



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:05 AM UTC

PDB ID : 7BUQ / pdb_00007buq
Title : mcGAS bound with 23-cGAMP
Authors : Wang, B.; Su, X.D.
Deposited on : 2020-04-07
Resolution : 3.09 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

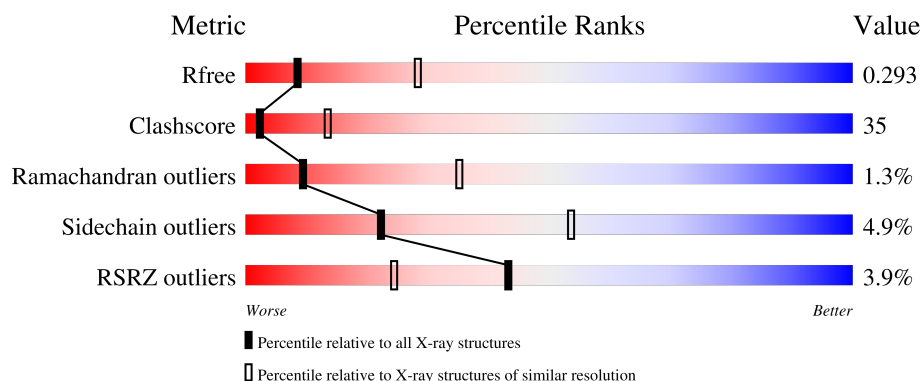
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	507	
1	B	507	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6070 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.

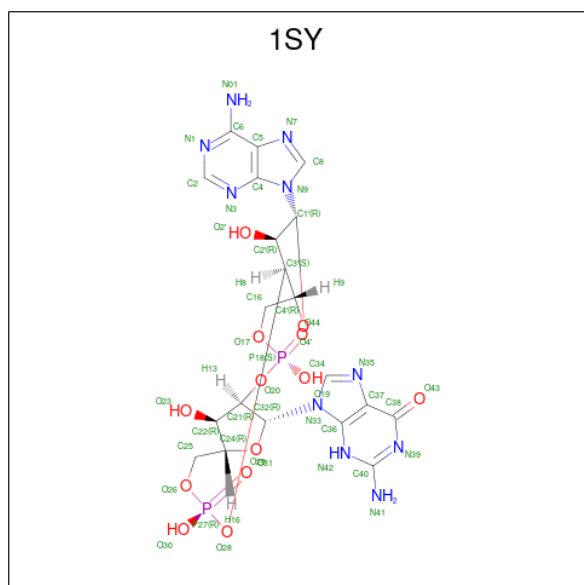
- Molecule 1 is a protein called Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2993	1924	509	547	13			
1	B	361	Total	C	N	O	S	0	0	0
			2984	1919	508	544	13			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is cGAMP (CCD ID: 1SY) (formula: C₂₀H₂₄N₁₀O₁₃P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
3	B	1	Total	C	N	O	P	0	0
			45	20	10	13	2		

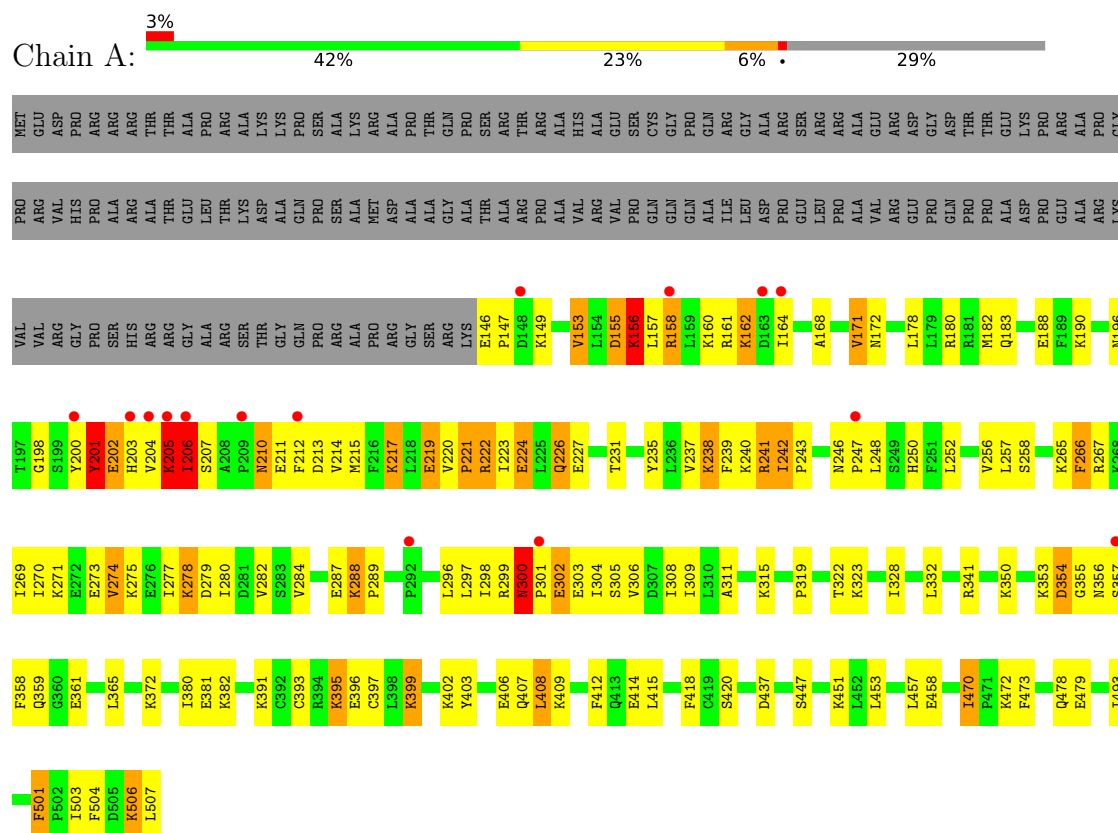
- Molecule 4 is water.

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

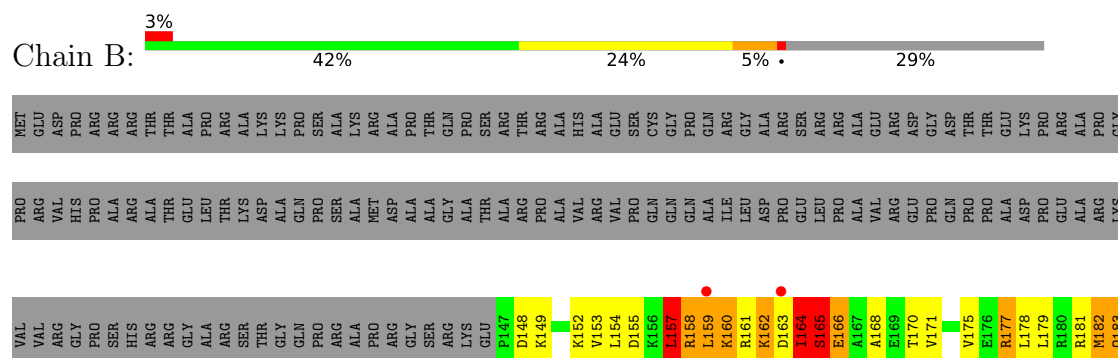
3 Residue-property plots

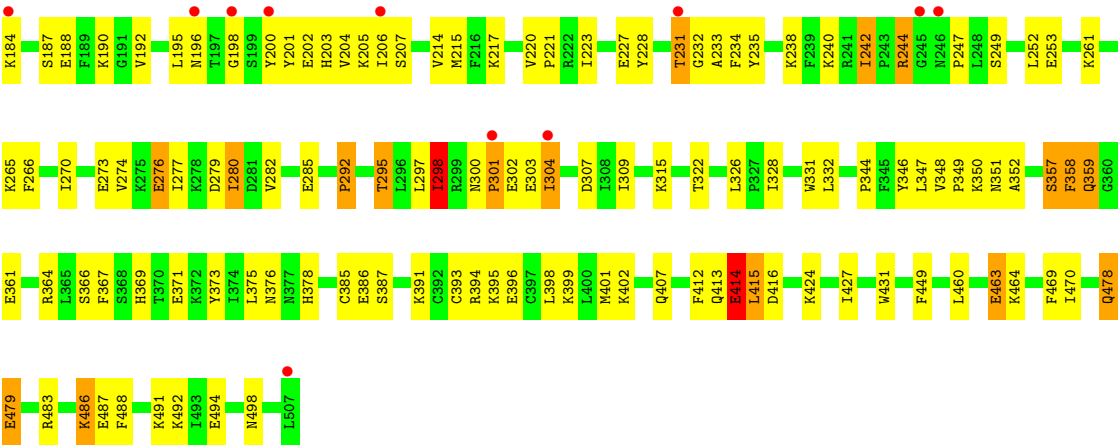
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Cyclic GMP-AMP synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.65Å 109.81Å 75.64Å 90.00° 94.13° 90.00°	Depositor
Resolution (Å)	37.72 – 3.09 37.72 – 3.09	Depositor EDS
% Data completeness (in resolution range)	97.2 (37.72-3.09) 97.1 (37.72-3.09)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.249 , 0.296 0.249 , 0.293	Depositor DCC
R_{free} test set	1403 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6070	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: 1SY, ZN

