



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:41 am BST

PDB ID : 2FZK  
Title : The Structure of Wild-Type E. Coli Aspartate Transcarbamoylase in Complex with Novel T State Inhibitors at 2.50 Resolution  
Authors : Heng, S.; Stieglitz, K.A.; Eldo, J.; Xia, J.; Cardia, J.P.; Kantrowitz, E.R.  
Deposited on : 2006-02-09  
Resolution : 2.50 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 : 2.11  
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) : 2.11

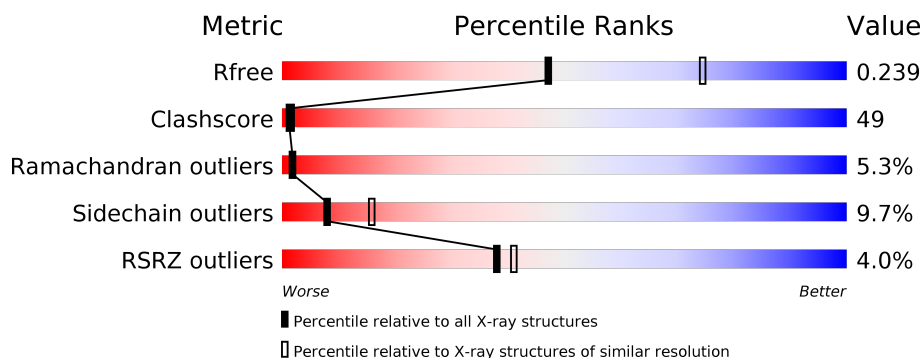
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	310	<div> <div>2%</div> <div> <div>44%</div> <div>51%</div> <div>5%</div> </div> </div>
1	C	310	<div> <div>3%</div> <div> <div>45%</div> <div>47%</div> <div>8%</div> </div> </div>
2	B	153	<div> <div>8%</div> <div> <div>17%</div> <div>58%</div> <div>21%</div> </div> </div>
2	D	153	<div> <div>5%</div> <div> <div>33%</div> <div>56%</div> <div>10%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EOZ	A	611	-	-	X	X
3	EOZ	C	612	-	-	X	-
5	CTP	B	901	-	-	X	-
5	CTP	D	902	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7855 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.

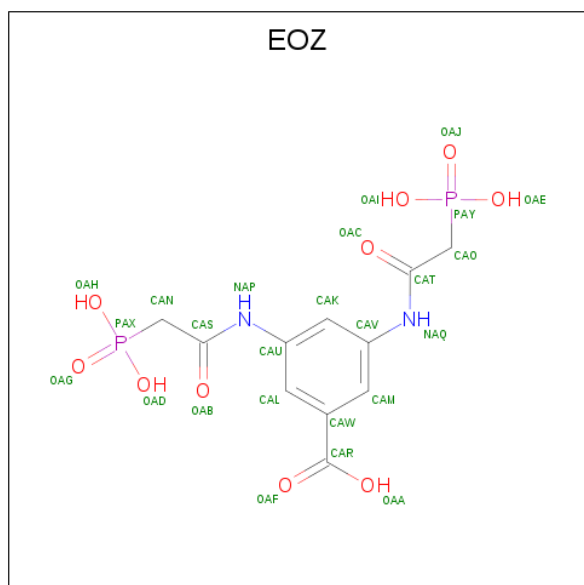
- Molecule 1 is a protein called Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	0	0
			1193	747	212	229	5			
2	D	152	Total	C	N	O	S	0	0	0
			1193	747	212	229	5			

- Molecule 3 is 3,5-BIS[(PHOSPHONOACETYL)AMINO]BENZOIC ACID (three-letter code: EOZ) (formula:  $C_{11}H_{14}N_2O_{10}P_2$ ).

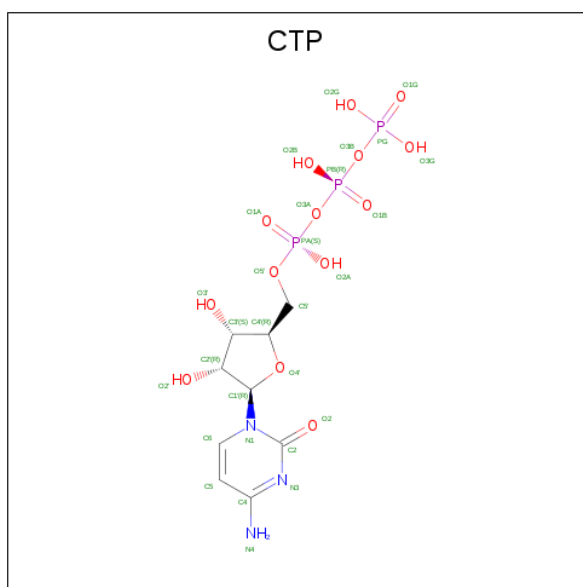


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	11	2	10	2		
3	C	1	Total	C	N	O	P	0	0
			25	11	2	10	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
5	D	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 6 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	161	Total	O	0	0
			161	161		


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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	87	Total 87	O 87	0	0
6	C	190	Total 190	O 190	0	0
6	D	91	Total 91	O 91	0	0

These plots are drawn for all protein, RNA and DNA 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.

- Chain A: 

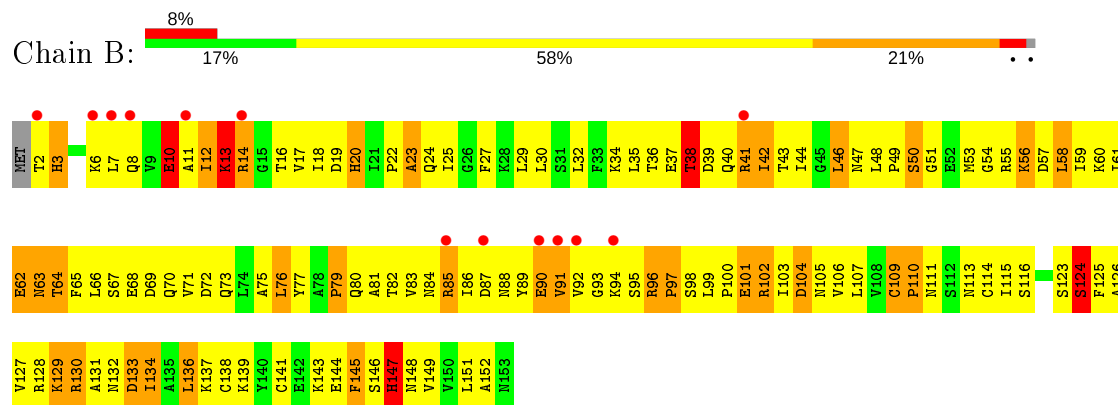


Item	Item	Item	Item	Item	Item	Item	Item	Item	Item
A1	B2	C3	D4	E5	F6	G7	H8	I9	J10
K11	L12	M13	N14	O15	P16	Q17	R18	S19	T20
U21	V22	W23	X24	Y25	Z26	A27	B28	C29	D30
E31	F32	G33	H34	I35	J36	K37	L38	M39	N40
O41	P42	Q43	R44	S45	T46	U47	V48	W49	X50
Y51	Z52	A53	B54	C55	D56	E57	F58	G59	H60
I61	J62	K63	L64	M65	N66	O67	P68	Q69	R70
S71	T72	U73	V74	W75	X76	Y77	Z78	A79	B80
C81	D82	E83	F84	G85	H86	I87	J88	K89	L90
M91	N92	O93	P94	Q95	R96	S97	T98	U99	V99

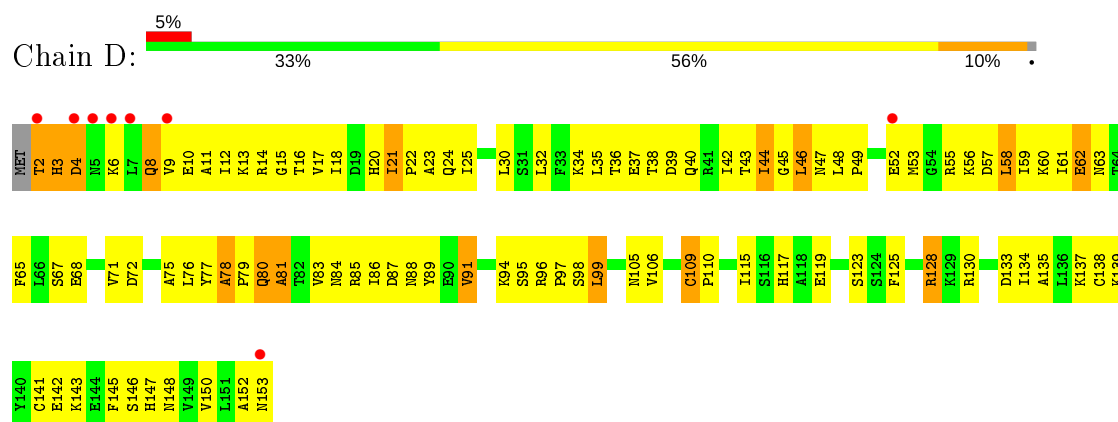
- Chain C:**

Node	Status
A1	Good
M2	Good
P3	Fair
L4	Fair
Y5	Good
Q6	Poor
K7	Good
H8	Marginal
I9	Good
J10	Fair
S11	Good
I12	Good
N13	Fair
D14	Marginal
L15	Fair
S16	Good
D19	Marginal
V23	Fair
L24	Fair
K29	Good
Q35	Poor
P36	Fair
E37	Good
L38	Fair
L39	Fair
K40	Good
H41	Marginal
K42	Good
V43	Fair
B54	Marginal
T55	Fair
R56	Fair
F59	Marginal
E60	Fair
H63	Marginal
L66	Fair
S74	Good
D75	Marginal
S76	Good
A77	Good
M78	Good
T79	Critical
S80	Good
L81	Fair
G82	Fair
K83	Good
K84	Good
G85	Fair
E86	Fair
V89	Fair
A92	Good
S93	Fair
T97	Fair
Y98	Good
V99	Fair
V103	Fair
H106	Marginal
P107	Fair
Q108	Poor
E109	Fair
A112	Good
R113	Good
L114	Fair
A115	Fair
T116	Fair
E117	Good
F118	Marginal
S119	Good
G120	Fair
N121	Fair
V122	Fair
G130	Fair
S131	Good
N132	Fair
Q133	Poor
H134	Marginal
P135	Fair
T136	Good
Q137	Poor
T138	Fair
L139	Fair
L140	Fair
D141	Marginal
L142	Fair
F143	Marginal
T144	Fair
L145	Fair
Q146	Good
E147	Good
T148	Fair
Q149	Fair
D153	Marginal
N154	Fair
L155	Fair
A158	Good
M159	Good
V160	Fair
G161	Fair
D162	Marginal
G163	Fair
K164	Good
V165	Fair
C166	Fair
R167	Fair
T168	Fair
V169	Fair
H170	Marginal
Q174	Poor
A175	Good
L176	Fair
A177	Good
K178	Good
F179	Marginal
D180	Marginal
G181	Fair
N182	Fair
Y185	Good
F186	Marginal
P195	Fair
Q196	Poor
R269	Good
L198	Fair
D200	Marginal
M201	Fair
L202	Fair
D203	Fair
E204	Good
K205	Fair
G206	Fair
D207	Marginal
L211	Fair
H212	Marginal
S213	Fair
S214	Fair
E217	Fair
V218	Good
A235	Good
V222	Fair
D223	Marginal
L224	Fair
M227	Fair
A301	Good
T228	Fair
R229	Marginal
V230	Fair
Q231	Marginal
K232	Fair
E233	Good
R234	Marginal
L235	Fair
S238	Fair
E239	Fair
Y240	Good
A241	Fair
M242	Good
V243	Good

- Molecule 2: Aspartate carbamoyltransferase regulatory chain



- Molecule 2: Aspartate carbamoyltransferase regulatory chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.90Å 120.90Å 141.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.45 – 2.50 28.45 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.45-2.50) 99.0 (28.45-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.01 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.211 , 0.239 0.211 , 0.239	Depositor DCC
$R_{free}$ test set	4218 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.247 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7855	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: EOZ, ZN, CTP

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	0.74	1/2461 (0.0%)	0.84	1/3339 (0.0%)
1	C	0.78	1/2461 (0.0%)	0.88	0/3339
2	B	0.65	1/1211 (0.1%)	0.94	3/1637 (0.2%)
2	D	0.69	1/1211 (0.1%)	0.91	4/1637 (0.2%)
All	All	0.73	4/7344 (0.1%)	0.88	8/9952 (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
2	B	0	1
2	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLU	CD-OE2	9.55	1.36	1.25
1	C	147	GLU	CD-OE2	8.06	1.34	1.25
2	D	109	CYS	C-N	6.03	1.45	1.34
2	B	109	CYS	C-N	5.35	1.44	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	109	CYS	C-N-CD	9.10	147.51	128.40
2	B	109	CYS	C-N-CD	8.91	147.12	128.40
2	D	110	PRO	CA-N-CD	-7.38	101.17	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	58	LEU	CA-CB-CG	7.16	131.77	115.30
2	B	110	PRO	CA-N-CD	-6.79	102.00	111.50
1	A	269	ARG	N-CA-C	-5.68	95.66	111.00
2	B	3	HIS	N-CA-C	5.55	125.99	111.00
2	D	110	PRO	N-CA-CB	5.03	109.34	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	109	CYS	Mainchain
2	D	109	CYS	Mainchain

