



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 10:17 PM EDT

PDB ID : 4KVM  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

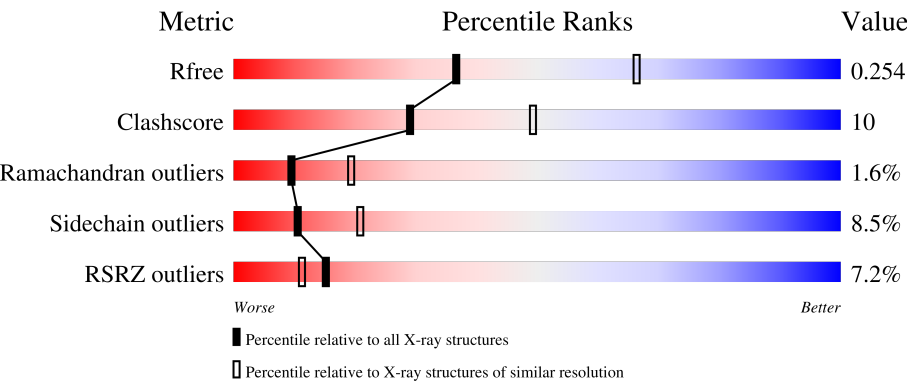
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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  $\geq 3$ , 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	<div><div>6%</div><div><div></div><div>72%</div><div>22%</div><div>• •</div></div></div>
1	B	734	<div><div>10%</div><div><div></div><div>74%</div><div>21%</div><div>• •</div></div></div>
1	C	734	<div><div>8%</div><div><div></div><div>72%</div><div>23%</div><div>• •</div></div></div>
1	D	734	<div><div>8%</div><div><div></div><div>72%</div><div>23%</div><div>• •</div></div></div>
2	E	156	<div><div>%</div><div><div></div><div>78%</div><div>18%</div><div>• •</div></div></div>

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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	B	806	-	-	-	X
4	CL	B	807	-	-	-	X
4	CL	B	813	-	-	-	X
4	CL	C	807	-	-	-	X
4	CL	C	810	-	-	X	-
4	CL	D	803	-	-	-	X
4	CL	D	805	-	-	-	X
4	CL	D	806	-	-	-	X
4	CL	D	811	-	-	X	-
4	CL	D	813	-	-	-	X
4	CL	F	201	-	-	-	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 (three-letter code: CL) (formula: Cl).

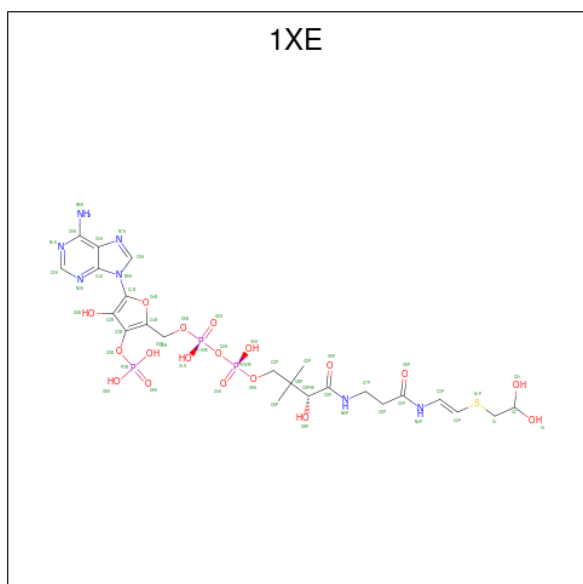
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	Cl	0	0
			14	14		
4	B	16	Total	Cl	0	0
			16	16		
4	C	13	Total	Cl	0	0
			13	13		
4	D	15	Total	Cl	0	0
			15	15		
4	E	3	Total	Cl	0	0
			3	3		
4	F	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: 1XE) (formula: C<sub>23</sub>H<sub>34</sub>N<sub>7</sub>O<sub>18</sub>P<sub>3</sub>S).



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		

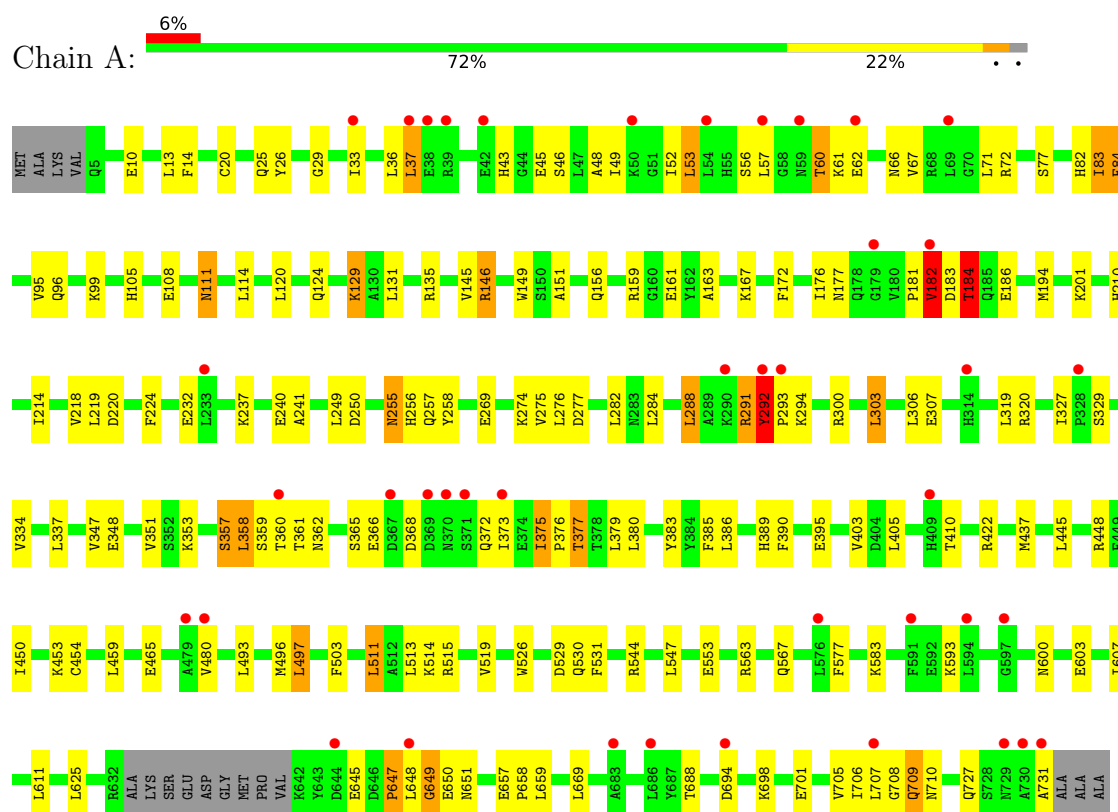
- Molecule 7 is water.

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		

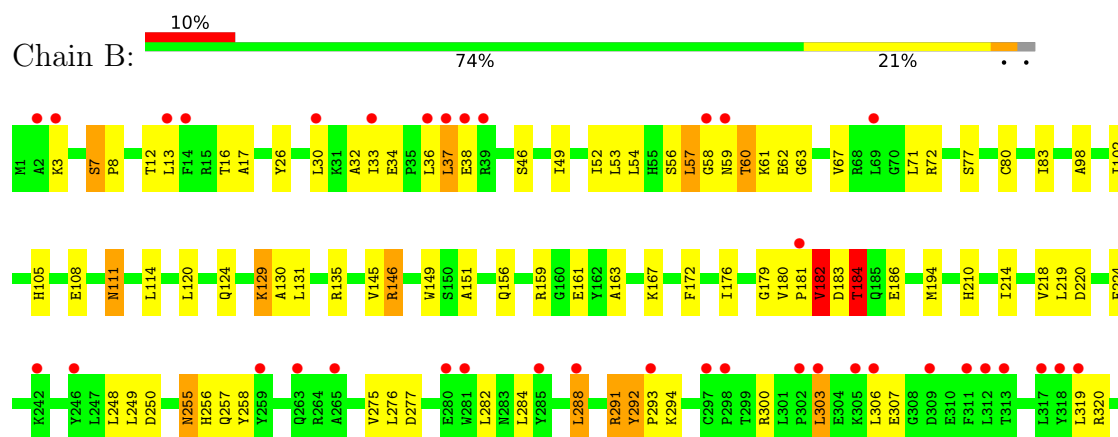
### 3 Residue-property plots

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.

