



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:15 am BST

PDB ID : 1B3O  
Title : TERNARY COMPLEX OF HUMAN TYPE-II INOSINE MONOPHOSPHATE DEHYDROGENASE WITH 6-CL-IMP AND SELENAZOLE ADENINE DINUCLEOTIDE  
Authors : Colby, T.D.; Vanderveen, K.; Strickler, M.D.; Goldstein, B.M.  
Deposited on : 1998-12-14  
Resolution : 2.90 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 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

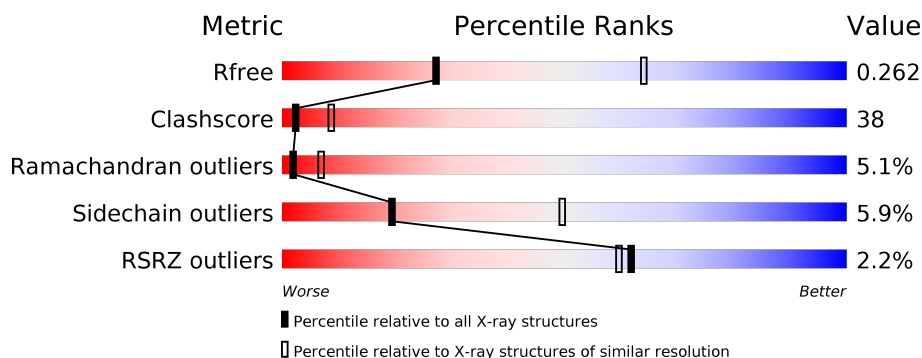
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	514	<div> <div> <div></div> <div>35%</div> <div>22%</div> <div>•</div> <div>40%</div> </div> </div>
1	B	514	<div> <div>2%</div> <div> <div></div> <div>38%</div> <div>35%</div> <div>7%</div> <div>•</div> <div>19%</div> </div> </div>

## 2 Entry composition [i](#)

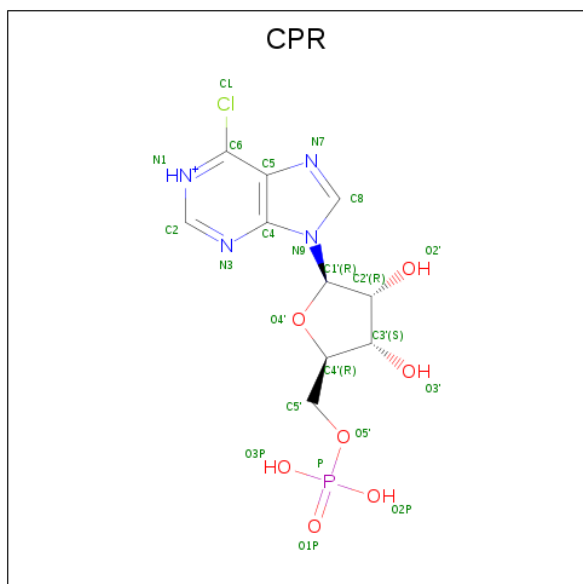
There are 5 unique types of molecules in this entry. The entry contains 5536 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (INOSINE MONOPHOSPHATE DEHYDROGENASE 2).

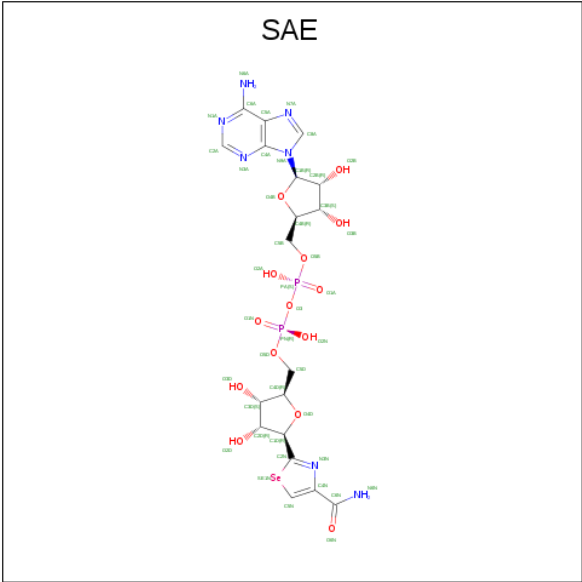
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	3
			2275	1434	389	439	13			
1	B	414	Total	C	N	O	S	0	0	4
			3085	1941	535	591	18			

- Molecule 2 is 6-CHLOROPURINE RIBOSIDE, 5'-MONOPHOSPHATE (three-letter code: CPR) (formula:  $C_{10}H_{13}ClN_4O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	4	7	1		

- Molecule 3 is SELENAZOLE-4-CARBOXYAMIDE-ADENINE DINUCLEOTIDE (three-letter code: SAE) (formula:  $C_{19}H_{25}N_7O_{14}P_2Se$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	Se	0	0
			43	19	7	14	2	1		
3	B	1	Total	C	N	O	P	Se	0	0
			43	19	7	14	2	1		

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	15	Total	X	15	0
			15	15		

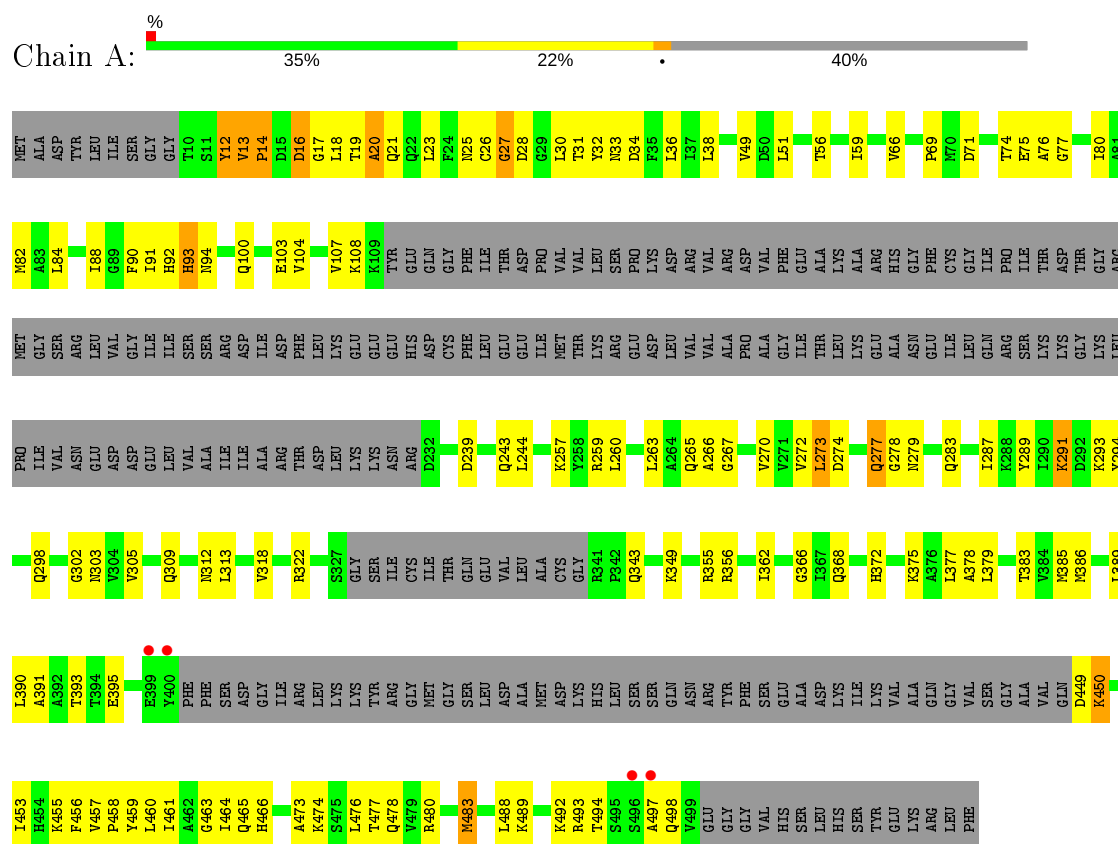
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	20	Total	O	0	0
			20	20		

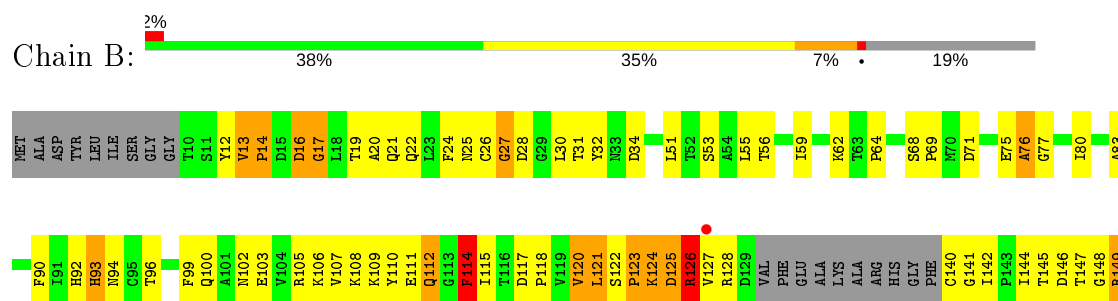
### 3 Residue-property plots [i](#)