## 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	2415	0	2422	176	0
1	C	2415	0	2422	237	0
2	B	1193	0	1207	184	0
2	D	1193	0	1207	124	0
3	A	25	0	9	16	0
3	C	25	0	9	35	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	29	0	12	13	0
5	D	29	0	12	10	0
6	A	161	0	0	19	0
6	B	87	0	0	20	0
6	C	190	0	0	22	0
6	D	91	0	0	12	0
All	All	7855	0	7300	723	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

All (723) 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)
2:B:99:LEU:HD12	2:B:100:PRO:HD2	1.26	1.18
1:C:137:GLN:HG3	1:C:296:ARG:NH2	1.59	1.17
1:A:94:VAL:HB	6:A:612:HOH:O	1.41	1.16
3:A:611:EOZ:HAN1	3:A:611:EOZ:HAL	1.29	1.14
1:C:168:THR:CG2	3:C:612:EOZ:HAP	1.60	1.13
1:C:231:GLN:NE2	1:C:234:ARG:HE	1.45	1.12
1:C:145:ILE:HD12	1:C:224:ILE:HG12	1.26	1.12
2:D:96:ARG:HD3	2:D:97:PRO:HD2	1.31	1.12
3:C:612:EOZ:HAN2	3:C:612:EOZ:HAK	1.21	1.11
2:D:11:ALA:HB1	5:D:902:CTP:HN41	1.06	1.11
1:C:10:ILE:HD11	1:C:116:THR:HG21	1.32	1.09
1:C:168:THR:HG22	3:C:612:EOZ:HAP	1.21	1.05
1:A:302:LEU:HD23	1:A:308:LEU:HD23	1.38	1.04
1:A:229:ARG:HB3	3:A:611:EOZ:OAG	1.58	1.01
2:D:2:THR:N	5:D:902:CTP:HO2'	1.59	0.98
1:C:168:THR:HB	3:C:612:EOZ:OAB	1.64	0.98
2:B:75:ALA:HB3	2:B:100:PRO:HD3	1.44	0.97
2:D:11:ALA:HB1	5:D:902:CTP:N4	1.78	0.97
2:D:13:LYS:HA	6:D:965:HOH:O	1.64	0.96
1:C:269:ARG:O	1:C:269:ARG:HD2	1.66	0.96
1:C:149:GLN:HE22	1:C:260:ASN:ND2	1.62	0.95
1:C:137:GLN:HB3	3:C:612:EOZ:PAX	2.06	0.94
2:D:13:LYS:O	2:D:87:ASP:HA	1.69	0.93
2:B:48:LEU:O	2:B:55:ARG:HA	1.68	0.92
1:C:137:GLN:NE2	1:C:140:LEU:HD21	1.85	0.92
2:B:67:SER:O	2:B:71:VAL:HG23	1.70	0.92
3:C:612:EOZ:HAN2	3:C:612:EOZ:CAK	1.93	0.91
2:D:21:ILE:HG12	2:D:57:ASP:O	1.70	0.91
2:B:6:LYS:HG3	2:B:7:LEU:HD12	1.51	0.90
1:C:266:PRO:CB	3:C:612:EOZ:OAD	2.18	0.90
1:C:231:GLN:HE21	1:C:234:ARG:HE	1.19	0.90
3:C:612:EOZ:CAN	3:C:612:EOZ:HAK	2.01	0.90
1:C:137:GLN:HG3	1:C:296:ARG:HH22	1.28	0.90
1:C:154:ASN:HD22	1:C:181:GLY:HA3	1.37	0.89
1:A:81:LEU:HD12	1:A:91:THR:HA	1.53	0.88
1:C:79:THR:OG1	1:C:84:LYS:HA	1.74	0.88
2:B:19:ASP:OD1	2:B:58:LEU:HD22	1.73	0.87
1:A:101:ALA:HB2	1:A:304:LEU:HD21	1.56	0.87
1:A:55:THR:OG1	3:A:611:EOZ:HAO2	1.74	0.87
2:B:130:ARG:C	2:B:132:ASN:H	1.78	0.87
2:D:48:LEU:O	2:D:55:ARG:HA	1.74	0.86
2:D:89:TYR:N	6:D:965:HOH:O	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:GLN:HG2	1:C:140:LEU:CD2	2.06	0.85
2:D:14:ARG:O	2:D:63:ASN:HA	1.75	0.85
1:A:145:ILE:HG23	1:A:224:ILE:HD12	1.59	0.84
1:A:265:HIS:H	1:A:288:GLN:HE22	1.24	0.84
2:D:96:ARG:HD3	2:D:97:PRO:CD	2.06	0.84
1:C:231:GLN:NE2	1:C:234:ARG:NE	2.26	0.83
2:D:2:THR:N	5:D:902:CTP:HO3'	1.76	0.83
1:A:92:ILE:HG12	1:A:115:ALA:HB1	1.61	0.83
1:C:137:GLN:HB2	3:C:612:EOZ:HAN1	1.60	0.83
1:C:168:THR:CG2	3:C:612:EOZ:NAP	2.41	0.83
2:B:103:ILE:O	2:B:124:SER:HA	1.79	0.82
2:D:3:HIS:CD2	2:D:3:HIS:H	1.95	0.82
1:A:223:ASP:O	1:A:261:MET:HA	1.80	0.82
1:A:29:LYS:HE3	6:A:639:HOH:O	1.78	0.82
2:B:2:THR:HG21	5:B:901:CTP:O1B	1.79	0.82
1:C:140:LEU:HD22	1:C:292:GLY:CA	2.09	0.82
1:C:145:ILE:HD12	1:C:224:ILE:CG1	2.09	0.81
1:C:162:ASP:OD2	1:C:165:TYR:HB2	1.79	0.81
2:B:44:ILE:HB	2:D:44:ILE:HG12	1.63	0.80
1:A:74:SER:O	1:A:76:SER:N	2.15	0.80
1:C:168:THR:HG21	3:C:612:EOZ:HAP	1.46	0.80
2:B:18:ILE:H	2:B:18:ILE:HD12	1.46	0.80
1:C:137:GLN:NE2	3:C:612:EOZ:OAG	2.15	0.79
1:C:137:GLN:CD	1:C:140:LEU:HD21	2.03	0.79
1:C:145:ILE:CD1	1:C:224:ILE:HG12	2.08	0.79
1:A:81:LEU:HD11	1:A:94:VAL:HG11	1.63	0.79
1:C:2:ASN:HD22	1:C:5:TYR:N	1.81	0.79
1:C:137:GLN:HG3	1:C:296:ARG:CZ	2.12	0.79
2:D:134:ILE:H	2:D:147:HIS:HD2	1.31	0.78
1:C:10:ILE:CD1	1:C:116:THR:HG21	2.11	0.78
2:D:75:ALA:HB3	6:D:968:HOH:O	1.83	0.78
1:C:231:GLN:HE22	1:C:234:ARG:HH11	1.32	0.78
2:D:49:PRO:HB3	6:D:905:HOH:O	1.83	0.77
1:A:269:ARG:C	1:A:269:ARG:HD2	2.03	0.77
1:A:51:ALA:HB2	1:A:75:ASP:HB3	1.63	0.77
1:A:229:ARG:NH2	1:A:268:PRO:HD2	1.99	0.77
1:A:145:ILE:HG12	1:A:224:ILE:HD13	1.66	0.77
1:A:243:VAL:HA	1:A:246:GLN:NE2	2.00	0.77
2:B:99:LEU:HD12	2:B:100:PRO:CD	2.13	0.77
2:B:71:VAL:O	2:B:97:PRO:HB3	1.85	0.76
1:C:81:LEU:O	1:C:86:GLU:HB3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:TYR:HD1	6:D:965:HOH:O	1.68	0.76
1:C:149:GLN:HE22	1:C:260:ASN:HD21	1.34	0.75
1:A:61:THR:O	1:A:65:ARG:HG2	1.87	0.75
1:A:183:ARG:HH21	1:A:208:ALA:HB1	1.52	0.75
2:D:72:ASP:OD1	2:D:98:SER:HB2	1.85	0.75
2:D:80:GLN:HG2	2:D:81:ALA:N	2.00	0.75
2:B:130:ARG:C	2:B:132:ASN:N	2.36	0.74
2:D:65:PHE:HD2	2:D:85:ARG:HE	1.36	0.74
2:B:68:GLU:O	2:B:71:VAL:HB	1.88	0.73
1:C:149:GLN:NE2	1:C:260:ASN:ND2	2.35	0.73
1:C:154:ASN:ND2	1:C:181:GLY:HA3	2.02	0.73
2:B:107:LEU:HB2	6:B:906:HOH:O	1.87	0.73
2:D:45:GLY:O	2:D:57:ASP:HA	1.89	0.73
3:A:611:EOZ:OAC	3:A:611:EOZ:HAK	1.87	0.73
2:B:11:ALA:HB1	5:B:901:CTP:N3	2.03	0.73
1:C:244:LYS:NZ	1:C:248:VAL:HG21	2.03	0.73
1:A:84:LYS:HA	6:A:661:HOH:O	1.88	0.72
3:A:611:EOZ:HAN1	3:A:611:EOZ:CAL	2.08	0.72
2:B:12:ILE:O	5:B:901:CTP:N4	2.20	0.72
2:B:41:ARG:O	2:B:62:GLU:HB2	1.90	0.72
1:C:54:ARG:HB3	3:C:612:EOZ:OAJ	1.90	0.72
2:B:86:ILE:HG12	2:B:91:VAL:HA	1.71	0.71
1:A:219:MET:CE	1:A:254:LEU:HD22	2.19	0.71
2:B:71:VAL:HG12	2:B:97:PRO:HG3	1.71	0.71
1:C:82:GLY:HA3	1:C:86:GLU:HB2	1.71	0.71
1:C:137:GLN:CD	3:C:612:EOZ:OAG	2.29	0.71
2:B:12:ILE:HD12	2:B:62:GLU:HG2	1.71	0.71
1:C:214:SER:OG	1:C:217:GLU:HG2	1.90	0.71
2:B:73:GLN:HG2	6:B:922:HOH:O	1.89	0.71
2:D:40:GLN:O	2:D:42:ILE:HG13	1.91	0.70
2:B:84:ASN:HB3	2:B:86:ILE:HG13	1.72	0.70
2:B:71:VAL:CG1	2:B:97:PRO:HG3	2.21	0.70
1:C:266:PRO:HB2	3:C:612:EOZ:OAD	1.91	0.70
1:C:137:GLN:CB	3:C:612:EOZ:PAX	2.79	0.70
1:C:137:GLN:HG2	1:C:140:LEU:HD23	1.72	0.70
2:D:76:LEU:HD21	2:D:134:ILE:HD12	1.74	0.70
2:B:44:ILE:HB	2:D:44:ILE:CG1	2.21	0.70
1:C:153:ASP:OD1	1:C:179:PHE:HB3	1.92	0.70
1:C:121:ASN:ND2	1:C:121:ASN:H	1.90	0.70
1:A:82:GLY:HA3	1:A:86:GLU:HG2	1.74	0.70
1:C:59:PHE:CE2	1:C:296:ARG:HG2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:THR:OG1	2:D:39:ASP:N	2.24	0.69
1:A:1:ALA:HB1	1:A:306:ARG:O	1.93	0.69
2:D:20:HIS:HA	2:D:56:LYS:HD2	1.72	0.69
1:A:32:ALA:HB3	6:A:656:HOH:O	1.91	0.69
2:D:65:PHE:CE2	2:D:85:ARG:HG2	2.28	0.69
2:D:15:GLY:HA3	2:D:62:GLU:HA	1.74	0.69
2:B:12:ILE:HD12	2:B:62:GLU:CG	2.22	0.69
2:D:21:ILE:HD13	2:D:21:ILE:N	2.06	0.69
1:C:136:THR:HB	1:C:296:ARG:HH21	1.58	0.69
1:C:137:GLN:HB2	3:C:612:EOZ:CAN	2.22	0.69
1:C:36:PRO:HG2	6:C:704:HOH:O	1.93	0.69
2:B:32:LEU:HD22	2:B:106:VAL:HB	1.73	0.68
1:C:242:ASN:O	1:C:244:LYS:N	2.25	0.68
2:D:115:ILE:HG13	2:D:119:GLU:HG3	1.76	0.68
2:D:128:ARG:O	2:D:128:ARG:HG2	1.93	0.68
2:B:19:ASP:O	2:B:20:HIS:HB2	1.93	0.68
1:C:279:LYS:HB3	1:C:279:LYS:NZ	2.09	0.68
1:C:137:GLN:HB3	3:C:612:EOZ:OAH	1.94	0.68
1:A:81:LEU:HD13	1:A:82:GLY:N	2.09	0.68
1:C:265:HIS:HE2	1:C:272:GLU:HG3	1.59	0.68
2:B:38:THR:HG21	6:B:980:HOH:O	1.92	0.67
1:A:136:THR:HG22	1:A:299:LEU:CD2	2.24	0.67
2:D:40:GLN:NE2	2:D:63:ASN:HB2	2.09	0.67
1:A:106:HIS:ND1	1:A:107:PRO:HD2	2.09	0.67
1:A:125:LEU:HD12	1:A:125:LEU:N	2.09	0.67
2:D:12:ILE:HG21	2:D:62:GLU:HB2	1.75	0.67
1:C:121:ASN:H	1:C:121:ASN:HD22	1.42	0.67
1:C:168:THR:HG21	3:C:612:EOZ:NAP	2.07	0.67
1:C:269:ARG:C	1:C:269:ARG:HD2	2.15	0.67
2:B:69:ASP:O	2:B:72:ASP:N	2.26	0.67
1:C:231:GLN:HE22	1:C:234:ARG:NH1	1.93	0.67
1:A:229:ARG:NH2	3:A:611:EOZ:OAH	2.26	0.66
1:A:1:ALA:HB2	1:A:306:ARG:HG3	1.77	0.66
2:B:22:PRO:HB2	2:B:25:ILE:HD12	1.78	0.66
2:B:13:LYS:H	2:B:13:LYS:HD2	1.59	0.66
1:C:137:GLN:CB	3:C:612:EOZ:HAN1	2.25	0.66
1:C:40:LYS:O	1:C:41:HIS:HB2	1.95	0.66
2:B:43:THR:O	2:B:44:ILE:HD13	1.96	0.66
1:C:269:ARG:HA	1:C:272:GLU:OE2	1.95	0.66
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.78	0.65
1:C:244:LYS:O	1:C:246:GLN:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:O	1:A:91:THR:HB	1.96	0.65
1:A:81:LEU:HD11	1:A:94:VAL:CG1	2.26	0.65
2:B:72:ASP:O	2:B:75:ALA:N	2.23	0.65
1:A:187:ILE:HG12	1:A:212:HIS:HB2	1.78	0.65
2:B:13:LYS:HA	2:B:89:TYR:H	1.62	0.65
1:A:219:MET:HE3	1:A:254:LEU:HD22	1.79	0.65
2:B:50:SER:HB2	2:B:54:GLY:H	1.62	0.65
1:C:149:GLN:NE2	1:C:260:ASN:HD21	1.95	0.65
