



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 03:52 PM EDT

PDB ID : 1RYW  
Title : C115S MurA liganded with reaction products  
Authors : Eschenburg, S.; Schonbrunn, E.  
Deposited on : 2003-12-22  
Resolution : 2.30 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

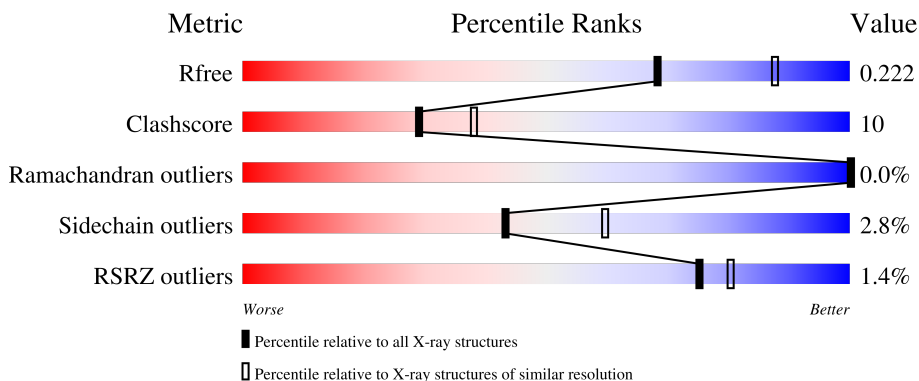
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.



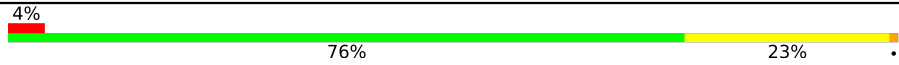

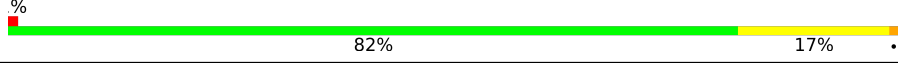
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	419	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="text-align: center;">80%      20%</p>
1	B	419	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="text-align: center;">82%      18%</p>
1	C	419	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="text-align: center;">82%      18%</p>
1	D	419	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="text-align: center;">79%      21%</p>
1	E	419	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="text-align: center;">83%      17%</p>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	419	 4% 76% 23%
1	G	419	 % 80% 20%
1	H	419	 % 82% 17%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 27527 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	3173	1996	560	603	14	0	6	0
1	B	419	3143	1976	554	600	13	0	0	0
1	C	419	3143	1976	554	600	13	0	0	0
1	D	419	3145	1977	554	601	13	0	1	0
1	E	419	3149	1979	555	602	13	0	2	0
1	F	419	3150	1980	557	600	13	0	1	0
1	G	419	3155	1983	557	602	13	0	2	0
1	H	419	3154	1983	557	600	14	0	2	0

There are 16 discrepancies between the modelled and reference sequences:

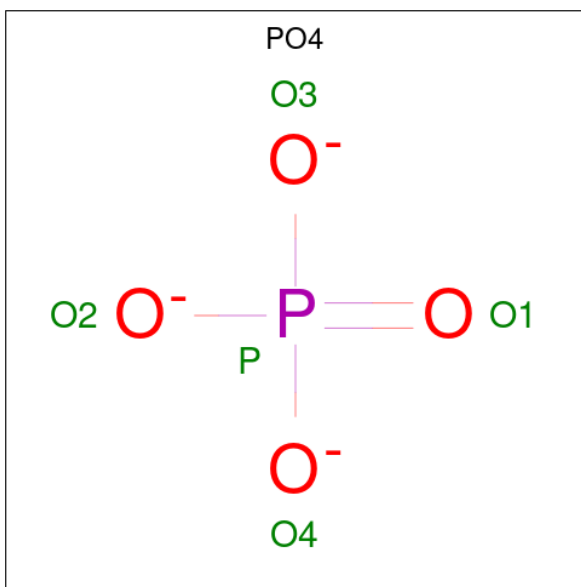
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	engineered mutation	UNP P33038
A	115	SER	CYS	engineered mutation	UNP P33038
B	67	IAS	ASN	engineered mutation	UNP P33038
B	115	SER	CYS	engineered mutation	UNP P33038
C	67	IAS	ASN	engineered mutation	UNP P33038
C	115	SER	CYS	engineered mutation	UNP P33038
D	67	IAS	ASN	engineered mutation	UNP P33038
D	115	SER	CYS	engineered mutation	UNP P33038
E	67	IAS	ASN	engineered mutation	UNP P33038
E	115	SER	CYS	engineered mutation	UNP P33038
F	67	IAS	ASN	engineered mutation	UNP P33038
F	115	SER	CYS	engineered mutation	UNP P33038
G	67	IAS	ASN	engineered mutation	UNP P33038

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	115	SER	CYS	engineered mutation	UNP P33038
H	67	IAS	ASN	engineered mutation	UNP P33038
H	115	SER	CYS	engineered mutation	UNP P33038

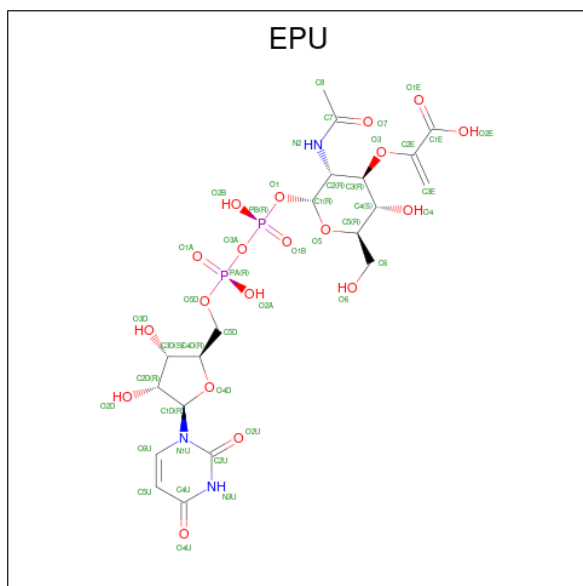
- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0

- Molecule 3 is URIDINE-DIPHOSPHATE-2(N-ACETYLGUCOSAMINYL) BUTYRIC

ACID (three-letter code: EPU) (formula:  $C_{20}H_{29}N_3O_{19}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	Total 44	C 20	N 3	O 19	P 2	0	0
3	B	1	Total 44	C 20	N 3	O 19	P 2	0	0
3	C	1	Total 44	C 20	N 3	O 19	P 2	0	0
3	D	1	Total 44	C 20	N 3	O 19	P 2	0	0
3	E	1	Total 44	C 20	N 3	O 19	P 2	0	0
3	F	1	Total 44	C 20	N 3	O 19	P 2	0	0
3	G	1	Total 44	C 20	N 3	O 19	P 2	0	0
3	H	1	Total 44	C 20	N 3	O 19	P 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

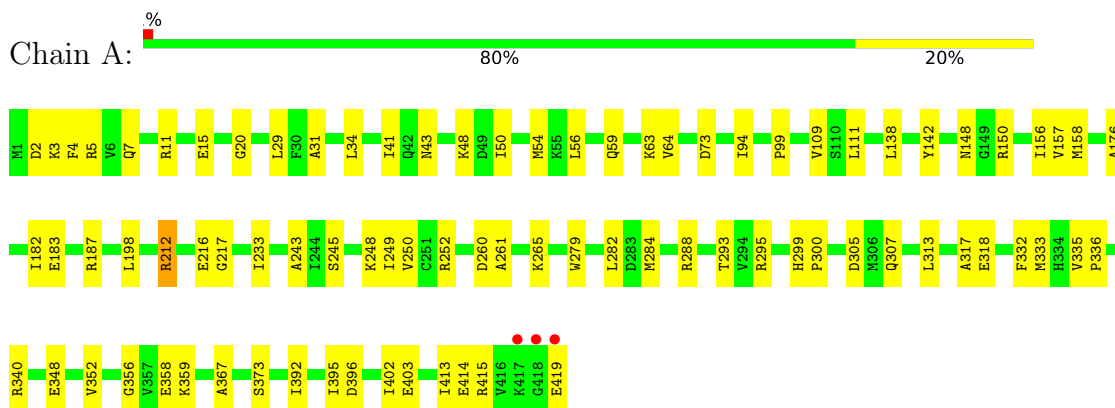
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	284	Total	O	0	0
			284	284		
5	B	253	Total	O	0	0
			253	253		
5	C	272	Total	O	0	0
			272	272		
5	D	208	Total	O	0	0
			208	208		
5	E	214	Total	O	0	0
			214	214		
5	F	136	Total	O	0	0
			136	136		
5	G	237	Total	O	0	0
			237	237		
5	H	212	Total	O	0	0
			212	212		



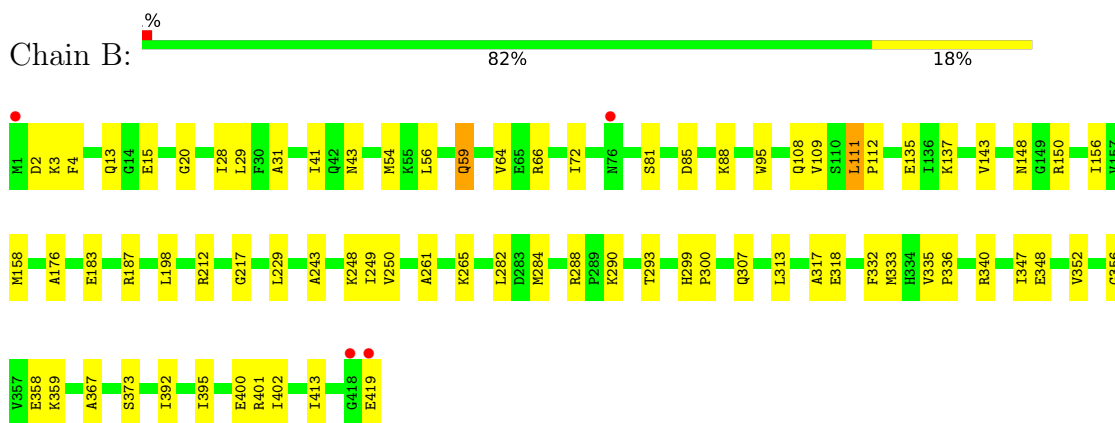
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

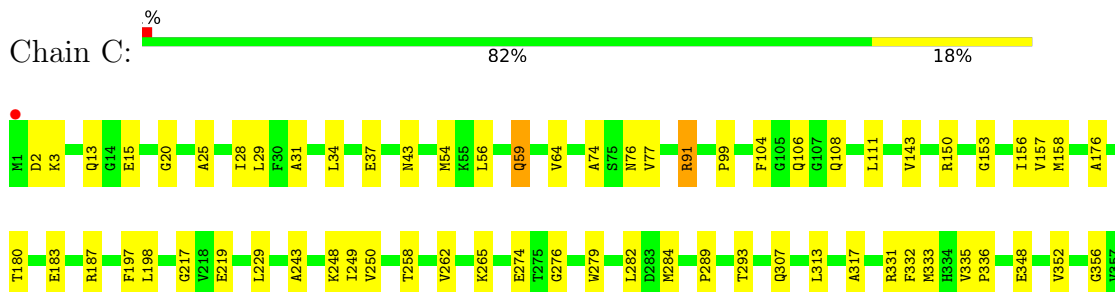
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

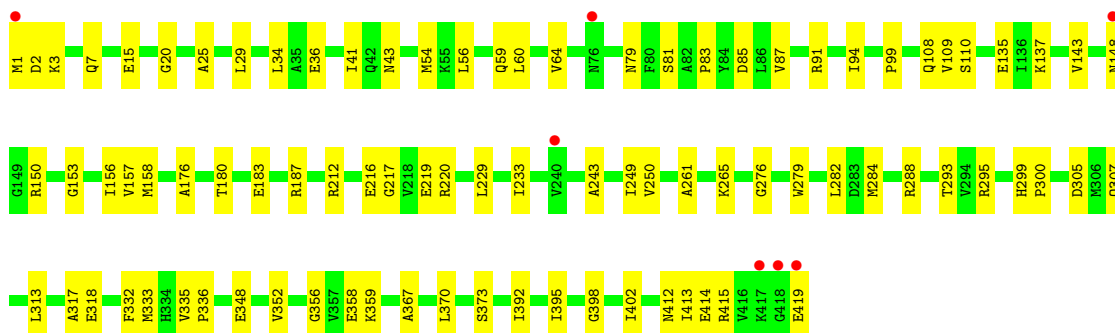
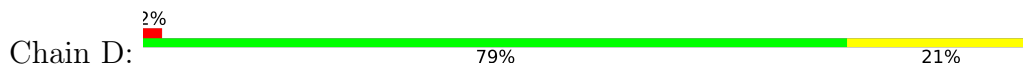


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

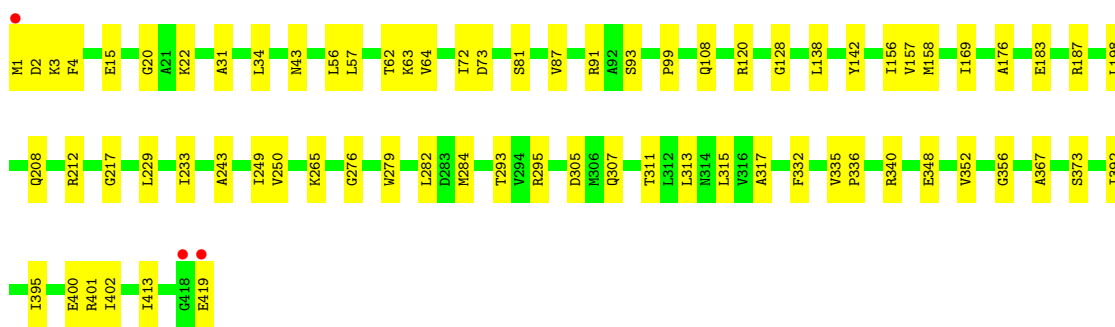
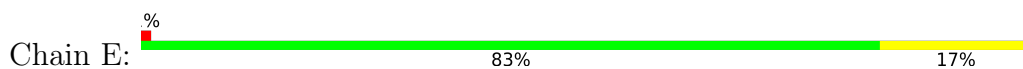




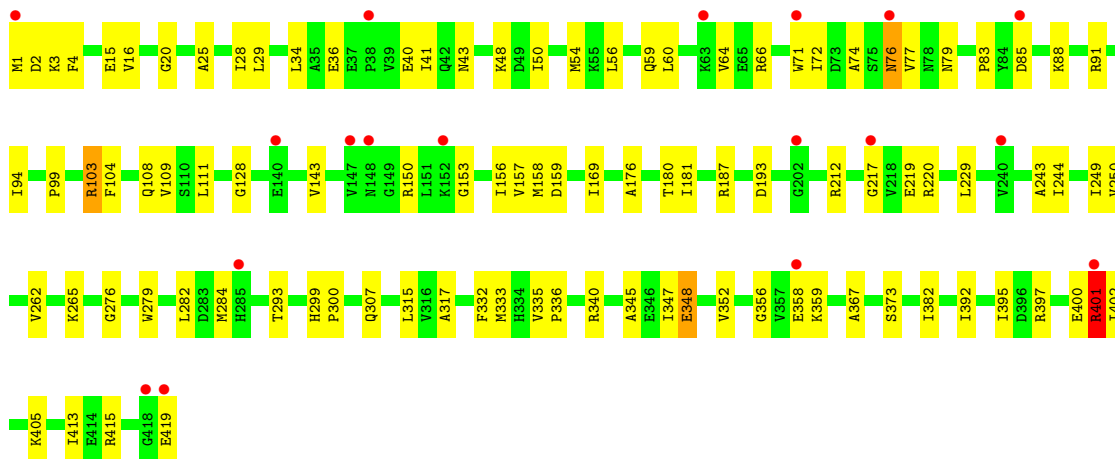
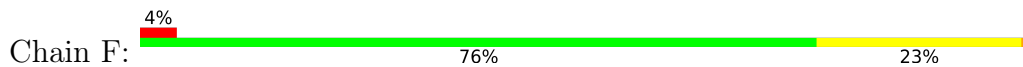
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase




• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

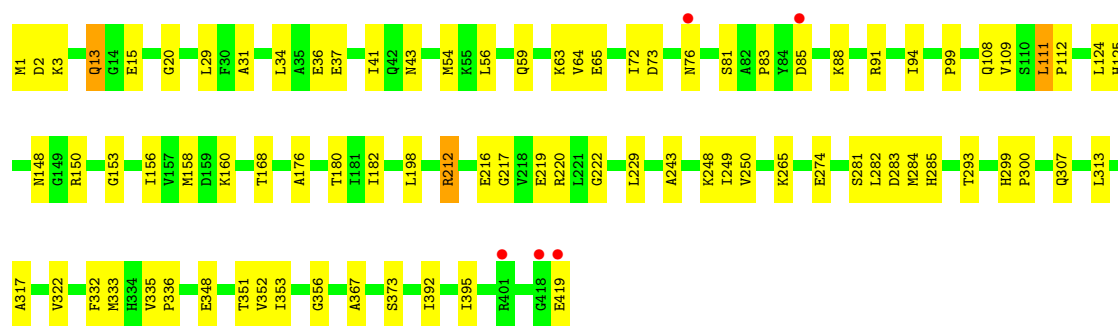


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase




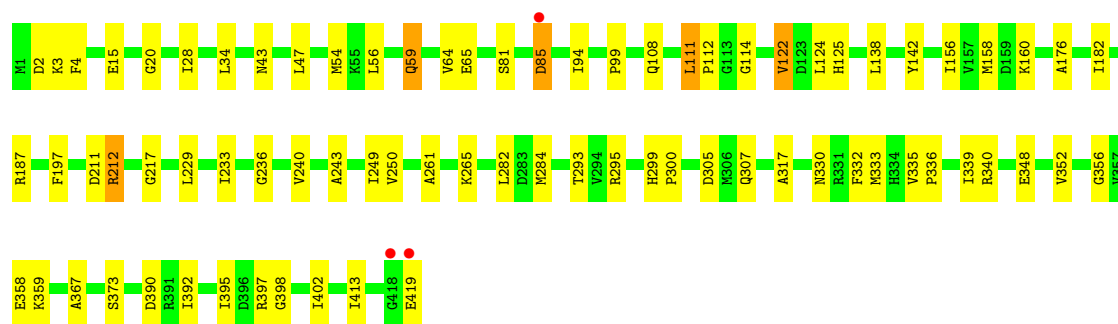
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain G:  %



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain H:  %



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.87Å 153.73Å 135.09Å 90.00° 104.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 29.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.30) 98.9 (29.92-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.31Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.178 , 0.225 0.177 , 0.222	Depositor DCC
$R_{free}$ test set	2801 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtrriage
Anisotropy	0.513	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	27527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7730e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, EPU, GOL, IAS

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	0.37	0/3233	0.62	0/4376
1	B	0.36	0/3179	0.61	0/4305
1	C	0.36	0/3179	0.61	0/4305
1	D	0.35	0/3185	0.59	0/4313
1	E	0.36	0/3193	0.61	0/4324
1	F	0.34	0/3190	0.60	0/4319
1	G	0.36	0/3199	0.61	0/4332
1	H	0.35	0/3198	0.62	0/4329
All	All	0.36	0/25556	0.61	0/34603

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3173	0	3253	70	0
1	B	3143	0	3216	56	0
1	C	3143	0	3216	58	0
1	D	3145	0	3217	61	0
1	E	3149	0	3219	49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3150	0	3225	75	0
1	G	3155	0	3227	67	0
1	H	3154	0	3230	56	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
2	G	10	0	0	0	0
2	H	5	0	0	1	0
3	A	44	0	26	2	0
3	B	44	0	26	2	0
3	C	44	0	26	2	0
3	D	44	0	26	1	0
3	E	44	0	26	3	0
3	F	44	0	26	1	0
3	G	44	0	26	1	0
3	H	44	0	26	3	0
4	A	12	0	16	5	0
4	B	12	0	16	3	0
4	C	30	0	40	7	0
4	D	12	0	16	1	0
4	E	12	0	16	2	0
4	F	6	0	8	1	0
4	G	6	0	8	2	0
4	H	12	0	16	3	0
5	A	284	0	0	7	0
5	B	253	0	0	3	0
5	C	272	0	0	4	0
5	D	208	0	0	3	0
5	E	214	0	0	2	0
5	F	136	0	0	1	0
5	G	237	0	0	7	0
5	H	212	0	0	3	0
All	All	27527	0	26147	498	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 10.

