



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:57 AM UTC

PDB ID : 7DSY / pdb_00007dsy
Title : Crystal Structure of RNase L in complex with KM05073
Authors : Tang, J.; Huang, H.
Deposited on : 2021-01-03
Resolution : 2.65 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

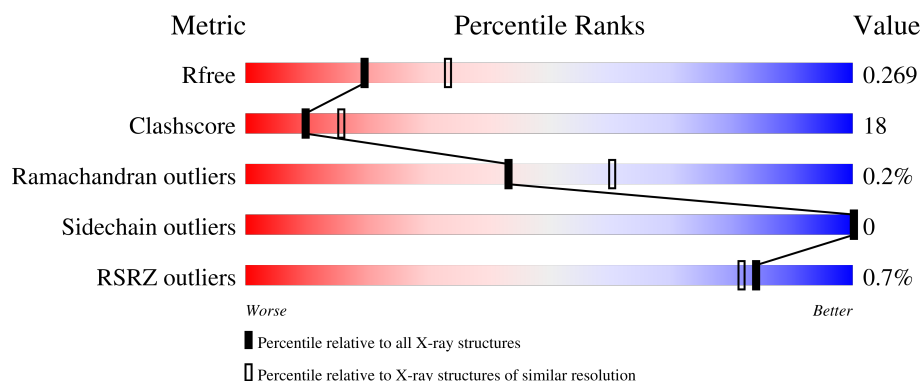
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	717	
1	b	717	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10986 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.

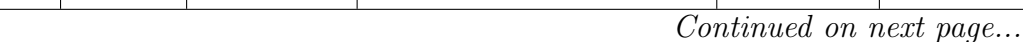
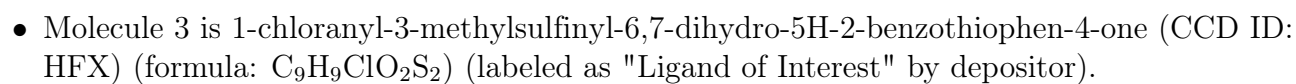
- Molecule 1 is a protein called Ribonuclease L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	672	Total	C	N	O	S	0	0	0
			5339	3353	942	1022	22			
1	b	676	Total	C	N	O	S	0	0	0
			5361	3365	947	1027	22			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	16	GLY	-	expression tag	UNP A5H025
a	17	ALA	-	expression tag	UNP A5H025
a	18	MET	-	expression tag	UNP A5H025
a	19	ASP	-	expression tag	UNP A5H025
a	20	PRO	-	expression tag	UNP A5H025
b	16	GLY	-	expression tag	UNP A5H025
b	17	ALA	-	expression tag	UNP A5H025
b	18	MET	-	expression tag	UNP A5H025
b	19	ASP	-	expression tag	UNP A5H025
b	20	PRO	-	expression tag	UNP A5H025

- Molecule 2 is 5'-O-MONOPHOSPHORYLADENYLYL(2'->5')ADENYLYL(2'->5')ADENOSINE (CCD ID: 25A) (formula: C₃₀H₃₈N₁₅O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	b	1	Total	C	Cl	O	S	0	0
			14	9	1	2	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	a	1	Total	O	P	0	0
			5	4	1		

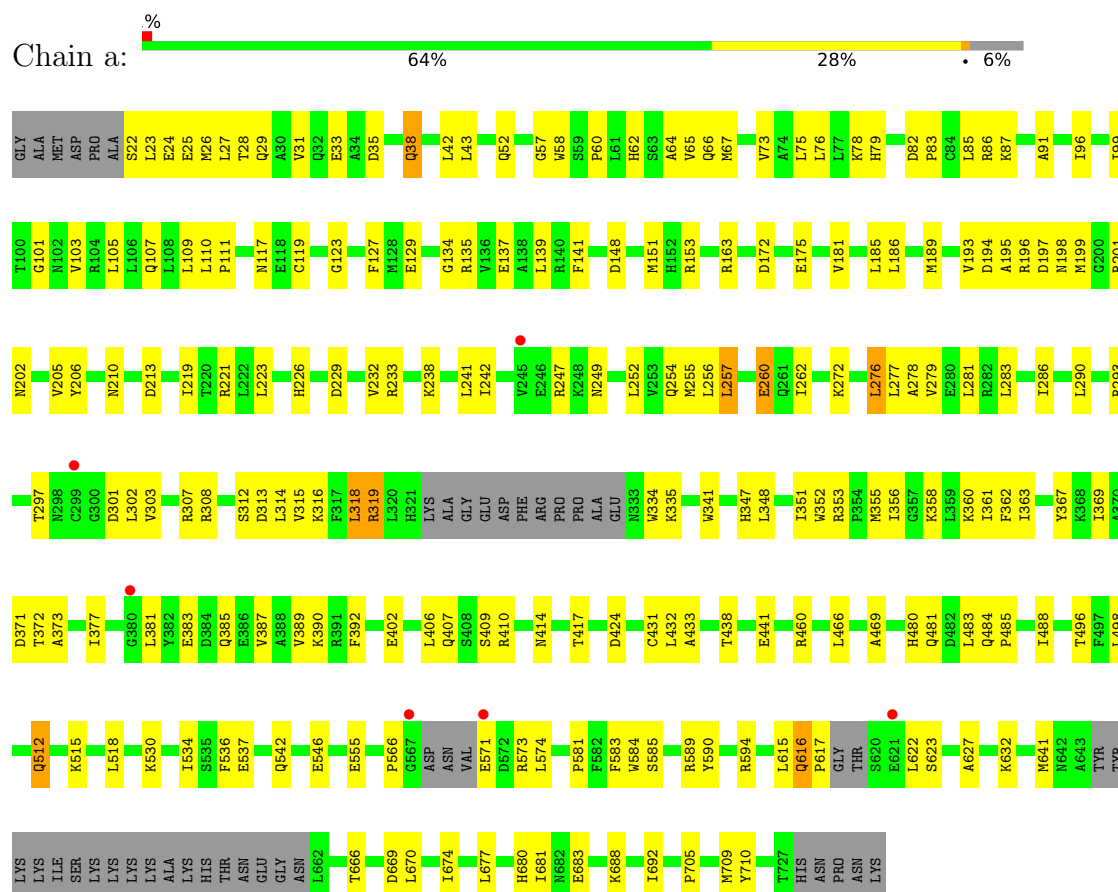
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	a	50	Total	O	0	0
			50	50		
5	b	69	Total	O	0	0
			69	69		

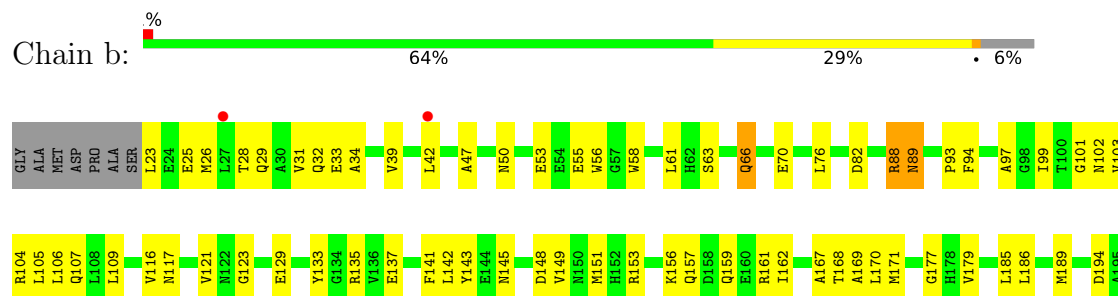
3 Residue-property plots

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: Ribonuclease L



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LYS	L289	R410	T538	L208	R196
LYS	L293	T417	Q542	L209	D197
ALA	R293		S543	N210	N198
LYS	S296			P211	M199
HIS	D301	S421	E546	D212	G200
THR			V547	D213	R201
ASN		L428	I548	L314	N202
GLY		H429		V315	A203
		V430	E555	K316	L204
N661			T556		
		A433	R557	L320	L208
T666				H321	L209
L667		T438	I560	LYS	N210
S688		L439	H561	ALA	P211
D689		Q440	H562	GLY	D212
L670		V451	E571	ASP	D213
L671			D572	PHE	
L672		E454	R573	ARG	K217
		L463	L574	PRO	L224
L677		L466	P581	ALA	D225
		I470	V584	GLY	H226
N686			S585	ASP	D229
K687		Y478	R589	PRO	V230
K688		S479	Y590	ALA	N231
K689		H480	R594	GLY	V232
K690		Q481	G597	GLU	R233
S691		D482	L615	N333	
I692		L483		K346	S237
I693		N487	G618	R350	K238
		I488	T619	K360	T239
K709		L489	SER	I369	P240
Y710		I490	GLU	A370	L241
K714			L622	D371	I242
			V629	T372	L243
N721				A373	
			I633	E374	R247
F724			D634	G375	V253
			S635	G376	Q254
T727			F636	I377	L256
HIS			V637	L381	L257
ASN			H641	Q385	E258
PRO			Y644	V389	Q259
ASN			TYR	K390	E263
ASN			LYS	Q401	V264
LYS			LYS	Q407	N265
			ILE		T273
			SER		L277
			LYS		L283
			LYS		E284
			LYS		E285
			LYS		I286

