C4'	2.12	1.57	1.51
3	A	501	AMP	O4'-C1'	2.01	1.46	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	614	GOL	O3-C3-C2	10.84	159.19	110.38
4	A	614	GOL	O2-C2-C3	7.24	139.16	109.18
4	A	614	GOL	O1-C1-C2	3.62	126.68	110.38
3	A	501	AMP	N6-C6-N1	3.15	125.40	118.38
3	C	503	AMP	N6-C6-N1	3.14	125.36	118.38
3	B	502	AMP	N6-C6-N1	3.00	125.06	118.38
3	B	502	AMP	C2-N1-C6	2.83	123.38	118.73
3	A	501	AMP	C2-N1-C6	2.80	123.33	118.73
3	C	503	AMP	C2-N1-C6	2.78	123.30	118.73
3	B	502	AMP	C4-C5-N7	2.72	113.69	110.58
3	C	503	AMP	C4-C5-N7	2.67	113.63	110.58
3	B	502	AMP	C5-N7-C8	-2.66	99.27	103.45
3	A	501	AMP	C4-C5-N7	2.66	113.62	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	AMP	N9-C8-N7	2.57	117.58	113.94
3	A	501	AMP	C5-N7-C8	-2.56	99.42	103.45
3	C	503	AMP	C5-N7-C8	-2.50	99.53	103.45
3	C	503	AMP	C3'-C2'-C1'	2.37	105.94	101.46
3	B	502	AMP	N3-C2-N1	-2.36	125.01	128.58
3	B	502	AMP	N9-C8-N7	2.27	117.16	113.94
3	A	501	AMP	C3'-C2'-C1'	2.26	105.73	101.46
3	C	503	AMP	C4'-O4'-C1'	2.17	114.26	109.47
3	C	503	AMP	N3-C2-N1	-2.10	125.40	128.58
3	B	502	AMP	O3'-C3'-C4'	-2.09	105.09	111.08
3	C	503	AMP	O3'-C3'-C4'	-2.08	105.11	111.08
3	C	503	AMP	N9-C8-N7	2.01	116.79	113.94

There are no chirality outliers.

All (15) torsion outliers are listed below:

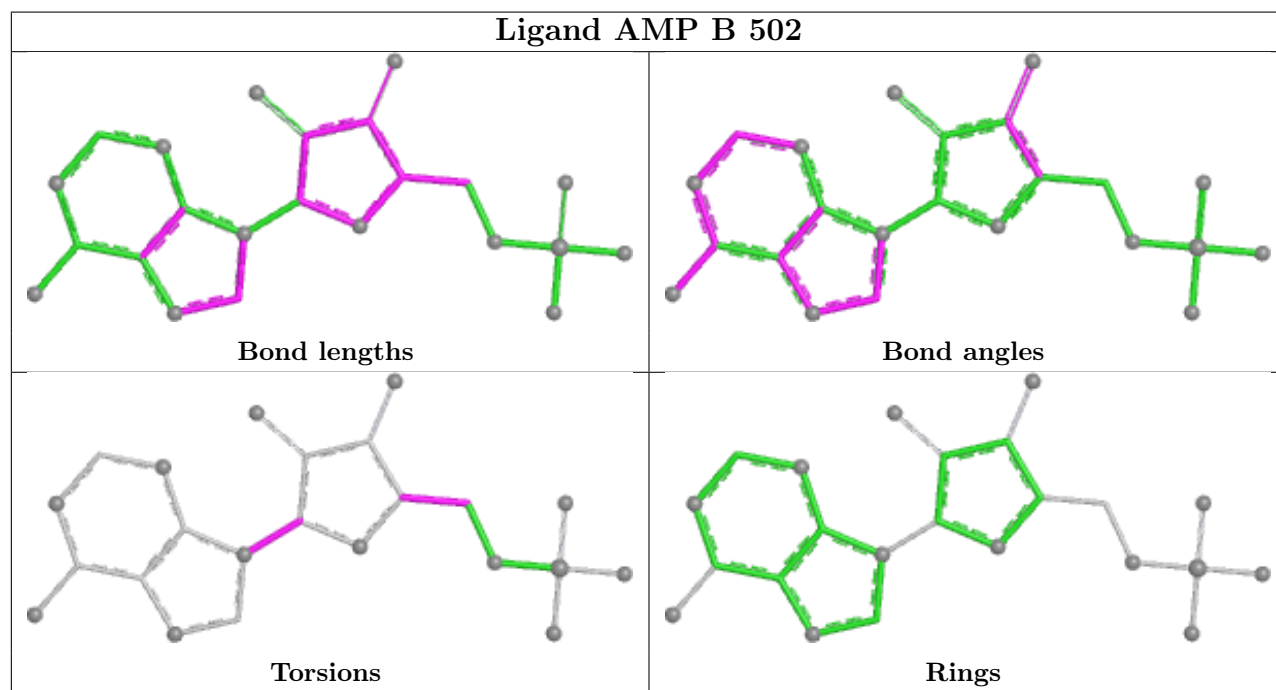
Mol	Chain	Res	Type	Atoms
4	A	614	GOL	C1-C2-C3-O3
4	A	614	GOL	O1-C1-C2-O2
3	B	502	AMP	C2'-C1'-N9-C8
3	C	503	AMP	C2'-C1'-N9-C8
3	A	501	AMP	C2'-C1'-N9-C8
3	B	502	AMP	C2'-C1'-N9-C4
3	C	503	AMP	C2'-C1'-N9-C4
3	A	501	AMP	O4'-C1'-N9-C4
3	A	501	AMP	O4'-C1'-N9-C8
3	A	501	AMP	C2'-C1'-N9-C4
3	B	502	AMP	O4'-C1'-N9-C8
3	C	503	AMP	O4'-C1'-N9-C8
3	A	501	AMP	O4'-C4'-C5'-O5'
3	B	502	AMP	O4'-C4'-C5'-O5'
3	C	503	AMP	O4'-C4'-C5'-O5'

