



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 06:22 AM EST

PDB ID : 1WVG
Title : Structure of CDP-D-glucose 4,6-dehydratase from Salmonella typhi
Authors : Koropatkin, N.M.; Holden, H.M.
Deposited on : 2004-12-15
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

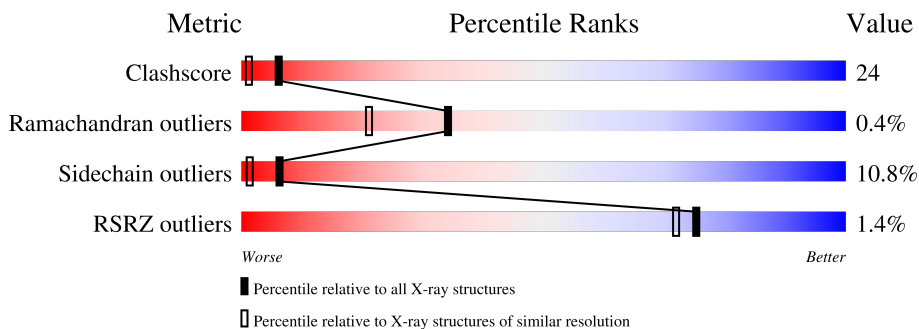
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	359	 62% 27% 8% ..
1	B	359	 3% 42% 43% 11% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6098 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.

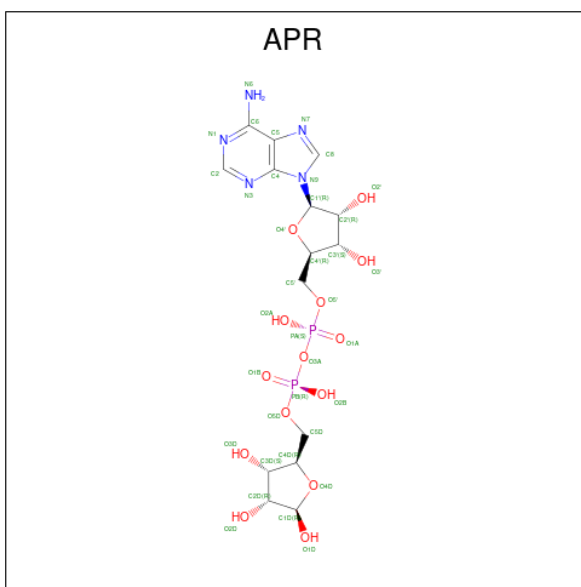
- Molecule 1 is a protein called CDP-glucose 4,6-dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	Total 2839	C 1818	N 490	O 518	S 13	0	2	0
1	B	350	Total 2827	C 1812	N 491	O 511	S 13	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	MET	conflict	UNP P26397
B	1003	SER	MET	conflict	UNP P26397

- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



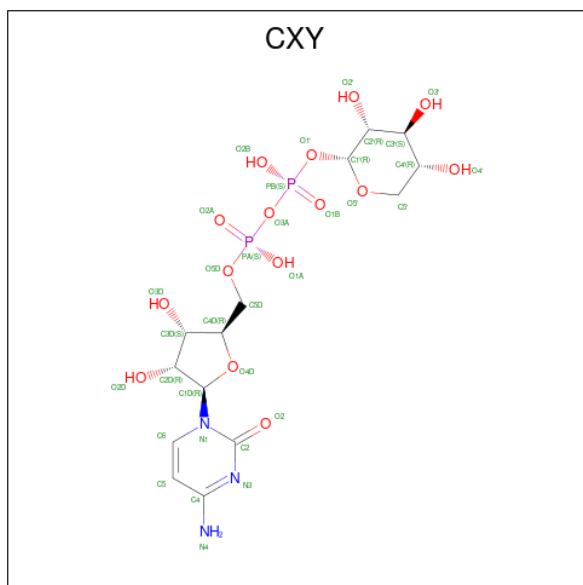
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 36	C 15	N 5	O 14	P 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	B	1	36	15	5	14	2	0	0

- Molecule 3 is CYTIDINE-5'-DIPHOSPHO-BETA-D-XYLOSE (three-letter code: CXY) (formula: C₁₄H₂₃N₃O₁₅P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	34	14	3	15	2	0	0

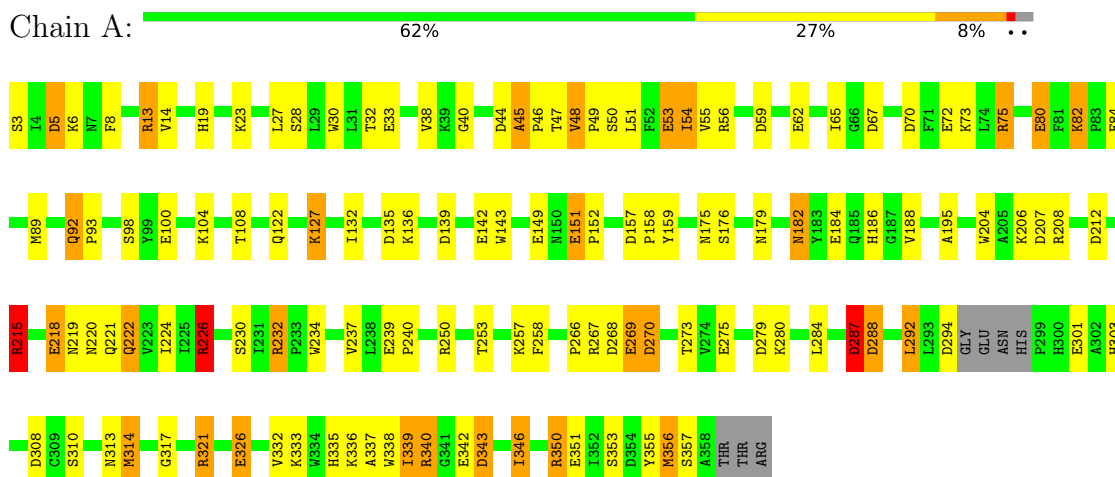
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	214	Total	O	0	0
			214	214		
4	B	112	Total	O	0	0
			112	112		