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.32Å 111.05Å 262.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.50 – 2.65 31.50 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.50-2.65) 99.7 (31.50-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.199 , 0.270 0.201 , 0.269	Depositor DCC
R_{free} test set	2568 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.3	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	0.95	EDS
Total number of atoms	10986	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: PO4, 25A, HFX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.44	0/5431	0.78	14/7330 (0.2%)
1	b	0.42	0/5455	0.73	6/7365 (0.1%)
All	All	0.43	0/10886	0.75	20/14695 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	537	GLU	N-CA-CB	-11.85	92.06	110.30
1	a	537	GLU	CB-CG-CD	-8.31	98.47	112.60
1	a	537	GLU	CA-CB-CG	8.08	130.26	114.10
1	b	506	LYS	CB-CG-CD	-7.15	94.85	111.30
1	a	615	LEU	CA-C-N	-6.99	113.19	122.56
1	a	615	LEU	C-N-CA	-6.99	113.19	122.56
1	a	257	LEU	CB-CG-CD1	-6.96	89.81	110.70
1	a	616	GLN	CA-CB-CG	6.56	127.23	114.10
1	b	88	ARG	CA-C-N	6.45	131.50	120.72
1	b	88	ARG	C-N-CA	6.45	131.50	120.72
1	b	66	GLN	CB-CG-CD	-6.32	101.86	112.60
1	b	506	LYS	CG-CD-CE	6.28	125.73	111.30
1	a	38	GLN	CA-CB-CG	6.10	126.31	114.10
1	a	512	GLN	CB-CA-C	-6.05	99.05	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	260	GLU	CA-C-N	-5.72	110.94	122.55
1	a	260	GLU	C-N-CA	-5.72	110.94	122.55
1	b	89	ASN	N-CA-CB	-5.59	101.11	110.39
1	a	536	PHE	CA-C-N	5.45	129.95	120.68
1	a	536	PHE	C-N-CA	5.45	129.95	120.68
1	a	276	LEU	CB-CG-CD2	-5.33	94.72	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	318	LEU	Peptide
1	a	616	GLN	Peptide