2:B:42:ILE:HD11	2:D:47:ASN:OD1	1.96	0.65
2:B:39:ASP:O	2:D:55:ARG:NH2	2.30	0.64
1:C:161:GLY:HA3	1:C:228:THR:HG22	1.78	0.64
2:D:68:GLU:O	2:D:72:ASP:OD2	2.15	0.64
1:C:307:ASP:HB3	6:C:738:HOH:O	1.98	0.64
1:A:216:GLU:HG2	6:A:687:HOH:O	1.98	0.64
1:C:140:LEU:HD22	1:C:292:GLY:HA2	1.76	0.64
2:B:98:SER:HA	6:B:913:HOH:O	1.97	0.64
2:D:22:PRO:HG3	2:D:80:GLN:OE1	1.97	0.64
2:B:125:PHE:HA	2:B:137:LYS:O	1.97	0.64
2:D:2:THR:N	5:D:902:CTP:C3'	2.61	0.64
1:C:108:GLN:HB2	6:C:655:HOH:O	1.98	0.64
1:C:2:ASN:ND2	1:C:5:TYR:N	2.45	0.64
2:B:103:ILE:HG21	2:B:107:LEU:HG	1.80	0.64
1:C:137:GLN:CG	1:C:140:LEU:HD21	2.28	0.64
1:A:94:VAL:HG13	1:A:95:ILE:N	2.13	0.63
1:C:251:ALA:HA	1:C:254:LEU:HD12	1.80	0.63
2:D:18:ILE:O	2:D:21:ILE:HD11	1.99	0.63
6:C:655:HOH:O	2:D:115:ILE:HD13	1.98	0.63
2:D:77:TYR:O	2:D:78:ALA:HB2	1.96	0.63
2:B:49:PRO:HA	2:B:54:GLY:O	1.99	0.63
2:B:127:VAL:HG22	2:B:136:LEU:HD23	1.79	0.63
2:D:9:VAL:HG12	2:D:10:GLU:H	1.63	0.63
1:A:81:LEU:CD1	1:A:91:THR:HA	2.25	0.63
1:A:194:MET:SD	1:A:195:PRO:HD2	2.39	0.62
1:C:132:ASN:ND2	1:C:133:GLN:HG2	2.14	0.62
3:C:612:EOZ:OAE	3:C:612:EOZ:NAQ	2.32	0.62
1:C:7:LYS:HE3	6:C:722:HOH:O	1.98	0.62
1:C:266:PRO:HB3	3:C:612:EOZ:OAD	1.99	0.62
2:B:84:ASN:HD22	2:B:91:VAL:CG1	2.11	0.62
1:A:81:LEU:CB	1:A:91:THR:HG23	2.30	0.62
2:B:131:ALA:O	2:B:132:ASN:HB3	2.00	0.62
2:D:22:PRO:HD2	2:D:25:ILE:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD11	1:A:254:LEU:HD21	1.79	0.62
2:B:94:LYS:NZ	5:B:901:CTP:O1A	2.22	0.62
2:D:67:SER:HA	6:D:980:HOH:O	2.00	0.61
1:C:12:ILE:HG22	1:C:133:GLN:OE1	2.00	0.61
1:C:82:GLY:HA3	1:C:86:GLU:CB	2.30	0.61
1:A:81:LEU:HB3	1:A:91:THR:HG23	1.81	0.61
2:B:84:ASN:HD22	2:B:91:VAL:HG13	1.64	0.61
1:C:201:MET:O	1:C:205:LYS:HG3	2.00	0.61
1:C:16:SER:O	1:C:19:ASP:HB2	1.99	0.61
1:C:79:THR:O	1:C:80:SER:HB2	1.99	0.61
1:A:59:PHE:CZ	1:A:136:THR:HG21	2.35	0.61
1:C:35:GLN:HB3	1:C:38:LEU:HB2	1.83	0.61
2:D:65:PHE:HD2	2:D:85:ARG:NE	1.99	0.61
2:B:34:LYS:HE3	6:B:920:HOH:O	1.98	0.61
5:B:901:CTP:H5'1	5:B:901:CTP:O1B	2.01	0.60
1:C:227:MET:HG3	1:C:273:ILE:HD11	1.83	0.60
1:A:145:ILE:HG12	1:A:224:ILE:CD1	2.29	0.60
1:C:140:LEU:CD2	1:C:292:GLY:HA2	2.30	0.60
2:D:2:THR:HB	2:D:56:LYS:HE3	1.83	0.60
2:B:96:ARG:HG3	6:B:935:HOH:O	2.00	0.60
1:C:140:LEU:CD2	1:C:292:GLY:CA	2.80	0.60
1:C:294:PHE:HE2	6:C:736:HOH:O	1.83	0.59
1:C:55:THR:N	3:C:612:EOZ:OAJ	2.31	0.59
2:D:17:VAL:HG13	2:D:60:LYS:HG2	1.84	0.59
2:B:128:ARG:O	2:B:134:ILE:HA	2.03	0.59
2:B:29:LEU:O	2:B:35:LEU:HD12	2.03	0.59
1:C:244:LYS:HZ2	1:C:248:VAL:HG21	1.66	0.59
2:B:42:ILE:HB	2:D:46:LEU:HD12	1.85	0.59
1:A:91:THR:O	1:A:94:VAL:HG12	2.02	0.59
1:C:83:LYS:O	1:C:84:LYS:HB2	2.02	0.59
2:D:21:ILE:H	2:D:21:ILE:HD13	1.66	0.59
2:B:44:ILE:CD1	2:B:59:ILE:HG23	2.32	0.59
1:C:230:VAL:O	1:C:232:LYS:N	2.36	0.59
1:C:309:VAL:HG13	1:C:309:VAL:O	2.03	0.59
1:C:56:ARG:O	1:C:60:GLU:HG3	2.02	0.59
1:A:251:ALA:O	1:A:254:LEU:HB2	2.03	0.59
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.84	0.59
1:C:59:PHE:O	1:C:63:MET:HG3	2.03	0.59
2:D:34:LYS:HA	6:D:973:HOH:O	2.02	0.59
2:B:16:THR:HG22	2:B:64:THR:O	2.02	0.58
2:D:77:TYR:O	2:D:78:ALA:CB	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PHE:HZ	1:A:136:THR:HG21	1.68	0.58
1:A:278:ASP:HB2	6:A:756:HOH:O	2.02	0.58
2:B:36:THR:HB	6:B:909:HOH:O	2.01	0.58
1:C:229:ARG:NH1	1:C:231:GLN:HA	2.18	0.58
1:C:40:LYS:HE3	1:C:41:HIS:CE1	2.38	0.58
1:A:114:LEU:C	1:A:114:LEU:HD23	2.23	0.58
2:D:40:GLN:HB3	2:D:62:GLU:O	2.03	0.58
1:A:5:TYR:CD2	1:A:306:ARG:HA	2.39	0.58
3:A:611:EOZ:OAC	3:A:611:EOZ:CAK	2.51	0.58
2:B:30:LEU:HD22	2:B:36:THR:HG23	1.86	0.58
1:C:137:GLN:HA	1:C:140:LEU:HG	1.85	0.58
1:A:309:VAL:HG12	1:A:310:LEU:HG	1.86	0.58
2:B:91:VAL:HG22	5:B:901:CTP:C6	2.39	0.58
2:D:30:LEU:HD23	2:D:35:LEU:HD12	1.86	0.58
1:A:293:ILE:O	1:A:297:GLN:HG3	2.03	0.57
1:A:1:ALA:HB2	1:A:306:ARG:CG	2.34	0.57
1:A:189:PRO:HG2	1:A:192:LEU:HB2	1.86	0.57
2:D:76:LEU:CD2	2:D:134:ILE:HD12	2.34	0.57
2:B:18:ILE:HD12	2:B:18:ILE:N	2.19	0.57
1:A:141:ASP:O	1:A:145:ILE:HG13	2.04	0.57
1:A:234:ARG:HD3	6:A:717:HOH:O	2.04	0.57
1:A:44:ILE:HD12	1:A:101:ALA:HB3	1.87	0.57
1:A:269:ARG:O	1:A:269:ARG:HD2	2.04	0.57
2:B:63:ASN:O	2:B:64:THR:HB	2.04	0.57
2:B:90:GLU:O	2:B:92:VAL:HG22	2.05	0.57
1:A:132:ASN:ND2	1:A:133:GLN:HE21	2.03	0.56
1:A:8:HIS:CE1	1:A:123:PRO:HA	2.39	0.56
2:B:2:THR:HG21	5:B:901:CTP:PB	2.45	0.56
1:C:267:LEU:HD22	1:C:268:PRO:HA	1.87	0.56
1:A:91:THR:O	1:A:95:ILE:HG12	2.04	0.56
2:D:128:ARG:HE	2:D:135:ALA:HB3	1.69	0.56
2:B:101:GLU:OE2	2:B:102:ARG:N	2.38	0.56
1:C:106:HIS:ND1	1:C:107:PRO:HD2	2.20	0.56
2:B:42:ILE:HD12	2:D:46:LEU:HB2	1.88	0.56
2:B:42:ILE:HG13	2:D:46:LEU:O	2.06	0.56
2:D:128:ARG:HE	2:D:135:ALA:CB	2.18	0.56
1:A:94:VAL:HG13	1:A:95:ILE:H	1.71	0.56
2:B:11:ALA:HB1	5:B:901:CTP:C4	2.39	0.56
1:A:219:MET:HE3	1:A:254:LEU:HA	1.88	0.56
1:C:137:GLN:CG	1:C:140:LEU:CD2	2.80	0.56
1:C:35:GLN:HE22	1:C:310:LEU:HD23	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:TYR:CE2	1:A:306:ARG:N	2.74	0.56
1:C:81:LEU:HD23	1:C:91:THR:HB	1.88	0.56
2:D:14:ARG:O	2:D:63:ASN:CA	2.51	0.56
1:C:43:VAL:HG12	1:C:99:VAL:HG12	1.88	0.55
1:A:229:ARG:CZ	3:A:611:EOZ:OAG	2.53	0.55
1:A:137:GLN:NE2	3:A:611:EOZ:OAI	2.31	0.55
1:C:160:VAL:O	1:C:228:THR:HG22	2.06	0.55
2:B:55:ARG:O	2:B:56:LYS:HB3	2.05	0.55
2:B:27:PHE:CD1	2:D:36:THR:HG21	2.42	0.55
2:D:23:ALA:HA	2:D:57:ASP:OD1	2.06	0.55
1:A:285:TYR:HA	1:A:288:GLN:HE21	1.72	0.55
1:A:279:LYS:NZ	6:A:737:HOH:O	2.39	0.55
1:C:11:SER:HB3	1:C:14:ASP:OD2	2.07	0.55
1:A:92:ILE:HG12	1:A:115:ALA:CB	2.34	0.55
1:A:40:LYS:O	1:A:41:HIS:HB2	2.05	0.55
2:B:71:VAL:O	2:B:97:PRO:CB	2.53	0.55
1:C:54:ARG:HB3	3:C:612:EOZ:PAY	2.47	0.55
1:C:63:MET:CE	1:C:103:VAL:HG21	2.36	0.54
2:B:34:LYS:HB3	2:B:37:GLU:HG3	1.89	0.54
1:C:24:LEU:HD22	1:C:143:PHE:HA	1.89	0.54
2:D:43:THR:C	2:D:44:ILE:HD13	2.28	0.54
1:A:236:ASP:OD2	1:A:239:GLU:HB2	2.07	0.54
2:D:44:ILE:HG23	2:D:59:ILE:HG12	1.89	0.54
1:A:35:GLN:HE22	1:A:310:LEU:HD12	1.72	0.54
2:B:101:GLU:HG2	6:B:927:HOH:O	2.08	0.54
2:B:47:ASN:HD22	2:B:55:ARG:HD2	1.73	0.54
2:D:45:GLY:O	2:D:48:LEU:HG	2.08	0.54
1:C:195:PRO:O	1:C:199:LEU:HG	2.08	0.54
1:C:196:GLN:OE1	1:C:199:LEU:HD12	2.08	0.54
2:B:67:SER:OG	2:B:70:GLN:HG3	2.08	0.54
2:B:89:TYR:HA	5:B:901:CTP:HN42	1.72	0.54
1:C:137:GLN:O	3:C:612:EOZ:HAN1	2.07	0.54
1:C:155:LEU:HB2	1:C:182:ASN:OD1	2.08	0.54
1:C:59:PHE:CE1	1:C:136:THR:HG21	2.42	0.54
2:B:82:THR:HG23	2:B:95:SER:O	2.08	0.54
1:C:74:SER:O	1:C:75:ASP:O	2.25	0.54
1:C:137:GLN:CB	3:C:612:EOZ:CAN	2.84	0.54
1:C:158:ALA:HA	1:C:185:TYR:HB2	1.90	0.54
1:C:186:PHE:HB2	1:C:211:LEU:HD23	1.90	0.54
1:C:137:GLN:CG	1:C:296:ARG:CZ	2.86	0.53
1:C:79:THR:O	1:C:80:SER:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ALA:O	1:C:116:THR:HG23	2.09	0.53
1:C:54:ARG:HD2	3:C:612:EOZ:HAO2	1.90	0.53
1:C:250:ARG:HB3	1:C:250:ARG:CZ	2.39	0.53
2:B:86:ILE:HD13	5:B:901:CTP:C4	2.44	0.53
1:C:244:LYS:O	1:C:247:PHE:N	2.39	0.53
1:C:266:PRO:CG	6:C:673:HOH:O	2.57	0.53
1:A:145:ILE:HG23	1:A:224:ILE:CD1	2.36	0.53
1:C:59:PHE:CZ	1:C:136:THR:HG21	2.44	0.53
1:C:140:LEU:C	1:C:140:LEU:HD12	2.28	0.53
1:C:1:ALA:N	6:C:665:HOH:O	2.42	0.53
1:C:231:GLN:HE22	1:C:234:ARG:NE	2.05	0.53
1:A:236:ASP:O	1:A:239:GLU:HB3	2.09	0.53
2:B:38:THR:HG23	2:B:42:ILE:HD13	1.91	0.53
2:B:130:ARG:O	2:B:132:ASN:N	2.42	0.53
2:B:40:GLN:O	2:B:42:ILE:HG12	2.09	0.53
1:C:231:GLN:HE22	1:C:234:ARG:HE	1.46	0.53
1:A:35:GLN:HE22	1:A:310:LEU:CD1	2.22	0.52
2:B:146:SER:O	2:B:149:VAL:N	2.37	0.52
2:B:136:LEU:HD12	2:B:147:HIS:HA	1.91	0.52
1:C:250:ARG:NH1	1:C:252:SER:OG	2.43	0.52
2:D:6:LYS:N	2:D:8:GLN:OE1	2.42	0.52
1:C:232:LYS:HG3	1:C:233:GLU:N	2.25	0.52
2:B:104:ASP:O	2:B:105:ASN:HB2	2.10	0.52
1:C:244:LYS:HD3	1:C:245:ALA:N	2.24	0.52
2:B:38:THR:OG1	2:B:39:ASP:N	2.42	0.52
2:B:76:LEU:CD1	2:B:151:LEU:HD21	2.39	0.52
2:B:136:LEU:CD1	2:B:147:HIS:HA	2.40	0.52
2:B:91:VAL:HG22	5:B:901:CTP:C5	2.44	0.52
1:C:140:LEU:HD22	1:C:292:GLY:HA3	1.91	0.52