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	1.23	17/3058 (0.6%)	1.08	31/4106 (0.8%)
1	B	1.03	9/3049 (0.3%)	1.02	24/4093 (0.6%)
All	All	1.13	26/6107 (0.4%)	1.05	55/8199 (0.7%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	350	LYS	C-O	-6.85	1.15	1.24
1	A	153	VAL	C-O	-6.48	1.16	1.24
1	A	350	LYS	C-O	-6.28	1.16	1.24
1	B	424	LYS	C-O	-6.16	1.17	1.24
1	A	217	LYS	C-O	-6.16	1.16	1.24
1	A	171	VAL	C-O	-6.14	1.16	1.24
1	B	464	LYS	CA-C	-5.87	1.47	1.53
1	A	190	LYS	CA-C	-5.84	1.45	1.52
1	A	470	ILE	C-O	-5.74	1.17	1.24
1	A	155	ASP	C-O	-5.65	1.16	1.24
1	A	382	LYS	C-O	-5.62	1.16	1.24
1	A	397	CYS	C-O	-5.59	1.17	1.24
1	B	460	LEU	C-O	-5.59	1.17	1.24
1	A	408	LEU	C-O	-5.51	1.16	1.24
1	A	399	LYS	C-O	-5.48	1.17	1.24
1	A	242	ILE	CA-C	-5.48	1.48	1.52
1	B	463	GLU	CA-C	-5.45	1.47	1.53
1	B	233	ALA	C-O	-5.41	1.17	1.24
1	A	219	GLU	CA-C	-5.31	1.46	1.52
1	A	224	GLU	C-O	-5.27	1.18	1.24
1	A	395	LYS	C-O	-5.26	1.17	1.24
1	A	224	GLU	CA-C	-5.26	1.46	1.52
1	A	190	LYS	C-O	-5.23	1.17	1.24
1	B	152	LYS	C-O	-5.05	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	MET	C-O	-5.02	1.17	1.24
1	B	157	LEU	CA-C	-5.00	1.46	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	THR	N-CA-C	-9.16	101.88	113.43
1	B	373	TYR	N-CA-C	-9.08	101.97	113.23
1	A	358	PHE	N-CA-C	8.22	122.64	107.60
1	A	206	ILE	CB-CA-C	-8.11	100.99	111.53
1	B	166	GLU	N-CA-C	-8.05	103.47	113.38
1	B	165	SER	N-CA-C	7.76	121.25	111.24
1	B	177	ARG	N-CA-C	-7.60	102.13	111.40
1	B	359	GLN	N-CA-C	7.44	119.03	111.07
1	B	149	LYS	N-CA-C	-7.39	104.77	114.31
1	A	201	TYR	N-CA-C	-7.31	95.80	108.52
1	A	222	ARG	N-CA-C	7.17	126.07	110.80
1	B	280	ILE	N-CA-C	6.99	118.22	108.23
1	B	242	ILE	CA-C-N	6.94	128.51	119.84
1	B	242	ILE	C-N-CA	6.94	128.51	119.84
1	B	414	GLU	N-CA-C	-6.83	104.56	113.17
1	A	156	LYS	N-CA-C	-6.80	104.99	113.28
1	A	354	ASP	N-CA-C	6.74	119.72	108.73
1	A	210	ASN	N-CA-C	6.67	125.02	110.80
1	A	355	GLY	N-CA-C	-6.53	107.21	115.31
1	B	164	ILE	N-CA-C	6.30	122.45	109.34
1	A	241	ARG	CA-C-N	-6.17	117.36	123.04
1	A	241	ARG	C-N-CA	-6.17	117.36	123.04
1	A	278	LYS	N-CA-C	6.12	123.84	110.80
1	A	162	LYS	N-CA-C	5.98	118.58	111.71
1	A	279	ASP	CA-C-N	-5.91	115.86	123.19
1	A	279	ASP	C-N-CA	-5.91	115.86	123.19
1	A	288	LYS	CA-C-N	5.90	125.83	119.76
1	A	288	LYS	C-N-CA	5.90	125.83	119.76
1	A	277	ILE	N-CA-C	-5.86	101.10	108.84
1	A	190	LYS	N-CA-C	-5.86	104.97	111.36
1	A	458	GLU	N-CA-C	-5.80	104.86	111.07
1	A	280	ILE	N-CA-C	5.74	116.21	108.17
1	B	231	THR	N-CA-C	-5.74	105.05	112.68
1	B	196	ASN	N-CA-C	-5.65	101.01	109.15
1	B	148	ASP	N-CA-C	-5.65	103.53	110.65
1	A	158	ARG	N-CA-C	-5.62	106.28	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	LYS	N-CA-C	-5.57	98.93	110.80
1	B	160	LYS	N-CA-C	5.48	122.48	110.80
1	A	226	GLN	N-CA-C	-5.37	99.98	108.73
1	B	266	PHE	N-CA-C	-5.35	105.35	111.07
1	B	295	THR	N-CA-C	5.34	118.25	109.76
1	A	501	PHE	CA-C-N	5.29	126.00	120.12
1	A	501	PHE	C-N-CA	5.29	126.00	120.12
1	B	298	ILE	N-CA-CB	5.28	119.31	110.86
1	B	416	ASP	N-CA-C	-5.26	106.09	112.88
1	A	353	LYS	N-CA-C	5.24	119.35	111.81
1	B	357	SER	N-CA-C	-5.22	99.67	110.80
1	A	357	SER	CB-CA-C	-5.22	110.54	116.54
1	B	183	GLN	N-CA-C	-5.14	105.26	112.25
1	A	242	ILE	N-CA-C	-5.12	102.02	108.05
1	B	153	VAL	CB-CA-C	-5.10	105.41	112.24
1	A	472	LYS	N-CA-C	5.09	116.91	111.36
1	A	266	PHE	N-CA-C	-5.08	105.63	111.07
1	B	358	PHE	N-CA-C	5.07	121.60	110.80
1	A	274	VAL	N-CA-C	5.04	118.13	111.17

There are no chirality outliers.

There are no planarity outliers.

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	2993	0	3039	214	0
1	B	2984	0	3034	215	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	45	0	22	14	0
3	B	45	0	22	13	0
4	A	1	0	0	0	0
All	All	6070	0	6117	432	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 35.