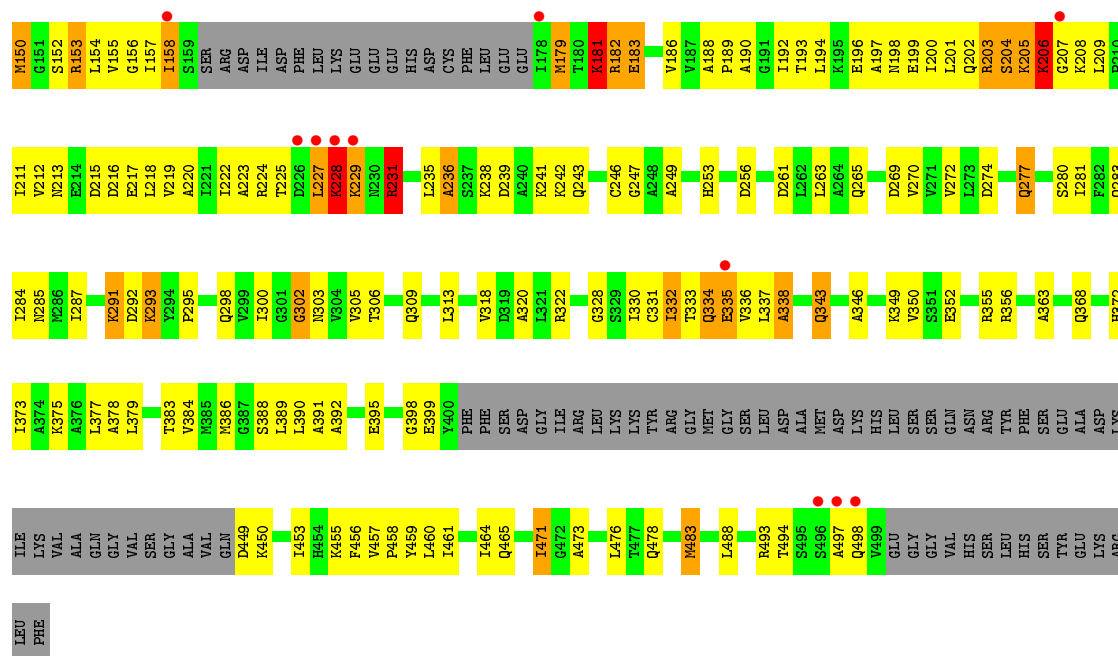
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

#### • Molecule 1: PROTEIN (INOSINE MONOPHOSPHATE DEHYDROGENASE 2)



#### • Molecule 1: PROTEIN (INOSINE MONOPHOSPHATE DEHYDROGENASE 2)





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.26 Å   142.26 Å   174.94 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	100.00 – 2.90 29.69 – 2.86	Depositor EDS
% Data completeness (in resolution range)	86.4 (100.00-2.90) 84.4 (29.69-2.86)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.85 Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.244   ,   0.270 0.234   ,   0.262	Depositor DCC
$R_{free}$ test set	3253 reflections (9.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29   ,   4.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5536	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: UNX, CPR, SAE

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	0.49	0/2308	0.77	0/3122
1	B	0.58	0/3125	0.85	2/4224 (0.0%)
All	All	0.54	0/5433	0.82	2/7346 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	181	LYS	N-CA-C	6.40	128.27	111.00
1	B	231	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Sidechain

### 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	2275	0	2294	129	0
1	B	3085	0	3161	285	0
2	A	22	0	11	1	0
2	B	22	0	11	2	0
3	A	43	0	23	4	0
3	B	43	0	23	4	0
4	B	15	0	0	0	0
5	A	11	0	0	0	0
5	B	20	0	0	0	0
All	All	5536	0	5523	417	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 38.