2:D:86:ILE:HG12	2:D:91:VAL:HA	1.92	0.52
2:B:86:ILE:HD13	5:B:901:CTP:C5	2.45	0.51
2:D:30:LEU:CD2	2:D:59:ILE:HD13	2.40	0.51
1:A:153:ASP:O	1:A:154:ASN:C	2.48	0.51
1:C:112:ALA:O	1:C:115:ALA:HB3	2.10	0.51
1:C:121:ASN:HD22	1:C:121:ASN:N	2.08	0.51
1:C:140:LEU:HD12	1:C:141:ASP:N	2.26	0.51
1:C:207:ILE:HD13	6:C:680:HOH:O	2.09	0.51
2:D:85:ARG:C	2:D:86:ILE:HG13	2.29	0.51
1:A:19:ASP:O	1:A:22:LEU:HB3	2.10	0.51
1:C:292:GLY:O	1:C:296:ARG:HB2	2.10	0.51
1:A:227:MET:HG3	1:A:273:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HD11	1:C:116:THR:CG2	2.22	0.51
1:C:266:PRO:HG2	6:C:673:HOH:O	2.10	0.51
2:D:13:LYS:HD3	6:D:965:HOH:O	2.10	0.51
2:B:48:LEU:HB3	2:B:49:PRO:CD	2.41	0.51
1:A:132:ASN:HD21	1:A:133:GLN:HE21	1.58	0.51
1:A:81:LEU:CG	1:A:91:THR:HG23	2.41	0.51
2:B:115:ILE:HG23	2:B:116:SER:N	2.26	0.51
1:C:267:LEU:CD2	1:C:268:PRO:HA	2.41	0.51
1:A:137:GLN:NE2	3:A:611:EOZ:OAC	2.43	0.50
3:C:612:EOZ:CAN	3:C:612:EOZ:CAK	2.70	0.50
2:D:16:THR:HG22	2:D:17:VAL:N	2.25	0.50
2:D:89:TYR:CD1	6:D:965:HOH:O	2.53	0.50
1:A:161:GLY:HA3	1:A:228:THR:OG1	2.12	0.50
2:B:18:ILE:H	2:B:18:ILE:CD1	2.20	0.50
2:B:91:VAL:HG11	2:B:94:LYS:HE3	1.92	0.50
2:B:96:ARG:HD2	6:B:935:HOH:O	2.10	0.50
2:B:134:ILE:O	2:B:147:HIS:HB3	2.11	0.50
2:D:62:GLU:O	2:D:63:ASN:HB2	2.10	0.50
2:D:3:HIS:O	2:D:4:ASP:CB	2.60	0.50
2:B:123:SER:HB2	2:B:125:PHE:CE1	2.47	0.50
1:C:168:THR:HA	6:C:712:HOH:O	2.10	0.50
1:C:168:THR:HG22	3:C:612:EOZ:NAP	2.06	0.50
1:C:77:ALA:HA	6:C:666:HOH:O	2.12	0.50
2:D:17:VAL:HG22	2:D:60:LYS:HG2	1.92	0.50
2:D:78:ALA:H	2:D:79:PRO:HD3	1.75	0.50
2:D:20:HIS:NE2	5:D:902:CTP:O1G	2.42	0.50
1:C:164:LYS:HA	1:C:195:PRO:HD3	1.93	0.50
1:C:301:ALA:O	1:C:305:ASN:HB2	2.11	0.50
2:D:67:SER:O	2:D:71:VAL:HG23	2.11	0.50
2:B:125:PHE:CD1	2:B:125:PHE:N	2.80	0.50
1:C:132:ASN:CG	1:C:133:GLN:HG2	2.33	0.50
1:C:54:ARG:CB	3:C:612:EOZ:OAJ	2.59	0.50
1:A:302:LEU:CD2	1:A:308:LEU:HD23	2.26	0.49
2:B:95:SER:O	2:B:97:PRO:HD3	2.12	0.49
1:A:83:LYS:NZ	1:A:83:LYS:HB3	2.26	0.49
2:B:19:ASP:O	2:B:20:HIS:CB	2.60	0.49
1:A:137:GLN:NE2	3:A:611:EOZ:PAY	2.84	0.49
1:A:152:LEU:HA	1:A:155:LEU:HD11	1.95	0.49
1:A:158:ALA:HB2	1:A:222:VAL:HG11	1.93	0.49
1:A:187:ILE:HA	1:A:212:HIS:O	2.12	0.49
1:C:276:ASP:N	6:C:620:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD11	1:A:254:LEU:CD2	2.43	0.49
2:D:17:VAL:HG22	2:D:60:LYS:CG	2.43	0.49
1:C:35:GLN:NE2	1:C:310:LEU:HD23	2.26	0.49
1:C:266:PRO:CA	3:C:612:EOZ:OAD	2.60	0.49
2:B:59:ILE:HG22	2:B:60:LYS:N	2.27	0.49
1:A:182:ASN:O	1:A:207:ILE:HG23	2.13	0.49
1:A:273:ILE:HG22	1:A:273:ILE:O	2.13	0.49
2:B:123:SER:HB2	2:B:125:PHE:HE1	1.77	0.49
2:D:145:PHE:HB2	2:D:150:VAL:CG2	2.43	0.49
2:B:46:LEU:N	2:B:46:LEU:HD23	2.28	0.49
2:D:9:VAL:HG12	2:D:10:GLU:N	2.28	0.49
2:D:16:THR:CG2	2:D:83:VAL:HG13	2.43	0.49
1:C:232:LYS:O	1:C:234:ARG:N	2.46	0.48
2:D:2:THR:N	5:D:902:CTP:O2'	2.35	0.48
1:C:239:GLU:O	1:C:243:VAL:HG22	2.13	0.48
2:B:146:SER:O	2:B:148:ASN:N	2.46	0.48
1:C:251:ALA:O	1:C:254:LEU:HB2	2.13	0.48
2:D:143:LYS:HB2	2:D:145:PHE:CZ	2.49	0.48
1:A:8:HIS:CE1	1:A:124:VAL:H	2.31	0.48
1:A:81:LEU:HG	1:A:91:THR:HG23	1.94	0.48
2:B:77:TYR:O	2:B:79:PRO:HD3	2.14	0.48
1:C:137:GLN:HB3	3:C:612:EOZ:OAG	2.12	0.48
1:A:47:CYS:O	1:A:104:MET:HA	2.14	0.48
1:A:189:PRO:HG3	1:A:192:LEU:HD12	1.94	0.48
2:B:32:LEU:HD13	2:B:77:TYR:CE2	2.49	0.48
2:D:84:ASN:HB3	2:D:86:ILE:HD11	1.95	0.48
1:A:92:ILE:HG21	1:A:118:PHE:HB2	1.94	0.48
1:A:164:LYS:HE2	1:A:165:TYR:CZ	2.49	0.48
1:A:255:HIS:CG	1:A:256:ASN:N	2.81	0.48
1:C:203:ASP:HA	6:C:754:HOH:O	2.13	0.48
2:D:2:THR:OG1	2:D:3:HIS:N	2.46	0.48
1:C:232:LYS:C	1:C:234:ARG:N	2.67	0.48
1:C:279:LYS:HZ2	1:C:279:LYS:HB3	1.78	0.48
1:C:40:LYS:HE3	1:C:41:HIS:NE2	2.29	0.48
1:A:195:PRO:HG2	1:A:198:ILE:HD12	1.94	0.47
2:B:90:GLU:HA	2:B:90:GLU:OE1	2.14	0.47
1:C:130:GLY:O	1:C:167:ARG:NH2	2.48	0.47
2:B:71:VAL:O	2:B:97:PRO:CG	2.62	0.47
1:C:9:ILE:HG21	1:C:299:LEU:HD21	1.95	0.47
2:B:101:GLU:HA	2:B:127:VAL:HB	1.95	0.47
2:B:133:ASP:O	2:B:133:ASP:CG	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:ILE:HG23	6:B:980:HOH:O	2.12	0.47
1:C:287:GLN:OE1	6:C:614:HOH:O	2.20	0.47
1:C:40:LYS:HE2	1:C:40:LYS:HB3	1.52	0.47
1:C:109:GLU:HB3	2:D:141:CYS:HA	1.95	0.47
1:C:83:LYS:O	1:C:84:LYS:CB	2.62	0.47
1:A:204:GLU:C	1:A:206:GLY:H	2.18	0.47
1:A:81:LEU:HG	1:A:95:ILE:HD11	1.96	0.47
1:C:166:GLY:O	1:C:169:VAL:HG22	2.14	0.47
1:C:54:ARG:NH2	3:C:612:EOZ:OAI	2.48	0.47
2:B:66:LEU:HD12	2:B:83:VAL:HG11	1.95	0.47
2:B:14:ARG:HA	2:B:88:ASN:H	1.78	0.47
1:C:265:HIS:NE2	1:C:272:GLU:HG3	2.28	0.47
2:D:84:ASN:HD22	2:D:91:VAL:HG13	1.80	0.47
1:A:174:GLN:HG2	1:A:201:MET:CE	2.45	0.47
1:A:199:LEU:HD22	1:A:209:TRP:CD2	2.49	0.47
1:C:308:LEU:HB2	1:C:310:LEU:HD11	1.97	0.47
1:A:229:ARG:NH2	3:A:611:EOZ:PAX	2.88	0.47
1:A:82:GLY:HA3	1:A:86:GLU:CG	2.42	0.47
1:C:238:SER:O	1:C:241:ALA:HB3	2.15	0.47
1:C:79:THR:CB	1:C:84:LYS:HA	2.45	0.47
2:D:15:GLY:CA	2:D:63:ASN:H	2.28	0.47
1:A:35:GLN:HB3	6:A:647:HOH:O	2.15	0.47
1:C:137:GLN:HE21	1:C:140:LEU:HD11	1.80	0.47
2:B:130:ARG:HG3	2:B:130:ARG:HH11	1.79	0.47
2:D:23:ALA:O	2:D:24:GLN:HB2	2.13	0.47
2:B:14:ARG:CA	2:B:88:ASN:H	2.27	0.46
2:D:2:THR:N	5:D:902:CTP:O3'	2.44	0.46
2:D:80:GLN:O	2:D:81:ALA:O	2.33	0.46
1:C:169:VAL:HG23	1:C:170:HIS:N	2.30	0.46
1:C:59:PHE:CD2	1:C:296:ARG:HG2	2.50	0.46
2:D:11:ALA:HB1	5:D:902:CTP:C4	2.47	0.46
2:D:3:HIS:CD2	2:D:3:HIS:N	2.70	0.46
1:A:17:ARG:HD3	1:A:179:PHE:CE1	2.51	0.46
1:A:187:ILE:HD13	1:A:215:ILE:HA	1.98	0.46
2:B:93:GLY:N	6:B:988:HOH:O	2.44	0.46
2:B:96:ARG:NH2	6:B:913:HOH:O	2.49	0.46
2:B:102:ARG:HG2	2:B:104:ASP:OD2	2.15	0.46
1:C:82:GLY:C	1:C:84:LYS:N	2.68	0.46
2:B:129:LYS:HA	2:B:134:ILE:HA	1.98	0.46
2:B:49:PRO:HD2	6:B:981:HOH:O	2.15	0.46
1:C:12:ILE:CG2	6:C:789:HOH:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:LYS:CG	1:C:233:GLU:N	2.78	0.46
2:D:148:ASN:O	2:D:152:ALA:HB2	2.16	0.46
1:A:219:MET:HE1	1:A:254:LEU:HD22	1.97	0.46
1:A:254:LEU:N	1:A:254:LEU:HD23	2.31	0.46
1:C:227:MET:O	1:C:266:PRO:HD2	2.16	0.46
2:B:22:PRO:O	2:B:23:ALA:C	2.54	0.46
1:C:39:LEU:N	1:C:66:LEU:O	2.40	0.46
2:D:2:THR:N	5:D:902:CTP:H3'	2.31	0.46
1:A:118:PHE:C	1:A:120:GLY:H	2.20	0.46
1:A:269:ARG:HH21	1:A:273:ILE:HG22	1.81	0.46
2:B:20:HIS:HB2	2:B:81:ALA:HA	1.98	0.46
2:D:49:PRO:HG3	6:D:947:HOH:O	2.15	0.46
1:A:8:HIS:HE1	1:A:123:PRO:HA	1.81	0.45
1:A:33:ASN:HA	1:A:34:PRO:HD2	1.69	0.45
1:C:252:SER:C	1:C:254:LEU:H	2.17	0.45
1:C:2:ASN:HD22	1:C:5:TYR:H	1.60	0.45
1:A:125:LEU:CD1	1:A:125:LEU:N	2.75	0.45
1:A:137:GLN:HE22	3:A:611:EOZ:PAY	2.39	0.45
1:A:108:GLN:HG2	2:B:113:ASN:O	2.17	0.45
1:C:266:PRO:O	1:C:267:LEU:HB2	2.15	0.45
2:D:88:ASN:O	2:D:89:TYR:HB2	2.15	0.45
1:A:189:PRO:CG	1:A:192:LEU:HD12	2.46	0.45
2:B:64:THR:HG21	6:B:919:HOH:O	2.16	0.45
1:C:121:ASN:ND2	1:C:121:ASN:N	2.59	0.45
1:A:5:TYR:CE2	1:A:306:ARG:HA	2.51	0.45
2:B:138:CYS:HB3	2:B:141:CYS:SG	2.56	0.45
2:B:48:LEU:HD12	2:B:58:LEU:HD23	1.98	0.45
1:C:231:GLN:HE22	1:C:234:ARG:CZ	2.28	0.45
1:C:35:GLN:NE2	1:C:309:VAL:O	2.50	0.45
1:A:244:LYS:HA	1:A:247:PHE:CE1	2.51	0.45
1:C:137:GLN:CB	3:C:612:EOZ:OAG	2.64	0.45
1:A:169:VAL:HG21	1:A:228:THR:HG21	1.99	0.45
2:B:130:ARG:HG3	2:B:130:ARG:NH1	2.32	0.45
2:B:14:ARG:O	2:B:63:ASN:OD1	2.35	0.45
2:B:71:VAL:HG13	2:B:97:PRO:HG3	1.97	0.45
1:C:145:ILE:O	1:C:149:GLN:HG2	2.16	0.45
6:A:660:HOH:O	2:B:143:LYS:HD3	2.17	0.45
1:A:31:LYS:HG3	1:A:294:PHE:CZ	2.52	0.45
2:B:111:ASN:HD22	2:B:114:CYS:HB2	1.82	0.45
1:A:163:LEU:CD1	1:A:186:PHE:HB3	2.47	0.45
1:A:41:HIS:HA	6:A:750:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:LYS:C	1:C:246:GLN:N	2.70	0.45
1:C:2:ASN:HB3	1:C:5:TYR:HB2	1.98	0.45
2:D:62:GLU:HG2	2:D:63:ASN:HD22	1.82	0.45
1:A:231:GLN:HB3	1:A:234:ARG:HG2	1.98	0.45
2:B:91:VAL:CG1	2:B:94:LYS:HE3	2.47	0.45
2:D:153:ASN:HA	6:D:924:HOH:O	2.17	0.45
2:D:3:HIS:O	2:D:4:ASP:HB2	2.17	0.45
1:A:43:VAL:HG22	1:A:69:SER:HB2	2.00	0.44
2:B:130:ARG:O	2:B:133:ASP:N	2.49	0.44
2:B:71:VAL:O	2:B:97:PRO:HG3	2.17	0.44
1:C:149:GLN:CG	1:C:224:ILE:HD11	2.48	0.44