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	5339	0	5258	178	0
1	b	5361	0	5261	202	0
2	a	67	0	29	4	0
2	b	67	0	29	5	0
3	a	14	0	0	1	0
3	b	14	0	0	0	0
4	a	5	0	0	0	0
5	a	50	0	0	6	0
5	b	69	0	0	6	0
All	All	10986	0	10577	376	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (376) 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:311:ASP:OD1	1:b:314:LEU:HD13	1.30	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:801:25A:O4'	2:a:801:25A:C1'	1.63	1.23
2:a:801:25A:OO'	2:a:801:25A:CL'	1.65	1.19
1:a:196:ARG:NH1	1:a:202:ASN:HB3	1.59	1.16
2:b:801:25A:OO'	2:b:801:25A:CL'	1.67	1.13
1:a:78:LYS:HE3	1:a:79:HIS:CE1	1.91	1.05
1:b:466:LEU:HD21	1:b:488:ILE:HD12	1.36	1.02
1:b:301:ASP:O	1:b:305:ILE:CD1	2.13	0.96
1:b:301:ASP:O	1:b:305:ILE:HD12	1.68	0.94
1:a:369:ILE:HB	1:a:377:ILE:CD1	1.98	0.93
1:b:311:ASP:CG	1:b:314:LEU:HD13	1.94	0.91
1:b:677:LEU:O	1:b:681:ILE:HG12	1.71	0.89
1:a:101:GLY:HA3	1:a:135:ARG:HG2	1.55	0.89
1:b:466:LEU:HD21	1:b:488:ILE:CD1	2.04	0.86
1:b:666:THR:HG23	1:b:669:ASP:H	1.41	0.85
1:a:196:ARG:HH22	1:a:232:VAL:HG11	1.42	0.85
1:a:666:THR:HG23	1:a:669:ASP:H	1.44	0.82
1:a:363:ILE:HG21	1:b:159:GLN:HE21	1.45	0.81
1:a:369:ILE:HB	1:a:377:ILE:HD12	1.62	0.81
1:b:478:TYR:OH	1:b:506:LYS:NZ	2.12	0.81
1:a:193:VAL:HG21	1:a:226:HIS:HB3	1.61	0.81
1:a:571:GLU:HA	1:a:573:ARG:HH11	1.45	0.80
1:b:254:GLN:HG3	1:b:289:LEU:HD11	1.64	0.79
1:b:168:THR:HG23	1:b:171:MET:H	1.48	0.78
1:a:369:ILE:HB	1:a:377:ILE:HD11	1.65	0.78
1:a:622:LEU:HD23	1:a:623:SER:H	1.49	0.78
1:a:438:THR:HG23	1:a:441:GLU:H	1.49	0.77
1:b:369:ILE:HB	1:b:377:ILE:HD13	1.67	0.76
1:a:383:GLU:OE2	1:b:407:GLN:NE2	2.19	0.76
1:a:196:ARG:HH11	1:a:202:ASN:HB3	1.51	0.75
1:a:334:TRP:C	1:a:335:LYS:HE2	2.11	0.75
1:a:319:ARG:HH22	1:b:34:ALA:HB3	1.51	0.74
1:b:153:ARG:NH2	1:b:167:ALA:HB3	2.02	0.74
1:b:101:GLY:HA3	1:b:135:ARG:HG2	1.70	0.74
1:b:377:ILE:HG22	1:b:390:LYS:HA	1.70	0.73
1:a:407:GLN:O	1:b:385:GLN:NE2	2.21	0.73
1:a:219:ILE:O	1:a:223:LEU:HD12	1.88	0.73
1:b:470:ILE:HG13	5:b:968:HOH:O	1.89	0.72
1:b:401:GLN:OE1	1:b:504:SER:OG	2.06	0.72
3:a:802:HFX:S1	5:a:921:HOH:O	2.48	0.72
1:b:555:GLU:HA	1:b:709:MET:HE3	1.71	0.71
1:a:334:TRP:O	1:a:335:LYS:HE2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:52:GLN:NE2	1:a:57:GLY:O	2.23	0.71
1:b:265:ASN:OD1	1:b:296:SER:HB3	1.91	0.70
1:b:548:ILE:HG23	1:b:557:ARG:HG3	1.71	0.70
1:a:307:ARG:HH21	2:b:801:25A:C26	2.04	0.70
1:b:224:LEU:HD13	1:b:259:GLN:HE21	1.56	0.70
1:a:213:ASP:OD2	1:a:249:ASN:ND2	2.24	0.70
1:a:35:ASP:HB3	1:a:38:GLN:HB2	1.74	0.69
1:a:196:ARG:NH1	1:a:202:ASN:CB	2.49	0.69
1:b:39:VAL:HA	1:b:42:LEU:HG	1.74	0.69
1:b:143:TYR:CD2	1:b:189:MET:HE2	2.26	0.69
1:a:260:GLU:HA	1:a:293:ARG:HH22	1.57	0.69
1:b:470:ILE:HD11	1:b:483:LEU:HD21	1.75	0.69
1:a:175:GLU:HB2	1:a:206:TYR:HB3	1.74	0.68
1:b:634:ASP:HB3	1:b:637:VAL:HG12	1.75	0.68
1:b:32:GLN:NE2	1:b:63:SER:OG	2.25	0.68
1:b:153:ARG:HH21	1:b:167:ALA:HB3	1.56	0.68
1:b:451:VAL:HG22	1:b:454:GLU:HB2	1.75	0.68
1:b:186:LEU:HD23	1:b:186:LEU:O	1.94	0.67
1:b:185:LEU:HA	1:b:189:MET:HG3	1.77	0.66
1:a:252:LEU:O	1:a:256:LEU:HD12	1.96	0.66
1:b:28:THR:O	1:b:31:VAL:HG12	1.95	0.66
1:b:438:THR:HG22	1:b:440:GLN:H	1.59	0.66
1:a:87:LYS:HE3	1:a:91:ALA:HB3	1.78	0.66
1:b:686:ASN:HB3	1:b:689:MET:HE2	1.78	0.66
1:a:585:SER:O	1:a:589:ARG:HG3	1.95	0.65
1:b:168:THR:HG22	1:b:171:MET:HE3	1.78	0.65
1:a:139:LEU:HD13	1:a:189:MET:HE1	1.79	0.65
1:b:369:ILE:HB	1:b:377:ILE:CD1	2.26	0.64
1:b:148:ASP:HB3	1:b:151:MET:HE3	1.78	0.64
1:a:194:ASP:O	1:a:196:ARG:HD3	1.96	0.64
1:b:542:GLN:HB3	1:b:546:GLU:HG3	1.78	0.64
1:a:387:VAL:HG23	1:a:432:LEU:O	1.98	0.64
1:a:137:GLU:OE2	1:a:137:GLU:N	2.26	0.64
1:a:286:ILE:O	1:a:290:LEU:HD12	1.98	0.64
1:b:231:ASN:HD21	1:b:263:GLU:HB2	1.63	0.64
1:a:360:LYS:HB3	1:a:381:LEU:HB2	1.81	0.63
1:b:421:SER:HB2	1:b:428:LEU:HD11	1.81	0.63
1:b:377:ILE:HD12	1:b:377:ILE:O	1.99	0.63
1:a:78:LYS:CE	1:a:79:HIS:CE1	2.79	0.62
1:b:213:ASP:O	1:b:217:LYS:HG3	1.98	0.62
1:a:58:TRP:CE3	1:a:62:HIS:HB3	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:312:SER:HA	1:a:315:VAL:HG12	1.80	0.62
1:b:283:LEU:HB3	1:b:286:ILE:HD13	1.81	0.62
1:a:22:SER:O	1:a:26:MET:HG3	2.00	0.62
1:b:89:ASN:O	1:b:121:VAL:HG22	1.99	0.61
1:a:301:ASP:OD2	1:a:303:VAL:HG12	2.00	0.61
1:a:196:ARG:CZ	1:a:202:ASN:HB3	2.28	0.61
1:b:58:TRP:HZ3	1:b:66:GLN:OE1	1.84	0.61
1:a:196:ARG:HH22	1:a:232:VAL:CG1	2.11	0.60
1:a:319:ARG:NH2	1:b:34:ALA:HB3	2.16	0.60
1:a:581:PRO:HA	1:a:584:TRP:CD1	2.35	0.60
1:b:273:THR:O	1:b:277:LEU:HD12	2.00	0.60
1:a:181:VAL:O	1:a:185:LEU:HD12	2.02	0.60
1:a:64:ALA:HA	1:a:67:MET:HE3	1.84	0.60
1:a:670:LEU:O	1:a:674:ILE:HG12	2.02	0.60
1:a:677:LEU:C	1:a:677:LEU:HD23	2.27	0.60
1:a:313:ASP:O	1:a:316:LYS:HG3	2.01	0.60
1:b:515:LYS:HD3	1:b:519:GLU:OE2	2.01	0.60
1:a:316:LYS:O	1:a:319:ARG:HB3	2.02	0.59
1:b:156:LYS:CD	1:b:157:GLN:H	2.15	0.59
1:b:58:TRP:CZ3	1:b:66:GLN:OE1	2.56	0.59
1:a:75:LEU:HD12	1:a:78:LYS:HG2	1.85	0.59
1:a:221:ARG:HH21	1:a:255:MET:HB3	1.67	0.59
1:a:24:GLU:OE1	1:a:24:GLU:N	2.35	0.59
1:b:466:LEU:CD2	1:b:488:ILE:HD12	2.21	0.59
1:a:387:VAL:HG21	1:a:431:CYS:HB3	1.84	0.58
1:b:253:VAL:O	1:b:257:LEU:HD12	2.03	0.58
1:b:466:LEU:CD2	1:b:488:ILE:CD1	2.79	0.58
1:b:143:TYR:CG	1:b:189:MET:HE2	2.38	0.58
1:a:555:GLU:HA	1:a:709:MET:HE3	1.86	0.58
1:a:249:ASN:HB3	1:a:252:LEU:HD23	1.86	0.58
1:b:585:SER:O	1:b:589:ARG:HG3	2.04	0.57
1:a:483:LEU:HD21	1:a:498:LEU:HD11	1.87	0.57
1:b:156:LYS:HE3	1:b:157:GLN:H	1.69	0.57
1:a:358:LYS:HD3	1:a:383:GLU:OE1	2.04	0.57
1:b:253:VAL:HG12	1:b:257:LEU:HD11	1.85	0.57
1:b:311:ASP:OD1	1:b:314:LEU:CD1	2.26	0.57
1:a:581:PRO:HA	1:a:584:TRP:CG	2.40	0.57
1:a:25:GLU:HA	1:a:28:THR:HG22	1.86	0.57
1:b:156:LYS:CE	1:b:157:GLN:H	2.18	0.57
1:b:265:ASN:OD1	1:b:296:SER:N	2.37	0.57
1:b:257:LEU:O	1:b:293:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:417:THR:HB	1:a:433:ALA:HB2	1.86	0.56
1:a:27:LEU:O	1:a:31:VAL:HG23	2.05	0.56
1:a:555:GLU:HG3	1:a:709:MET:HE3	1.88	0.56
1:a:392:PHE:HZ	1:a:402:GLU:OE1	1.89	0.56
1:b:186:LEU:HD21	1:b:226:HIS:CG	2.41	0.56
1:b:629:TRP:HE3	1:b:633:ILE:HD11	1.71	0.56
1:a:127:PHE:CE1	1:a:139:LEU:HD22	2.41	0.56
1:b:159:GLN:O	1:b:162:ILE:HG12	2.05	0.56
1:b:410:ARG:HD2	5:b:902:HOH:O	2.06	0.56
1:b:257:LEU:HD22	1:b:293:ARG:HG2	1.86	0.56
1:b:521:LEU:HD13	5:b:968:HOH:O	2.06	0.55
1:a:260:GLU:HA	1:a:293:ARG:NH2	2.19	0.55
1:a:341:TRP:CH2	1:a:369:ILE:HG23	2.40	0.55
1:a:363:ILE:HG21	1:b:159:GLN:NE2	2.17	0.55
1:a:627:ALA:O	1:a:632:LYS:NZ	2.39	0.55
1:a:238:LYS:HZ1	1:a:242:ILE:HG22	1.72	0.54
1:b:677:LEU:HG	1:b:681:ILE:HD11	1.89	0.54
1:b:123:GLY:HA3	1:b:153:ARG:HG2	1.90	0.54
1:a:137:GLU:H	1:a:137:GLU:CD	2.13	0.54
1:b:254:GLN:CG	1:b:289:LEU:HD11	2.34	0.54
1:a:566:PRO:HB2	1:a:573:ARG:HD3	1.90	0.54
1:b:224:LEU:HD11	1:b:256:LEU:HD23	1.89	0.54
1:b:123:GLY:C	1:b:153:ARG:HG2	2.33	0.54
1:b:94:PHE:HD1	1:b:109:LEU:CD1	2.21	0.53
1:a:356:ILE:HD13	1:a:424:ASP:HB3	1.89	0.53
1:b:286:ILE:HD12	1:b:286:ILE:H	1.73	0.53
1:a:134:GLY:HA2	1:a:181:VAL:HG21	1.89	0.53
1:a:99:ILE:O	1:a:135:ARG:NH1	2.41	0.53
1:a:414:ASN:HB2	1:a:469:ALA:HB2	1.90	0.53
1:b:636:PHE:CE1	1:b:688:LYS:HG3	2.43	0.53
1:a:590:TYR:CZ	1:a:594:ARG:HD2	2.42	0.53
1:b:293:ARG:O	1:b:293:ARG:HG3	2.09	0.53
1:b:590:TYR:CZ	1:b:594:ARG:HD2	2.43	0.53
1:b:141:PHE:O	1:b:145:ASN:ND2	2.34	0.53
1:b:177:GLY:O	1:b:179:VAL:N	2.42	0.53
1:a:409:SER:HB3	5:a:909:HOH:O	2.09	0.53
1:b:231:ASN:ND2	1:b:263:GLU:HB2	2.23	0.53
1:b:101:GLY:HA3	1:b:135:ARG:CG	2.38	0.52
1:a:347:HIS:O	1:a:351:ILE:HG23	2.10	0.52
1:a:73:VAL:HG11	1:a:105:LEU:HD23	1.91	0.52
1:b:305:ILE:HD12	1:b:305:ILE:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:466:LEU:HD21	1:a:488:ILE:HG12	1.91	0.52
1:a:148:ASP:HB3	1:a:151:MET:HE3	1.90	0.51
1:a:279:VAL:HG22	1:a:314:LEU:HD11	1.92	0.51
2:b:801:25A:OF'	2:b:801:25A:H18	2.10	0.51
2:a:801:25A:C26	1:b:307:ARG:NH1	2.73	0.51
1:a:348:LEU:HB2	1:a:367:TYR:CE1	2.45	0.51
1:b:53:GLU:OE2	1:b:58:TRP:HD1	1.92	0.51
1:b:137:GLU:OE2	1:b:137:GLU:N	2.38	0.51
1:b:629:TRP:CE2	1:b:670:LEU:HB2	2.45	0.51
1:a:460:ARG:HD2	1:a:583:PHE:HA	1.91	0.51
1:a:680:HIS:ND1	1:a:683:GLU:OE1	2.35	0.51
1:b:677:LEU:CG	1:b:681:ILE:HD11	2.41	0.51
1:a:314:LEU:HD23	1:a:314:LEU:O	2.10	0.51
1:a:66:GLN:NE2	1:b:307:ARG:O	2.44	0.51
1:a:117:ASN:HB3	1:a:151:MET:HE1	1.93	0.51
1:a:221:ARG:NH2	1:a:255:MET:HB3	2.25	0.51
1:a:254:GLN:HA	1:a:257:LEU:HD12	1.92	0.51
1:a:86:ARG:NH2	1:a:119:CYS:O	2.44	0.51
1:a:196:ARG:NH2	1:a:232:VAL:HG11	2.18	0.51