All (417) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:HH12	1:B:109:LYS:HG2	1.18	1.06
1:B:181:LYS:HE2	1:B:181:LYS:H	1.20	1.01
1:B:224:ARG:HB3	1:B:227:LEU:HD11	1.46	0.97
1:B:227:LEU:HD13	1:B:228:LYS:N	1.80	0.96
1:B:198:ASN:HA	1:B:201:LEU:HD12	1.44	0.95
1:B:122:SER:N	1:B:148:GLY:HA2	1.81	0.94
1:B:270:VAL:HG12	1:B:298:GLN:HB2	1.49	0.94
1:B:201:LEU:HD22	1:B:206:LYS:HA	1.52	0.92
1:B:207:GLY:O	1:B:223:ALA:HA	1.70	0.90
1:A:270:VAL:HG12	1:A:298:GLN:HB2	1.54	0.90
1:A:277:GLN:C	1:A:277:GLN:HE21	1.75	0.89
1:B:203:ARG:HH21	1:B:205:LYS:HB2	1.39	0.88
1:B:212:VAL:HG11	1:B:216:ASP:HA	1.57	0.87
1:B:343:GLN:HE21	1:B:343:GLN:HA	1.40	0.87
1:B:239:ASP:OD2	1:B:243:GLN:HB2	1.75	0.86
1:B:198:ASN:O	1:B:201:LEU:HB2	1.76	0.85
1:B:203:ARG:NE	1:B:205:LYS:H	1.74	0.85
1:B:224:ARG:HB3	1:B:227:LEU:CD1	2.07	0.84
1:B:291:LYS:HA	1:B:291:LYS:HE2	1.60	0.83
1:B:277:GLN:C	1:B:277:GLN:HE21	1.82	0.82
1:B:204:SER:C	1:B:206:LYS:H	1.83	0.81
1:B:368:GLN:H	1:B:372:HIS:HD2	1.26	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLU:OE2	1:B:92:HIS:HE1	1.63	0.81
1:A:368:GLN:H	1:A:372:HIS:HD2	1.26	0.81
1:B:330:ILE:HG23	1:B:335:GLU:HB2	1.62	0.81
1:B:198:ASN:HB3	1:B:224:ARG:HH12	1.46	0.80
1:A:283:GLN:HE22	1:A:302:GLY:HA3	1.46	0.80
1:A:473:ALA:HA	1:A:478:GLN:NE2	1.97	0.79
1:A:239:ASP:OD2	1:A:243:GLN:HB2	1.83	0.79
1:B:92:HIS:HD2	1:B:94:ASN:HB3	1.45	0.79
1:B:203:ARG:HD2	1:B:204:SER:N	1.97	0.79
1:B:114:PHE:O	1:B:115:ILE:HD13	1.83	0.78
1:B:330:ILE:HG12	1:B:335:GLU:HG2	1.65	0.78
1:B:483:MET:HB3	1:B:488:LEU:HD23	1.63	0.78
1:A:16:ASP:HB2	1:A:489:LYS:HG3	1.65	0.78
1:B:153:ARG:HA	1:B:216:ASP:O	1.83	0.78
1:A:493:ARG:HE	1:A:498:GLN:HG2	1.48	0.78
1:B:204:SER:O	1:B:206:LYS:N	2.16	0.78
1:B:207:GLY:O	1:B:208:LYS:HD2	1.84	0.77
1:B:111:GLU:O	1:B:112:GLN:HG2	1.84	0.77
1:B:181:LYS:CE	1:B:181:LYS:H	1.98	0.77
1:A:31:THR:HG22	1:A:32:TYR:N	2.01	0.76
1:B:213:ASN:OD1	1:B:217:GLU:HB2	1.85	0.76
1:B:144:ILE:HG12	1:B:156:GLY:CA	2.16	0.76
1:B:181:LYS:HE2	1:B:181:LYS:N	2.00	0.76
1:B:12:TYR:CE2	1:B:14:PRO:HA	2.22	0.75
1:A:291:LYS:HE2	1:A:291:LYS:HA	1.69	0.74
1:B:144:ILE:HD11	1:B:179:MET:SD	2.28	0.74
1:B:203:ARG:NH1	1:B:204:SER:HB3	2.04	0.73
1:B:204:SER:O	1:B:206:LYS:HG3	1.88	0.73
1:B:261:ASP:O	1:B:265:GLN:HG3	1.87	0.73
1:A:473:ALA:HA	1:A:478:GLN:HE21	1.54	0.73
1:B:105:ARG:HH12	1:B:109:LYS:CG	2.00	0.73
1:B:115:ILE:HG22	1:B:118:PRO:HD3	1.70	0.72
1:B:31:THR:HG22	1:B:32:TYR:N	2.03	0.72
1:B:207:GLY:HA2	1:B:224:ARG:H	1.54	0.72
1:B:283:GLN:HE22	1:B:302:GLY:HA3	1.54	0.72
1:B:337:LEU:O	1:B:338:ALA:HB2	1.89	0.72
1:A:92:HIS:HD2	1:A:94:ASN:HB3	1.54	0.72
1:B:203:ARG:HD2	1:B:203:ARG:C	2.09	0.72
1:A:16:ASP:CB	1:A:489:LYS:HG3	2.20	0.72
1:B:471:ILE:HD12	1:B:488:LEU:HD13	1.71	0.71
1:A:26:CYS:HB3	1:A:28:ASP:OD2	1.89	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:MET:CE	1:B:220:ALA:HA	2.21	0.70
1:A:277:GLN:HE22	1:A:279:ASN:N	1.89	0.70
1:B:155:VAL:HG12	1:B:155:VAL:O	1.92	0.70
1:A:277:GLN:HE22	1:A:279:ASN:H	1.39	0.69
1:B:157:ILE:O	1:B:158:ILE:HG23	1.91	0.69
1:B:197:ALA:O	1:B:201:LEU:HG	1.92	0.69
1:B:227:LEU:C	1:B:227:LEU:HD13	2.12	0.69
1:B:105:ARG:NH1	1:B:109:LYS:HG2	2.02	0.69
1:B:120:VAL:HG11	1:B:150:MET:HB2	1.74	0.69
1:B:331:CYS:O	1:B:332:ILE:HB	1.92	0.69
1:A:270:VAL:CG1	1:A:298:GLN:HB2	2.22	0.69
1:A:283:GLN:O	1:A:287:ILE:HG12	1.93	0.69
1:A:31:THR:HG22	1:A:33:ASN:H	1.56	0.69
1:A:386:MET:CE	1:A:389:LEU:HD23	2.23	0.69
1:B:198:ASN:CB	1:B:224:ARG:HH12	2.05	0.69
1:B:193:THR:HG23	1:B:196:GLU:H	1.58	0.69
1:B:157:ILE:HG22	1:B:158:ILE:N	2.08	0.68
1:B:203:ARG:HG3	1:B:204:SER:H	1.57	0.68
1:B:305:VAL:H	1:B:309:GLN:NE2	1.92	0.68
1:B:283:GLN:O	1:B:287:ILE:HG12	1.94	0.68
1:B:494:THR:O	1:B:497:ALA:HB3	1.93	0.67
1:A:75:GLU:O	1:A:77:GLY:N	2.27	0.67
1:B:333:THR:O	1:B:334:GLN:HB3	1.95	0.67
1:A:456:PHE:O	1:A:459:TYR:HB3	1.95	0.67
1:B:206:LYS:HD2	1:B:206:LYS:C	2.16	0.67
1:A:483:MET:HB3	1:A:488:LEU:HD23	1.78	0.66
1:B:120:VAL:HG21	1:B:150:MET:N	2.11	0.66
1:B:211:ILE:O	1:B:218:LEU:HD12	1.95	0.66
1:B:203:ARG:NH2	1:B:205:LYS:HB2	2.09	0.66
1:B:473:ALA:HA	1:B:478:GLN:NE2	2.11	0.66
1:B:378:ALA:O	1:B:483:MET:HG2	1.95	0.66
1:A:31:THR:CG2	1:A:32:TYR:N	2.60	0.65
1:A:51:LEU:HD12	1:A:461:ILE:HG23	1.77	0.65
1:B:227:LEU:O	1:B:227:LEU:HD22	1.97	0.65
1:B:225:THR:HG22	1:B:225:THR:O	1.97	0.65
1:B:16:ASP:O	1:B:17:GLY:O	2.13	0.65
1:B:144:ILE:HG13	1:B:144:ILE:O	1.97	0.65
1:B:112:GLN:OE1	1:B:243:GLN:HG2	1.96	0.65
1:B:333:THR:O	1:B:333:THR:HG22	1.97	0.65
1:A:305:VAL:H	1:A:309:GLN:NE2	1.95	0.64
1:B:121:LEU:HA	1:B:148:GLY:O	1.97	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:O	1:A:108:LYS:HG2	1.98	0.64
1:A:494:THR:N	1:A:497:ALA:HB3	2.12	0.63
1:A:305:VAL:H	1:A:309:GLN:HE22	1.46	0.63
1:A:449:ASP:O	1:A:450:LYS:O	2.15	0.63
1:B:12:TYR:HE2	1:B:14:PRO:HA	1.62	0.63
1:B:303:ASN:OD1	1:B:322:ARG:HD3	1.99	0.63
1:B:203:ARG:CD	1:B:204:SER:N	2.62	0.63
1:B:75:GLU:O	1:B:77:GLY:N	2.32	0.62
1:B:69:PRO:HG3	1:B:90:PHE:HB2	1.82	0.62
1:B:471:ILE:HD12	1:B:488:LEU:CD1	2.29	0.62
1:B:204:SER:C	1:B:206:LYS:N	2.54	0.61
1:B:203:ARG:CG	1:B:204:SER:N	2.62	0.61
1:B:51:LEU:HD12	1:B:461:ILE:HG23	1.80	0.61
1:B:238:LYS:HA	1:B:243:GLN:O	2.00	0.61
1:B:64:PRO:HA	1:B:383:THR:HG22	1.82	0.61
1:B:457:VAL:O	1:B:461:ILE:HG13	2.00	0.61
1:B:142:ILE:HD12	1:B:142:ILE:N	2.16	0.60
1:A:69:PRO:HG3	1:A:90:PHE:HB2	1.82	0.60
1:B:201:LEU:CD2	1:B:206:LYS:HA	2.29	0.60
1:B:100:GLN:HG2	1:B:263:LEU:HD21	1.82	0.60
1:B:121:LEU:C	1:B:148:GLY:HA2	2.21	0.60
1:B:203:ARG:HD2	1:B:204:SER:HB3	1.83	0.60
1:B:212:VAL:CG1	1:B:216:ASP:HA	2.31	0.60
1:B:144:ILE:HG12	1:B:156:GLY:HA3	1.82	0.60
1:B:12:TYR:O	1:B:13:VAL:O	2.20	0.60
1:B:31:THR:HG22	1:B:32:TYR:H	1.66	0.60
1:B:337:LEU:O	1:B:338:ALA:CB	2.48	0.60
1:B:395:GLU:OE1	1:B:395:GLU:N	2.35	0.59
1:B:75:GLU:OE2	1:B:92:HIS:CE1	2.52	0.59
1:A:25:ASN:OD1	1:A:349:LYS:HE2	2.03	0.59
1:B:22:GLN:O	1:B:26:CYS:SG	2.60	0.59
1:B:55:LEU:HG	1:B:56:THR:HG23	1.83	0.58
1:B:150:MET:HE2	1:B:220:ALA:HA	1.84	0.58
1:A:74:THR:O	1:A:75:GLU:HG3	2.04	0.58
1:B:270:VAL:CG1	1:B:298:GLN:HB2	2.29	0.58
1:A:368:GLN:H	1:A:372:HIS:CD2	2.15	0.58
1:A:378:ALA:O	1:A:483:MET:HG2	2.04	0.58
1:A:303:ASN:CG	3:A:600:SAE:H62N	2.08	0.57
1:B:460:LEU:O	1:B:464:ILE:HG13	2.04	0.57
1:A:377:LEU:HD13	1:A:476:LEU:HD13	1.86	0.57
1:B:239:ASP:CG	1:B:243:GLN:HB2	2.25	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ASP:O	1:B:295:PRO:HD3	2.03	0.57
1:B:118:PRO:HD2	1:B:150:MET:SD	2.44	0.57
1:B:368:GLN:H	1:B:372:HIS:CD2	2.15	0.57
1:B:12:TYR:C	1:B:13:VAL:HG13	2.25	0.57
1:A:31:THR:CG2	1:A:32:TYR:H	2.18	0.56
1:A:75:GLU:HA	1:A:91:ILE:HD12	1.87	0.56
1:A:366:GLY:O	1:A:368:GLN:HG3	2.05	0.56
1:B:386:MET:CE	1:B:389:LEU:HD23	2.34	0.56
1:B:31:THR:CG2	1:B:32:TYR:N	2.69	0.56
1:A:493:ARG:NE	1:A:498:GLN:HG2	2.19	0.56
1:B:182:ARG:O	1:B:182:ARG:HD3	2.05	0.56
1:A:100:GLN:HG2	1:A:263:LEU:HD21	1.88	0.56
1:B:198:ASN:CA	1:B:224:ARG:HH12	2.18	0.56
1:B:157:ILE:CG2	1:B:158:ILE:N	2.68	0.56
1:A:477:THR:HA	1:A:480:ARG:NH1	2.21	0.56
1:B:62:LYS:HB3	1:B:235:LEU:HD22	1.88	0.56
1:A:33:ASN:OD1	1:A:372:HIS:HE1	1.89	0.56
1:A:395:GLU:H	1:A:395:GLU:CD	2.08	0.56
1:A:277:GLN:NE2	1:A:279:ASN:H	2.02	0.55
1:B:103:GLU:OE1	1:B:106:LYS:HE3	2.07	0.55
1:A:303:ASN:ND2	3:A:600:SAE:H62N	2.03	0.55
1:B:144:ILE:CG1	1:B:144:ILE:O	2.54	0.55
1:A:273:LEU:HD11	1:A:287:ILE:HD13	1.88	0.55
1:A:270:VAL:HG12	1:A:298:GLN:CB	2.32	0.55
1:B:291:LYS:CE	1:B:291:LYS:HA	2.34	0.55
1:B:333:THR:O	1:B:334:GLN:CB	2.55	0.55
1:A:272:VAL:HG13	1:A:272:VAL:O	2.07	0.55
1:B:291:LYS:CA	1:B:291:LYS:HE2	2.35	0.55
1:B:125:ASP:O	1:B:126:ARG:HD2	2.06	0.54
1:A:12:TYR:O	1:A:13:VAL:O	2.26	0.54
1:A:26:CYS:O	1:A:28:ASP:N	2.40	0.54
1:B:144:ILE:CD1	1:B:156:GLY:HA3	2.36	0.54
1:B:199:GLU:O	1:B:202:GLN:N	2.32	0.54
1:B:212:VAL:CG1	1:B:215:ASP:O	2.55	0.54
1:B:150:MET:HE1	1:B:220:ALA:HA	1.88	0.54
1:B:277:GLN:C	1:B:277:GLN:NE2	2.57	0.54
1:B:108:LYS:HB3	1:B:243:GLN:NE2	2.23	0.54
1:B:92:HIS:CD2	1:B:94:ASN:HB3	2.35	0.54
1:B:13:VAL:O	1:B:13:VAL:HG22	2.06	0.54
1:A:390:LEU:O	1:A:393:THR:HG23	2.08	0.54
1:B:25:ASN:OD1	1:B:349:LYS:HE2	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:GLN:O	1:B:335:GLU:HB2	2.08	0.54
1:B:456:PHE:O	1:B:459:TYR:HB3	2.08	0.53
1:A:257:LYS:O	1:A:260:LEU:HB3	2.07	0.53
1:B:154:LEU:HD12	1:B:218:LEU:HD13	1.91	0.53
1:B:190:ALA:HB2	1:B:219:VAL:HG11	1.90	0.53
1:B:26:CYS:O	1:B:28:ASP:N	2.41	0.53
1:A:313:LEU:O	1:A:318:VAL:HG13	2.09	0.53
1:A:80:ILE:HG13	1:A:107:VAL:HG22	1.91	0.53
1:B:122:SER:OG	1:B:148:GLY:N	2.41	0.53
1:B:203:ARG:HG3	1:B:204:SER:N	2.20	0.53
1:A:74:THR:HG22	1:A:91:ILE:HD13	1.90	0.53
1:B:330:ILE:HG12	1:B:335:GLU:CG	2.36	0.53
1:A:36:LEU:HG	1:A:493:ARG:HD3	1.91	0.52
1:A:277:GLN:C	1:A:277:GLN:NE2	2.56	0.52
1:A:493:ARG:HH21	1:A:498:GLN:HG2	1.74	0.52
1:B:203:ARG:HD2	1:B:204:SER:CB	2.40	0.52
1:B:207:GLY:H	1:B:224:ARG:HB2	1.75	0.52
1:B:343:GLN:NE2	1:B:343:GLN:HA	2.19	0.52
1:A:277:GLN:HE21	1:A:278:GLY:N	2.08	0.52
1:B:145:THR:OG1	1:B:146:ASP:N	2.43	0.52
1:B:328:GLY:HA2	2:B:631:CPR:O1P	2.09	0.52
1:A:93:HIS:HB3	1:A:100:GLN:HE22	1.75	0.52
1:B:26:CYS:O	1:B:27:GLY:C	2.47	0.52
1:A:19:THR:O	1:A:20:ALA:C	2.47	0.52
