



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:24 AM UTC

PDB ID : 4KVM / pdb_00004kvm
Title : The NatA (Naa10p/Naa15p) amino-terminal acetyltransferase complex bound to a bisubstrate analog
Authors : Liszczak, G.P.; Marmorstein, R.Q.
Deposited on : 2013-05-22
Resolution : 2.60 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

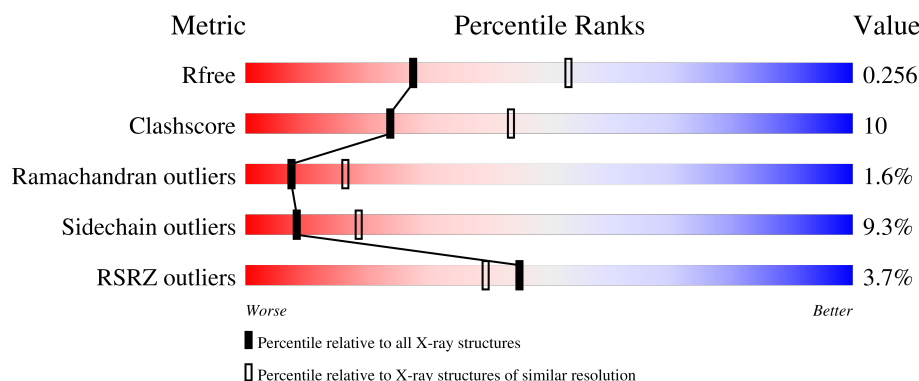
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	734	4% 71% 23% ...
1	B	734	4% 72% 22% ...
1	C	734	4% 70% 24% ...
1	D	734	4% 70% 23% ...
2	E	156	% 76% 20% ..

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Mol	Chain	Length	Quality of chain
2	F	156	
2	G	156	
2	H	156	
3	I	4	
3	J	4	
3	K	4	
3	L	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	810	-	-	X	-
4	CL	A	814	-	-	X	-
4	CL	C	810	-	-	X	-
4	CL	C	812	-	-	-	X
4	CL	D	811	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28749 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 N-terminal acetyltransferase A complex subunit nat1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	3	0
			5782	3689	976	1099	18			
1	B	722	Total	C	N	O	S	0	1	0
			5777	3686	971	1102	18			
1	C	717	Total	C	N	O	S	0	1	0
			5753	3671	968	1096	18			
1	D	718	Total	C	N	O	S	0	1	0
			5766	3681	970	1097	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	ALA	-	expression tag	UNP O74985
A	731	ALA	-	expression tag	UNP O74985
A	732	ALA	-	expression tag	UNP O74985
A	733	ALA	-	expression tag	UNP O74985
A	734	ALA	-	expression tag	UNP O74985
B	730	ALA	-	expression tag	UNP O74985
B	731	ALA	-	expression tag	UNP O74985
B	732	ALA	-	expression tag	UNP O74985
B	733	ALA	-	expression tag	UNP O74985
B	734	ALA	-	expression tag	UNP O74985
C	730	ALA	-	expression tag	UNP O74985
C	731	ALA	-	expression tag	UNP O74985
C	732	ALA	-	expression tag	UNP O74985
C	733	ALA	-	expression tag	UNP O74985
C	734	ALA	-	expression tag	UNP O74985
D	730	ALA	-	expression tag	UNP O74985
D	731	ALA	-	expression tag	UNP O74985
D	732	ALA	-	expression tag	UNP O74985
D	733	ALA	-	expression tag	UNP O74985
D	734	ALA	-	expression tag	UNP O74985

- Molecule 2 is a protein called N-terminal acetyltransferase A complex catalytic subunit ard1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	153	Total	C	N	O	S	0	1	0
			1247	790	221	225	11			
2	F	153	Total	C	N	O	S	0	0	0
			1239	785	220	224	10			
2	G	153	Total	C	N	O	S	0	0	0
			1239	785	220	224	10			
2	H	153	Total	C	N	O	S	0	0	0
			1239	785	220	224	10			

- Molecule 3 is a protein called bisubstrate analog inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			26	14	4	8			
3	J	4	Total	C	N	O	0	0	0
			26	14	4	8			
3	K	4	Total	C	N	O	0	0	0
			26	14	4	8			
3	L	4	Total	C	N	O	0	0	0
			26	14	4	8			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

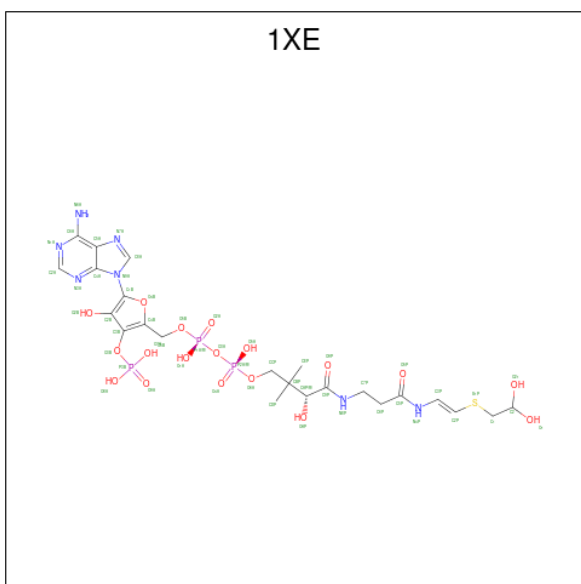
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	Cl	0	0
			14	14		
4	B	16	Total	Cl	0	0
			16	16		
4	C	13	Total	Cl	0	0
			13	13		
4	D	15	Total	Cl	0	0
			15	15		
4	E	3	Total	Cl	0	0
			3	3		
4	F	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is [5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonooxy)furan-2-yl]methyl (3R)-4-{[3-({(E)-2-[(2,2-dihydroxyethyl)sulfanyl]ethenyl}amino)-3-oxopropyl]amino}-3-hydroxy-2,2-dimethyl-4-oxobutyl dihydrogen diphosphate (CCD ID: 1XE) (formula: $C_{23}H_{34}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
6	J	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
6	K	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
6	L	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

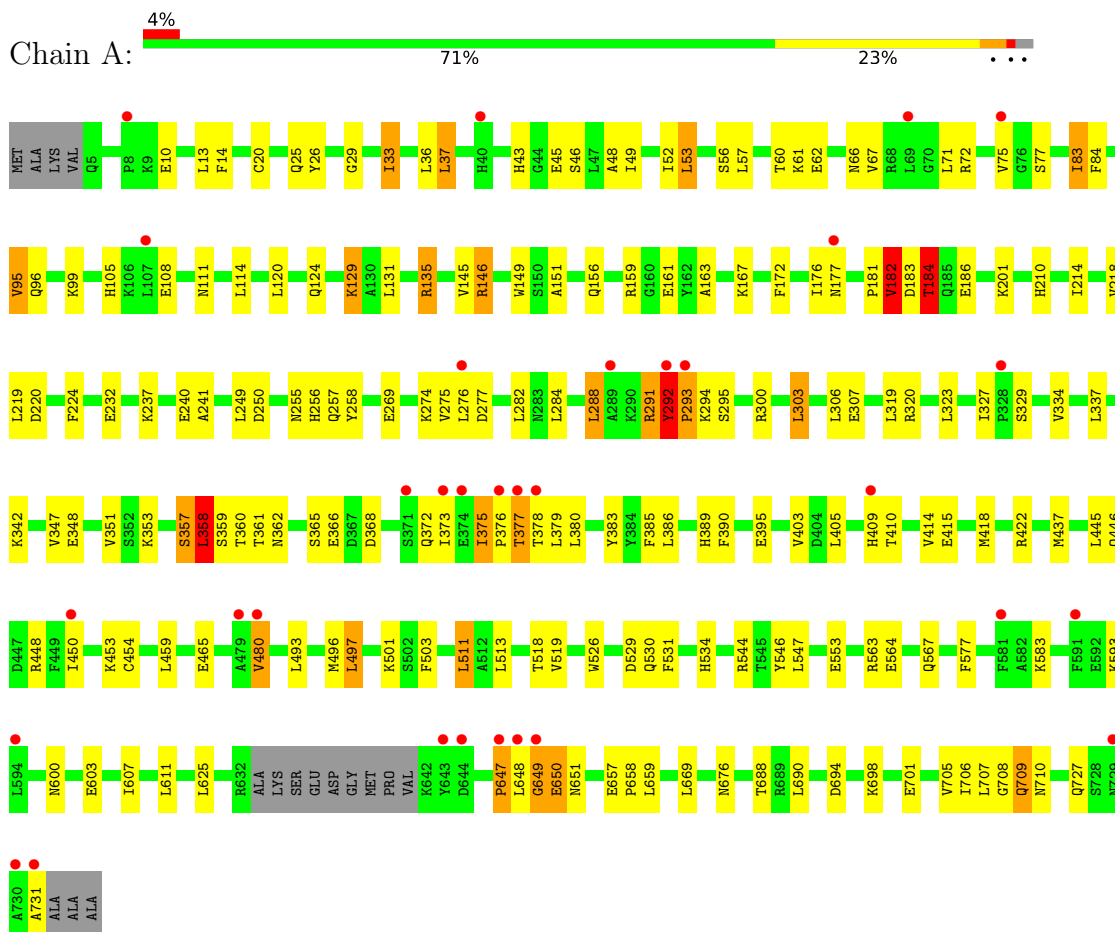
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	79	Total	O	0	0
			79	79		
7	B	50	Total	O	0	0
			50	50		
7	C	80	Total	O	0	0
			80	80		
7	D	64	Total	O	0	0
			64	64		
7	E	20	Total	O	0	0
			20	20		
7	F	6	Total	O	0	0
			6	6		
7	G	5	Total	O	0	0
			5	5		
7	H	18	Total	O	0	0
			18	18		
7	I	1	Total	O	0	0
			1	1		
7	J	1	Total	O	0	0
			1	1		
7	L	1	Total	O	0	0
			1	1		

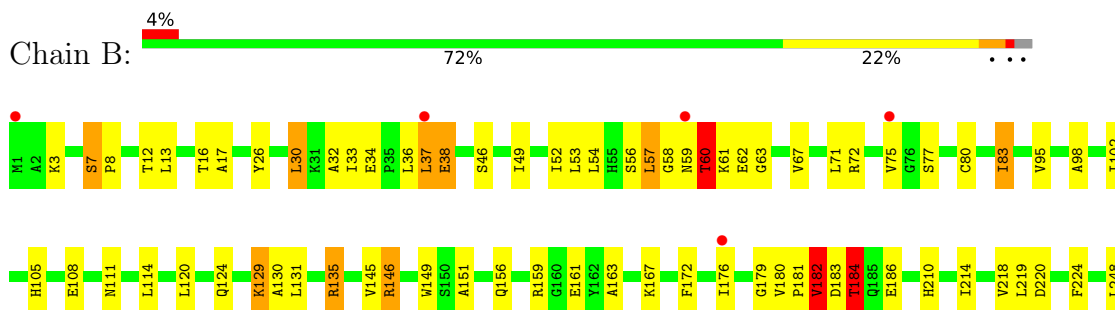
3 Residue-property plots [i](#)

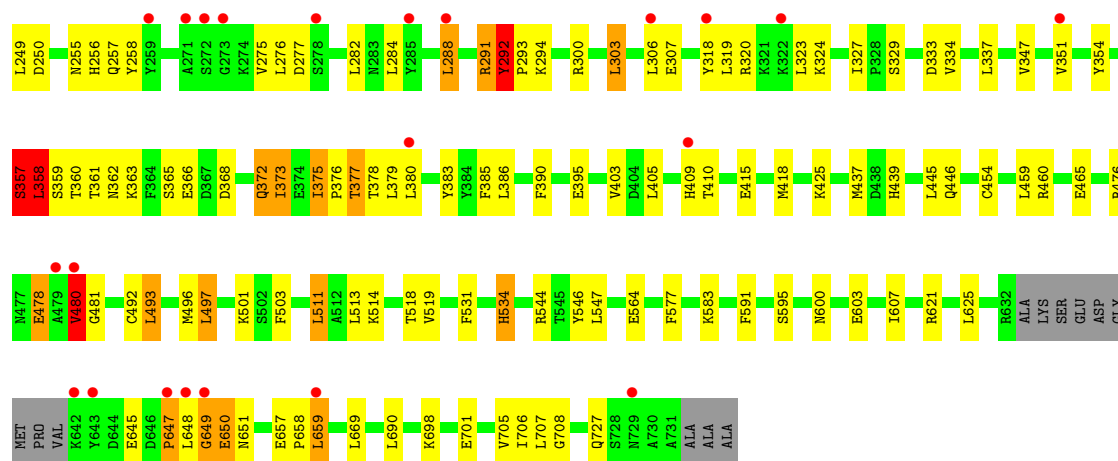
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: N-terminal acetyltransferase A complex subunit nat1