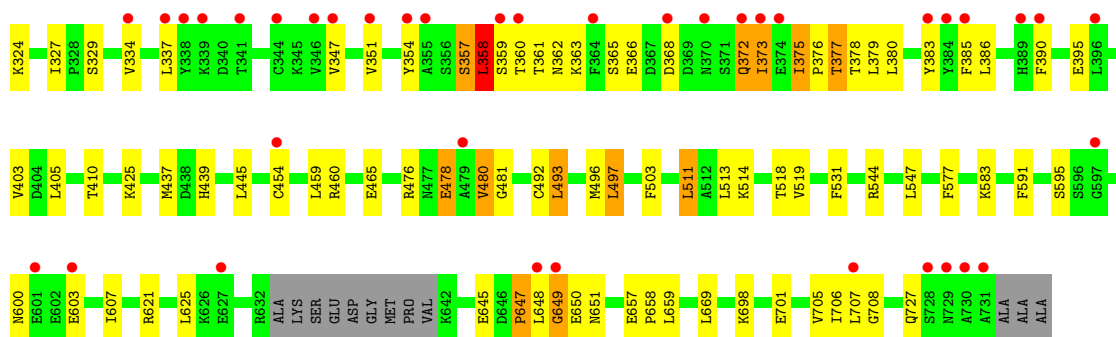
- Molecule 1: N-terminal acetyltransferase A complex subunit nat1



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



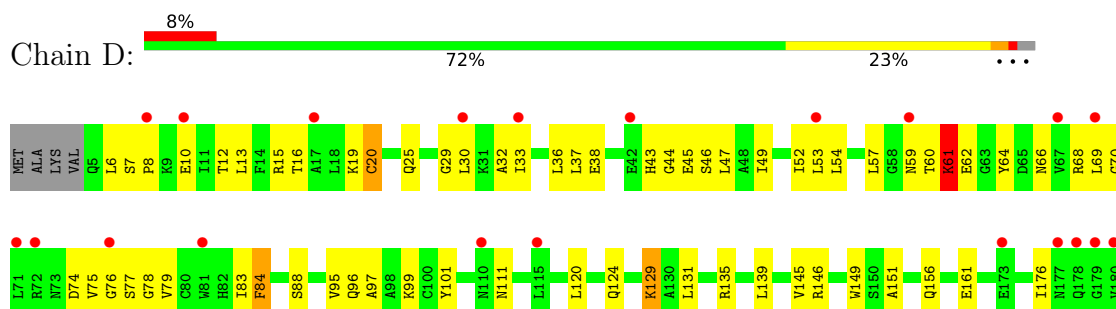




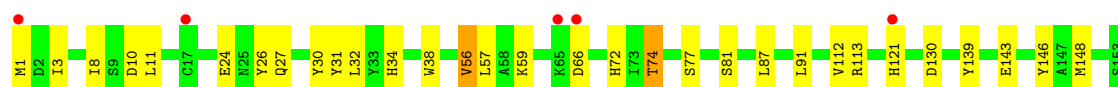
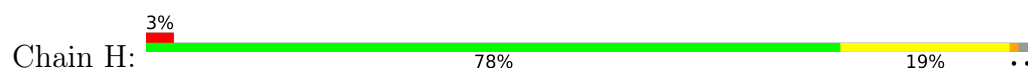
• Molecule 1: N-terminal acetyltransferase A complex subunit nat1



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







THR  
LEU  
LYS

- Molecule 3: bisubstrate analog inhibitor



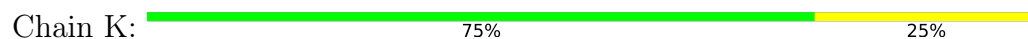
There are no outlier residues recorded for this chain.

- Molecule 3: bisubstrate analog inhibitor



S5122  
E5125

- Molecule 3: bisubstrate analog inhibitor



S5122  
E5125

- Molecule 3: bisubstrate analog inhibitor



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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.222 , 0.260 0.214 , 0.254	Depositor DCC
$R_{free}$ test set	6916 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.7	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 1XE, SO4

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	0.45	0/5896	0.59	1/7952 (0.0%)
1	B	0.40	0/5891	0.56	0/7948
1	C	0.41	0/5867	0.55	0/7915
1	D	0.43	0/5881	0.56	0/7934
2	E	0.52	0/1277	0.63	0/1722
2	F	0.40	0/1269	0.56	0/1712
2	G	0.41	0/1269	0.56	0/1712
2	H	0.48	0/1269	0.62	0/1712
3	I	0.71	0/25	0.74	0/32
3	J	0.50	0/25	0.58	0/32
3	K	0.34	0/25	0.43	0/32
3	L	0.63	0/25	0.65	0/32
All	All	0.43	0/28719	0.57	1/38735 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	THR	N-CA-C	-5.16	97.08	111.00

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
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	124	1
1	B	5777	0	5697	114	0
1	C	5753	0	5675	123	0
1	D	5766	0	5691	115	0
2	E	1247	0	1233	21	0
2	F	1239	0	1223	13	0
2	G	1239	0	1223	19	0
2	H	1239	0	1223	15	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	22	0
7	D	64	0	0	10	0
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	542	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 (542) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:514:LYS:NZ	1:C:645:GLU:OE1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:129[A]:LYS:NZ	4:A:811:CL:CL	2.58	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:MET:HE2	1:B:518:THR:HG21	1.86	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:D:183:ASP:OD2	7:D:930:HOH:O	2.18	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:C:255:ASN:C	1:C:255:ASN:HD22	2.09	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: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:A:255:ASN:C	1:A:255:ASN:HD22	2.11	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:D:84:PHE:O	1:D:88:SER:OG	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:255:ASN:C	1:B:255:ASN:HD22	2.13	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:A:593:LYS:NZ	7:A:968:HOH:O	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:A:292:TYR:C	1:A:294:LYS:H	2.12	0.52
1:B:292:TYR:C	1:B:294:LYS:H	2.13	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:292:TYR:C	1:C:294:LYS:H	2.13	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
1:A:514:LYS:NZ	1:A:645:GLU:OE1	2.25	0.51
1:A:437:MET:HE2	1:A:450:ILE:HD11	1.91	0.51
1:D:255:ASN:C	1:D:255:ASN:HD22	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129[A]:LYS:H	1:A:129[A]:LYS:CD	2.24	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: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
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:D:292:TYR:C	1:D:294:LYS:H	2.14	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:C:377:THR:O	1:C:377:THR:OG1	2.26	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:327:ILE:HG22	1:C:329:SER:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:437:MET:HE2	1:D:450:ILE:HD11	1.95	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:D:534:HIS:HD1	1:D:546:TYR:HH	1.54	0.48
1:A:10:GLU:O	1:A:14:PHE:N	2.38	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
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:476:ARG:HG2	1:B:478:GLU:HG2	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:358:LEU:HD13	1:B:358:LEU:HA	1.81	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: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
2:F:56:VAL:CG1	2:F:91:LEU:HB3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:496:MET:HE1	1:D:515:ARG:HD3	1.99	0.45
1:D:694:ASP:N	1:D:694:ASP:OD1	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: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: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
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: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: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
2:E:1[A]:MET:HB3	2:E:1[A]:MET:HE3	1.79	0.44
2:E:1[B]:MET:CE	2:E:48:PRO:HD3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:478:GLU:HG2	1:B:478:GLU:H	1.41	0.44
1:A:496:MET:HE3	1:A:515:ARG:HD3	2.00	0.43
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: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:A:292:TYR:C	1:A:294:LYS:N	2.72	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:709:GLN:HE21	1:D:709:GLN:HB3	1.61	0.43
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: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
1:D:292:TYR:C	1:D:294:LYS:N	2.73	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: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: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: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:C:673:GLY:HA3	1:C:680:TYR:CZ	2.55	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
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
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:A:437:MET:HE2	1:A:450:ILE:CD1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:292:TYR:C	1:B:294:LYS:N	2.73	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:292:TYR:C	1:C:294:LYS:N	2.73	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1[B]:MET:HE3	2:E:48:PRO:HD3	2.03	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:C:496:MET:HE1	1:C:515:ARG:HD3	2.03	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:C:368:ASP:N	1:C:368:ASP:OD1	2.54	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:C:7:SER:HA	1:C:8:PRO:HD3	1.88	0.40
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

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	717/734 (98%)	658 (92%)	46 (6%)	13 (2%)	8	16
1	B	719/734 (98%)	660 (92%)	45 (6%)	14 (2%)	8	15
1	C	714/734 (97%)	660 (92%)	42 (6%)	12 (2%)	9	18
1	D	715/734 (97%)	657 (92%)	43 (6%)	15 (2%)	7	13
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
All	All	3477/3576 (97%)	3225 (93%)	198 (6%)	54 (2%)	9	19