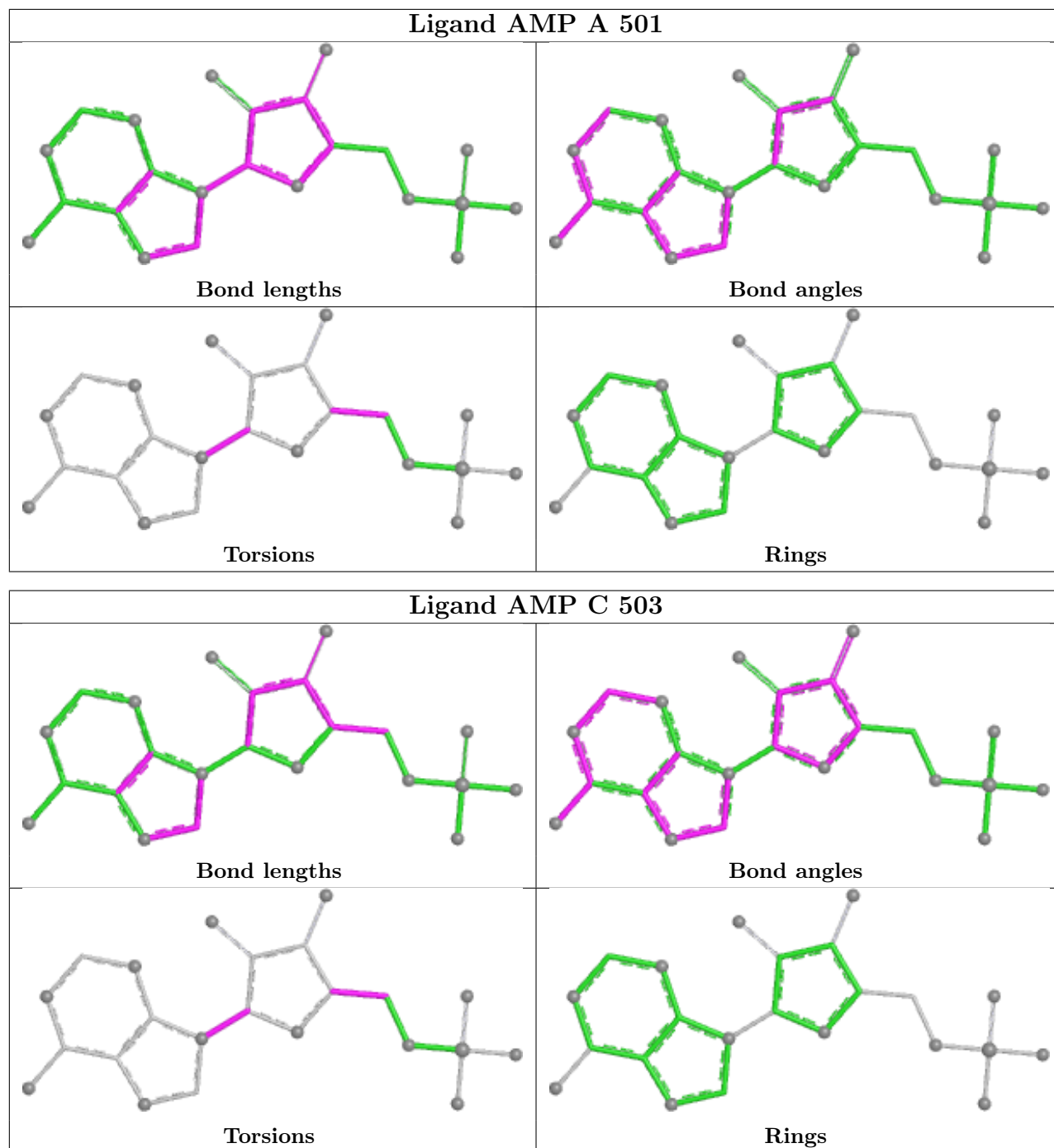
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	AMP	2	0
3	A	501	AMP	1	0
3	C	503	AMP	3	0