1:A:343:GLN:HA	1:A:343:GLN:NE2	2.24	0.52
1:B:56:THR:OG1	1:B:59:ILE:HG12	2.10	0.51
1:B:343:GLN:HE21	1:B:343:GLN:CA	2.10	0.51
1:B:212:VAL:HG13	1:B:217:GLU:O	2.10	0.51
1:B:196:GLU:O	1:B:199:GLU:HB2	2.10	0.51
1:B:270:VAL:HG12	1:B:298:GLN:CB	2.33	0.51
1:B:193:THR:HG22	1:B:196:GLU:CD	2.31	0.51
1:B:127:VAL:HG22	1:B:128:ARG:H	1.75	0.51
1:B:355:ARG:HG3	1:B:356:ARG:N	2.25	0.51
1:A:494:THR:H	1:A:497:ALA:HB3	1.75	0.50
1:B:140:CYS:SG	1:B:141:GLY:N	2.83	0.50
1:B:198:ASN:HB3	1:B:224:ARG:NH1	2.20	0.50
1:A:283:GLN:HE22	1:A:302:GLY:CA	2.22	0.50
1:B:346:ALA:O	1:B:350:VAL:HG23	2.11	0.50
1:B:181:LYS:HG2	1:B:183:GLU:HG2	1.93	0.50
1:B:493:ARG:NH2	1:B:498:GLN:HG2	2.25	0.50
1:A:395:GLU:N	1:A:395:GLU:CD	2.64	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:TYR:O	1:B:13:VAL:HG13	2.11	0.50
1:B:375:LYS:O	1:B:379:LEU:HG	2.11	0.50
1:B:218:LEU:HD11	1:B:220:ALA:O	2.12	0.50
1:B:76:ALA:O	1:B:80:ILE:HG13	2.11	0.50
1:B:120:VAL:O	1:B:121:LEU:HB3	2.12	0.50
1:B:71:ASP:HB3	1:B:92:HIS:CD2	2.46	0.50
1:A:84:LEU:HD23	1:A:244:LEU:HD21	1.92	0.49
1:B:190:ALA:HA	1:B:211:ILE:CG2	2.42	0.49
1:B:313:LEU:O	1:B:318:VAL:HG22	2.12	0.49
1:B:157:ILE:CG2	1:B:158:ILE:H	2.26	0.49
1:B:212:VAL:HG12	1:B:215:ASP:O	2.12	0.49
1:B:228:LYS:HB2	1:B:228:LYS:NZ	2.27	0.49
1:B:461:ILE:O	1:B:465:GLN:HG3	2.12	0.49
1:B:186:VAL:HG13	1:B:205:LYS:NZ	2.28	0.49
1:B:203:ARG:HH11	1:B:204:SER:HB3	1.77	0.49
1:B:227:LEU:HD22	1:B:227:LEU:C	2.33	0.49
1:B:206:LYS:HD2	1:B:207:GLY:N	2.28	0.49
1:A:277:GLN:NE2	1:A:278:GLY:N	2.60	0.49
1:B:306:THR:OG1	1:B:309:GLN:HG3	2.13	0.49
1:B:31:THR:CG2	1:B:32:TYR:H	2.24	0.49
1:B:336:VAL:HG23	1:B:336:VAL:O	2.13	0.49
1:B:377:LEU:HD13	1:B:476:LEU:HD13	1.95	0.48
1:B:115:ILE:O	1:B:117:ASP:N	2.47	0.48
1:B:203:ARG:HE	1:B:205:LYS:CB	2.26	0.48
1:B:203:ARG:O	1:B:204:SER:HB2	2.13	0.48
1:B:227:LEU:CD1	1:B:227:LEU:N	2.76	0.48
1:B:368:GLN:N	1:B:372:HIS:HD2	2.05	0.48
1:A:477:THR:HA	1:A:480:ARG:HH11	1.78	0.48
1:B:19:THR:HG22	1:B:21:GLN:H	1.79	0.48
1:B:386:MET:HE2	1:B:389:LEU:HD23	1.96	0.48
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.78	0.48
1:B:224:ARG:NE	1:B:225:THR:H	2.11	0.48
1:B:212:VAL:HG12	1:B:213:ASN:N	2.29	0.48
1:A:455:LYS:C	1:A:458:PRO:HD2	2.33	0.48
1:B:115:ILE:HG22	1:B:118:PRO:CD	2.42	0.48
1:B:127:VAL:HG22	1:B:128:ARG:N	2.28	0.48
1:B:283:GLN:HE22	1:B:302:GLY:CA	2.24	0.48
1:B:150:MET:HG2	1:B:150:MET:O	2.14	0.47
1:B:193:THR:HG22	1:B:196:GLU:OE2	2.13	0.47
1:A:103:GLU:OE1	1:A:103:GLU:HA	2.14	0.47
3:B:601:SAE:PN	3:B:601:SAE:H51A	2.54	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:HIS:CD2	1:B:93:HIS:H	2.31	0.47
1:A:343:GLN:HE21	1:A:343:GLN:HA	1.79	0.47
1:B:28:ASP:HB3	1:B:30:LEU:HG	1.95	0.47
1:A:265:GLN:C	1:A:267:GLY:H	2.16	0.47
1:B:80:ILE:HG13	1:B:107:VAL:HG22	1.97	0.47
1:A:100:GLN:OE1	1:A:259:ARG:HD3	2.15	0.47
1:A:31:THR:HG22	1:A:32:TYR:H	1.74	0.47
1:B:144:ILE:CG1	1:B:156:GLY:HA3	2.44	0.47
1:B:198:ASN:CB	1:B:224:ARG:NH1	2.75	0.47
1:A:291:LYS:HA	1:A:291:LYS:CE	2.41	0.47
1:B:105:ARG:NH1	1:B:105:ARG:HG2	2.30	0.47
1:A:56:THR:OG1	1:A:59:ILE:HG12	2.14	0.47
1:B:494:THR:H	1:B:497:ALA:CB	2.27	0.47
1:A:18:LEU:N	1:A:18:LEU:HD22	2.29	0.47
1:A:26:CYS:O	1:A:27:GLY:C	2.54	0.47
1:A:66:VAL:O	1:A:385:MET:HA	2.15	0.47
1:B:363:ALA:HB3	1:B:384:VAL:HG22	1.96	0.47
1:B:121:LEU:C	1:B:121:LEU:HD22	2.35	0.46
1:B:125:ASP:O	1:B:126:ARG:CD	2.63	0.46
1:A:19:THR:O	1:A:21:GLN:N	2.47	0.46
1:B:205:LYS:O	1:B:206:LYS:O	2.33	0.46
1:B:213:ASN:ND2	1:B:215:ASP:OD2	2.48	0.46
1:B:494:THR:H	1:B:497:ALA:HB2	1.81	0.46
1:B:124:LYS:H	1:B:124:LYS:HD2	1.80	0.46
1:B:51:LEU:CD1	1:B:461:ILE:HG23	2.45	0.46
1:A:80:ILE:HG23	1:A:244:LEU:CD1	2.46	0.46
1:B:303:ASN:HA	1:B:322:ARG:O	2.16	0.46
1:B:455:LYS:C	1:B:458:PRO:HD2	2.36	0.46
1:B:471:ILE:HG13	1:B:471:ILE:O	2.15	0.46
3:A:600:SAE:H51A	3:A:600:SAE:PN	2.55	0.46
1:B:203:ARG:CZ	1:B:204:SER:HB3	2.45	0.46
1:B:13:VAL:O	1:B:13:VAL:CG2	2.63	0.46
1:B:453:ILE:HG23	1:B:457:VAL:HG23	1.97	0.46
1:B:390:LEU:O	1:B:392:ALA:N	2.49	0.46
1:B:388:SER:N	2:B:631:CPR:O3P	2.38	0.46
1:B:96:THR:OG1	1:B:99:PHE:HB2	2.15	0.46
1:A:303:ASN:OD1	1:A:322:ARG:HD3	2.16	0.46
1:A:483:MET:CB	1:A:488:LEU:HD23	2.45	0.46
1:A:23:LEU:HD11	1:A:492:LYS:CG	2.46	0.46
1:A:460:LEU:O	1:A:464:ILE:HG13	2.16	0.46
1:A:303:ASN:HA	1:A:322:ARG:O	2.16	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ALA:HB1	1:B:192:ILE:HD13	1.98	0.45
1:A:75:GLU:OE2	1:A:92:HIS:HE1	1.98	0.45
1:B:300:ILE:HG12	1:B:320:ALA:HB3	1.97	0.45
1:B:303:ASN:CG	3:B:601:SAE:H62N	2.20	0.45
1:A:26:CYS:C	1:A:28:ASP:N	2.70	0.45
1:B:227:LEU:CD1	1:B:227:LEU:C	2.82	0.45
1:B:90:PHE:HA	1:B:247:GLY:O	2.17	0.45
1:B:398:GLY:O	1:B:399:GLU:C	2.54	0.45
1:A:483:MET:HB3	1:A:488:LEU:CD2	2.44	0.45
1:B:154:LEU:N	1:B:216:ASP:O	2.48	0.45
1:A:343:GLN:HE21	1:A:343:GLN:CA	2.29	0.45
1:A:12:TYR:HE2	1:A:14:PRO:HA	1.82	0.45
1:B:115:ILE:C	1:B:117:ASP:H	2.20	0.45
1:B:181:LYS:O	1:B:182:ARG:CB	2.62	0.45
1:B:20:ALA:O	1:B:24:PHE:HD2	1.99	0.45
1:A:293:LYS:O	1:A:294:TYR:CG	2.70	0.45
1:B:157:ILE:HG22	1:B:158:ILE:H	1.80	0.45
1:A:395:GLU:OE1	1:A:453:ILE:HG12	2.17	0.44
1:B:386:MET:HE3	1:B:389:LEU:HD23	1.98	0.44
1:A:13:VAL:HA	1:A:14:PRO:HD3	1.85	0.44
1:A:23:LEU:O	1:A:28:ASP:OD2	2.35	0.44
1:B:246:CYS:N	1:B:269:ASP:OD2	2.37	0.44
1:A:28:ASP:HB3	1:A:30:LEU:HD21	1.98	0.44
1:A:49:VAL:HA	1:A:474:LYS:O	2.17	0.44
1:B:198:ASN:CA	1:B:224:ARG:NH1	2.80	0.44
1:A:273:LEU:HD12	1:A:287:ILE:HD11	1.99	0.44
1:B:125:ASP:HB3	1:B:126:ARG:H	1.40	0.44
1:B:281:ILE:HG13	1:B:285:ASN:ND2	2.33	0.44
1:B:225:THR:O	1:B:225:THR:CG2	2.64	0.44
1:B:334:GLN:CD	3:B:601:SAE:SE1N	3.06	0.44
1:A:355:ARG:HG3	1:A:356:ARG:N	2.32	0.44
1:A:71:ASP:HB3	1:A:92:HIS:CD2	2.53	0.44
1:B:249:ALA:HB1	1:B:274:ASP:HB2	2.00	0.44
1:B:280:SER:O	1:B:284:ILE:HG13	2.18	0.44
1:B:147:THR:C	1:B:149:ARG:H	2.22	0.43
1:A:277:GLN:NE2	1:A:279:ASN:N	2.61	0.43
1:A:375:LYS:O	1:A:379:LEU:HG	2.18	0.43
1:B:112:GLN:OE1	1:B:243:GLN:CG	2.64	0.43
1:B:199:GLU:O	1:B:200:ILE:C	2.56	0.43
1:B:494:THR:N	1:B:497:ALA:HB3	2.34	0.43
1:A:343:GLN:CA	1:A:343:GLN:NE2	2.82	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:H	1:A:93:HIS:CD2	2.36	0.43
1:A:69:PRO:HG3	1:A:90:PHE:CB	2.48	0.43
1:B:144:ILE:CD1	1:B:179:MET:SD	3.04	0.43
1:B:213:ASN:C	1:B:215:ASP:H	2.22	0.43
1:B:203:ARG:CD	1:B:203:ARG:C	2.79	0.43
1:B:272:VAL:HG13	1:B:272:VAL:O	2.19	0.43
1:B:122:SER:CB	1:B:123:PRO:HD2	2.49	0.43
1:A:108:LYS:HG3	1:A:266:ALA:O	2.19	0.43
1:A:362:ILE:HG12	1:A:383:THR:OG1	2.19	0.43
1:B:153:ARG:HH11	1:B:153:ARG:HB2	1.84	0.43
1:B:219:VAL:O	1:B:220:ALA:HB2	2.19	0.43
1:A:13:VAL:HG23	1:A:13:VAL:O	2.18	0.42
1:A:395:GLU:OE1	1:A:453:ILE:N	2.49	0.42
1:B:62:LYS:CB	1:B:235:LEU:HD22	2.49	0.42
1:B:30:LEU:HD22	1:B:34:ASP:HB3	1.99	0.42
1:B:303:ASN:ND2	3:B:601:SAE:H62N	2.16	0.42
1:B:102:ASN:O	1:B:106:LYS:HG3	2.19	0.42
1:B:144:ILE:HG12	1:B:156:GLY:C	2.40	0.42
1:B:53:SER:OG	1:B:64:PRO:HB3	2.20	0.42
1:A:28:ASP:HB3	1:A:30:LEU:CD2	2.49	0.42
1:A:461:ILE:O	1:A:465:GLN:HG3	2.19	0.42
1:B:202:GLN:CG	1:B:203:ARG:N	2.82	0.42
1:B:111:GLU:HG3	1:B:242:LYS:O	2.20	0.42
1:B:373:ILE:HG21	1:B:464:ILE:HD11	2.02	0.42
1:B:120:VAL:HG23	1:B:121:LEU:N	2.34	0.42
1:A:90:PHE:CD1	1:A:90:PHE:N	2.87	0.42
1:A:108:LYS:O	1:A:243:GLN:NE2	2.53	0.42
1:B:203:ARG:HE	1:B:205:LYS:HB3	1.83	0.42
1:B:203:ARG:CZ	1:B:205:LYS:H	2.31	0.41
1:A:312:ASN:HD22	1:A:312:ASN:N	2.18	0.41
1:B:343:GLN:NE2	1:B:343:GLN:CA	2.81	0.41
1:B:68:SER:HA	1:B:69:PRO:HD3	1.81	0.41
1:A:463:GLY:O	1:A:466:HIS:HB3	2.21	0.41
1:A:80:ILE:HG12	1:A:107:VAL:HG13	2.01	0.41
1:B:155:VAL:O	1:B:155:VAL:CG1	2.63	0.41
1:B:193:THR:CG2	1:B:196:GLU:HG3	2.50	0.41
1:B:293:LYS:O	1:B:293:LYS:HG2	2.20	0.41
1:A:19:THR:HG22	1:A:21:GLN:H	1.85	0.41
1:B:194:LEU:HD23	1:B:222:ILE:HD13	2.02	0.41
1:B:198:ASN:HA	1:B:224:ARG:NH1	2.36	0.41
1:B:110:TYR:HE2	1:B:117:ASP:OD1	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ILE:CG2	1:B:118:PRO:HD3	2.45	0.41
1:B:181:LYS:H	1:B:181:LYS:CD	2.34	0.41
1:B:142:ILE:N	1:B:142:ILE:CD1	2.82	0.41
1:B:188:ALA:HA	1:B:189:PRO:HD3	1.87	0.41
1:B:199:GLU:O	1:B:202:GLN:HB3	2.21	0.41
1:B:199:GLU:O	1:B:202:GLN:CB	2.68	0.41
1:B:218:LEU:CD1	1:B:220:ALA:O	2.69	0.41
1:A:293:LYS:O	1:A:293:LYS:HG2	2.21	0.41
1:B:253:HIS:O	1:B:256:ASP:HB2	2.20	0.41
1:A:273:LEU:HD11	1:A:287:ILE:CD1	2.50	0.41
1:A:31:THR:N	1:A:34:ASP:OD2	2.46	0.41
1:A:455:LYS:HA	1:A:455:LYS:HD3	1.91	0.41
1:A:457:VAL:O	1:A:461:ILE:HG13	2.21	0.41
1:A:16:ASP:HB3	1:A:489:LYS:HG3	2.02	0.41
1:B:225:THR:O	1:B:228:LYS:HD3	2.22	0.40
1:A:492:LYS:HB3	1:A:492:LYS:HE2	1.84	0.40
1:B:141:GLY:O	1:B:208:LYS:HG2	2.21	0.40
1:B:146:ASP:HB3	1:B:152:SER:OG	2.21	0.40
1:B:352:GLU:O	1:B:355:ARG:HG2	2.21	0.40
1:B:494:THR:N	1:B:497:ALA:CB	2.84	0.40
1:A:272:VAL:O	1:A:274:ASP:N	2.55	0.40
1:A:82:MET:HG3	1:A:88:ILE:H	1.87	0.40
1:B:231:ARG:H	1:B:231:ARG:HG3	1.36	0.40
1:B:83:ALA:O	1:B:236:ALA:HA	2.21	0.40
1:A:265:GLN:C	1:A:267:GLY:N	2.74	0.40
2:A:631:CPR:O2'	3:A:600:SAE:N6N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/514 (58%)	249 (83%)	39 (13%)	11 (4%)	3	13
1	B	406/514 (79%)	304 (75%)	77 (19%)	25 (6%)	1	4
All	All	705/1028 (69%)	553 (78%)	116 (16%)	36 (5%)	2	7