All (498) 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:G:81:SER:HB2	1:G:108:GLN:HE21	1.40	0.86
1:B:54:MET:HE3	1:B:66:ARG:HB3	1.57	0.85
1:G:13:GLN:HG2	1:G:248:LYS:H	1.41	0.84
1:A:150:ARG:HD3	5:A:1069:HOH:O	1.78	0.83
1:C:54:MET:HG2	1:C:64:VAL:HG11	1.60	0.83
1:B:400:GLU:O	1:B:401:ARG:HG2	1.79	0.83
1:F:54:MET:HE1	1:F:66:ARG:HB3	1.62	0.81
1:A:252:ARG:HH12	4:A:2472:GOL:H11	1.43	0.80
1:C:15:GLU:HG2	1:C:250:VAL:HB	1.62	0.80
1:D:15:GLU:HG2	1:D:250:VAL:HB	1.64	0.79
1:B:150:ARG:HD3	5:B:1116:HOH:O	1.83	0.79
1:H:295[B]:ARG:HD2	5:H:769:HOH:O	1.81	0.79
1:F:15:GLU:HG2	1:F:250:VAL:HB	1.65	0.79
1:H:15:GLU:HG2	1:H:250:VAL:HB	1.65	0.79
1:D:87:VAL:HG21	1:D:110:SER:HB3	1.66	0.76
1:A:2:ASP:HB3	1:A:392:ILE:HD11	1.66	0.74
1:E:15:GLU:HG2	1:E:250:VAL:HB	1.69	0.74
1:G:15:GLU:HG2	1:G:250:VAL:HB	1.69	0.74
1:G:322:VAL:HG13	5:G:429:HOH:O	1.87	0.74
1:B:15:GLU:HG2	1:B:250:VAL:HB	1.72	0.71
1:H:54[A]:MET:HG2	1:H:64:VAL:HG11	1.71	0.71
1:C:2:ASP:HB3	1:C:392:ILE:HD11	1.73	0.70
1:E:157:VAL:HA	1:E:183:GLU:HB3	1.73	0.70
1:D:295:ARG:HD2	5:D:1448:HOH:O	1.93	0.69
1:A:54[B]:MET:HG2	1:A:64:VAL:HG11	1.75	0.68
1:D:150:ARG:NH1	1:D:219:GLU:HA	2.09	0.68
1:H:2:ASP:HB3	1:H:392:ILE:HD11	1.75	0.67
1:G:243:ALA:HA	1:G:284:MET:CG	2.24	0.67
1:A:243:ALA:HA	1:A:284:MET:CG	2.25	0.67
1:C:106:GLN:HE21	1:C:108:GLN:HE22	1.43	0.66
1:E:2:ASP:HB3	1:E:392:ILE:HD11	1.76	0.66
1:H:243:ALA:HA	1:H:284:MET:CG	2.26	0.66
1:D:2:ASP:HB3	1:D:392:ILE:HD11	1.76	0.66
1:F:332:PHE:CZ	1:F:352:VAL:HG23	2.31	0.65
1:H:94:ILE:HG12	1:H:122:VAL:HG21	1.77	0.65
1:G:36:GLU:OE1	1:G:220:ARG:HD2	1.96	0.65
1:A:15:GLU:HG2	1:A:250:VAL:HB	1.80	0.64
1:A:358:GLU:HG3	1:A:359:LYS:HG2	1.78	0.64
1:B:135:GLU:OE2	1:B:137:LYS:HE3	1.96	0.64
1:F:109:VAL:O	1:F:143:VAL:HG12	1.97	0.64
1:H:122:VAL:HG22	1:H:125:HIS:CD2	2.33	0.64
1:D:243:ALA:HA	1:D:284:MET:CG	2.28	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:GLN:O	1:D:59:GLN:HG2	1.99	0.63
1:E:332:PHE:CZ	1:E:352:VAL:HG23	2.32	0.63
1:A:156:ILE:HG22	1:A:158:MET:CE	2.29	0.63
1:H:81:SER:HB2	1:H:108:GLN:HE21	1.63	0.62
1:D:54:MET:HG2	1:D:64:VAL:HG11	1.81	0.62
1:A:265:LYS:HE3	1:A:293:THR:O	1.99	0.62
1:G:2:ASP:HB3	1:G:392:ILE:HD11	1.82	0.62
1:F:85:ASP:HA	1:F:88:LYS:HE2	1.81	0.62
1:B:212:ARG:HG2	5:B:475:HOH:O	1.99	0.61
1:G:37[B]:GLU:HG2	1:G:220:ARG:HH22	1.65	0.61
1:F:36:GLU:HB2	1:F:220:ARG:NH2	2.14	0.61
1:D:358:GLU:HG3	1:D:359:LYS:HG2	1.83	0.61
1:G:243:ALA:HA	1:G:284:MET:HG3	1.81	0.60
1:C:332:PHE:CZ	1:C:352:VAL:HG23	2.36	0.60
1:E:87:VAL:HG22	1:E:93[A]:SER:OG	2.01	0.60
1:H:395:ILE:HD11	1:H:402:ILE:HD13	1.82	0.60
3:E:6450:EPU:O1B	4:E:6471:GOL:H11	2.02	0.60
1:F:335:VAL:HB	1:F:336:PRO:HD3	1.83	0.60
1:B:243:ALA:HA	1:B:284:MET:CG	2.32	0.59
1:D:216:GLU:HG3	5:D:1231:HOH:O	2.02	0.59
1:C:150:ARG:NH1	1:C:219:GLU:HA	2.17	0.59
1:A:295[B]:ARG:HD2	5:A:1725:HOH:O	2.03	0.59
1:B:2:ASP:HB3	1:B:392:ILE:HD11	1.85	0.59
1:F:243:ALA:HA	1:F:284:MET:CG	2.33	0.59
3:G:8450:EPU:O1B	4:G:8471:GOL:H11	2.03	0.59
1:C:243:ALA:HA	1:C:284:MET:CG	2.33	0.58
1:E:243:ALA:HA	1:E:284:MET:CG	2.32	0.58
1:F:4:PHE:CD1	1:F:413:ILE:HD11	2.39	0.58
1:A:243:ALA:HA	1:A:284:MET:HG2	1.85	0.58
3:A:2450:EPU:O1B	4:A:2471:GOL:H11	2.04	0.58
1:B:158:MET:HE2	1:B:158:MET:HA	1.85	0.58
1:D:36:GLU:OE1	1:D:220:ARG:HD2	2.02	0.58
1:D:176:ALA:O	1:D:217:GLY:HA3	2.04	0.58
1:B:183:GLU:OE2	1:B:212:ARG:HB2	2.04	0.57
3:H:9450:EPU:H82	4:H:9471:GOL:H32	1.85	0.57
3:B:3450:EPU:O1B	4:B:3471:GOL:H11	2.04	0.57
1:F:59:GLN:O	1:F:59:GLN:HG2	2.05	0.57
1:H:156:ILE:HG22	1:H:158:MET:HE3	1.86	0.57
1:H:367:ALA:HB1	1:H:373:SER:HB3	1.87	0.57
1:B:111:LEU:HD23	1:B:112:PRO:HD2	1.87	0.57
1:G:59:GLN:HE22	1:G:83:PRO:HG3	1.67	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LYS:HE3	1:B:293:THR:O	2.04	0.57
1:B:367:ALA:HB1	1:B:373:SER:HB3	1.87	0.57
1:G:31:ALA:HB1	1:G:198:LEU:HD21	1.85	0.57
1:G:64:VAL:HG13	1:G:72:ILE:CD1	2.35	0.57
1:H:333:MET:O	1:H:336:PRO:HD2	2.05	0.56
1:E:138:LEU:HD12	1:E:142:TYR:O	2.05	0.56
1:H:332:PHE:CZ	1:H:352:VAL:HG23	2.41	0.56
1:F:59:GLN:HE22	1:F:83:PRO:HD3	1.69	0.56
1:F:176:ALA:O	1:F:217:GLY:HA3	2.05	0.56
1:G:54:MET:CE	1:G:64:VAL:HG12	2.35	0.56
1:G:335:VAL:HB	1:G:336:PRO:HD3	1.88	0.56
1:D:413:ILE:HG22	1:D:414:GLU:N	2.21	0.56
3:C:4450:EPU:H82	4:C:4471:GOL:H32	1.88	0.56
1:A:403:GLU:HB3	5:A:1512:HOH:O	2.04	0.56
1:C:335:VAL:HB	1:C:336:PRO:HD3	1.88	0.56
1:E:295:ARG:NH1	5:E:1167:HOH:O	2.39	0.56
1:H:156:ILE:HG22	1:H:158:MET:CE	2.35	0.56
1:A:3:LYS:HE3	1:A:419:GLU:OXT	2.06	0.55
1:C:393:TYR:OH	4:C:3473:GOL:H12	2.06	0.55
1:G:64:VAL:HG13	1:G:72:ILE:HD13	1.88	0.55
1:C:331:ARG:H	4:C:4474:GOL:C3	2.19	0.55
1:F:2:ASP:HB3	1:F:392:ILE:HD11	1.88	0.55
1:F:395:ILE:HD13	1:F:402:ILE:HG21	1.89	0.55
1:G:317:ALA:O	1:G:356:GLY:HA3	2.06	0.55
1:C:392:ILE:O	1:C:395:ILE:HG22	2.07	0.55
1:G:37[A]:GLU:HG3	1:G:220:ARG:HH22	1.71	0.55
1:D:83:PRO:O	1:D:87:VAL:HG13	2.06	0.55
1:D:288:ARG:HD3	1:D:318:GLU:HG3	1.89	0.55
1:C:91:ARG:NH2	5:C:1762:HOH:O	2.40	0.55
1:C:13:GLN:HA	1:C:248:LYS:O	2.07	0.54
1:A:392:ILE:O	1:A:395:ILE:HG22	2.07	0.54
1:B:340:ARG:HG2	1:B:340:ARG:HH11	1.70	0.54
1:B:156:ILE:HG22	1:B:158:MET:CE	2.38	0.54
1:D:243:ALA:HA	1:D:284:MET:HG3	1.88	0.54
1:D:317:ALA:O	1:D:356:GLY:HA3	2.07	0.54
1:G:212:ARG:O	1:G:212:ARG:HG3	2.08	0.54
3:C:4450:EPU:O1B	4:C:4471:GOL:H11	2.08	0.54
1:F:358:GLU:HG3	1:F:359:LYS:HG2	1.90	0.54
1:H:265:LYS:HE3	1:H:293:THR:O	2.07	0.54
1:C:54:MET:HG2	1:C:64:VAL:CG1	2.35	0.54
1:C:331:ARG:H	4:C:4474:GOL:H31	1.72	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:VAL:HG23	5:C:456:HOH:O	2.07	0.54
1:F:392:ILE:O	1:F:395:ILE:HG22	2.07	0.54
1:A:4:PHE:CD1	1:A:413[A]:ILE:HD11	2.43	0.54
1:G:111:LEU:HD23	1:G:112:PRO:HD2	1.89	0.53
1:E:335:VAL:HB	1:E:336:PRO:HD3	1.90	0.53
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.90	0.53
1:B:332:PHE:CZ	1:B:352:VAL:HG23	2.43	0.53
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.91	0.53
1:D:135:GLU:OE2	1:D:137:LYS:HE3	2.07	0.53
1:F:29:LEU:HD23	1:F:41:ILE:HD12	1.88	0.53
1:F:64:VAL:HG13	1:F:72:ILE:HD13	1.91	0.53
1:G:37[B]:GLU:HG2	1:G:220:ARG:NH2	2.24	0.53
1:E:62:THR:HG22	1:E:64:VAL:HG23	1.90	0.53
1:F:181:ILE:HG21	1:F:212:ARG:HH11	1.73	0.53
1:G:332:PHE:CZ	1:G:352:VAL:HG23	2.43	0.53
1:B:317:ALA:O	1:B:356:GLY:HA3	2.08	0.53
1:D:332:PHE:CZ	1:D:352:VAL:HG23	2.44	0.53
1:A:138:LEU:HD12	1:A:142:TYR:O	2.08	0.53
1:B:3:LYS:HE3	1:B:419:GLU:OXT	2.08	0.53
1:F:333:MET:O	1:F:336:PRO:HD2	2.09	0.53
1:A:156:ILE:HG22	1:A:158:MET:HE3	1.90	0.52
1:B:156:ILE:HG22	1:B:158:MET:HE3	1.91	0.52
1:C:56:LEU:C	1:C:56:LEU:HD23	2.29	0.52
1:A:282:LEU:C	1:A:282:LEU:HD23	2.30	0.52
5:G:852:HOH:O	1:H:114:GLY:HA3	2.08	0.52
1:A:29:LEU:HD23	1:A:41:ILE:HD12	1.91	0.52
1:C:3:LYS:HE3	1:C:419:GLU:OXT	2.10	0.52
1:C:258:THR:HG22	5:C:986:HOH:O	2.09	0.52
1:H:249:ILE:HG12	1:H:250:VAL:N	2.24	0.52
1:C:156:ILE:HG22	1:C:158:MET:CE	2.39	0.52
1:D:392:ILE:O	1:D:395:ILE:HG22	2.09	0.52
1:A:317:ALA:O	1:A:356:GLY:HA3	2.09	0.52
1:F:64:VAL:HG13	1:F:72:ILE:CD1	2.39	0.52
1:F:367:ALA:HB1	1:F:373:SER:HB3	1.92	0.52
1:G:54:MET:HE2	1:G:64:VAL:HG12	1.91	0.52
1:G:91:ARG:NH2	5:G:870:HOH:O	2.40	0.52
1:D:150:ARG:HH12	1:D:219:GLU:HA	1.74	0.52
1:D:395:ILE:HD11	1:D:402:ILE:HD13	1.91	0.52
1:A:333:MET:O	1:A:336:PRO:HD2	2.10	0.51
1:F:243:ALA:HA	1:F:284:MET:HG3	1.91	0.51
3:H:9450:EPU:O1B	4:H:9471:GOL:H11	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:GLU:C	1:E:401:ARG:HG2	2.30	0.51
1:G:150:ARG:NH1	1:G:219:GLU:HA	2.25	0.51
1:B:20:GLY:HA3	1:B:43:ASN:O	2.11	0.51
1:A:158:MET:HE2	1:A:158:MET:HA	1.92	0.51
1:C:289:PRO:HD3	5:C:1098:HOH:O	2.11	0.51
1:G:156:ILE:HG22	1:G:158:MET:HE3	1.93	0.51
1:H:392:ILE:O	1:H:395:ILE:HG22	2.10	0.51
1:C:77:VAL:HB	1:C:104:PHE:CZ	2.45	0.51
1:C:367:ALA:HB1	1:C:373:SER:HB3	1.91	0.51
1:E:392:ILE:O	1:E:395:ILE:HG22	2.11	0.51
1:F:3:LYS:HE3	1:F:419:GLU:OXT	2.10	0.51
1:E:4:PHE:CD1	1:E:413:ILE:HD11	2.46	0.51
1:A:252:ARG:NH1	4:A:2472:GOL:H11	2.22	0.51
3:A:2450:EPU:H82	4:A:2471:GOL:H32	1.93	0.51
1:A:295[B]:ARG:NH1	5:A:1725:HOH:O	2.43	0.51
1:B:158:MET:HA	1:B:158:MET:CE	2.41	0.51
1:H:176:ALA:O	1:H:217:GLY:HA3	2.12	0.50
1:E:56:LEU:C	1:E:56:LEU:HD23	2.30	0.50
1:C:317:ALA:O	1:C:356:GLY:HA3	2.11	0.50
1:D:59:GLN:NE2	1:D:81:SER:O	2.44	0.50
1:F:265:LYS:HE3	1:F:293:THR:O	2.11	0.50
1:F:332:PHE:CE1	1:F:352:VAL:HG23	2.46	0.50
1:B:395:ILE:HD13	1:B:402:ILE:HG21	1.94	0.50
1:F:249:ILE:HG12	1:F:250:VAL:N	2.25	0.50
1:G:333:MET:O	1:G:336:PRO:HD2	2.12	0.50
1:A:332:PHE:CZ	1:A:352:VAL:HG23	2.45	0.50
1:B:395:ILE:HD11	1:B:402:ILE:HD13	1.93	0.50
1:A:176:ALA:O	1:A:217:GLY:HA3	2.12	0.50
1:D:87:VAL:CG2	1:D:110:SER:HB3	2.40	0.50
1:D:212:ARG:HG2	5:D:493:HOH:O	2.11	0.50
1:E:3:LYS:HE3	1:E:419:GLU:OXT	2.12	0.50
1:H:243:ALA:HA	1:H:284:MET:HG2	1.94	0.50
1:B:54:MET:HE2	1:B:64:VAL:CG1	2.42	0.50
1:E:340:ARG:HG2	1:E:340:ARG:HH11	1.76	0.50
1:H:124:LEU:HD11	1:H:160:LYS:HB2	1.93	0.50
1:H:335:VAL:O	1:H:339:ILE:HG13	2.12	0.50
1:B:81:SER:HB2	1:B:108:GLN:HE21	1.76	0.50
1:F:153:GLY:HA2	1:F:180:THR:OG1	2.12	0.50
1:G:282:LEU:C	1:G:282:LEU:HD23	2.31	0.50
1:C:31:ALA:HB1	1:C:198:LEU:HD21	1.94	0.49
1:E:138:LEU:HA	1:E:142:TYR:O	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ALA:O	1:E:217:GLY:HA3	2.12	0.49
1:B:392:ILE:O	1:B:395:ILE:HG22	2.12	0.49
1:F:56:LEU:C	1:F:56:LEU:HD23	2.32	0.49
1:F:262:VAL:HG23	5:F:624:HOH:O	2.11	0.49
1:B:249:ILE:HG12	1:B:250:VAL:N	2.27	0.49
1:B:333:MET:O	1:B:336:PRO:HD2	2.12	0.49
1:G:367:ALA:HB1	1:G:373:SER:HB3	1.94	0.49
1:B:29:LEU:HD23	1:B:41:ILE:HD12	1.93	0.49
1:B:109:VAL:O	1:B:143:VAL:HG12	2.13	0.49
1:E:313:LEU:HD23	1:E:313:LEU:C	2.32	0.49
1:F:20:GLY:HA3	1:F:43:ASN:O	2.12	0.49
1:F:48:LYS:HB3	1:F:397:ARG:HD3	1.94	0.49
1:B:290:LYS:HE2	5:B:669:HOH:O	2.12	0.49
1:G:156:ILE:HG22	1:G:158:MET:CE	2.43	0.49
1:H:111:LEU:HD23	1:H:112:PRO:HD2	1.94	0.49
1:A:260:ASP:OD2	1:D:212:ARG:NH2	2.46	0.49
1:F:54:MET:HE3	1:F:64:VAL:HG12	1.94	0.49
1:H:54[A]:MET:CE	1:H:64:VAL:HG12	2.43	0.49
1:C:249:ILE:HG12	1:C:250:VAL:N	2.28	0.49
1:D:282:LEU:HD23	1:D:282:LEU:C	2.32	0.49
1:A:48:LYS:HG3	5:A:796:HOH:O	2.13	0.49
1:A:279:TRP:CE2	4:A:2472:GOL:H12	2.48	0.48
1:G:85:ASP:HA	1:G:88:LYS:HE2	1.95	0.48
1:A:261:ALA:HA	1:D:157:VAL:HG11	1.94	0.48
1:D:335:VAL:HB	1:D:336:PRO:HD3	1.96	0.48
1:F:340:ARG:HH11	1:F:340:ARG:HG2	1.78	0.48
1:H:138:LEU:HD12	1:H:142:TYR:O	2.13	0.48
1:G:392:ILE:O	1:G:395:ILE:HG22	2.13	0.48
1:H:122:VAL:HG13	1:H:122:VAL:O	2.13	0.48
1:H:212:ARG:HG3	1:H:212:ARG:O	2.12	0.48
1:B:56:LEU:HD23	1:B:56:LEU:C	2.33	0.48
1:C:358:GLU:HG3	1:C:359:LYS:HG2	1.94	0.48
1:E:265:LYS:HE3	1:E:293:THR:O	2.13	0.48
1:E:34:LEU:HD21	1:E:99:PRO:HA	1.95	0.48
1:G:3:LYS:HE3	1:G:419:GLU:OXT	2.13	0.48
1:A:243:ALA:HA	1:A:284:MET:HG3	1.95	0.48
1:B:54:MET:HE2	1:B:64:VAL:HG12	1.96	0.48
1:F:150:ARG:NH1	1:F:219:GLU:HA	2.29	0.48
3:F:7450:EPU:O1B	4:F:7471:GOL:H11	2.14	0.48
1:A:413[B]:ILE:HG22	1:A:414:GLU:N	2.29	0.48
1:C:243:ALA:HA	1:C:284:MET:HG2	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:ILE:CG2	1:D:414:GLU:N	2.77	0.47
1:H:54[A]:MET:HE2	1:H:64:VAL:HG12	1.96	0.47
1:H:233:ILE:HD12	1:H:305:ASP:HB2	1.96	0.47
1:H:243:ALA:HA	1:H:284:MET:HG3	1.94	0.47