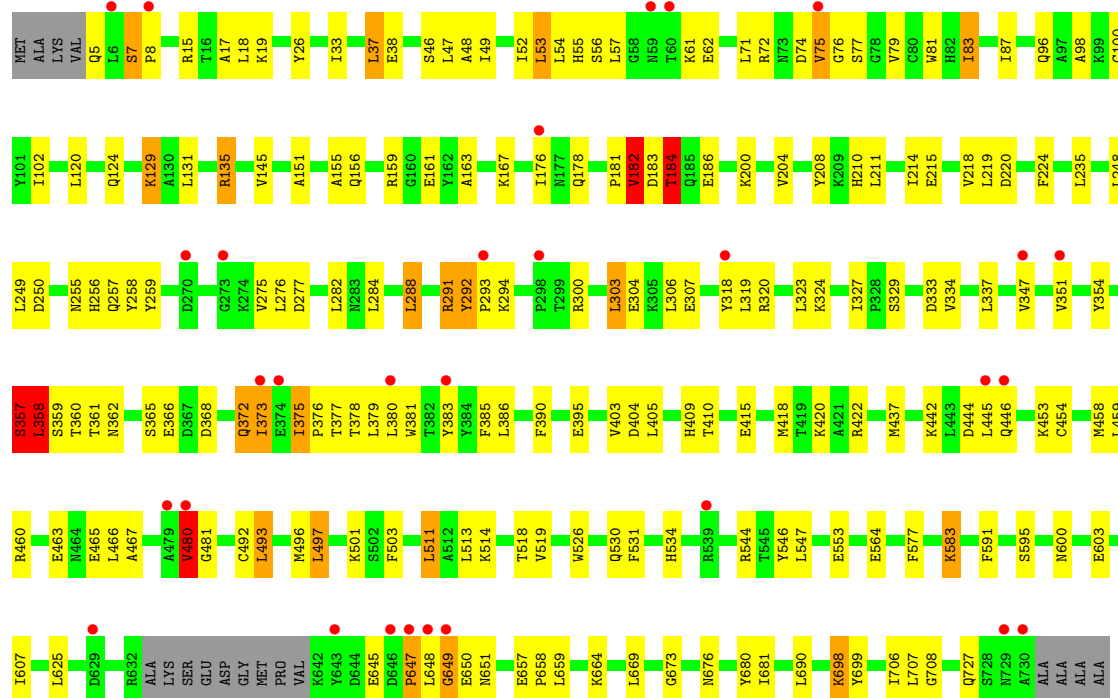


- Molecule 1: N-terminal acetyltransferase A complex subunit nat1

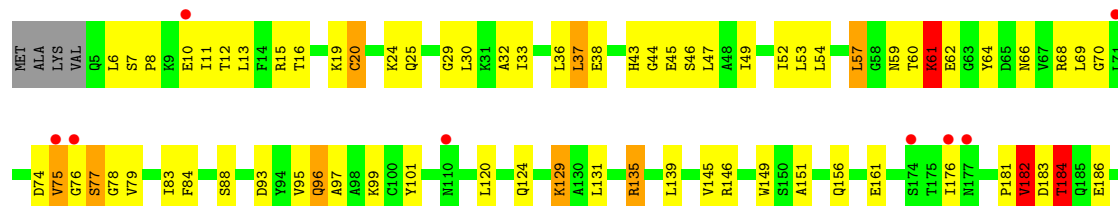


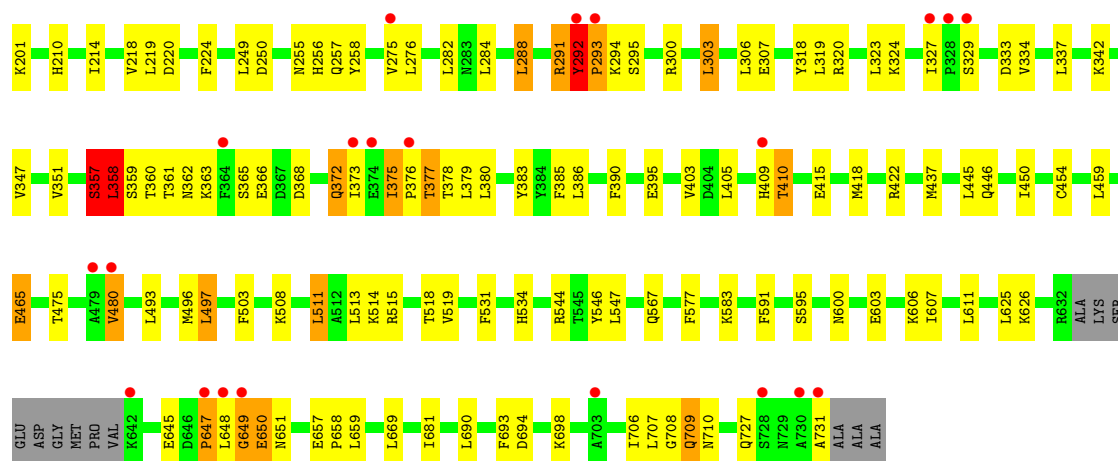


• Molecule 1: N-terminal acetyltransferase A complex subunit nat1

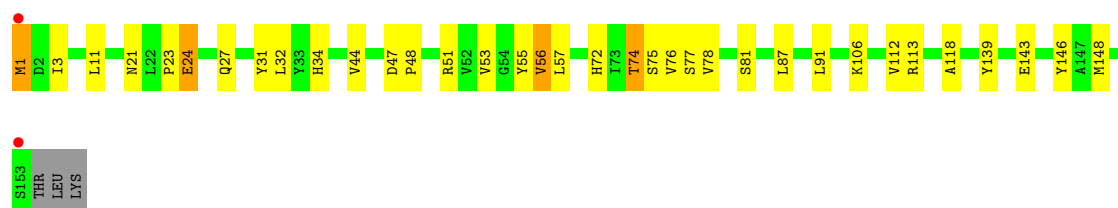
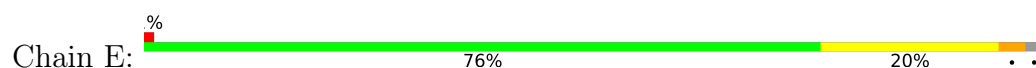


• Molecule 1: N-terminal acetyltransferase A complex subunit nat1

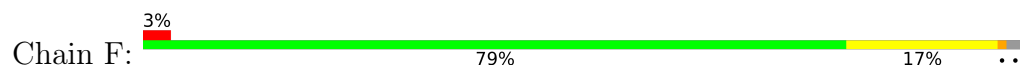




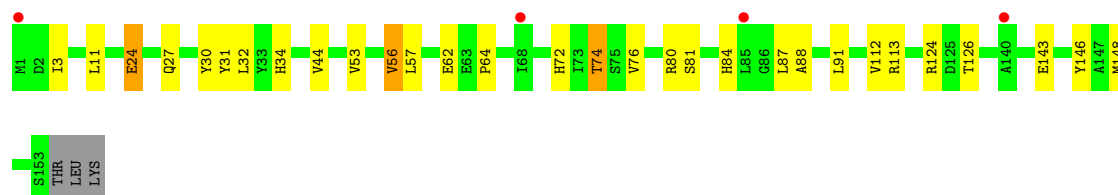
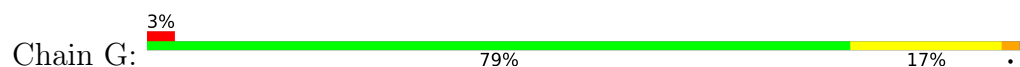
- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



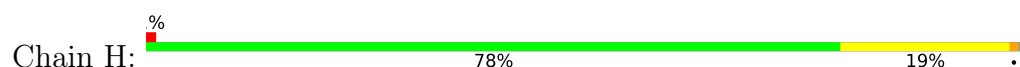
- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



LYS

- Molecule 3: bisubstrate analog inhibitor

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: bisubstrate analog inhibitor

Chain J:  50% 50%

S5122

E5125

- Molecule 3: bisubstrate analog inhibitor

Chain K:  25% 75% 25%

S5122

E5125

- Molecule 3: bisubstrate analog inhibitor

Chain L:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.44Å 119.38Å 134.06Å 80.20° 76.60° 70.42°	Depositor
Resolution (Å)	49.59 – 2.60 49.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.59-2.60) 89.8 (49.59-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.222 , 0.260 0.218 , 0.256	Depositor DCC
R_{free} test set	6916 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28749	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: CL, SO4, 1XE

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	0.56	0/5896	0.88	8/7952 (0.1%)
1	B	0.50	0/5891	0.85	7/7948 (0.1%)
1	C	0.52	0/5867	0.86	8/7915 (0.1%)
1	D	0.54	1/5881 (0.0%)	0.87	8/7934 (0.1%)
2	E	0.64	0/1277	0.92	0/1722
2	F	0.51	0/1269	0.85	0/1712
2	G	0.52	0/1269	0.84	0/1712
2	H	0.59	0/1269	0.90	0/1712
3	I	0.93	0/25	1.09	0/32
3	J	0.66	0/25	0.59	0/32
3	K	0.32	0/25	0.78	0/32
3	L	0.50	0/25	0.84	0/32
All	All	0.54	1/28719 (0.0%)	0.87	31/38735 (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
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	410	THR	CA-CB	5.84	1.59	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	VAL	N-CA-C	9.04	119.07	110.30
1	C	75	VAL	N-CA-C	8.51	119.30	110.36
1	D	75	VAL	N-CA-C	7.76	117.83	110.30
1	B	75	VAL	N-CA-C	7.71	118.25	110.23
1	A	33	ILE	CB-CA-C	-7.25	105.55	111.71
1	D	57	LEU	N-CA-C	-6.46	105.43	113.38
1	D	77	SER	CB-CA-C	-6.41	109.19	116.63
1	C	650	GLU	N-CA-C	6.15	120.95	113.38
1	A	650	GLU	N-CA-C	5.93	120.67	113.38
1	A	342	LYS	N-CA-C	-5.83	105.83	113.12
1	D	650	GLU	N-CA-C	5.71	120.40	113.38
1	A	676	ASN	CA-C-N	5.53	125.24	119.82
1	A	676	ASN	C-N-CA	5.53	125.24	119.82
1	B	650	GLU	N-CA-C	5.46	120.10	113.38
1	A	358	LEU	N-CA-C	5.38	122.27	110.80
1	D	342	LYS	N-CA-C	-5.31	106.48	113.12
1	A	414	VAL	N-CA-C	5.30	116.66	110.62
1	C	676	ASN	CA-C-N	5.27	124.98	119.82
1	C	676	ASN	C-N-CA	5.27	124.98	119.82
1	C	7	SER	CA-C-N	5.22	124.40	118.97
1	C	7	SER	C-N-CA	5.22	124.40	118.97
1	D	357	SER	CA-C-N	5.21	131.09	121.70
1	D	357	SER	C-N-CA	5.21	131.09	121.70
1	D	693	PHE	N-CA-C	5.17	117.82	111.82
1	C	357	SER	CA-C-N	5.13	130.94	121.70
1	C	357	SER	C-N-CA	5.13	130.94	121.70
1	B	357	SER	CA-C-N	5.11	130.90	121.70
1	B	357	SER	C-N-CA	5.11	130.90	121.70
1	B	534	HIS	N-CA-C	-5.11	107.02	113.20
1	B	292	TYR	CA-C-N	5.06	126.16	119.84
1	B	292	TYR	C-N-CA	5.06	126.16	119.84

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	357	SER	Peptide
1	A	649	GLY	Peptide
1	B	357	SER	Peptide
1	B	649	GLY	Peptide
1	C	357	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	649	GLY	Peptide
1	D	357	SER	Peptide
1	D	649	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5782	0	5705	129	1
1	B	5777	0	5697	119	0
1	C	5753	0	5675	128	0
1	D	5766	0	5691	122	0
2	E	1247	0	1233	22	0
2	F	1239	0	1223	13	0
2	G	1239	0	1223	19	0
2	H	1239	0	1223	16	0
3	I	26	0	20	0	0
3	J	26	0	20	2	0
3	K	26	0	20	1	0
3	L	26	0	20	0	0
4	A	14	0	0	10	0
4	B	16	0	0	3	0
4	C	13	0	0	4	0
4	D	15	0	0	7	0
4	E	3	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	1	0
4	H	1	0	0	0	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0
6	I	51	0	29	5	0
6	J	51	0	30	2	0
6	K	51	0	30	7	0
6	L	51	0	29	3	0
7	A	79	0	0	19	0
7	B	50	0	0	6	0
7	C	80	0	0	23	0
7	D	64	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	20	0	0	3	0
7	F	6	0	0	1	0
7	G	5	0	0	0	1
7	H	18	0	0	1	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	L	1	0	0	0	0
All	All	28749	0	27868	566	1

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 10.