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





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	409/425 (96%)	0.72	21 (5%) 33 17	26, 45, 73, 94	0
1	B	407/425 (95%)	1.05	52 (12%) 7 5	31, 50, 73, 87	0
1	C	415/425 (97%)	1.87	171 (41%) 0 1	26, 46, 77, 91	0
All	All	1231/1275 (96%)	1.22	244 (19%) 3 2	26, 46, 74, 94	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	67	PRO	6.7
1	C	11	LEU	6.0
1	C	89	GLY	5.6
1	C	-6	SER	5.4
1	C	409	GLY	5.3
1	C	114	SER	5.1
1	C	120	ASN	5.1
1	C	98	CYS	4.9
1	C	68	ASP	4.8
1	B	16	ASN	4.4
1	C	382	GLN	4.2
1	C	164	ALA	4.1
1	C	24	ASP	4.1
1	C	134	ALA	4.1
1	C	79	PRO	4.0
1	C	25	PHE	4.0
1	A	249	ASN	3.8
1	C	347	PHE	3.8
1	C	62	SER	3.7
1	C	163	ASP	3.7
1	C	10	ASP	3.6
1	C	75	TYR	3.6
1	C	-7	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	8	ILE	3.6
1	C	34	ILE	3.5
1	C	72	ASN	3.5
1	C	416	LYS	3.5
1	B	345	PRO	3.5
1	C	64	CYS	3.5
1	C	23	VAL	3.4
1	B	204	GLN	3.4
1	B	10	ASP	3.4
1	C	76	THR	3.4
1	C	123	PHE	3.4
1	C	185	SER	3.4
1	C	107	ILE	3.3
1	C	142	ASN	3.3
1	C	4	ASN	3.3
1	C	238	GLY	3.2
1	A	71	ARG	3.2
1	C	118	LEU	3.2
1	C	94	PHE	3.2
1	B	184	ALA	3.2
1	C	129	GLY	3.1
1	C	342	PHE	3.1
1	C	256	LEU	3.1
1	B	201	GLU	3.1
1	B	8	ILE	3.1
1	C	63	HIS	3.1
1	C	315	ALA	3.1
1	C	83	THR	3.1
1	C	214	ALA	3.1
1	C	218	ASP	3.1
1	C	55	ALA	3.1
1	C	237	GLY	3.1
1	C	177	GLY	3.0
1	A	322	ASN	3.0
1	B	56	SER	3.0
1	C	44	LEU	3.0
1	C	95	LEU	3.0
1	C	12	LYS	3.0
1	C	124	HIS	3.0
1	C	156	LEU	3.0
1	C	349	LYS	3.0
1	C	117	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	56	SER	2.9
1	B	295	ALA	2.9
1	C	39	ARG	2.9
1	C	82	GLU	2.9
1	C	54	GLY	2.9
1	C	160	PHE	2.9
1	C	293	ASN	2.9
1	B	6	LEU	2.9
1	C	47	ILE	2.9
1	C	286	LYS	2.9
1	C	399	LEU	2.9
1	C	119	GLU	2.8
1	C	162	ASN	2.8
1	C	5	LYS	2.8
1	C	149	PHE	2.8
1	C	92	VAL	2.8
1	B	202	ASN	2.8
1	C	77	LEU	2.8
1	C	130	LYS	2.8
1	A	285	PHE	2.8
1	C	41	THR	2.8
1	C	338	PRO	2.8
1	B	181	ASN	2.7
1	C	251	LYS	2.7
1	C	103	VAL	2.7
1	B	307	PRO	2.7
1	C	158	ASP	2.7
1	C	314	ASP	2.7
1	B	331	LYS	2.7
1	A	10	ASP	2.7
1	C	171	ALA	2.7
1	C	27	VAL	2.7
1	C	187	PHE	2.7
1	C	291	PHE	2.7
1	C	19	VAL	2.7
1	C	14	ILE	2.7
1	C	184	ALA	2.7
1	C	366	ALA	2.7
1	C	413	LEU	2.7
1	A	-1	HIS	2.7
1	C	40	ILE	2.6
1	C	200	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	74	LYS	2.6
1	A	380	GLU	2.6
1	C	20	LEU	2.6
1	B	7	SER	2.6
1	B	294	ASN	2.6