1:B:282:LEU:C	1:B:282:LEU:HD23	2.34	0.47
1:F:317:ALA:O	1:F:356:GLY:HA3	2.14	0.47
1:A:358:GLU:HG2	1:G:13:GLN:NE2	2.29	0.47
1:B:299:HIS:CG	1:B:300:PRO:HA	2.49	0.47
1:C:56:LEU:HD23	1:C:56:LEU:O	2.13	0.47
3:B:3450:EPU:H82	4:B:3471:GOL:H32	1.96	0.47
1:C:91:ARG:HD3	4:C:4471:GOL:O2	2.14	0.47
1:D:265:LYS:CE	1:D:293:THR:O	2.62	0.47
1:D:333:MET:O	1:D:336:PRO:HD2	2.15	0.47
1:H:59:GLN:HE21	1:H:59:GLN:HB3	1.48	0.47
1:D:56:LEU:HD23	1:D:56:LEU:C	2.35	0.47
1:E:243:ALA:HA	1:E:284:MET:HG3	1.97	0.47
1:F:244:ILE:HD12	1:F:382:ILE:HD13	1.95	0.47
1:C:395:ILE:HD13	1:C:402:ILE:HG21	1.97	0.47
1:A:156:ILE:CG2	1:A:158:MET:HE1	2.45	0.47
1:C:265:LYS:HE3	1:C:293:THR:O	2.15	0.47
1:F:94:ILE:HA	1:F:109:VAL:HG11	1.96	0.47
1:G:353:ILE:HG12	5:G:429:HOH:O	2.15	0.47
1:A:5:ARG:HH12	1:A:7:GLN:NE2	2.13	0.47
1:G:108:GLN:NE2	5:G:1729:HOH:O	2.46	0.47
1:H:3:LYS:HE3	1:H:419:GLU:OXT	2.15	0.47
1:D:1:MET:N	1:D:419:GLU:HA	2.30	0.46
1:F:29:LEU:HD23	1:F:41:ILE:CD1	2.45	0.46
1:H:299:HIS:CG	1:H:300:PRO:HA	2.50	0.46
1:B:288:ARG:HD3	1:B:318:GLU:HG3	1.96	0.46
1:E:265:LYS:CE	1:E:293:THR:O	2.62	0.46
1:F:109:VAL:O	1:F:143:VAL:CG1	2.64	0.46
1:D:2:ASP:OD2	1:D:415:ARG:HD3	2.15	0.46
1:E:120:ARG:HA	3:E:6450:EPU:O2D	2.16	0.46
1:F:395:ILE:HD11	1:F:402:ILE:HD13	1.96	0.46
1:A:54[B]:MET:CE	1:A:64:VAL:HG12	2.45	0.46
1:A:156:ILE:HG22	1:A:158:MET:HE1	1.98	0.46
1:C:176:ALA:O	1:C:217:GLY:HA3	2.16	0.46
1:D:7:GLN:HB2	1:D:412:ASN:HB3	1.96	0.46
1:E:317:ALA:O	1:E:356:GLY:HA3	2.15	0.46
1:A:265:LYS:CE	1:A:293:THR:O	2.64	0.46
1:C:59:GLN:HE21	1:C:59:GLN:HB3	1.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:ILE:HD12	1:E:305:ASP:HB2	1.98	0.46
1:B:400:GLU:C	1:B:401:ARG:HG2	2.36	0.46
1:D:20:GLY:HA3	1:D:43:ASN:O	2.15	0.46
1:D:25:ALA:O	1:D:29:LEU:HG	2.15	0.46
1:G:176:ALA:O	1:G:217:GLY:HA3	2.16	0.46
1:D:395:ILE:HD13	1:D:402:ILE:HG21	1.98	0.46
1:F:400:GLU:O	1:F:401:ARG:HG2	2.15	0.46
1:G:20:GLY:HA3	1:G:43:ASN:O	2.15	0.46
1:A:249:ILE:HG12	1:A:250:VAL:N	2.31	0.45
1:D:60:LEU:HA	1:D:79:ASN:HB3	1.98	0.45
1:E:158:MET:HA	1:E:158:MET:HE2	1.98	0.45
1:E:282:LEU:C	1:E:282:LEU:HD23	2.37	0.45
1:E:367:ALA:HB1	1:E:373:SER:HB3	1.98	0.45
1:H:56:LEU:C	1:H:56:LEU:HD23	2.36	0.45
1:A:395:ILE:HD11	1:A:402:ILE:HD13	1.98	0.45
1:E:276:GLY:HA3	1:E:279:TRP:NE1	2.31	0.45
1:F:397:ARG:NH1	1:F:397:ARG:HG3	2.30	0.45
1:G:243:ALA:HA	1:G:284:MET:HG2	1.96	0.45
1:H:395:ILE:HD13	1:H:402:ILE:HG21	1.97	0.45
1:H:397:ARG:HH12	2:H:9461:PO4:P	2.38	0.45
1:D:370:LEU:HD21	1:D:398:GLY:HA3	1.97	0.45
1:G:91:ARG:HG3	4:G:8471:GOL:O3	2.16	0.45
1:D:3:LYS:HE3	1:D:419:GLU:OXT	2.17	0.45
1:F:156:ILE:HG22	1:F:158:MET:HE3	1.96	0.45
1:H:158:MET:HA	1:H:158:MET:HE2	1.97	0.45
1:B:85:ASP:O	1:B:88:LYS:HG2	2.16	0.45
1:C:158:MET:HA	1:C:158:MET:HE2	1.99	0.45
1:H:3:LYS:HG2	1:H:390:ASP:HA	1.99	0.45
1:H:340:ARG:HH11	1:H:340:ARG:HG2	1.81	0.45
1:A:233:ILE:HD12	1:A:305:ASP:HB2	1.98	0.45
1:E:249:ILE:HG12	1:E:250:VAL:N	2.32	0.45
1:E:332:PHE:CE1	1:E:352:VAL:HG23	2.52	0.45
1:G:1:MET:N	1:G:419:GLU:HA	2.31	0.45
1:A:288:ARG:NH1	1:A:318[B]:GLU:OE2	2.50	0.45
1:D:94:ILE:HA	1:D:109:VAL:HG11	1.97	0.45
1:D:367:ALA:HB1	1:D:373:SER:HB3	1.99	0.45
1:F:16:VAL:CG2	1:F:405:LYS:HD3	2.46	0.45
1:F:34:LEU:HD21	1:F:99:PRO:HA	1.98	0.45
1:H:317:ALA:O	1:H:356:GLY:HA3	2.17	0.45
1:A:31:ALA:HB1	1:A:198:LEU:HD21	1.97	0.45
1:A:299:HIS:CG	1:A:300:PRO:HA	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:LEU:HA	1:F:79:ASN:HB3	1.98	0.45
1:F:76:ASN:HD22	1:F:76:ASN:C	2.19	0.45
1:F:299:HIS:CG	1:F:300:PRO:HA	2.52	0.45
1:H:47:LEU:HD13	1:H:398:GLY:HA2	1.98	0.45
1:H:358:GLU:HG3	1:H:359:LYS:HG2	1.99	0.45
1:A:367:ALA:HB1	1:A:373:SER:HB3	1.97	0.45
3:D:5450:EPU:O1B	4:D:5471:GOL:H11	2.17	0.45
1:G:34:LEU:HD21	1:G:99:PRO:HA	1.99	0.45
1:B:28:ILE:HG22	1:B:41:ILE:HD13	1.98	0.45
1:D:29:LEU:HD23	1:D:41:ILE:HD12	1.99	0.45
1:F:2:ASP:OD2	1:F:415:ARG:HD3	2.17	0.45
1:D:156:ILE:HG22	1:D:158:MET:HE3	1.98	0.44
1:E:22:LYS:NZ	2:E:6461:PO4:O2	2.46	0.44
1:A:11:ARG:HG3	1:A:245:SER:O	2.18	0.44
1:G:249:ILE:HG12	1:G:250:VAL:N	2.31	0.44
1:B:143:VAL:HG13	1:B:143:VAL:O	2.16	0.44
1:D:313:LEU:C	1:D:313:LEU:HD23	2.37	0.44
1:G:313:LEU:HD23	1:G:313:LEU:C	2.37	0.44
3:H:9450:EPU:H82	4:H:9471:GOL:C3	2.46	0.44
1:D:54:MET:CE	1:D:64:VAL:HG12	2.47	0.44
1:D:156:ILE:HG22	1:D:158:MET:CE	2.47	0.44
1:E:81:SER:HA	1:E:108:GLN:O	2.17	0.44
1:G:63:LYS:HB2	1:G:73:ASP:HB3	1.99	0.44
1:G:94:ILE:HA	1:G:109:VAL:HG11	1.99	0.44
1:G:274:GLU:HB2	1:G:281:SER:OG	2.18	0.44
1:F:40:GLU:HG3	1:F:71:TRP:NE1	2.33	0.44
1:B:4:PHE:CD1	1:B:413:ILE:HD11	2.53	0.44
1:C:395:ILE:HD11	1:C:402:ILE:HD13	2.00	0.44
1:D:54:MET:HE2	1:D:64:VAL:HG12	2.00	0.44
1:E:276:GLY:HA3	1:E:279:TRP:CE2	2.53	0.44
1:F:315:LEU:HD21	1:F:345:ALA:HB2	2.00	0.44
1:A:63:LYS:HB2	1:A:73:ASP:HB3	2.00	0.44
1:G:56:LEU:HD23	1:G:56:LEU:C	2.38	0.44
1:A:295[A]:ARG:HD2	5:A:1725:HOH:O	2.17	0.44
1:C:74:ALA:O	1:C:77:VAL:HG23	2.18	0.43
1:B:313:LEU:HD23	1:B:313:LEU:C	2.39	0.43
1:C:276:GLY:HA3	1:C:279:TRP:CE2	2.53	0.43
1:F:56:LEU:O	1:F:60:LEU:HG	2.18	0.43
1:A:50:ILE:O	1:A:54[A]:MET:HG3	2.17	0.43
1:E:1:MET:N	1:E:419:GLU:HA	2.33	0.43
1:F:16:VAL:HG23	1:F:405:LYS:HD3	2.00	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:VAL:HG22	1:H:125:HIS:CG	2.53	0.43
1:H:282:LEU:C	1:H:282:LEU:HD23	2.37	0.43
1:A:56:LEU:C	1:A:56:LEU:HD23	2.38	0.43
1:C:156:ILE:HG22	1:C:158:MET:HE3	2.00	0.43
1:D:276:GLY:HA3	1:D:279:TRP:NE1	2.34	0.43
1:F:128:GLY:HA3	1:F:169:ILE:CD1	2.49	0.43
1:G:220:ARG:HH21	1:G:222:GLY:HA2	1.83	0.43
1:G:37[A]:GLU:HG3	1:G:220:ARG:NH2	2.32	0.43
1:G:248:LYS:HA	1:G:282:LEU:O	2.19	0.43
1:G:125:HIS:HD2	1:G:168:THR:OG1	2.00	0.43
1:B:64:VAL:HG13	1:B:72:ILE:HD13	2.00	0.43
1:G:353:ILE:HA	5:G:429:HOH:O	2.18	0.43
1:E:158:MET:HA	1:E:158:MET:CE	2.49	0.43
1:G:29:LEU:HD23	1:G:41:ILE:HD12	2.00	0.43
1:H:335:VAL:HB	1:H:336:PRO:HD3	2.00	0.43
1:D:233:ILE:HD12	1:D:305:ASP:HB2	2.01	0.43
3:E:6450:EPU:H82	4:E:6471:GOL:H32	2.01	0.43
1:F:128:GLY:HA3	1:F:169:ILE:HD11	2.00	0.43
1:H:85:ASP:OD1	1:H:85:ASP:N	2.48	0.43
1:B:261:ALA:HA	1:C:157:VAL:HG11	2.01	0.43
1:D:249:ILE:HG12	1:D:250:VAL:N	2.33	0.43
1:F:150:ARG:HH12	1:F:219:GLU:HA	1.83	0.42
1:C:2:ASP:CB	1:C:392:ILE:HD11	2.45	0.42
1:C:332:PHE:CE1	1:C:352:VAL:HG23	2.54	0.42
1:B:59:GLN:HE21	1:B:59:GLN:HB3	1.54	0.42
1:C:158:MET:CE	1:C:158:MET:HA	2.50	0.42
1:E:156:ILE:HG22	1:E:158:MET:CE	2.49	0.42
1:F:347:ILE:HG12	1:F:352:VAL:HG22	2.01	0.42
1:A:34:LEU:HD21	1:A:99:PRO:HA	2.00	0.42
1:A:94:ILE:HA	1:A:109:VAL:HG11	2.02	0.42
1:B:358:GLU:HG3	1:B:359:LYS:HG2	2.02	0.42
1:D:299:HIS:CG	1:D:300:PRO:HA	2.54	0.42
1:E:20:GLY:HA3	1:E:43:ASN:O	2.18	0.42
1:F:276:GLY:HA3	1:F:279:TRP:NE1	2.35	0.42
1:F:54:MET:HE3	1:F:64:VAL:CG1	2.50	0.42
1:F:74:ALA:O	1:F:77:VAL:HG23	2.19	0.42
1:G:153:GLY:HA2	1:G:180:THR:OG1	2.20	0.42
1:A:413[B]:ILE:CG2	1:A:414:GLU:N	2.83	0.42
1:E:128:GLY:HA3	1:E:169:ILE:CD1	2.49	0.42
1:E:212:ARG:CD	5:E:1769:HOH:O	2.68	0.42
1:G:265:LYS:CE	1:G:293:THR:O	2.68	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:ILE:HG23	1:H:197:PHE:CD2	2.54	0.42
1:B:347:ILE:HG12	1:B:352:VAL:HG22	2.02	0.42
1:D:34:LEU:HD21	1:D:99:PRO:HA	2.00	0.42
1:F:28:ILE:HG22	1:F:41:ILE:HD13	2.00	0.42
1:F:282:LEU:C	1:F:282:LEU:HD23	2.40	0.42
1:A:248:LYS:HA	1:A:282:LEU:O	2.20	0.42
1:B:81:SER:HB2	1:B:108:GLN:NE2	2.34	0.42
1:D:153:GLY:HA2	1:D:180:THR:OG1	2.19	0.42
1:H:330:ASN:ND2	5:H:839:HOH:O	2.52	0.42
1:A:20:GLY:HA3	1:A:43:ASN:O	2.20	0.42
1:A:158:MET:CE	1:A:158:MET:HA	2.49	0.42
1:F:103:ARG:HD2	1:F:104:PHE:CZ	2.55	0.42
1:F:156:ILE:HG22	1:F:158:MET:CE	2.50	0.42
1:F:157:VAL:HG11	1:H:261:ALA:HA	2.02	0.42
1:G:124:LEU:HD11	1:G:160:LYS:HB2	2.01	0.42
1:C:156:ILE:CG2	1:C:158:MET:HE1	2.50	0.42
1:C:243:ALA:HA	1:C:284:MET:HG3	2.00	0.42
1:A:313:LEU:C	1:A:313:LEU:HD23	2.41	0.41
1:C:333:MET:O	1:C:336:PRO:HD2	2.20	0.41
1:F:54:MET:CE	1:F:64:VAL:HG12	2.50	0.41
1:G:125:HIS:HE1	5:G:420:HOH:O	2.02	0.41
1:H:20:GLY:HA3	1:H:43:ASN:O	2.20	0.41
1:D:332:PHE:CE1	1:D:352:VAL:HG23	2.55	0.41
1:F:265:LYS:CE	1:F:293:THR:O	2.68	0.41
1:H:4:PHE:CD1	1:H:413:ILE:HD11	2.55	0.41
1:A:29:LEU:HD23	1:A:41:ILE:CD1	2.50	0.41
1:A:359:LYS:HD2	5:A:571:HOH:O	2.21	0.41
1:E:63:LYS:HB2	1:E:73:ASP:HB3	2.01	0.41
1:F:348:GLU:HG2	1:G:351:THR:HG21	2.02	0.41
1:E:395:ILE:HD13	1:E:402:ILE:HG21	2.01	0.41
1:F:1:MET:N	1:F:419:GLU:HA	2.35	0.41
1:C:34:LEU:HD21	1:C:99:PRO:HA	2.01	0.41
1:C:265:LYS:CE	1:C:293:THR:O	2.68	0.41
1:C:403:GLU:HG2	1:C:404:ASP:N	2.35	0.41
1:A:2:ASP:CB	1:A:392:ILE:HD11	2.43	0.41
1:C:282:LEU:C	1:C:282:LEU:HD23	2.41	0.41
1:B:243:ALA:HA	1:B:284:MET:HG3	2.01	0.41
1:B:367:ALA:HB1	1:B:373:SER:CB	2.49	0.41
1:B:13:GLN:HA	1:B:248:LYS:O	2.20	0.41
1:B:176:ALA:O	1:B:217:GLY:HA3	2.21	0.41
1:C:25:ALA:O	1:C:29:LEU:HG	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ILE:HG23	1:C:197:PHE:CD2	2.56	0.41
1:C:391:ARG:HH12	4:C:2473:GOL:H12	1.86	0.41
1:E:156:ILE:HG22	1:E:158:MET:HE3	2.01	0.41
1:E:208:GLN:O	1:E:208:GLN:HG2	2.21	0.41
1:F:400:GLU:O	1:F:401:ARG:C	2.59	0.41
1:H:34:LEU:HD21	1:H:99:PRO:HA	2.03	0.41
1:A:396:ASP:CG	1:A:415:ARG:HH22	2.24	0.41
1:B:31:ALA:HB1	1:B:198:LEU:HD21	2.02	0.41
1:C:265:LYS:HD2	1:C:265:LYS:HA	1.92	0.41
1:C:313:LEU:C	1:C:313:LEU:HD23	2.41	0.41
1:E:31:ALA:HB1	1:E:198:LEU:HD21	2.03	0.41
1:E:57:LEU:O	1:E:62:THR:HB	2.20	0.41
1:F:25:ALA:O	1:F:29:LEU:HG	2.21	0.41
1:F:50:ILE:O	1:F:54:MET:HG3	2.20	0.41
1:F:56:LEU:HD23	1:F:56:LEU:O	2.20	0.41
1:G:2:ASP:CB	1:G:392:ILE:HD11	2.50	0.41
1:G:282:LEU:HD23	1:G:283:ASP:N	2.36	0.41
1:H:392:ILE:H	1:H:392:ILE:HG13	1.71	0.41
1:B:332:PHE:CE1	1:B:352:VAL:HG23	2.56	0.41
1:C:20:GLY:HA3	1:C:43:ASN:O	2.20	0.41
1:D:29:LEU:HD23	1:D:41:ILE:CD1	2.51	0.41
1:A:157:VAL:HG11	1:D:261:ALA:HA	2.03	0.40
1:D:265:LYS:HA	1:D:265:LYS:HD2	1.84	0.40
1:E:64:VAL:HG22	1:E:72:ILE:CD1	2.51	0.40
1:F:397:ARG:HG3	1:F:397:ARG:HH11	1.86	0.40
1:H:236:GLY:O	1:H:240:VAL:HG23	2.21	0.40
1:G:54:MET:HE3	1:G:64:VAL:HG12	2.03	0.40
1:G:158:MET:CE	1:G:158:MET:HA	2.50	0.40
1:C:153:GLY:HA2	1:C:180:THR:OG1	2.21	0.40
1:C:156:ILE:HG22	1:C:158:MET:HE1	2.03	0.40
1:A:318[A]:GLU:HG2	1:G:285:HIS:O	2.21	0.40
1:A:340:ARG:HH11	1:A:340:ARG:HG2	1.87	0.40
1:D:81:SER:HA	1:D:108:GLN:O	2.22	0.40
1:G:158:MET:HA	1:G:158:MET:HE2	2.02	0.40
1:G:182:ILE:O	1:G:212:ARG:HA	2.22	0.40
1:G:299:HIS:CG	1:G:300:PRO:HA	2.57	0.40
1:H:182:ILE:O	1:H:212:ARG:HA	2.22	0.40
1:H:295[A]:ARG:HD2	5:H:769:HOH:O	2.21	0.40
1:A:332:PHE:CE1	1:A:352:VAL:HG23	2.57	0.40
1:B:95:TRP:CZ2	4:B:3471:GOL:H12	2.56	0.40
1:E:311:THR:O	1:E:315:LEU:HG	2.22	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:GLN:HE21	1:G:13:GLN:HB3	1.52	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	421/419 (100%)	413 (98%)	8 (2%)	0	100	100
1	B	415/419 (99%)	404 (97%)	11 (3%)	0	100	100
1	C	415/419 (99%)	407 (98%)	8 (2%)	0	100	100
1	D	416/419 (99%)	405 (97%)	11 (3%)	0	100	100
1	E	417/419 (100%)	408 (98%)	9 (2%)	0	100	100
1	F	416/419 (99%)	399 (96%)	16 (4%)	1 (0%)	47	58
1	G	417/419 (100%)	409 (98%)	8 (2%)	0	100	100
1	H	417/419 (100%)	408 (98%)	9 (2%)	0	100	100
All	All	3334/3352 (100%)	3253 (98%)	80 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	401	ARG