All (566) 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:A:237:LYS:O	7:A:957:HOH:O	1.83	0.96
1:C:211:LEU:O	7:C:942:HOH:O	1.86	0.92
1:A:291:ARG:NH2	4:A:813:CL:CL	2.39	0.92
1:A:129[B]:LYS:NZ	4:A:805:CL:CL	2.41	0.91
1:C:463:GLU:O	7:C:915:HOH:O	1.90	0.90
1:D:606:LYS:NZ	4:D:802:CL:CL	2.42	0.89
1:A:567:GLN:OE1	7:A:912:HOH:O	1.93	0.87
1:B:647:PRO:HB3	1:B:651:ASN:HB2	1.59	0.84
1:C:647:PRO:HB3	1:C:651:ASN:HB2	1.60	0.84
4:C:808:CL:CL	7:C:901:HOH:O	2.34	0.82
1:D:647:PRO:HB3	1:D:651:ASN:HB2	1.61	0.81
1:D:465:GLU:OE2	7:D:952:HOH:O	1.97	0.80
1:A:647:PRO:HB3	1:A:651:ASN:HB2	1.62	0.80
1:D:731:ALA:O	7:D:901:HOH:O	2.00	0.78
1:B:57:LEU:HD12	1:B:58:GLY:H	1.47	0.78
1:B:108:GLU:O	7:B:913:HOH:O	2.02	0.77
1:A:108:GLU:O	7:A:930:HOH:O	2.02	0.77
1:A:232:GLU:HB3	7:A:957:HOH:O	1.85	0.76
1:D:77:SER:OG	1:D:78:GLY:N	2.18	0.75
1:D:358:LEU:HD12	1:D:379:LEU:HG	1.69	0.75
1:A:183:ASP:HB3	1:A:186:GLU:HB2	1.70	0.73
1:A:181:PRO:HA	1:A:182:VAL:HG22	1.71	0.73
1:D:181:PRO:HA	1:D:182:VAL:HG22	1.71	0.73
1:A:241:ALA:N	7:A:957:HOH:O	2.20	0.73
1:C:52:ILE:HB	1:C:83:ILE:HD11	1.70	0.73
1:B:358:LEU:HD12	1:B:379:LEU:HG	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:GLU:OE2	7:C:955:HOH:O	2.08	0.72
1:C:181:PRO:HA	1:C:182:VAL:HG22	1.70	0.72
1:A:358:LEU:HD12	1:A:379:LEU:HG	1.72	0.71
1:C:358:LEU:HD12	1:C:379:LEU:HG	1.72	0.71
1:A:526:TRP:O	7:A:914:HOH:O	2.06	0.71
1:B:181:PRO:HA	1:B:182:VAL:HG22	1.71	0.71
1:D:650:GLU:OE1	7:D:903:HOH:O	2.09	0.71
2:E:106:LYS:HE2	7:E:315:HOH:O	1.91	0.71
1:C:467:ALA:N	7:C:915:HOH:O	2.22	0.70
1:D:320:ARG:NH1	1:D:368:ASP:OD2	2.18	0.70
1:C:458:MET:HB3	7:C:915:HOH:O	1.89	0.70
2:G:84:HIS:NE2	6:K:5201:1XE:H1	2.07	0.69
1:C:526:TRP:O	7:C:955:HOH:O	2.11	0.68
1:B:183:ASP:HB3	1:B:186:GLU:HB2	1.74	0.68
1:A:553:GLU:OE2	7:A:914:HOH:O	2.11	0.68
1:A:320:ARG:NH1	1:A:368:ASP:OD2	2.20	0.67
1:C:129:LYS:H	1:C:129:LYS:HD2	1.59	0.67
1:D:567:GLN:OE1	7:D:942:HOH:O	2.12	0.67
2:E:24:GLU:OE2	7:E:319:HOH:O	2.11	0.67
1:A:62:GLU:O	1:A:66:ASN:ND2	2.27	0.67
1:B:320:ARG:NH1	1:B:368:ASP:OD2	2.19	0.67
1:D:475:THR:O	7:D:964:HOH:O	2.11	0.67
1:A:177:ASN:HA	1:B:621:ARG:HH21	1.58	0.67
1:B:650:GLU:OE1	7:B:934:HOH:O	2.13	0.67
1:C:54:LEU:HD13	1:C:62:GLU:HG3	1.76	0.66
1:B:497:LEU:HD13	1:B:519:VAL:HG21	1.76	0.66
1:C:320:ARG:NH1	1:C:368:ASP:OD2	2.20	0.66
1:A:269:GLU:HG3	1:A:274:LYS:HA	1.77	0.66
1:D:124:GLN:HG3	1:D:531:PHE:CD1	2.31	0.66
1:D:183:ASP:HB3	1:D:186:GLU:HB2	1.78	0.66
1:B:390:PHE:HD1	1:B:395:GLU:HG3	1.61	0.65
1:A:497:LEU:HD13	1:A:519:VAL:HG21	1.78	0.65
1:A:563:ARG:NH1	4:A:814:CL:CL	2.62	0.65
1:D:422:ARG:NH2	4:D:811:CL:CL	2.67	0.65
1:A:709:GLN:HG2	1:A:710:ASN:H	1.61	0.65
1:D:124:GLN:HG3	1:D:531:PHE:HD1	1.61	0.65
1:D:497:LEU:HD13	1:D:519:VAL:HG21	1.80	0.64
2:E:51:ARG:HD2	7:E:312:HOH:O	1.97	0.64
1:A:688:THR:O	7:A:927:HOH:O	2.15	0.64
1:C:124:GLN:HG3	1:C:531:PHE:CD1	2.33	0.64
1:D:709:GLN:HG2	1:D:710:ASN:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ASP:HB3	1:C:186:GLU:HB2	1.79	0.64
1:D:61:LYS:HD3	1:D:64:TYR:HB2	1.80	0.64
2:E:77:SER:HB2	6:I:5201:1XE:H24	1.80	0.64
1:C:390:PHE:HD1	1:C:395:GLU:HG3	1.62	0.63
2:E:118:ALA:HA	6:I:5201:1XE:N7A	2.12	0.63
1:A:659:LEU:HD22	1:A:659:LEU:H	1.63	0.63
1:C:5:GLN:NE2	7:C:903:HOH:O	2.27	0.63
1:C:659:LEU:HD22	1:C:659:LEU:H	1.64	0.63
1:A:422:ARG:NH2	4:A:810:CL:CL	2.69	0.63
1:D:390:PHE:HD1	1:D:395:GLU:HG3	1.63	0.63
1:A:563:ARG:HD2	4:A:814:CL:CL	2.36	0.63
1:B:124:GLN:HG3	1:B:531:PHE:CD1	2.34	0.63
2:E:56:VAL:HG12	2:E:91:LEU:HB3	1.80	0.62
1:A:390:PHE:HD1	1:A:395:GLU:HG3	1.64	0.62
1:D:156:GLN:HG3	1:D:161:GLU:HB2	1.80	0.62
2:F:56:VAL:HG12	2:F:91:LEU:HB3	1.80	0.62
2:G:56:VAL:HG12	2:G:91:LEU:HB3	1.81	0.62
1:A:124:GLN:HG3	1:A:531:PHE:CD1	2.35	0.62
1:A:709:GLN:HG2	1:A:710:ASN:N	2.15	0.62
1:B:129[A]:LYS:H	1:B:129[A]:LYS:HD2	1.65	0.62
1:D:659:LEU:H	1:D:659:LEU:HD22	1.64	0.62
2:H:56:VAL:HG12	2:H:91:LEU:HB3	1.81	0.62
1:C:183:ASP:O	1:C:184:THR:HB	1.98	0.62
1:A:183:ASP:O	1:A:184:THR:HB	1.98	0.61
1:A:156:GLN:HG3	1:A:161:GLU:HB2	1.81	0.61
1:D:183:ASP:O	1:D:184:THR:HB	1.98	0.61
1:A:48:ALA:HB1	1:A:83:ILE:HD12	1.82	0.61
1:A:124:GLN:HG3	1:A:531:PHE:HD1	1.65	0.61
1:A:292:TYR:O	1:A:294:LYS:N	2.34	0.61
1:B:124:GLN:HG3	1:B:531:PHE:HD1	1.66	0.61
1:D:709:GLN:HG2	1:D:710:ASN:N	2.16	0.60
1:A:250:ASP:OD2	1:A:291:ARG:NH1	2.34	0.60
1:B:183:ASP:O	1:B:184:THR:HB	1.99	0.60
1:C:215:GLU:HB2	7:C:942:HOH:O	2.01	0.60
1:D:359:SER:OG	1:D:360:THR:N	2.35	0.60
2:E:112:VAL:HG12	6:I:5201:1XE:S1P	2.40	0.60
1:C:496:MET:HE2	1:C:518:THR:HG21	1.84	0.60
1:C:497:LEU:HD13	1:C:519:VAL:HG21	1.82	0.60
1:C:124:GLN:HG3	1:C:531:PHE:HD1	1.65	0.60
1:A:52:ILE:HB	1:A:83:ILE:HG13	1.83	0.60
1:B:659:LEU:H	1:B:659:LEU:HD22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLN:HG3	1:B:161:GLU:HB2	1.82	0.60
1:B:292:TYR:O	1:B:294:LYS:N	2.34	0.60
1:C:304:GLU:O	7:C:948:HOH:O	2.16	0.59
2:E:34:HIS:NE2	2:E:74:THR:HG21	2.18	0.59
1:C:255:ASN:C	1:C:255:ASN:HD22	2.09	0.59
1:C:292:TYR:O	1:C:294:LYS:N	2.35	0.59
1:D:503:PHE:CD2	1:D:511:LEU:HB3	2.37	0.59
1:A:359:SER:OG	1:A:360:THR:N	2.36	0.59
1:B:390:PHE:CD1	1:B:395:GLU:HG3	2.36	0.59
2:H:34:HIS:NE2	2:H:74:THR:HG21	2.18	0.59
1:B:13:LEU:HD22	1:B:32:ALA:HB1	1.82	0.59
2:G:84:HIS:CD2	6:K:5201:1XE:H1	2.38	0.59
1:C:444:ASP:OD1	2:G:80:ARG:NH2	2.33	0.59
1:C:503:PHE:CD2	1:C:511:LEU:HB3	2.37	0.59
1:C:156:GLN:HG3	1:C:161:GLU:HB2	1.83	0.59
1:A:503:PHE:CD2	1:A:511:LEU:HB3	2.38	0.59
1:D:292:TYR:O	1:D:294:LYS:N	2.36	0.59
1:A:255:ASN:C	1:A:255:ASN:HD22	2.11	0.58
1:B:496:MET:HE2	1:B:518:THR:HG21	1.85	0.58
1:C:390:PHE:CD1	1:C:395:GLU:HG3	2.37	0.58
1:D:390:PHE:CD1	1:D:395:GLU:HG3	2.38	0.58
1:D:496:MET:HE2	1:D:518:THR:HG21	1.84	0.58
1:A:71:LEU:HD22	1:A:84:PHE:HD2	1.68	0.58
1:A:159[B]:ARG:NH2	4:A:807:CL:CL	2.74	0.58
1:A:496:MET:HE2	1:A:518:THR:HG21	1.85	0.58
1:C:250:ASP:OD2	1:C:291:ARG:NH1	2.37	0.58
1:D:47:LEU:HD13	1:D:69:LEU:HB3	1.85	0.58
1:A:390:PHE:CD1	1:A:395:GLU:HG3	2.38	0.58
1:C:135:ARG:HD2	7:C:937:HOH:O	2.04	0.58
1:C:359:SER:OG	1:C:360:THR:N	2.35	0.58
1:B:359:SER:OG	1:B:360:THR:N	2.36	0.58
1:C:466:LEU:HB3	7:C:915:HOH:O	2.03	0.57
2:F:34:HIS:NE2	2:F:74:THR:HG21	2.19	0.57
1:B:250:ASP:OD2	1:B:291:ARG:NH1	2.38	0.57
1:D:250:ASP:OD2	1:D:291:ARG:NH1	2.37	0.57
1:B:33:ILE:HG13	1:B:37:LEU:HD21	1.85	0.57
1:A:146[B]:ARG:HB3	1:A:172:PHE:CZ	2.39	0.57
1:C:178:GLN:OE1	7:C:918:HOH:O	2.18	0.57
2:H:77:SER:HB2	6:L:5201:1XE:H24	1.85	0.57
1:A:292:TYR:C	1:A:294:LYS:H	2.12	0.56
1:B:255:ASN:C	1:B:255:ASN:HD22	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ASP:OD2	7:D:930:HOH:O	2.18	0.56
1:B:292:TYR:C	1:B:294:LYS:H	2.13	0.56
1:C:292:TYR:C	1:C:294:LYS:H	2.13	0.56
2:G:124:ARG:HD3	4:G:201:CL:CL	2.42	0.56
1:A:67:VAL:HG22	1:A:83:ILE:HD11	1.87	0.56
2:F:112:VAL:HG12	6:J:5201:1XE:S1P	2.46	0.56
1:A:437:MET:HG2	1:A:454:CYS:HA	1.87	0.56
1:C:577:PHE:CD1	1:C:659:LEU:HD21	2.41	0.56
1:B:503:PHE:CD2	1:B:511:LEU:HB3	2.41	0.56
1:D:255:ASN:C	1:D:255:ASN:HD22	2.13	0.56
1:D:625:LEU:HB3	1:D:648:LEU:HG	1.87	0.56
1:B:129[A]:LYS:H	1:B:129[A]:LYS:CD	2.19	0.55
1:A:351:VAL:HG23	1:A:386:LEU:HD21	1.89	0.55
1:A:625:LEU:HB3	1:A:648:LEU:HG	1.88	0.55
1:D:577:PHE:CD1	1:D:659:LEU:HD21	2.41	0.55
1:A:146[B]:ARG:HH22	1:A:182:VAL:HG12	1.72	0.55
1:D:135:ARG:HD3	1:D:151:ALA:HB1	1.89	0.54
1:D:292:TYR:C	1:D:294:LYS:H	2.14	0.54
1:C:422:ARG:NH2	4:C:810:CL:CL	2.77	0.54
1:D:201:LYS:NZ	4:D:809:CL:CL	2.70	0.54
1:C:37:LEU:HD13	1:C:47:LEU:HD23	1.89	0.54
1:B:135:ARG:HD3	1:B:151:ALA:HB1	1.88	0.54
1:B:625:LEU:HB3	1:B:648:LEU:HG	1.90	0.54
1:C:625:LEU:HB3	1:C:648:LEU:HG	1.90	0.54
1:B:114:LEU:HD12	7:B:913:HOH:O	2.08	0.54
1:C:17:ALA:HB1	1:C:33:ILE:HD11	1.90	0.54
1:A:114:LEU:HD12	7:A:930:HOH:O	2.08	0.53
1:A:129[A]:LYS:H	1:A:129[A]:LYS:HD2	1.73	0.53
2:G:34:HIS:NE2	2:G:74:THR:HG21	2.22	0.53
1:C:381:TRP:HB3	7:C:949:HOH:O	2.07	0.53
2:G:126:THR:HG21	6:K:5201:1XE:P3B	2.49	0.53
1:C:182:VAL:HG23	1:C:184:THR:H	1.74	0.53
1:C:235:LEU:HD11	7:C:941:HOH:O	2.08	0.53
1:C:52:ILE:HD12	1:C:83:ILE:HG12	1.91	0.53
1:D:15:ARG:HD3	1:D:19:LYS:HE2	1.90	0.53
1:A:237:LYS:NZ	4:A:812:CL:CL	2.68	0.53
1:B:111:ASN:HB3	7:B:913:HOH:O	2.08	0.53
1:A:334:VAL:HG13	1:A:337:LEU:HD12	1.91	0.53
1:B:577:PHE:CD1	1:B:659:LEU:HD21	2.44	0.53
1:C:48:ALA:HB1	1:C:83:ILE:HG21	1.90	0.53
1:C:534:HIS:HD1	1:C:546:TYR:HH	1.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:VAL:HG23	1:D:386:LEU:HD21	1.91	0.53
1:C:664:LYS:NZ	7:C:926:HOH:O	2.42	0.53
1:D:437:MET:HG2	1:D:454:CYS:HA	1.90	0.53
1:A:43:HIS:ND1	1:A:46:SER:OG	2.41	0.52
2:G:113:ARG:NH1	2:G:143:GLU:OE2	2.39	0.52
1:B:476:ARG:HH21	1:B:478:GLU:HG3	1.73	0.52
1:B:514:LYS:NZ	1:B:645:GLU:OE1	2.29	0.52
1:B:34:GLU:O	1:B:38:GLU:HB2	2.09	0.52
1:D:60:THR:O	1:D:62:GLU:N	2.42	0.52
1:A:201:LYS:HE3	4:A:803:CL:CL	2.47	0.52
1:A:577:PHE:CD1	1:A:659:LEU:HD21	2.43	0.52
1:B:282:LEU:HD21	1:B:306:LEU:HD21	1.91	0.52
1:C:282:LEU:HD21	1:C:306:LEU:HD21	1.91	0.52
1:B:351:VAL:HG23	1:B:386:LEU:HD21	1.91	0.52
1:D:324:LYS:HB3	4:D:810:CL:CL	2.47	0.52
1:B:706:ILE:O	1:B:708:GLY:N	2.43	0.52
1:C:351:VAL:HG23	1:C:386:LEU:HD21	1.91	0.52
1:D:52:ILE:HD12	1:D:83:ILE:HG23	1.92	0.52
1:B:357:SER:N	1:B:359:SER:H	2.08	0.52
1:C:357:SER:N	1:C:359:SER:H	2.08	0.51
1:B:327:ILE:HG22	1:B:329:SER:H	1.75	0.51
1:A:383:TYR:CZ	1:A:405:LEU:HD13	2.45	0.51
2:G:84:HIS:HE2	6:K:5201:1XE:H1	1.75	0.51
1:A:135:ARG:HD2	7:A:925:HOH:O	2.10	0.51
1:D:291:ARG:NH2	7:D:932:HOH:O	2.42	0.51
1:D:357:SER:N	1:D:359:SER:H	2.08	0.51
1:C:49:ILE:O	1:C:53:LEU:HD22	2.10	0.51
1:C:334:VAL:HG13	1:C:337:LEU:HD12	1.92	0.51
1:C:437:MET:HG2	1:C:454:CYS:HA	1.93	0.51
1:A:129[A]:LYS:H	1:A:129[A]:LYS:CD	2.24	0.51
1:C:501:LYS:NZ	1:C:564:GLU:OE1	2.33	0.51
1:B:182:VAL:HG23	1:B:184:THR:H	1.76	0.50
2:H:113:ARG:NH1	2:H:143:GLU:OE2	2.40	0.50
1:D:146:ARG:NH1	4:D:807:CL:CL	2.79	0.50
2:E:113:ARG:NH1	2:E:143:GLU:OE2	2.38	0.50
1:B:288:LEU:O	1:B:291:ARG:HB3	2.11	0.50
1:D:13:LEU:HD12	1:D:36:LEU:HD11	1.93	0.50
2:F:113:ARG:NH1	2:F:143:GLU:OE2	2.41	0.50
1:A:534:HIS:ND1	1:A:546:TYR:OH	2.39	0.50
1:C:204:VAL:HG12	7:C:941:HOH:O	2.11	0.50
2:G:112:VAL:HG12	6:K:5201:1XE:S1P	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ARG:HD3	1:C:151:ALA:HB1	1.92	0.50
1:D:383:TYR:CZ	1:D:405:LEU:HD13	2.47	0.50
2:G:24:GLU:HG3	3:K:5122:SER:OG	2.11	0.50
1:A:220:ASP:OD2	1:A:544:ARG:NH2	2.45	0.50
1:D:79:VAL:O	1:D:83:ILE:HG12	2.11	0.50
1:A:129[A]:LYS:NZ	4:A:811:CL:CL	2.58	0.50
1:A:706:ILE:O	1:A:708:GLY:N	2.44	0.50
1:D:365:SER:OG	1:D:366:GLU:N	2.45	0.50
1:A:184:THR:CG2	1:A:219:LEU:HD11	2.41	0.49
1:C:259:TYR:HA	7:C:947:HOH:O	2.11	0.49
1:D:282:LEU:HD21	1:D:306:LEU:HD21	1.93	0.49
1:C:46:SER:HA	1:C:49:ILE:HG12	1.93	0.49
1:D:706:ILE:O	1:D:708:GLY:N	2.45	0.49
2:G:88:ALA:HB3	6:K:5201:1XE:O2A	2.12	0.49
2:H:112:VAL:HG12	6:L:5201:1XE:S1P	2.52	0.49
1:A:357:SER:N	1:A:359:SER:H	2.11	0.49
1:B:30:LEU:O	1:B:34:GLU:HG2	2.13	0.49
1:C:319:LEU:HD21	1:C:334:VAL:HG21	1.95	0.49
1:D:184:THR:CG2	1:D:219:LEU:HD11	2.42	0.49
1:B:52:ILE:HB	1:B:83:ILE:HD13	1.94	0.49
1:C:155:ALA:HB2	7:C:937:HOH:O	2.13	0.49
1:A:111:ASN:HB3	7:A:930:HOH:O	2.13	0.49
1:A:530:GLN:N	7:A:914:HOH:O	2.31	0.49
1:B:334:VAL:HG13	1:B:337:LEU:HD12	1.94	0.49
1:B:383:TYR:CZ	1:B:405:LEU:HD13	2.48	0.49
1:D:603:GLU:O	1:D:607:ILE:HG12	2.12	0.49
1:D:351:VAL:HG21	1:D:385:PHE:CE2	2.48	0.49
1:A:357:SER:OG	1:A:358:LEU:N	2.46	0.48
1:C:291:ARG:NH2	4:C:801:CL:CL	2.83	0.48
1:C:318:TYR:OH	1:C:333:ASP:OD2	2.22	0.48
1:C:327:ILE:HG22	1:C:329:SER:H	1.78	0.48
1:A:135:ARG:HD3	1:A:151:ALA:HB1	1.94	0.48
1:A:288:LEU:O	1:A:291:ARG:HB3	2.13	0.48
1:A:351:VAL:HG21	1:A:385:PHE:CE2	2.49	0.48
1:B:105:HIS:HD2	7:B:913:HOH:O	1.95	0.48
1:C:383:TYR:CZ	1:C:405:LEU:HD13	2.48	0.48
1:A:10:GLU:O	1:A:14:PHE:N	2.38	0.48
1:A:501:LYS:NZ	1:A:564:GLU:OE1	2.41	0.48
1:B:377:THR:O	1:B:377:THR:OG1	2.27	0.48
1:C:75:VAL:N	1:C:76:GLY:HA3	2.28	0.48
1:C:358:LEU:HD13	1:C:358:LEU:HA	1.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:GLU:OE2	1:C:657:GLU:N	2.47	0.48
1:D:44:GLY:HA2	1:D:70:GLY:HA2	1.95	0.48
1:B:319:LEU:HD21	1:B:334:VAL:HG21	1.96	0.48
1:C:71:LEU:HD11	1:C:81:TRP:CD2	2.49	0.48
1:B:318:TYR:OH	1:B:333:ASP:OD2	2.23	0.48
1:B:476:ARG:HG2	1:B:478:GLU:HG2	1.94	0.48
1:B:534:HIS:ND1	1:B:546:TYR:OH	2.38	0.48
1:D:534:HIS:ND1	1:D:546:TYR:OH	2.35	0.48
1:B:184:THR:CG2	1:B:219:LEU:HD11	2.44	0.48