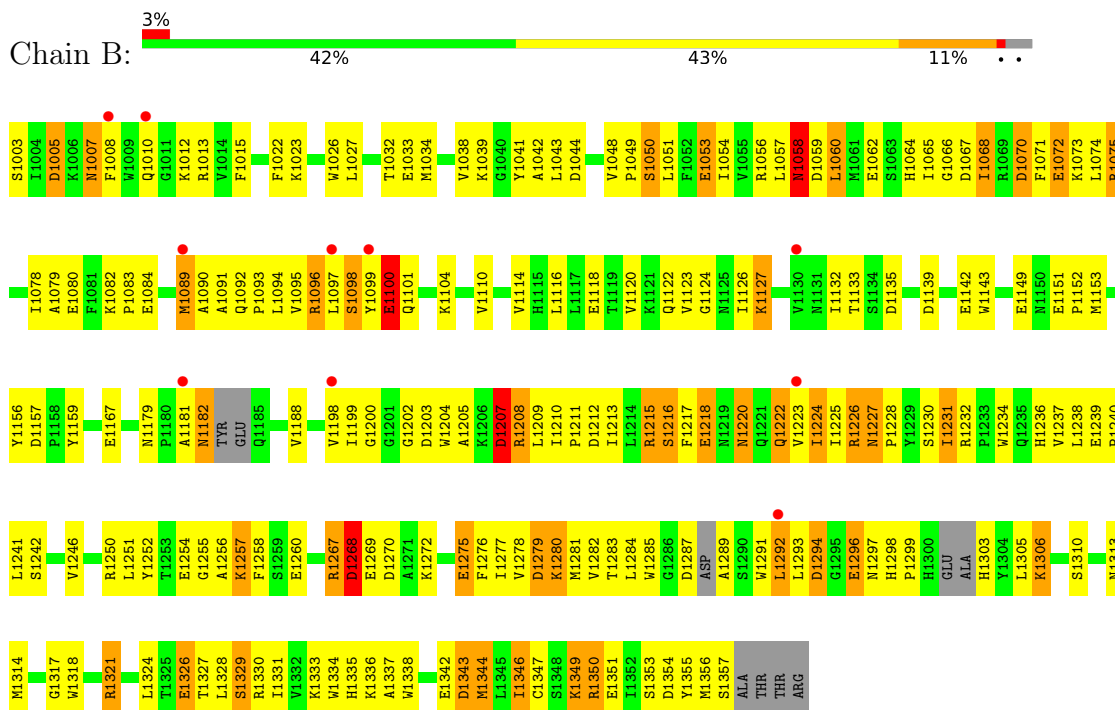
3 Residue-property plots

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

- Molecule 1: CDP-glucose 4,6-dehydratase



- Molecule 1: CDP-glucose 4,6-dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.90Å 93.90Å 152.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.80 34.52 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-1.80) 93.8 (34.52-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.82 (at 1.81Å)	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.201 , 0.270 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 118.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6098	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: APR, CXY

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	0.93	17/2921 (0.6%)	1.37	46/3961 (1.2%)
1	B	0.93	17/2919 (0.6%)	1.41	38/3956 (1.0%)
All	All	0.93	34/5840 (0.6%)	1.39	84/7917 (1.1%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1100	GLU	CD-OE2	7.23	1.33	1.25
1	B	1342	GLU	CD-OE2	6.94	1.33	1.25
1	A	33	GLU	CD-OE2	6.77	1.33	1.25
1	A	72	GLU	CD-OE2	6.75	1.33	1.25
1	A	218	GLU	CD-OE2	6.75	1.33	1.25
1	A	53	GLU	CD-OE2	6.58	1.32	1.25
1	B	1254	GLU	CD-OE2	6.46	1.32	1.25
1	B	1062	GLU	CD-OE2	6.44	1.32	1.25
1	B	1080	GLU	CD-OE2	6.33	1.32	1.25
1	B	1053	GLU	CD-OE2	6.32	1.32	1.25
1	A	184	GLU	CD-OE2	6.06	1.32	1.25
1	B	1351	GLU	CD-OE2	6.05	1.32	1.25
1	A	149	GLU	CD-OE2	5.85	1.32	1.25
1	B	1142	GLU	CD-OE2	5.73	1.31	1.25
1	A	62	GLU	CD-OE2	5.71	1.31	1.25
1	B	1072	GLU	CD-OE2	5.68	1.31	1.25
1	B	1326	GLU	CD-OE2	5.65	1.31	1.25
1	B	1084	GLU	CD-OE2	5.64	1.31	1.25
1	A	351	GLU	CD-OE2	5.60	1.31	1.25
1	A	301	GLU	CD-OE2	5.52	1.31	1.25
1	A	80	GLU	CD-OE2	5.50	1.31	1.25
1	B	1260	GLU	CD-OE2	5.50	1.31	1.25
1	B	1149	GLU	CD-OE2	5.48	1.31	1.25
1	A	326	GLU	CD-OE2	5.47	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	GLU	CD-OE2	5.45	1.31	1.25
1	B	1218	GLU	CD-OE2	5.45	1.31	1.25
1	B	1275	GLU	CD-OE2	5.42	1.31	1.25
1	A	275	GLU	CD-OE2	5.32	1.31	1.25
1	B	1151	GLU	CD-OE2	5.25	1.31	1.25
1	A	239	GLU	CD-OE2	5.24	1.31	1.25
1	A	151	GLU	CD-OE2	5.20	1.31	1.25
1	B	1351	GLU	CD-OE1	-5.19	1.20	1.25
1	A	100	GLU	CD-OE2	5.16	1.31	1.25
1	A	142	GLU	CD-OE2	5.08	1.31	1.25

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1208	ARG	NE-CZ-NH1	10.61	125.60	120.30
1	A	67	ASP	CB-CG-OD2	-10.19	109.13	118.30
1	B	1226	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	59	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	A	270	ASP	CB-CG-OD2	-8.48	110.67	118.30
1	B	1267	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	5	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	B	1139	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	288	ASP	CB-CG-OD2	-7.97	111.12	118.30
1	B	1270	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	B	1350	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	67	ASP	CB-CG-OD1	7.66	125.19	118.30
1	B	1343	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	207	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	B	1067	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	B	1070	ASP	CB-CG-OD1	7.15	124.74	118.30
1	A	270	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	157	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	287	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	B	1067	ASP	CB-CG-OD1	6.90	124.51	118.30
1	B	1267	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	212	ASP	CB-CG-OD1	6.77	124.39	118.30
1	B	1203	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	B	1343	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	B	1044	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	B	1070	ASP	N-CA-CB	6.66	122.59	110.60
1	A	215	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	5	ASP	CB-CG-OD1	6.61	124.25	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1279	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	B	1139	ASP	CB-CG-OD1	6.52	124.16	118.30
1	B	1070	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	45	ALA	N-CA-CB	6.26	118.87	110.10
1	A	59	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	1075	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	314	MET	CB-CA-C	-6.17	98.05	110.40
1	B	1268	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	279	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	208	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	343	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	1232	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	B	1135	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	1059	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	B	1270	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	253	THR	CA-CB-CG2	-5.96	104.06	112.40
1	B	1005	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	222	GLN	N-CA-CB	5.92	121.26	110.60
1	B	1058	ASN	N-CA-CB	5.88	121.18	110.60
1	A	207	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	350	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	13	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	294	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	B	1059	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	288	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	44	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	294	ASP	CB-CG-OD1	5.76	123.49	118.30
1	B	1279	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	268	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	B	1212	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	B	1215	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	1354	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	A	250	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	92	GLN	N-CA-C	-5.56	95.98	111.00
1	A	287	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	279	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	1207	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	1268	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	56	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	1153	MET	CG-SD-CE	5.33	108.72	100.20
1	A	157	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	1203	ASP	CB-CG-OD1	5.29	123.06	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1215	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	232	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	1294	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	343	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	139	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	1208	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	308	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	70[A]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	70[B]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	226	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	48	VAL	N-CA-CB	5.12	122.76	111.50
1	A	70[A]	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	70[B]	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	215	ARG	NE-CZ-NH2	-5.08	117.76	120.30