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/329 (102%)	325 (97%)	10 (3%)	41	57
1	B	329/329 (100%)	322 (98%)	7 (2%)	53	70
1	C	329/329 (100%)	317 (96%)	12 (4%)	35	49
1	D	330/329 (100%)	321 (97%)	9 (3%)	44	61
1	E	331/329 (101%)	326 (98%)	5 (2%)	65	79
1	F	330/329 (100%)	318 (96%)	12 (4%)	35	49
1	G	331/329 (101%)	321 (97%)	10 (3%)	41	57
1	H	331/329 (101%)	320 (97%)	11 (3%)	38	53
All	All	2646/2632 (100%)	2570 (97%)	76 (3%)	43	58

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	111	LEU
1	A	148	ASN
1	A	183	GLU
1	A	187	ARG
1	A	212[A]	ARG
1	A	212[B]	ARG
1	A	216	GLU
1	A	307	GLN
1	A	348	GLU
1	B	59	GLN
1	B	111	LEU
1	B	148	ASN
1	B	187	ARG
1	B	229	LEU
1	B	307	GLN
1	B	348	GLU
1	C	37	GLU
1	C	59	GLN
1	C	76	ASN
1	C	91	ARG
1	C	111	LEU
1	C	143	VAL
1	C	183	GLU
1	C	187	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	229	LEU
1	C	274	GLU
1	C	307	GLN
1	C	348	GLU
1	D	85	ASP
1	D	91	ARG
1	D	143	VAL
1	D	148	ASN
1	D	183	GLU
1	D	187	ARG
1	D	229	LEU
1	D	307	GLN
1	D	348	GLU
1	E	91	ARG
1	E	187	ARG
1	E	229	LEU
1	E	307	GLN
1	E	348	GLU
1	F	76	ASN
1	F	91	ARG
1	F	103	ARG
1	F	108	GLN
1	F	111	LEU
1	F	159	ASP
1	F	187	ARG
1	F	193	ASP
1	F	229	LEU
1	F	307	GLN
1	F	348	GLU
1	F	401	ARG
1	G	13	GLN
1	G	65	GLU
1	G	76	ASN
1	G	111	LEU
1	G	148	ASN
1	G	212	ARG
1	G	216	GLU
1	G	229	LEU
1	G	307	GLN
1	G	348	GLU
1	H	59	GLN
1	H	65	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	85	ASP
1	H	111	LEU
1	H	122	VAL
1	H	187	ARG
1	H	211	ASP
1	H	212	ARG
1	H	229	LEU
1	H	307	GLN
1	H	348	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	148	ASN
1	A	330	ASN
1	B	13	GLN
1	B	106	GLN
1	B	108	GLN
1	B	148	ASN
1	B	330	ASN
1	B	364	GLN
1	C	76	ASN
1	C	106	GLN
1	C	330	ASN
1	C	344	HIS
1	D	79	ASN
1	D	148	ASN
1	D	344	HIS
1	E	108	GLN
1	E	330	ASN
1	F	7	GLN
1	F	76	ASN
1	F	253	ASN
1	G	76	ASN
1	G	108	GLN
1	G	125	HIS
1	G	148	ASN
1	G	330	ASN
1	H	59	GLN
1	H	108	GLN
1	H	148	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	330	ASN
1	H	344	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	IAS	A	67	1	6,7,8	1.02	0	6,8,10	0.94	0
1	IAS	F	67	1	6,7,8	0.98	0	6,8,10	1.09	0
1	IAS	B	67	1	6,7,8	0.94	0	6,8,10	1.03	0
1	IAS	C	67	1	6,7,8	0.99	0	6,8,10	1.09	0
1	IAS	D	67	1	6,7,8	0.88	0	6,8,10	1.16	0
1	IAS	H	67	1	6,7,8	0.94	0	6,8,10	1.17	0
1	IAS	G	67	1	6,7,8	0.88	0	6,8,10	1.13	0
1	IAS	E	67	1	6,7,8	0.90	0	6,8,10	1.09	0

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
1	IAS	A	67	1	-	0/7/7/8	-
1	IAS	F	67	1	-	2/7/7/8	-
1	IAS	B	67	1	-	0/7/7/8	-
1	IAS	C	67	1	-	0/7/7/8	-
1	IAS	D	67	1	-	0/7/7/8	-
1	IAS	H	67	1	-	0/7/7/8	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IAS	G	67	1	-	0/7/7/8	-
1	IAS	E	67	1	-	0/7/7/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	67	IAS	OXT-C-CA-CB
1	F	67	IAS	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	C	4461	-	4,4,4	1.66	0	6,6,6	0.44	0
3	EPU	D	5450	-	43,46,46	1.93	18 (41%)	61,69,69	1.39	10 (16%)
3	EPU	B	3450	-	43,46,46	1.99	17 (39%)	61,69,69	1.40	7 (11%)
4	GOL	C	2473	-	5,5,5	0.40	0	5,5,5	0.54	0
4	GOL	C	4474	-	5,5,5	0.44	0	5,5,5	0.45	0
4	GOL	B	3471	-	5,5,5	0.38	0	5,5,5	0.35	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	E	6471	-	5,5,5	0.48	0	5,5,5	0.38	0
2	PO4	A	2461	-	4,4,4	1.71	1 (25%)	6,6,6	0.40	0
2	PO4	G	8461	-	4,4,4	1.68	0	6,6,6	0.46	0
3	EPU	E	6450	-	43,46,46	2.03	18 (41%)	61,69,69	1.46	9 (14%)
3	EPU	C	4450	-	43,46,46	1.99	18 (41%)	61,69,69	1.34	8 (13%)
4	GOL	C	4471	-	5,5,5	0.38	0	5,5,5	0.35	0
2	PO4	D	5461	-	4,4,4	1.68	0	6,6,6	0.43	0
4	GOL	D	5471	-	5,5,5	0.47	0	5,5,5	0.39	0
4	GOL	E	8472	-	5,5,5	0.46	0	5,5,5	0.54	0
3	EPU	G	8450	-	43,46,46	1.99	15 (34%)	61,69,69	1.39	7 (11%)
2	PO4	G	8462	-	4,4,4	1.58	0	6,6,6	0.45	0
4	GOL	C	3473	-	5,5,5	0.47	0	5,5,5	0.50	0
4	GOL	H	9471	-	5,5,5	0.44	0	5,5,5	0.43	0
4	GOL	C	4472	-	5,5,5	0.51	0	5,5,5	0.49	0
4	GOL	H	9472	-	5,5,5	0.44	0	5,5,5	0.53	0
2	PO4	F	7461	-	4,4,4	1.71	0	6,6,6	0.45	0
3	EPU	A	2450	-	43,46,46	1.87	18 (41%)	61,69,69	1.38	9 (14%)
4	GOL	A	2472	-	5,5,5	0.68	0	5,5,5	0.51	0
3	EPU	H	9450	-	43,46,46	1.91	14 (32%)	61,69,69	1.36	7 (11%)
2	PO4	B	3461	-	4,4,4	1.73	0	6,6,6	0.43	0
4	GOL	B	3472	-	5,5,5	0.51	0	5,5,5	0.49	0
2	PO4	E	6461	-	4,4,4	1.64	0	6,6,6	0.45	0
4	GOL	G	8471	-	5,5,5	0.41	0	5,5,5	0.32	0
4	GOL	A	2471	-	5,5,5	0.52	0	5,5,5	0.36	0
4	GOL	F	7471	-	5,5,5	0.46	0	5,5,5	0.39	0
4	GOL	D	5472	-	5,5,5	0.47	0	5,5,5	0.58	0
3	EPU	F	7450	-	43,46,46	1.92	17 (39%)	61,69,69	1.38	8 (13%)
2	PO4	H	9461	-	4,4,4	1.73	1 (25%)	6,6,6	0.45	0

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	EPU	D	5450	-	-	8/32/71/71	0/3/3/3
3	EPU	B	3450	-	-	10/32/71/71	0/3/3/3
4	GOL	C	2473	-	-	0/4/4/4	-
4	GOL	C	4474	-	-	0/4/4/4	-
4	GOL	B	3471	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	6471	-	-	0/4/4/4	-
3	EPU	E	6450	-	-	7/32/71/71	0/3/3/3
3	EPU	C	4450	-	-	8/32/71/71	0/3/3/3
4	GOL	C	4471	-	-	0/4/4/4	-
4	GOL	D	5471	-	-	0/4/4/4	-
4	GOL	E	8472	-	-	0/4/4/4	-
3	EPU	G	8450	-	-	8/32/71/71	0/3/3/3
4	GOL	C	3473	-	-	0/4/4/4	-
4	GOL	H	9471	-	-	0/4/4/4	-
4	GOL	C	4472	-	-	0/4/4/4	-
4	GOL	H	9472	-	-	0/4/4/4	-
3	EPU	A	2450	-	-	9/32/71/71	0/3/3/3
4	GOL	A	2472	-	-	0/4/4/4	-
3	EPU	H	9450	-	-	10/32/71/71	0/3/3/3
4	GOL	B	3472	-	-	0/4/4/4	-
4	GOL	G	8471	-	-	0/4/4/4	-
4	GOL	A	2471	-	-	0/4/4/4	-
4	GOL	F	7471	-	-	0/4/4/4	-
4	GOL	D	5472	-	-	0/4/4/4	-
3	EPU	F	7450	-	-	9/32/71/71	0/3/3/3

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	9450	EPU	C2E-C1E	4.78	1.54	1.49
3	E	6450	EPU	C2E-C1E	4.62	1.53	1.49
3	C	4450	EPU	C2E-C1E	4.54	1.53	1.49
3	B	3450	EPU	C2E-C1E	4.39	1.53	1.49
3	G	8450	EPU	C2E-C1E	4.39	1.53	1.49
3	G	8450	EPU	O2D-C2D	4.19	1.52	1.43
3	D	5450	EPU	O2D-C2D	4.19	1.52	1.43
3	C	4450	EPU	O2D-C2D	4.14	1.52	1.43
3	B	3450	EPU	O2D-C2D	4.03	1.52	1.43
3	E	6450	EPU	O2D-C2D	3.92	1.52	1.43
3	F	7450	EPU	O2D-C2D	3.91	1.52	1.43
3	F	7450	EPU	C2E-C1E	3.82	1.53	1.49
3	A	2450	EPU	C2E-C1E	3.80	1.53	1.49
3	A	2450	EPU	O2D-C2D	3.77	1.51	1.43
3	H	9450	EPU	O2D-C2D	3.61	1.51	1.43
3	D	5450	EPU	C2E-C1E	3.47	1.52	1.49
3	F	7450	EPU	C1-C2	3.47	1.58	1.53