1:B:255:ASN:O	1:B:257:GLN:N	2.47	0.48
1:C:15:ARG:O	1:C:19:LYS:HG2	2.13	0.48
1:D:10:GLU:HG2	1:D:36:LEU:HD13	1.96	0.48
1:D:30:LEU:HG	1:D:53:LEU:HD12	1.94	0.48
1:D:514:LYS:NZ	1:D:645:GLU:OE1	2.23	0.48
1:B:347:VAL:O	1:B:351:VAL:HG22	2.14	0.48
1:C:288:LEU:O	1:C:291:ARG:HB3	2.14	0.48
1:D:16:THR:O	1:D:20:CYS:N	2.47	0.48
1:C:351:VAL:HG21	1:C:385:PHE:CE2	2.49	0.47
1:A:379:LEU:HD23	1:A:379:LEU:HA	1.80	0.47
1:D:415:GLU:HG3	1:D:418:MET:HE2	1.96	0.47
1:A:37:LEU:HD21	1:A:46:SER:HB3	1.96	0.47
1:D:220:ASP:OD2	1:D:544:ARG:NH2	2.47	0.47
1:D:319:LEU:HD21	1:D:334:VAL:HG21	1.95	0.47
1:D:422:ARG:CZ	4:D:811:CL:CL	3.00	0.47
1:A:319:LEU:HD21	1:A:334:VAL:HG21	1.96	0.47
1:C:33:ILE:HG22	1:C:37:LEU:HG	1.96	0.47
1:C:255:ASN:O	1:C:257:GLN:N	2.47	0.47
1:A:365:SER:OG	1:A:366:GLU:N	2.48	0.47
1:D:97:ALA:O	1:D:101:TYR:HD2	1.97	0.47
2:H:113:ARG:HB3	2:H:139:TYR:CE2	2.50	0.47
1:A:129[B]:LYS:H	1:A:129[B]:LYS:HG3	1.47	0.47
1:A:347:VAL:O	1:A:351:VAL:HG22	2.14	0.47
1:B:437:MET:HG2	1:B:454:CYS:HA	1.97	0.47
1:A:327:ILE:HG22	1:A:329:SER:H	1.79	0.47
1:B:13:LEU:HD12	1:B:36:LEU:HD21	1.96	0.47
1:D:327:ILE:HG22	1:D:329:SER:H	1.79	0.47
2:E:23:PRO:HD2	2:E:24:GLU:OE2	2.14	0.47
2:F:22:LEU:HD21	6:J:5201:1XE:N4P	2.29	0.47
1:B:365:SER:OG	1:B:366:GLU:N	2.47	0.47
1:D:255:ASN:O	1:D:257:GLN:N	2.47	0.47
1:D:288:LEU:O	1:D:291:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:LEU:HD13	1:B:358:LEU:HA	1.81	0.47
1:B:415:GLU:HG3	1:B:418:MET:HE2	1.97	0.47
1:A:292:TYR:C	1:A:294:LYS:N	2.72	0.47
1:C:362:ASN:HB3	1:C:375:ILE:H	1.80	0.47
1:A:282:LEU:HD21	1:A:306:LEU:HD21	1.96	0.46
1:A:422:ARG:CZ	4:A:810:CL:CL	3.00	0.46
1:B:129[B]:LYS:HE3	1:B:130:ALA:N	2.19	0.46
1:A:593:LYS:NZ	7:A:968:HOH:O	2.43	0.46
1:B:184:THR:HG22	1:B:219:LEU:HD11	1.97	0.46
1:C:163:ALA:O	1:C:167:LYS:HG2	2.15	0.46
1:C:706:ILE:O	1:C:708:GLY:N	2.49	0.46
1:D:292:TYR:C	1:D:294:LYS:N	2.73	0.46
2:F:56:VAL:CG1	2:F:91:LEU:HB3	2.45	0.46
1:A:437:MET:HE2	1:A:450:ILE:HD11	1.97	0.46
1:B:71:LEU:HD13	1:B:80:CYS:HB3	1.97	0.46
1:C:347:VAL:O	1:C:351:VAL:HG22	2.15	0.46
1:C:365:SER:OG	1:C:366:GLU:N	2.48	0.46
1:A:362:ASN:HB3	1:A:375:ILE:H	1.80	0.46
1:C:530:GLN:N	7:C:955:HOH:O	2.30	0.46
1:D:515:ARG:NH2	7:D:963:HOH:O	2.46	0.46
2:H:10:ASP:HA	7:H:308:HOH:O	2.15	0.46
1:A:377:THR:O	1:A:377:THR:OG1	2.28	0.46
1:C:300:ARG:O	1:C:303:LEU:HB2	2.16	0.46
1:D:275:VAL:HA	1:D:276:LEU:HA	1.60	0.46
1:D:377:THR:O	1:D:377:THR:OG1	2.28	0.46
2:E:56:VAL:CG1	2:E:91:LEU:HB3	2.45	0.46
1:A:453:LYS:HA	1:A:453:LYS:HD3	1.79	0.46
1:D:95:VAL:O	1:D:99:LYS:HG3	2.15	0.46
1:A:105:HIS:HD2	7:A:930:HOH:O	1.98	0.46
1:B:460:ARG:HD2	4:B:813:CL:CL	2.53	0.46
1:C:184:THR:CG2	1:C:219:LEU:HD11	2.46	0.46
2:E:113:ARG:HB3	2:E:139:TYR:CE2	2.51	0.46
1:A:95:VAL:O	1:A:99:LYS:HG3	2.16	0.45
1:B:362:ASN:HB3	1:B:375:ILE:H	1.81	0.45
1:C:81:TRP:O	1:C:100:CYS:HB3	2.15	0.45
1:D:363:LYS:NZ	1:D:372:GLN:O	2.43	0.45
1:D:657:GLU:HB2	7:D:960:HOH:O	2.17	0.45
1:A:362:ASN:ND2	1:A:375:ILE:O	2.44	0.45
1:D:362:ASN:HB3	1:D:375:ILE:H	1.81	0.45
1:B:7:SER:HA	1:B:8:PRO:HD3	1.84	0.45
1:B:300:ARG:O	1:B:303:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LYS:HE2	1:D:68:ARG:HH12	1.81	0.45
1:D:12:THR:O	1:D:16:THR:HG23	2.17	0.45
2:F:74:THR:O	3:J:5122:SER:HA	2.16	0.45
1:A:275:VAL:HA	1:A:276:LEU:HA	1.61	0.45
1:B:220:ASP:OD2	1:B:544:ARG:NH2	2.48	0.45
1:B:351:VAL:HG21	1:B:385:PHE:CE2	2.51	0.45
1:B:439:HIS:HD2	4:B:801:CL:CL	2.36	0.45
1:C:248:LEU:HB3	1:C:258:TYR:CE1	2.51	0.45
1:A:45:GLU:O	1:A:49:ILE:HG13	2.16	0.45
1:A:184:THR:HG22	1:A:219:LEU:HD11	1.99	0.45
1:C:422:ARG:CZ	4:C:810:CL:CL	3.01	0.45
1:D:43:HIS:ND1	1:D:46:SER:OG	2.44	0.45
1:A:210:HIS:CE1	1:A:214:ILE:HD13	2.51	0.45
1:D:362:ASN:ND2	1:D:375:ILE:O	2.45	0.45
1:B:476:ARG:NH2	1:B:478:GLU:HG3	2.31	0.45
1:D:694:ASP:OD1	1:D:694:ASP:N	2.50	0.45
1:A:603:GLU:O	1:A:607:ILE:HG12	2.16	0.45
1:A:657:GLU:HA	1:A:658:PRO:HD2	1.82	0.45
1:B:218:VAL:HG21	1:B:224:PHE:CD1	2.52	0.45
1:C:218:VAL:HG21	1:C:224:PHE:CD1	2.52	0.45
1:C:415:GLU:HG3	1:C:418:MET:HE2	1.99	0.45
1:C:534:HIS:ND1	1:C:546:TYR:OH	2.31	0.45
1:D:75:VAL:N	1:D:76:GLY:HA3	2.32	0.45
1:A:496:MET:HE2	1:A:518:THR:CG2	2.47	0.45
1:B:163:ALA:O	1:B:167:LYS:HG2	2.17	0.45
1:A:218:VAL:HG21	1:A:224:PHE:CD1	2.52	0.44
1:A:650:GLU:HA	7:A:962:HOH:O	2.17	0.44
1:D:45:GLU:O	1:D:49:ILE:HG12	2.16	0.44
1:B:292:TYR:C	1:B:294:LYS:N	2.73	0.44
1:D:534:HIS:HD1	1:D:546:TYR:HH	1.58	0.44
2:G:56:VAL:CG1	2:G:91:LEU:HB3	2.47	0.44
2:G:84:HIS:CD2	6:K:5201:1XE:C2A	3.00	0.44
1:B:54:LEU:HD13	1:B:62:GLU:HB3	1.99	0.44
1:C:292:TYR:C	1:C:294:LYS:N	2.73	0.44
1:D:74:ASP:OD2	1:D:77:SER:HB2	2.18	0.44
1:A:657:GLU:O	1:A:657:GLU:HG2	2.18	0.44
1:D:358:LEU:HD13	1:D:358:LEU:HA	1.78	0.44
2:E:78:VAL:H	6:I:5201:1XE:H22	1.65	0.44
1:A:415:GLU:HG3	1:A:418:MET:HE2	2.00	0.44
1:B:63:GLY:O	1:B:67:VAL:HG23	2.17	0.44
1:B:480:VAL:HB	1:B:481:GLY:H	1.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1[B]:MET:CE	2:E:48:PRO:HD3	2.47	0.44
1:A:694:ASP:OD1	1:A:694:ASP:N	2.51	0.44
1:C:52:ILE:HB	1:C:83:ILE:CD1	2.44	0.44
1:C:55:HIS:CD2	1:C:87:ILE:HB	2.53	0.44
1:C:210:HIS:CE1	1:C:214:ILE:HD13	2.52	0.44
2:H:56:VAL:CG1	2:H:91:LEU:HB3	2.47	0.44
1:B:98:ALA:O	1:B:102:ILE:HG12	2.18	0.44
2:E:1[B]:MET:HE2	2:E:47:ASP:HA	1.99	0.44
1:B:478:GLU:HG2	1:B:478:GLU:H	1.41	0.44
1:B:372:GLN:HB3	1:B:373:ILE:H	1.63	0.43
2:F:113:ARG:HB3	2:F:139:TYR:CE2	2.52	0.43
2:H:11:LEU:HD22	2:H:31:TYR:HB3	1.99	0.43
1:B:363:LYS:HA	1:B:363:LYS:HD2	1.83	0.43
1:C:460:ARG:HD2	7:C:954:HOH:O	2.16	0.43
1:D:657:GLU:HA	1:D:658:PRO:HD2	1.83	0.43
1:B:58:GLY:HA2	1:B:59:ASN:HA	1.50	0.43
1:D:218:VAL:HG21	1:D:224:PHE:CD1	2.53	0.43
1:C:18:LEU:HD21	1:C:49:ILE:HD12	2.00	0.43
1:C:79:VAL:O	1:C:83:ILE:HG22	2.19	0.43
1:C:220:ASP:OD2	1:C:544:ARG:NH2	2.49	0.43
1:C:657:GLU:HA	1:C:658:PRO:HD2	1.81	0.43
1:D:84:PHE:O	1:D:88:SER:OG	2.20	0.43
1:D:210:HIS:CE1	1:D:214:ILE:HD13	2.53	0.43
2:F:11:LEU:HD22	2:F:31:TYR:HB3	1.99	0.43
2:G:30:TYR:CZ	2:G:34:HIS:HE1	2.36	0.43
1:A:149:TRP:CE3	1:A:172:PHE:HB2	2.53	0.43
1:A:249:LEU:CD1	1:A:258:TYR:HB3	2.48	0.43
1:C:200:LYS:HD2	1:C:200:LYS:HA	1.89	0.43
1:B:275:VAL:HA	1:B:276:LEU:HA	1.61	0.43
1:C:480:VAL:HB	1:C:481:GLY:H	1.56	0.43
1:A:240:GLU:HB2	7:A:957:HOH:O	2.17	0.43
1:C:98:ALA:O	1:C:102:ILE:HG12	2.18	0.43
1:C:275:VAL:HA	1:C:276:LEU:HA	1.62	0.43
1:A:26:TYR:CZ	1:A:56:SER:HB3	2.54	0.43
1:D:54:LEU:HD13	1:D:62:GLU:HG3	1.99	0.43
1:D:291:ARG:O	1:D:292:TYR:C	2.62	0.43
1:A:13:LEU:HB3	1:A:36:LEU:HD11	2.01	0.43
1:A:255:ASN:O	1:A:257:GLN:N	2.51	0.43
1:C:282:LEU:HD23	1:C:282:LEU:HA	1.90	0.43
1:C:415:GLU:OE1	2:G:80:ARG:HD3	2.19	0.43
1:C:442:LYS:NZ	7:C:916:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD12	1:A:53:LEU:HA	1.76	0.43
1:B:657:GLU:HA	1:B:658:PRO:HD2	1.83	0.43
1:C:372:GLN:HB3	1:C:373:ILE:H	1.63	0.43
1:D:709:GLN:HE21	1:D:709:GLN:HB3	1.61	0.43
1:A:293:PRO:C	1:A:295:SER:H	2.27	0.42
1:A:657:GLU:HB2	7:A:979:HOH:O	2.19	0.42
1:B:379:LEU:HD23	1:B:379:LEU:HA	1.79	0.42
1:C:583:LYS:H	1:C:583:LYS:HG3	1.62	0.42
1:D:93:ASP:CG	1:D:96:GLN:HB2	2.44	0.42
1:D:129:LYS:HE3	4:D:806:CL:CL	2.56	0.42
1:D:657:GLU:N	1:D:657:GLU:OE2	2.52	0.42
1:C:492:CYS:O	1:C:496:MET:HG2	2.20	0.42
2:G:11:LEU:HD22	2:G:31:TYR:HB3	2.00	0.42
1:A:448:ARG:HH11	2:E:23:PRO:HA	1.83	0.42
1:A:709:GLN:HE21	1:A:709:GLN:HB3	1.62	0.42
1:B:248:LEU:HB3	1:B:258:TYR:CE1	2.54	0.42
1:C:208:TYR:HB2	7:C:941:HOH:O	2.20	0.42
1:C:514:LYS:NZ	1:C:645:GLU:OE1	2.23	0.42
1:D:300:ARG:O	1:D:303:LEU:HB2	2.19	0.42
1:D:334:VAL:HG13	1:D:337:LEU:HD12	2.01	0.42
1:D:607:ILE:O	1:D:611:LEU:HG	2.19	0.42
1:A:105:HIS:CD2	7:A:930:HOH:O	2.71	0.42
1:A:291:ARG:O	1:A:292:TYR:C	2.63	0.42
1:A:300:ARG:O	1:A:303:LEU:HB2	2.20	0.42
1:A:607:ILE:O	1:A:611:LEU:HG	2.20	0.42
1:D:626:LYS:HG2	1:D:648:LEU:HD23	2.01	0.42
2:E:55:TYR:OH	2:E:75:SER:OG	2.35	0.42
2:H:121:HIS:HB3	6:L:5201:1XE:C8A	2.49	0.42
1:B:57:LEU:CD1	1:B:58:GLY:H	2.26	0.42
1:D:184:THR:HG22	1:D:219:LEU:HD11	2.02	0.42
1:D:657:GLU:O	1:D:657:GLU:HG2	2.20	0.42
1:B:405:LEU:HD23	1:B:405:LEU:HA	1.90	0.42
1:C:184:THR:HG22	1:C:219:LEU:HD11	2.01	0.42
1:C:354:TYR:O	1:C:358:LEU:HB2	2.19	0.42
2:H:112:VAL:HG23	2:H:146:TYR:HB2	2.01	0.42
1:A:437:MET:HE2	1:A:450:ILE:CD1	2.49	0.42
1:C:673:GLY:HA3	1:C:680:TYR:CZ	2.55	0.42
1:D:437:MET:HE2	1:D:450:ILE:HD11	2.02	0.42
1:D:591:PHE:O	1:D:595:SER:HB2	2.19	0.42
2:F:112:VAL:HG23	2:F:146:TYR:HB2	2.02	0.42
1:B:249:LEU:CD1	1:B:258:TYR:HB3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:GLU:O	1:B:607:ILE:HG12	2.20	0.42
1:A:353:LYS:HB3	1:A:353:LYS:HE2	1.79	0.42
1:C:71:LEU:HD11	1:C:81:TRP:CE2	2.55	0.42
1:C:591:PHE:O	1:C:595:SER:HB2	2.19	0.42
1:D:318:TYR:OH	1:D:333:ASP:OD2	2.26	0.42
2:E:112:VAL:HG23	2:E:146:TYR:HB2	2.01	0.42
2:G:112:VAL:HG23	2:G:146:TYR:HB2	2.02	0.42
1:B:105:HIS:CD2	7:B:913:HOH:O	2.70	0.42
1:D:47:LEU:HB3	1:D:66:ASN:O	2.20	0.41
1:B:60:THR:O	1:B:63:GLY:N	2.51	0.41
1:D:37:LEU:HD21	1:D:46:SER:HB3	2.01	0.41
2:E:1[A]:MET:HB3	2:E:1[A]:MET:HE3	1.85	0.41
2:H:30:TYR:CE1	2:H:34:HIS:HE1	2.37	0.41
1:B:129[B]:LYS:H	1:B:129[B]:LYS:HG3	1.47	0.41
1:B:657:GLU:OE2	1:B:657:GLU:N	2.54	0.41
1:D:7:SER:HA	1:D:8:PRO:HD3	1.78	0.41
1:A:657:GLU:N	1:A:657:GLU:OE2	2.53	0.41
1:B:149:TRP:CE3	1:B:172:PHE:HB2	2.54	0.41
1:C:405:LEU:HD23	1:C:405:LEU:HA	1.91	0.41
1:A:701:GLU:O	1:A:705:VAL:HG23	2.20	0.41
1:B:37:LEU:HD23	1:B:37:LEU:N	2.35	0.41
1:B:354:TYR:O	1:B:358:LEU:HB2	2.20	0.41
1:B:493:LEU:HD12	1:B:493:LEU:HA	1.88	0.41
1:D:13:LEU:HD22	1:D:32:ALA:HB1	2.03	0.41
1:D:249:LEU:CD1	1:D:258:TYR:HB3	2.50	0.41
1:D:508:LYS:NZ	7:D:952:HOH:O	2.53	0.41
2:E:21:ASN:HB3	6:I:5201:1XE:H24	2.02	0.41
1:A:348:GLU:HB2	1:A:389:HIS:NE2	2.36	0.41
1:C:181:PRO:HA	1:C:182:VAL:CG2	2.45	0.41
1:C:404:ASP:OD1	1:C:420:LYS:NZ	2.50	0.41
1:C:493:LEU:HD12	1:C:493:LEU:HA	1.90	0.41
2:H:8:ILE:HD13	2:H:8:ILE:HA	1.91	0.41
1:B:146:ARG:HB2	1:B:172:PHE:CZ	2.56	0.41
1:C:159:ARG:NH1	1:C:161:GLU:HG3	2.35	0.41
1:D:181:PRO:HA	1:D:182:VAL:CG2	2.46	0.41
1:D:347:VAL:O	1:D:351:VAL:HG22	2.21	0.41
1:D:405:LEU:HD23	1:D:405:LEU:HA	1.85	0.41
2:F:62:GLU:O	2:F:64:PRO:HD3	2.20	0.41
2:H:60:MET:HE3	2:H:60:MET:HB3	1.92	0.41
1:A:181:PRO:HA	1:A:182:VAL:CG2	2.46	0.41
1:B:210:HIS:CE1	1:B:214:ILE:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ASN:ND2	1:B:375:ILE:O	2.46	0.41
1:B:511:LEU:HD12	1:B:511:LEU:HA	1.85	0.41
1:C:362:ASN:ND2	1:C:375:ILE:O	2.46	0.41
2:H:30:TYR:CZ	2:H:34:HIS:HE1	2.38	0.41
1:A:29:GLY:O	1:A:33:ILE:HG13	2.21	0.41
1:A:529:ASP:N	7:A:914:HOH:O	2.53	0.41
1:B:135:ARG:CD	1:B:151:ALA:HB1	2.51	0.41
1:B:591:PHE:O	1:B:595:SER:HB2	2.20	0.41
1:B:701:GLU:O	1:B:705:VAL:HG23	2.21	0.41
1:C:324:LYS:HG2	1:C:375:ILE:HD13	2.03	0.41
1:C:454:CYS:SG	1:C:458:MET:HE3	2.61	0.41
1:D:293:PRO:C	1:D:295:SER:H	2.28	0.41
1:D:437:MET:HE2	1:D:450:ILE:CD1	2.51	0.41
1:D:496:MET:HE2	1:D:518:THR:CG2	2.50	0.41
2:E:11:LEU:HD22	2:E:31:TYR:HB3	2.02	0.41
2:G:62:GLU:O	2:G:64:PRO:HD3	2.20	0.41
2:H:38:TRP:CZ3	2:H:59:LYS:HB2	2.56	0.41
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.98	0.41
1:B:26:TYR:HD2	1:B:57:LEU:HD23	1.86	0.41
1:B:425:LYS:NZ	4:B:814:CL:CL	2.68	0.41
1:C:26:TYR:CZ	1:C:56:SER:HB3	2.56	0.41
1:D:29:GLY:O	1:D:33:ILE:HG13	2.21	0.41
2:F:15:GLN:HG3	2:F:31:TYR:CE1	2.56	0.41
1:A:182:VAL:HG23	1:A:184:THR:H	1.86	0.40
1:C:249:LEU:CD1	1:C:258:TYR:HB3	2.52	0.40
1:C:453:LYS:HD3	1:C:453:LYS:HA	1.80	0.40
1:C:603:GLU:O	1:C:607:ILE:HG12	2.22	0.40
2:F:30:TYR:CZ	2:F:34:HIS:HE1	2.39	0.40
1:B:324:LYS:HG2	1:B:375:ILE:HD13	2.03	0.40
1:B:12:THR:O	1:B:16:THR:HG23	2.21	0.40
1:B:17:ALA:CB	1:B:33:ILE:HD13	2.52	0.40
1:B:37:LEU:HD22	1:B:46:SER:HB3	2.02	0.40
1:B:501:LYS:NZ	1:B:564:GLU:OE1	2.42	0.40
1:D:324:LYS:HG2	1:D:375:ILE:HD13	2.04	0.40
1:D:379:LEU:HA	1:D:379:LEU:HD23	1.81	0.40
2:E:47:ASP:HB2	2:E:48:PRO:HD2	2.04	0.40
1:B:129[A]:LYS:HD2	1:B:129[A]:LYS:N	2.34	0.40
1:B:179:GLY:HA3	1:B:180:VAL:HA	1.62	0.40
1:B:492:CYS:O	1:B:496:MET:HG2	2.22	0.40
1:B:706:ILE:C	1:B:708:GLY:H	2.30	0.40
1:C:7:SER:HA	1:C:8:PRO:HD3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:LEU:HD11	1:D:149:TRP:CE2	2.57	0.40
7:F:305:HOH:O	3:J:5122:SER:HB2	2.21	0.40
1:A:163:ALA:O	1:A:167:LYS:HG2	2.21	0.40
1:B:181:PRO:HA	1:B:182:VAL:CG2	2.46	0.40
1:C:698:LYS:HG3	1:C:699:TYR:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:ALA:O	7:G:304:HOH:O[1_556]	2.08	0.12