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

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Mol	Chain	Res	Type
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
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%)	558 (91%)	53 (9%)	10	20
1	B	610/638 (96%)	559 (92%)	51 (8%)	11	21
1	C	609/638 (96%)	561 (92%)	48 (8%)	12	24
1	D	610/638 (96%)	562 (92%)	48 (8%)	12	24
2	E	133/135 (98%)	118 (89%)	15 (11%)	6	10
2	F	132/135 (98%)	118 (89%)	14 (11%)	6	12
2	G	132/135 (98%)	119 (90%)	13 (10%)	8	15
2	H	132/135 (98%)	117 (89%)	15 (11%)	5	10
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
3	L	3/3 (100%)	3 (100%)	0	100	100
All	All	2981/3104 (96%)	2723 (91%)	258 (9%)	10	20

All (258) 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	82	HIS
1	A	83	ILE
1	A	84	PHE
1	A	96	GLN
1	A	111	ASN
1	A	120	LEU
1	A	129[A]	LYS

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Mol	Chain	Res	Type
1	A	129[B]	LYS
1	A	131	LEU
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	194	MET
1	A	255	ASN
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	361	THR
1	A	372	GLN
1	A	375	ILE
1	A	377	THR
1	A	380	LEU
1	A	403	VAL
1	A	410	THR
1	A	445	LEU
1	A	459	LEU
1	A	465	GLU
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	698	LYS
1	A	707	LEU
1	A	709	GLN
1	A	727	GLN
1	B	7	SER
1	B	37	LEU
1	B	49	ILE

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Mol	Chain	Res	Type
1	B	53	LEU
1	B	56	SER
1	B	57	LEU
1	B	61	LYS
1	B	72	ARG
1	B	111	ASN
1	B	120	LEU
1	B	129[A]	LYS
1	B	129[B]	LYS
1	B	131	LEU
1	B	145	VAL
1	B	146	ARG
1	B	159	ARG
1	B	176	ILE
1	B	182	VAL
1	B	184	THR
1	B	194	MET
1	B	255	ASN
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	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	410	THR
1	B	445	LEU
1	B	459	LEU
1	B	465	GLU
1	B	478	GLU
1	B	493	LEU
1	B	497	LEU
1	B	511	LEU
1	B	513	LEU
1	B	547	LEU

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Mol	Chain	Res	Type
1	B	583	LYS
1	B	600	ASN
1	B	669	LEU
1	B	698	LYS
1	B	707	LEU
1	B	727	GLN
1	C	38	GLU
1	C	53	LEU
1	C	72	ARG
1	C	74	ASP
1	C	83	ILE
1	C	96	GLN
1	C	111	ASN
1	C	120	LEU
1	C	129	LYS
1	C	131	LEU
1	C	145	VAL
1	C	176	ILE
1	C	182	VAL
1	C	184	THR
1	C	194	MET
1	C	255	ASN
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	358	LEU
1	C	361	THR
1	C	372	GLN
1	C	375	ILE
1	C	377	THR
1	C	380	LEU
1	C	403	VAL
1	C	410	THR
1	C	445	LEU
1	C	459	LEU
1	C	465	GLU
1	C	493	LEU
1	C	497	LEU
1	C	511	LEU

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Mol	Chain	Res	Type
1	C	513	LEU
1	C	517	SER
1	C	539[A]	ARG
1	C	539[B]	ARG
1	C	547	LEU
1	C	583	LYS
1	C	600	ASN
1	C	669	LEU
1	C	690	LEU
1	C	698	LYS
1	C	707	LEU
1	C	727	GLN
1	D	20	CYS
1	D	38	GLU
1	D	57	LEU
1	D	61	LYS
1	D	84	PHE
1	D	96	GLN
1	D	111	ASN
1	D	120	LEU
1	D	129	LYS
1	D	131	LEU
1	D	145	VAL
1	D	176	ILE
1	D	182	VAL
1	D	184	THR
1	D	194	MET
1	D	255	ASN
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	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

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Mol	Chain	Res	Type
1	D	410	THR
1	D	445	LEU
1	D	459	LEU
1	D	465	GLU
1	D	493	LEU
1	D	497	LEU
1	D	511	LEU
1	D	513	LEU
1	D	539[A]	ARG
1	D	539[B]	ARG
1	D	547	LEU
1	D	583	LYS
1	D	600	ASN
1	D	669	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	26	TYR
2	E	27	GLN
2	E	32	LEU
2	E	56	VAL
2	E	57	LEU
2	E	66	ASP
2	E	72	HIS
2	E	74	THR
2	E	81	SER
2	E	130	ASP
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	53	VAL
2	F	56	VAL
2	F	57	LEU
2	F	66	ASP

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Mol	Chain	Res	Type
2	F	72	HIS
2	F	74	THR
2	F	81	SER
2	F	130	ASP
2	F	148	MET
2	G	3	ILE
2	G	24	GLU
2	G	26	TYR
2	G	27	GLN
2	G	32	LEU
2	G	56	VAL
2	G	57	LEU
2	G	66	ASP
2	G	72	HIS
2	G	74	THR
2	G	81	SER
2	G	130	ASP
2	G	148	MET
2	H	1	MET
2	H	3	ILE
2	H	24	GLU
2	H	26	TYR
2	H	27	GLN
2	H	32	LEU
2	H	56	VAL
2	H	57	LEU
2	H	66	ASP
2	H	72	HIS
2	H	74	THR
2	H	81	SER
2	H	87	LEU
2	H	130	ASP
2	H	148	MET
3	J	5125	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	111	ASN
1	A	255	ASN
1	A	600	ASN

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Mol	Chain	Res	Type
1	A	709	GLN
1	B	111	ASN
1	B	255	ASN
1	B	439	HIS
1	B	600	ASN
1	C	111	ASN
1	C	255	ASN
1	C	256	HIS
1	C	600	ASN
1	D	111	ASN
1	D	255	ASN
1	D	600	ASN
1	D	709	GLN
2	E	27	GLN
2	G	27	GLN
2	H	27	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 monosaccharides 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
5	SO4	A	815	-	4,4,4	0.20	0	6,6,6	0.17	0
6	1XE	I	5201	3	43,53,54	2.49	13 (30%)	45,78,80	2.82	16 (35%)
5	SO4	D	816	-	4,4,4	0.18	0	6,6,6	0.22	0
6	1XE	K	5201	3	43,53,54	2.49	11 (25%)	45,78,80	2.47	14 (31%)
6	1XE	J	5201	3	43,53,54	2.51	12 (27%)	45,78,80	2.14	15 (33%)
6	1XE	L	5201	3	43,53,54	2.42	11 (25%)	45,78,80	2.39	14 (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
6	1XE	I	5201	3	-	17/42/51/52	0/3/3/3
6	1XE	L	5201	3	-	17/42/51/52	0/3/3/3
6	1XE	K	5201	3	-	16/42/51/52	0/3/3/3
6	1XE	J	5201	3	-	17/42/51/52	0/3/3/3