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	2839	0	2756	95	1
1	B	2827	0	2753	187	1
2	A	36	0	21	2	0
2	B	36	0	21	4	0
3	A	34	0	19	2	0
4	A	214	0	0	7	0
4	B	112	0	0	2	0
All	All	6098	0	5570	278	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (278) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:TRP:HE1	1:A:356:MET:HE2	1.04	1.12
1:B:1236:HIS:HD2	1:B:1238:LEU:H	1.04	0.94
1:B:1022:PHE:CZ	1:B:1237[C]:VAL:HG11	2.03	0.93
1:A:186:HIS:HD2	1:A:188:VAL:H	1.17	0.93
1:A:30:TRP:NE1	1:A:356:MET:HE2	1.85	0.90
1:B:1049:PRO:HB2	1:B:1054:ILE:HD11	1.54	0.88
1:B:1224:ILE:HG23	1:B:1292:LEU:HD13	1.57	0.87
1:B:1211:PRO:HB2	1:B:1215:ARG:NH1	1.90	0.86
1:B:1236:HIS:CD2	1:B:1238:LEU:H	1.92	0.86
1:B:1094:LEU:HD23	1:B:1096:ARG:HE	1.39	0.86
1:B:1057:LEU:HA	1:B:1060:LEU:HD12	1.59	0.85
1:B:1093:PRO:HB3	2:B:1400:APR:HR'3	1.59	0.84
1:A:47:THR:O	4:A:2020:HOH:O	1.97	0.83
1:A:215:ARG:NH2	1:A:219:ASN:HD22	1.77	0.83
1:B:1198:VAL:CG1	1:B:1237[C]:VAL:HG12	2.09	0.81
1:B:1321:ARG:HG3	1:B:1355:TYR:CZ	2.17	0.80
1:B:1224:ILE:HG23	1:B:1292:LEU:CD1	2.13	0.79
1:B:1008:PHE:O	1:B:1012:LYS:HE2	1.83	0.79
1:B:1208:ARG:HB3	1:B:1211:PRO:HG2	1.65	0.79
1:B:1051:LEU:HD13	1:B:1202:GLY:HA3	1.63	0.78
1:B:1198:VAL:HG13	1:B:1237[C]:VAL:HG12	1.66	0.78
1:B:1049:PRO:HG2	1:B:1204:TRP:CE2	2.20	0.77
1:B:1199:ILE:O	1:B:1237[C]:VAL:HG13	1.85	0.77
1:B:1326:GLU:O	1:B:1330:ARG:HG3	1.85	0.77
1:A:215:ARG:CZ	1:A:219:ASN:HD22	1.97	0.76
1:B:1127:LYS:HG3	1:B:1252:TYR:CE1	2.22	0.74
1:B:1208:ARG:CB	1:B:1211:PRO:HG2	2.17	0.74
1:A:104:LYS:HE2	1:A:108:THR:OG1	1.89	0.72
1:A:30:TRP:HE1	1:A:356:MET:CE	1.96	0.72
1:B:1049:PRO:CB	1:B:1054:ILE:HD11	2.19	0.71
1:B:1091:ALA:HB3	2:B:1400:APR:HR'4	1.72	0.71
1:A:135:ASP:HB3	1:A:195:ALA:O	1.92	0.70
1:B:1215:ARG:O	1:B:1218:GLU:HG2	1.90	0.70
1:A:218:GLU:HG2	1:A:339:ILE:HD11	1.73	0.70
1:A:182:ASN:HD22	1:A:186:HIS:CE1	2.09	0.70
1:A:48:VAL:CG1	1:A:49:PRO:HA	2.22	0.69
1:B:1022:PHE:CZ	1:B:1237[B]:VAL:HG21	2.28	0.69
1:A:48:VAL:HG13	1:A:49:PRO:HA	1.75	0.68
1:B:1097:LEU:HD21	1:B:1101:GLN:HB2	1.76	0.68
1:B:1236:HIS:HD2	1:B:1238:LEU:N	1.87	0.67
1:A:310:SER:O	1:A:314:MET:HG2	1.95	0.67
1:B:1058:ASN:O	1:B:1058:ASN:ND2	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1216:SER:CB	1:B:1223:VAL:HG22	2.25	0.66
1:A:224:ILE:HG12	1:A:292:LEU:HD23	1.78	0.65
1:B:1094:LEU:N	1:B:1094:LEU:HD12	2.12	0.65
1:B:1205:ALA:C	1:B:1215:ARG:HH22	1.99	0.65
1:A:48:VAL:HG22	4:A:2020:HOH:O	1.95	0.65
1:A:313:ASN:O	1:A:317:GLY:HA2	1.98	0.64
1:A:346:ILE:HD13	1:A:346:ILE:N	2.13	0.64
1:B:1027:LEU:HD23	1:B:1089:MET:CE	2.29	0.63
1:A:50:SER:HB3	4:A:2020:HOH:O	1.98	0.63
1:B:1023:LYS:NZ	2:B:1400:APR:O1D	2.28	0.63
1:A:182:ASN:ND2	4:A:1718:HOH:O	2.32	0.62
1:B:1224:ILE:HA	1:B:1292:LEU:HD12	1.81	0.62
1:B:1074:LEU:HD12	1:B:1074:LEU:O	1.99	0.62
1:A:6:LYS:HE2	1:A:356:MET:HE1	1.81	0.62
1:A:179:ASN:HB3	1:A:182:ASN:HD21	1.64	0.62
1:B:1272:LYS:HG3	1:B:1324:LEU:HD23	1.82	0.62
1:B:1075:ARG:NH1	1:B:1122:GLN:OE1	2.30	0.61
1:B:1209:LEU:O	1:B:1209:LEU:HD12	1.99	0.61
1:B:1280:LYS:NZ	1:B:1283:THR:HG21	2.14	0.61
1:A:186:HIS:CD2	1:A:188:VAL:H	2.08	0.61
1:B:1022:PHE:CE2	1:B:1237[C]:VAL:HG11	2.36	0.61
1:B:1224:ILE:HA	1:B:1292:LEU:CD1	2.32	0.60
1:A:6:LYS:HG3	4:A:2096:HOH:O	2.01	0.60
1:A:267:ARG:HB2	1:A:269:GLU:OE2	2.01	0.60
1:A:284:LEU:HB3	1:A:332:VAL:HG21	1.84	0.59
1:A:51:LEU:O	1:A:55:VAL:HG22	2.02	0.59
1:A:136:LYS:HD3	4:A:2335:HOH:O	2.04	0.58
1:B:1071:PHE:HZ	1:B:1122:GLN:NE2	2.02	0.58
1:B:1054:ILE:HD13	1:B:1204:TRP:CH2	2.38	0.58
1:A:19:HIS:CG	1:A:40:GLY:HA3	2.38	0.58
1:B:1049:PRO:HB2	1:B:1054:ILE:CD1	2.30	0.58
1:B:1094:LEU:HB3	1:B:1096:ARG:HG3	1.85	0.58
1:B:1231:ILE:HG23	1:B:1272:LYS:O	2.04	0.58
1:B:1209:LEU:HD11	1:B:1213:ILE:HD11	1.87	0.57
1:B:1013:ARG:NH2	1:B:1082:LYS:O	2.37	0.57
1:B:1208:ARG:HB3	1:B:1211:PRO:CG	2.34	0.57
1:B:1097:LEU:CD2	1:B:1101:GLN:HB2	2.33	0.57
1:B:1334:TRP:O	1:B:1344:MET:HE2	2.05	0.57
1:B:1038:VAL:HG12	1:B:1039:LYS:N	2.19	0.56
1:B:1267:ARG:HB3	1:B:1269[A]:GLU:OE1	2.05	0.56
1:A:343:ASP:OD2	1:A:346:ILE:HG12	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1284:LEU:HD23	1:B:1329:SER:HA	1.85	0.56
1:B:1297:ASN:O	1:B:1299:PRO:HD3	2.06	0.56
1:A:321:ARG:HD3	1:A:355:TYR:CZ	2.41	0.56
1:B:1179:ASN:OD1	1:B:1181:ALA:HB3	2.05	0.56