2:D:16:THR:CG2	2:D:17:VAL:N	2.79	0.44
1:A:299:LEU:HA	1:A:299:LEU:HD12	1.84	0.44
1:A:175:ALA:O	1:A:178:LYS:HB2	2.17	0.44
1:C:137:GLN:HE21	1:C:140:LEU:HD21	1.77	0.44
1:C:232:LYS:C	1:C:234:ARG:H	2.21	0.44
1:C:23:VAL:HG11	1:C:139:LEU:HD22	1.99	0.44
2:D:22:PRO:O	2:D:25:ILE:HG22	2.18	0.44
2:D:46:LEU:HA	2:D:57:ASP:OD2	2.17	0.44
1:A:218:VAL:O	1:A:219:MET:C	2.55	0.44
1:A:77:ALA:HA	6:A:622:HOH:O	2.17	0.44
2:B:104:ASP:OD1	2:B:124:SER:HB2	2.17	0.44
2:B:151:LEU:O	2:B:152:ALA:C	2.55	0.44
2:B:62:GLU:O	2:B:63:ASN:O	2.36	0.44
1:A:209:TRP:HZ3	1:A:211:LEU:HG	1.83	0.44
2:B:23:ALA:HA	2:B:57:ASP:OD2	2.17	0.44
1:C:24:LEU:HD22	1:C:143:PHE:CA	2.48	0.44
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.89	0.44
1:C:75:ASP:CG	1:C:76:SER:N	2.71	0.44
1:A:236:ASP:HA	6:A:757:HOH:O	2.17	0.44
3:A:611:EOZ:CAL	3:A:611:EOZ:CAN	2.83	0.44
2:B:126:ALA:HB3	2:B:137:LYS:HB3	1.99	0.44
1:A:161:GLY:HA3	1:A:228:THR:HG1	1.83	0.44
1:A:225:LEU:C	1:A:225:LEU:HD12	2.38	0.44
1:A:59:PHE:O	1:A:63:MET:HG3	2.18	0.44
2:B:61:ILE:HG22	2:B:64:THR:CG2	2.48	0.44
2:B:85:ARG:HB2	2:B:93:GLY:O	2.18	0.44
1:C:154:ASN:N	1:C:154:ASN:ND2	2.66	0.44
2:D:2:THR:HB	2:D:56:LYS:CE	2.46	0.44
1:A:113:ARG:O	1:A:116:THR:HB	2.18	0.44
1:A:199:LEU:HD22	1:A:209:TRP:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ASP:CG	2:B:124:SER:HB2	2.39	0.44
2:B:115:ILE:CG2	2:B:116:SER:N	2.81	0.44
1:C:235:LEU:HD22	1:C:239:GLU:OE2	2.18	0.44
1:A:261:MET:O	1:A:282:HIS:CD2	2.71	0.43
1:A:78:ASN:O	1:A:79:THR:C	2.56	0.43
1:A:94:VAL:CG1	1:A:95:ILE:N	2.81	0.43
2:B:138:CYS:O	2:B:139:LYS:C	2.55	0.43
2:D:128:ARG:HA	6:D:946:HOH:O	2.18	0.43
1:A:59:PHE:CE2	1:A:296:ARG:HG2	2.52	0.43
1:A:47:CYS:HB3	1:A:73:PHE:CZ	2.53	0.43
2:B:110:PRO:HG2	2:B:145:PHE:CE2	2.54	0.43
2:B:46:LEU:HA	2:B:57:ASP:HA	2.01	0.43
2:D:133:ASP:HB2	2:D:147:HIS:CD2	2.54	0.43
2:D:99:LEU:H	2:D:99:LEU:HG	1.36	0.43
1:C:134:HIS:N	1:C:135:PRO:CD	2.82	0.43
1:C:93:SER:O	1:C:97:THR:HG23	2.18	0.43
1:A:219:MET:HG2	6:A:687:HOH:O	2.19	0.43
2:B:72:ASP:O	2:B:75:ALA:CB	2.67	0.43
2:B:73:GLN:CG	6:B:922:HOH:O	2.60	0.43
2:B:92:VAL:HG23	2:B:92:VAL:O	2.18	0.43
2:D:130:ARG:NH2	2:D:146:SER:HB2	2.33	0.43
1:A:76:SER:HB2	1:A:80:SER:OG	2.19	0.43
2:B:20:HIS:O	2:B:81:ALA:HB2	2.18	0.43
1:C:114:LEU:O	1:C:117:GLU:HB2	2.19	0.43
1:C:162:ASP:N	1:C:228:THR:CG2	2.82	0.43
1:C:244:LYS:CD	1:C:245:ALA:N	2.81	0.43
1:A:87:THR:HG23	6:A:616:HOH:O	2.19	0.43
2:B:103:ILE:CG2	2:B:107:LEU:HG	2.47	0.43
1:C:229:ARG:CZ	1:C:231:GLN:HG2	2.48	0.43
1:A:162:ASP:HB2	1:A:230:VAL:HA	1.99	0.43
1:A:265:HIS:H	1:A:288:GLN:NE2	2.05	0.43
2:B:69:ASP:O	2:B:72:ASP:HB2	2.17	0.43
2:B:14:ARG:N	2:B:88:ASN:HA	2.33	0.43
1:A:112:ALA:CB	1:A:126:ASN:HB2	2.49	0.42
1:A:221:GLU:HG2	1:A:221:GLU:H	1.60	0.42
1:C:176:LEU:C	1:C:178:LYS:H	2.22	0.42
1:C:272:GLU:CD	1:C:272:GLU:H	2.22	0.42
2:B:107:LEU:O	2:B:123:SER:OG	2.20	0.42
2:B:147:HIS:ND1	2:B:151:LEU:HD12	2.34	0.42
2:B:22:PRO:O	2:B:23:ALA:O	2.37	0.42
2:B:87:ASP:O	2:B:88:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:ARG:O	2:D:86:ILE:HG13	2.19	0.42
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.53	0.42
2:B:10:GLU:HG3	6:B:926:HOH:O	2.19	0.42
1:C:266:PRO:HG3	6:C:673:HOH:O	2.19	0.42
2:D:32:LEU:O	2:D:106:VAL:HG12	2.20	0.42
2:B:60:LYS:HE2	5:B:901:CTP:O2	2.19	0.42
2:B:61:ILE:HG22	2:B:64:THR:HG22	2.01	0.42
2:B:70:GLN:HA	6:B:922:HOH:O	2.19	0.42
1:C:185:TYR:CD1	1:C:218:VAL:HG21	2.54	0.42
1:C:185:TYR:CE1	1:C:218:VAL:HG22	2.55	0.42
1:C:228:THR:HG23	1:C:229:ARG:O	2.18	0.42
1:C:284:TRP:HA	1:C:287:GLN:OE1	2.19	0.42
1:A:228:THR:O	1:A:272:GLU:HG2	2.20	0.42
1:A:38:LEU:HD11	1:A:305:ASN:ND2	2.35	0.42
2:B:127:VAL:HG22	2:B:136:LEU:CD2	2.48	0.42
2:B:72:ASP:O	2:B:73:GLN:C	2.58	0.42
1:C:160:VAL:HG12	1:C:161:GLY:N	2.34	0.42
1:A:40:LYS:HD2	1:A:40:LYS:HA	1.94	0.42
2:B:101:GLU:HG3	6:B:942:HOH:O	2.19	0.42
2:B:84:ASN:ND2	2:B:91:VAL:CG1	2.79	0.42
1:A:199:LEU:HD11	6:A:634:HOH:O	2.19	0.42
1:C:222:VAL:O	1:C:261:MET:HG2	2.19	0.42
1:C:306:ARG:NH2	6:C:717:HOH:O	2.52	0.42
1:C:82:GLY:CA	1:C:86:GLU:HB2	2.46	0.42
2:D:44:ILE:HA	2:D:58:LEU:O	2.20	0.42
2:D:45:GLY:N	2:D:58:LEU:O	2.53	0.42
1:A:114:LEU:O	1:A:114:LEU:HD23	2.20	0.41
2:B:23:ALA:O	2:B:24:GLN:HB2	2.20	0.41
2:B:84:ASN:HB3	2:B:86:ILE:CG1	2.45	0.41
2:B:84:ASN:HD21	2:B:94:LYS:CE	2.33	0.41
1:C:243:VAL:HG23	1:C:243:VAL:O	2.20	0.41
2:D:30:LEU:HD21	2:D:59:ILE:HD13	2.02	0.41
1:A:269:ARG:O	1:A:270:VAL:HB	2.20	0.41
1:C:132:ASN:ND2	1:C:133:GLN:HE21	2.18	0.41
1:C:2:ASN:HA	1:C:3:PRO:HD3	1.85	0.41
2:D:87:ASP:OD1	2:D:88:ASN:N	2.54	0.41
1:A:95:ILE:O	1:A:99:VAL:HG22	2.21	0.41
2:B:17:VAL:CG2	2:B:60:LYS:HG2	2.49	0.41
1:C:114:LEU:HG	1:C:118:PHE:HE1	1.86	0.41
1:A:227:MET:O	1:A:266:PRO:HD2	2.21	0.41
1:C:132:ASN:ND2	6:C:729:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ASN:ND2	6:C:789:HOH:O	2.53	0.41
1:C:240:TYR:HA	1:C:243:VAL:CG2	2.51	0.41
2:D:81:ALA:O	2:D:96:ARG:NE	2.53	0.41
1:A:9:ILE:N	1:A:9:ILE:HD12	2.36	0.41
2:B:100:PRO:HA	6:B:942:HOH:O	2.19	0.41
2:B:13:LYS:HD3	6:B:934:HOH:O	2.19	0.41
2:B:44:ILE:HD12	2:B:59:ILE:HG23	2.01	0.41
2:B:79:PRO:HB2	2:B:80:GLN:H	1.70	0.41
3:C:612:EOZ:OAC	3:C:612:EOZ:HAK	2.20	0.41
2:B:111:ASN:ND2	2:B:114:CYS:HB2	2.36	0.41
1:C:267:LEU:HD23	1:C:267:LEU:HA	1.73	0.41
1:C:79:THR:HG23	1:C:84:LYS:HG2	2.03	0.41
2:D:61:ILE:HG23	2:D:61:ILE:O	2.20	0.41
1:C:84:LYS:HB2	1:C:84:LYS:NZ	2.35	0.41
1:A:24:LEU:HD22	1:A:143:PHE:HB2	2.03	0.41
1:C:174:GLN:HG3	6:C:779:HOH:O	2.19	0.41
1:C:251:ALA:N	1:C:277:VAL:HG22	2.34	0.41
1:C:145:ILE:HD11	1:C:264:LEU:HD11	2.03	0.41
1:C:276:ASP:HB3	6:C:620:HOH:O	2.21	0.41
1:A:307:ASP:HB2	6:A:755:HOH:O	2.21	0.41
1:A:79:THR:HA	6:A:664:HOH:O	2.21	0.41
2:B:64:THR:CG2	2:B:64:THR:O	2.68	0.41
1:C:175:ALA:O	1:C:178:LYS:HB2	2.21	0.41
1:C:231:GLN:O	1:C:234:ARG:HB3	2.21	0.41
1:A:12:ILE:HA	1:A:15:LEU:HD12	2.02	0.41
1:A:1:ALA:HB1	1:A:306:ARG:C	2.40	0.41
1:A:83:LYS:O	1:A:84:LYS:HE2	2.21	0.41
2:B:124:SER:C	2:B:125:PHE:CD1	2.94	0.41
2:B:44:ILE:HG22	2:B:46:LEU:CD2	2.51	0.41
2:B:90:GLU:O	2:B:92:VAL:N	2.54	0.41
1:C:240:TYR:CD1	1:C:240:TYR:C	2.94	0.41
1:C:2:ASN:OD1	1:C:302:LEU:HD22	2.21	0.41
2:D:139:LYS:HB3	2:D:139:LYS:HE2	1.82	0.41
1:A:229:ARG:NH2	3:A:611:EOZ:OAG	2.54	0.41
1:A:256:ASN:ND2	6:A:630:HOH:O	2.45	0.41
1:C:132:ASN:HD21	1:C:133:GLN:HE21	1.69	0.41
1:C:229:ARG:HH12	1:C:231:GLN:HA	1.84	0.41
1:C:229:ARG:NH2	1:C:231:GLN:HG2	2.36	0.41
1:A:234:ARG:O	1:A:235:LEU:HD23	2.21	0.40
1:A:140:LEU:HD13	1:A:288:GLN:O	2.20	0.40
1:A:39:LEU:HB2	1:A:68:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:LYS:HD2	2:D:37:GLU:OE1	2.21	0.40
2:B:17:VAL:HG12	2:B:17:VAL:O	2.21	0.40
2:B:50:SER:HB2	2:B:54:GLY:N	2.33	0.40
1:C:114:LEU:HD23	1:C:114:LEU:C	2.42	0.40
2:D:138:CYS:O	2:D:142:GLU:HA	2.21	0.40
1:A:168:THR:HG21	3:A:611:EOZ:HAP	1.86	0.40
2:B:30:LEU:HA	2:B:35:LEU:HB2	2.04	0.40
2:B:72:ASP:OD2	2:B:98:SER:O	2.39	0.40
2:B:84:ASN:ND2	2:B:94:LYS:HE3	2.37	0.40
1:C:4:LEU:O	1:C:303:VAL:HA	2.20	0.40
2:D:125:PHE:HA	2:D:137:LYS:O	2.22	0.40
2:D:3:HIS:HD2	2:D:3:HIS:H	1.60	0.40
1:A:146:GLN:O	1:A:146:GLN:HG2	2.20	0.40
1:A:218:VAL:O	1:A:221:GLU:N	2.55	0.40
1:A:4:LEU:HA	1:A:4:LEU:HD23	1.89	0.40
2:B:16:THR:CG2	2:B:64:THR:O	2.67	0.40
1:C:119:SER:HB2	1:C:122:VAL:HB	2.01	0.40
1:C:270:VAL:HG23	1:C:271:ASP:N	2.36	0.40
2:D:40:GLN:HA	2:D:40:GLN:NE2	2.36	0.40
1:A:102:ILE:O	1:A:125:LEU:N	2.43	0.40
2:B:137:LYS:HB2	2:B:144:GLU:HG3	2.03	0.40
2:B:29:LEU:C	2:B:35:LEU:HD12	2.42	0.40
1:C:8:HIS:CD2	1:C:116:THR:HB	2.56	0.40
1:C:24:LEU:CD2	1:C:143:PHE:HB2	2.52	0.40
2:D:78:ALA:N	2:D:79:PRO:HD3	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	308/310 (99%)	267 (87%)	31 (10%)	10 (3%)	<b>4</b> <b>5</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	308/310 (99%)	262 (85%)	32 (10%)	14 (4%)	2	3
2	B	150/153 (98%)	102 (68%)	29 (19%)	19 (13%)	0	0
2	D	150/153 (98%)	111 (74%)	33 (22%)	6 (4%)	3	3
All	All	916/926 (99%)	742 (81%)	125 (14%)	49 (5%)	2	2