All (47) 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
6	L	5201	1XE	C9P-N8P	6.83	1.48	1.33
6	K	5201	1XE	C9P-N8P	6.78	1.48	1.33
6	J	5201	1XE	C9P-N8P	6.75	1.48	1.33
6	J	5201	1XE	C1-S1P	-6.68	1.73	1.81
6	I	5201	1XE	C9P-N8P	6.55	1.47	1.33
6	I	5201	1XE	C5P-N4P	6.05	1.48	1.37
6	L	5201	1XE	C5P-N4P	6.04	1.48	1.37
6	J	5201	1XE	C5P-N4P	5.77	1.48	1.37
6	K	5201	1XE	C5P-N4P	5.61	1.47	1.37
6	K	5201	1XE	C1-S1P	-4.75	1.75	1.81
6	K	5201	1XE	O3B-C3B	-4.12	1.33	1.40
6	I	5201	1XE	C1-S1P	-4.01	1.76	1.81
6	I	5201	1XE	C3P-N4P	3.79	1.50	1.40
6	L	5201	1XE	C1-S1P	-3.77	1.76	1.81
6	J	5201	1XE	C3P-N4P	3.47	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	5201	1XE	C3P-N4P	3.40	1.49	1.40
6	K	5201	1XE	C3P-N4P	3.32	1.49	1.40
6	K	5201	1XE	C6A-N6A	3.29	1.46	1.34
6	K	5201	1XE	O2B-C2B	3.26	1.44	1.37
6	L	5201	1XE	O2B-C2B	3.21	1.44	1.37
6	J	5201	1XE	CDP-CBP	-3.16	1.46	1.53
6	I	5201	1XE	C8A-N9A	-3.13	1.33	1.36
6	I	5201	1XE	O2B-C2B	3.10	1.44	1.37
6	J	5201	1XE	O2B-C2B	3.05	1.44	1.37
6	L	5201	1XE	C6A-N6A	3.05	1.45	1.34
6	I	5201	1XE	C6A-N6A	3.00	1.45	1.34
6	I	5201	1XE	CDP-CBP	-2.99	1.47	1.53
6	J	5201	1XE	C6A-N6A	2.98	1.44	1.34
6	L	5201	1XE	CDP-CBP	-2.95	1.47	1.53
6	I	5201	1XE	O3B-C3B	-2.91	1.35	1.40
6	K	5201	1XE	CDP-CBP	-2.84	1.47	1.53
6	K	5201	1XE	C8A-N9A	-2.76	1.33	1.36
6	J	5201	1XE	O3B-C3B	-2.54	1.36	1.40
6	L	5201	1XE	C8A-N9A	-2.49	1.34	1.36
6	I	5201	1XE	O5P-C5P	2.44	1.28	1.23
6	J	5201	1XE	C8A-N9A	-2.38	1.34	1.36
6	J	5201	1XE	P2A-O4A	2.35	1.59	1.50
6	I	5201	1XE	P2A-O4A	2.29	1.59	1.50
6	K	5201	1XE	C5B-C4B	-2.28	1.48	1.50
6	L	5201	1XE	P2A-O4A	2.13	1.58	1.50
6	I	5201	1XE	P3B-O3B	-2.04	1.56	1.59
6	J	5201	1XE	O5P-C5P	2.02	1.27	1.23
6	L	5201	1XE	O3B-C3B	-2.00	1.37	1.40

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	5201	1XE	O5B-C5B-C4B	8.59	125.26	109.44
6	I	5201	1XE	C7P-C6P-C5P	8.02	125.72	112.36
6	I	5201	1XE	C7P-N8P-C9P	-7.83	108.62	122.59
6	L	5201	1XE	C1-S1P-C2P	7.25	112.24	100.33
6	K	5201	1XE	C1-S1P-C2P	7.17	112.11	100.33
6	I	5201	1XE	C6P-C7P-N8P	6.65	125.31	111.90
6	L	5201	1XE	O5B-C5B-C4B	6.06	120.59	109.44
6	L	5201	1XE	C6P-C7P-N8P	6.05	124.11	111.90
6	I	5201	1XE	C1-S1P-C2P	5.76	109.80	100.33
6	K	5201	1XE	O6A-CCP-CBP	5.22	118.94	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	5201	1XE	C3P-N4P-C5P	-5.00	113.78	123.35
6	J	5201	1XE	C1-S1P-C2P	4.48	107.68	100.33
6	J	5201	1XE	C3P-C2P-S1P	-4.43	115.50	124.22
6	K	5201	1XE	P2A-O3A-P1A	-4.42	117.67	132.83
6	J	5201	1XE	N3A-C2A-N1A	-4.27	122.00	128.68
6	I	5201	1XE	N3A-C2A-N1A	-4.24	122.05	128.68
6	I	5201	1XE	O5B-C5B-C4B	4.17	117.11	109.44
6	J	5201	1XE	C6P-C5P-N4P	4.16	123.49	114.94
6	I	5201	1XE	C6P-C5P-N4P	4.08	123.32	114.94
6	L	5201	1XE	N3A-C2A-N1A	-4.04	122.36	128.68
6	L	5201	1XE	CDP-CBP-CCP	3.99	114.74	108.23
6	L	5201	1XE	C6P-C5P-N4P	3.98	123.12	114.94
6	J	5201	1XE	O6A-CCP-CBP	3.97	116.93	110.55
6	I	5201	1XE	O6A-CCP-CBP	3.90	116.82	110.55
6	I	5201	1XE	P2A-O3A-P1A	-3.80	119.79	132.83
6	L	5201	1XE	C7P-N8P-C9P	-3.75	115.89	122.59
6	J	5201	1XE	CDP-CBP-CAP	3.68	115.20	108.82
6	K	5201	1XE	C6P-C5P-N4P	3.64	122.43	114.94
6	J	5201	1XE	P2A-O3A-P1A	-3.59	120.50	132.83
6	I	5201	1XE	O5P-C5P-N4P	-3.41	115.90	122.47
6	K	5201	1XE	C8A-N9A-C1B	3.40	129.81	125.24
6	K	5201	1XE	N3A-C2A-N1A	-3.29	123.53	128.68
6	K	5201	1XE	C3P-N4P-C5P	-3.26	117.11	123.35
6	L	5201	1XE	C3P-C2P-S1P	-3.26	117.80	124.22
6	L	5201	1XE	O5P-C5P-N4P	-3.04	116.60	122.47
6	I	5201	1XE	CAP-C9P-N8P	3.02	122.58	116.58
6	L	5201	1XE	C3P-N4P-C5P	-2.93	117.74	123.35
6	K	5201	1XE	C4A-C5A-N7A	-2.83	106.45	109.40
6	J	5201	1XE	O5B-C5B-C4B	2.60	114.23	109.44
6	K	5201	1XE	O5P-C5P-N4P	-2.58	117.50	122.47
6	J	5201	1XE	CEP-CBP-CDP	-2.56	103.94	109.17
6	J	5201	1XE	O5P-C5P-N4P	-2.53	117.58	122.47
6	K	5201	1XE	C3P-C2P-S1P	-2.49	119.33	124.22
6	I	5201	1XE	C4A-C5A-N7A	-2.46	106.83	109.40
6	K	5201	1XE	CDP-CBP-CCP	2.38	112.11	108.23
6	I	5201	1XE	C3P-C2P-S1P	-2.33	119.63	124.22
6	J	5201	1XE	O21-C2-C1	2.33	120.01	110.83
6	K	5201	1XE	P3B-O3B-C3B	-2.26	115.88	123.96
6	J	5201	1XE	CDP-CBP-CCP	2.24	111.89	108.23
6	K	5201	1XE	C7P-C6P-C5P	2.22	116.05	112.36
6	L	5201	1XE	C2-C1-S1P	2.19	121.57	113.06
6	J	5201	1XE	C7P-N8P-C9P	-2.18	118.70	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	5201	1XE	CAP-C9P-N8P	2.13	120.82	116.58
6	L	5201	1XE	CDP-CBP-CAP	2.12	112.50	108.82
6	I	5201	1XE	O9P-C9P-N8P	-2.12	118.45	122.99
6	L	5201	1XE	P2A-O3A-P1A	-2.11	125.59	132.83
6	L	5201	1XE	C7P-C6P-C5P	2.10	115.85	112.36
6	I	5201	1XE	CDP-CBP-CCP	2.09	111.65	108.23
6	I	5201	1XE	P3B-O3B-C3B	-2.01	116.76	123.96

There are no chirality outliers.

All (67) 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	CCP-O6A-P2A-O3A
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	C5B-O5B-P1A-O1A
6	J	5201	1XE	C5B-O5B-P1A-O2A
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	CCP-O6A-P2A-O3A
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	CCP-O6A-P2A-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	I	5201	1XE	CDP-CBP-CCP-O6A