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	14	PRO
1	A	17	GLY
1	A	76	ALA
1	A	450	LYS
1	B	14	PRO
1	B	17	GLY
1	B	76	ALA
1	B	114	PHE
1	B	205	LYS
1	B	206	LYS
1	B	228	LYS
1	B	229	LYS
1	B	332	ILE
1	B	334	GLN
1	B	335	GLU
1	B	450	LYS
1	A	16	ASP
1	A	27	GLY
1	B	13	VAL
1	B	27	GLY
1	B	123	PRO
1	B	126	ARG
1	B	150	MET
1	B	204	SER
1	B	302	GLY
1	B	338	ALA
1	B	391	ALA
1	A	20	ALA
1	A	273	LEU
1	A	391	ALA
1	B	125	ASP
1	B	236	ALA
1	B	293	LYS
1	B	181	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	289	TYR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/420 (58%)	237 (98%)	5 (2%)	53	81
1	B	333/420 (79%)	304 (91%)	29 (9%)	10	30
All	All	575/840 (68%)	541 (94%)	34 (6%)	19	49

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	93	HIS
1	A	277	GLN
1	A	291	LYS
1	A	483	MET
1	B	16	ASP
1	B	93	HIS
1	B	112	GLN
1	B	114	PHE
1	B	120	VAL
1	B	121	LEU
1	B	124	LYS
1	B	126	ARG
1	B	149	ARG
1	B	153	ARG
1	B	158	ILE
1	B	179	MET
1	B	181	LYS
1	B	182	ARG
1	B	183	GLU
1	B	203	ARG
1	B	206	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	209	LEU
1	B	227	LEU
1	B	228	LYS
1	B	229	LYS
1	B	231	ARG
1	B	241	LYS
1	B	277	GLN
1	B	291	LYS
1	B	343	GLN
1	B	449	ASP
1	B	471	ILE
1	B	483	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	94	ASN
1	A	243	GLN
1	A	265	GLN
1	A	277	GLN
1	A	283	GLN
1	A	285	ASN
1	A	309	GLN
1	A	312	ASN
1	A	343	GLN
1	A	372	HIS
1	A	478	GLN
1	B	92	HIS
1	B	93	HIS
1	B	94	ASN
1	B	243	GLN
1	B	265	GLN
1	B	277	GLN
1	B	283	GLN
1	B	285	ASN
1	B	309	GLN
1	B	312	ASN
1	B	343	GLN
1	B	372	HIS
1	B	478	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 15 are unknown - 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	SAE	A	600	-	38,47,47	1.16	2 (5%)	42,72,72	1.93	13 (30%)
2	CPR	A	631	-	20,24,25	1.35	3 (15%)	21,36,38	3.06	7 (33%)
3	SAE	B	601	-	38,47,47	1.16	2 (5%)	42,72,72	1.94	12 (28%)
2	CPR	B	631	1	20,24,25	1.48	5 (25%)	21,36,38	3.04	7 (33%)