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	9450	EPU	C1-C2	3.26	1.58	1.53
3	B	3450	EPU	C4-C3	3.12	1.60	1.52
3	D	5450	EPU	C2U-N1U	3.09	1.43	1.38
3	E	6450	EPU	C4-C3	3.08	1.60	1.52
3	G	8450	EPU	C6U-N1U	3.06	1.45	1.38
3	D	5450	EPU	C1-C2	3.02	1.58	1.53
3	C	4450	EPU	C4-C3	3.01	1.60	1.52
3	B	3450	EPU	C6U-N1U	3.00	1.45	1.38
3	A	2450	EPU	C1-C2	2.98	1.58	1.53
3	E	6450	EPU	C6U-N1U	2.97	1.45	1.38
3	G	8450	EPU	C6U-C5U	2.97	1.41	1.35
3	B	3450	EPU	C6U-C5U	2.96	1.41	1.35
3	B	3450	EPU	C1-C2	2.91	1.57	1.53
3	E	6450	EPU	C3D-C4D	2.91	1.60	1.53
3	C	4450	EPU	C6U-N1U	2.91	1.45	1.38
3	F	7450	EPU	C6U-N1U	2.89	1.45	1.38
3	F	7450	EPU	C3D-C4D	2.84	1.60	1.53
3	F	7450	EPU	C6U-C5U	2.83	1.41	1.35
3	E	6450	EPU	C2-N2	2.81	1.50	1.45
3	E	6450	EPU	C1-C2	2.80	1.57	1.53
3	E	6450	EPU	C6U-C5U	2.80	1.41	1.35
3	D	5450	EPU	C3D-C4D	2.79	1.60	1.53
3	C	4450	EPU	C3D-C4D	2.79	1.60	1.53
3	C	4450	EPU	C6U-C5U	2.79	1.41	1.35
3	G	8450	EPU	C4-C3	2.77	1.59	1.52
3	H	9450	EPU	C3D-C4D	2.76	1.60	1.53
3	C	4450	EPU	C2-N2	2.76	1.50	1.45
3	A	2450	EPU	C4-C3	2.76	1.59	1.52
3	G	8450	EPU	C3D-C4D	2.75	1.60	1.53
3	G	8450	EPU	C1-C2	2.73	1.57	1.53
3	D	5450	EPU	C1D-N1U	2.73	1.55	1.47
3	A	2450	EPU	C6U-N1U	2.72	1.44	1.38
3	C	4450	EPU	C1-C2	2.72	1.57	1.53
3	F	7450	EPU	C4-C3	2.68	1.59	1.52
3	G	8450	EPU	PB-O1B	-2.66	1.41	1.50
3	B	3450	EPU	C3D-C4D	2.63	1.59	1.53
3	E	6450	EPU	O5-C1	2.62	1.48	1.41
3	D	5450	EPU	C4-C3	2.61	1.59	1.52
3	E	6450	EPU	O5-C5	2.60	1.50	1.44
3	H	9450	EPU	C6U-N1U	2.59	1.44	1.38
3	H	9450	EPU	C4-C3	2.59	1.59	1.52
3	A	2450	EPU	C3D-C4D	2.58	1.59	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5450	EPU	C6U-N1U	2.57	1.44	1.38
3	D	5450	EPU	O3D-C3D	2.56	1.49	1.43
3	C	4450	EPU	O4-C4	2.55	1.49	1.43
3	A	2450	EPU	C6U-C5U	2.54	1.40	1.35
3	G	8450	EPU	O5-C5	2.54	1.50	1.44
3	G	8450	EPU	C3E-C2E	2.53	1.38	1.31
3	F	7450	EPU	O3D-C3D	2.52	1.48	1.43
3	E	6450	EPU	C3E-C2E	2.49	1.38	1.31
3	C	4450	EPU	O3D-C3D	2.49	1.48	1.43
3	H	9450	EPU	C3E-C2E	2.49	1.38	1.31
3	B	3450	EPU	C2U-N1U	2.47	1.42	1.38
3	E	6450	EPU	O4-C4	2.44	1.48	1.43
3	B	3450	EPU	O3D-C3D	2.44	1.48	1.43
3	A	2450	EPU	C1D-N1U	2.40	1.54	1.47
3	C	4450	EPU	O5-C1	2.40	1.48	1.41
3	F	7450	EPU	O5-C5	2.39	1.50	1.44
3	D	5450	EPU	C6U-C5U	2.38	1.40	1.35
3	H	9450	EPU	O5-C1	2.38	1.47	1.41
3	C	4450	EPU	O5-C5	2.38	1.50	1.44
3	A	2450	EPU	C3E-C2E	2.37	1.38	1.31
3	A	2450	EPU	C2-N2	2.36	1.49	1.45
3	F	7450	EPU	C2-N2	2.36	1.49	1.45
3	A	2450	EPU	O4-C4	2.35	1.48	1.43
3	D	5450	EPU	C3E-C2E	2.35	1.38	1.31
3	B	3450	EPU	O5-C1	2.35	1.47	1.41
3	C	4450	EPU	PB-O1B	-2.34	1.42	1.50
3	A	2450	EPU	PB-O1B	-2.33	1.42	1.50
3	B	3450	EPU	O4-C4	2.32	1.48	1.43
3	E	6450	EPU	C3-C2	2.31	1.56	1.53
3	G	8450	EPU	C5U-C4U	2.30	1.48	1.43
3	C	4450	EPU	C2U-N1U	2.30	1.42	1.38
3	B	3450	EPU	C1D-N1U	2.28	1.54	1.47
3	H	9450	EPU	O3D-C3D	2.28	1.48	1.43
3	H	9450	EPU	PB-O1B	-2.28	1.42	1.50
3	D	5450	EPU	O4-C4	2.27	1.48	1.43
3	G	8450	EPU	C2U-N1U	2.27	1.42	1.38
3	D	5450	EPU	C5D-C4D	2.26	1.58	1.51
3	E	6450	EPU	C1D-N1U	2.26	1.54	1.47
3	E	6450	EPU	PB-O2B	-2.25	1.44	1.55
3	B	3450	EPU	C3E-C2E	2.24	1.38	1.31
3	G	8450	EPU	O5-C1	2.24	1.47	1.41
3	C	4450	EPU	C3E-C2E	2.24	1.38	1.31

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	7450	EPU	C3E-C2E	2.22	1.38	1.31
3	B	3450	EPU	PB-O1	-2.21	1.54	1.60
3	A	2450	EPU	O6-C6	2.21	1.51	1.42
3	F	7450	EPU	PB-O2B	-2.21	1.45	1.55
3	D	5450	EPU	O5-C1	2.20	1.47	1.41
3	F	7450	EPU	PB-O1B	-2.20	1.43	1.50
3	D	5450	EPU	PB-O2B	-2.20	1.45	1.55
3	H	9450	EPU	C6U-C5U	2.20	1.40	1.35
3	D	5450	EPU	PB-O1B	-2.19	1.43	1.50
3	D	5450	EPU	C2-N2	2.19	1.49	1.45
3	C	4450	EPU	C5U-C4U	2.19	1.48	1.43
3	H	9450	EPU	O5-C5	2.18	1.49	1.44
3	A	2450	EPU	C2U-N1U	2.17	1.41	1.38
3	B	3450	EPU	PB-O1B	-2.17	1.43	1.50
3	G	8450	EPU	O3D-C3D	2.17	1.48	1.43
3	G	8450	EPU	O4-C4	2.16	1.48	1.43
3	F	7450	EPU	O4-C4	2.13	1.48	1.43
3	C	4450	EPU	C1D-N1U	2.13	1.53	1.47
3	A	2450	EPU	O5-C5	2.12	1.49	1.44
3	H	9450	EPU	C2U-N1U	2.11	1.41	1.38
3	E	6450	EPU	PB-O1	-2.10	1.55	1.60
3	F	7450	EPU	C1D-N1U	2.10	1.53	1.47
3	E	6450	EPU	O3D-C3D	2.10	1.47	1.43
3	E	6450	EPU	PB-O1B	-2.09	1.43	1.50
2	H	9461	PO4	P-O3	-2.08	1.48	1.54
3	H	9450	EPU	O6-C6	2.07	1.51	1.42
3	A	2450	EPU	PB-O2B	-2.07	1.45	1.55
3	F	7450	EPU	PB-O1	-2.07	1.55	1.60
3	A	2450	EPU	C5U-C4U	2.03	1.48	1.43
3	A	2450	EPU	O5-C1	2.03	1.47	1.41
3	C	4450	EPU	O6-C6	2.03	1.51	1.42
3	D	5450	EPU	O6-C6	2.02	1.50	1.42
3	B	3450	EPU	PB-O2B	-2.02	1.45	1.55
3	B	3450	EPU	C3-C2	2.01	1.56	1.53
2	A	2461	PO4	P-O2	-2.00	1.48	1.54
3	F	7450	EPU	O1E-C1E	2.00	1.28	1.22

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3450	EPU	O3A-PB-O1	3.67	109.89	102.48
3	D	5450	EPU	O3A-PB-O1	3.62	109.79	102.48

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	6450	EPU	O3D-C3D-C4D	3.60	121.46	111.05
3	E	6450	EPU	O3A-PB-O1	3.58	109.70	102.48
3	C	4450	EPU	O3A-PB-O1	3.54	109.61	102.48
3	G	8450	EPU	O3A-PB-O1	3.51	109.57	102.48
3	H	9450	EPU	O3A-PB-O1	3.50	109.55	102.48
3	F	7450	EPU	O3A-PB-O1	3.47	109.48	102.48
3	H	9450	EPU	C2D-C3D-C4D	-3.45	95.94	102.64
3	G	8450	EPU	C2D-C3D-C4D	-3.45	95.94	102.64
3	F	7450	EPU	C2D-C3D-C4D	-3.42	96.00	102.64
3	C	4450	EPU	C2D-C3D-C4D	-3.39	96.05	102.64
3	A	2450	EPU	C2D-C3D-C4D	-3.37	96.09	102.64
3	E	6450	EPU	C2D-C3D-C4D	-3.36	96.11	102.64
3	D	5450	EPU	C2D-C3D-C4D	-3.36	96.12	102.64
3	B	3450	EPU	C2D-C3D-C4D	-3.36	96.12	102.64
3	A	2450	EPU	O3D-C3D-C4D	3.31	120.61	111.05
3	A	2450	EPU	O3A-PB-O1	3.28	109.11	102.48
3	B	3450	EPU	O3D-C3D-C4D	3.24	120.41	111.05
3	F	7450	EPU	O3D-C3D-C4D	3.21	120.33	111.05
3	C	4450	EPU	O3D-C3D-C4D	3.19	120.27	111.05
3	G	8450	EPU	O3D-C3D-C4D	3.15	120.15	111.05
3	H	9450	EPU	O3D-C3D-C4D	2.99	119.70	111.05
3	D	5450	EPU	O3D-C3D-C4D	2.94	119.55	111.05
3	E	6450	EPU	O3D-C3D-C2D	-2.89	102.47	111.82
3	B	3450	EPU	N3U-C2U-N1U	2.79	118.60	114.89
3	G	8450	EPU	N3U-C2U-N1U	2.79	118.59	114.89
3	A	2450	EPU	N3U-C2U-N1U	2.77	118.56	114.89
3	D	5450	EPU	C1D-N1U-C2U	2.72	122.49	117.57
3	E	6450	EPU	N3U-C2U-N1U	2.65	118.40	114.89
3	E	6450	EPU	O1E-C1E-C2E	-2.64	117.80	121.79
3	B	3450	EPU	O3D-C3D-C2D	-2.64	103.29	111.82
3	H	9450	EPU	O3D-C3D-C2D	-2.60	103.43	111.82
3	C	4450	EPU	N3U-C2U-N1U	2.59	118.32	114.89
3	G	8450	EPU	O3D-C3D-C2D	-2.54	103.60	111.82
3	E	6450	EPU	O2E-C1E-C2E	2.49	118.16	113.91
3	A	2450	EPU	O3D-C3D-C2D	-2.42	103.99	111.82
3	H	9450	EPU	N3U-C2U-N1U	2.42	118.10	114.89
3	D	5450	EPU	C6U-N1U-C2U	-2.40	117.92	120.99
3	D	5450	EPU	O3D-C3D-C2D	-2.38	104.13	111.82
3	F	7450	EPU	N3U-C2U-N1U	2.37	118.03	114.89
3	C	4450	EPU	O3D-C3D-C2D	-2.37	104.17	111.82
3	A	2450	EPU	C1D-N1U-C2U	2.37	121.85	117.57
3	F	7450	EPU	O3D-C3D-C2D	-2.34	104.25	111.82

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5450	EPU	N3U-C2U-N1U	2.32	117.97	114.89
3	B	3450	EPU	C6U-N1U-C2U	-2.27	118.09	120.99
3	G	8450	EPU	O2D-C2D-C1D	2.25	117.54	110.02
3	A	2450	EPU	C6U-N1U-C2U	-2.23	118.14	120.99
3	F	7450	EPU	C6U-N1U-C2U	-2.22	118.15	120.99
3	D	5450	EPU	O2D-C2D-C1D	2.20	117.37	110.02
3	E	6450	EPU	C6U-N1U-C2U	-2.16	118.22	120.99
3	C	4450	EPU	O2D-C2D-C1D	2.14	117.17	110.02
3	G	8450	EPU	C6U-N1U-C2U	-2.14	118.26	120.99
3	F	7450	EPU	C1D-N1U-C2U	2.13	121.42	117.57
3	H	9450	EPU	C1D-N1U-C2U	2.12	121.42	117.57
3	B	3450	EPU	O2D-C2D-C1D	2.12	117.11	110.02
3	A	2450	EPU	O2D-C2D-C1D	2.09	117.02	110.02
3	F	7450	EPU	O2D-C2D-C1D	2.08	116.96	110.02
3	C	4450	EPU	C6U-N1U-C2U	-2.07	118.34	120.99
3	E	6450	EPU	O2D-C2D-C1D	2.05	116.87	110.02
3	D	5450	EPU	O1E-C1E-C2E	-2.04	118.72	121.79
3	D	5450	EPU	O2E-C1E-C2E	2.04	117.38	113.91
3	H	9450	EPU	O2D-C2D-C1D	2.02	116.77	110.02
3	C	4450	EPU	O2D-C2D-C3D	2.01	118.32	111.82
3	A	2450	EPU	O2D-C2D-C3D	2.01	118.31	111.82

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2450	EPU	C5D-O5D-PA-O1A
3	A	2450	EPU	C5D-O5D-PA-O2A
3	A	2450	EPU	O1E-C1E-C2E-C3E
3	A	2450	EPU	O2E-C1E-C2E-C3E
3	B	3450	EPU	C5D-O5D-PA-O1A
3	B	3450	EPU	C5D-O5D-PA-O2A
3	B	3450	EPU	O1E-C1E-C2E-O3
3	B	3450	EPU	O1E-C1E-C2E-C3E
3	B	3450	EPU	O2E-C1E-C2E-C3E
3	C	4450	EPU	C5D-O5D-PA-O1A
3	C	4450	EPU	C5D-O5D-PA-O2A
3	C	4450	EPU	O1E-C1E-C2E-C3E
3	C	4450	EPU	O2E-C1E-C2E-C3E
3	D	5450	EPU	C5D-O5D-PA-O1A
3	D	5450	EPU	C5D-O5D-PA-O2A
3	D	5450	EPU	O1E-C1E-C2E-C3E

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	D	5450	EPU	O2E-C1E-C2E-C3E
3	E	6450	EPU	C5D-O5D-PA-O1A
3	E	6450	EPU	C5D-O5D-PA-O2A
3	E	6450	EPU	O2E-C1E-C2E-O3
3	F	7450	EPU	C5D-O5D-PA-O1A
3	F	7450	EPU	C5D-O5D-PA-O2A
3	F	7450	EPU	O1E-C1E-C2E-O3
3	F	7450	EPU	O1E-C1E-C2E-C3E
3	F	7450	EPU	O2E-C1E-C2E-C3E
3	G	8450	EPU	C5D-O5D-PA-O1A
3	G	8450	EPU	C5D-O5D-PA-O2A
3	G	8450	EPU	O1E-C1E-C2E-O3
3	G	8450	EPU	O1E-C1E-C2E-C3E
3	G	8450	EPU	O2E-C1E-C2E-C3E
3	H	9450	EPU	C5D-O5D-PA-O1A
3	H	9450	EPU	C5D-O5D-PA-O2A
3	H	9450	EPU	O1E-C1E-C2E-C3E
3	H	9450	EPU	O2E-C1E-C2E-C3E
3	A	2450	EPU	O1E-C1E-C2E-O3
3	C	4450	EPU	O1E-C1E-C2E-O3
3	D	5450	EPU	O1E-C1E-C2E-O3
3	A	2450	EPU	C5D-O5D-PA-O3A
3	B	3450	EPU	C5D-O5D-PA-O3A
3	C	4450	EPU	C5D-O5D-PA-O3A
3	D	5450	EPU	C5D-O5D-PA-O3A
3	E	6450	EPU	C5D-O5D-PA-O3A
3	F	7450	EPU	C5D-O5D-PA-O3A
3	G	8450	EPU	C5D-O5D-PA-O3A
3	H	9450	EPU	C5D-O5D-PA-O3A
3	H	9450	EPU	O1E-C1E-C2E-O3
3	A	2450	EPU	O2E-C1E-C2E-O3
3	B	3450	EPU	O2E-C1E-C2E-O3
3	C	4450	EPU	O2E-C1E-C2E-O3
3	D	5450	EPU	O2E-C1E-C2E-O3
3	F	7450	EPU	O2E-C1E-C2E-O3
3	G	8450	EPU	O2E-C1E-C2E-O3
3	H	9450	EPU	O2E-C1E-C2E-O3
3	B	3450	EPU	PB-O3A-PA-O2A
3	E	6450	EPU	PB-O3A-PA-O1A
3	F	7450	EPU	PB-O3A-PA-O2A
3	H	9450	EPU	PB-O3A-PA-O1A
3	H	9450	EPU	C3-C2-N2-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	2450	EPU	PB-O3A-PA-O2A
3	B	3450	EPU	PB-O3A-PA-O1A
3	C	4450	EPU	PB-O3A-PA-O2A
3	D	5450	EPU	PB-O3A-PA-O2A
3	F	7450	EPU	PB-O3A-PA-O1A
3	G	8450	EPU	PB-O3A-PA-O2A
3	H	9450	EPU	PB-O3A-PA-O2A
3	A	2450	EPU	C3-C2-N2-C7
3	B	3450	EPU	C3-C2-N2-C7
3	E	6450	EPU	C3-C2-N2-C7
3	E	6450	EPU	O1E-C1E-C2E-O3