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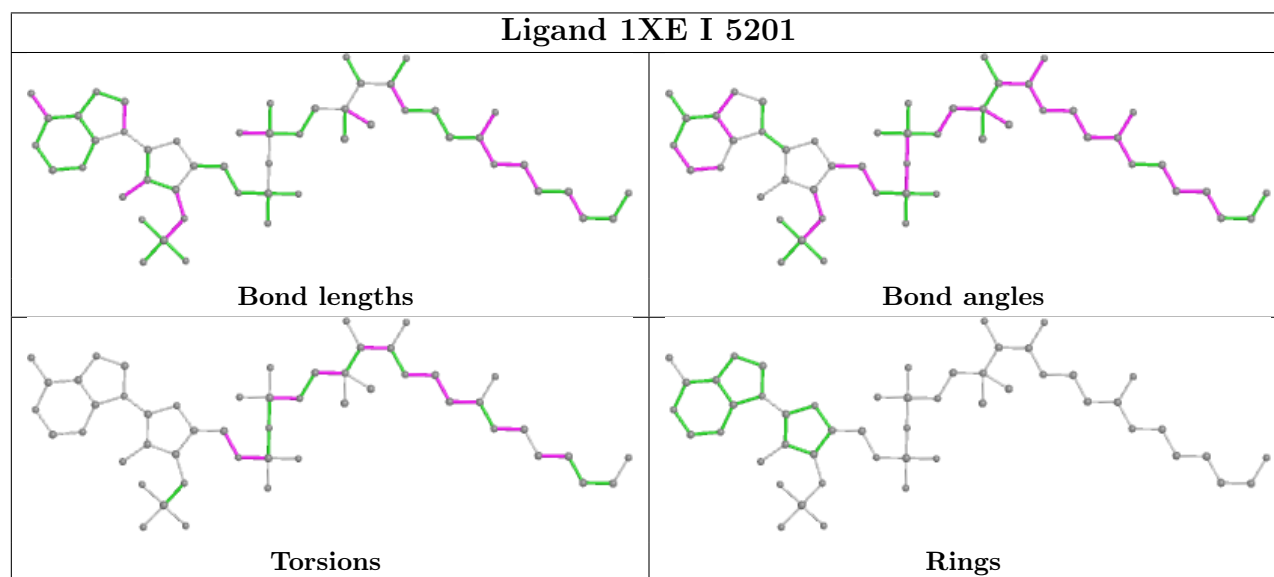
Mol	Chain	Res	Type	Atoms
6	K	5201	1XE	OAP-CAP-CBP-CEP
6	J	5201	1XE	P1A-O3A-P2A-O4A
6	K	5201	1XE	O9P-C9P-CAP-CBP
6	I	5201	1XE	C3P-C2P-S1P-C1
6	J	5201	1XE	C3P-C2P-S1P-C1
6	K	5201	1XE	C3P-C2P-S1P-C1
6	K	5201	1XE	N8P-C9P-CAP-CBP
6	I	5201	1XE	C6P-C7P-N8P-C9P
6	K	5201	1XE	C2P-C3P-N4P-C5P
6	L	5201	1XE	C2P-C3P-N4P-C5P
6	J	5201	1XE	C3B-O3B-P3B-O9A
6	I	5201	1XE	O5P-C5P-C6P-C7P
6	I	5201	1XE	N4P-C5P-C6P-C7P
6	J	5201	1XE	C5B-O5B-P1A-O3A
6	L	5201	1XE	C5B-O5B-P1A-O3A
6	I	5201	1XE	CCP-O6A-P2A-O4A
6	I	5201	1XE	CCP-O6A-P2A-O5A
6	K	5201	1XE	CCP-O6A-P2A-O5A
6	L	5201	1XE	CCP-O6A-P2A-O4A
6	L	5201	1XE	CCP-O6A-P2A-O5A
6	J	5201	1XE	CAP-CBP-CCP-O6A
6	K	5201	1XE	OAP-CAP-CBP-CCP
6	L	5201	1XE	CAP-CBP-CCP-O6A
6	I	5201	1XE	CEP-CBP-CCP-O6A
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	C2-C1-S1P-C2P
6	J	5201	1XE	CEP-CBP-CCP-O6A
6	J	5201	1XE	C2P-C3P-N4P-C5P
6	I	5201	1XE	N8P-C9P-CAP-OAP
6	J	5201	1XE	C9P-CAP-CBP-CDP
6	K	5201	1XE	C9P-CAP-CBP-CDP
6	I	5201	1XE	C5B-O5B-P1A-O3A
6	L	5201	1XE	P1A-O3A-P2A-O4A
6	L	5201	1XE	P1A-O3A-P2A-O5A
6	L	5201	1XE	CEP-CBP-CCP-O6A

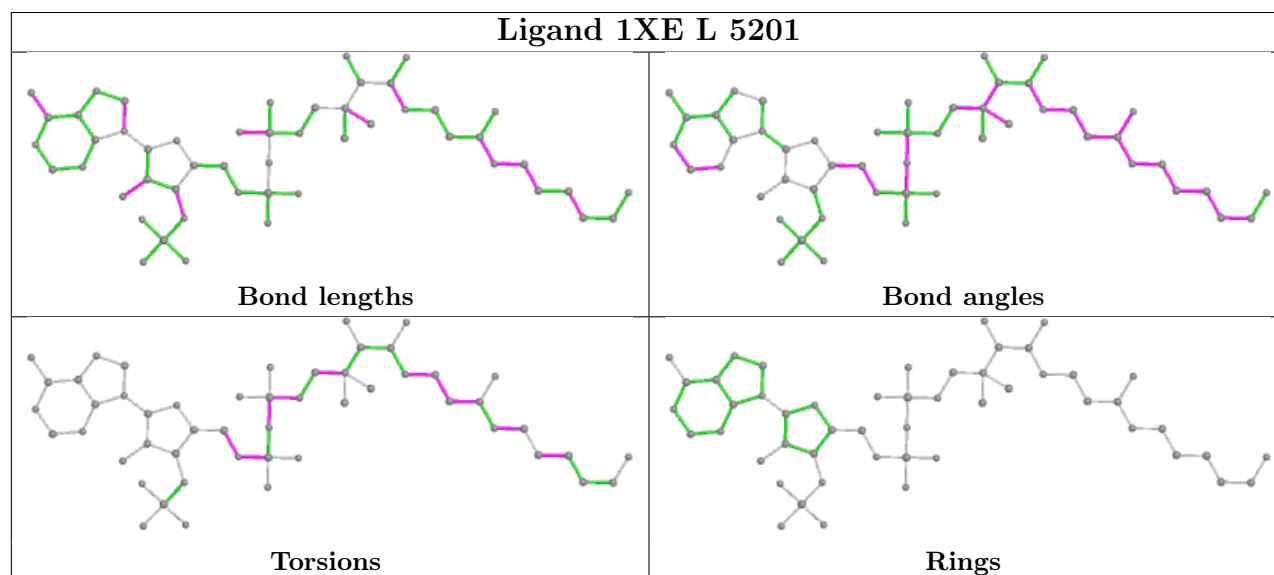
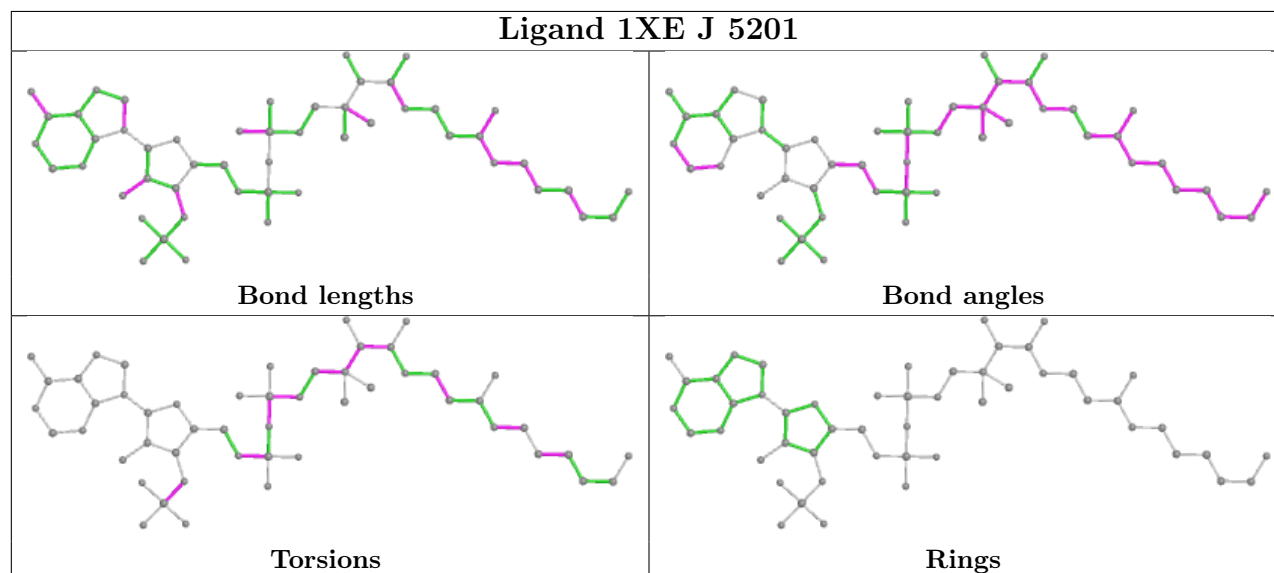
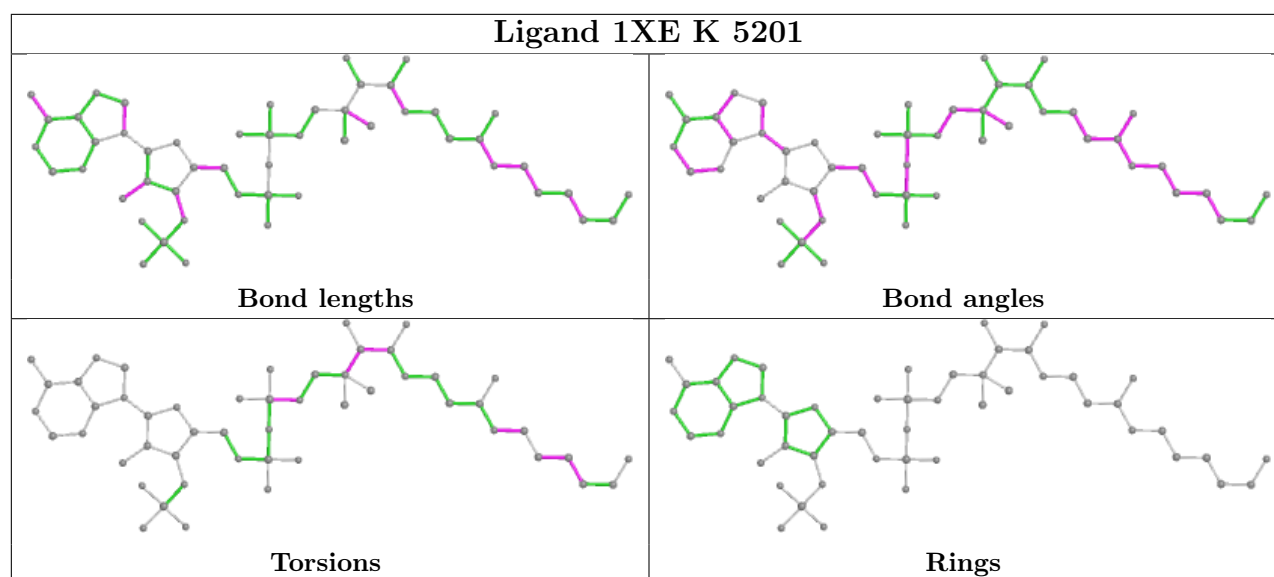
There are no ring outliers.