1	C	113	ASN	2.6
1	B	396	GLY	2.6
1	C	69	GLY	2.6
1	A	246	VAL	2.6
1	C	169	HIS	2.6
1	C	220	ILE	2.6
1	C	-1	HIS	2.6
1	A	283	VAL	2.6
1	C	141	ALA	2.6
1	C	146	VAL	2.6
1	C	348	ALA	2.6
1	B	1	HIS	2.5
1	C	398	SER	2.5
1	A	2	LEU	2.5
1	C	99	VAL	2.5
1	C	48	ASN	2.5
1	C	412	ALA	2.5
1	C	299	PHE	2.5
1	C	307	PRO	2.5
1	B	86	GLY	2.5
1	C	396	GLY	2.5
1	C	381	GLN	2.5
1	C	110	ALA	2.5
1	C	174	SER	2.5
1	B	34	ILE	2.5
1	C	104	GLU	2.5
1	C	267	GLU	2.5
1	C	66	ARG	2.5
1	C	172	HIS	2.5
1	C	81	ALA	2.4
1	A	218	ASP	2.4
1	B	251	LYS	2.4
1	C	292	ASP	2.4
1	B	323	TYR	2.4
1	C	176	VAL	2.4
1	B	168	ALA	2.4
1	B	73	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	354	CYS	2.4
1	C	380	GLU	2.4
1	C	245	LYS	2.4
1	C	115	VAL	2.4
1	C	353	GLU	2.4
1	C	60	LEU	2.4
1	B	413	LEU	2.4
1	C	132	VAL	2.4
1	C	86	GLY	2.4
1	B	389	SER	2.4
1	A	238	GLY	2.3
1	C	65	GLY	2.3
1	C	101	LYS	2.3
1	B	24	ASP	2.3
1	C	302	ASP	2.3
1	C	265	VAL	2.3
1	C	351	SER	2.3
1	C	121	LEU	2.3
1	C	128	GLU	2.3
1	C	385	LYS	2.3
1	C	173	SER	2.3
1	B	31	ASN	2.3
1	C	38	ASN	2.3
1	B	302	ASP	2.3
1	C	15	LYS	2.3
1	C	22	ARG	2.3
1	C	61	ILE	2.3
1	C	255	SER	2.3
1	C	36	ASP	2.3
1	B	146	VAL	2.3
1	C	194	GLU	2.3
1	C	33	ILE	2.3
1	C	377	SER	2.3
1	C	221	GLN	2.3
1	C	303	GLU	2.2
1	B	252	ILE	2.2
1	C	288	ALA	2.2
1	B	144	GLU	2.2
1	C	304	GLU	2.2
1	B	185	SER	2.2
1	C	137	ASN	2.2
1	B	321	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	406	GLU	2.2
1	C	29	ILE	2.2
1	B	13	ASP	2.2
1	C	3	GLY	2.2
1	A	138	LYS	2.2
1	B	167	THR	2.2
1	B	306	ILE	2.2
1	B	90	GLU	2.2
1	C	96	ASN	2.2
1	C	50	LEU	2.2
1	A	330	SER	2.2
1	A	6	LEU	2.2
1	C	111	LYS	2.2
1	C	415	ASN	2.2
1	B	37	THR	2.1
1	C	106	LYS	2.1
1	B	171	ALA	2.1
1	B	89	GLY	2.1
1	B	4	ASN	2.1
1	C	248	ASN	2.1
1	A	325	ASP	2.1
1	B	23	VAL	2.1
1	B	178	VAL	2.1
1	C	391	VAL	2.1
1	B	2	LEU	2.1
1	A	272	ALA	2.1
1	A	255	SER	2.1
1	C	312	GLY	2.1
1	B	14	ILE	2.1
1	B	61	ILE	2.1
1	C	153	LEU	2.1
1	C	16	ASN	2.1
1	A	227	LEU	2.1
1	C	178	VAL	2.1
1	C	246	VAL	2.1
1	C	18	LYS	2.1
1	C	290	ASN	2.1
1	C	90	GLU	2.1
1	A	276	ASN	2.0
1	C	310	TRP	2.0
1	C	308	ASP	2.0
1	C	100	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	198	LYS	2.0
1	B	364	LYS	2.0
1	C	259	GLU	2.0
1	B	391	VAL	2.0
1	C	84	LEU	2.0
1	C	26	ASN	2.0
1	C	42	ALA	2.0
1	C	295	ALA	2.0
1	C	289	ASP	2.0
1	C	357	LEU	2.0
1	C	252	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