All (432) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HG23	1:B:399:LYS:CG	1.47	1.42
1:B:164:ILE:CD1	1:B:202:GLU:HA	1.56	1.35
1:A:223:ILE:CD1	1:A:239:PHE:HE1	1.41	1.33
1:A:300:ASN:HB3	1:A:301:PRO:CD	1.55	1.33
1:A:300:ASN:CB	1:A:301:PRO:HD3	1.52	1.30
1:B:164:ILE:HD11	1:B:202:GLU:CG	1.66	1.25
1:B:182:MET:HE1	1:B:270:ILE:HG12	1.24	1.19
1:B:198:GLY:CA	1:B:201:TYR:HE1	1.56	1.19
1:A:296:LEU:HB2	1:A:306:VAL:CG2	1.75	1.17
1:A:265:LYS:HG2	1:A:269:ILE:CD1	1.74	1.16
1:B:207:SER:CB	1:B:402:LYS:HG3	1.76	1.15
1:B:198:GLY:HA3	1:B:201:TYR:CE1	1.80	1.15
1:B:207:SER:HB3	1:B:402:LYS:HG3	1.26	1.14
1:A:205:LYS:O	1:A:402:LYS:HD2	1.47	1.14
1:A:243:PRO:HD2	1:A:246:ASN:HD22	1.11	1.14
1:B:285:GLU:CG	1:B:297:LEU:HD23	1.78	1.13
1:A:203:HIS:ND1	1:A:207:SER:HB2	1.62	1.13
3:A:602:1SY:H8	3:A:602:1SY:H18	1.13	1.12
1:B:463:GLU:HG2	1:B:486:LYS:HE3	1.19	1.12
1:B:206:ILE:CG2	1:B:399:LYS:HG2	1.81	1.09
1:B:181:ARG:HG2	1:B:273:GLU:OE2	1.52	1.09
1:A:223:ILE:CD1	1:A:239:PHE:CE1	2.34	1.09
1:B:164:ILE:CD1	1:B:202:GLU:HG3	1.83	1.08
1:B:198:GLY:CA	1:B:201:TYR:CE1	2.36	1.08
1:A:162:LYS:HG3	1:B:387:SER:OG	1.52	1.08
1:B:206:ILE:HG23	1:B:399:LYS:HG2	1.12	1.08
1:B:198:GLY:HA3	1:B:201:TYR:HE1	1.03	1.07
1:A:160:LYS:HD3	1:A:203:HIS:CB	1.85	1.06
1:B:207:SER:HB3	1:B:402:LYS:CG	1.84	1.06
1:B:171:VAL:O	1:B:175:VAL:HG23	1.55	1.06
3:B:602:1SY:H18	3:B:602:1SY:H8	1.13	1.06
1:B:206:ILE:CG2	1:B:399:LYS:CG	2.37	1.02
1:A:409:LYS:HE3	1:A:418:PHE:O	1.59	1.02
1:A:161:ARG:HH22	1:B:201:TYR:HE2	1.06	1.01
1:A:223:ILE:HD12	1:A:239:PHE:HE1	1.21	1.01
1:B:164:ILE:HG21	1:B:205:LYS:HG3	1.42	1.01
1:B:300:ASN:HB3	1:B:301:PRO:HD3	1.41	1.00
1:A:447:SER:O	1:A:451:LYS:HG3	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PRO:HG3	1:A:246:ASN:HD21	1.23	1.00
1:B:164:ILE:HD13	1:B:202:GLU:HA	1.02	1.00
1:B:182:MET:HE1	1:B:270:ILE:CG1	1.91	0.99
1:A:296:LEU:HB2	1:A:306:VAL:HG23	1.40	0.99
1:A:205:LYS:C	1:A:402:LYS:NZ	2.22	0.98
1:B:164:ILE:CD1	1:B:202:GLU:CA	2.41	0.98
1:A:206:ILE:HA	1:A:402:LYS:HD3	1.45	0.97
1:A:223:ILE:HD13	1:A:239:PHE:HE1	1.27	0.96
1:B:206:ILE:HG23	1:B:399:LYS:HG3	1.43	0.96
1:B:285:GLU:HG3	1:B:297:LEU:HD23	1.48	0.95
1:B:244:ARG:HE	1:B:244:ARG:HA	1.27	0.95
1:B:179:LEU:O	1:B:183:GLN:HG3	1.66	0.94
1:A:204:VAL:CG1	1:A:395:LYS:HE2	1.98	0.93
1:B:309:ILE:CD1	3:B:602:1SY:N42	2.31	0.93
1:A:203:HIS:CG	1:A:207:SER:HB2	2.04	0.92
3:B:602:1SY:H18	3:B:602:1SY:C3'	1.99	0.91
1:B:463:GLU:HG2	1:B:486:LYS:CE	2.00	0.91
1:A:146:GLU:HB2	1:A:147:PRO:HD2	1.52	0.91
1:A:223:ILE:HD12	1:A:239:PHE:CE1	2.01	0.91
1:B:164:ILE:HD11	1:B:202:GLU:HG3	0.91	0.90
1:B:164:ILE:O	1:B:168:ALA:HB3	1.70	0.90
1:A:300:ASN:CB	1:A:301:PRO:CD	2.29	0.89
1:B:207:SER:HB3	1:B:402:LYS:CB	2.03	0.88
1:A:146:GLU:HB2	1:A:147:PRO:CD	2.03	0.88
1:A:205:LYS:C	1:A:402:LYS:HZ3	1.81	0.87
1:A:172:ASN:HA	1:A:200:TYR:OH	1.74	0.87
1:B:158:ARG:O	1:B:158:ARG:NH2	2.07	0.87
1:B:201:TYR:CE2	1:B:203:HIS:ND1	2.42	0.87
1:B:201:TYR:CE2	1:B:203:HIS:CE1	2.63	0.86
1:A:265:LYS:HG2	1:A:269:ILE:HD11	1.55	0.86
1:A:160:LYS:HD3	1:A:203:HIS:HB2	1.57	0.86
3:B:602:1SY:O17	3:B:602:1SY:H4	1.76	0.86
1:B:201:TYR:CZ	1:B:203:HIS:ND1	2.44	0.85
1:B:244:ARG:HA	1:B:244:ARG:NE	1.87	0.85
1:B:159:LEU:HD12	1:B:159:LEU:H	1.41	0.84
1:A:205:LYS:O	1:A:402:LYS:CD	2.25	0.84
1:A:160:LYS:CD	1:A:203:HIS:HB2	2.08	0.84
1:B:164:ILE:HG12	1:B:205:LYS:HZ3	1.42	0.84
1:A:223:ILE:HD13	1:A:239:PHE:CE1	2.05	0.83
1:B:164:ILE:HG21	1:B:205:LYS:CG	2.08	0.83
1:B:463:GLU:CG	1:B:486:LYS:HE3	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:HH12	1:B:277:ILE:HG21	1.40	0.83
3:A:602:1SY:H18	3:A:602:1SY:C3'	2.04	0.83
1:A:149:LYS:O	1:A:153:VAL:HG23	1.80	0.82
1:A:219:GLU:OE2	1:A:315:LYS:HD2	1.78	0.82
1:A:219:GLU:OE2	1:A:315:LYS:HG3	1.79	0.82
1:A:206:ILE:HA	1:A:402:LYS:CD	2.09	0.81
1:A:203:HIS:ND1	1:A:207:SER:CB	2.44	0.81
1:B:297:LEU:HA	1:B:304:ILE:O	1.80	0.80
1:A:203:HIS:CE1	1:A:207:SER:CB	2.64	0.80
1:A:243:PRO:HD2	1:A:246:ASN:ND2	1.94	0.80
1:A:153:VAL:O	1:A:157:LEU:HG	1.82	0.80
1:A:265:LYS:CG	1:A:269:ILE:CD1	2.58	0.79
1:A:160:LYS:HD3	1:A:203:HIS:CG	2.17	0.79
1:B:181:ARG:NH1	1:B:277:ILE:HG21	1.97	0.79
1:B:181:ARG:NH1	1:B:277:ILE:CG2	2.47	0.78
1:A:265:LYS:HG2	1:A:269:ILE:HD13	1.64	0.78
1:B:285:GLU:HG2	1:B:297:LEU:HD23	1.63	0.78
1:B:300:ASN:CB	1:B:301:PRO:HD3	2.13	0.78
1:B:478:GLN:H	1:B:478:GLN:NE2	1.82	0.77
1:B:171:VAL:O	1:B:175:VAL:CG2	2.32	0.77
1:B:367:PHE:O	1:B:371:GLU:HG3	1.84	0.77
1:B:164:ILE:HD11	1:B:202:GLU:CA	2.11	0.77
1:B:203:HIS:NE2	1:B:376:ASN:ND2	2.33	0.76
1:A:248:LEU:N	1:A:248:LEU:HD22	2.02	0.75
3:A:602:1SY:H8	3:A:602:1SY:C25	2.06	0.75
1:B:164:ILE:HG21	1:B:205:LYS:HB2	1.68	0.75
1:B:414:GLU:HG3	1:B:414:GLU:O	1.84	0.75
1:A:219:GLU:OE2	1:A:315:LYS:CD	2.35	0.74
1:A:300:ASN:HB3	1:A:301:PRO:HD3	0.77	0.74
1:A:204:VAL:HG13	1:A:395:LYS:HE2	1.70	0.73
1:A:171:VAL:HG12	1:A:200:TYR:CE1	2.23	0.73
1:A:203:HIS:CE1	1:A:207:SER:HB2	2.24	0.73
1:B:187:SER:O	1:B:190:LYS:HG2	1.89	0.73
1:B:203:HIS:CE1	1:B:376:ASN:HD21	2.06	0.73
1:A:206:ILE:N	1:A:402:LYS:HZ3	1.86	0.72
1:B:164:ILE:HG12	1:B:205:LYS:NZ	2.03	0.72
1:B:220:VAL:HB	1:B:221:PRO:HD2	1.70	0.72
1:B:164:ILE:HD11	1:B:202:GLU:CB	2.19	0.72
1:B:195:LEU:HD21	1:B:346:TYR:OH	1.90	0.72
1:B:207:SER:OG	1:B:402:LYS:HG3	1.89	0.71
1:A:219:GLU:OE2	1:A:315:LYS:CG	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:1SY:O29	3:B:602:1SY:O2'	2.04	0.71
1:B:292:PRO:HB2	1:B:349:PRO:HG2	1.73	0.71
1:B:276:GLU:HG3	1:B:276:GLU:O	1.89	0.71
1:B:154:LEU:HD11	1:B:396:GLU:HB3	1.72	0.71
1:A:402:LYS:O	1:A:406:GLU:HG3	1.90	0.70
1:B:300:ASN:HB3	1:B:301:PRO:CD	2.21	0.70
1:B:234:PHE:CD2	1:B:352:ALA:HB2	2.25	0.70
3:B:602:1SY:H8	3:B:602:1SY:C25	2.07	0.70
1:A:196:ASN:OD1	1:A:372:LYS:NZ	2.24	0.70
1:A:203:HIS:CD2	1:A:207:SER:OG	2.45	0.70
1:A:205:LYS:C	1:A:402:LYS:HZ2	1.98	0.70
1:A:206:ILE:HG12	1:A:420:SER:CB	2.22	0.70
1:A:160:LYS:CG	1:A:203:HIS:HD2	2.06	0.69
1:B:198:GLY:HA2	1:B:201:TYR:CE1	2.26	0.69
1:B:164:ILE:HG21	1:B:205:LYS:CB	2.23	0.69
1:A:203:HIS:CG	1:A:207:SER:CB	2.76	0.68
1:A:160:LYS:O	1:A:164:ILE:HG22	1.92	0.68
1:B:206:ILE:HG23	1:B:399:LYS:CD	2.20	0.68
1:A:171:VAL:CG1	1:A:200:TYR:CE1	2.76	0.68
1:A:202:GLU:HG2	1:A:202:GLU:O	1.93	0.67
1:A:223:ILE:HG21	1:A:237:VAL:HG22	1.76	0.67
1:B:253:GLU:OE1	1:B:261:LYS:HE3	1.95	0.67
1:A:188:GLU:HG2	1:A:250:HIS:HE1	1.60	0.67
1:A:300:ASN:HB2	1:A:301:PRO:HD3	1.69	0.67
1:A:222:ARG:HD3	1:A:222:ARG:N	2.10	0.66
1:A:221:PRO:CG	1:A:246:ASN:HD21	2.06	0.66