4 monomers are involved in 17 short contacts:

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

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





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	718/734 (97%)	0.35	41 (5%) 23 18	55, 89, 162, 258	0
1	B	722/734 (98%)	0.64	75 (10%) 6 4	52, 109, 199, 296	0
1	C	717/734 (97%)	0.56	56 (7%) 13 9	52, 104, 191, 257	0
1	D	718/734 (97%)	0.41	57 (7%) 12 9	56, 95, 180, 280	0
2	E	153/156 (98%)	0.36	2 (1%) 77 73	51, 72, 139, 167	0
2	F	153/156 (98%)	0.57	7 (4%) 32 26	58, 104, 168, 207	0
2	G	153/156 (98%)	0.72	9 (5%) 22 17	59, 110, 179, 215	0
2	H	153/156 (98%)	0.36	5 (3%) 46 39	52, 78, 137, 182	0
3	I	4/4 (100%)	0.09	0 100 100	60, 65, 80, 111	0
3	J	4/4 (100%)	0.25	0 100 100	80, 92, 100, 125	0
3	K	4/4 (100%)	0.25	0 100 100	90, 93, 130, 151	0
3	L	4/4 (100%)	0.03	0 100 100	65, 66, 88, 108	0
All	All	3503/3576 (97%)	0.49	252 (7%) 15 11	51, 96, 181, 296	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	731	ALA	17.1
1	C	730	ALA	16.0
1	B	730	ALA	10.4
1	C	370	ASN	9.9
1	A	38	GLU	8.5
1	B	374	GLU	7.8
1	C	351	VAL	7.6
1	C	37	LEU	6.9
1	B	351	VAL	6.8
1	C	371	SER	6.5
1	B	355	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
1	D	730	ALA	6.0
1	B	306	LEU	5.9
1	B	318	TYR	5.7
2	F	66	ASP	5.7
1	A	730	ALA	5.6
1	B	39	ARG	5.6
1	C	59	ASN	5.6
1	C	390	PHE	5.5
1	A	731	ALA	5.5
2	G	66	ASP	5.4
1	A	597	GLY	5.4
1	D	371	SER	5.3
1	B	281	TRP	5.3
1	B	370	ASN	5.3
1	D	731	ALA	5.2
1	C	312	LEU	5.2
1	D	59	ASN	5.2
1	A	42	GLU	4.9
1	B	38	GLU	4.9
1	B	69	LEU	4.9
1	D	729	ASN	4.9
1	D	76	GLY	4.9
1	D	179	GLY	4.8
1	C	181	PRO	4.8
1	C	383	TYR	4.8
1	B	364	PHE	4.5
1	D	71	LEU	4.4
1	B	372	GLN	4.4
2	G	134	ILE	4.4
1	B	347	VAL	4.3
1	C	347	VAL	4.3
1	A	370	ASN	4.3
1	B	293	PRO	4.2
1	C	306	LEU	4.2
1	C	39	ARG	4.2
1	A	729	ASN	4.1
1	C	374	GLU	4.1
1	C	480	VAL	4.1
1	D	374	GLU	4.1
1	C	33	ILE	4.0
1	A	369	ASP	4.0
1	B	305	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	13	LEU	3.9
1	A	373	ILE	3.9
1	D	10	GLU	3.9
1	D	72	ARG	3.9
1	C	318	TYR	3.9
1	B	479	ALA	3.9
1	B	259	TYR	3.9
1	A	591	PHE	3.8
1	A	182	VAL	3.8
1	D	182	VAL	3.8
1	B	368	ASP	3.8
1	C	13	LEU	3.8
1	C	364	PHE	3.8
1	D	648	LEU	3.7
1	A	648	LEU	3.6
1	B	729	ASN	3.6
1	C	293	PRO	3.6
1	B	390	PHE	3.6
1	B	288	LEU	3.6
1	D	409	HIS	3.6
1	D	292	TYR	3.6
1	B	59	ASN	3.5
1	B	383	TYR	3.5
1	A	409	HIS	3.4
2	E	1[A]	MET	3.4
1	C	707	LEU	3.4
1	A	39	ARG	3.4
1	C	57	LEU	3.4
1	A	59	ASN	3.4
1	B	359	SER	3.3
1	A	480	VAL	3.3
1	C	259	TYR	3.3
2	H	66	ASP	3.3
1	C	38	GLU	3.3
1	D	363	LYS	3.3
1	B	311	PHE	3.3
1	B	58	GLY	3.2
1	B	37	LEU	3.2
1	C	368	ASP	3.2
1	B	3	LYS	3.2
1	A	37	LEU	3.2
1	A	594	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	312	LEU	3.2
1	B	246	TYR	3.2
1	C	649	GLY	3.2
1	C	354	TYR	3.2
2	H	65	LYS	3.1
1	B	346	VAL	3.1
1	C	311	PHE	3.1
1	D	370	ASN	3.1
1	D	728	SER	3.1
1	C	479	ALA	3.1
1	A	694	ASP	3.1
1	C	648	LEU	3.1
1	D	373	ILE	3.0
1	B	263	GLN	3.0
1	C	246	TYR	3.0
1	D	81	TRP	3.0
1	D	177	ASN	3.0
1	D	178	GLN	2.9
1	B	265	ALA	2.9
1	B	298	PRO	2.9
1	B	313	THR	2.9
1	B	2	ALA	2.9
1	B	648	LEU	2.9
1	B	338	TYR	2.9
1	D	233	LEU	2.9
1	D	33	ILE	2.8
1	B	36	LEU	2.8
1	A	33	ILE	2.8
1	D	693	PHE	2.8
1	D	42	GLU	2.8
1	D	69	LEU	2.8
1	A	371	SER	2.8
1	D	369	ASP	2.8
1	D	480	VAL	2.8
2	F	146	TYR	2.8
1	D	715	ILE	2.8
1	D	30	LEU	2.8
1	A	293	PRO	2.7
1	C	369	ASP	2.7
2	G	146	TYR	2.7
1	B	242	LYS	2.7
1	A	57	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	181	PRO	2.7
1	C	627	GLU	2.7
2	G	1	MET	2.7
1	B	360	THR	2.7
1	A	686	LEU	2.7
1	B	319	LEU	2.7
1	D	53	LEU	2.7