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	SAE	A	600	-	-	3/18/62/62	0/5/5/5
2	CPR	A	631	-	-	5/6/26/26	0/3/3/3
3	SAE	B	601	-	-	3/18/62/62	0/5/5/5
2	CPR	B	631	1	-	0/6/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	SAE	O4B-C1B	4.46	1.47	1.41
3	A	600	SAE	O4B-C1B	4.43	1.47	1.41
2	A	631	CPR	C2-N3	3.14	1.37	1.32
2	B	631	CPR	C2-N3	2.79	1.36	1.32
2	B	631	CPR	C6-N1	2.70	1.37	1.32
2	B	631	CPR	O4'-C1'	2.64	1.44	1.41
3	B	601	SAE	C2A-N3A	2.50	1.36	1.32
3	A	600	SAE	C2A-N3A	2.47	1.36	1.32
2	A	631	CPR	O4'-C1'	2.45	1.44	1.41
2	B	631	CPR	C5-N7	-2.32	1.31	1.38
2	B	631	CPR	P-O3P	-2.22	1.46	1.54
2	A	631	CPR	C6-N1	2.06	1.36	1.32

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	631	CPR	C6-N1-C2	8.66	128.25	115.84
2	B	631	CPR	N1-C2-N3	-8.42	116.87	127.65
2	B	631	CPR	C6-N1-C2	8.26	127.68	115.84
2	A	631	CPR	N1-C2-N3	-8.18	117.18	127.65
3	B	601	SAE	N3A-C2A-N1A	-5.84	119.56	128.68
3	A	600	SAE	N3A-C2A-N1A	-5.81	119.59	128.68
3	A	600	SAE	O4B-C4B-C5B	-4.70	93.91	109.37
3	B	601	SAE	O4B-C4B-C5B	-4.70	93.92	109.37
3	B	601	SAE	O3B-C3B-C2B	3.92	124.52	111.82
3	A	600	SAE	O3B-C3B-C2B	3.92	124.50	111.82
2	A	631	CPR	O2P-P-O5'	-3.67	96.96	106.73
2	B	631	CPR	O4'-C1'-C2'	-3.29	102.12	106.93
2	B	631	CPR	C3'-C2'-C1'	3.29	105.93	100.98
3	B	601	SAE	O4B-C4B-C3B	3.24	111.52	105.11
3	A	600	SAE	O4B-C4B-C3B	3.24	111.52	105.11
2	A	631	CPR	O3'-C3'-C4'	3.17	120.22	111.05
2	B	631	CPR	O3'-C3'-C4'	3.09	119.98	111.05
3	A	600	SAE	O5D-C5D-C4D	2.85	118.81	108.99
3	B	601	SAE	O5D-C5D-C4D	2.85	118.80	108.99
2	B	631	CPR	C5'-C4'-C3'	-2.70	105.06	115.18
3	B	601	SAE	C2A-N1A-C6A	2.70	123.37	118.75
3	A	600	SAE	C2A-N1A-C6A	2.66	123.31	118.75
3	A	600	SAE	C5B-C4B-C3B	-2.65	105.24	115.18
2	A	631	CPR	C2'-C3'-C4'	-2.65	97.49	102.64
3	B	601	SAE	C5B-C4B-C3B	-2.64	105.28	115.18
3	A	600	SAE	O5D-PN-O1N	2.56	119.06	109.07

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	SAE	O5D-PN-O1N	2.54	119.00	109.07
3	B	601	SAE	O4B-C1B-C2B	-2.43	103.37	106.93
3	A	600	SAE	O4B-C1B-C2B	-2.43	103.38	106.93
3	B	601	SAE	C4A-C5A-N7A	2.42	111.92	109.40
3	B	601	SAE	O6N-C6N-C4N	2.41	121.63	119.61
3	A	600	SAE	C4A-C5A-N7A	2.41	111.91	109.40
2	A	631	CPR	O4'-C1'-C2'	-2.37	103.47	106.93
3	A	600	SAE	O6N-C6N-C4N	2.36	121.59	119.61
2	A	631	CPR	C3'-C2'-C1'	2.31	104.46	100.98
3	A	600	SAE	C5A-C6A-N6A	2.21	123.71	120.35
3	B	601	SAE	C5A-C6A-N6A	2.20	123.70	120.35
2	B	631	CPR	C2'-C3'-C4'	-2.06	98.63	102.64
3	A	600	SAE	O2B-C2B-C3B	2.00	118.30	111.82

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	631	CPR	C5'-O5'-P-O2P
2	A	631	CPR	C5'-O5'-P-O3P
2	A	631	CPR	C3'-C4'-C5'-O5'
2	A	631	CPR	C5'-O5'-P-O1P
3	A	600	SAE	PN-O3-PA-O5B
3	B	601	SAE	PN-O3-PA-O5B
2	A	631	CPR	O4'-C4'-C5'-O5'
3	A	600	SAE	PA-O3-PN-O1N
3	A	600	SAE	PA-O3-PN-O2N
3	B	601	SAE	PA-O3-PN-O1N
3	B	601	SAE	PA-O3-PN-O2N

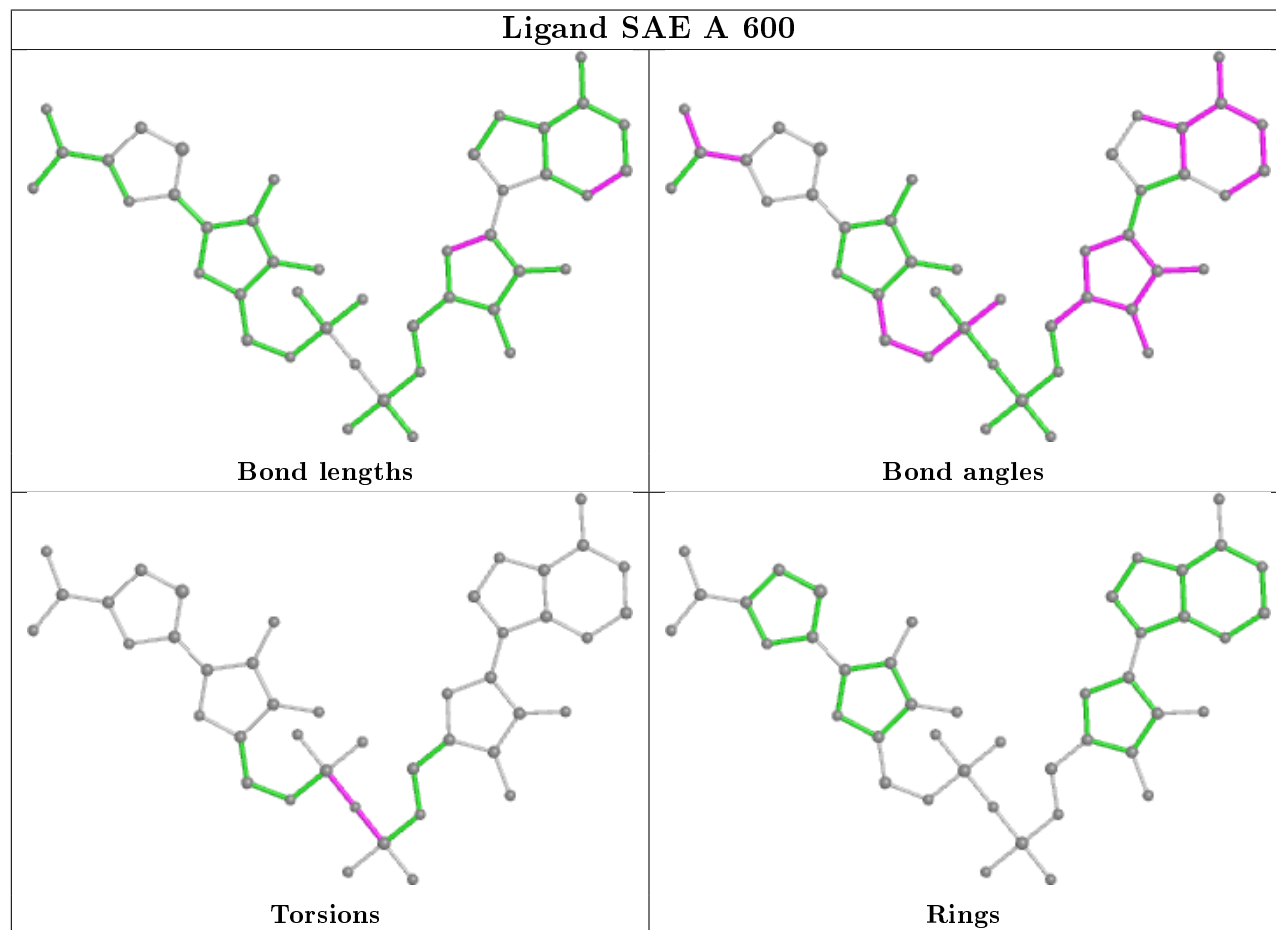
There are no ring outliers.