1:a:279:VAL:HG21	1:a:302:LEU:HD12	1.93	0.51
1:b:253:VAL:HG12	1:b:257:LEU:CD1	2.41	0.50
1:b:99:ILE:HG12	1:b:129:GLU:HB3	1.92	0.50
1:b:194:ASP:OD1	1:b:229:ASP:HB2	2.12	0.50
1:a:361:ILE:HD12	1:a:389:VAL:HG11	1.94	0.50
1:a:107:GLN:HG2	1:a:141:PHE:CZ	2.47	0.49
1:a:410:ARG:HD2	5:a:905:HOH:O	2.11	0.49
1:b:530:LYS:NZ	5:b:913:HOH:O	2.45	0.49
1:b:677:LEU:HG	1:b:681:ILE:CD1	2.42	0.49
1:b:229:ASP:HB3	1:b:232:VAL:HG23	1.95	0.49
1:b:629:TRP:O	1:b:633:ILE:HD12	2.12	0.49
1:b:170:LEU:HD22	1:b:203:ALA:CB	2.42	0.49
1:a:369:ILE:CB	1:a:377:ILE:HD11	2.40	0.49
1:a:677:LEU:O	1:a:681:ILE:HG12	2.12	0.49
1:b:186:LEU:HD21	1:b:226:HIS:ND1	2.27	0.49
1:b:106:LEU:HD12	1:b:142:LEU:HD21	1.95	0.49
1:a:107:GLN:HG2	1:a:141:PHE:CE2	2.47	0.49
1:a:272:LYS:HG2	1:a:276:LEU:CD2	2.43	0.49
1:a:571:GLU:HA	1:a:573:ARG:NH1	2.22	0.49
1:b:55:GLU:HG2	1:b:56:TRP:CD1	2.48	0.48
1:b:196:ARG:HD3	1:b:202:ASN:HB3	1.95	0.48
1:b:94:PHE:CZ	1:b:116:VAL:HG23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:186:LEU:HD21	1:b:226:HIS:CE1	2.49	0.48
1:b:721:MET:HG3	1:b:724:PHE:CD2	2.48	0.48
1:a:303:VAL:CG2	1:a:315:VAL:HG23	2.44	0.48
1:a:414:ASN:CB	1:a:469:ALA:HB2	2.44	0.48
1:a:153:ARG:NH2	1:a:172:ASP:OD1	2.47	0.48
1:a:372:THR:CG2	1:a:377:ILE:HG23	2.44	0.47
1:b:53:GLU:CG	1:b:58:TRP:HB2	2.44	0.47
1:b:265:ASN:OD1	1:b:296:SER:CB	2.61	0.47
1:b:285:GLU:HG2	5:b:963:HOH:O	2.14	0.47
1:a:43:LEU:HD11	1:a:76:LEU:HD23	1.96	0.47
1:b:634:ASP:HB3	1:b:637:VAL:CG1	2.43	0.47
1:a:38:GLN:O	1:a:42:LEU:HG	2.15	0.47
1:b:210:ASN:HD22	1:b:211:PRO:N	2.12	0.47
1:a:186:LEU:HD22	1:a:193:VAL:HG22	1.97	0.47
1:b:199:MET:HE3	1:b:199:MET:HB2	1.86	0.47
1:b:530:LYS:HD2	1:b:530:LYS:HA	1.59	0.47
1:b:633:ILE:HG22	1:b:637:VAL:HG13	1.97	0.47
1:b:50:ASN:HD21	1:b:82:ASP:H	1.62	0.47
1:a:233:ARG:HA	1:a:233:ARG:HD3	1.74	0.47
1:b:117:ASN:HB3	1:b:151:MET:HE1	1.97	0.47
1:b:156:LYS:HD2	1:b:157:GLN:H	1.80	0.47
1:a:358:LYS:NZ	5:a:903:HOH:O	2.43	0.46
1:b:239:THR:HG22	1:b:242:ILE:HG13	1.96	0.46
1:a:688:LYS:O	1:a:692:ILE:HD12	2.15	0.46
1:b:94:PHE:HZ	1:b:116:VAL:HG23	1.80	0.46
1:b:257:LEU:O	1:b:293:ARG:NH2	2.48	0.46
1:a:202:ASN:OD1	1:a:205:VAL:HG23	2.15	0.46
1:b:372:THR:HG22	1:b:376:GLY:N	2.30	0.46
1:b:372:THR:HG23	1:b:374:GLU:H	1.80	0.46
1:b:490:ILE:HA	1:b:495:GLY:O	2.15	0.46
1:b:153:ARG:HH21	1:b:167:ALA:CB	2.27	0.46
1:b:284:GLU:HA	1:b:314:LEU:HD11	1.96	0.46
1:b:505:ILE:CD1	1:b:513:LYS:HD3	2.46	0.46
1:b:257:LEU:HB3	1:b:293:ARG:NH1	2.31	0.46
1:a:87:LYS:NZ	2:a:801:25A:OMP	2.45	0.46
1:a:677:LEU:HD21	1:a:681:ILE:HD11	1.96	0.46
1:b:97:ALA:HB1	1:b:106:LEU:HD22	1.98	0.46
1:b:525:VAL:HB	1:b:560:ILE:CD1	2.46	0.46
1:a:542:GLN:HB3	1:a:546:GLU:HB2	1.97	0.46
1:b:23:LEU:O	1:b:26:MET:HE2	2.16	0.46
1:b:197:ASP:OD1	1:b:201:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:417:THR:HB	1:b:433:ALA:HB2	1.98	0.46
1:a:390:LYS:HD3	1:a:402:GLU:OE1	2.16	0.46
1:b:224:LEU:HB3	1:b:259:GLN:NE2	2.30	0.45
1:b:186:LEU:CD2	1:b:226:HIS:CE1	2.99	0.45
1:b:243:LEU:O	1:b:247:ARG:HB2	2.16	0.45
1:a:87:LYS:CE	1:a:91:ALA:HB3	2.45	0.45
1:a:617:PRO:HD2	1:a:710:TYR:OH	2.17	0.45
1:a:518:LEU:HD11	1:a:573:ARG:HD2	1.98	0.45
1:b:490:ILE:HD12	1:b:496:THR:HG22	1.99	0.45
1:b:148:ASP:CB	1:b:151:MET:HE3	2.46	0.45
1:a:705:PRO:O	5:a:901:HOH:O	2.20	0.45
1:a:512:GLN:NE2	1:a:515:LYS:HB2	2.31	0.45
1:b:346:LYS:HB3	1:b:350:ARG:NH2	2.31	0.45
1:a:496:THR:HG23	5:a:936:HOH:O	2.16	0.45
1:b:537:GLU:OE1	1:b:537:GLU:N	2.47	0.45
1:a:438:THR:HG22	1:a:441:GLU:OE1	2.17	0.44
1:a:555:GLU:HG3	1:a:709:MET:CE	2.46	0.44
1:b:688:LYS:O	1:b:692:ILE:HD12	2.17	0.44
1:a:99:ILE:CG1	1:a:129:GLU:HB3	2.48	0.44
1:a:197:ASP:OD2	1:a:206:TYR:OH	2.29	0.44
1:a:371:ASP:OD2	1:a:371:ASP:N	2.49	0.44
1:a:484:GLN:HG2	1:a:485:PRO:HD2	1.98	0.44
1:b:23:LEU:O	1:b:26:MET:HG3	2.17	0.44
1:b:61:LEU:HD23	1:b:93:PRO:HG2	1.99	0.44
1:b:254:GLN:O	1:b:258:GLU:HG3	2.18	0.44
1:a:83:PRO:HB3	1:a:109:LEU:HD22	1.98	0.44
1:b:103:VAL:O	1:b:107:GLN:HG3	2.17	0.44
1:b:320:LEU:O	1:b:321:HIS:ND1	2.50	0.44
1:b:370:ALA:HB3	1:b:377:ILE:HD11	1.98	0.44
1:a:65:VAL:HG12	1:a:96:ILE:HG22	1.99	0.44
1:a:82:ASP:HB3	1:a:85:LEU:HB2	2.00	0.44
1:b:385:GLN:NE2	5:b:917:HOH:O	2.50	0.44
1:b:687:LYS:HA	1:b:687:LYS:HD3	1.86	0.44
1:b:505:ILE:HD13	1:b:513:LYS:HD3	1.98	0.44
1:b:581:PRO:HA	1:b:584:TRP:CD1	2.52	0.44
1:a:196:ARG:NH2	1:a:229:ASP:HB3	2.32	0.44
1:a:195:ALA:C	1:a:196:ARG:HD3	2.43	0.44
1:a:307:ARG:HH21	2:b:801:25A:C25	2.30	0.44
1:a:316:LYS:C	1:a:319:ARG:HB3	2.43	0.43
1:a:512:GLN:CD	1:a:512:GLN:O	2.62	0.43
1:a:641:MET:HB2	1:a:641:MET:HE3	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:377:ILE:HG22	1:b:390:LYS:CA	2.45	0.43
1:a:99:ILE:HG12	1:a:129:GLU:HB3	1.99	0.43
1:b:581:PRO:HA	1:b:584:TRP:CG	2.53	0.43
1:a:260:GLU:CA	1:a:293:ARG:HH22	2.27	0.43
1:b:76:LEU:HD23	1:b:76:LEU:HA	1.71	0.43
1:b:562:HIS:CB	1:b:573:ARG:HH11	2.32	0.43
1:b:29:GLN:NE2	1:b:33:GLU:OE2	2.50	0.43
1:b:70:GLU:OE1	1:b:104:ARG:NH1	2.51	0.43
1:a:197:ASP:OD2	1:a:201:ARG:HB2	2.19	0.43
1:b:233:ARG:NH1	1:b:237:SER:OG	2.52	0.43
1:b:710:TYR:CZ	1:b:714:LYS:HE2	2.54	0.43
1:b:194:ASP:O	1:b:194:ASP:OD2	2.37	0.43
1:a:247:ARG:HG2	1:a:249:ASN:HB2	2.00	0.43
1:b:311:ASP:CG	1:b:314:LEU:CD1	2.82	0.43
1:b:377:ILE:HA	1:b:389:VAL:O	2.18	0.43
1:b:693:ILE:HD13	1:b:693:ILE:HA	1.83	0.43
1:a:123:GLY:C	1:a:153:ARG:HG2	2.43	0.42
1:b:543:SER:O	1:b:547:VAL:HG23	2.18	0.42
1:a:581:PRO:HB2	1:a:709:MET:HE1	2.01	0.42
1:b:88:ARG:HH11	1:b:88:ARG:HG2	1.84	0.42
1:a:31:VAL:HG21	1:a:60:PRO:HB3	2.00	0.42
1:a:283:LEU:HB3	1:a:286:ILE:HB	2.01	0.42
1:b:390:LYS:HB3	1:b:430:VAL:HG13	2.01	0.42
1:b:123:GLY:CA	1:b:153:ARG:HG2	2.49	0.42
1:b:360:LYS:HB3	1:b:381:LEU:HB2	2.00	0.42
1:b:479:SER:OG	1:b:481:GLN:NE2	2.50	0.42
1:a:574:LEU:HA	1:a:574:LEU:HD23	1.76	0.42
1:a:530:LYS:HG3	1:a:534:ILE:HD13	2.02	0.42
1:a:622:LEU:CD2	1:a:623:SER:H	2.26	0.42
1:b:312:SER:O	1:b:316:LYS:HG3	2.19	0.42
1:a:110:LEU:N	1:a:111:PRO:HD2	2.35	0.42
1:a:355:MET:HE3	1:a:355:MET:HB3	1.72	0.42
1:b:346:LYS:HB3	1:b:350:ARG:HH21	1.84	0.42
1:a:210:ASN:O	1:a:247:ARG:NH1	2.52	0.42
1:a:385:GLN:NE2	1:b:407:GLN:HB3	2.34	0.42
1:b:149:VAL:HG21	1:b:189:MET:HB2	2.01	0.42
1:b:462:ILE:HG12	1:b:496:THR:HG21	2.01	0.42
1:b:482:ASP:O	1:b:487:ASN:ND2	2.53	0.42
1:a:52:GLN:OE1	1:a:85:LEU:HD11	2.20	0.42
1:a:297:THR:HG21	1:a:318:LEU:HD11	2.00	0.42
1:a:372:THR:HG21	1:a:377:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:801:25A:H8	2:b:801:25A:H5'2	2.02	0.41
1:a:103:VAL:O	1:a:107:GLN:HG3	2.21	0.41
1:b:143:TYR:CE1	1:b:189:MET:HB3	2.55	0.41
1:a:373:ALA:O	1:b:161:ARG:HD2	2.21	0.41
1:b:104:ARG:HH11	1:b:104:ARG:HB3	1.85	0.41
1:a:67:MET:HE3	1:a:67:MET:HB2	1.86	0.41
1:a:406:LEU:HD23	1:a:406:LEU:HA	1.94	0.41
1:b:370:ALA:H	1:b:377:ILE:HD12	1.86	0.41
1:b:538:THR:O	1:b:542:GLN:HG3	2.21	0.41
1:b:556:THR:O	1:b:560:ILE:HG12	2.21	0.41
1:a:241:LEU:HB2	1:a:262:ILE:HD11	2.03	0.41
1:b:168:THR:OG1	1:b:169:ALA:N	2.53	0.41
1:b:555:GLU:HG3	1:b:709:MET:HE3	2.03	0.41
1:b:615:LEU:HB3	1:b:667:LEU:HD23	2.03	0.41
1:a:277:LEU:O	1:a:281:LEU:HD12	2.20	0.41
1:a:308:ARG:HD3	1:a:352:TRP:CZ3	2.55	0.41
1:a:688:LYS:HD2	1:a:692:ILE:HD11	2.02	0.41
1:b:156:LYS:HE3	1:b:157:GLN:N	2.35	0.41
1:b:311:ASP:OD2	1:b:314:LEU:HD13	2.19	0.41
1:a:163:ARG:O	1:a:199:MET:HG3	2.21	0.41
1:a:381:LEU:HD23	1:a:381:LEU:HA	1.87	0.41
1:b:99:ILE:HG23	1:b:133:TYR:CD2	2.56	0.41
1:b:463:LEU:HA	1:b:463:LEU:HD23	1.77	0.41
1:b:555:GLU:HG3	1:b:709:MET:CE	2.50	0.41
1:b:641:MET:HE2	1:b:641:MET:HB2	1.92	0.41
1:b:687:LYS:NZ	1:b:690:LYS:HD3	2.36	0.41
1:a:29:GLN:O	1:a:33:GLU:HG3	2.21	0.41
1:a:377:ILE:HD12	1:a:377:ILE:O	2.21	0.41
1:b:105:LEU:O	1:b:109:LEU:HG	2.21	0.41
1:b:372:THR:HG22	1:b:376:GLY:CA	2.50	0.41
1:b:574:LEU:HD23	1:b:574:LEU:HA	1.75	0.41
1:a:341:TRP:CZ2	1:a:369:ILE:HG23	2.56	0.40
1:a:353:ARG:CD	1:a:362:PHE:HB2	2.51	0.40
1:a:278:ALA:HA	1:a:283:LEU:HD12	2.03	0.40
1:b:25:GLU:OE1	1:b:47:ALA:HA	2.22	0.40
1:b:204:LEU:O	1:b:208:LEU:HD12	2.21	0.40
1:b:240:PRO:HA	1:b:243:LEU:HD12	2.04	0.40
1:b:525:VAL:HB	1:b:560:ILE:HD11	2.02	0.40
1:b:669:ASP:HA	1:b:672:LYS:HB3	2.03	0.40
1:a:23:LEU:HB3	1:a:24:GLU:OE1	2.21	0.40
1:a:480:HIS:O	1:a:481:GLN:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:139:LEU:HD13	1:a:189:MET:CE	2.51	0.40
1:a:163:ARG:HD2	1:a:198:ASN:O	2.21	0.40
1:a:307:ARG:HG2	1:b:66:GLN:HE21	1.85	0.40
1:b:102:ASN:HB3	1:b:105:LEU:HD13	2.03	0.40
1:a:530:LYS:HD2	1:a:530:LYS:HA	1.80	0.40
1:b:286:ILE:HD12	1:b:286:ILE:N	2.36	0.40