1:B:309:ILE:HD12	3:B:602:1SY:C40	2.26	0.66
1:B:280:ILE:O	1:B:280:ILE:HD12	1.95	0.66
1:A:274:VAL:HG22	1:A:282:VAL:O	1.96	0.66
1:A:243:PRO:CD	1:A:246:ASN:HD22	2.00	0.66
1:B:159:LEU:HD12	1:B:159:LEU:N	2.07	0.65
1:A:238:LYS:HD2	1:A:256:VAL:HG22	1.78	0.65
1:B:483:ARG:HA	1:B:486:LYS:HG3	1.78	0.65
1:B:478:GLN:H	1:B:478:GLN:CD	2.05	0.65
1:A:409:LYS:HE2	1:A:415:LEU:O	1.96	0.65
1:A:258:SER:HA	1:A:361:GLU:HG2	1.78	0.64
1:B:274:VAL:CG2	1:B:282:VAL:CG1	2.74	0.64
1:B:285:GLU:CG	1:B:297:LEU:CD2	2.67	0.64
1:B:177:ARG:NH2	1:B:279:ASP:OD2	2.30	0.64
1:A:210:ASN:HB2	1:A:211:GLU:OE2	1.97	0.64
1:A:238:LYS:HD2	1:A:256:VAL:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLU:O	1:A:287:GLU:HG3	1.98	0.64
1:B:309:ILE:HD12	3:B:602:1SY:N42	2.12	0.64
1:B:206:ILE:CG2	1:B:399:LYS:HG3	2.17	0.64
1:A:284:VAL:HG12	1:A:296:LEU:HD23	1.80	0.64
1:A:252:LEU:HD12	1:A:257:LEU:HA	1.79	0.63
1:B:195:LEU:HG	1:B:217:LYS:HD3	1.80	0.63
1:B:351:ASN:HD22	1:B:351:ASN:C	2.05	0.63
1:B:274:VAL:CG2	1:B:282:VAL:HG13	2.28	0.63
1:B:164:ILE:O	1:B:168:ALA:CB	2.47	0.63
1:A:160:LYS:CD	1:A:203:HIS:CB	2.66	0.62
1:A:309:ILE:CD1	3:A:602:1SY:N42	2.62	0.62
1:A:160:LYS:HD3	1:A:203:HIS:HB3	1.79	0.62
1:A:503:ILE:O	1:A:503:ILE:HG12	1.98	0.62
1:B:285:GLU:HG3	1:B:297:LEU:CD2	2.26	0.62
1:B:297:LEU:CD1	1:B:303:GLU:HG3	2.30	0.62
1:A:223:ILE:O	1:A:240:LYS:NZ	2.32	0.62
1:A:168:ALA:HB1	1:A:200:TYR:CB	2.30	0.62
1:A:274:VAL:HG13	1:A:275:LYS:HG2	1.81	0.61
1:B:393:CYS:HA	1:B:396:GLU:OE1	2.00	0.61
1:A:265:LYS:CG	1:A:269:ILE:HD11	2.25	0.61
1:A:188:GLU:OE1	1:A:250:HIS:CE1	2.54	0.61
1:A:298:ILE:HG22	1:A:298:ILE:O	1.99	0.61
1:A:407:GLN:HB3	1:A:503:ILE:HD11	1.83	0.61
1:B:198:GLY:C	1:B:201:TYR:HE1	2.08	0.61
1:A:203:HIS:HA	1:A:207:SER:HA	1.83	0.61
1:A:188:GLU:N	1:A:188:GLU:OE2	2.31	0.61
1:A:265:LYS:O	1:A:269:ILE:HD12	2.01	0.61
1:B:195:LEU:HD21	1:B:346:TYR:CZ	2.36	0.61
1:A:306:VAL:HG23	1:A:306:VAL:O	2.00	0.61
1:A:409:LYS:CE	1:A:418:PHE:O	2.43	0.60
1:B:228:TYR:HB3	1:B:234:PHE:O	2.02	0.60
1:A:246:ASN:OD1	1:A:247:PRO:HD2	2.01	0.60
1:A:160:LYS:HD3	1:A:203:HIS:CD2	2.37	0.60
1:A:205:LYS:CA	1:A:402:LYS:HZ2	2.15	0.59
1:A:309:ILE:HD11	3:A:602:1SY:H20	1.84	0.59
1:A:206:ILE:CA	1:A:402:LYS:HD3	2.28	0.59
1:B:297:LEU:HD12	1:B:303:GLU:HG3	1.84	0.59
1:A:160:LYS:HG3	1:A:203:HIS:HD2	1.68	0.59
1:B:164:ILE:CG2	1:B:205:LYS:HB2	2.32	0.59
1:A:160:LYS:HD2	1:A:203:HIS:HB2	1.84	0.59
1:B:182:MET:CE	1:B:270:ILE:HG12	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ILE:CD1	3:B:602:1SY:H24	2.13	0.59
1:A:309:ILE:HD12	3:A:602:1SY:N42	2.18	0.59
1:B:181:ARG:CZ	1:B:277:ILE:HG23	2.34	0.58
1:A:319:PRO:HG2	1:A:365:LEU:HD11	1.84	0.58
1:B:274:VAL:HG22	1:B:282:VAL:HG13	1.86	0.58
1:B:161:ARG:HA	1:B:165:SER:CB	2.34	0.58
1:B:181:ARG:NH1	1:B:277:ILE:HG23	2.18	0.58
1:B:181:ARG:CZ	1:B:277:ILE:CG2	2.82	0.58
1:A:231:THR:O	1:A:473:PHE:HD2	1.87	0.58
1:A:223:ILE:HG23	1:A:237:VAL:HG13	1.86	0.58
3:A:602:1SY:H13	3:A:602:1SY:H10	1.86	0.58
1:A:161:ARG:NH2	1:B:203:HIS:HE1	2.02	0.58
3:A:602:1SY:O29	3:A:602:1SY:O2'	2.15	0.58
1:A:274:VAL:CG2	1:A:282:VAL:O	2.51	0.57
1:B:220:VAL:HB	1:B:221:PRO:CD	2.33	0.57
1:A:168:ALA:HB1	1:A:200:TYR:HB3	1.85	0.57
1:B:309:ILE:HD13	3:B:602:1SY:N42	2.18	0.57
1:B:487:GLU:O	1:B:491:LYS:HG2	2.04	0.57
1:B:184:LYS:HE3	1:B:273:GLU:OE1	2.05	0.57
1:A:328:ILE:HB	1:A:332:LEU:HB2	1.86	0.57
1:A:158:ARG:NH1	1:B:386:GLU:O	2.31	0.57
1:B:181:ARG:CG	1:B:273:GLU:OE2	2.40	0.57
1:B:203:HIS:CE1	1:B:376:ASN:ND2	2.72	0.56
1:B:207:SER:HB3	1:B:402:LYS:HB3	1.86	0.56
1:A:161:ARG:NH2	1:B:201:TYR:CE2	2.66	0.56
1:B:358:PHE:N	1:B:358:PHE:CD1	2.72	0.56
1:A:188:GLU:CG	1:A:250:HIS:HE1	2.17	0.56
1:A:222:ARG:HD3	1:A:222:ARG:H	1.71	0.56
1:B:348:VAL:HG21	1:B:364:ARG:NH2	2.20	0.56
1:A:146:GLU:CB	1:A:147:PRO:CD	2.77	0.56
1:A:223:ILE:C	1:A:240:LYS:HZ2	2.14	0.56
1:B:315:LYS:HG2	1:B:344:PRO:HG3	1.88	0.56
1:B:164:ILE:CD1	1:B:202:GLU:CG	2.59	0.55
1:B:201:TYR:CZ	1:B:203:HIS:CE1	2.91	0.55
1:A:172:ASN:HA	1:A:200:TYR:CZ	2.40	0.55
1:A:205:LYS:O	1:A:402:LYS:CE	2.54	0.55
1:B:274:VAL:CG2	1:B:282:VAL:HG11	2.37	0.55
1:B:298:ILE:H	1:B:304:ILE:HG22	1.72	0.55
1:A:220:VAL:HB	1:A:223:ILE:HD11	1.89	0.55
1:B:161:ARG:HA	1:B:165:SER:HB2	1.88	0.55
1:B:351:ASN:CG	1:B:359:GLN:O	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLU:HB2	1:A:437:ASP:OD2	2.06	0.55
1:A:211:GLU:HG2	1:A:305:SER:OG	2.07	0.54
1:A:206:ILE:HG12	1:A:420:SER:HB2	1.88	0.54
1:A:205:LYS:C	1:A:402:LYS:HD2	2.29	0.54
1:B:309:ILE:HD13	3:B:602:1SY:C36	2.38	0.54
1:B:378:HIS:CD2	1:B:394:ARG:HD2	2.43	0.54
1:A:265:LYS:O	1:A:269:ILE:CD1	2.55	0.54
1:A:160:LYS:CG	1:A:203:HIS:CD2	2.87	0.54
1:A:171:VAL:CG1	1:A:200:TYR:HE1	2.20	0.54
1:B:161:ARG:HG2	1:B:165:SER:HB3	1.90	0.54
1:B:200:TYR:OH	1:B:214:VAL:CG2	2.55	0.54
1:B:231:THR:HG21	1:B:234:PHE:HB2	1.90	0.53
1:A:309:ILE:HD13	3:A:602:1SY:C36	2.39	0.53
1:B:285:GLU:CD	1:B:297:LEU:HD23	2.33	0.53
1:B:280:ILE:HD12	1:B:280:ILE:C	2.34	0.53
1:A:210:ASN:ND2	1:A:211:GLU:H	2.07	0.53
1:A:210:ASN:HD22	1:A:211:GLU:H	1.54	0.52
1:A:160:LYS:HG3	1:A:203:HIS:CD2	2.44	0.52
1:A:252:LEU:CD1	1:A:257:LEU:HA	2.39	0.52
1:B:265:LYS:O	1:B:265:LYS:HD3	2.09	0.52
1:A:266:PHE:O	1:A:270:ILE:HG13	2.09	0.52
1:A:309:ILE:CD1	3:A:602:1SY:H20	2.38	0.52
1:B:175:VAL:HG21	1:B:200:TYR:OH	2.10	0.52
1:A:180:ARG:HA	1:A:183:GLN:HG3	1.91	0.52
1:A:270:ILE:HG22	1:A:270:ILE:O	2.10	0.52
1:B:412:PHE:CE2	1:B:492:LYS:HE3	2.45	0.52
1:A:267:ARG:O	1:A:271:LYS:HD3	2.10	0.51
1:B:195:LEU:HD12	1:B:215:MET:HE3	1.92	0.51
1:B:309:ILE:HD11	3:B:602:1SY:H24	1.76	0.51
1:B:358:PHE:HD1	1:B:358:PHE:H	1.56	0.51
1:A:161:ARG:NH1	1:B:201:TYR:CD2	2.77	0.51
1:B:159:LEU:CD1	1:B:159:LEU:C	2.84	0.51
1:B:182:MET:HE1	1:B:270:ILE:HG13	1.90	0.51
1:A:274:VAL:HG22	1:A:274:VAL:O	2.10	0.51
1:A:172:ASN:CG	1:A:200:TYR:HE2	2.20	0.50
1:A:155:ASP:O	1:A:158:ARG:HG2	2.11	0.50
1:B:200:TYR:N	1:B:200:TYR:CD1	2.79	0.50
1:A:149:LYS:O	1:A:149:LYS:HG3	2.11	0.50
1:A:296:LEU:HB2	1:A:306:VAL:HG22	1.84	0.50
1:B:300:ASN:CB	1:B:301:PRO:CD	2.85	0.50
1:A:198:GLY:O	1:B:166:GLU:OE2	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:602:1SY:H1	3:A:602:1SY:O19	2.12	0.49
1:B:303:GLU:O	1:B:303:GLU:HG2	2.13	0.49
1:B:347:LEU:HA	1:B:364:ARG:O	2.13	0.49
1:B:206:ILE:O	1:B:399:LYS:HG2	2.12	0.49
1:B:285:GLU:CD	1:B:297:LEU:CD2	2.85	0.49
1:B:394:ARG:HB3	1:B:431:TRP:CZ2	2.48	0.49
3:A:602:1SY:H10	3:A:602:1SY:C21	2.42	0.49
1:B:494:GLU:O	1:B:498:ASN:ND2	2.45	0.49
1:B:158:ARG:HH21	1:B:159:LEU:HA	1.77	0.48