4 monomers are involved in 10 short contacts:

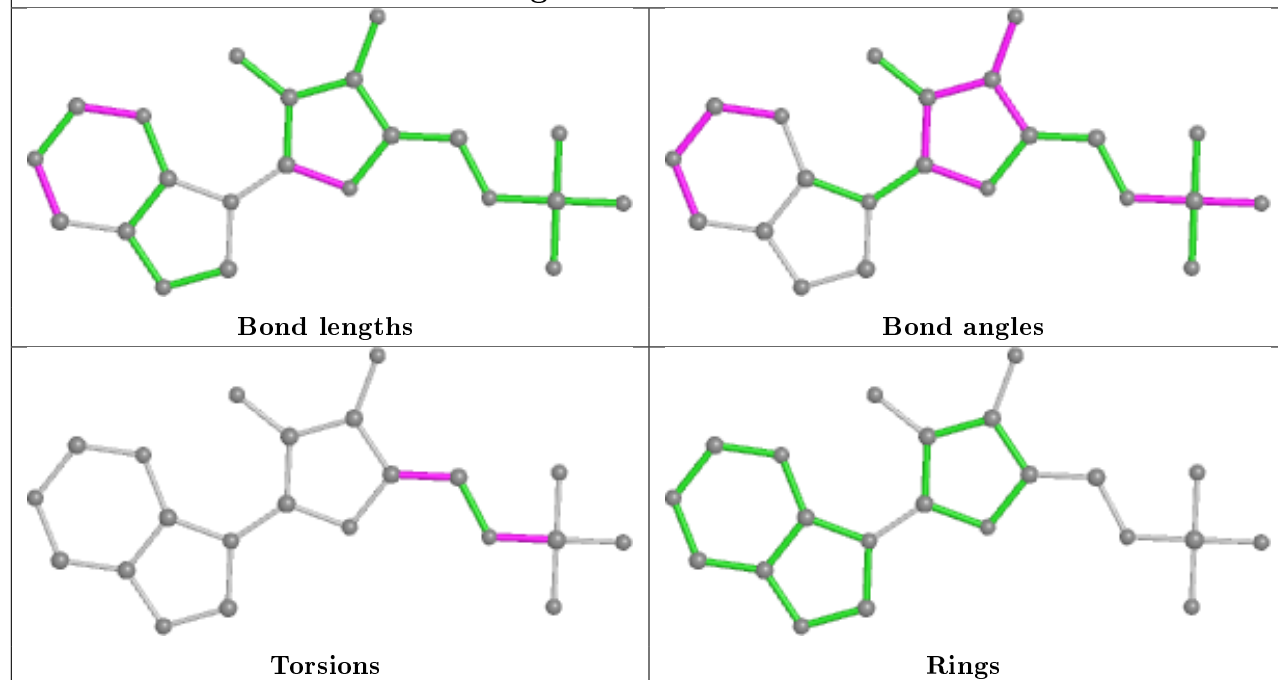
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	SAE	4	0
2	A	631	CPR	1	0
3	B	601	SAE	4	0
2	B	631	CPR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

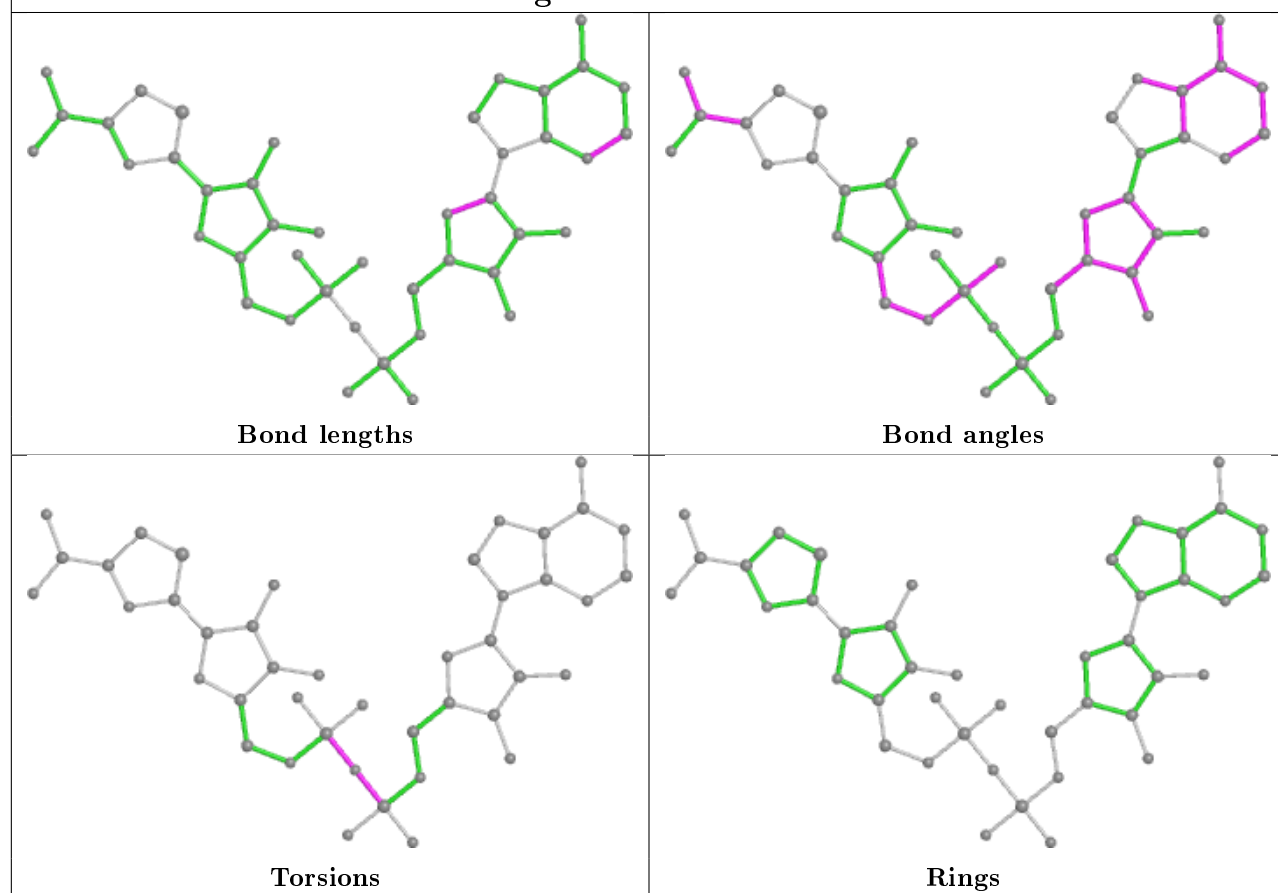
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

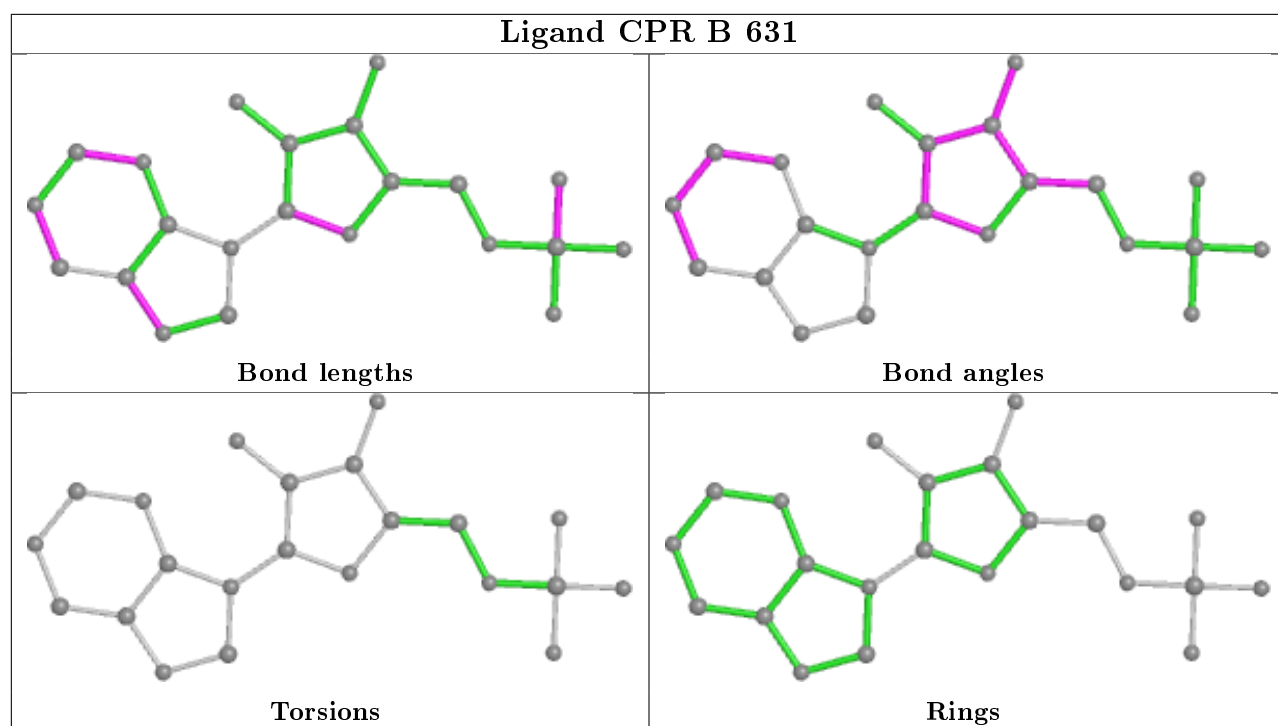


## Ligand CPR A 631



## Ligand SAE B 601





## 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	307/514 (59%)	-0.05	4 (1%) 77 77	12, 32, 55, 88	0
1	B	414/514 (80%)	0.12	12 (2%) 51 47	14, 35, 81, 95	0
All	All	721/1028 (70%)	0.05	16 (2%) 62 59	12, 34, 78, 95	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	497	ALA	4.6
1	A	400	TYR	4.4
1	B	497	ALA	3.9
1	B	228	LYS	3.3
1	B	498	GLN	3.0
1	B	227	LEU	2.9
1	B	127	VAL	2.8
1	A	496	SER	2.7
1	B	178	ILE	2.6
1	B	229	LYS	2.6
1	B	335	GLU	2.6
1	A	399	GLU	2.5
1	B	496	SER	2.5
1	B	207	GLY	2.2
1	B	158	ILE	2.2
1	B	226	ASP	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