There are no symmetry-related clashes.

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	662/717 (92%)	638 (96%)	23 (4%)	1 (0%)	43 60
1	b	668/717 (93%)	639 (96%)	27 (4%)	2 (0%)	36 52
All	All	1330/1434 (93%)	1277 (96%)	50 (4%)	3 (0%)	43 60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	319	ARG
1	b	618	GLY
1	b	571	GLU

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	575/617 (93%)	575 (100%)	0	100	100
1	b	574/617 (93%)	574 (100%)	0	100	100
All	All	1149/1234 (93%)	1149 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	107	GLN
1	a	122	ASN
1	a	178	HIS
1	a	198	ASN
1	a	440	GLN
1	a	453	ASN
1	b	32	GLN
1	b	210	ASN
1	b	249	ASN
1	b	259	GLN
1	b	292	HIS
1	b	481	GLN
1	b	684	GLN
1	b	716	GLN

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](#)

5 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	25A	a	801	-	75,75,75	3.33	28 (37%)	111,116,116	2.16	32 (28%)
3	HFX	b	802	-	12,15,15	1.25	1 (8%)	12,22,22	1.23	1 (8%)
4	PO4	a	803	-	4,4,4	0.89	0	6,6,6	0.72	0
3	HFX	a	802	-	12,15,15	1.27	1 (8%)	12,22,22	1.26	1 (8%)
2	25A	b	801	-	75,75,75	3.30	29 (38%)	111,116,116	2.14	35 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	25A	a	801	-	-	7/40/88/88	0/9/9/9
3	HFX	a	802	-	-	0/0/14/14	0/2/2/2
3	HFX	b	802	-	-	0/0/14/14	0/2/2/2
2	25A	b	801	-	-	6/40/88/88	0/9/9/9

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	801	25A	OO'-CL'	10.85	1.67	1.42
2	a	801	25A	OO'-CL'	10.36	1.65	1.42
2	a	801	25A	O4'-C1'	9.36	1.63	1.42
2	b	801	25A	O4'-C1'	9.21	1.63	1.42
2	a	801	25A	OE'-CB'	9.10	1.63	1.42
2	b	801	25A	OE'-CB'	8.58	1.61	1.42
2	a	801	25A	CC'-CB'	-7.72	1.34	1.53
2	b	801	25A	CC'-CB'	-7.34	1.35	1.53
2	b	801	25A	C2'-C1'	-7.29	1.35	1.53
2	a	801	25A	C2'-C1'	-7.12	1.35	1.53
2	a	801	25A	CM'-CL'	-6.45	1.33	1.53
2	b	801	25A	CM'-CL'	-6.43	1.33	1.53
2	b	801	25A	O4'-C4'	-6.40	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	801	25A	OO'-CO'	-6.23	1.31	1.45
2	a	801	25A	O4'-C4'	-6.19	1.31	1.45
2	a	801	25A	C16-N16	6.03	1.49	1.34
2	b	801	25A	C16-N16	6.02	1.49	1.34
2	a	801	25A	OO'-CO'	-5.96	1.31	1.45
2	a	801	25A	OE'-CE'	-5.80	1.32	1.45
2	a	801	25A	P-O3P	5.60	1.67	1.50
2	a	801	25A	C26-N26	5.34	1.47	1.34
2	b	801	25A	OE'-CE'	-5.24	1.33	1.45
2	b	801	25A	P-O3P	5.23	1.66	1.50
2	b	801	25A	C26-N26	5.21	1.47	1.34
2	a	801	25A	OD'-CD'	-4.87	1.30	1.43
2	b	801	25A	ON'-CN'	-4.19	1.32	1.43
2	a	801	25A	ON'-CN'	-4.11	1.32	1.43
2	b	801	25A	OD'-CD'	-4.02	1.33	1.43
3	b	802	HFX	C2-C8	-3.85	1.36	1.45
2	b	801	25A	C5-C4	-3.84	1.32	1.39
3	a	802	HFX	C2-C8	-3.75	1.37	1.45
2	b	801	25A	C6-N6	3.64	1.43	1.34
2	b	801	25A	O3'-C3'	-3.40	1.34	1.43
2	a	801	25A	C25-N27	-3.38	1.32	1.39
2	a	801	25A	O3'-C3'	-3.35	1.34	1.43
2	a	801	25A	C5-C4	-3.33	1.33	1.39
2	b	801	25A	P1-O2'	3.27	1.69	1.59
2	a	801	25A	C5-N7	-2.93	1.33	1.39
2	b	801	25A	OM'-CM'	2.86	1.50	1.43
2	a	801	25A	OM'-CM'	2.83	1.50	1.43
2	a	801	25A	P1-O2'	2.83	1.67	1.59
2	a	801	25A	C15-C14	-2.62	1.34	1.39
2	b	801	25A	C18-N17	2.58	1.36	1.31
2	a	801	25A	C6-N6	2.56	1.40	1.34
2	b	801	25A	C25-N27	-2.56	1.34	1.39
2	a	801	25A	C8-N9	-2.46	1.33	1.37
2	b	801	25A	C25-C24	-2.41	1.34	1.39
2	b	801	25A	C8-N9	-2.40	1.33	1.37
2	a	801	25A	C28-N27	2.40	1.36	1.31
2	b	801	25A	P2-OC'	2.39	1.66	1.59
2	b	801	25A	C28-N27	2.38	1.36	1.31
2	b	801	25A	C28-N29	-2.33	1.33	1.37
2	a	801	25A	C3'-C4'	2.25	1.58	1.53
2	b	801	25A	C5-N7	-2.25	1.35	1.39
2	a	801	25A	C28-N29	-2.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	a	801	25A	C25-C24	-2.19	1.35	1.39
2	b	801	25A	C3'-C4'	2.14	1.58	1.53
2	b	801	25A	C15-C14	-2.06	1.35	1.39
2	a	801	25A	C18-N17	2.01	1.35	1.31