1:B:231:THR:HG23	1:B:232:GLY:N	2.28	0.48
1:A:172:ASN:CB	1:A:200:TYR:CE2	2.96	0.48
1:A:239:PHE:CD2	1:A:242:ILE:CD1	2.96	0.48
1:A:213:ASP:N	1:A:213:ASP:OD1	2.46	0.48
1:B:182:MET:HB2	1:B:182:MET:HE3	1.76	0.48
1:B:295:THR:HG22	1:B:307:ASP:HA	1.95	0.48
1:A:224:GLU:HB2	1:A:240:LYS:HD2	1.95	0.48
1:B:344:PRO:O	1:B:369:HIS:NE2	2.47	0.48
1:A:178:LEU:HD13	1:A:182:MET:HE3	1.96	0.48
1:A:205:LYS:C	1:A:402:LYS:CD	2.85	0.48
1:A:210:ASN:HD22	1:A:211:GLU:N	2.12	0.48
1:A:322:THR:O	1:A:341:ARG:NH2	2.46	0.47
1:A:211:GLU:CG	1:A:305:SER:OG	2.61	0.47
1:A:223:ILE:CG2	1:A:237:VAL:HG13	2.44	0.47
1:B:223:ILE:HD12	1:B:238:LYS:O	2.14	0.47
1:A:267:ARG:HB2	1:A:267:ARG:CZ	2.44	0.47
1:B:178:LEU:O	1:B:182:MET:HB3	2.15	0.47
1:B:479:GLU:N	1:B:479:GLU:CD	2.72	0.47
1:A:252:LEU:HD13	1:A:257:LEU:HD12	1.96	0.47
1:B:274:VAL:HG22	1:B:282:VAL:CG1	2.43	0.47
1:A:201:TYR:CE2	1:B:202:GLU:OE2	2.68	0.47
1:A:217:LYS:HA	1:A:311:ALA:O	2.15	0.47
1:A:453:LEU:CD1	1:A:501:PHE:HZ	2.28	0.47
1:A:453:LEU:HD11	1:A:501:PHE:CZ	2.50	0.47
1:B:200:TYR:OH	1:B:214:VAL:HG21	2.14	0.47
1:B:304:ILE:HD12	1:B:304:ILE:HA	1.76	0.47
1:B:328:ILE:HD12	1:B:332:LEU:HB2	1.96	0.47
1:A:164:ILE:HD11	1:A:212:PHE:CE1	2.49	0.47
1:B:181:ARG:O	1:B:184:LYS:HD2	2.15	0.47
1:B:378:HIS:HD2	1:B:394:ARG:HD2	1.80	0.47
1:A:196:ASN:CG	1:A:372:LYS:NZ	2.72	0.47
1:B:274:VAL:HG23	1:B:282:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ILE:HD11	3:B:602:1SY:N42	2.27	0.46
1:A:354:ASP:C	1:A:356:ASN:N	2.73	0.46
1:B:188:GLU:HG3	1:B:247:PRO:HB2	1.96	0.46
1:B:214:VAL:HG12	1:B:215:MET:N	2.31	0.46
1:B:158:ARG:O	1:B:158:ARG:CD	2.64	0.46
1:B:178:LEU:O	1:B:182:MET:CB	2.64	0.46
1:B:181:ARG:HG2	1:B:181:ARG:O	2.15	0.46
1:A:391:LYS:HE3	1:A:391:LYS:HB3	1.78	0.46
1:B:358:PHE:HB3	1:B:361:GLU:HB2	1.97	0.46
1:A:196:ASN:CG	1:A:372:LYS:HZ3	2.24	0.46
1:A:412:PHE:HB3	1:A:414:GLU:OE1	2.16	0.46
1:B:280:ILE:C	1:B:280:ILE:CD1	2.89	0.46
1:A:354:ASP:C	1:A:356:ASN:H	2.22	0.45
1:B:249:SER:HA	1:B:252:LEU:HD13	1.98	0.45
1:A:395:LYS:O	1:A:399:LYS:HG3	2.15	0.45
1:A:206:ILE:HG12	1:A:420:SER:OG	2.16	0.45
1:A:265:LYS:CG	1:A:269:ILE:HD12	2.46	0.45
1:B:159:LEU:HD13	1:B:159:LEU:O	2.16	0.45
1:B:200:TYR:OH	1:B:214:VAL:HG22	2.15	0.45
1:A:156:LYS:C	1:A:158:ARG:H	2.24	0.45
1:A:470:ILE:HG22	1:A:473:PHE:H	1.81	0.45
1:B:407:GLN:HE21	1:B:407:GLN:HA	1.81	0.45
1:B:401:MET:HG2	1:B:449:PHE:HE1	1.82	0.45
1:B:412:PHE:CD2	1:B:488:PHE:HZ	2.35	0.45
1:A:223:ILE:C	1:A:240:LYS:NZ	2.75	0.45
1:A:227:GLU:HA	1:A:235:TYR:CD2	2.52	0.45
1:B:228:TYR:CB	1:B:234:PHE:O	2.65	0.45
1:B:358:PHE:HD2	1:B:361:GLU:HB2	1.82	0.45
1:A:354:ASP:O	1:A:359:GLN:HG2	2.16	0.44
1:A:478:GLN:HG3	1:A:479:GLU:OE1	2.17	0.44
1:B:201:TYR:O	1:B:201:TYR:CG	2.70	0.44
1:B:346:TYR:HD1	1:B:369:HIS:CE1	2.36	0.44
1:A:214:VAL:CG1	1:A:308:ILE:HD13	2.48	0.44
1:B:201:TYR:HD1	1:B:201:TYR:H	1.65	0.44
1:B:231:THR:HG23	1:B:232:GLY:H	1.82	0.44
1:B:204:VAL:O	1:B:204:VAL:HG22	2.17	0.44
1:A:202:GLU:OE2	1:A:212:PHE:HD1	2.00	0.44
1:B:164:ILE:CG2	1:B:205:LYS:HG3	2.31	0.44
1:B:168:ALA:HA	1:B:171:VAL:HG23	2.00	0.44
1:A:172:ASN:HB2	1:A:200:TYR:CE2	2.53	0.44
1:A:507:LEU:N	1:A:507:LEU:HD22	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HA	1:A:402:LYS:HD2	1.97	0.43
1:B:351:ASN:ND2	1:B:359:GLN:O	2.51	0.43
1:B:358:PHE:N	1:B:358:PHE:HD1	2.11	0.43
1:A:149:LYS:O	1:A:153:VAL:CG2	2.61	0.43
1:B:195:LEU:HD11	1:B:346:TYR:CZ	2.53	0.43
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.54	0.43
1:B:292:PRO:HB3	1:B:349:PRO:O	2.19	0.43
1:A:403:TYR:OH	1:A:506:LYS:HD3	2.18	0.43
1:A:162:LYS:CG	1:B:387:SER:OG	2.43	0.43
1:A:273:GLU:OE2	1:A:273:GLU:N	2.52	0.43
1:B:168:ALA:HA	1:B:171:VAL:CG2	2.48	0.43
1:A:408:LEU:HD23	1:A:408:LEU:HA	1.82	0.43
1:B:292:PRO:CB	1:B:349:PRO:HG2	2.46	0.43
1:A:205:LYS:CA	1:A:402:LYS:NZ	2.76	0.43
1:B:158:ARG:NH2	1:B:159:LEU:HA	2.33	0.42
1:B:322:THR:HG22	1:B:470:ILE:HG12	2.00	0.42
1:A:203:HIS:CE1	1:A:207:SER:HG	2.37	0.42
1:A:453:LEU:CD1	1:A:501:PHE:CZ	3.03	0.42
1:B:178:LEU:O	1:B:178:LEU:HD12	2.18	0.42
1:B:398:LEU:HD13	1:B:427:ILE:HG21	2.01	0.42
1:A:196:ASN:HD21	1:A:372:LYS:HZ1	1.66	0.42
1:A:200:TYR:C	1:A:202:GLU:N	2.76	0.42
1:A:171:VAL:HG11	1:A:200:TYR:CE1	2.55	0.42
1:A:182:MET:HE3	1:A:182:MET:HB2	1.87	0.42
1:A:359:GLN:H	1:A:359:GLN:HG3	1.41	0.42
1:B:270:ILE:O	1:B:270:ILE:HG22	2.20	0.42
1:A:309:ILE:CD1	3:A:602:1SY:H24	2.30	0.42
1:B:478:GLN:NE2	1:B:478:GLN:N	2.60	0.42
1:B:412:PHE:CD1	1:B:412:PHE:N	2.88	0.42
1:A:215:MET:SD	3:A:602:1SY:N39	2.93	0.41
1:A:221:PRO:HG3	1:A:246:ASN:ND2	2.08	0.41
1:A:457:LEU:HD21	1:A:493:ILE:HB	2.02	0.41
1:B:159:LEU:O	1:B:162:LYS:O	2.37	0.41
1:B:179:LEU:HD11	1:B:192:VAL:HG13	2.02	0.41
1:B:375:LEU:O	1:B:395:LYS:HE3	2.20	0.41
1:B:198:GLY:C	1:B:201:TYR:CE1	2.91	0.41
1:A:214:VAL:HG12	1:A:308:ILE:HD13	2.02	0.41
1:B:385:CYS:HA	1:B:391:LYS:HD2	2.02	0.41
1:A:168:ALA:HB1	1:A:200:TYR:HB2	2.01	0.41
1:A:203:HIS:NE2	1:A:207:SER:OG	2.45	0.41
1:B:227:GLU:HA	1:B:235:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LYS:O	1:A:402:LYS:NZ	2.49	0.41
1:B:155:ASP:O	1:B:158:ARG:HG3	2.21	0.41
1:B:331:TRP:HH2	1:B:431:TRP:HE3	1.68	0.41
1:A:205:LYS:HA	1:A:402:LYS:HZ2	1.86	0.41
1:A:252:LEU:HD12	1:A:257:LEU:CA	2.47	0.41
1:A:296:LEU:HB2	1:A:306:VAL:HG21	1.86	0.41
1:A:304:ILE:HG23	1:A:304:ILE:HD12	1.75	0.41
1:B:205:LYS:CG	1:B:205:LYS:O	2.69	0.41
1:A:172:ASN:CA	1:A:200:TYR:CZ	3.04	0.41
1:B:326:LEU:HD13	1:B:469:PHE:CE2	2.56	0.41
1:B:195:LEU:HD11	1:B:346:TYR:CE2	2.56	0.40
1:B:415:LEU:HD12	1:B:415:LEU:HA	1.85	0.40
1:A:160:LYS:HB3	1:A:160:LYS:HE2	1.81	0.40
1:A:203:HIS:CE1	1:A:207:SER:OG	2.75	0.40
1:A:298:ILE:HB	1:A:304:ILE:HB	2.03	0.40
1:A:323:LYS:O	1:A:323:LYS:HG2	2.20	0.40
1:A:470:ILE:HG22	1:A:470:ILE:O	2.21	0.40
1:B:346:TYR:CD1	1:B:369:HIS:CE1	3.10	0.40
1:A:198:GLY:N	1:A:372:LYS:HD2	2.36	0.40
1:A:288:LYS:HA	1:A:289:PRO:HD3	1.87	0.40
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.77	0.40
1:B:412:PHE:HD2	1:B:488:PHE:HZ	1.69	0.40
1:A:393:CYS:HA	1:A:396:GLU:HB2	2.02	0.40
1:A:403:TYR:HD2	1:A:504:PHE:CE1	2.39	0.40
1:B:348:VAL:HG13	1:B:366:SER:HB2	2.02	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	360/507 (71%)	317 (88%)	38 (11%)	5 (1%)	9 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	359/507 (71%)	314 (88%)	41 (11%)	4 (1%)	11	39
All	All	719/1014 (71%)	631 (88%)	79 (11%)	9 (1%)	9	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	LYS
1	A	300	ASN
1	B	160	LYS
1	A	302	GLU
1	B	357	SER
1	A	205	LYS
1	B	292	PRO
1	B	301	PRO
1	A	221	PRO