1	A	576	LEU	2.7
1	C	338	TYR	2.7
1	B	303	LEU	2.6
1	D	721	TYR	2.6
1	B	354	TYR	2.6
1	B	337	LEU	2.6
1	B	603	GLU	2.6
2	G	135	GLU	2.6
1	B	396	LEU	2.6
1	C	282	LEU	2.6
1	A	290	LYS	2.6
1	B	280	GLU	2.6
1	B	649	GLY	2.5
1	A	233	LEU	2.5
2	G	153	SER	2.5
1	B	30	LEU	2.5
1	A	314	HIS	2.5
1	A	707	LEU	2.5
1	D	279	ALA	2.5
1	B	597	GLY	2.5
1	D	364	PHE	2.5
1	C	285	TYR	2.5
1	C	373	ILE	2.5
2	H	121	HIS	2.4
1	C	69	LEU	2.4
1	D	17	ALA	2.4
1	C	224	PHE	2.4
1	A	328	PRO	2.4
1	C	647	PRO	2.4
1	A	683	ALA	2.4
1	B	385	PHE	2.4
1	D	293	PRO	2.4
1	D	267	GLY	2.4
1	A	292	TYR	2.4
1	B	33	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	373	ILE	2.4
1	A	479	ALA	2.4
2	F	123	TYR	2.4
2	G	123	TYR	2.4
1	C	32	ALA	2.4
1	D	329	SER	2.4
1	B	707	LEU	2.4
1	D	115	LEU	2.3
1	B	297	CYS	2.3
1	A	54	LEU	2.3
1	C	281	TRP	2.3
1	D	180	VAL	2.3
1	A	360	THR	2.3
1	D	360	THR	2.3
1	D	725	LYS	2.3
1	B	317	LEU	2.3
1	C	319	LEU	2.3
1	D	700	LEU	2.3
1	C	355	ALA	2.3
1	A	69	LEU	2.3
2	F	85	LEU	2.3
1	B	302	PRO	2.2
2	F	112	VAL	2.2
1	D	692	ASN	2.2
2	F	86	GLY	2.2
1	C	315	VAL	2.2
1	B	285	TYR	2.2
1	B	339	LYS	2.2
1	D	67	VAL	2.2
1	D	351	VAL	2.2
1	B	14	PHE	2.2
1	D	720	PHE	2.2
1	B	384	TYR	2.1
1	B	309	ASP	2.1
1	D	173	GLU	2.1
1	C	317	LEU	2.1
1	B	728	SER	2.1
2	F	117	ARG	2.1
1	A	179	GLY	2.1
1	D	8	PRO	2.1
2	G	137	LYS	2.1
1	C	372	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	309	ASP	2.1
2	H	1	MET	2.1
1	B	334	VAL	2.1
1	C	211	LEU	2.1
2	G	122	LEU	2.1
1	C	710	ASN	2.1
1	A	644	ASP	2.1
1	C	344	CYS	2.1
1	D	416	LEU	2.1
1	A	62	GLU	2.1
1	C	305	LYS	2.1
1	B	389	HIS	2.1
1	D	707	LEU	2.1
1	D	110	ASN	2.1
1	B	454	CYS	2.1
1	C	727	GLN	2.1
1	B	627	GLU	2.1
2	H	17	CYS	2.1
1	A	50	LYS	2.1
1	C	35	PRO	2.0
1	D	479	ALA	2.0
1	B	601	GLU	2.0
1	D	686	LEU	2.0
1	B	344	CYS	2.0
2	E	66	ASP	2.0
1	B	341	THR	2.0
1	D	714	VAL	2.0
1	C	398	LYS	2.0
1	A	367	ASP	2.0
1	C	288	LEU	2.0
1	D	238	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	CL	B	808	1/1	-0.35	0.18	161,161,161,161	0
4	CL	D	805	1/1	0.08	1.56	288,288,288,288	0
4	CL	C	813	1/1	0.09	0.24	137,137,137,137	0
4	CL	A	812	1/1	0.10	0.27	141,141,141,141	0
4	CL	D	803	1/1	0.30	0.43	118,118,118,118	0
4	CL	C	803	1/1	0.48	0.17	129,129,129,129	0
4	CL	B	806	1/1	0.54	0.63	151,151,151,151	0
4	CL	F	201	1/1	0.56	0.92	148,148,148,148	0
4	CL	A	804	1/1	0.57	0.09	143,143,143,143	0
4	CL	B	807	1/1	0.58	0.66	140,140,140,140	0
4	CL	B	813	1/1	0.59	0.88	145,145,145,145	0
4	CL	E	202	1/1	0.59	0.31	102,102,102,102	0
4	CL	A	807	1/1	0.59	0.30	148,148,148,148	0
4	CL	D	806	1/1	0.64	0.48	139,139,139,139	0
4	CL	C	807	1/1	0.67	0.41	125,125,125,125	0
4	CL	D	804	1/1	0.67	0.20	132,132,132,132	0
4	CL	D	802	1/1	0.70	0.17	149,149,149,149	0
4	CL	D	807	1/1	0.71	0.30	173,173,173,173	0
4	CL	D	810	1/1	0.71	0.30	157,157,157,157	0
4	CL	B	815	1/1	0.74	0.27	192,192,192,192	0
4	CL	D	812	1/1	0.74	0.21	138,138,138,138	0
4	CL	D	809	1/1	0.75	0.24	127,127,127,127	0
4	CL	C	804	1/1	0.76	0.22	118,118,118,118	0
4	CL	G	201	1/1	0.76	0.14	133,133,133,133	0
4	CL	D	813	1/1	0.79	0.41	130,130,130,130	0
4	CL	A	809	1/1	0.79	0.15	125,125,125,125	0
4	CL	A	808	1/1	0.79	0.36	113,113,113,113	0
4	CL	B	801	1/1	0.79	0.14	127,127,127,127	0
4	CL	A	811	1/1	0.80	0.67	188,188,188,188	0
4	CL	C	801	1/1	0.81	0.09	111,111,111,111	0
4	CL	C	812	1/1	0.81	0.75	126,126,126,126	0
4	CL	B	804	1/1	0.81	0.41	107,107,107,107	0
4	CL	B	816	1/1	0.81	0.11	107,107,107,107	0
4	CL	C	808	1/1	0.83	0.26	110,110,110,110	0
4	CL	B	805	1/1	0.83	0.23	108,108,108,108	0
4	CL	C	809	1/1	0.85	0.11	151,151,151,151	0