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	801	25A	N16-C16-N11	-6.15	104.69	118.38
2	b	801	25A	C25-C24-N23	-5.71	118.85	126.72
2	a	801	25A	C25-C24-N23	-5.47	119.19	126.72
2	a	801	25A	N1-C2-N3	-5.40	120.41	128.58
2	b	801	25A	N21-C22-N23	-5.39	120.43	128.58
2	a	801	25A	N16-C16-N11	-5.38	106.40	118.38
2	a	801	25A	N6-C6-N1	-5.18	106.84	118.38
2	a	801	25A	N21-C22-N23	-5.13	120.82	128.58
2	b	801	25A	N6-C6-N1	-5.12	106.97	118.38
2	b	801	25A	C15-C16-N16	5.10	135.92	123.29
2	a	801	25A	C5-C4-N3	-4.99	119.84	126.72
2	b	801	25A	N1-C2-N3	-4.87	121.22	128.58
2	a	801	25A	N19-C18-N17	-4.82	107.10	113.94
2	b	801	25A	N11-C12-N13	-4.77	121.36	128.58
2	b	801	25A	C15-C14-N13	-4.76	120.16	126.72
2	b	801	25A	C5-C4-N3	-4.74	120.19	126.72
2	a	801	25A	N11-C12-N13	-4.70	121.47	128.58
2	a	801	25A	C15-C14-N13	-4.29	120.81	126.72
2	a	801	25A	C15-C16-N16	4.11	133.45	123.29
2	b	801	25A	C5-C6-N6	3.97	133.12	123.29
2	a	801	25A	C5-C6-N6	3.97	133.12	123.29
2	b	801	25A	N19-C18-N17	-3.92	108.37	113.94
2	a	801	25A	N29-C28-N27	-3.88	108.43	113.94
2	b	801	25A	N9-C8-N7	-3.71	108.67	113.94
2	b	801	25A	C22-N23-C24	3.71	120.89	111.83
2	b	801	25A	N26-C26-N21	-3.67	110.19	118.38
2	a	801	25A	O5'-P-O3P	3.55	116.03	106.44
2	a	801	25A	N9-C8-N7	-3.50	108.97	113.94
2	b	801	25A	N29-C28-N27	-3.47	109.01	113.94
2	a	801	25A	C22-N23-C24	3.39	120.11	111.83
2	a	801	25A	C14-N19-C18	3.35	109.25	105.74
3	a	802	HFX	C1-S1-C4	-3.26	91.20	94.73
2	a	801	25A	N23-C24-N29	3.21	132.62	127.17
3	b	802	HFX	C1-S1-C4	-3.11	91.36	94.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	801	25A	C2-N3-C4	3.11	119.42	111.83
2	a	801	25A	N3-C4-N9	3.09	132.43	127.17
2	b	801	25A	CP'-CO'-CN'	-3.07	104.16	115.21
2	b	801	25A	N23-C24-N29	3.05	132.36	127.17
2	b	801	25A	C2-N3-C4	3.05	119.27	111.83
2	b	801	25A	C15-N17-C18	2.98	108.13	103.45
2	a	801	25A	C15-N17-C18	2.96	108.10	103.45
2	a	801	25A	N26-C26-N21	-2.90	111.91	118.38
2	b	801	25A	C12-N13-C14	2.84	118.77	111.83
2	a	801	25A	C25-N27-C28	2.79	107.83	103.45
2	a	801	25A	C12-N13-C14	2.78	118.61	111.83
2	a	801	25A	N13-C14-N19	2.77	131.88	127.17
2	b	801	25A	C25-C24-N29	2.73	108.79	105.81
2	a	801	25A	CN'-CM'-CL'	2.63	106.45	101.46
2	b	801	25A	C15-C14-N19	2.61	108.66	105.81
2	b	801	25A	N3-C4-N9	2.61	131.61	127.17
2	b	801	25A	C5-N7-C8	2.57	107.50	103.45
2	a	801	25A	C26-C25-C24	2.54	120.64	117.18
2	b	801	25A	C14-C15-N17	-2.51	107.72	110.58
2	b	801	25A	C25-N27-C28	2.48	107.34	103.45
2	a	801	25A	C6-C5-C4	2.39	120.44	117.18
2	a	801	25A	C5-N7-C8	2.39	107.20	103.45
2	b	801	25A	C24-C25-N27	-2.38	107.86	110.58
2	b	801	25A	N13-C14-N19	2.36	131.18	127.17
2	b	801	25A	C25-C26-N26	2.35	129.09	123.29
2	b	801	25A	C5'-C4'-C3'	-2.35	106.77	115.21
2	b	801	25A	C2'-C3'-C4'	2.30	106.93	101.99
2	b	801	25A	C5-C4-N9	2.19	108.20	105.81
2	a	801	25A	C25-C24-N29	2.17	108.18	105.81
2	b	801	25A	C16-C15-C14	2.12	120.07	117.18
2	b	801	25A	C26-C25-C24	2.09	120.04	117.18
2	a	801	25A	C24-C25-N27	-2.06	108.22	110.58
2	a	801	25A	CP'-CO'-CN'	-2.06	107.79	115.21
2	b	801	25A	C6-C5-C4	2.06	119.99	117.18
2	a	801	25A	C14-C15-N17	-2.06	108.23	110.58

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	a	801	25A	OO'-CO'-CP'-OP'
2	b	801	25A	OO'-CO'-CP'-OP'

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Mol	Chain	Res	Type	Atoms
2	a	801	25A	CN'-CO'-CP'-OP'
2	b	801	25A	CN'-CO'-CP'-OP'
2	b	801	25A	OE'-CE'-CF'-OF'
2	a	801	25A	C2'-C1'-N9-C8
2	b	801	25A	CD'-CE'-CF'-OF'
2	b	801	25A	CC'-OC'-P2-OMP
2	a	801	25A	CP'-OP'-P2-OC'
2	a	801	25A	CP'-OP'-P2-OMP
2	a	801	25A	C2'-C1'-N9-C4
2	b	801	25A	CC'-OC'-P2-OLP
2	a	801	25A	O4'-C1'-N9-C8

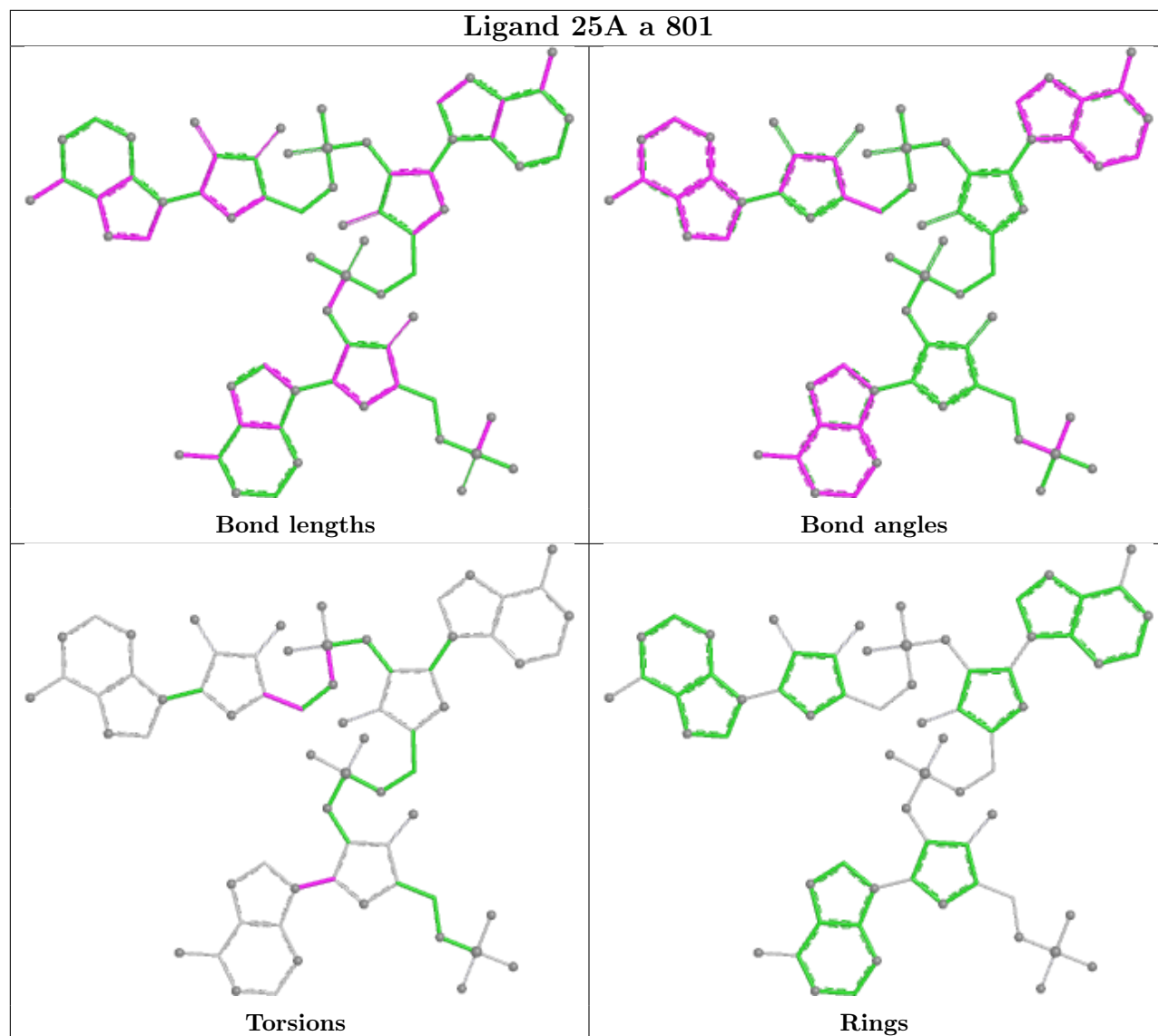
There are no ring outliers.