5.3.2 Protein sidechains [i](#)

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	335/447 (75%)	322 (96%)	13 (4%)	28	60
1	B	334/447 (75%)	314 (94%)	20 (6%)	17	47
All	All	669/894 (75%)	636 (95%)	33 (5%)	22	53

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	LYS
1	A	201	TYR
1	A	202	GLU
1	A	205	LYS
1	A	206	ILE
1	A	226	GLN
1	A	238	LYS

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Mol	Chain	Res	Type
1	A	241	ARG
1	A	299	ARG
1	A	300	ASN
1	A	302	GLU
1	A	303	GLU
1	A	380	ILE
1	B	157	LEU
1	B	158	ARG
1	B	159	LEU
1	B	162	LYS
1	B	163	ASP
1	B	164	ILE
1	B	165	SER
1	B	240	LYS
1	B	242	ILE
1	B	244	ARG
1	B	276	GLU
1	B	298	ILE
1	B	302	GLU
1	B	304	ILE
1	B	413	GLN
1	B	414	GLU
1	B	415	LEU
1	B	478	GLN
1	B	479	GLU
1	B	486	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	194	GLN
1	A	210	ASN
1	A	246	ASN
1	A	250	HIS
1	A	356	ASN
1	A	376	ASN
1	B	172	ASN
1	B	183	GLN
1	B	210	ASN
1	B	250	HIS
1	B	351	ASN

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Mol	Chain	Res	Type
1	B	376	ASN
1	B	407	GLN
1	B	439	GLN
1	B	444	ASN
1	B	478	GLN
1	B	498	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	1SY	B	602	-	51,51,51	2.86	20 (39%)	70,80,80	1.90	21 (30%)
3	1SY	A	602	-	51,51,51	3.22	27 (52%)	70,80,80	2.32	25 (35%)

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	1SY	B	602	-	-	12/30/62/62	0/6/7/7
3	1SY	A	602	-	-	14/30/62/62	0/6/7/7

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	1SY	C4-N3	8.98	1.51	1.34
3	A	602	1SY	C36-N42	7.91	1.51	1.37
3	A	602	1SY	C2-N3	7.80	1.47	1.33
3	B	602	1SY	C4-N3	7.75	1.48	1.34
3	B	602	1SY	C36-N42	7.04	1.49	1.37
3	B	602	1SY	C2-N3	6.47	1.45	1.33
3	A	602	1SY	C36-N33	-5.70	1.31	1.37
3	B	602	1SY	C36-N33	-5.67	1.31	1.37
3	B	602	1SY	C2-N1	5.59	1.43	1.33
3	A	602	1SY	C5-C6	5.44	1.56	1.41
3	A	602	1SY	C40-N41	4.89	1.45	1.34
3	A	602	1SY	C21-C32	-4.72	1.41	1.53
3	A	602	1SY	C2-N1	4.57	1.42	1.33
3	A	602	1SY	C6-N01	4.54	1.45	1.34
3	A	602	1SY	C37-N35	-4.31	1.30	1.39
3	B	602	1SY	O43-C38	-4.30	1.15	1.23
3	A	602	1SY	C40-N39	3.87	1.42	1.33
3	B	602	1SY	C40-N41	3.83	1.43	1.34
3	B	602	1SY	C6-N01	3.82	1.44	1.34
3	A	602	1SY	C5-C4	-3.76	1.32	1.39
3	B	602	1SY	C5-N7	-3.72	1.32	1.39
3	A	602	1SY	C37-C36	-3.63	1.32	1.38
3	B	602	1SY	C37-C36	-3.61	1.32	1.38
3	B	602	1SY	C21-C32	-3.51	1.44	1.53
3	B	602	1SY	C37-N35	-3.51	1.32	1.39
3	A	602	1SY	O43-C38	-3.36	1.17	1.23
3	B	602	1SY	C5-C6	3.35	1.50	1.41
3	A	602	1SY	C3'-C4'	-3.31	1.44	1.52
3	B	602	1SY	C40-N39	3.26	1.41	1.33
3	A	602	1SY	P18-O20	3.17	1.68	1.59
3	A	602	1SY	P27-O26	3.12	1.71	1.59
3	A	602	1SY	C5-N7	-3.06	1.33	1.39
3	B	602	1SY	C5-C4	-2.94	1.33	1.39
3	B	602	1SY	C3'-C4'	-2.93	1.45	1.52
3	A	602	1SY	C40-N42	2.60	1.43	1.37
3	A	602	1SY	C8-N9	-2.47	1.33	1.37
3	B	602	1SY	C4-N9	-2.47	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	1SY	C38-N39	2.39	1.42	1.38
3	A	602	1SY	C38-C37	2.32	1.51	1.45
3	A	602	1SY	C8-N7	2.29	1.36	1.31
3	B	602	1SY	P27-O26	2.22	1.68	1.59
3	A	602	1SY	C34-N33	-2.22	1.32	1.37
3	A	602	1SY	C6-N1	2.12	1.41	1.35
3	B	602	1SY	C40-N42	2.03	1.42	1.37
3	B	602	1SY	C6-N1	2.02	1.41	1.35
3	A	602	1SY	O31-C32	2.02	1.46	1.42
3	A	602	1SY	P27-O28	2.01	1.65	1.59

