



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:47 PM UTC

PDB ID : 1WVG / pdb_00001wvg
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

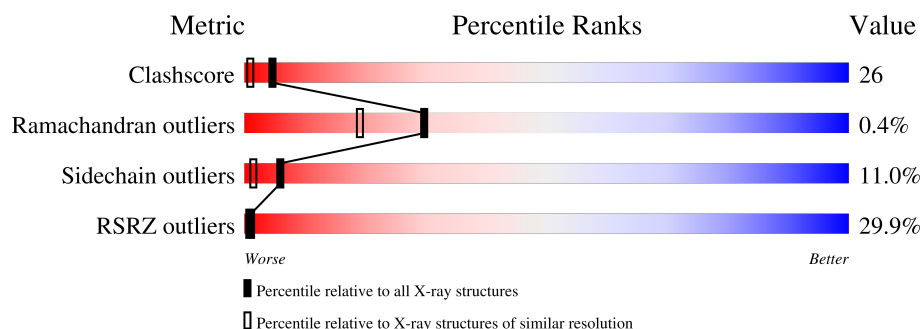
1 Overall quality at a glance

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	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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	
1	B	359	

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.

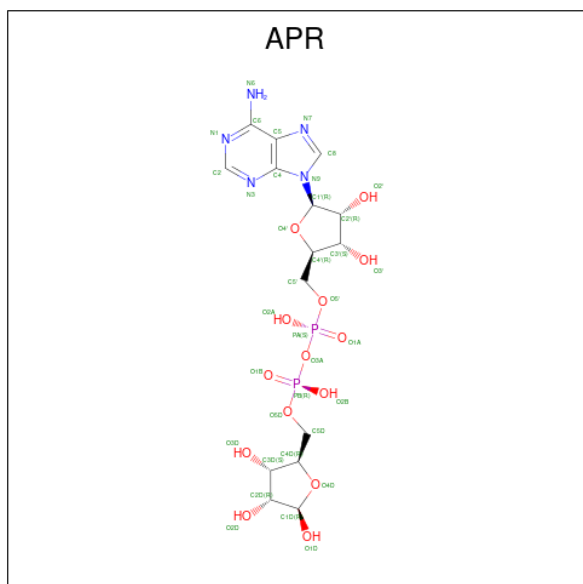
- Molecule 1 is a protein called CDP-glucose 4,6-dehydratase.

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

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 (CCD ID: APR) (formula: C₁₅H₂₃N₅O₁₄P₂).



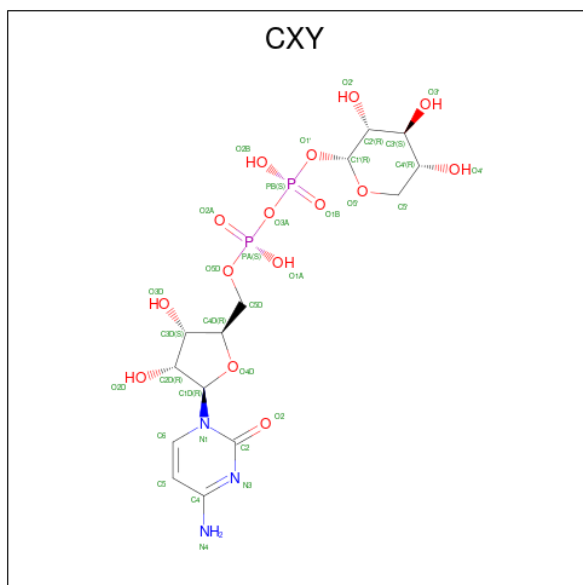
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

Continued on next page...

Continued from previous page...

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

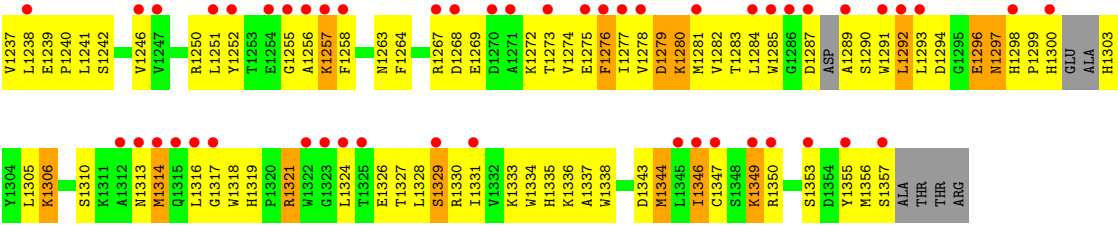
- Molecule 3 is CYTIDINE-5'-DIPHOSPHO-BETA-D-XYLOSE (CCD ID: CXY) (formula: $C_{14}H_{23}N_3O_{15}P_2$).