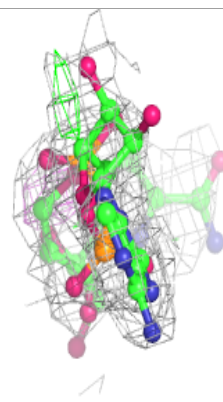
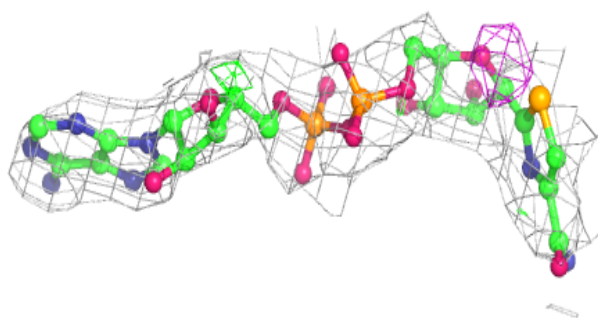
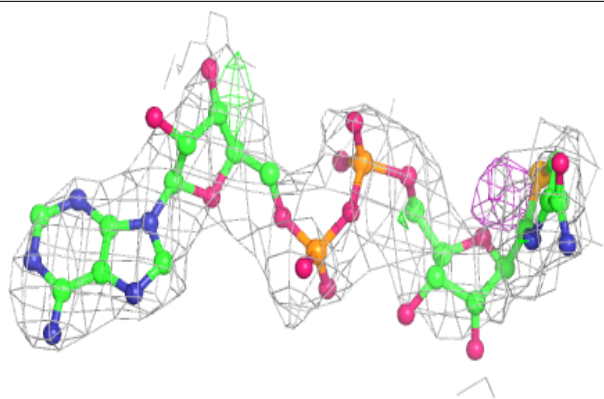
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	UNX	B	639	1/1	-	-	20,20,20,20	1
4	UNX	B	641	1/1	-	-	20,20,20,20	1
4	UNX	B	643	1/1	-	-	20,20,20,20	1
4	UNX	B	644	1/1	-	-	20,20,20,20	1
4	UNX	B	637	1/1	-	-	20,20,20,20	1
4	UNX	B	640	1/1	-	-	20,20,20,20	1
4	UNX	B	633	1/1	-	-	20,20,20,20	1
3	SAE	B	601	43/43	0.86	0.26	54,76,87,89	43
2	CPR	A	631	22/23	0.95	0.18	30,36,55,57	0
4	UNX	B	642	1/1	-	-	20,20,20,20	1
4	UNX	B	646	1/1	-	-	20,20,20,20	1
2	CPR	B	631	22/23	0.97	0.17	26,31,53,54	0
4	UNX	B	638	1/1	-	-	20,20,20,20	1
4	UNX	B	636	1/1	-	-	20,20,20,20	1
3	SAE	A	600	43/43	0.88	0.30	55,71,91,96	43
4	UNX	B	635	1/1	-	-	20,20,20,20	1
4	UNX	B	634	1/1	-	-	20,20,20,20	1
4	UNX	B	645	1/1	-	-	20,20,20,20	1
4	UNX	B	632	1/1	-	-	20,20,20,20	1

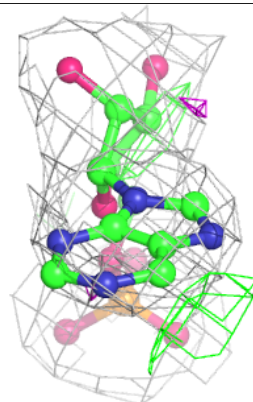
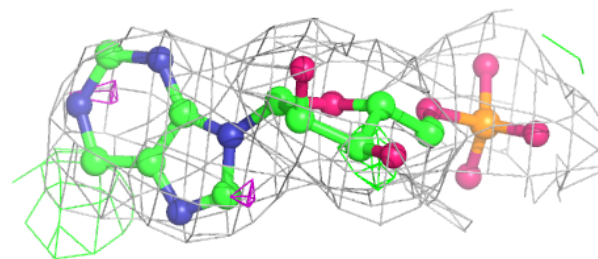
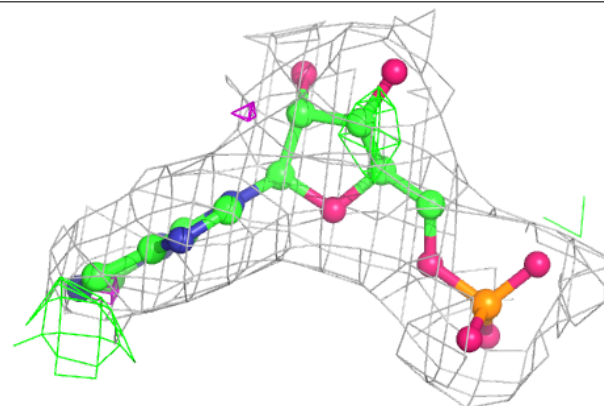
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SAE B 601:**

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

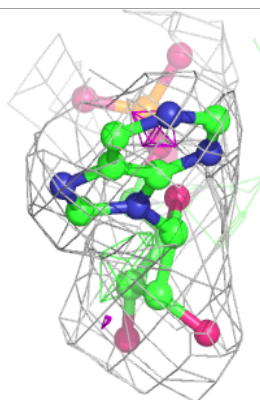
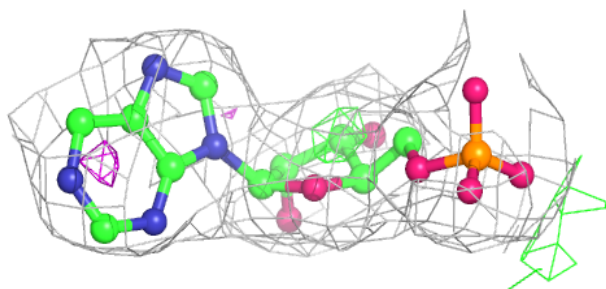
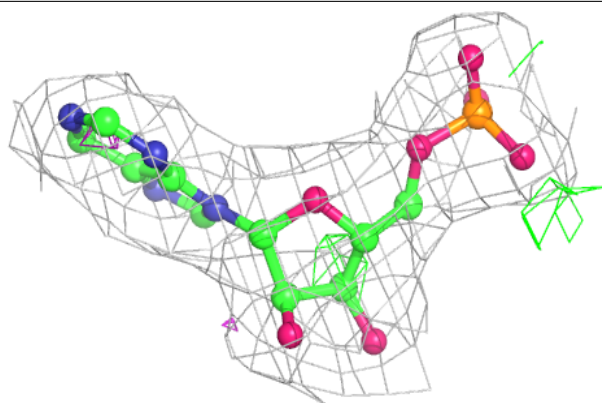
**Electron density around CPR A 631:**

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

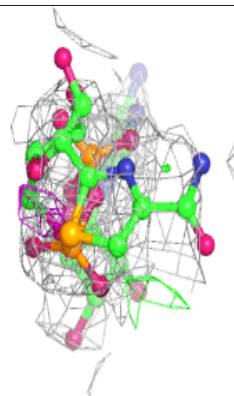
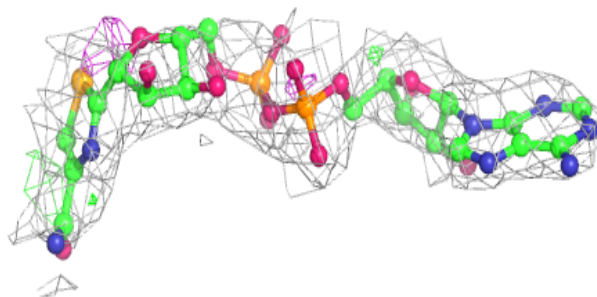
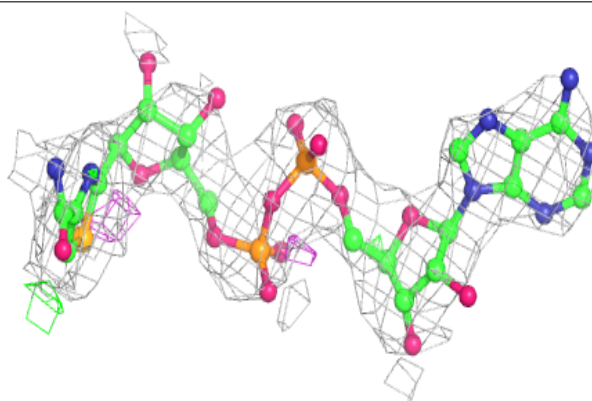


**Electron density around CPR B 631:**

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

**Electron density around SAE A 600:**

$2mF_o-DF_c$  (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.