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	1SY	N3-C2-N1	-8.22	116.14	128.58
3	A	602	1SY	C5-C4-N3	-6.11	118.31	126.72
3	B	602	1SY	N3-C2-N1	-5.93	119.61	128.58
3	A	602	1SY	O31-C24-C22	-5.64	93.96	105.15
3	A	602	1SY	C2-N3-C4	5.33	124.85	111.83
3	A	602	1SY	C2'-C1'-N9	5.07	125.91	113.30
3	B	602	1SY	O31-C24-C22	-5.00	95.24	105.15
3	B	602	1SY	C5-C4-N3	-4.36	120.71	126.72
3	A	602	1SY	N9-C8-N7	-4.10	108.12	113.94
3	B	602	1SY	C37-C36-N33	3.61	107.92	106.25
3	B	602	1SY	O20-P18-O44	3.57	121.22	109.81
3	A	602	1SY	N3-C4-N9	3.40	132.95	127.17
3	A	602	1SY	O20-P18-O44	3.28	120.30	109.81
3	A	602	1SY	N42-C40-N39	-3.28	117.31	123.32
3	B	602	1SY	C2-N3-C4	3.07	119.32	111.83
3	A	602	1SY	O28-P27-O29	-3.04	100.09	109.81
3	B	602	1SY	C5-C6-N01	-3.03	115.78	123.29
3	B	602	1SY	N3-C4-N9	2.91	132.11	127.17
3	A	602	1SY	C5-N7-C8	2.90	108.01	103.45
3	A	602	1SY	C22-C21-C32	-2.85	97.34	102.81
3	B	602	1SY	N42-C40-N39	-2.70	118.38	123.32
3	A	602	1SY	C5-C4-N9	2.68	108.73	105.81
3	B	602	1SY	C22-C21-C32	-2.67	97.70	102.81
3	B	602	1SY	N33-C34-N35	-2.64	108.51	113.40
3	A	602	1SY	C5-C6-N1	2.63	124.19	117.51
3	A	602	1SY	O31-C32-N33	-2.60	102.48	108.36
3	A	602	1SY	C37-C36-N33	2.57	107.44	106.25
3	B	602	1SY	O28-P27-O29	-2.47	101.92	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	1SY	N01-C6-N1	2.43	123.79	118.38
3	B	602	1SY	C2'-C3'-C4'	2.40	107.45	103.24
3	A	602	1SY	O19-P18-O44	-2.37	101.44	112.44
3	A	602	1SY	C5-C6-N01	-2.34	117.48	123.29
3	A	602	1SY	N33-C34-N35	-2.33	109.08	113.40
3	B	602	1SY	N9-C8-N7	-2.33	110.64	113.94
3	B	602	1SY	C3'-C2'-C1'	2.32	104.99	99.89
3	B	602	1SY	C6-C5-C4	2.28	120.29	117.18
3	B	602	1SY	O26-C25-C24	2.26	116.70	108.99
3	B	602	1SY	O19-P18-O44	-2.25	102.00	112.44
3	A	602	1SY	O26-C25-C24	2.19	116.45	108.99
3	B	602	1SY	O4'-C4'-C3'	2.15	109.45	104.92
3	A	602	1SY	O20-C21-C32	2.13	117.56	110.05
3	A	602	1SY	C16-C4'-C3'	-2.11	107.35	114.38
3	A	602	1SY	O30-P27-O26	2.09	117.03	107.57
3	B	602	1SY	O30-P27-O26	2.07	116.96	107.57
3	A	602	1SY	C4-C5-N7	-2.06	108.23	110.58
3	A	602	1SY	C3'-C2'-C1'	2.01	104.30	99.89

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	1SY	O4'-C1'-N9-C4
3	A	602	1SY	O4'-C1'-N9-C8
3	A	602	1SY	O17-C16-C4'-O4'
3	A	602	1SY	C16-O17-P18-O44
3	A	602	1SY	C21-O20-P18-O17
3	A	602	1SY	C25-O26-P27-O29
3	B	602	1SY	C21-O20-P18-O17
3	B	602	1SY	C25-O26-P27-O29
3	A	602	1SY	O17-C16-C4'-C3'
3	B	602	1SY	O17-C16-C4'-O4'
3	B	602	1SY	C22-C24-C25-O26
3	B	602	1SY	O31-C24-C25-O26
3	A	602	1SY	C2'-C3'-O28-P27
3	B	602	1SY	C2'-C3'-O28-P27
3	A	602	1SY	C22-C24-C25-O26
3	A	602	1SY	O31-C24-C25-O26
3	B	602	1SY	O17-C16-C4'-C3'
3	A	602	1SY	C4'-C3'-O28-P27
3	B	602	1SY	C4'-C3'-O28-P27

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Mol	Chain	Res	Type	Atoms
3	A	602	1SY	C16-O17-P18-O19
3	A	602	1SY	C16-O17-P18-O20
3	A	602	1SY	C25-O26-P27-O28
3	B	602	1SY	C16-O17-P18-O44
3	B	602	1SY	C25-O26-P27-O28
3	B	602	1SY	C21-O20-P18-O44
3	B	602	1SY	C3'-O28-P27-O29

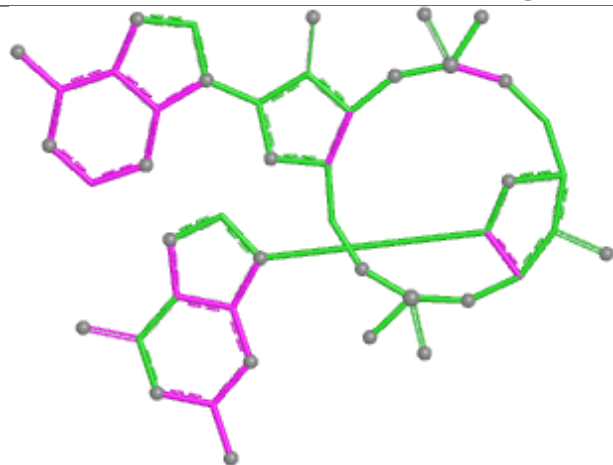
There are no ring outliers.

2 monomers are involved in 27 short contacts:

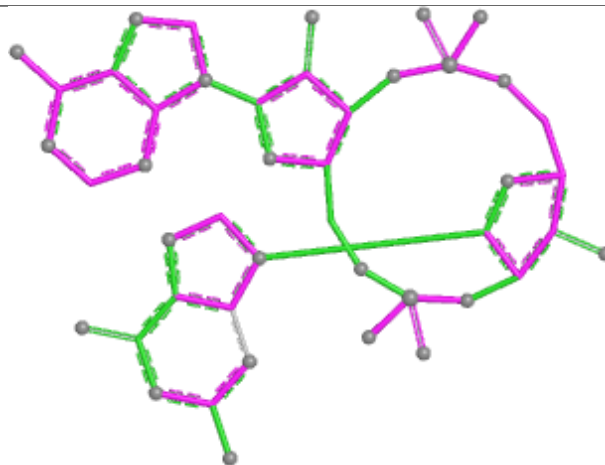
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	1SY	13	0
3	A	602	1SY	14	0

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.