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	717/734 (98%)	658 (92%)	46 (6%)	13 (2%)	6	14
1	B	719/734 (98%)	660 (92%)	45 (6%)	14 (2%)	6	13
1	C	714/734 (97%)	660 (92%)	42 (6%)	12 (2%)	7	15
1	D	715/734 (97%)	657 (92%)	43 (6%)	15 (2%)	5	11
2	E	151/156 (97%)	144 (95%)	7 (5%)	0	100	100
2	F	151/156 (97%)	147 (97%)	4 (3%)	0	100	100
2	G	151/156 (97%)	146 (97%)	5 (3%)	0	100	100
2	H	151/156 (97%)	145 (96%)	6 (4%)	0	100	100
3	I	2/4 (50%)	2 (100%)	0	0	100	100
3	J	2/4 (50%)	2 (100%)	0	0	100	100
3	K	2/4 (50%)	2 (100%)	0	0	100	100
3	L	2/4 (50%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3477/3576 (97%)	3225 (93%)	198 (6%)	54 (2%)	7	16

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	VAL
1	A	184	THR
1	A	256	HIS
1	A	293	PRO
1	A	358	LEU
1	A	373	ILE
1	B	182	VAL
1	B	256	HIS
1	B	293	PRO
1	B	373	ILE
1	C	182	VAL
1	C	256	HIS
1	C	293	PRO
1	C	373	ILE
1	D	25	GLN
1	D	182	VAL
1	D	184	THR
1	D	256	HIS
1	D	373	ILE
1	A	647	PRO
1	B	184	THR
1	B	358	LEU
1	B	647	PRO
1	C	184	THR
1	C	358	LEU
1	C	647	PRO
1	D	61	LYS
1	D	293	PRO
1	D	358	LEU
1	D	647	PRO
1	A	376	PRO
1	B	60	THR
1	B	376	PRO
1	C	77	SER
1	C	376	PRO
1	D	59	ASN
1	D	376	PRO

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Mol	Chain	Res	Type
1	D	6	LEU
1	A	77	SER
1	B	649	GLY
1	C	649	GLY
1	A	25	GLN
1	A	649	GLY
1	B	3	LYS
1	B	77	SER
1	D	649	GLY
1	A	480	VAL
1	B	480	VAL
1	C	480	VAL
1	D	480	VAL
1	A	292	TYR
1	D	292	TYR
1	B	292	TYR
1	C	292	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	611/638 (96%)	554 (91%)	57 (9%)	8	18
1	B	610/638 (96%)	550 (90%)	60 (10%)	7	17
1	C	609/638 (96%)	557 (92%)	52 (8%)	10	22
1	D	610/638 (96%)	558 (92%)	52 (8%)	10	22
2	E	133/135 (98%)	117 (88%)	16 (12%)	5	10
2	F	132/135 (98%)	117 (89%)	15 (11%)	5	11
2	G	132/135 (98%)	118 (89%)	14 (11%)	6	14
2	H	132/135 (98%)	117 (89%)	15 (11%)	5	11
3	I	3/3 (100%)	3 (100%)	0	100	100
3	J	3/3 (100%)	2 (67%)	1 (33%)	0	0
3	K	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	3/3 (100%)	3 (100%)	0	100	100
All	All	2981/3104 (96%)	2699 (90%)	282 (10%)	8	18

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	CYS
1	A	37	LEU
1	A	53	LEU
1	A	57	LEU
1	A	60	THR
1	A	61	LYS
1	A	72	ARG
1	A	83	ILE
1	A	95	VAL
1	A	96	GLN
1	A	120	LEU
1	A	129[A]	LYS
1	A	129[B]	LYS
1	A	131	LEU
1	A	135	ARG
1	A	145	VAL
1	A	146[A]	ARG
1	A	146[B]	ARG
1	A	176	ILE
1	A	182	VAL
1	A	184	THR
1	A	277	ASP
1	A	284	LEU
1	A	288	LEU
1	A	291	ARG
1	A	292	TYR
1	A	303	LEU
1	A	307	GLU
1	A	323	LEU
1	A	358	LEU
1	A	361	THR
1	A	372	GLN
1	A	375	ILE
1	A	377	THR
1	A	378	THR
1	A	380	LEU

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Mol	Chain	Res	Type
1	A	403	VAL
1	A	409	HIS
1	A	410	THR
1	A	445	LEU
1	A	446	GLN
1	A	459	LEU
1	A	465	GLU
1	A	480	VAL
1	A	493	LEU
1	A	497	LEU
1	A	511	LEU
1	A	513	LEU
1	A	547	LEU
1	A	583	LYS
1	A	600	ASN
1	A	669	LEU
1	A	690	LEU
1	A	698	LYS
1	A	707	LEU
1	A	709	GLN
1	A	727	GLN
1	B	7	SER
1	B	30	LEU
1	B	37	LEU
1	B	38	GLU
1	B	49	ILE
1	B	53	LEU
1	B	56	SER
1	B	57	LEU
1	B	60	THR
1	B	61	LYS
1	B	72	ARG
1	B	83	ILE
1	B	95	VAL
1	B	120	LEU
1	B	129[A]	LYS
1	B	129[B]	LYS
1	B	131	LEU
1	B	135	ARG
1	B	145	VAL
1	B	146	ARG
1	B	159	ARG

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Mol	Chain	Res	Type
1	B	176	ILE
1	B	182	VAL
1	B	184	THR
1	B	277	ASP
1	B	284	LEU
1	B	288	LEU
1	B	291	ARG
1	B	303	LEU
1	B	307	GLU
1	B	323	LEU
1	B	358	LEU
1	B	361	THR
1	B	372	GLN
1	B	375	ILE
1	B	377	THR
1	B	378	THR
1	B	380	LEU
1	B	403	VAL
1	B	409	HIS
1	B	410	THR
1	B	445	LEU
1	B	446	GLN
1	B	459	LEU
1	B	465	GLU
1	B	478	GLU
1	B	480	VAL
1	B	493	LEU
1	B	497	LEU
1	B	511	LEU
1	B	513	LEU
1	B	547	LEU
1	B	583	LYS
1	B	600	ASN
1	B	659	LEU
1	B	669	LEU
1	B	690	LEU
1	B	698	LYS
1	B	707	LEU
1	B	727	GLN
1	C	37	LEU
1	C	38	GLU
1	C	53	LEU

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Mol	Chain	Res	Type
1	C	57	LEU
1	C	61	LYS
1	C	72	ARG
1	C	74	ASP
1	C	83	ILE
1	C	96	GLN
1	C	120	LEU
1	C	129	LYS
1	C	131	LEU
1	C	135	ARG
1	C	145	VAL
1	C	176	ILE
1	C	182	VAL
1	C	184	THR
1	C	277	ASP
1	C	284	LEU
1	C	288	LEU
1	C	291	ARG
1	C	303	LEU
1	C	307	GLU
1	C	323	LEU
1	C	358	LEU
1	C	361	THR
1	C	372	GLN
1	C	375	ILE
1	C	377	THR
1	C	378	THR
1	C	380	LEU
1	C	403	VAL
1	C	409	HIS
1	C	410	THR
1	C	445	LEU
1	C	446	GLN
1	C	459	LEU
1	C	465	GLU
1	C	480	VAL
1	C	493	LEU
1	C	497	LEU
1	C	511	LEU
1	C	513	LEU
1	C	547	LEU
1	C	583	LYS

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Mol	Chain	Res	Type
1	C	600	ASN
1	C	669	LEU
1	C	681	ILE
1	C	690	LEU
1	C	698	LYS
1	C	707	LEU
1	C	727	GLN
1	D	11	ILE
1	D	20	CYS
1	D	24	LYS
1	D	37	LEU
1	D	38	GLU
1	D	57	LEU
1	D	61	LYS
1	D	96	GLN
1	D	120	LEU
1	D	129	LYS
1	D	131	LEU
1	D	135	ARG
1	D	145	VAL
1	D	176	ILE
1	D	182	VAL
1	D	184	THR
1	D	284	LEU
1	D	288	LEU
1	D	291	ARG
1	D	292	TYR
1	D	303	LEU
1	D	307	GLU
1	D	323	LEU
1	D	358	LEU
1	D	361	THR
1	D	372	GLN
1	D	375	ILE
1	D	377	THR
1	D	378	THR
1	D	380	LEU
1	D	403	VAL
1	D	409	HIS
1	D	410	THR
1	D	445	LEU
1	D	446	GLN