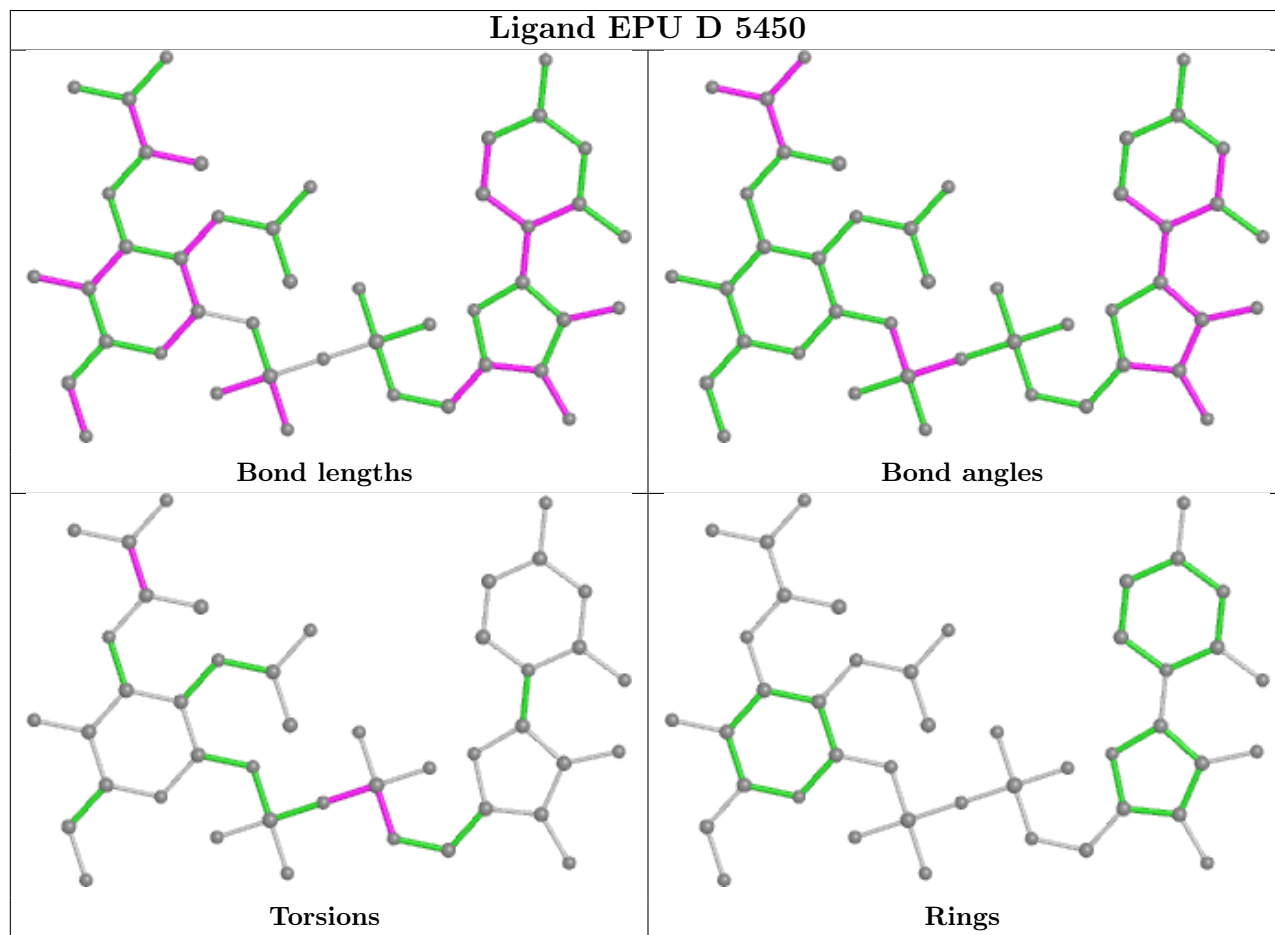
There are no ring outliers.

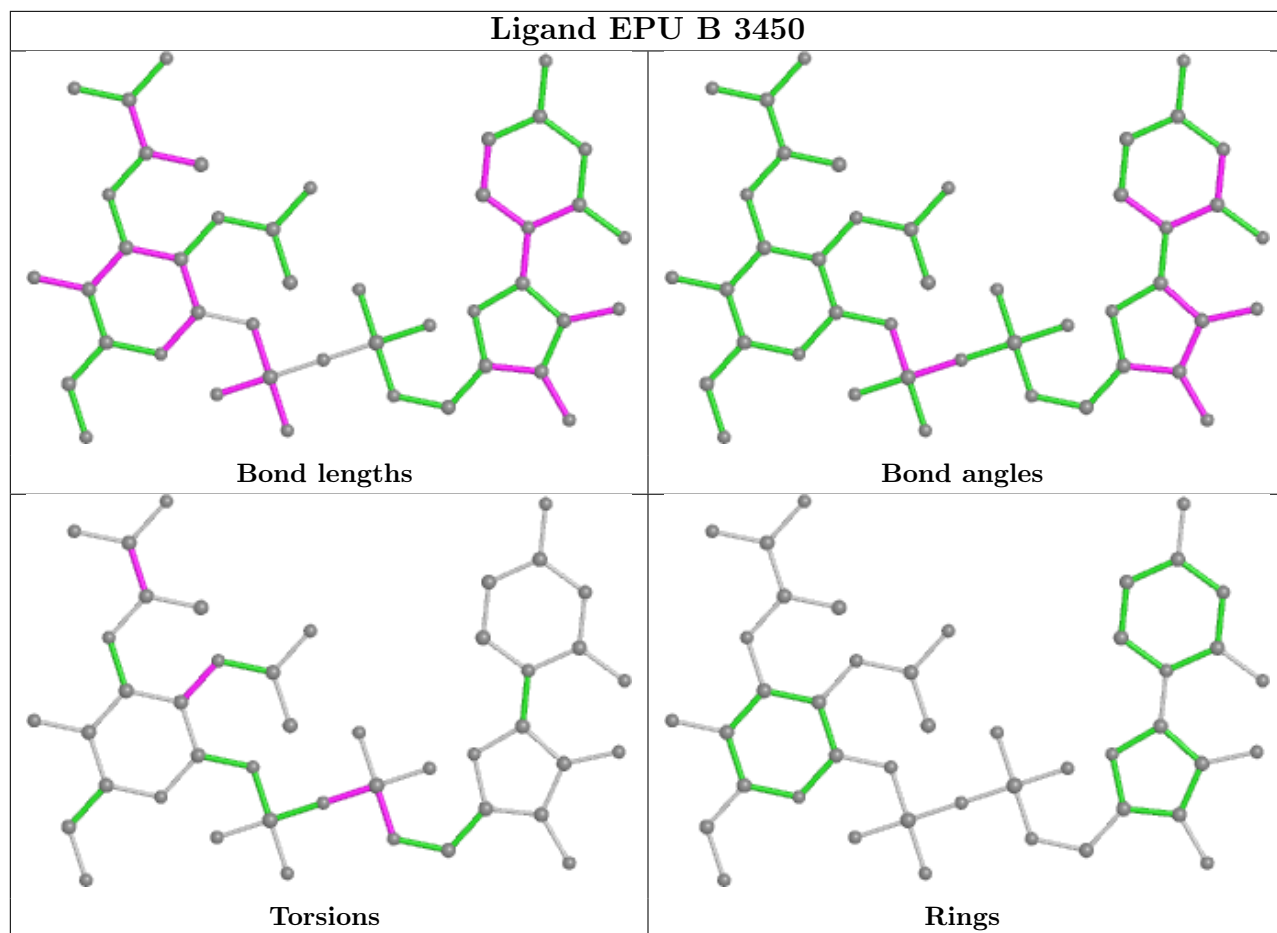
22 monomers are involved in 27 short contacts:

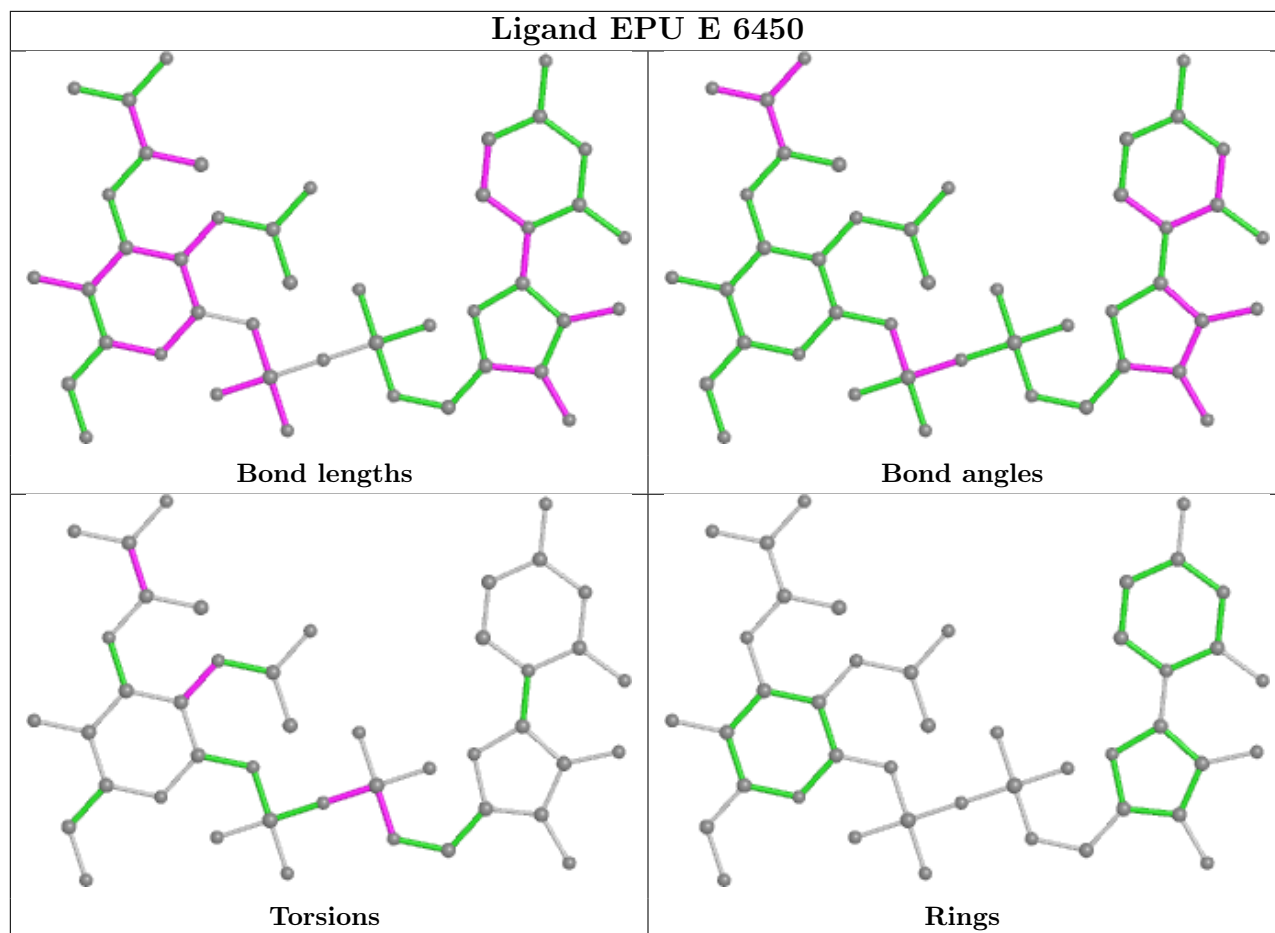
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5450	EPU	1	0
3	B	3450	EPU	2	0
4	C	2473	GOL	1	0
4	C	4474	GOL	2	0
4	B	3471	GOL	3	0
4	E	6471	GOL	2	0
3	E	6450	EPU	3	0
3	C	4450	EPU	2	0
4	C	4471	GOL	3	0
4	D	5471	GOL	1	0
3	G	8450	EPU	1	0
4	C	3473	GOL	1	0
4	H	9471	GOL	3	0
3	A	2450	EPU	2	0
4	A	2472	GOL	3	0
3	H	9450	EPU	3	0
2	E	6461	PO4	1	0
4	G	8471	GOL	2	0
4	A	2471	GOL	2	0
4	F	7471	GOL	1	0
3	F	7450	EPU	1	0
2	H	9461	PO4	1	0

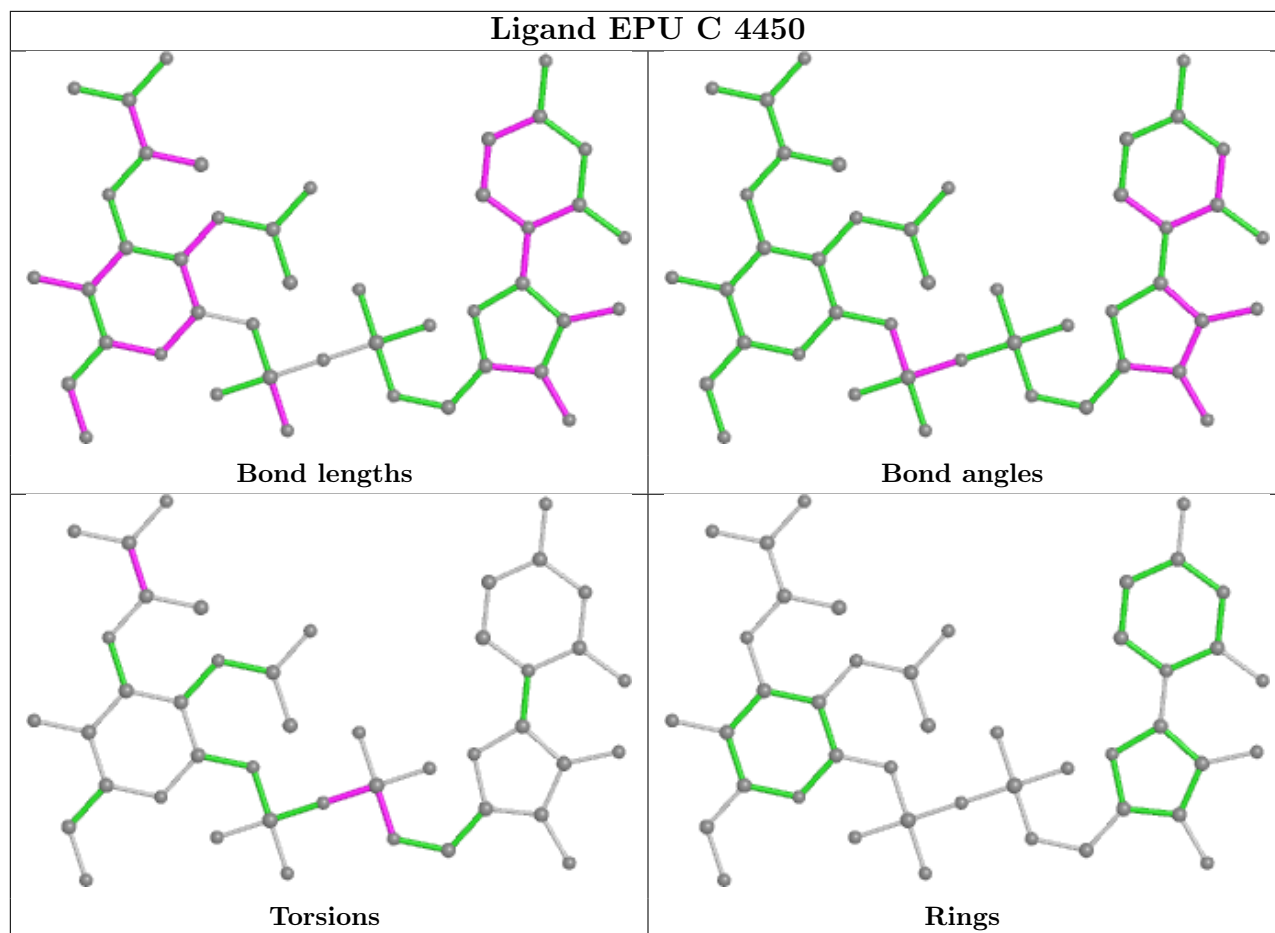
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

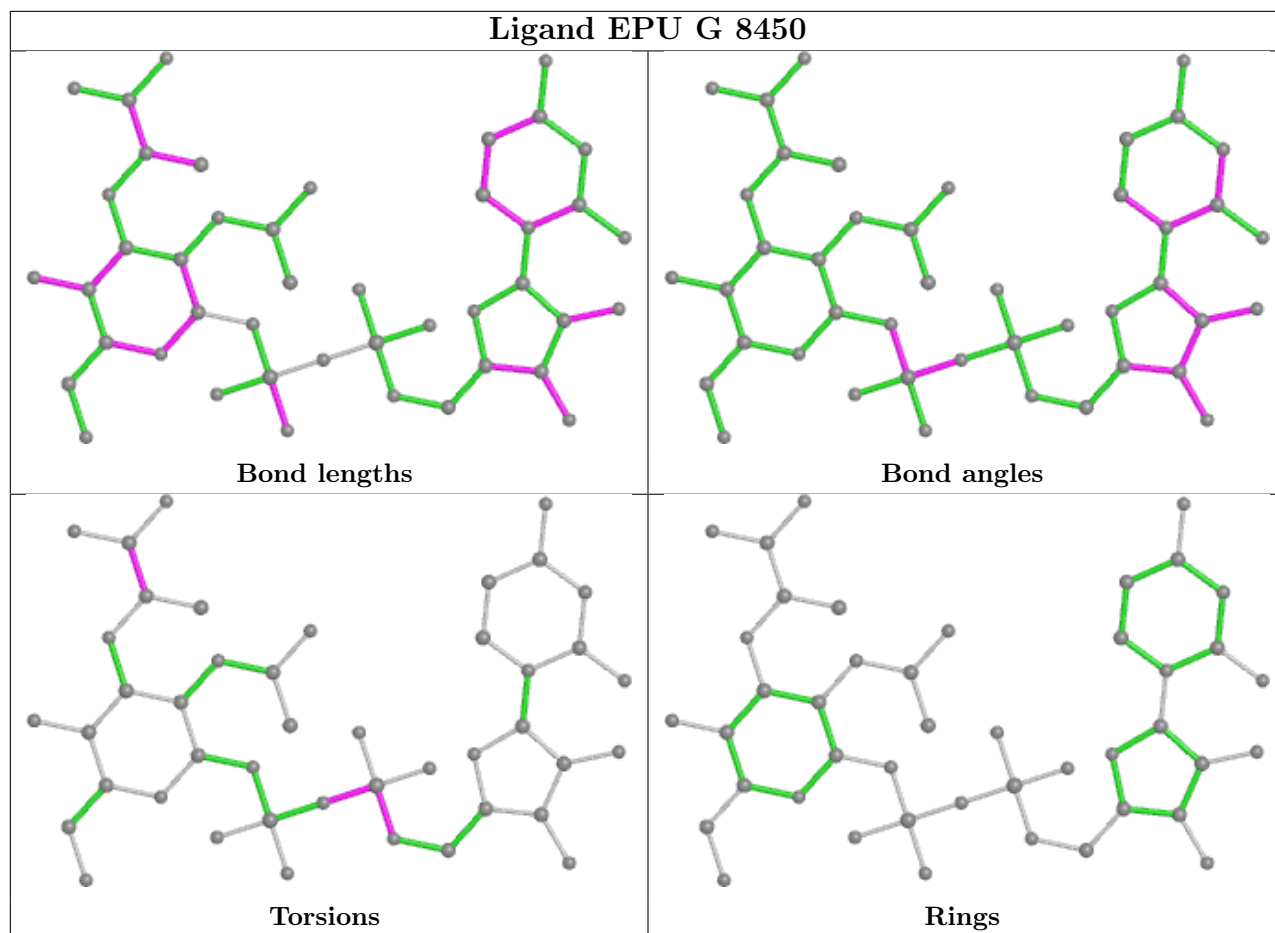
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