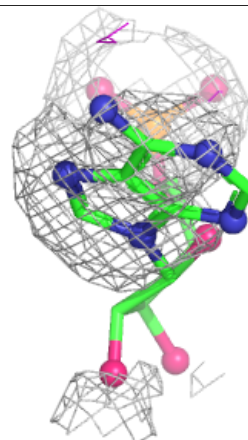
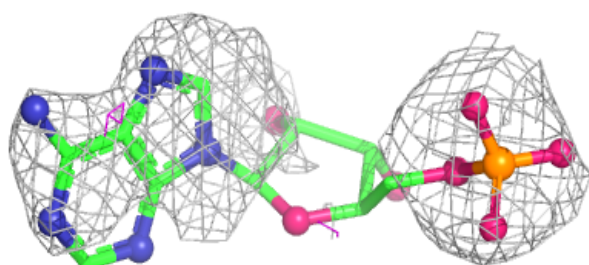
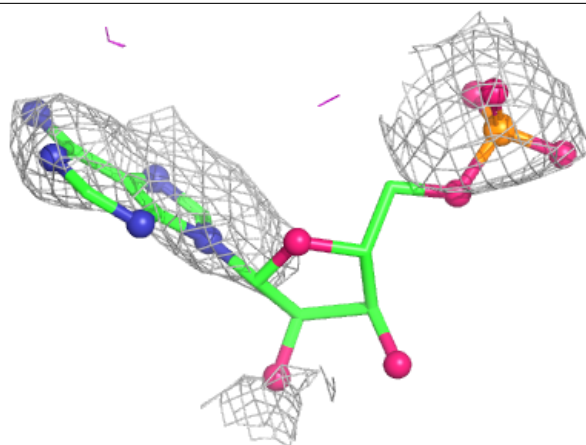
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	C	604	5/5	0.54	0.33	108,108,109,110	0
4	GOL	A	614	6/6	0.61	0.26	61,64,65,67	0
2	SO4	B	606	5/5	0.63	0.18	93,94,95,95	0
3	AMP	C	503	23/23	0.66	0.26	104,115,117,117	0
3	AMP	A	501	23/23	0.70	0.29	103,109,113,113	0
3	AMP	B	502	23/23	0.77	0.27	110,125,126,126	0
2	SO4	A	605	5/5	0.80	0.14	98,99,99,99	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.