3 monomers are involved in 10 short contacts:

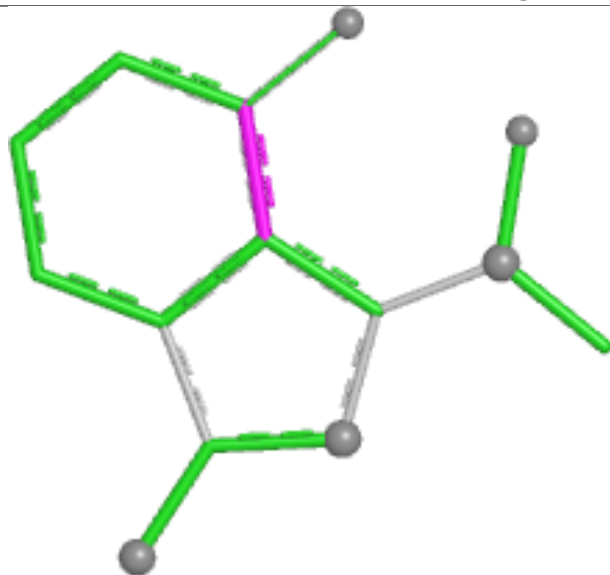
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	a	801	25A	4	0
3	a	802	HFX	1	0
2	b	801	25A	5	0