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASP
1	A	270	VAL
1	A	306	ARG
2	B	3	HIS
2	B	8	GLN
2	B	10	GLU
2	B	13	LYS
2	B	20	HIS
2	B	41	ARG
2	B	63	ASN
2	B	64	THR
2	B	134	ILE
1	C	75	ASP
1	C	80	SER
1	C	243	VAL
1	C	245	ALA
2	D	78	ALA
2	D	81	ALA
2	D	117	HIS
1	A	79	THR
2	B	23	ALA
2	B	79	PRO
2	B	147	HIS
1	C	78	ASN
1	C	81	LEU
1	C	84	LYS
1	C	138	THR
2	D	4	ASP
2	D	123	SER
1	A	232	LYS
1	C	218	VAL
1	A	81	LEU
2	B	50	SER

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Mol	Chain	Res	Type
2	B	56	LYS
2	B	91	VAL
1	C	231	GLN
1	C	233	GLU
1	A	134	HIS
1	A	190	ASP
2	B	38	THR
2	B	51	GLY
2	B	97	PRO
2	B	124	SER
1	C	2	ASN
1	C	242	ASN
1	A	119	SER
1	A	154	ASN
1	C	120	GLY
2	D	91	VAL

### 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	261/261 (100%)	245 (94%)	16 (6%)	18	36
1	C	261/261 (100%)	240 (92%)	21 (8%)	12	23
2	B	136/137 (99%)	111 (82%)	25 (18%)	1	2
2	D	136/137 (99%)	121 (89%)	15 (11%)	6	12
All	All	794/796 (100%)	717 (90%)	77 (10%)	8	16

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	PHE
1	A	79	THR
1	A	81	LEU
1	A	84	LYS
1	A	124	VAL

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Mol	Chain	Res	Type
1	A	197	TYR
1	A	219	MET
1	A	225	LEU
1	A	231	GLN
1	A	236	ASP
1	A	237	PRO
1	A	254	LEU
1	A	267	LEU
1	A	269	ARG
1	A	285	TYR
1	A	310	LEU
2	B	10	GLU
2	B	12	ILE
2	B	13	LYS
2	B	14	ARG
2	B	38	THR
2	B	42	ILE
2	B	46	LEU
2	B	53	MET
2	B	58	LEU
2	B	62	GLU
2	B	65	PHE
2	B	76	LEU
2	B	85	ARG
2	B	90	GLU
2	B	96	ARG
2	B	101	GLU
2	B	102	ARG
2	B	104	ASP
2	B	124	SER
2	B	129	LYS
2	B	130	ARG
2	B	133	ASP
2	B	136	LEU
2	B	145	PHE
2	B	147	HIS
1	C	7	LYS
1	C	29	LYS
1	C	59	PHE
1	C	76	SER
1	C	78	ASN
1	C	83	LYS

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Mol	Chain	Res	Type
1	C	91	THR
1	C	121	ASN
1	C	136	THR
1	C	138	THR
1	C	140	LEU
1	C	168	THR
1	C	174	GLN
1	C	180	ASP
1	C	213	SER
1	C	218	VAL
1	C	233	GLU
1	C	260	ASN
1	C	269	ARG
1	C	279	LYS
1	C	285	TYR
2	D	2	THR
2	D	3	HIS
2	D	8	GLN
2	D	21	ILE
2	D	44	ILE
2	D	46	LEU
2	D	52	GLU
2	D	53	MET
2	D	62	GLU
2	D	80	GLN
2	D	94	LYS
2	D	95	SER
2	D	99	LEU
2	D	105	ASN
2	D	128	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	13	ASN
1	A	21	ASN
1	A	35	GLN
1	A	64	HIS
1	A	132	ASN
1	A	146	GLN
1	A	149	GLN