1:B:1072:GLU:OE1	1:B:1075:ARG:NH2	2.39	0.56
1:B:1123:VAL:HG12	1:B:1124:GLY:O	2.06	0.56
1:B:1199:ILE:HG13	1:B:1331:ILE:HD11	1.88	0.56
1:B:1277:ILE:O	1:B:1281:MET:HG2	2.06	0.56
1:B:1267:ARG:HB3	1:B:1269[B]:GLU:HG2	1.88	0.55
1:A:303:HIS:HB3	4:A:1742:HOH:O	2.06	0.55
1:B:1022:PHE:HZ	1:B:1237[C]:VAL:HG11	1.67	0.55
1:B:1205:ALA:O	1:B:1215:ARG:NH2	2.36	0.55
1:B:1242:SER:O	1:B:1246:VAL:HG23	2.05	0.55
1:B:1275:GLU:O	1:B:1278:VAL:HG12	2.07	0.55
1:A:179:ASN:HB3	1:A:182:ASN:ND2	2.21	0.54
1:A:13:ARG:NE	1:A:82:LYS:O	2.40	0.54
1:B:1005:ASP:O	1:B:1008:PHE:HB3	2.07	0.54
1:B:1101:GLN:HB3	1:B:1104:LYS:HB3	1.89	0.54
1:B:1118:GLU:HG3	1:B:1122:GLN:HE21	1.72	0.54
1:A:337:ALA:O	1:A:342:GLU:HB2	2.07	0.54
1:A:219:ASN:O	1:A:221:GLN:HG3	2.07	0.54
1:B:1278:VAL:O	1:B:1281:MET:HB2	2.08	0.54
1:B:1272:LYS:HB2	1:B:1324:LEU:CD2	2.38	0.53
1:A:27:LEU:HD23	1:A:89:MET:CE	2.38	0.53
1:B:1116:LEU:C	1:B:1116:LEU:HD13	2.29	0.53
1:B:1005:ASP:OD2	1:B:1008:PHE:HB2	2.08	0.53
1:B:1097:LEU:HD23	1:B:1097:LEU:C	2.29	0.53
1:B:1098:SER:HB3	1:B:1159:TYR:HB2	1.89	0.53
1:B:1310:SER:O	1:B:1314:MET:HB2	2.08	0.53
1:B:1210:ILE:N	1:B:1211:PRO:HD2	2.24	0.53
1:B:1337:ALA:HB3	1:B:1344:MET:HE1	1.91	0.53
1:A:6:LYS:HE2	1:A:356:MET:CE	2.38	0.53
1:B:1049:PRO:HG2	1:B:1204:TRP:CD2	2.44	0.52
1:B:1199:ILE:C	1:B:1237[C]:VAL:HG13	2.29	0.52
1:A:179:ASN:O	1:A:186:HIS:HE1	1.92	0.52
1:A:48:VAL:HA	1:A:49:PRO:C	2.30	0.52
1:B:1328:LEU:O	1:B:1331:ILE:HB	2.09	0.52
1:A:49:PRO:HG2	1:A:204:TRP:CE2	2.44	0.51
1:A:127:LYS:HD3	1:A:127:LYS:N	2.25	0.51
1:A:230:SER:O	1:A:273:THR:HA	2.09	0.51
1:B:1305:LEU:HD23	1:B:1306:LYS:N	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:N	1:A:54:ILE:HD13	2.25	0.51
1:B:1091:ALA:O	1:B:1093:PRO:HD3	2.10	0.51
1:B:1100:GLU:HB2	1:B:1101:GLN:HE21	1.75	0.51
1:A:93:PRO:HA	1:A:159:TYR:CE1	2.45	0.51
1:B:1224:ILE:HG22	1:B:1294:ASP:HB3	1.93	0.51
1:B:1346:ILE:HG22	1:B:1347:CYS:N	2.25	0.51
1:B:1071:PHE:CZ	1:B:1122:GLN:NE2	2.79	0.50
1:B:1068:ILE:HD13	1:B:1090:ALA:HB3	1.92	0.50
1:B:1198:VAL:CG1	1:B:1237[B]:VAL:HG13	2.41	0.50
1:A:179:ASN:CB	1:A:182:ASN:HD21	2.25	0.50
1:A:232:ARG:HB2	1:A:234:TRP:CE2	2.47	0.50
1:B:1285:TRP:CD1	1:B:1289:ALA:HB2	2.46	0.50
1:A:13:ARG:N	1:A:84:GLU:OE1	2.29	0.50
1:A:27:LEU:HD23	1:A:89:MET:HE2	1.93	0.50
1:B:1010:GLN:HG3	1:B:1034:MET:O	2.12	0.50
1:B:1224:ILE:CG2	1:B:1294:ASP:HB3	2.42	0.50
1:B:1278:VAL:O	1:B:1282:VAL:HG23	2.12	0.50
1:B:1200:GLY:HA2	1:B:1331:ILE:HG12	1.94	0.49
1:B:1224:ILE:HA	1:B:1292:LEU:O	2.12	0.49
1:A:218:GLU:CG	1:A:339:ILE:HD11	2.40	0.49
1:B:1336:LYS:O	1:B:1337:ALA:C	2.50	0.49
1:A:337:ALA:HB1	1:A:342:GLU:HG3	1.94	0.49
1:B:1234:TRP:CD1	1:B:1277:ILE:HD11	2.48	0.49
1:B:1305:LEU:HD23	1:B:1305:LEU:C	2.32	0.49
1:A:226:ARG:HG2	1:A:226:ARG:HH11	1.78	0.49
1:A:336:LYS:O	1:A:340:ARG:HG3	2.12	0.49
1:B:1222:GLN:HG3	1:B:1291:TRP:HA	1.93	0.49
1:B:1313:ASN:HA	1:B:1318:TRP:O	2.12	0.49
1:B:1228:PRO:HG3	1:B:1293:LEU:HD11	1.95	0.49
1:B:1280:LYS:HD2	1:B:1284:LEU:CD1	2.43	0.49
1:B:1027:LEU:HD23	1:B:1089:MET:HE1	1.94	0.49
1:B:1327:THR:O	1:B:1331:ILE:HG13	2.12	0.49
1:B:1007:ASN:OD1	1:B:1007:ASN:N	2.46	0.48
1:B:1222:GLN:NE2	1:B:1292:LEU:HG	2.28	0.48
1:A:346:ILE:HD12	1:A:346:ILE:HA	1.65	0.48
1:B:1275:GLU:O	1:B:1279:ASP:OD2	2.30	0.48
1:A:14:VAL:O	1:A:38:VAL:HA	2.14	0.48
1:B:1126:ILE:O	1:B:1188:VAL:HG22	2.13	0.48
1:B:1198:VAL:HG12	1:B:1237[C]:VAL:HG12	1.95	0.48
1:B:1070:ASP:OD1	1:B:1073:LYS:HG3	2.14	0.48
1:B:1280:LYS:O	1:B:1284:LEU:HD13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1294:ASP:OD1	1:B:1296:GLU:HG3	2.13	0.48
1:B:1272:LYS:HB3	1:B:1276:PHE:CD2	2.49	0.48
1:A:186:HIS:HD2	1:A:188:VAL:N	1.99	0.47
1:A:215:ARG:HD3	1:A:215:ARG:C	2.34	0.47
1:A:182:ASN:HD22	1:A:186:HIS:HE1	1.60	0.47
1:B:1272:LYS:CG	1:B:1324:LEU:HD23	2.44	0.47
1:B:1057:LEU:HA	1:B:1060:LEU:CD1	2.38	0.47
1:B:1297:ASN:C	1:B:1299:PRO:HD3	2.34	0.47
1:A:266:PRO:HB2	1:A:270:ASP:HB2	1.96	0.47
1:B:1127:LYS:HE2	1:B:1252:TYR:CZ	2.50	0.47
1:B:1329:SER:O	1:B:1333:LYS:HG3	2.14	0.47
1:A:104:LYS:HE2	1:A:108:THR:HG1	1.77	0.47
1:A:257:LYS:HD3	1:A:258:PHE:CZ	2.49	0.47
1:B:1097:LEU:O	1:B:1100:GLU:N	2.46	0.47
1:B:1015:PHE:CZ	1:B:1078:ILE:HG13	2.50	0.46
1:A:28:SER:O	1:A:32:THR:HG23	2.16	0.46
1:A:132:ILE:N	1:A:132:ILE:HD12	2.30	0.46