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Mol	Chain	Res	Type
1	D	459	LEU
1	D	465	GLU
1	D	480	VAL
1	D	493	LEU
1	D	497	LEU
1	D	511	LEU
1	D	513	LEU
1	D	547	LEU
1	D	583	LYS
1	D	600	ASN
1	D	669	LEU
1	D	681	ILE
1	D	690	LEU
1	D	698	LYS
1	D	707	LEU
1	D	709	GLN
1	D	727	GLN
2	E	1[A]	MET
2	E	1[B]	MET
2	E	3	ILE
2	E	24	GLU
2	E	27	GLN
2	E	32	LEU
2	E	44	VAL
2	E	53	VAL
2	E	56	VAL
2	E	57	LEU
2	E	72	HIS
2	E	74	THR
2	E	76	VAL
2	E	81	SER
2	E	87	LEU
2	E	148	MET
2	F	1	MET
2	F	3	ILE
2	F	24	GLU
2	F	27	GLN
2	F	32	LEU
2	F	44	VAL
2	F	53	VAL
2	F	56	VAL
2	F	57	LEU

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Mol	Chain	Res	Type
2	F	72	HIS
2	F	74	THR
2	F	76	VAL
2	F	81	SER
2	F	87	LEU
2	F	148	MET
2	G	3	ILE
2	G	24	GLU
2	G	27	GLN
2	G	32	LEU
2	G	44	VAL
2	G	53	VAL
2	G	56	VAL
2	G	57	LEU
2	G	72	HIS
2	G	74	THR
2	G	76	VAL
2	G	81	SER
2	G	87	LEU
2	G	148	MET
2	H	1	MET
2	H	3	ILE
2	H	24	GLU
2	H	27	GLN
2	H	32	LEU
2	H	44	VAL
2	H	53	VAL
2	H	56	VAL
2	H	57	LEU
2	H	72	HIS
2	H	74	THR
2	H	76	VAL
2	H	81	SER
2	H	87	LEU
2	H	148	MET
3	J	5125	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	111	ASN

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Mol	Chain	Res	Type
1	A	255	ASN
1	A	263	GLN
1	A	388	GLN
1	A	600	ASN
1	A	663	GLN
1	A	685	GLN
1	A	709	GLN
1	B	66	ASN
1	B	105	HIS
1	B	111	ASN
1	B	255	ASN
1	B	263	GLN
1	B	439	HIS
1	B	600	ASN
1	B	663	GLN
1	C	111	ASN
1	C	255	ASN
1	C	256	HIS
1	C	263	GLN
1	C	287	GLN
1	C	600	ASN
1	C	663	GLN
1	D	25	GLN
1	D	96	GLN
1	D	111	ASN
1	D	255	ASN
1	D	263	GLN
1	D	600	ASN
1	D	663	GLN
1	D	709	GLN
2	E	27	GLN
2	F	27	GLN
2	G	27	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 64 are monoatomic - leaving 6 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$
6	1XE	I	5201	3	47,53,54	2.42	15 (31%)	62,78,80	3.11	23 (37%)
5	SO4	A	815	-	4,4,4	0.31	0	6,6,6	0.17	0
6	1XE	L	5201	3	47,53,54	2.39	12 (25%)	62,78,80	2.50	21 (33%)
6	1XE	J	5201	3	47,53,54	2.39	16 (34%)	62,78,80	2.63	22 (35%)
5	SO4	D	816	-	4,4,4	0.30	0	6,6,6	0.21	0
6	1XE	K	5201	3	47,53,54	2.42	13 (27%)	62,78,80	2.58	20 (32%)

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
6	1XE	J	5201	3	-	18/45/51/52	0/3/3/3
6	1XE	I	5201	3	-	18/45/51/52	0/3/3/3
6	1XE	L	5201	3	-	19/45/51/52	0/3/3/3
6	1XE	K	5201	3	-	19/45/51/52	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	5201	1XE	C3P-C2P	8.20	1.50	1.31
6	K	5201	1XE	C3P-C2P	8.00	1.50	1.31
6	I	5201	1XE	C3P-C2P	7.86	1.50	1.31
6	J	5201	1XE	C3P-C2P	7.48	1.49	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	5201	1XE	C9P-N8P	6.36	1.48	1.33
6	K	5201	1XE	C9P-N8P	6.31	1.48	1.33
6	J	5201	1XE	C9P-N8P	6.29	1.48	1.33
6	I	5201	1XE	C5P-N4P	6.17	1.48	1.37
6	L	5201	1XE	C5P-N4P	6.15	1.48	1.37
6	I	5201	1XE	C9P-N8P	6.10	1.47	1.33
6	J	5201	1XE	C5P-N4P	5.88	1.48	1.37
6	K	5201	1XE	C5P-N4P	5.72	1.47	1.37
6	K	5201	1XE	C6A-N6A	4.64	1.46	1.34
6	L	5201	1XE	C6A-N6A	4.29	1.45	1.34
6	I	5201	1XE	C6A-N6A	4.22	1.45	1.34
6	J	5201	1XE	C6A-N6A	4.20	1.44	1.34
6	I	5201	1XE	C3P-N4P	3.69	1.50	1.40
6	K	5201	1XE	O4B-C4B	-3.42	1.30	1.38
6	J	5201	1XE	C3P-N4P	3.37	1.49	1.40
6	J	5201	1XE	O4B-C4B	-3.36	1.30	1.38
6	J	5201	1XE	CDP-CBP	-3.34	1.46	1.53
6	L	5201	1XE	C3P-N4P	3.30	1.49	1.40
6	K	5201	1XE	O5B-C5B	3.28	1.46	1.43
6	K	5201	1XE	C3P-N4P	3.23	1.49	1.40
6	K	5201	1XE	O2B-C2B	3.22	1.44	1.33
6	L	5201	1XE	O5B-C5B	3.21	1.46	1.43
6	L	5201	1XE	O2B-C2B	3.18	1.44	1.33
6	I	5201	1XE	CDP-CBP	-3.16	1.47	1.53
6	J	5201	1XE	O5B-C5B	3.14	1.46	1.43
6	L	5201	1XE	CDP-CBP	-3.12	1.47	1.53
6	I	5201	1XE	O2B-C2B	3.11	1.44	1.33
6	I	5201	1XE	O4B-C4B	-3.10	1.31	1.38
6	J	5201	1XE	O2B-C2B	3.08	1.44	1.33
6	K	5201	1XE	CDP-CBP	-3.01	1.47	1.53
6	I	5201	1XE	C8A-N9A	-2.92	1.33	1.37
6	K	5201	1XE	P2A-O3A	-2.86	1.56	1.59
6	I	5201	1XE	O5B-C5B	2.80	1.46	1.43
6	K	5201	1XE	C4A-N9A	-2.65	1.36	1.39
6	K	5201	1XE	C8A-N9A	-2.64	1.33	1.37
6	L	5201	1XE	O4B-C4B	-2.62	1.32	1.38
6	J	5201	1XE	O4B-C1B	-2.52	1.31	1.37
6	I	5201	1XE	O5P-C5P	2.51	1.28	1.23
6	L	5201	1XE	C3B-C4B	2.45	1.40	1.35
6	J	5201	1XE	C1-S1P	-2.45	1.73	1.81
6	L	5201	1XE	C8A-N9A	-2.43	1.34	1.37
6	J	5201	1XE	P2A-O4A	2.43	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	5201	1XE	C3B-C4B	2.41	1.39	1.35
6	I	5201	1XE	P2A-O4A	2.37	1.59	1.50
6	J	5201	1XE	C8A-N9A	-2.35	1.34	1.37
6	L	5201	1XE	P2A-O4A	2.21	1.58	1.50
6	J	5201	1XE	C4A-N9A	-2.21	1.37	1.39
6	I	5201	1XE	O4B-C1B	-2.15	1.32	1.37
6	I	5201	1XE	C5A-N7A	-2.09	1.35	1.39
6	J	5201	1XE	O5P-C5P	2.07	1.27	1.23
6	K	5201	1XE	P2A-O4A	2.07	1.58	1.50
6	I	5201	1XE	P3B-O3B	-2.04	1.56	1.59

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	5201	1XE	N9A-C8A-N7A	-10.48	107.92	113.88
6	J	5201	1XE	N9A-C8A-N7A	-9.42	108.52	113.88
6	K	5201	1XE	N9A-C8A-N7A	-9.07	108.72	113.88
6	L	5201	1XE	N9A-C8A-N7A	-8.17	109.23	113.88
6	J	5201	1XE	C4A-N9A-C8A	8.14	109.14	105.35
6	I	5201	1XE	C7P-C6P-C5P	8.00	125.72	112.39
6	I	5201	1XE	C4A-N9A-C8A	7.98	109.06	105.35
6	I	5201	1XE	C7P-N8P-C9P	-7.75	108.62	122.55
6	L	5201	1XE	C4A-N9A-C8A	6.91	108.57	105.35
6	K	5201	1XE	C4A-N9A-C8A	6.31	108.29	105.35
6	I	5201	1XE	C6P-C7P-N8P	6.25	125.31	112.00
6	K	5201	1XE	C4B-O4B-C1B	6.17	112.72	106.16
6	I	5201	1XE	C5A-C4A-N3A	-5.93	118.56	126.72
6	L	5201	1XE	C6P-C7P-N8P	5.69	124.11	112.00
6	K	5201	1XE	O6A-CCP-CBP	5.22	118.94	110.55
6	J	5201	1XE	C4B-O4B-C1B	5.16	111.65	106.16
6	K	5201	1XE	C5A-C4A-N3A	-5.14	119.65	126.72
6	J	5201	1XE	C3P-N4P-C5P	-5.04	113.78	123.48
6	L	5201	1XE	C5A-C4A-N3A	-4.93	119.93	126.72
6	K	5201	1XE	C5A-C4A-N9A	4.77	107.59	105.06
6	I	5201	1XE	N3A-C4A-N9A	4.76	135.30	126.38
6	J	5201	1XE	C5A-C4A-N3A	-4.68	120.27	126.72
6	I	5201	1XE	C4B-O4B-C1B	4.44	110.88	106.16
6	J	5201	1XE	N3A-C2A-N1A	-4.35	122.00	128.58
6	I	5201	1XE	N3A-C2A-N1A	-4.32	122.05	128.58
6	J	5201	1XE	C6P-C5P-N4P	4.30	123.49	114.96
6	I	5201	1XE	C6P-C5P-N4P	4.22	123.32	114.96
6	I	5201	1XE	C5A-N7A-C8A	4.19	110.04	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	5201	1XE	C6P-C5P-N4P	4.11	123.12	114.96
6	L	5201	1XE	N3A-C2A-N1A	-4.11	122.36	128.58
6	J	5201	1XE	O6A-CCP-CBP	3.97	116.93	110.55
6	L	5201	1XE	CDP-CBP-CCP	3.95	114.74	108.22
6	I	5201	1XE	O6A-CCP-CBP	3.90	116.82	110.55
6	L	5201	1XE	N3A-C4A-N9A	3.84	133.58	126.38
6	L	5201	1XE	C4B-O4B-C1B	3.79	110.20	106.16
6	J	5201	1XE	CDP-CBP-CAP	3.77	115.20	108.77
6	K	5201	1XE	C6P-C5P-N4P	3.77	122.43	114.96
6	L	5201	1XE	C7P-N8P-C9P	-3.70	115.89	122.55
6	J	5201	1XE	N3A-C4A-N9A	3.70	133.32	126.38
6	K	5201	1XE	C4A-C5A-N7A	-3.62	106.45	110.58
6	I	5201	1XE	C2A-N3A-C4A	3.62	120.66	111.83
6	K	5201	1XE	C5A-N7A-C8A	3.49	108.94	103.45
6	K	5201	1XE	C4A-N9A-C1B	-3.49	121.81	128.49
6	I	5201	1XE	O5P-C5P-N4P	-3.47	115.90	122.43
6	K	5201	1XE	N3A-C4A-N9A	3.41	132.76	126.38
6	L	5201	1XE	C1-S1P-C2P	3.40	112.24	100.75
6	K	5201	1XE	C1-S1P-C2P	3.36	112.11	100.75
6	K	5201	1XE	N3A-C2A-N1A	-3.33	123.53	128.58
6	K	5201	1XE	C3P-N4P-C5P	-3.31	117.11	123.48
6	K	5201	1XE	C2A-N3A-C4A	3.30	119.88	111.83
6	J	5201	1XE	C5A-N7A-C8A	3.28	108.61	103.45
6	K	5201	1XE	P3B-O3B-C3B	-3.28	115.88	123.01
6	I	5201	1XE	C4A-C5A-N7A	-3.28	106.83	110.58
6	J	5201	1XE	C2A-N3A-C4A	3.27	119.81	111.83
6	L	5201	1XE	C2A-N3A-C4A	3.25	119.76	111.83
6	I	5201	1XE	CAP-C9P-N8P	3.21	122.58	116.48
6	L	5201	1XE	C5A-N7A-C8A	3.11	108.34	103.45
6	L	5201	1XE	O5P-C5P-N4P	-3.10	116.60	122.43
6	L	5201	1XE	C3P-N4P-C5P	-2.99	117.74	123.48
6	I	5201	1XE	P3B-O3B-C3B	-2.88	116.76	123.01
6	J	5201	1XE	C4A-C5A-N7A	-2.86	107.31	110.58
6	L	5201	1XE	C4A-C5A-N7A	-2.82	107.36	110.58
6	L	5201	1XE	O5A-P2A-O3A	2.77	114.77	107.27
6	L	5201	1XE	C5A-C4A-N9A	2.69	106.49	105.06
6	I	5201	1XE	C1-S1P-C2P	2.68	109.80	100.75
6	J	5201	1XE	CEP-CBP-CDP	-2.64	103.94	109.20
6	K	5201	1XE	O5P-C5P-N4P	-2.62	117.50	122.43
6	J	5201	1XE	O5P-C5P-N4P	-2.58	117.58	122.43
6	J	5201	1XE	C5A-C4A-N9A	2.54	106.41	105.06
6	K	5201	1XE	CDP-CBP-CCP	2.35	112.11	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	5201	1XE	O21-C2-C1	2.35	120.01	110.82
6	J	5201	1XE	CAP-C9P-N8P	2.29	120.82	116.48
6	J	5201	1XE	CDP-CBP-CCP	2.22	111.89	108.22
6	K	5201	1XE	C7P-C6P-C5P	2.20	116.05	112.39
6	L	5201	1XE	CDP-CBP-CAP	2.19	112.50	108.77
6	I	5201	1XE	C3B-C2B-C1B	-2.15	104.38	107.45
6	K	5201	1XE	O4B-C1B-C2B	-2.14	107.54	110.95
6	I	5201	1XE	O9P-C9P-N8P	-2.14	118.45	122.98
6	J	5201	1XE	C7P-N8P-C9P	-2.14	118.70	122.55
6	L	5201	1XE	C2-C1-S1P	2.13	121.57	112.33
6	L	5201	1XE	C7P-C6P-C5P	2.08	115.85	112.39
6	I	5201	1XE	CDP-CBP-CCP	2.07	111.65	108.22
6	J	5201	1XE	C1-S1P-C2P	2.05	107.68	100.75
6	J	5201	1XE	C4A-N9A-C1B	-2.05	124.57	128.49
6	I	5201	1XE	C5A-C4A-N9A	2.04	106.14	105.06
6	I	5201	1XE	C3P-N4P-C5P	-2.00	119.63	123.48