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Mol	Chain	Res	Type
1	A	174	GLN
1	A	246	GLN
1	A	288	GLN
1	A	291	ASN
1	A	297	GLN
2	B	8	GLN
2	B	20	HIS
2	B	24	GLN
2	B	40	GLN
2	B	47	ASN
2	B	84	ASN
2	B	132	ASN
1	C	2	ASN
1	C	13	ASN
1	C	21	ASN
1	C	33	ASN
1	C	35	GLN
1	C	78	ASN
1	C	121	ASN
1	C	132	ASN
1	C	154	ASN
1	C	174	GLN
1	C	231	GLN
1	C	260	ASN
1	C	291	ASN
2	D	40	GLN
2	D	63	ASN
2	D	84	ASN
2	D	105	ASN
2	D	117	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EOZ	C	612	-	23,25,25	2.19	7 (30%)	32,37,37	0.71	0
5	CTP	B	901	-	23,30,30	1.77	6 (26%)	30,47,47	1.68	6 (20%)
5	CTP	D	902	-	23,30,30	1.80	6 (26%)	30,47,47	1.57	5 (16%)
3	EOZ	A	611	-	23,25,25	2.26	7 (30%)	32,37,37	1.11	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EOZ	C	612	-	-	6/18/22/22	0/1/1/1
5	CTP	B	901	-	-	2/20/38/38	0/2/2/2
5	CTP	D	902	-	-	3/20/38/38	0/2/2/2
3	EOZ	A	611	-	-	2/18/22/22	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	611	EOZ	CAW-CAR	6.42	1.53	1.47
3	C	612	EOZ	CAW-CAR	6.41	1.53	1.47
3	A	611	EOZ	CAV-NAQ	-4.14	1.33	1.41
3	A	611	EOZ	CAU-NAP	-4.04	1.33	1.41
5	D	902	CTP	C6-N1	3.95	1.40	1.35
3	C	612	EOZ	CAV-NAQ	-3.91	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	612	EOZ	CAU-NAP	-3.89	1.33	1.41
5	B	901	CTP	C6-N1	3.88	1.40	1.35
5	B	901	CTP	PG-O1G	3.38	1.61	1.50
5	D	902	CTP	PG-O1G	3.38	1.61	1.50
5	D	902	CTP	C4-N3	3.26	1.40	1.35
5	B	901	CTP	C4-N3	3.18	1.40	1.35
3	C	612	EOZ	PAY-OAI	3.17	1.62	1.54
3	A	611	EOZ	PAY-OAI	3.10	1.62	1.54
3	C	612	EOZ	PAY-OAE	3.07	1.62	1.54
3	A	611	EOZ	PAY-OAE	3.04	1.61	1.54
5	B	901	CTP	PB-O1B	3.01	1.61	1.50
5	D	902	CTP	PB-O1B	2.99	1.61	1.50
5	B	901	CTP	PA-O1A	2.98	1.61	1.50
5	D	902	CTP	PA-O1A	2.96	1.61	1.50
3	A	611	EOZ	PAX-OAH	2.95	1.61	1.54
3	A	611	EOZ	PAX-OAD	2.90	1.61	1.54
3	C	612	EOZ	PAX-OAH	2.53	1.60	1.54
3	C	612	EOZ	PAX-OAD	2.40	1.60	1.54
5	D	902	CTP	O4'-C1'	2.40	1.44	1.41
5	B	901	CTP	O4'-C1'	2.01	1.43	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	902	CTP	C2-N3-C4	4.31	120.71	116.34
5	B	901	CTP	PB-O3A-PA	-4.22	118.34	132.83
5	B	901	CTP	C2-N3-C4	4.12	120.52	116.34
5	B	901	CTP	PB-O3B-PG	-4.11	118.74	132.83
5	D	902	CTP	PB-O3B-PG	-3.69	120.16	132.83
3	A	611	EOZ	CAV-NAQ-CAT	-3.01	122.23	127.50
5	D	902	CTP	PB-O3A-PA	-2.92	122.80	132.83
5	B	901	CTP	O4'-C1'-C2'	-2.72	102.94	106.93
5	D	902	CTP	O3G-PG-O3B	2.63	113.47	104.64
5	D	902	CTP	N4-C4-N3	2.50	120.44	116.49
5	B	901	CTP	O3G-PG-O3B	2.45	112.84	104.64
5	B	901	CTP	N4-C4-N3	2.44	120.35	116.49
3	A	611	EOZ	CAU-NAP-CAS	2.23	131.40	127.50
3	A	611	EOZ	CAN-CAS-NAP	2.14	119.09	114.36

There are no chirality outliers.

All (13) torsion outliers are listed below:

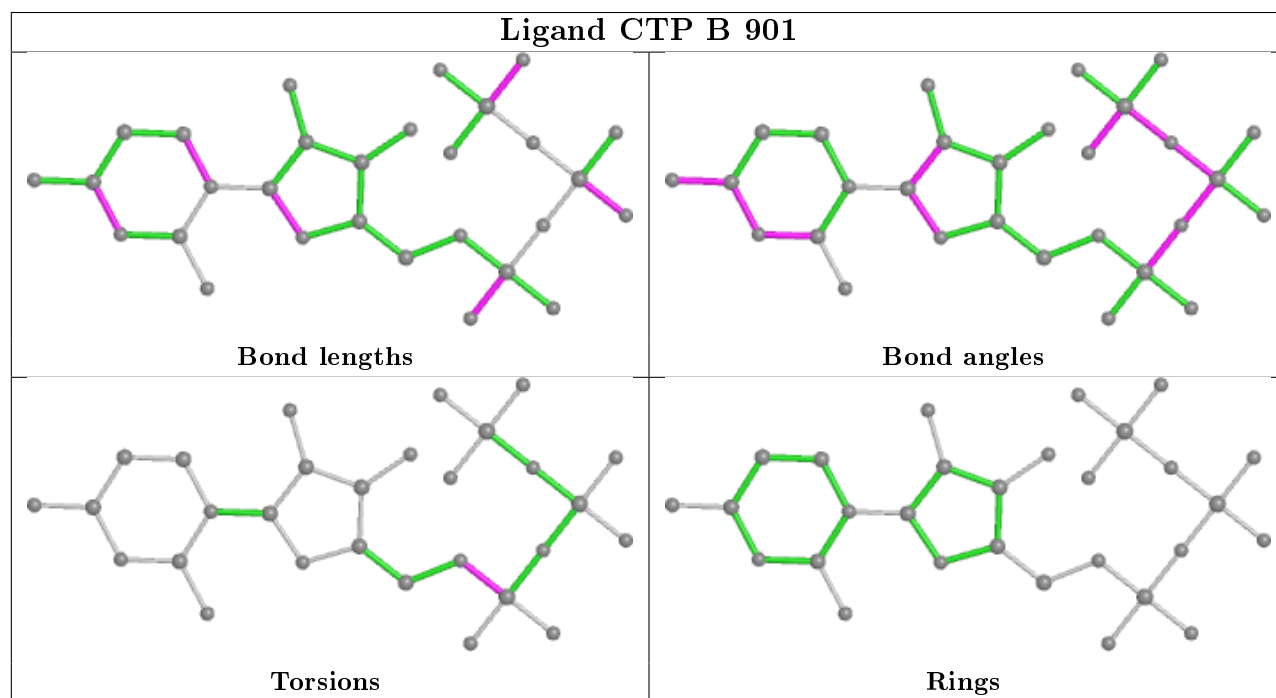
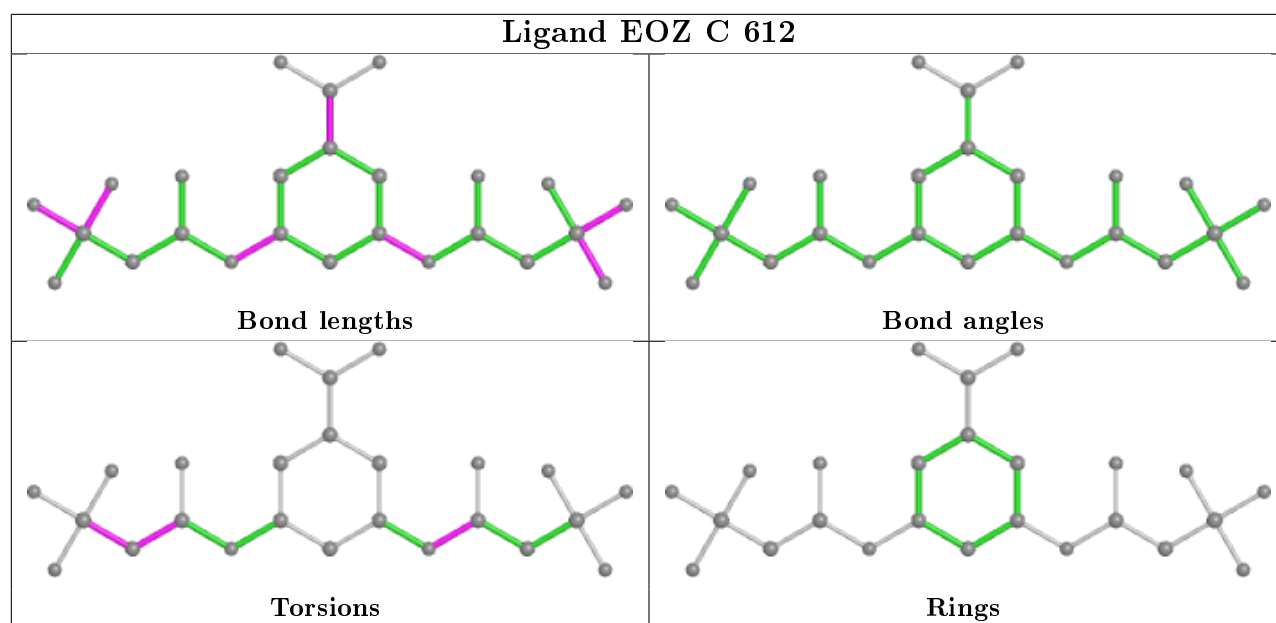
Mol	Chain	Res	Type	Atoms
3	C	612	EOZ	CAN-CAS-NAP-CAU
3	C	612	EOZ	PAY-CAO-CAT-NAQ
3	C	612	EOZ	PAY-CAO-CAT-OAC
3	C	612	EOZ	CAT-CAO-PAY-OAE
3	A	611	EOZ	CAN-CAS-NAP-CAU
3	C	612	EOZ	OAB-CAS-NAP-CAU
3	A	611	EOZ	OAB-CAS-NAP-CAU
3	C	612	EOZ	CAT-CAO-PAY-OAI
5	B	901	CTP	C5'-O5'-PA-O3A
5	D	902	CTP	PA-O3A-PB-O1B
5	B	901	CTP	C5'-O5'-PA-O2A
5	D	902	CTP	O4'-C4'-C5'-O5'
5	D	902	CTP	C5'-O5'-PA-O3A

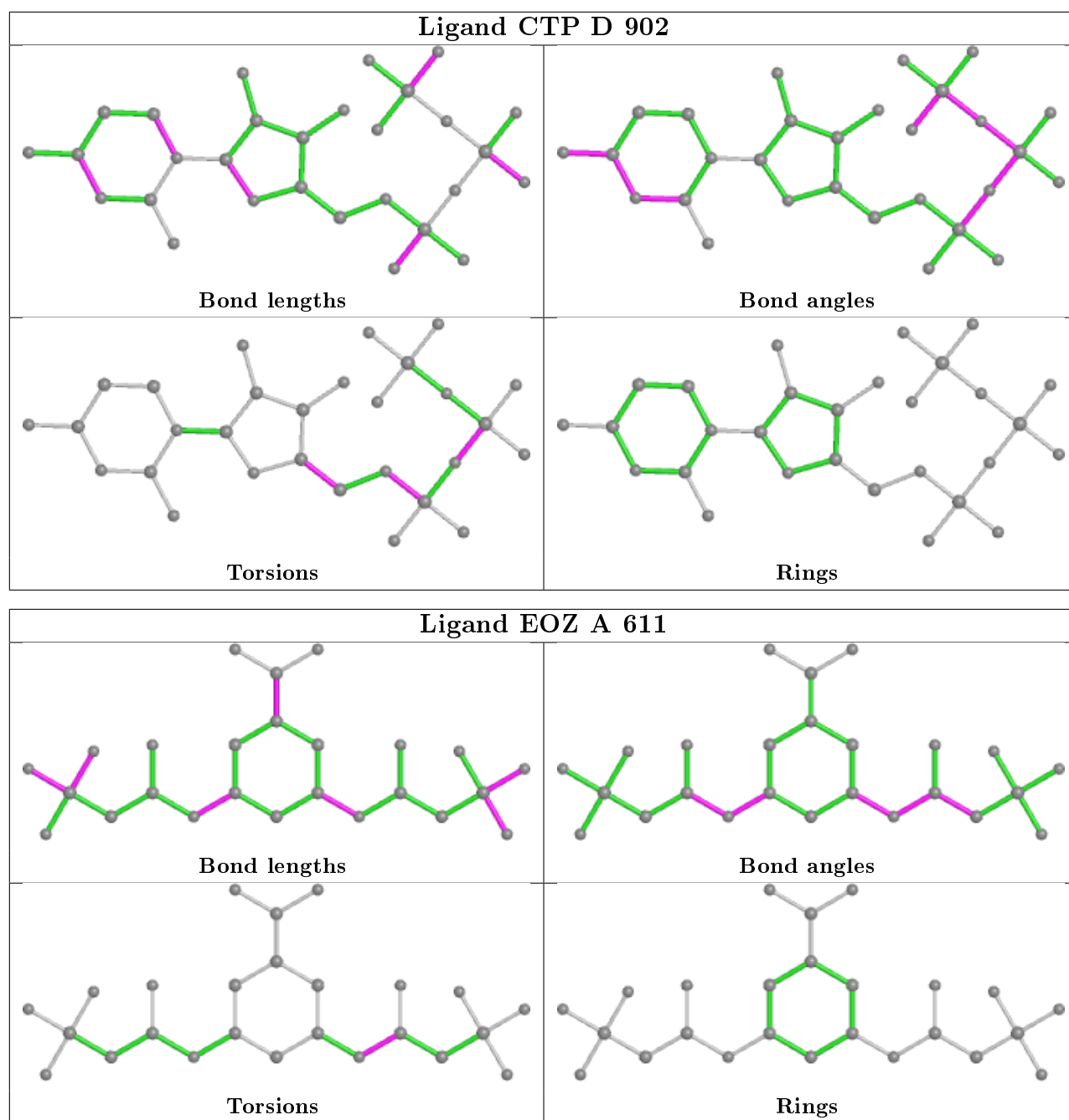
There are no ring outliers.