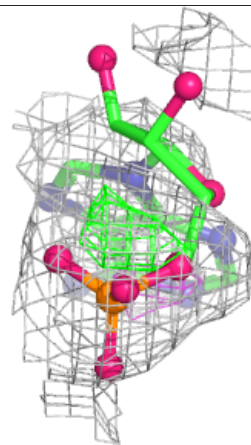
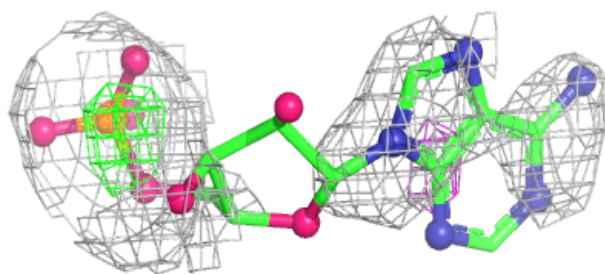
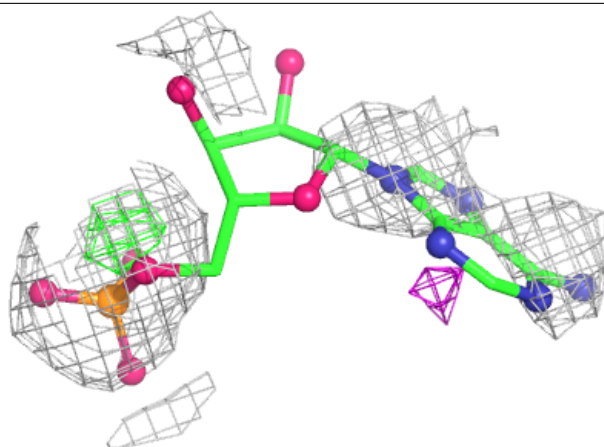
Electron density around AMP C 503:

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



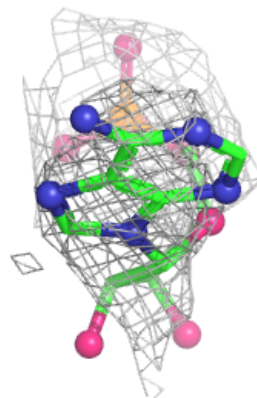
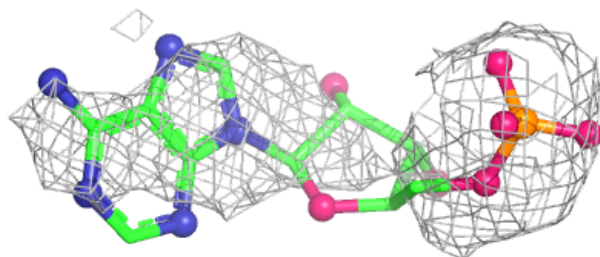
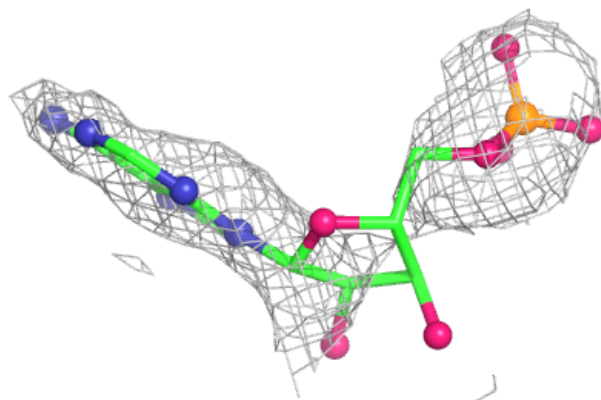
Electron density around AMP A 501:

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



Electron density around AMP B 502:

$2mF_o-DF_c$ (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.