1:A:6:LYS:NZ	1:A:356:MET:HE3	2.30	0.46
1:A:176:SER:HB3	1:B:1099:TYR:CE2	2.50	0.46
1:B:1054:ILE:CD1	1:B:1204:TRP:CZ3	2.98	0.46
1:B:1239:GLU:HB2	1:B:1240:PRO:HD3	1.96	0.46
1:B:1257:LYS:H	1:B:1257:LYS:HG2	1.31	0.46
1:A:75:ARG:HD3	1:A:122:GLN:OE1	2.15	0.46
1:B:1132:ILE:HD12	1:B:1132:ILE:N	2.31	0.46
1:B:1225:ILE:CG1	1:B:1291:TRP:CE3	2.98	0.46
1:B:1343:ASP:OD2	1:B:1346:ILE:HD12	2.15	0.46
1:B:1321:ARG:HG3	1:B:1355:TYR:CE1	2.50	0.46
1:B:1326:GLU:HG2	1:B:1330:ARG:HD2	1.98	0.46
1:A:321:ARG:HD3	1:A:355:TYR:CE2	2.50	0.46
1:B:1096:ARG:NH1	1:B:1207:ASP:HB2	2.31	0.46
1:A:215:ARG:NH2	1:A:219:ASN:ND2	2.56	0.46
1:B:1228:PRO:HD2	1:B:1298:HIS:HB3	1.98	0.46
1:B:1091:ALA:CB	2:B:1400:APR:HR'4	2.43	0.45
1:B:1152:PRO:HA	4:B:2060:HOH:O	2.15	0.45
1:B:1268:ASP:CG	1:B:1306:LYS:HZ2	2.20	0.45
1:B:1209:LEU:HD11	1:B:1213:ILE:CD1	2.45	0.45
1:B:1043:LEU:HD23	1:B:1066:GLY:O	2.15	0.45
1:B:1074:LEU:HD12	1:B:1074:LEU:C	2.36	0.45
1:B:1120:VAL:HG22	1:B:1126:ILE:HD13	1.98	0.45
1:B:1216:SER:OG	1:B:1223:VAL:HG22	2.17	0.45
1:B:1027:LEU:HD23	1:B:1089:MET:HE2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:NZ	1:A:356:MET:CE	2.79	0.45
1:B:1335:HIS:O	1:B:1338:TRP:HB3	2.16	0.45
1:A:232:ARG:HB2	1:A:234:TRP:CZ2	2.52	0.45
1:A:237:VAL:O	1:A:240:PRO:HD2	2.17	0.45
1:B:1198:VAL:HG11	1:B:1237[B]:VAL:HG13	1.98	0.45
1:B:1234:TRP:CD1	1:B:1277:ILE:CD1	3.00	0.45
1:A:13:ARG:NH2	1:A:82:LYS:O	2.49	0.45
1:A:47:THR:O	1:A:50:SER:HB3	2.17	0.45
1:A:267:ARG:HB2	1:A:269:GLU:CD	2.37	0.45
1:B:1313:ASN:O	1:B:1317:GLY:HA2	2.17	0.45
1:A:45:ALA:HB1	1:A:46:PRO:HD2	1.99	0.44
1:B:1051:LEU:HD13	1:B:1202:GLY:CA	2.42	0.44
1:B:1225:ILE:HB	1:B:1291:TRP:CZ3	2.53	0.44
1:A:175:ASN:HB3	1:B:1156:TYR:CZ	2.53	0.44
1:B:1013:ARG:NE	1:B:1082:LYS:O	2.46	0.44
1:B:1094:LEU:N	1:B:1094:LEU:CD1	2.81	0.44
1:B:1280:LYS:HZ2	1:B:1283:THR:HG21	1.79	0.44
1:B:1223:VAL:O	1:B:1292:LEU:N	2.30	0.44
1:A:136:LYS:NZ	3:A:401:CXY:H5B	2.33	0.44
1:B:1022:PHE:HZ	1:B:1237[B]:VAL:HG21	1.78	0.44
1:B:1095:VAL:HG13	1:B:1157:ASP:OD2	2.18	0.44
1:B:1110:VAL:O	1:B:1114:VAL:HG23	2.17	0.44
1:A:151:GLU:HB3	1:A:152:PRO:HD2	2.00	0.44
1:B:1050:SER:OG	1:B:1053:GLU:HG2	2.17	0.44
1:A:6:LYS:CE	1:A:356:MET:HE1	2.48	0.43
1:B:1013:ARG:HB3	1:B:1083:PRO:HA	1.99	0.43
1:B:1179:ASN:HB3	1:B:1182:ASN:OD1	2.18	0.43
1:A:335:HIS:O	1:A:338:TRP:HB3	2.18	0.43
1:B:1079:ALA:HB2	1:B:1123:VAL:HG22	1.99	0.43
1:B:1227:ASN:HD21	1:B:1230:SER:HB2	1.83	0.43
1:B:1346:ILE:O	1:B:1349:LYS:HB2	2.18	0.43
1:A:45:ALA:HA	1:A:46:PRO:HD3	1.90	0.43
1:B:1032:THR:O	1:B:1033:GLU:C	2.55	0.43
1:B:1211:PRO:HB2	1:B:1215:ARG:HH12	1.77	0.43
1:B:1226:ARG:O	1:B:1298:HIS:ND1	2.50	0.43
1:B:1038:VAL:CG1	1:B:1039:LYS:N	2.82	0.43
1:B:1298:HIS:HA	1:B:1299:PRO:HD2	1.88	0.43
1:B:1251:LEU:O	1:B:1255:GLY:HA2	2.18	0.43
1:B:1022:PHE:HE1	1:B:1026:TRP:HE1	1.66	0.43
1:B:1250:ARG:HD3	1:B:1250:ARG:HA	1.69	0.43
1:B:1258:PHE:N	1:B:1258:PHE:CD1	2.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1276:PHE:HA	1:B:1279:ASP:OD2	2.19	0.43
1:B:1209:LEU:HD12	1:B:1209:LEU:C	2.39	0.43
1:A:50:SER:OG	1:A:53:GLU:HG2	2.19	0.42
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.71	0.42
1:B:1280:LYS:HD2	1:B:1284:LEU:HD11	1.99	0.42
1:A:5:ASP:O	1:A:8:PHE:HB3	2.19	0.42
1:A:136:LYS:HZ3	3:A:401:CXY:H5B	1.83	0.42
1:A:65:ILE:HD13	1:A:65:ILE:HA	1.71	0.42
1:A:23:LYS:HG3	2:A:400:APR:H5R1	2.02	0.42
1:A:152:PRO:HB3	1:B:1152:PRO:HB3	2.01	0.42
1:A:332:VAL:HG12	1:A:333:LYS:N	2.35	0.42
1:B:1042:ALA:O	1:B:1065:ILE:HA	2.19	0.42
1:B:1133:THR:HG21	1:B:1167:GLU:HG2	2.00	0.42
1:B:1048:VAL:HA	1:B:1049:PRO:HA	1.94	0.41
1:B:1227:ASN:ND2	1:B:1230:SER:HB2	2.35	0.41
1:B:1303:HIS:HD2	4:B:2510:HOH:O	2.02	0.41
1:B:1256:ALA:O	1:B:1257:LYS:C	2.58	0.41
1:B:1217:PHE:CD2	1:B:1285:TRP:HB2	2.56	0.41
1:B:1216:SER:HB3	1:B:1223:VAL:HG22	2.02	0.41
1:A:6:LYS:HZ1	1:A:356:MET:HE3	1.86	0.41
1:A:23:LYS:HE2	2:A:400:APR:O4D	2.21	0.41
1:A:27:LEU:CD2	1:A:89:MET:CE	2.98	0.41
1:A:98:SER:HB2	1:A:158:PRO:HB2	2.02	0.41
1:A:176:SER:HB3	1:B:1099:TYR:HE2	1.85	0.41
1:B:1054:ILE:HD13	1:B:1204:TRP:CZ3	2.56	0.41
1:B:1280:LYS:CD	1:B:1284:LEU:CD1	3.00	0.40
1:A:321:ARG:HB2	1:A:355:TYR:CE1	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:SER:OG	1:B:1220:ASN:ND2[6_655]	2.17	0.03