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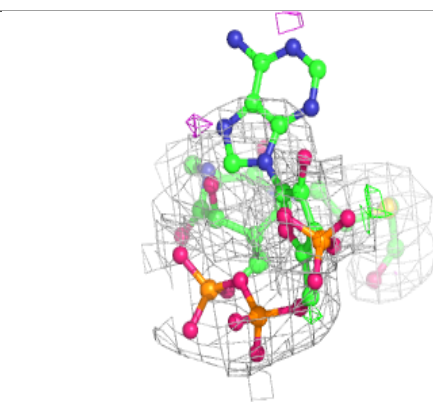
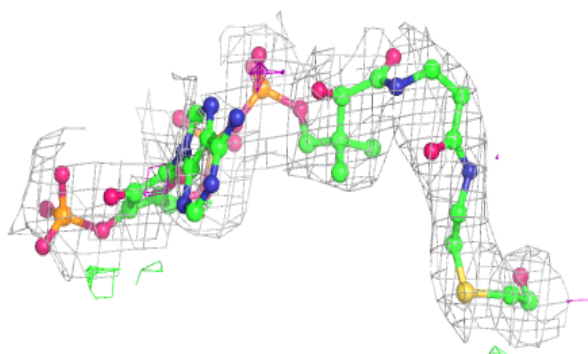
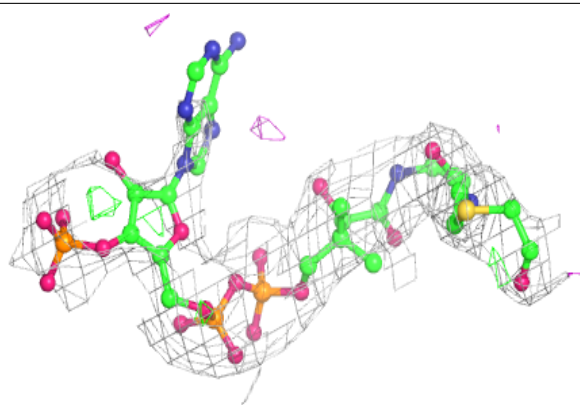
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	C	806	1/1	0.85	0.13	117,117,117,117	0
4	CL	B	814	1/1	0.85	0.17	141,141,141,141	0
4	CL	C	805	1/1	0.85	0.11	119,119,119,119	0
4	CL	A	806	1/1	0.87	0.17	145,145,145,145	0
4	CL	E	203	1/1	0.87	0.14	110,110,110,110	0
4	CL	B	809	1/1	0.87	0.19	109,109,109,109	0
4	CL	D	815	1/1	0.87	0.26	105,105,105,105	0
4	CL	A	810	1/1	0.88	0.41	86,86,86,86	0
4	CL	D	808	1/1	0.89	0.39	131,131,131,131	0
4	CL	B	812	1/1	0.89	0.34	112,112,112,112	0
6	1XE	J	5201	51/52	0.89	0.20	67,142,228,241	0
6	1XE	K	5201	51/52	0.89	0.21	53,128,279,303	0
4	CL	A	814	1/1	0.90	0.10	120,120,120,120	0
4	CL	B	803	1/1	0.91	0.12	99,99,99,99	0
4	CL	A	805	1/1	0.91	0.24	138,138,138,138	0
4	CL	B	810	1/1	0.92	0.30	99,99,99,99	0
5	SO4	D	816	5/5	0.92	0.14	80,110,119,124	0
4	CL	A	803	1/1	0.92	0.08	99,99,99,99	0
4	CL	D	801	1/1	0.92	0.11	93,93,93,93	0
4	CL	C	802	1/1	0.93	0.33	106,106,106,106	0
6	1XE	I	5201	51/52	0.93	0.22	49,92,190,217	0
4	CL	C	811	1/1	0.94	0.19	94,94,94,94	0
4	CL	H	201	1/1	0.94	0.27	84,84,84,84	0
6	1XE	L	5201	51/52	0.94	0.21	49,92,179,181	0
4	CL	D	814	1/1	0.95	0.54	110,110,110,110	0
4	CL	C	810	1/1	0.95	0.35	97,97,97,97	0
4	CL	A	801	1/1	0.95	0.49	96,96,96,96	0
4	CL	A	813	1/1	0.96	0.18	124,124,124,124	0
4	CL	A	802	1/1	0.97	0.19	93,93,93,93	0
4	CL	E	201	1/1	0.97	0.26	79,79,79,79	0
5	SO4	A	815	5/5	0.98	0.12	88,104,110,121	0
4	CL	B	811	1/1	0.98	0.37	99,99,99,99	0
4	CL	D	811	1/1	0.98	0.23	73,73,73,73	0
4	CL	B	802	1/1	0.99	0.33	96,96,96,96	0

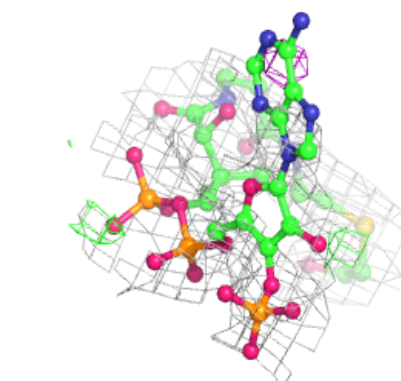
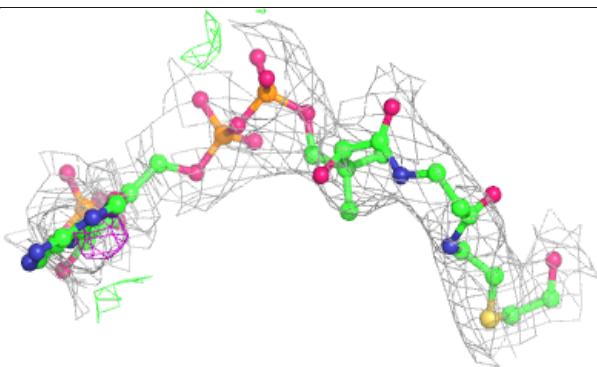
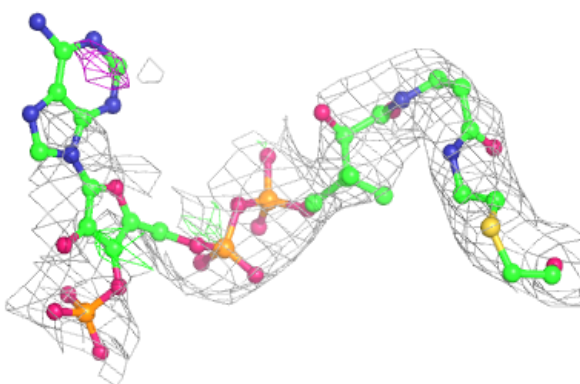
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

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

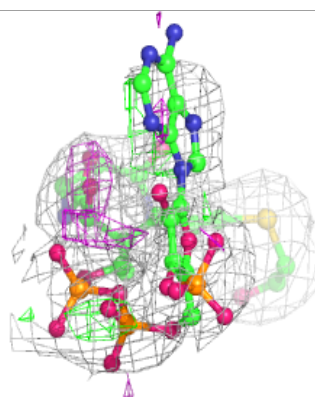
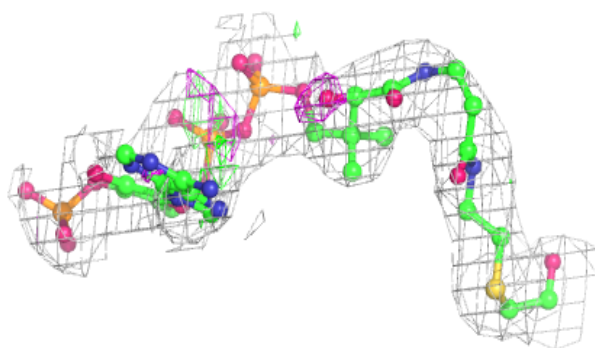
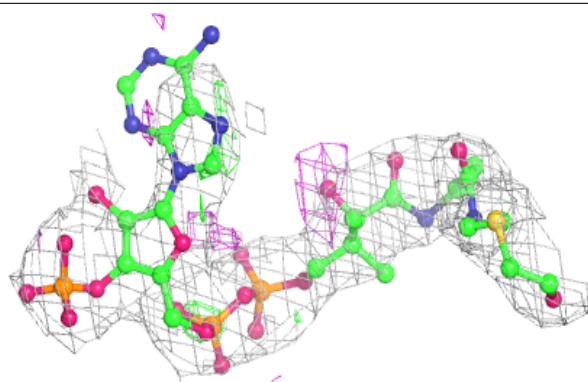
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



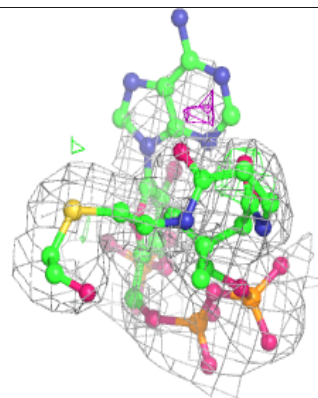
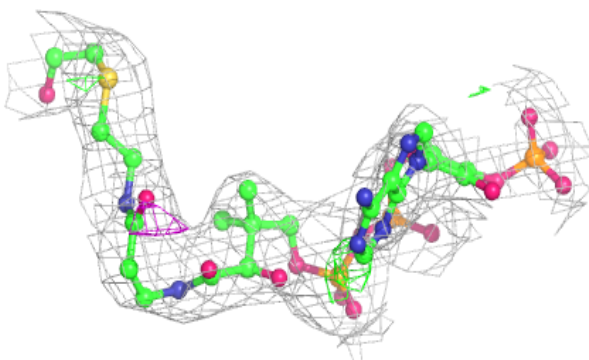
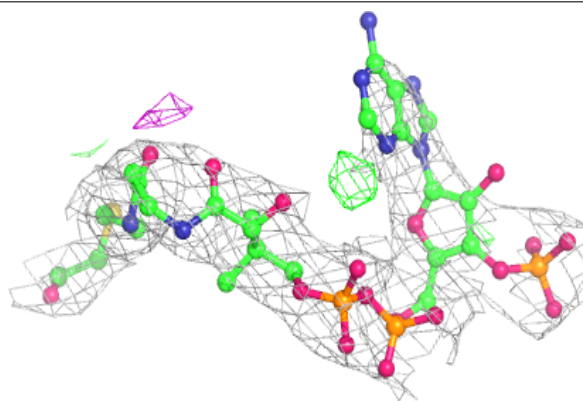


**Electron density around 1XE I 5201:**

$2mF_o-DF_c$  (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.