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	5201	1XE	C4B-C5B-O5B-P1A
6	I	5201	1XE	C5B-O5B-P1A-O1A
6	I	5201	1XE	C5B-O5B-P1A-O2A
6	I	5201	1XE	C5B-O5B-P1A-O3A
6	I	5201	1XE	CDP-CBP-CCP-O6A
6	I	5201	1XE	CAP-CBP-CCP-O6A
6	I	5201	1XE	C5P-C6P-C7P-N8P
6	I	5201	1XE	C2P-C3P-N4P-C5P
6	J	5201	1XE	C3B-C4B-C5B-O5B
6	J	5201	1XE	O4B-C4B-C5B-O5B
6	J	5201	1XE	C5B-O5B-P1A-O1A
6	J	5201	1XE	C5B-O5B-P1A-O2A
6	J	5201	1XE	C5B-O5B-P1A-O3A
6	J	5201	1XE	CCP-O6A-P2A-O3A
6	J	5201	1XE	CCP-O6A-P2A-O4A
6	J	5201	1XE	C9P-CAP-CBP-CCP
6	J	5201	1XE	C9P-CAP-CBP-CEP
6	J	5201	1XE	N8P-C9P-CAP-OAP
6	J	5201	1XE	C5P-C6P-C7P-N8P
6	K	5201	1XE	O4B-C1B-N9A-C4A
6	K	5201	1XE	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
6	K	5201	1XE	CCP-O6A-P2A-O4A
6	K	5201	1XE	C9P-CAP-CBP-CCP
6	K	5201	1XE	C9P-CAP-CBP-CEP
6	K	5201	1XE	N8P-C9P-CAP-OAP
6	L	5201	1XE	C4B-C5B-O5B-P1A
6	L	5201	1XE	C5B-O5B-P1A-O1A
6	L	5201	1XE	C5B-O5B-P1A-O2A
6	L	5201	1XE	C5B-O5B-P1A-O3A
6	L	5201	1XE	C5P-C6P-C7P-N8P
6	L	5201	1XE	C3P-C2P-S1P-C1
6	L	5201	1XE	C6P-C7P-N8P-C9P
6	J	5201	1XE	O9P-C9P-CAP-OAP
6	K	5201	1XE	O9P-C9P-CAP-OAP
6	K	5201	1XE	OAP-CAP-CBP-CEP
6	J	5201	1XE	P1A-O3A-P2A-O4A
6	K	5201	1XE	O9P-C9P-CAP-CBP
6	K	5201	1XE	N8P-C9P-CAP-CBP
6	I	5201	1XE	C3P-C2P-S1P-C1
6	J	5201	1XE	C3P-C2P-S1P-C1
6	K	5201	1XE	C3P-C2P-S1P-C1
6	K	5201	1XE	C2P-C3P-N4P-C5P
6	L	5201	1XE	C2P-C3P-N4P-C5P
6	I	5201	1XE	O5P-C5P-C6P-C7P
6	I	5201	1XE	C6P-C7P-N8P-C9P
6	I	5201	1XE	CEP-CBP-CCP-O6A
6	J	5201	1XE	CEP-CBP-CCP-O6A
6	I	5201	1XE	N4P-C5P-C6P-C7P
6	J	5201	1XE	CAP-CBP-CCP-O6A
6	L	5201	1XE	CAP-CBP-CCP-O6A
6	I	5201	1XE	CCP-O6A-P2A-O3A
6	I	5201	1XE	CCP-O6A-P2A-O4A
6	I	5201	1XE	CCP-O6A-P2A-O5A
6	K	5201	1XE	CCP-O6A-P2A-O3A
6	K	5201	1XE	CCP-O6A-P2A-O5A
6	K	5201	1XE	OAP-CAP-CBP-CCP
6	L	5201	1XE	CCP-O6A-P2A-O3A
6	L	5201	1XE	CCP-O6A-P2A-O4A
6	L	5201	1XE	CCP-O6A-P2A-O5A
6	L	5201	1XE	O5P-C5P-C6P-C7P
6	K	5201	1XE	OAP-CAP-CBP-CDP
6	L	5201	1XE	N4P-C5P-C6P-C7P
6	K	5201	1XE	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
6	K	5201	1XE	C2-C1-S1P-C2P
6	I	5201	1XE	N8P-C9P-CAP-OAP
6	J	5201	1XE	C2P-C3P-N4P-C5P
6	I	5201	1XE	C3B-O3B-P3B-O7A
6	J	5201	1XE	C9P-CAP-CBP-CDP
6	K	5201	1XE	C9P-CAP-CBP-CDP
6	L	5201	1XE	P1A-O3A-P2A-O4A
6	L	5201	1XE	P1A-O3A-P2A-O5A
6	L	5201	1XE	CDP-CBP-CCP-O6A
6	L	5201	1XE	CEP-CBP-CCP-O6A
6	L	5201	1XE	N8P-C9P-CAP-OAP

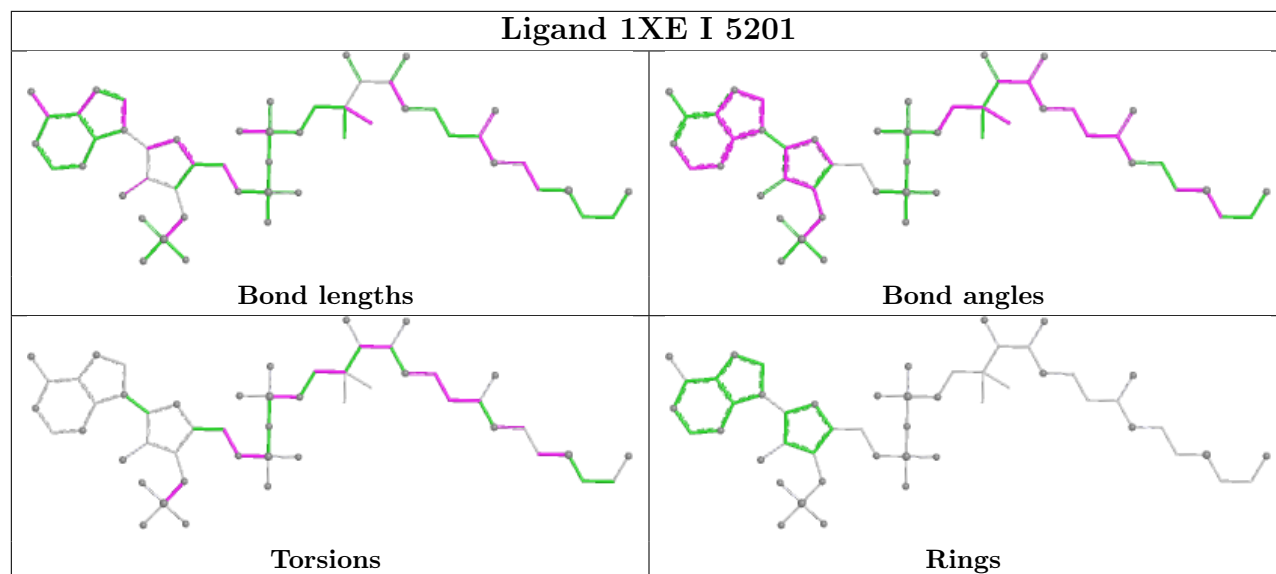
There are no ring outliers.

4 monomers are involved in 17 short contacts:

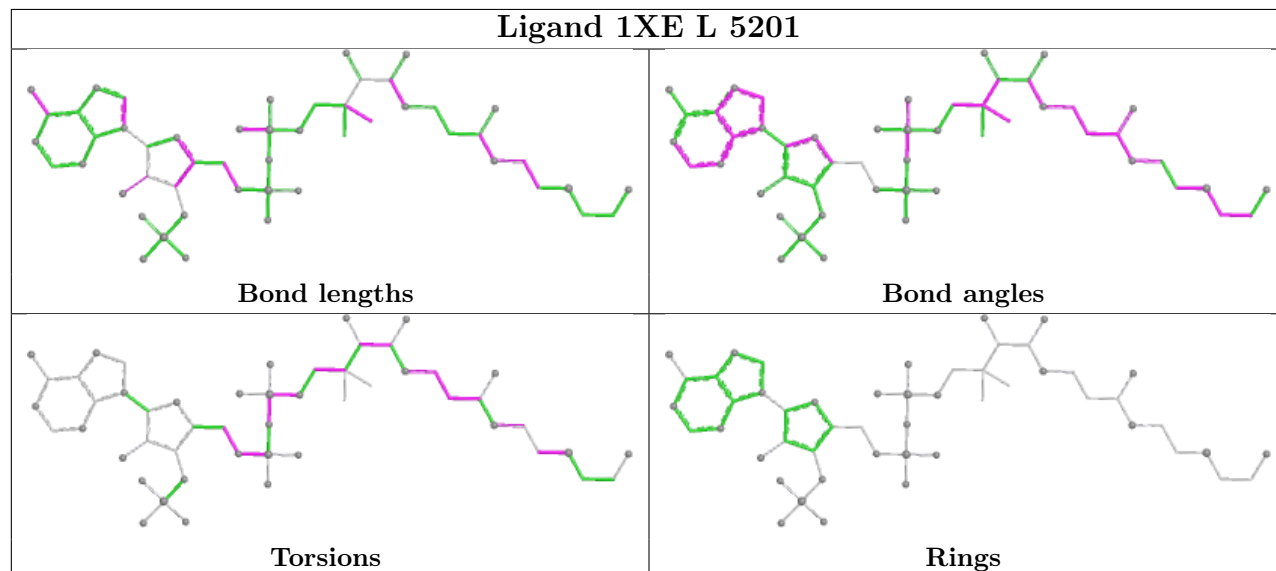
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	5201	1XE	5	0
6	L	5201	1XE	3	0
6	J	5201	1XE	2	0
6	K	5201	1XE	7	0

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.