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	349/359 (97%)	335 (96%)	12 (3%)	2 (1%)	25	12
1	B	346/359 (96%)	322 (93%)	23 (7%)	1 (0%)	41	27
All	All	695/718 (97%)	657 (94%)	35 (5%)	3 (0%)	34	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	B	1098	SER
1	A	287	ASP

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	303/309 (98%)	277 (91%)	26 (9%)	10	3
1	B	304/309 (98%)	265 (87%)	39 (13%)	4	1
All	All	607/618 (98%)	542 (89%)	65 (11%)	6	1

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	A	73	LYS
1	A	75	ARG
1	A	80	GLU
1	A	82	LYS
1	A	92	GLN
1	A	127	LYS
1	A	143	TRP
1	A	182	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	LYS
1	A	215	ARG
1	A	222	GLN
1	A	226	ARG
1	A	280	LYS
1	A	287	ASP
1	A	288	ASP
1	A	292	LEU
1	A	321	ARG
1	A	326	GLU
1	A	339	ILE
1	A	340	ARG
1	A	346	ILE
1	A	350	ARG
1	A	353	SER
1	A	356	MET
1	A	357	SER
1	B	1003	SER
1	B	1007	ASN
1	B	1041	TYR
1	B	1050	SER
1	B	1056	ARG
1	B	1058	ASN
1	B	1060	LEU
1	B	1064	HIS
1	B	1068	ILE
1	B	1089	MET
1	B	1092	GLN
1	B	1096	ARG
1	B	1100	GLU
1	B	1127	LYS
1	B	1143	TRP
1	B	1182	ASN
1	B	1207	ASP
1	B	1216	SER
1	B	1220	ASN
1	B	1222	GLN
1	B	1224	ILE
1	B	1227	ASN
1	B	1231	ILE
1	B	1257	LYS
1	B	1268	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1280	LYS
1	B	1287	ASP
1	B	1292	LEU
1	B	1296	GLU
1	B	1306	LYS
1	B	1321	ARG
1	B	1329	SER
1	B	1344	MET
1	B	1346	ILE
1	B	1349	LYS
1	B	1350	ARG
1	B	1353	SER
1	B	1356	MET
1	B	1357	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	64	HIS
1	A	182	ASN
1	A	186	HIS
1	A	219	ASN
1	A	300	HIS
1	A	315	GLN
1	B	1010	GLN
1	B	1058	ASN
1	B	1101	GLN
1	B	1197	ASN
1	B	1219	ASN
1	B	1222	GLN
1	B	1236	HIS
1	B	1303	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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	APR	A	400	-	34,39,39	0.91	2 (5%)	40,60,60	1.26	3 (7%)
2	APR	B	1400	-	34,39,39	0.87	1 (2%)	40,60,60	1.31	5 (12%)
3	CXY	A	401	-	33,36,36	1.27	4 (12%)	50,55,55	1.48	7 (14%)

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
2	APR	A	400	-	-	5/18/54/54	0/4/4/4
2	APR	B	1400	-	-	6/18/54/54	0/4/4/4
3	CXY	A	401	-	-	4/21/54/54	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	CXY	C4-N4	-4.55	1.23	1.33
3	A	401	CXY	C4-N3	3.16	1.40	1.34
2	B	1400	APR	O4D-C1D	-2.41	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	APR	O4D-C1D	-2.37	1.40	1.43
3	A	401	CXY	O5'-C1'	2.26	1.46	1.41
2	A	400	APR	O1D-C1D	2.04	1.46	1.39
3	A	401	CXY	O3D-C3D	2.02	1.47	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	CXY	C5-C4-N3	-4.53	113.63	121.33
2	A	400	APR	C5-C6-N6	4.34	126.95	120.35
3	A	401	CXY	C4-N3-C2	4.08	126.84	120.25
3	A	401	CXY	O3A-PB-O1'	3.50	109.54	102.48
3	A	401	CXY	C5-C4-N4	3.43	125.97	120.57
2	B	1400	APR	C5-C6-N1	-2.64	114.38	120.35
2	B	1400	APR	O1D-C1D-O4D	-2.55	107.87	111.13
3	A	401	CXY	N1-C2-N3	-2.53	114.20	118.81
2	B	1400	APR	N6-C6-N1	2.44	123.63	118.57
2	A	400	APR	O4'-C1'-C2'	-2.39	103.44	106.93
2	B	1400	APR	C2'-C3'-C4'	-2.37	98.03	102.64
3	A	401	CXY	C6-C5-C4	2.35	121.30	117.50
3	A	401	CXY	C2D-C3D-C4D	-2.27	98.23	102.64
2	B	1400	APR	O4'-C1'-C2'	-2.08	103.88	106.93
2	A	400	APR	O2D-C2D-C3D	-2.08	105.11	111.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	APR	C5D-O5D-PB-O1B
2	A	400	APR	C5D-O5D-PB-O2B
2	B	1400	APR	C5D-O5D-PB-O2B
2	B	1400	APR	O4D-C4D-C5D-O5D
3	A	401	CXY	C1'-O1'-PB-O3A
2	B	1400	APR	C3D-C4D-C5D-O5D
2	B	1400	APR	C5D-O5D-PB-O3A
2	B	1400	APR	C5D-O5D-PB-O1B
3	A	401	CXY	PA-O3A-PB-O2B
3	A	401	CXY	O4D-C4D-C5D-O5D
2	A	400	APR	C5D-O5D-PB-O3A
2	A	400	APR	O4'-C4'-C5'-O5'
2	A	400	APR	PA-O3A-PB-O1B
3	A	401	CXY	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