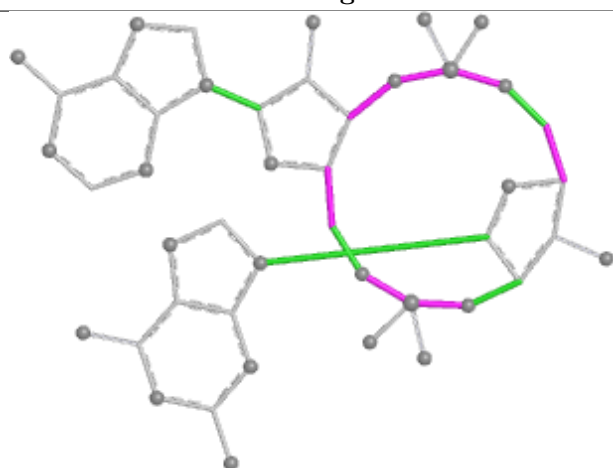
Ligand 1SY B 602



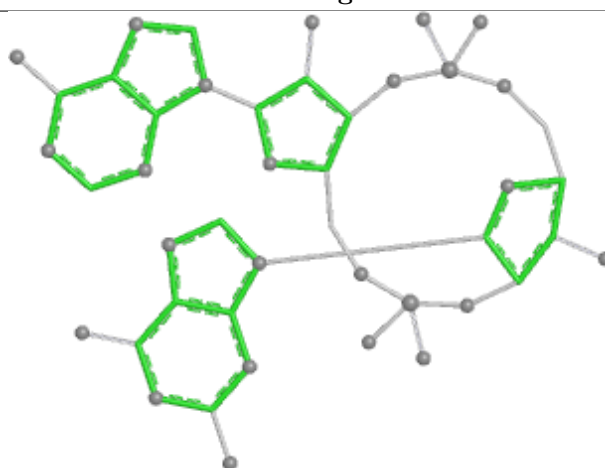
Bond lengths



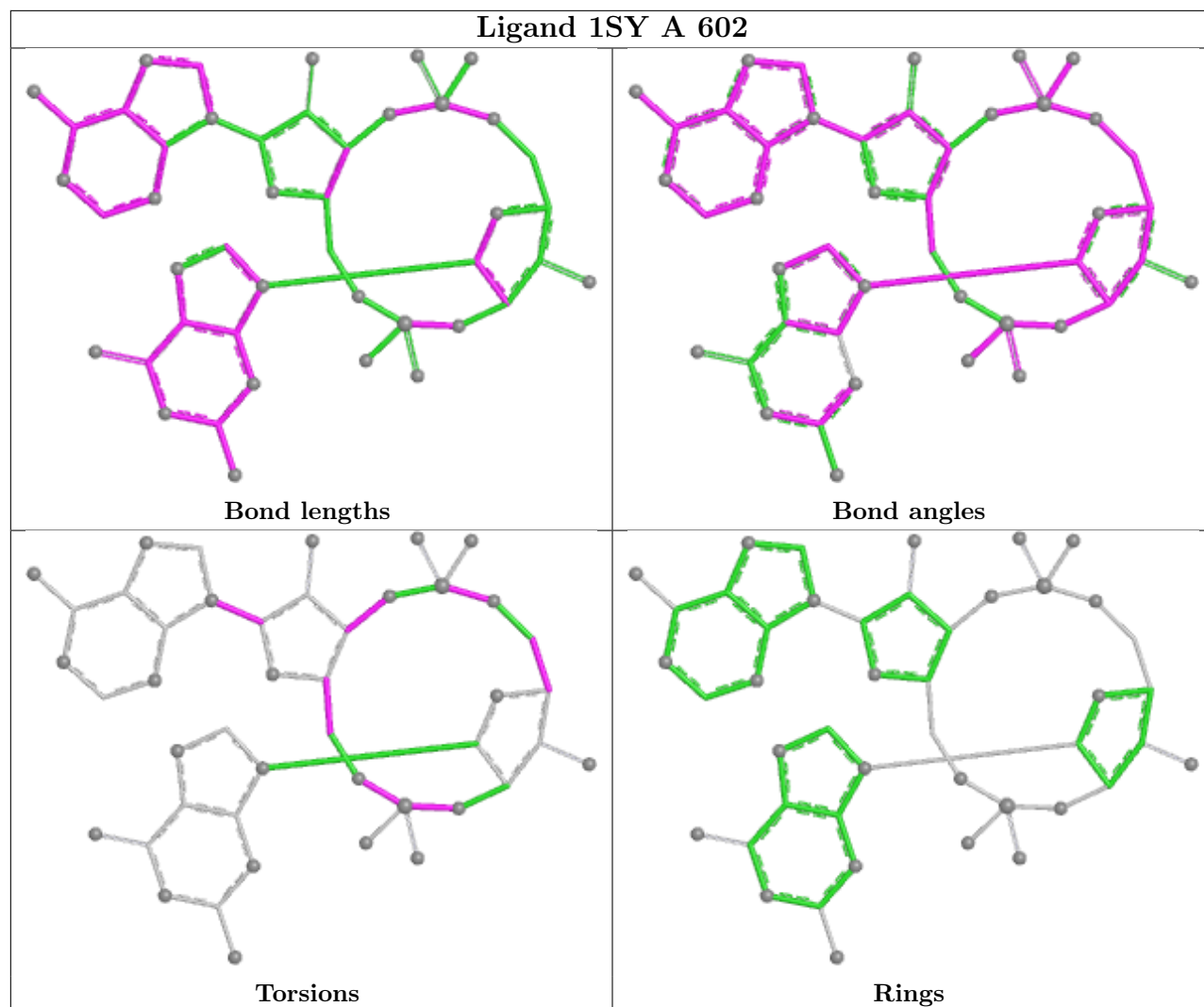
Bond angles



Torsions



Rings



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	362/507 (71%)	0.18	15 (4%)	41 23	26, 55, 122, 284	0
1	B	361/507 (71%)	0.29	13 (3%)	46 26	27, 54, 138, 259	0
All	All	723/1014 (71%)	0.24	28 (3%)	43 24	26, 55, 131, 284	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	ILE	5.1
1	B	200	TYR	4.1
1	B	231	THR	4.0
1	A	206	ILE	3.8
1	A	357	SER	3.4
1	A	203	HIS	3.4
1	A	301	PRO	3.3
1	A	200	TYR	3.3
1	A	209	PRO	3.3
1	A	158	ARG	3.2
1	B	301	PRO	3.1
1	B	159	LEU	3.0
1	A	164	ILE	2.8
1	A	205	LYS	2.8
1	A	292	PRO	2.5
1	A	212	PHE	2.4
1	B	507	LEU	2.4
1	A	247	PRO	2.3
1	B	245	GLY	2.3
1	B	163	ASP	2.3
1	B	304	ILE	2.2
1	A	204	VAL	2.2
1	A	163	ASP	2.2
1	B	196	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	198	GLY	2.1
1	B	184	LYS	2.1
1	B	246	ASN	2.1
1	A	148	ASP	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](#)

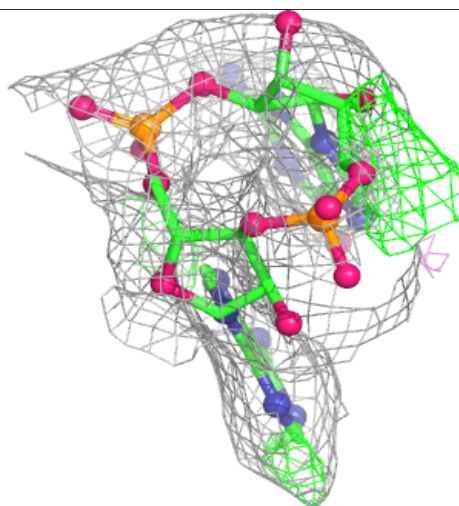
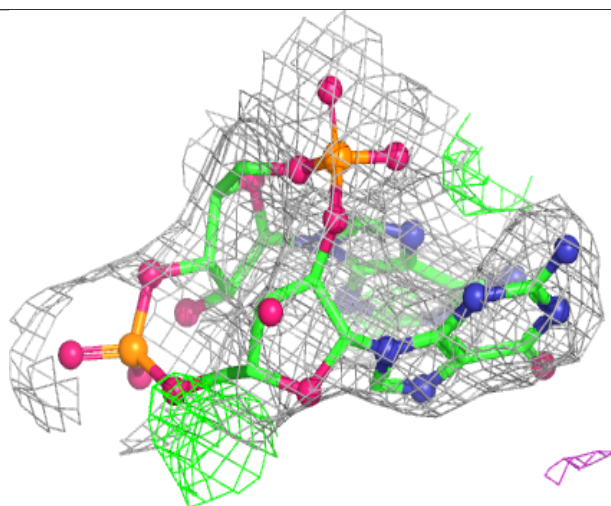
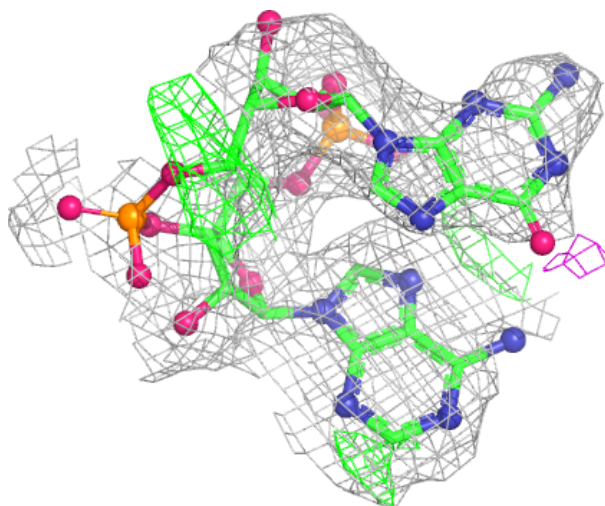
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	1SY	B	602	45/45	0.60	0.16	100,101,102,103	0
3	1SY	A	602	45/45	0.62	0.16	158,160,160,161	0
2	ZN	A	601	1/1	0.99	0.04	46,46,46,46	0
2	ZN	B	601	1/1	1.00	0.01	45,45,45,45	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.

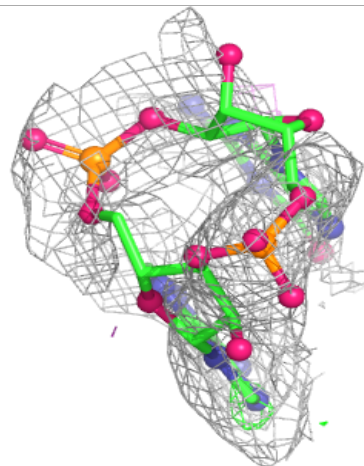
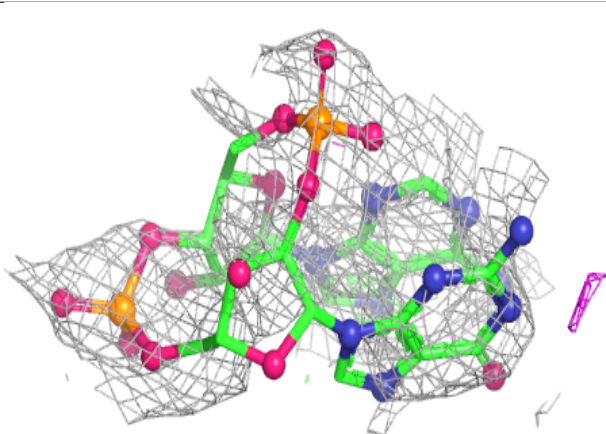
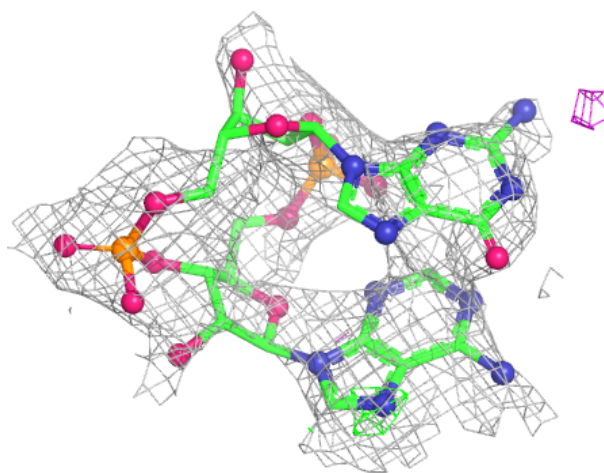
Electron density around 1SY B 602:

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



Electron density around 1SY A 602:

$2mF_o-DF_c$ (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.