4 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	612	EOZ	35	0
5	B	901	CTP	13	0
5	D	902	CTP	10	0
3	A	611	EOZ	16	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	310/310 (100%)	-0.25	7 (2%) 60 63	26, 44, 76, 99	0
1	C	310/310 (100%)	-0.24	9 (2%) 51 55	20, 38, 67, 108	0
2	B	152/153 (99%)	0.46	13 (8%) 10 10	32, 70, 106, 109	0
2	D	152/153 (99%)	0.08	8 (5%) 26 28	26, 63, 116, 124	1 (0%)
All	All	924/926 (99%)	-0.07	37 (4%) 38 41	20, 46, 94, 124	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	81	LEU	8.2
2	D	2	THR	7.6
2	B	7	LEU	7.5
1	A	81	LEU	7.2
1	C	80	SER	5.3
1	C	82	GLY	5.3
2	B	6	LYS	5.2
1	C	83	LYS	5.2
1	A	309	VAL	4.8
1	A	80	SER	4.3
2	D	153	ASN	4.1
2	D	4	ASP	3.8
2	D	5	ASN	3.5
2	B	92	VAL	3.4
1	C	137	GLN	3.3
1	C	79	THR	3.2
2	B	8	GLN	3.2
1	A	77	ALA	3.0
2	B	85	ARG	3.0
1	A	79	THR	3.0
2	B	41	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	243	VAL	2.9
2	B	87	ASP	2.9
2	B	11	ALA	2.9
2	D	6	LYS	2.8
1	C	1	ALA	2.8
2	B	91	VAL	2.7
2	D	9	VAL	2.7
1	A	76	SER	2.4
2	B	90	GLU	2.3
2	D	7	LEU	2.3
1	A	247	PHE	2.2
2	B	2	THR	2.2
2	D	52	GLU	2.1
2	B	14	ARG	2.1
1	C	78	ASN	2.1
2	B	94	LYS	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](#)

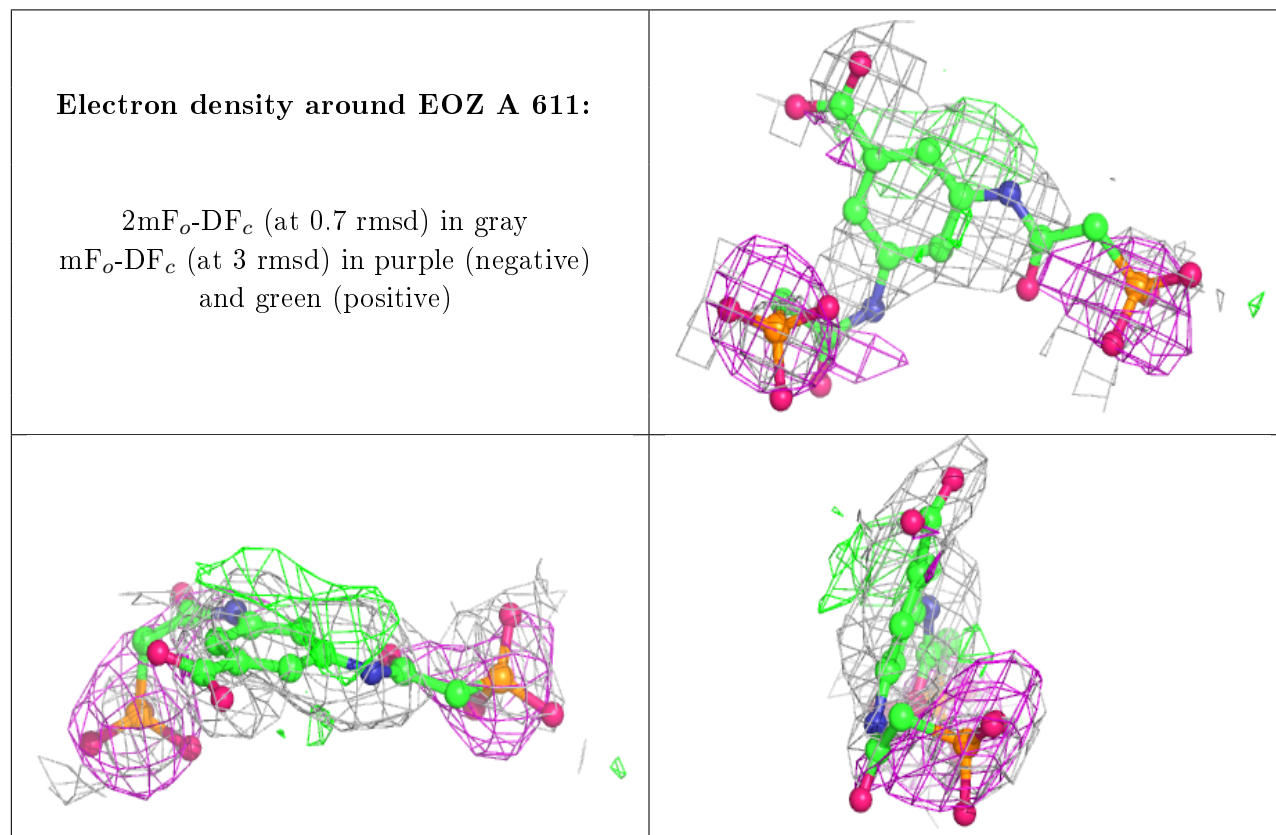
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

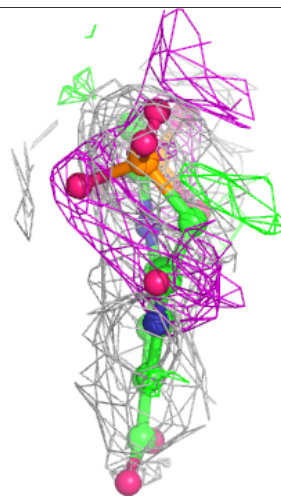
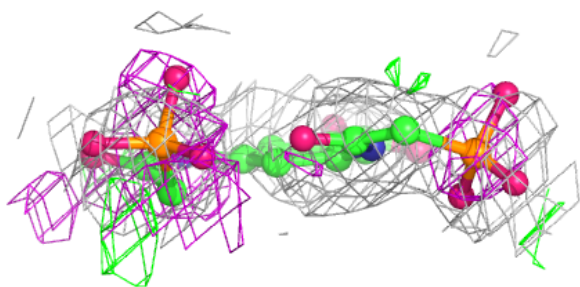
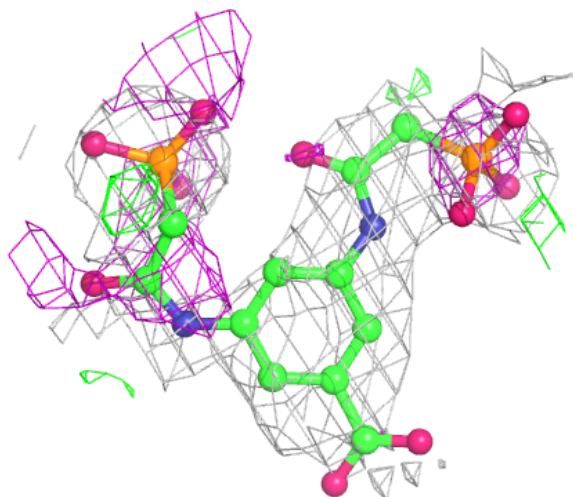
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EOZ	A	611	25/25	0.64	0.46	53,56,60,63	25
3	EOZ	C	612	25/25	0.77	0.36	49,56,63,68	25
5	CTP	D	902	29/29	0.84	0.17	74,82,96,98	29
5	CTP	B	901	29/29	0.85	0.16	86,91,95,100	29
4	ZN	D	154	1/1	0.99	0.18	50,50,50,50	0
4	ZN	B	154	1/1	0.99	0.14	50,50,50,50	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.



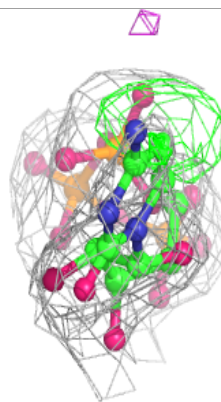
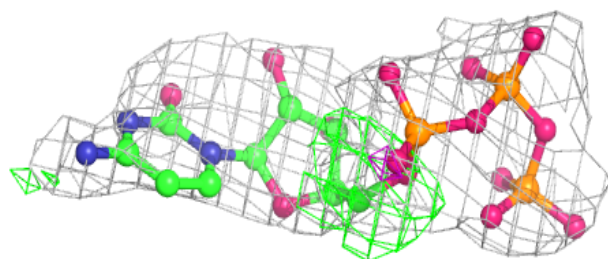
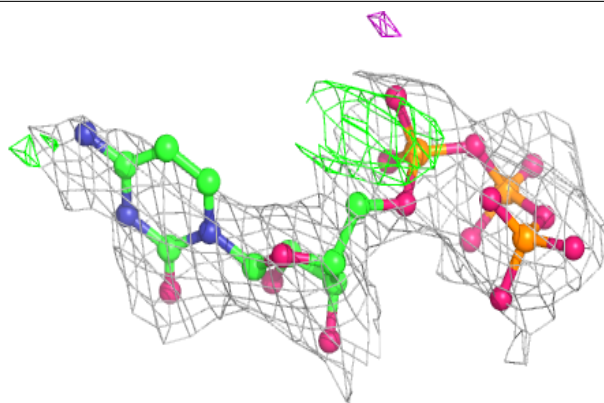
**Electron density around EOZ C 612:**

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

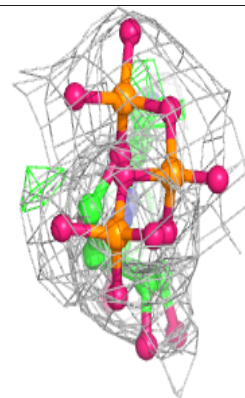
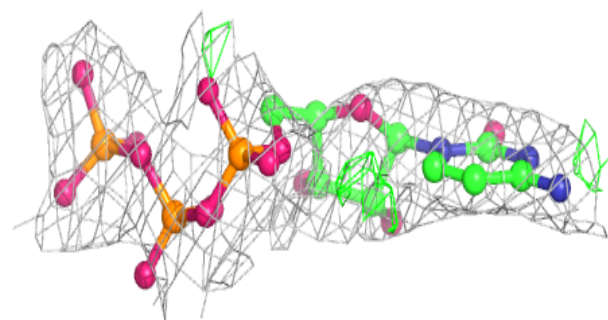
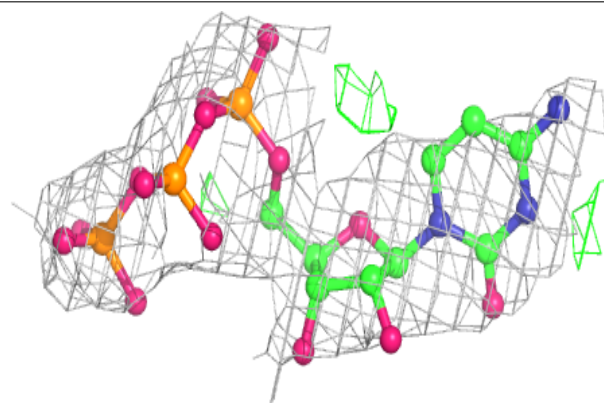


**Electron density around CTP D 902:**

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

**Electron density around CTP B 901:**

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



## 6.5 Other polymers

There are no such residues in this entry.