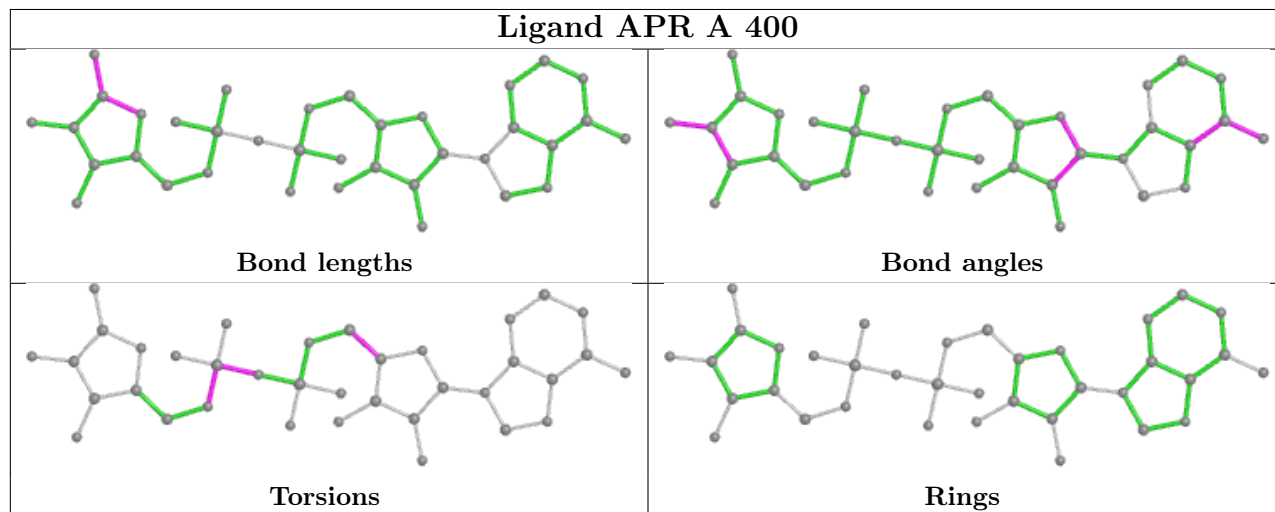
Mol	Chain	Res	Type	Atoms
2	B	1400	APR	O4'-C4'-C5'-O5'

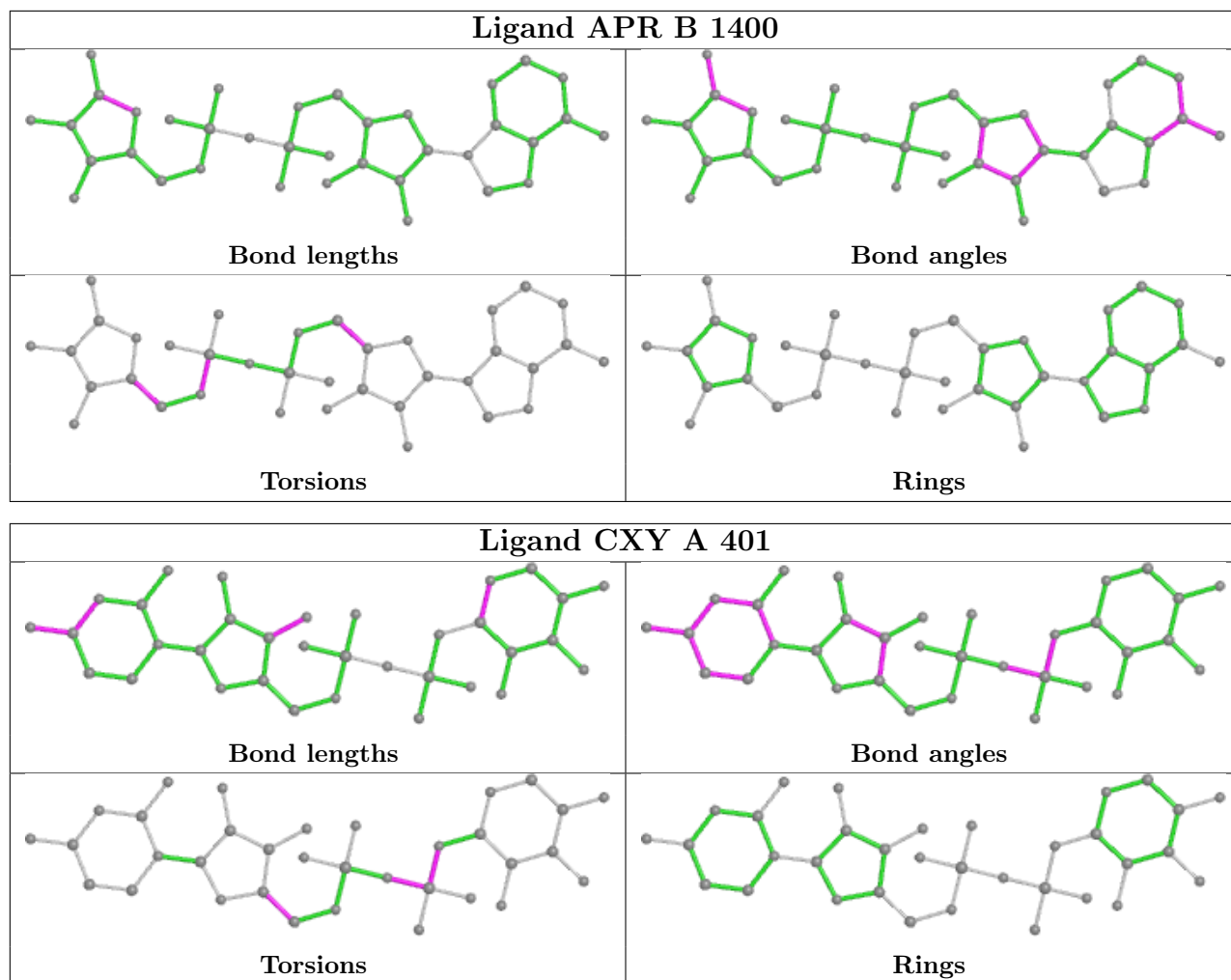
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	APR	2	0
2	B	1400	APR	4	0
3	A	401	CXY	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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	352/359 (98%)	-0.43	0 100 100	15, 28, 62, 76	0
1	B	350/359 (97%)	-0.05	10 (2%) 51 46	17, 39, 72, 96	0
All	All	702/718 (97%)	-0.24	10 (1%) 75 72	15, 34, 67, 96	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1097	LEU	3.3
1	B	1181	ALA	3.1
1	B	1010	GLN	2.8
1	B	1008	PHE	2.5
1	B	1292	LEU	2.4
1	B	1223	VAL	2.4
1	B	1099	TYR	2.2
1	B	1198	VAL	2.1
1	B	1089	MET	2.1
1	B	1130	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