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

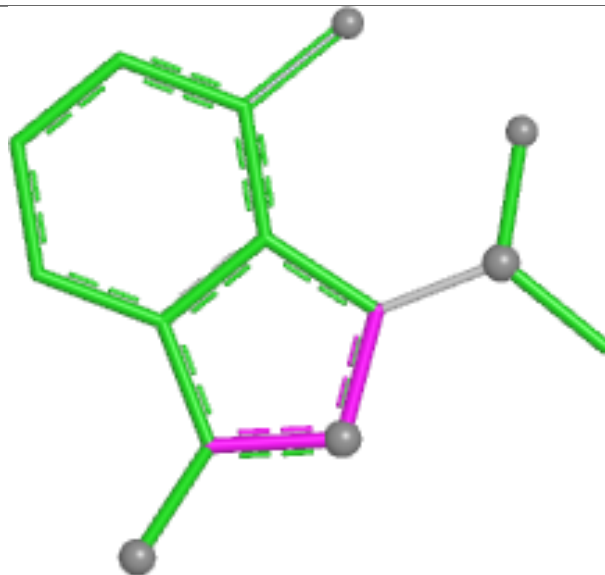
Ligand 25A a 801



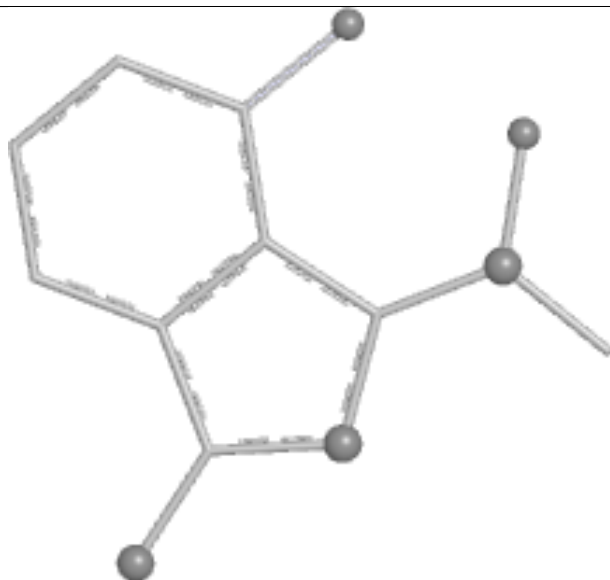
Ligand HFX b 802



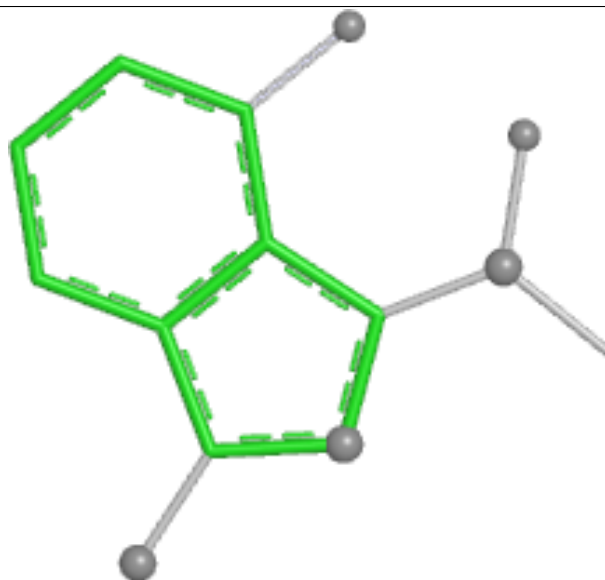
Bond lengths



Bond angles

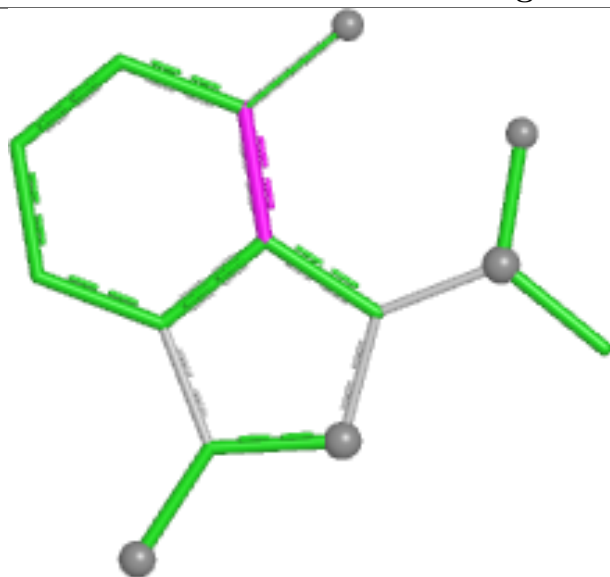


Torsions

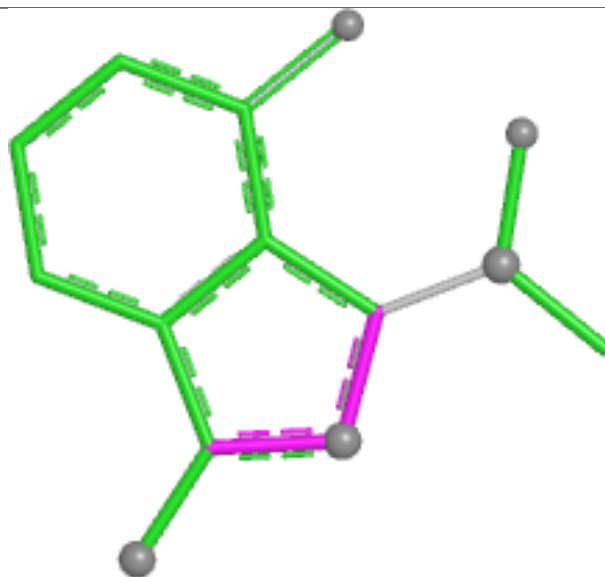


Rings

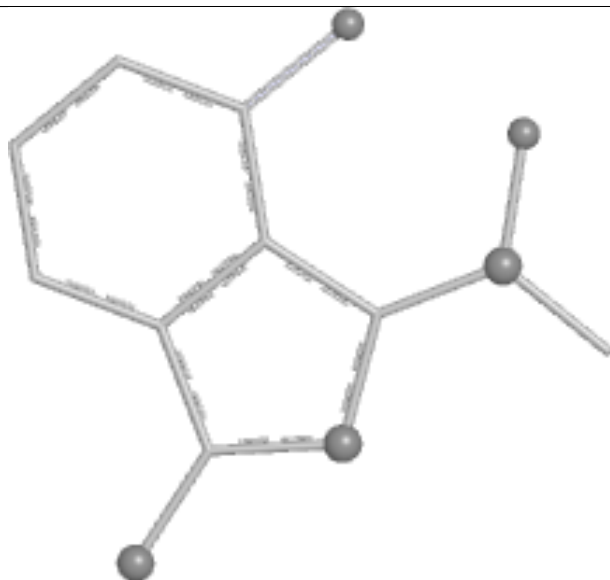
Ligand HFX a 802



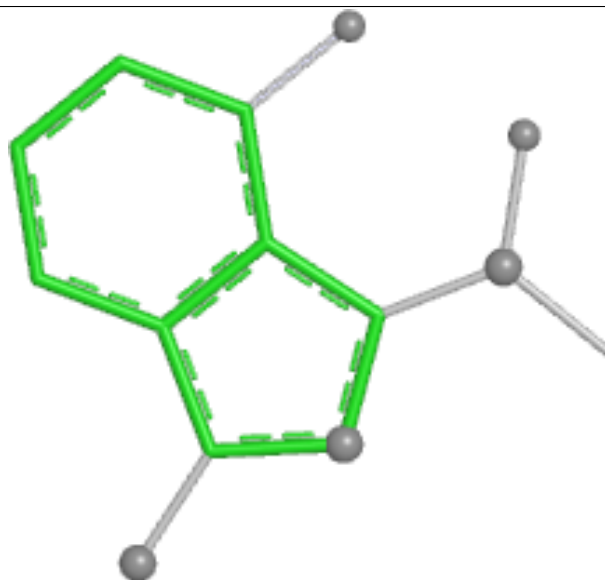
Bond lengths



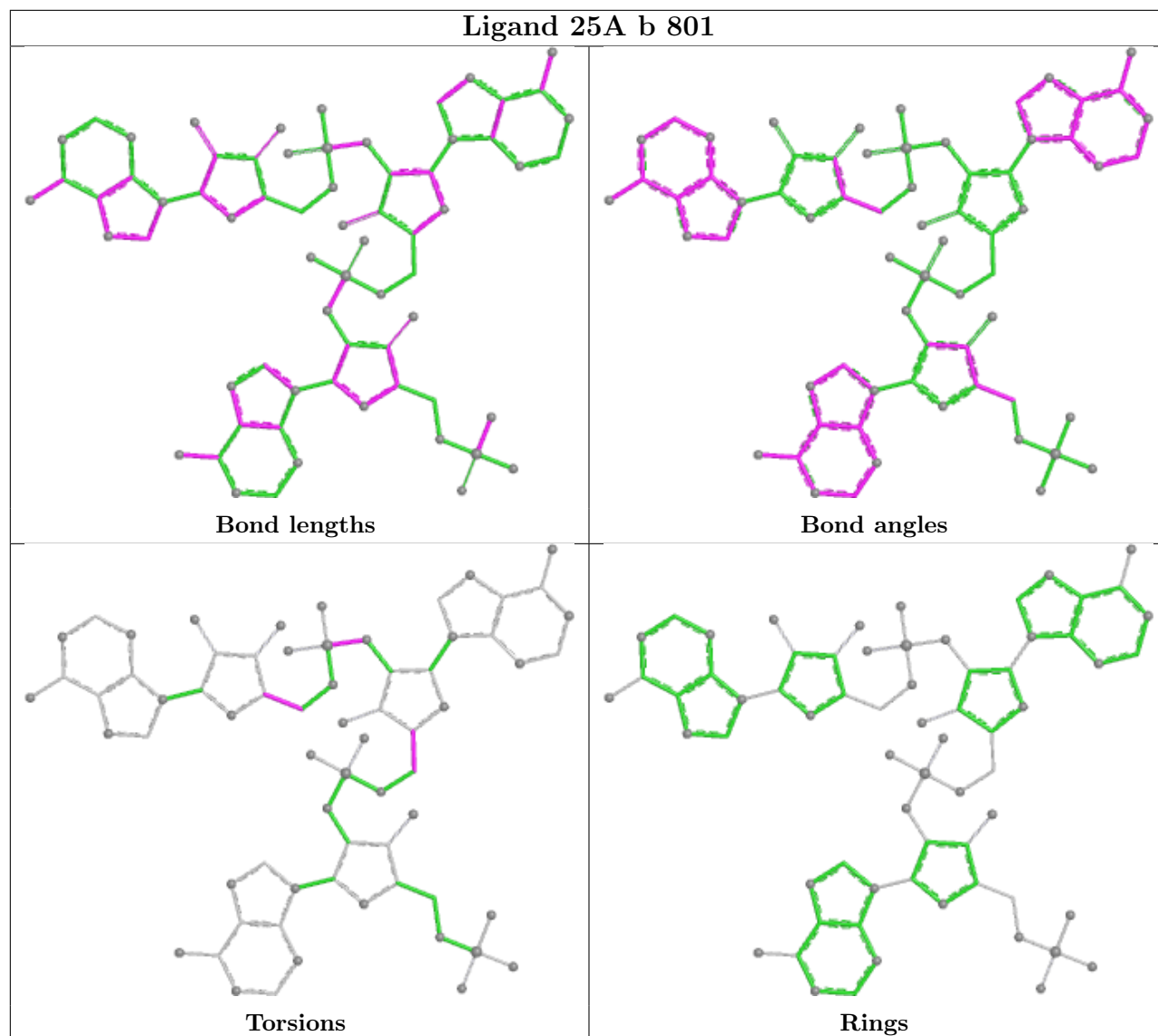
Bond angles



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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	a	672/717 (93%)	-0.19	6 (0%) 81 78	59, 98, 146, 195	0
1	b	676/717 (94%)	-0.18	4 (0%) 85 83	59, 102, 173, 219	0
All	All	1348/1434 (94%)	-0.18	10 (0%) 84 82	59, 100, 161, 219	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	567	GLY	3.6
1	a	571	GLU	3.1
1	a	245	VAL	2.8
1	a	299	CYS	2.7
1	b	42	LEU	2.6
1	a	621	GLU	2.5
1	a	380	GLY	2.4
1	b	597	GLY	2.3
1	b	619	THR	2.2
1	b	27	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

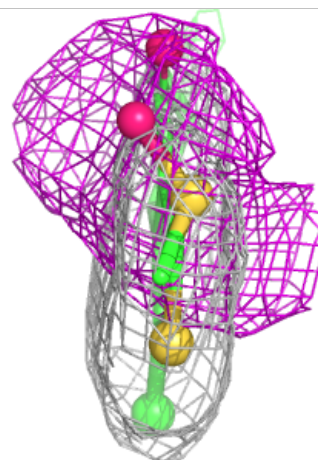
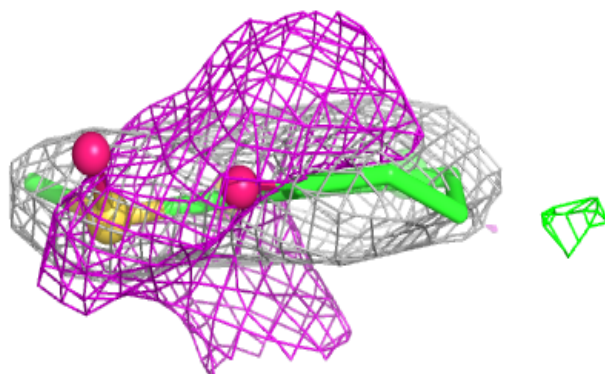
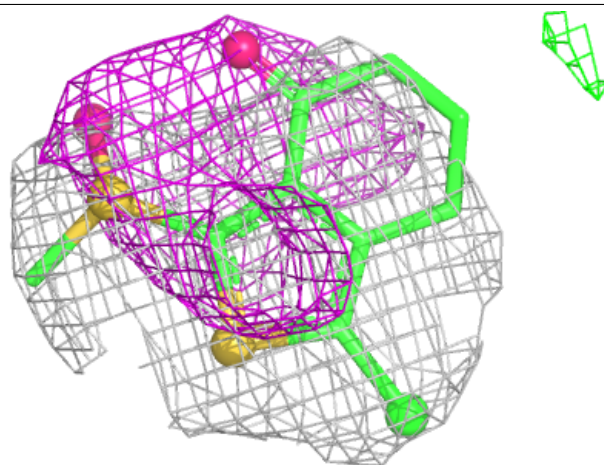
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HFX	a	802	14/14	0.85	0.12	66,108,127,127	0
3	HFX	b	802	14/14	0.89	0.12	82,98,115,116	0
2	25A	b	801	67/67	0.94	0.08	85,110,127,131	0
2	25A	a	801	67/67	0.95	0.07	61,84,102,105	0
4	PO4	a	803	5/5	0.96	0.05	72,73,92,106	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.

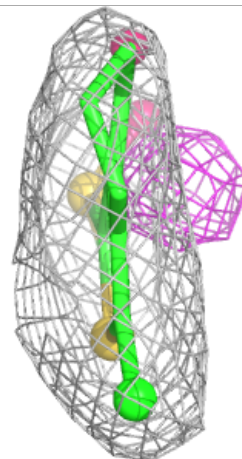
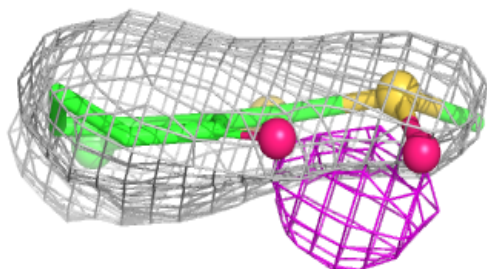
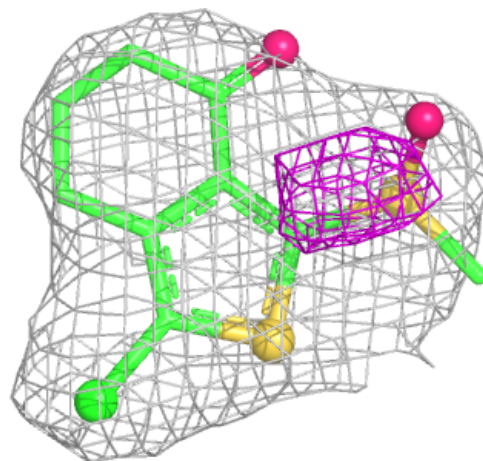
Electron density around HFX a 802:

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



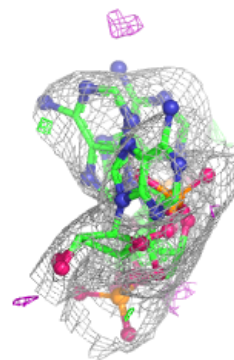
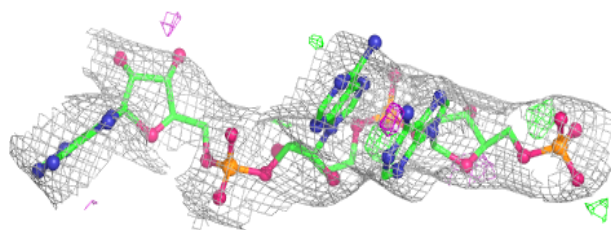
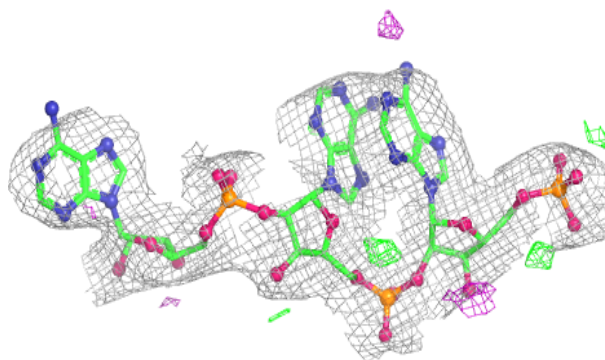
Electron density around HFX b 802:

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

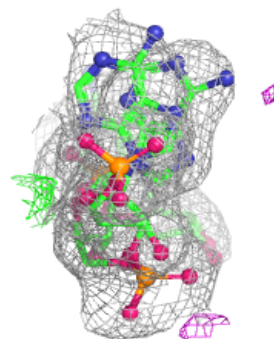
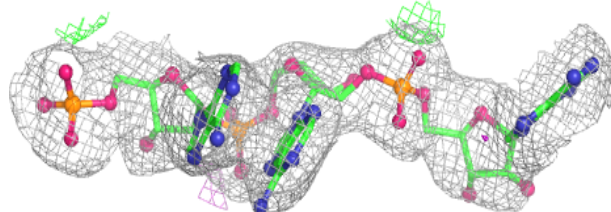
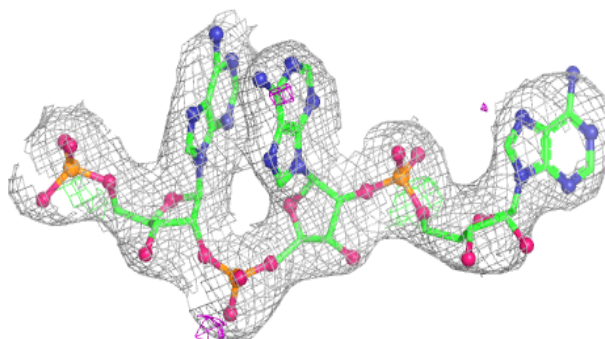


Electron density around 25A b 801:

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

**Electron density around 25A a 801:**

$2mF_o-DF_c$ (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.