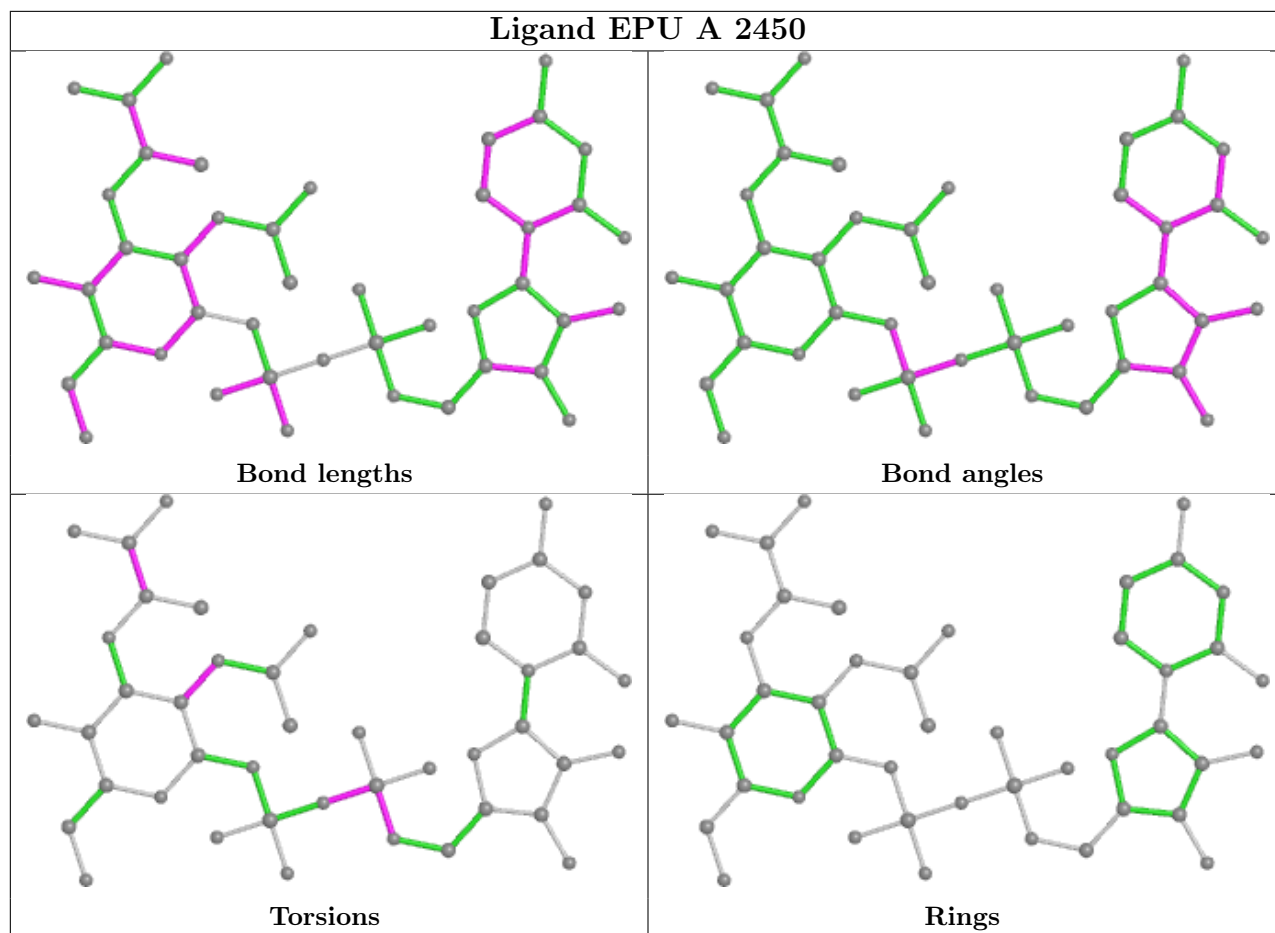


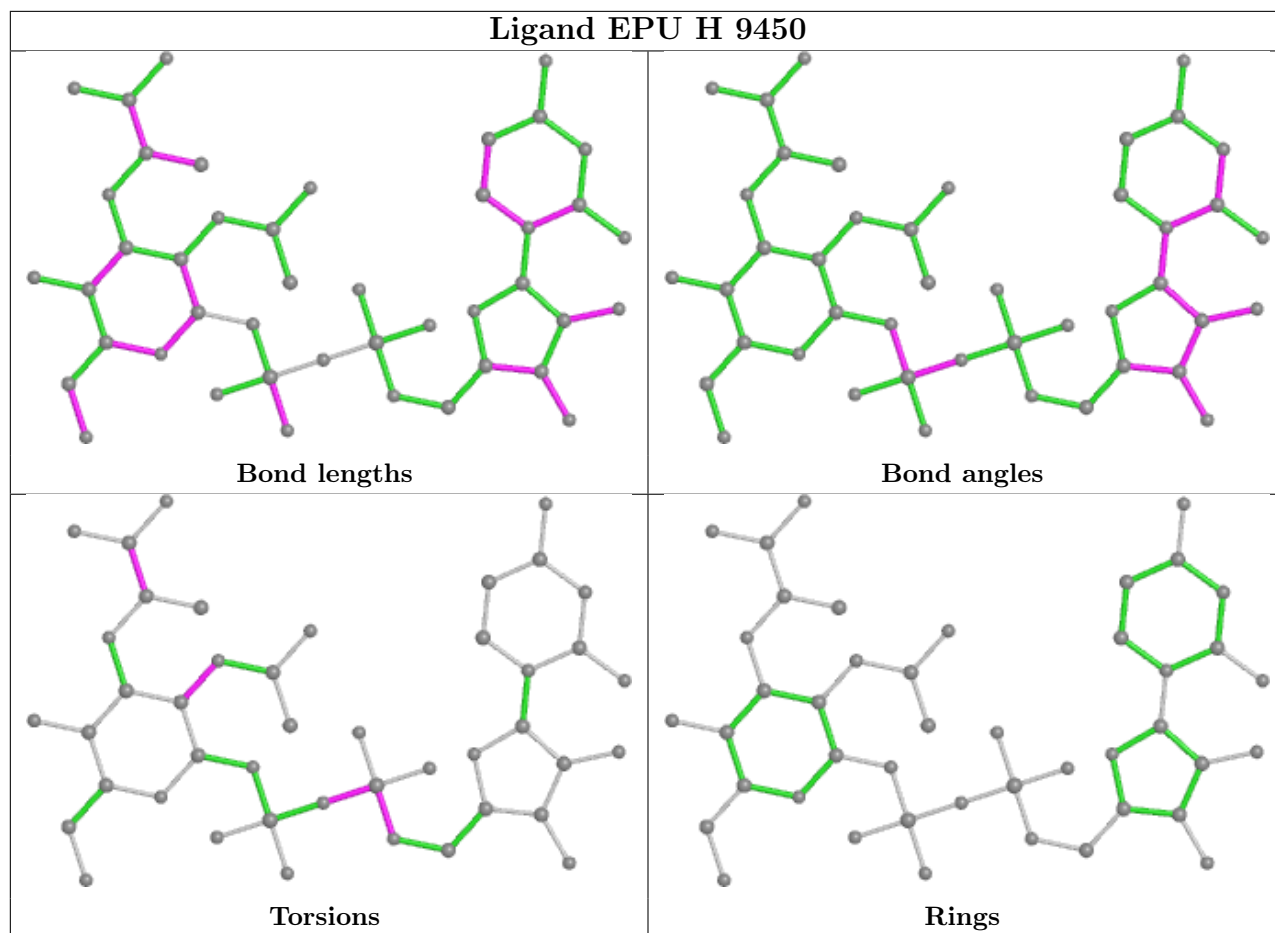




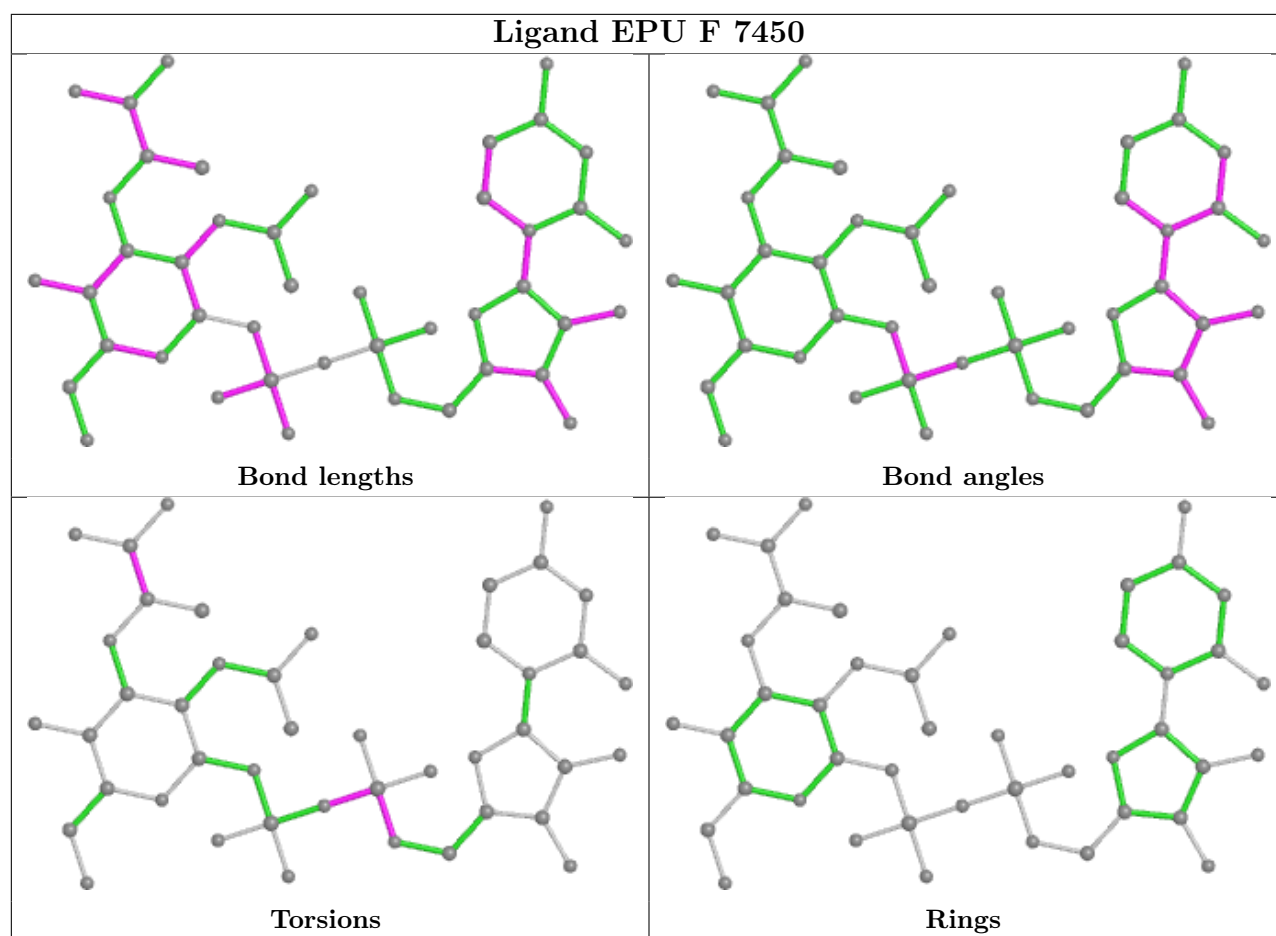












## 5.7 Other polymers [i](#)

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	418/419 (99%)	-0.42	3 (0%) 87 91	7, 18, 33, 94	0
1	B	418/419 (99%)	-0.16	4 (0%) 82 86	10, 21, 38, 93	0
1	C	418/419 (99%)	-0.35	5 (1%) 79 83	9, 20, 35, 91	0
1	D	418/419 (99%)	-0.15	7 (1%) 70 76	10, 23, 40, 93	0
1	E	418/419 (99%)	-0.20	3 (0%) 87 91	12, 22, 36, 92	0
1	F	418/419 (99%)	0.26	18 (4%) 35 42	14, 29, 47, 95	0
1	G	418/419 (99%)	-0.19	5 (1%) 79 83	10, 22, 39, 94	0
1	H	418/419 (99%)	-0.27	3 (0%) 87 91	10, 21, 37, 92	0
All	All	3344/3352 (99%)	-0.19	48 (1%) 75 80	7, 22, 39, 95	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	418	GLY	9.2
1	F	419	GLU	8.8
1	A	419	GLU	7.5
1	H	419	GLU	7.0
1	B	419	GLU	6.6
1	A	418	GLY	6.5
1	G	419	GLU	6.5
1	D	419	GLU	6.1
1	E	419	GLU	6.0
1	F	418	GLY	5.9
1	H	418	GLY	5.7
1	B	418	GLY	5.2
1	C	419	GLU	5.1
1	G	418	GLY	5.1
1	C	418	GLY	4.8
1	F	147	VAL	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	418	GLY	3.9
1	D	417	LYS	3.5
1	F	148	ASN	3.2
1	D	76	ASN	3.2
1	F	1	MET	3.0
1	G	76	ASN	2.6
1	E	1	MET	2.6
1	F	401	ARG	2.6
1	F	76	ASN	2.5
1	C	1	MET	2.5
1	C	401	ARG	2.4
1	G	85	ASP	2.4
1	A	417	LYS	2.4
1	F	71	TRP	2.4
1	D	148	ASN	2.3
1	F	217	GLY	2.3
1	B	1	MET	2.2
1	F	38	PRO	2.2
1	F	285	HIS	2.2
1	F	358	GLU	2.2
1	F	152	LYS	2.2
1	D	1	MET	2.2
1	C	417	LYS	2.2
1	D	240	VAL	2.2
1	F	63	LYS	2.1
1	F	240	VAL	2.1
1	F	140	GLU	2.1
1	B	76	ASN	2.1
1	H	85	ASP	2.1
1	F	85	ASP	2.1
1	F	202	GLY	2.0
1	G	401	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	IAS	F	67	8/9	0.81	0.30	34,36,38,41	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	IAS	B	67	8/9	0.93	0.15	23,26,29,35	0
1	IAS	D	67	8/9	0.95	0.17	24,27,29,31	0
1	IAS	E	67	8/9	0.96	0.19	22,26,28,34	0
1	IAS	C	67	8/9	0.96	0.14	20,21,28,28	0
1	IAS	H	67	8/9	0.96	0.13	18,22,24,24	0
1	IAS	G	67	8/9	0.97	0.14	21,23,25,28	0
1	IAS	A	67	8/9	0.97	0.09	13,16,17,18	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.