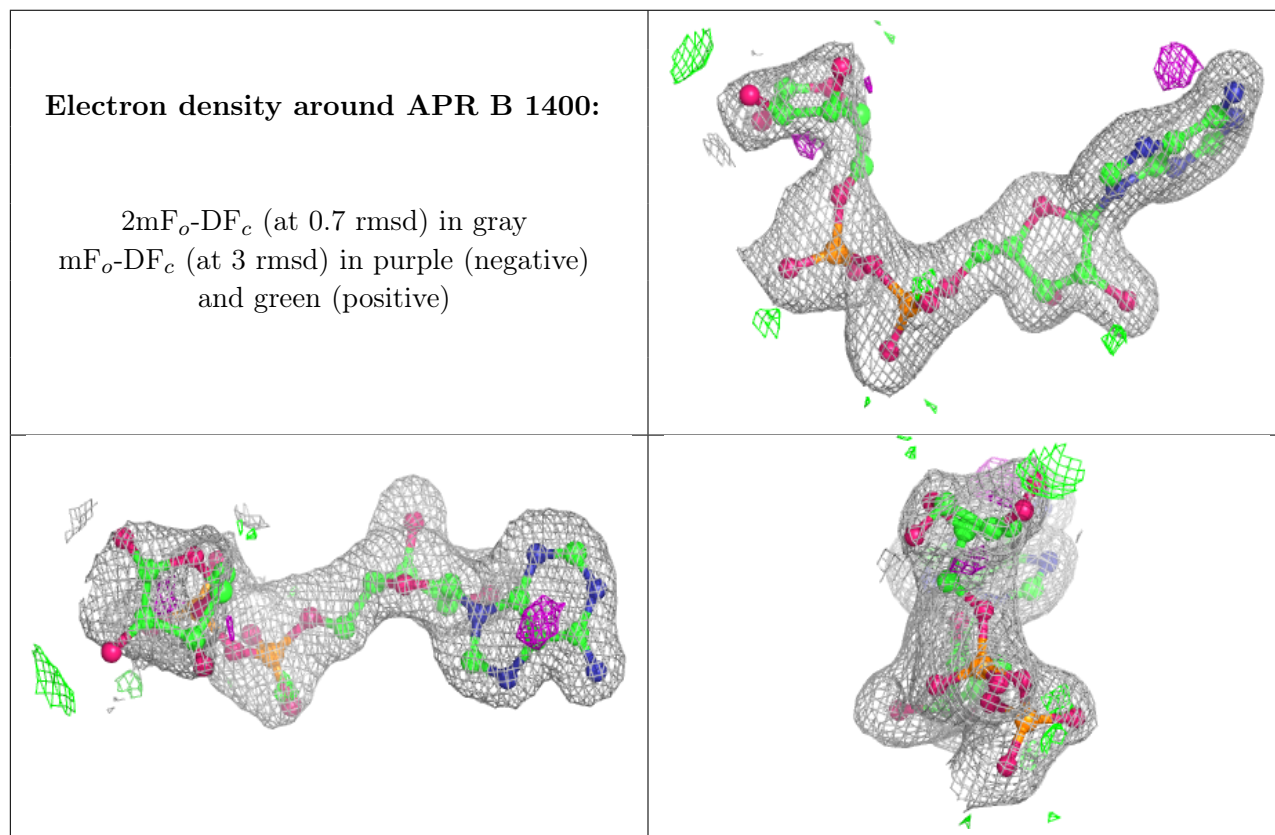
There are no monosaccharides in this entry.

6.4 Ligands [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

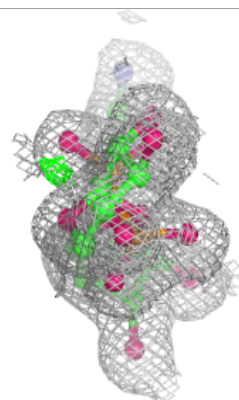
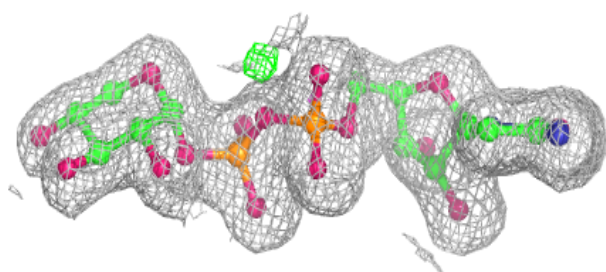
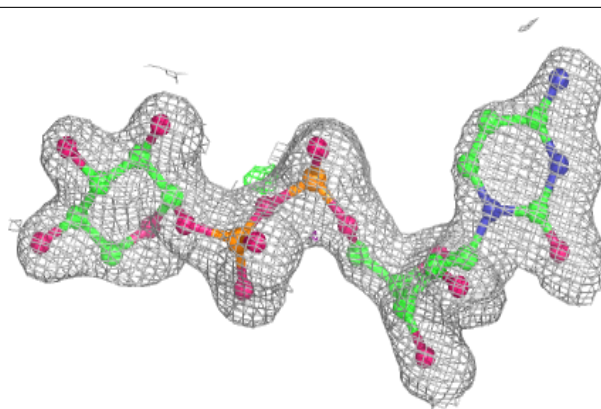
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	APR	B	1400	36/36	0.94	0.10	17,33,100,100	0
3	CXY	A	401	34/34	0.97	0.08	17,26,35,41	0
2	APR	A	400	36/36	0.98	0.09	11,23,40,80	0

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.

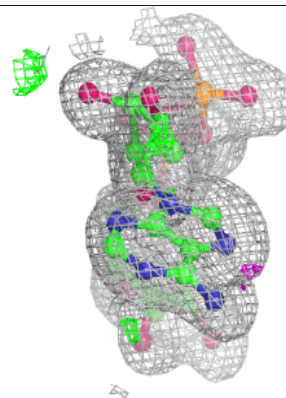
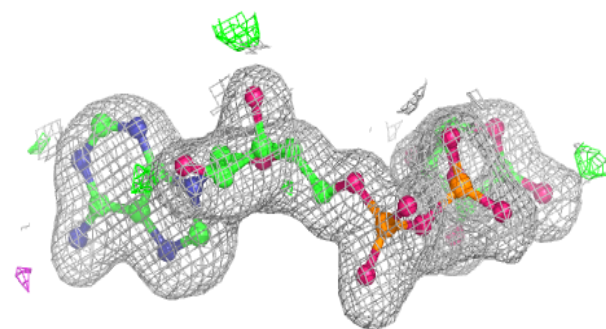
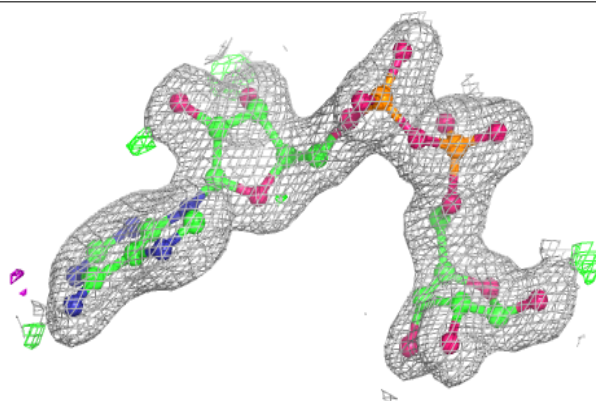


Electron density around CXY A 401:

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

**Electron density around APR A 400:**

$2mF_o-DF_c$ (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.