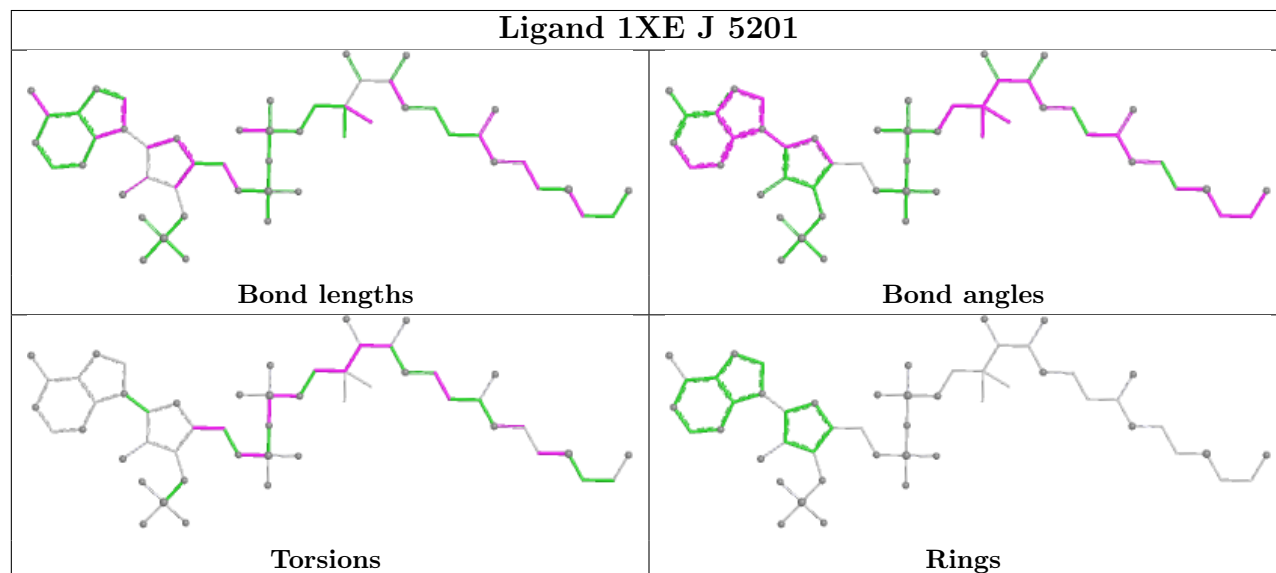
Ligand 1XE I 5201

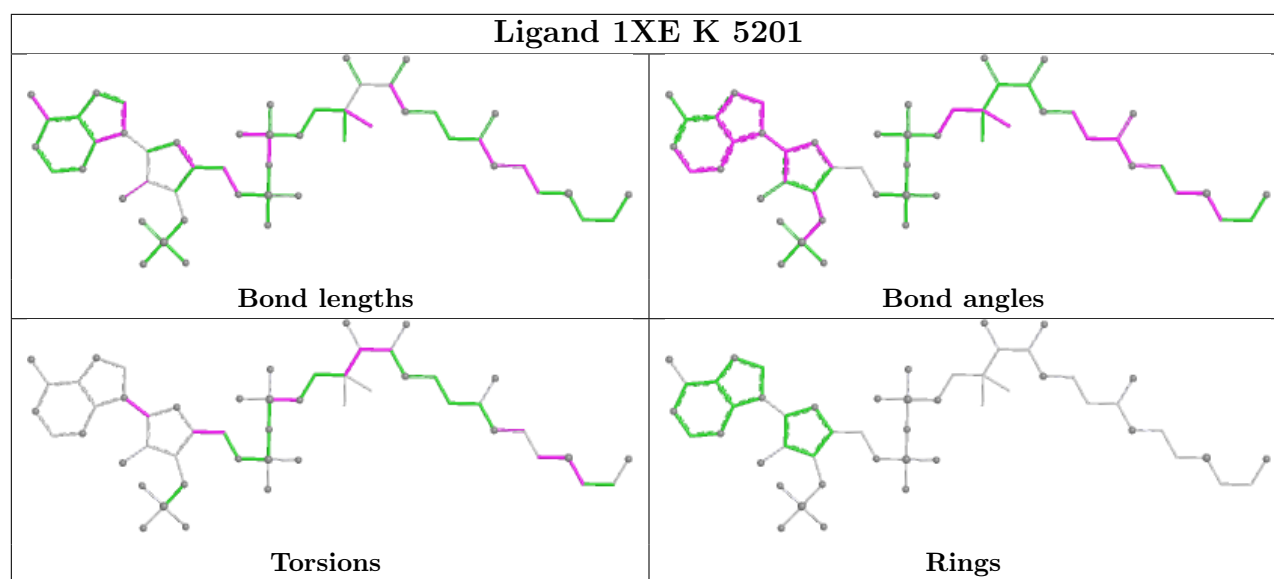


Ligand 1XE L 5201



Ligand 1XE J 5201





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	718/734 (97%)	0.22	32 (4%)	38	32	31, 89, 162, 258	3 (0%)
1	B	722/734 (98%)	0.32	27 (3%)	45	39	40, 109, 199, 296	1 (0%)
1	C	717/734 (97%)	0.36	30 (4%)	40	35	42, 104, 191, 257	1 (0%)
1	D	718/734 (97%)	0.20	29 (4%)	42	37	44, 95, 180, 280	1 (0%)
2	E	153/156 (98%)	0.05	2 (1%)	75	71	50, 72, 139, 167	1 (0%)
2	F	153/156 (98%)	0.31	4 (2%)	57	51	58, 104, 168, 207	0
2	G	153/156 (98%)	0.34	4 (2%)	57	51	59, 110, 179, 215	0
2	H	153/156 (98%)	0.00	1 (0%)	84	82	52, 78, 137, 182	0
3	I	4/4 (100%)	0.16	0	100	100	60, 65, 80, 111	0
3	J	4/4 (100%)	0.76	0	100	100	80, 92, 100, 125	0
3	K	4/4 (100%)	1.07	1 (25%)	2	1	90, 93, 130, 151	0
3	L	4/4 (100%)	0.28	0	100	100	65, 66, 88, 108	0
All	All	3503/3576 (97%)	0.26	130 (3%)	45	39	31, 96, 181, 296	7 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1[A]	MET	9.6
1	D	731	ALA	6.9
1	C	480	VAL	5.2
1	C	649	GLY	5.0
1	D	480	VAL	4.3
2	G	1	MET	4.3
1	A	731	ALA	4.3
1	B	649	GLY	4.3
1	C	539[A]	ARG	4.0
1	D	649	GLY	4.0
1	A	293	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	373	ILE	3.8
1	D	648	LEU	3.8
1	D	373	ILE	3.8
1	C	730	ALA	3.7
1	B	479	ALA	3.7
1	A	480	VAL	3.6
2	H	1	MET	3.5
1	C	479	ALA	3.4
2	F	1	MET	3.4
1	C	729	ASN	3.4
1	B	729	ASN	3.3
1	B	480	VAL	3.3
1	B	259	TYR	3.3
1	B	318	TYR	3.2
1	C	647	PRO	3.1
1	A	730	ALA	3.1
1	A	374	GLU	3.1
1	C	383	TYR	3.1
1	D	328	PRO	3.0
1	D	75	VAL	3.0
1	A	328	PRO	3.0
1	C	273	GLY	3.0
1	D	647	PRO	2.9
1	B	273	GLY	2.9
1	B	176	ILE	2.9
1	A	647	PRO	2.9
2	E	153	SER	2.8
1	B	75	VAL	2.8
1	C	75	VAL	2.8
1	D	71	LEU	2.8
1	B	648	LEU	2.8
1	B	643	TYR	2.8
1	D	76	GLY	2.8
1	C	373	ILE	2.8
1	A	648	LEU	2.8
1	B	285	TYR	2.7
1	A	376	PRO	2.7
1	C	298	PRO	2.7
1	A	69	LEU	2.7
1	A	649	GLY	2.6
1	C	176	ILE	2.6
1	C	648	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	110	ASN	2.6
2	G	140	ALA	2.6
1	A	643	TYR	2.6
1	C	293	PRO	2.6
1	A	409	HIS	2.6
1	B	647	PRO	2.5
1	A	289	ALA	2.5
2	F	153	SER	2.5
1	A	594	LEU	2.5
1	D	730	ALA	2.5
1	A	292	TYR	2.5
1	D	327	ILE	2.5
1	A	479	ALA	2.4
1	D	728	SER	2.4
1	A	40	HIS	2.4
1	A	591	PHE	2.4
2	F	44	VAL	2.4
1	B	306	LEU	2.4
1	D	409	HIS	2.4
1	D	329	SER	2.4
2	G	68	ILE	2.4
1	C	6	LEU	2.4
2	G	85	LEU	2.4
1	D	292	TYR	2.4
1	A	371	SER	2.3
1	D	174	SER	2.3
1	D	275	VAL	2.3
1	B	380	LEU	2.2
1	B	659	LEU	2.2
3	K	5125	GLU	2.2
1	A	729	ASN	2.2
1	C	318	TYR	2.2
1	A	377	THR	2.2
1	B	288	LEU	2.2
1	C	629	ASP	2.2
1	C	646	ASP	2.2
1	C	59	ASN	2.2
1	D	177	ASN	2.2
1	D	479	ALA	2.2
1	B	409	HIS	2.2
1	C	446	GLN	2.2
1	C	643	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	276	LEU	2.2
1	B	272	SER	2.2
1	D	374	GLU	2.2
1	B	351	VAL	2.2
1	B	642	LYS	2.2
1	A	177	ASN	2.2
1	C	60	THR	2.2
2	F	85	LEU	2.2
1	D	10	GLU	2.2
1	A	644	ASP	2.1
1	B	278	SER	2.1
1	B	1	MET	2.1
1	D	176	ILE	2.1
1	A	581	PHE	2.1
1	C	347	VAL	2.1
1	B	271	ALA	2.1
1	A	107	LEU	2.1
1	B	37	LEU	2.1
1	C	374	GLU	2.1
1	D	293	PRO	2.1
1	A	75	VAL	2.1
1	A	378	THR	2.1
1	B	322	LYS	2.1
1	A	8	PRO	2.1
1	C	8	PRO	2.1
1	C	351	VAL	2.0
1	D	364	PHE	2.0
1	D	703	ALA	2.0
1	B	59	ASN	2.0
1	A	450	ILE	2.0
1	D	642	LYS	2.0
1	C	380	LEU	2.0
1	C	445	LEU	2.0
1	C	270	ASP	2.0
1	D	376	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

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($\text{\AA}^2$)	Q<0.9
4	CL	A	811	1/1	0.29	0.17	188,188,188,188	0
4	CL	A	807	1/1	0.45	0.10	148,148,148,148	0
4	CL	D	810	1/1	0.51	0.10	157,157,157,157	0
4	CL	A	804	1/1	0.53	0.14	143,143,143,143	0
4	CL	B	808	1/1	0.54	0.12	161,161,161,161	0
4	CL	A	812	1/1	0.57	0.08	141,141,141,141	0
4	CL	C	809	1/1	0.62	0.14	151,151,151,151	0
4	CL	B	806	1/1	0.66	0.22	151,151,151,151	0
4	CL	B	813	1/1	0.66	0.15	145,145,145,145	0
4	CL	D	803	1/1	0.67	0.21	118,118,118,118	0
4	CL	A	806	1/1	0.69	0.11	145,145,145,145	0
4	CL	C	813	1/1	0.69	0.13	137,137,137,137	0
4	CL	F	201	1/1	0.69	0.22	148,148,148,148	0
4	CL	D	812	1/1	0.70	0.14	138,138,138,138	0
4	CL	D	804	1/1	0.71	0.07	132,132,132,132	0
4	CL	B	807	1/1	0.72	0.16	140,140,140,140	0
4	CL	D	813	1/1	0.73	0.20	130,130,130,130	0
4	CL	D	807	1/1	0.75	0.14	173,173,173,173	0
4	CL	G	201	1/1	0.76	0.10	133,133,133,133	0
4	CL	C	803	1/1	0.77	0.10	129,129,129,129	0
4	CL	A	809	1/1	0.78	0.10	125,125,125,125	0
4	CL	C	812	1/1	0.79	0.64	126,126,126,126	0
4	CL	E	203	1/1	0.79	0.10	110,110,110,110	0
4	CL	D	802	1/1	0.80	0.08	149,149,149,149	0
4	CL	B	816	1/1	0.82	0.16	107,107,107,107	0
4	CL	B	815	1/1	0.83	0.20	192,192,192,192	0
4	CL	D	808	1/1	0.84	0.11	131,131,131,131	0
5	SO4	D	816	5/5	0.84	0.11	80,110,119,124	0
4	CL	D	805	1/1	0.85	0.13	288,288,288,288	0
4	CL	B	805	1/1	0.85	0.17	108,108,108,108	0
4	CL	A	808	1/1	0.85	0.21	113,113,113,113	0
4	CL	B	814	1/1	0.85	0.13	141,141,141,141	0

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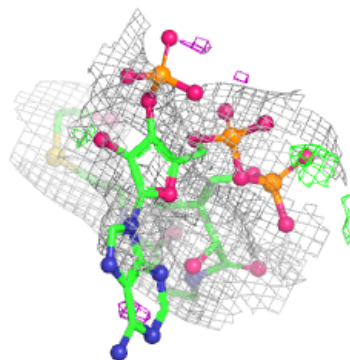
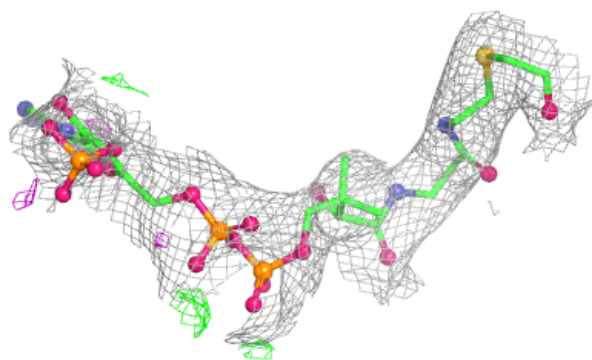
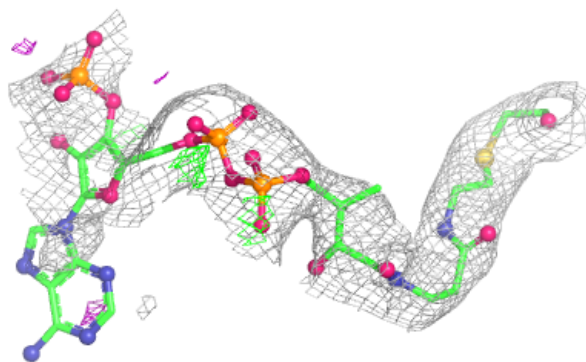
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	A	814	1/1	0.85	0.09	120,120,120,120	0
6	1XE	K	5201	51/52	0.85	0.13	53,128,279,303	0
4	CL	C	807	1/1	0.86	0.18	125,125,125,125	0
4	CL	B	803	1/1	0.86	0.12	99,99,99,99	0
4	CL	C	805	1/1	0.86	0.12	119,119,119,119	0
4	CL	C	804	1/1	0.87	0.10	118,118,118,118	0
4	CL	B	801	1/1	0.87	0.10	127,127,127,127	0
4	CL	A	805	1/1	0.88	0.12	138,138,138,138	0
4	CL	D	806	1/1	0.88	0.08	139,139,139,139	0
4	CL	D	809	1/1	0.88	0.07	127,127,127,127	0
4	CL	D	815	1/1	0.88	0.13	105,105,105,105	0
6	1XE	J	5201	51/52	0.88	0.12	67,142,228,241	0
4	CL	E	202	1/1	0.88	0.13	102,102,102,102	0
4	CL	B	809	1/1	0.89	0.13	109,109,109,109	0
4	CL	C	808	1/1	0.90	0.12	110,110,110,110	0
4	CL	A	813	1/1	0.90	0.08	124,124,124,124	0
4	CL	C	802	1/1	0.90	0.19	106,106,106,106	0
4	CL	D	814	1/1	0.90	0.38	110,110,110,110	0
4	CL	B	812	1/1	0.91	0.16	112,112,112,112	0
6	1XE	I	5201	51/52	0.91	0.13	49,92,190,217	0
4	CL	C	801	1/1	0.92	0.06	111,111,111,111	0
5	SO4	A	815	5/5	0.92	0.08	88,104,110,121	0
4	CL	B	804	1/1	0.92	0.16	107,107,107,107	0
6	1XE	L	5201	51/52	0.92	0.11	49,92,179,181	0
4	CL	D	801	1/1	0.93	0.09	93,93,93,93	0
4	CL	C	810	1/1	0.93	0.23	97,97,97,97	0
4	CL	E	201	1/1	0.94	0.16	79,79,79,79	0
4	CL	A	803	1/1	0.94	0.06	99,99,99,99	0
4	CL	B	810	1/1	0.94	0.15	99,99,99,99	0
4	CL	B	802	1/1	0.94	0.27	96,96,96,96	0
4	CL	C	806	1/1	0.94	0.12	117,117,117,117	0
4	CL	H	201	1/1	0.94	0.11	84,84,84,84	0
4	CL	A	801	1/1	0.95	0.22	96,96,96,96	0
4	CL	C	811	1/1	0.95	0.19	94,94,94,94	0
4	CL	B	811	1/1	0.95	0.26	99,99,99,99	0
4	CL	A	810	1/1	0.97	0.22	86,86,86,86	0
4	CL	A	802	1/1	0.98	0.12	93,93,93,93	0
4	CL	D	811	1/1	0.98	0.09	73,73,73,73	0

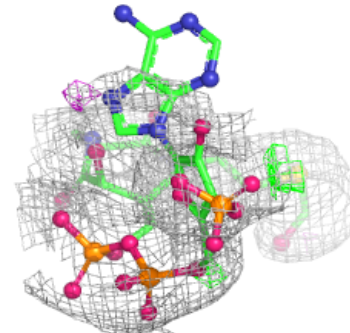
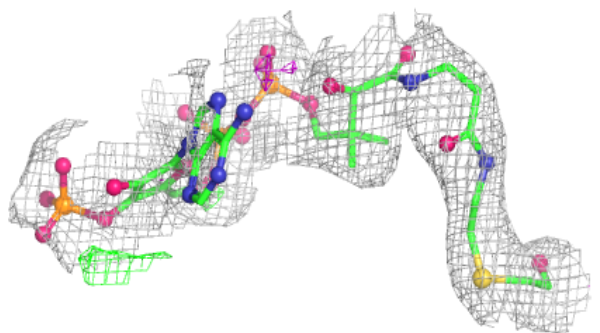
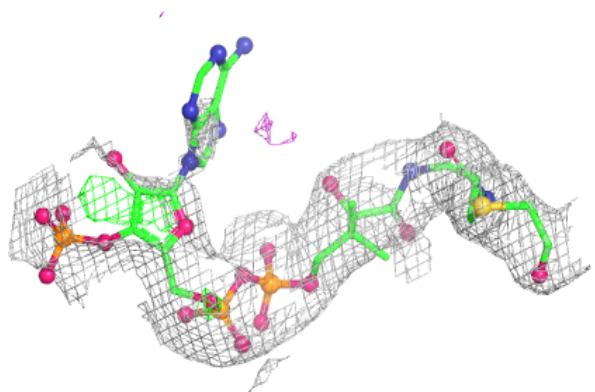
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1XE K 5201:

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

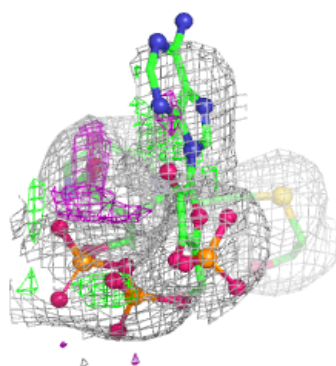
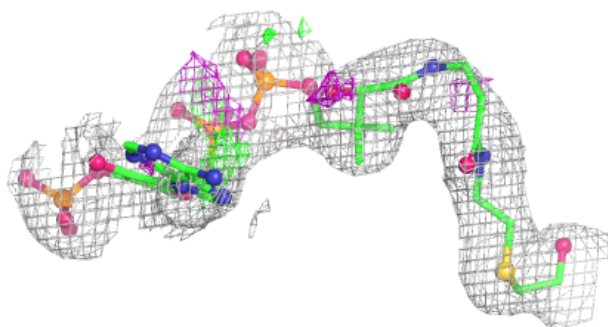
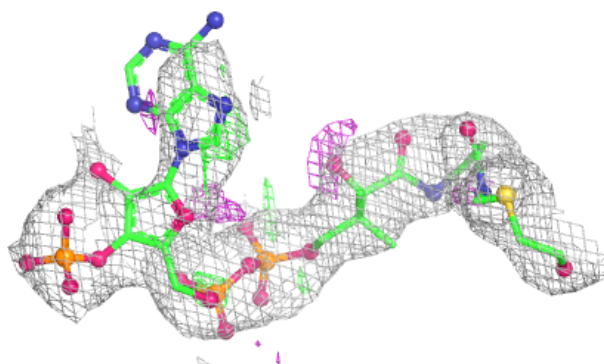
**Electron density around 1XE J 5201:**

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

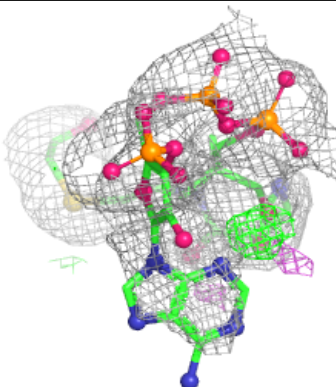
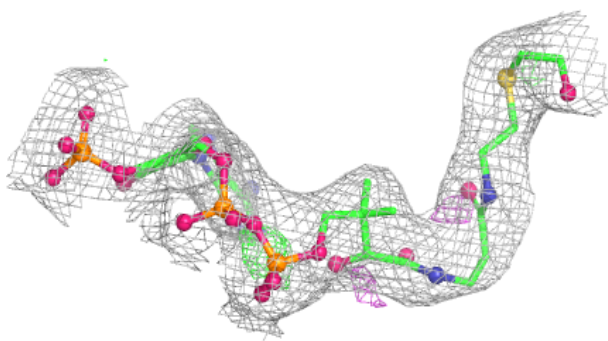
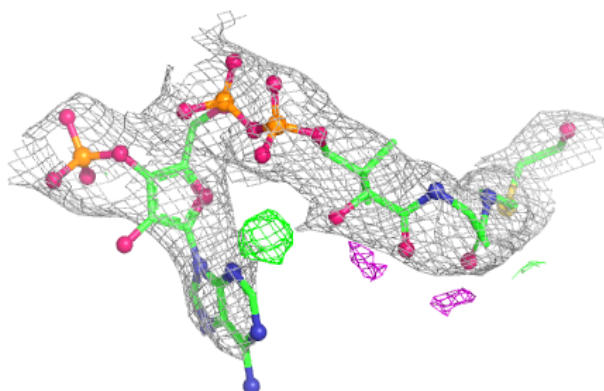


Electron density around 1XE I 5201:

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

**Electron density around 1XE L 5201:**

$2mF_o-DF_c$ (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.