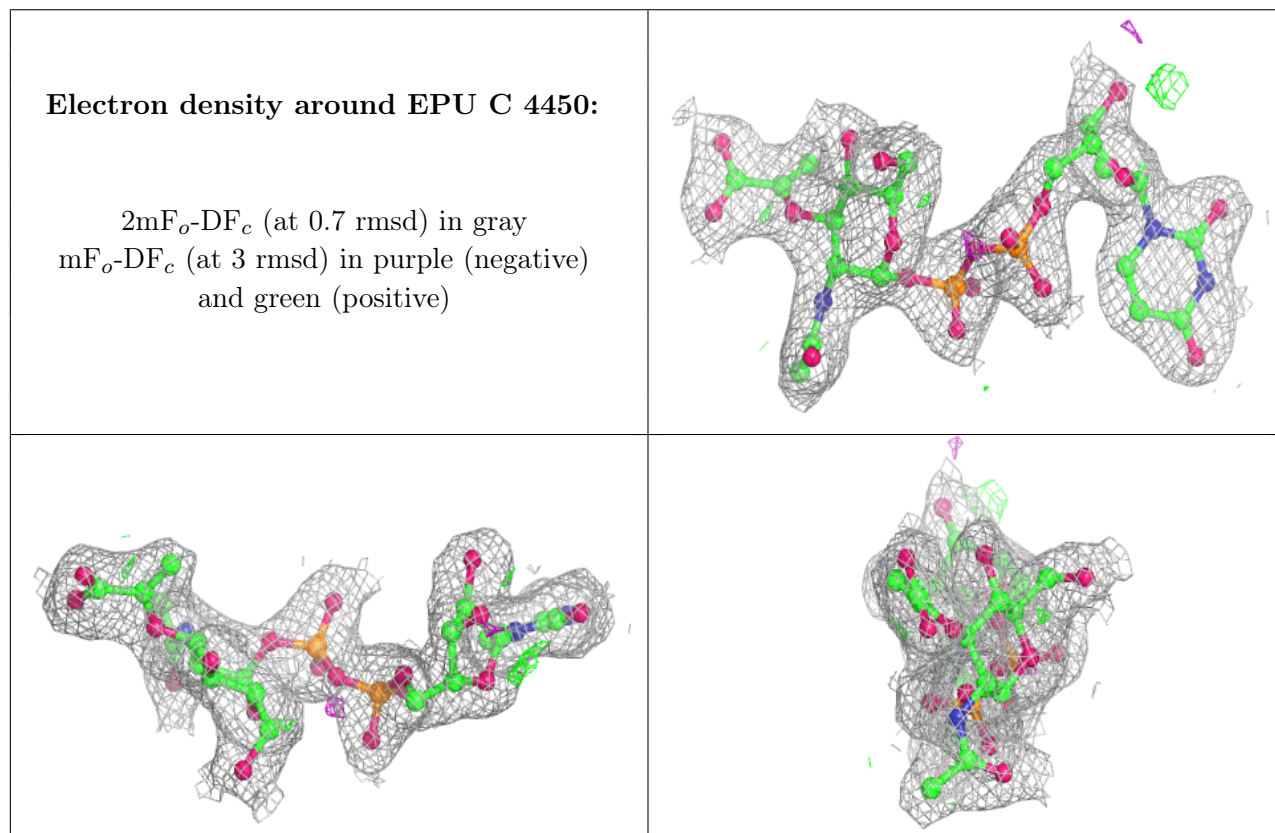
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	G	8462	5/5	0.74	0.22	91,92,93,93	0
4	GOL	C	4472	6/6	0.79	0.34	47,52,56,57	0
4	GOL	A	2472	6/6	0.81	0.25	43,46,46,50	0
4	GOL	C	3473	6/6	0.82	0.22	54,56,60,66	0
4	GOL	E	8472	6/6	0.82	0.34	51,56,59,61	0
4	GOL	C	2473	6/6	0.83	0.18	45,48,49,51	0
4	GOL	B	3472	6/6	0.85	0.27	53,55,55,58	0
4	GOL	F	7471	6/6	0.86	0.26	38,40,41,44	0
4	GOL	H	9472	6/6	0.86	0.29	40,47,50,52	0
4	GOL	D	5472	6/6	0.88	0.30	44,46,47,47	0
4	GOL	E	6471	6/6	0.89	0.23	23,27,30,33	0
4	GOL	A	2471	6/6	0.89	0.24	21,25,26,32	0
4	GOL	D	5471	6/6	0.90	0.26	24,29,34,38	0
4	GOL	C	4474	6/6	0.90	0.21	32,39,41,43	0
2	PO4	F	7461	5/5	0.91	0.21	64,65,66,70	0
4	GOL	G	8471	6/6	0.92	0.25	26,28,28,38	0
2	PO4	G	8461	5/5	0.92	0.19	50,52,55,58	0
2	PO4	B	3461	5/5	0.94	0.18	46,48,51,52	0
4	GOL	B	3471	6/6	0.94	0.22	23,25,27,32	0
4	GOL	C	4471	6/6	0.94	0.20	16,21,25,28	0
4	GOL	H	9471	6/6	0.94	0.22	24,28,30,36	0

Continued on next page...

Continued from previous page...

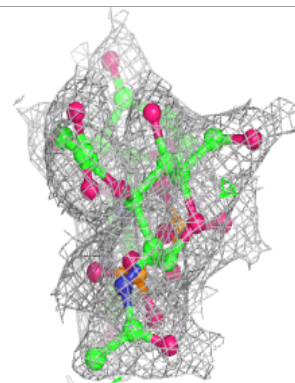
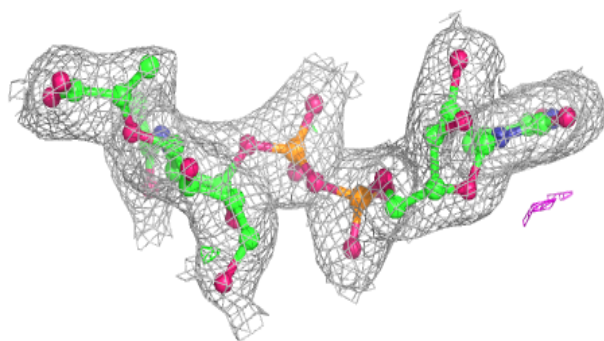
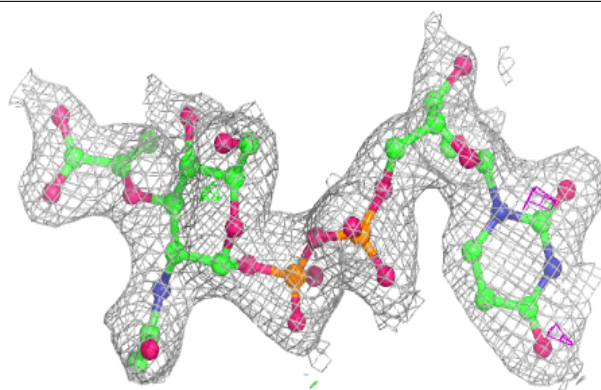
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	D	5461	5/5	0.94	0.17	54,55,58,61	0
2	PO4	A	2461	5/5	0.96	0.18	34,35,41,46	0
2	PO4	E	6461	5/5	0.96	0.15	47,50,50,52	0
2	PO4	H	9461	5/5	0.96	0.13	42,44,47,50	0
2	PO4	C	4461	5/5	0.96	0.15	42,45,48,50	0
3	EPU	C	4450	44/44	0.97	0.12	7,14,21,28	0
3	EPU	F	7450	44/44	0.97	0.13	14,21,27,29	0
3	EPU	G	8450	44/44	0.97	0.12	6,16,23,26	0
3	EPU	B	3450	44/44	0.97	0.11	8,16,20,24	0
3	EPU	A	2450	44/44	0.98	0.12	9,14,18,26	0
3	EPU	D	5450	44/44	0.98	0.10	10,17,27,31	0
3	EPU	H	9450	44/44	0.98	0.11	1,15,22,24	0
3	EPU	E	6450	44/44	0.98	0.11	8,15,21,22	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.

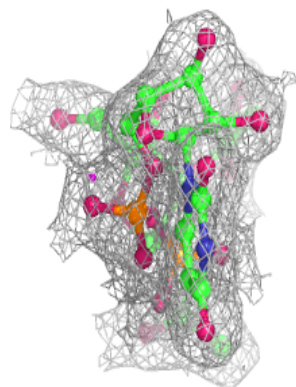
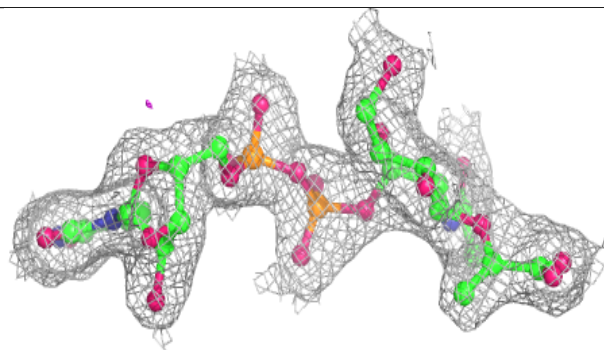
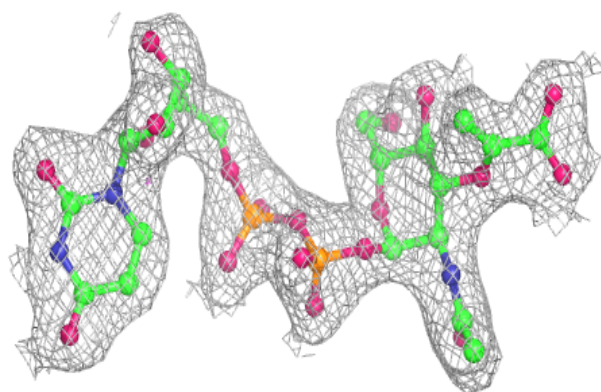


**Electron density around EPU F 7450:**

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

**Electron density around EPU G 8450:**

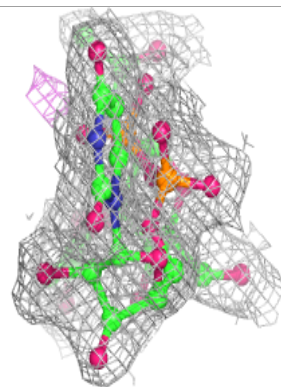
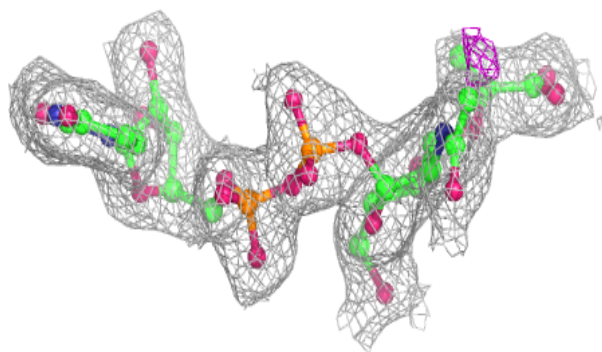
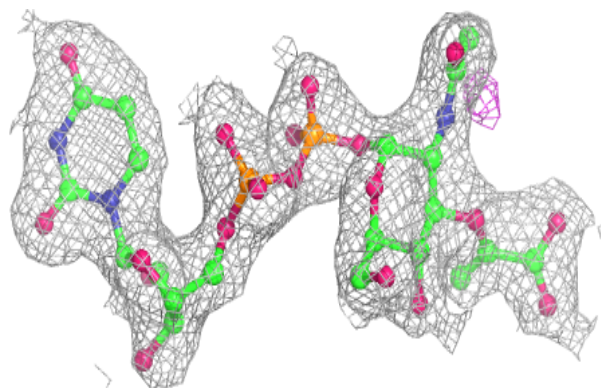
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



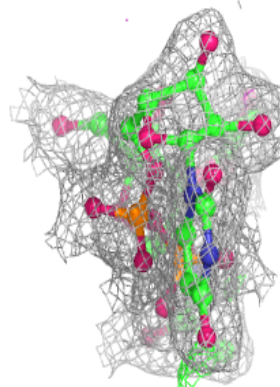
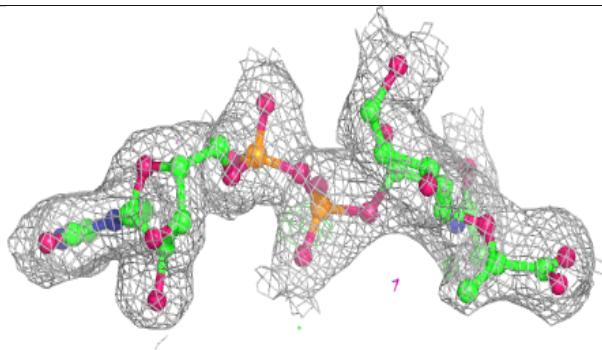
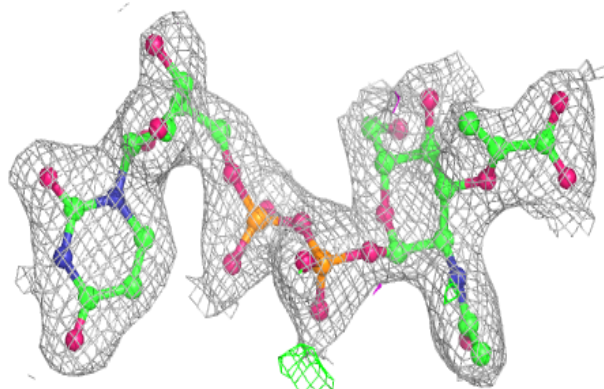


**Electron density around EPU B 3450:**

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

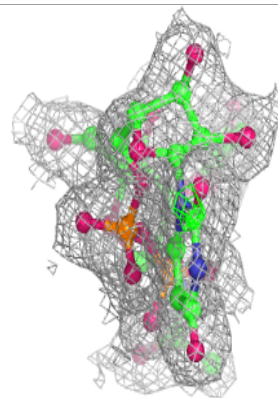
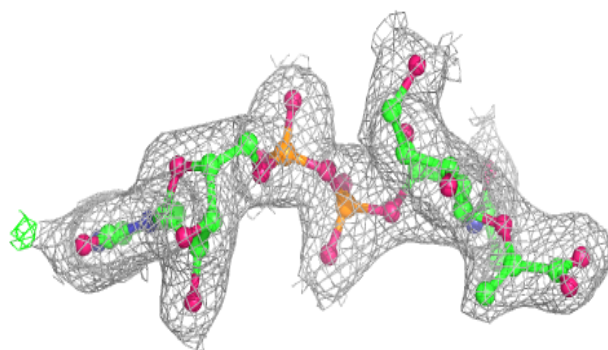
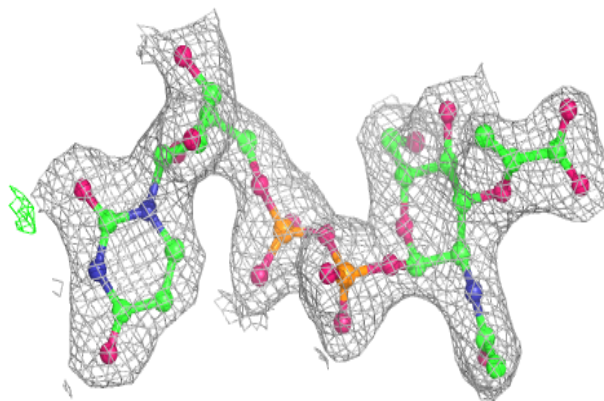
**Electron density around EPU A 2450:**

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

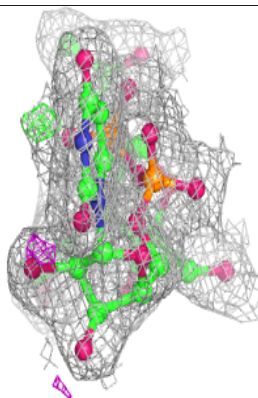
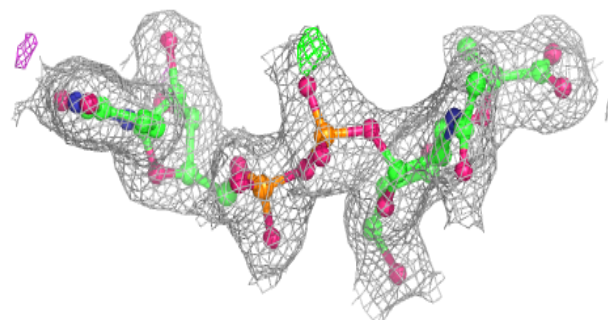
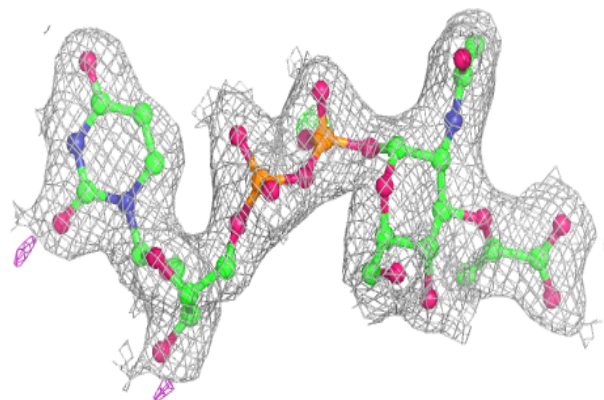


**Electron density around EPU D 5450:**

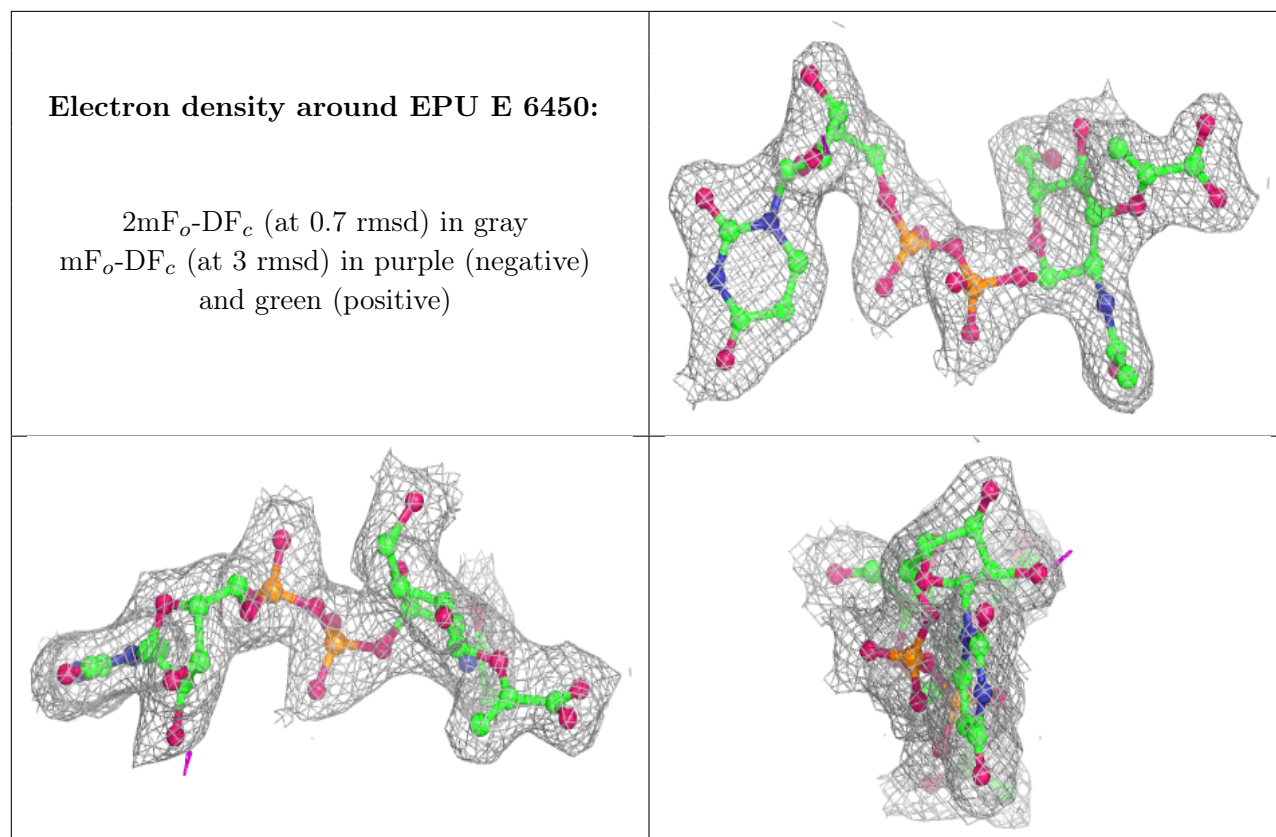
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around EPU H 9450:**

$2mF_o-DF_c$  (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.