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

- 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		



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 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-1.80) 93.8 (50.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.82 (at 1.81Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.201 , 0.270 0.267 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 118.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6098	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

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

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	1.07	1/2921 (0.0%)	1.62	28/3961 (0.7%)
1	B	1.06	0/2919	1.65	36/3956 (0.9%)
All	All	1.06	1/5840 (0.0%)	1.64	64/7917 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	LYS	C-O	-5.64	1.21	1.23

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASN	CA-CB-CG	-9.91	102.69	112.60
1	A	188	VAL	N-CA-C	8.59	120.65	108.36
1	B	1227	ASN	CA-C-N	8.29	128.77	119.32
1	B	1227	ASN	C-N-CA	8.29	128.77	119.32
1	A	48	VAL	N-CA-CB	8.25	122.76	111.21
1	A	315	GLN	N-CA-C	8.20	120.30	111.36
1	A	314	MET	CB-CA-C	-8.13	98.05	110.90
1	A	257	LYS	N-CA-C	7.92	119.91	111.28
1	B	1287	ASP	CA-CB-CG	7.89	120.49	112.60
1	A	209	LEU	N-CA-C	7.51	119.16	110.97
1	A	9	TRP	N-CA-C	7.40	119.42	111.36
1	A	300	HIS	N-CA-C	7.34	121.31	110.30
1	B	1070	ASP	N-CA-CB	7.26	122.59	110.53
1	B	1125	ASN	N-CA-C	7.07	121.85	113.23
1	A	288	ASP	CA-CB-CG	6.86	119.46	112.60
1	B	1038	VAL	N-CA-C	6.85	119.59	108.97
1	B	1034	MET	N-CA-C	6.81	121.44	113.20
1	A	222	GLN	N-CA-CB	6.66	121.26	110.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1319	HIS	CA-CB-CG	-6.61	107.19	113.80
1	A	227	ASN	CA-C-N	6.59	127.11	119.47
1	A	227	ASN	C-N-CA	6.59	127.11	119.47
1	B	1236	HIS	CA-CB-CG	-6.49	107.31	113.80
1	B	1145	TRP	N-CA-C	6.44	119.58	110.50
1	B	1223	VAL	N-CA-C	6.38	117.76	108.58
1	A	164	GLY	N-CA-C	-6.30	105.19	112.50
1	A	92	GLN	N-CA-C	-6.26	95.98	109.81
1	A	94	LEU	N-CA-C	6.19	119.92	109.76
1	B	1316	LEU	N-CA-C	-6.14	105.58	114.12
1	A	233	PRO	N-CA-CB	6.09	107.11	102.36
1	A	266	PRO	CB-CA-C	-6.06	101.78	110.75
1	B	1058	ASN	N-CA-CB	5.97	121.18	110.32
1	B	1092	GLN	N-CA-C	-5.83	98.04	108.47
1	B	1047	THR	N-CA-C	5.81	117.05	108.86
1	B	1071	PHE	CA-CB-CG	-5.75	108.05	113.80
1	A	135	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	5	ASP	CA-C-N	5.67	128.15	120.38
1	A	5	ASP	C-N-CA	5.67	128.15	120.38
1	B	1314	MET	N-CA-C	5.67	117.27	111.14
1	B	1014	VAL	N-CA-C	5.62	115.94	107.80
1	B	1138	TYR	N-CA-C	5.55	118.33	110.50
1	B	1263	ASN	CA-CB-CG	5.53	118.13	112.60
1	B	1276	PHE	CA-C-O	5.52	126.61	120.82
1	A	234	TRP	N-CA-C	5.49	118.31	110.24
1	B	1300	HIS	CA-CB-CG	-5.44	108.36	113.80
1	B	1177	PHE	N-CA-C	5.39	120.51	113.88
1	B	1279	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	1049	PRO	N-CA-CB	5.38	108.51	102.60
1	A	38	VAL	N-CA-C	5.34	116.67	108.71
1	A	103	ILE	N-CA-C	5.30	115.51	110.42
1	B	1273	THR	N-CA-CB	5.27	118.42	110.42
1	B	1297	ASN	CA-CB-CG	-5.20	107.40	112.60
1	B	1264	PHE	CA-CB-CG	-5.16	108.64	113.80
1	B	1032	THR	N-CA-C	-5.15	105.36	111.69
1	B	1065	ILE	N-CA-CB	5.14	116.86	111.00
1	A	290	SER	CA-C-N	-5.13	114.20	122.82
1	A	290	SER	C-N-CA	-5.13	114.20	122.82
1	B	1005	ASP	N-CA-C	5.11	116.64	108.41
1	A	84	GLU	N-CA-C	-5.08	107.47	113.97
1	A	211	PRO	N-CA-CB	5.04	108.88	103.33
1	B	1084	GLU	N-CA-C	-5.04	107.81	114.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1233	PRO	N-CA-CB	5.02	105.91	102.35
1	B	1290	SER	O-C-N	-5.00	118.28	123.29
1	B	1290	SER	CA-C-N	-5.00	113.67	121.87
1	B	1290	SER	C-N-CA	-5.00	113.67	121.87

There are no chirality outliers.

There are no planarity outliers.

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	2839	0	2756	97	1
1	B	2827	0	2753	203	1
2	A	36	0	21	2	0
2	B	36	0	21	4	0
3	A	34	0	19	1	0
4	A	214	0	0	7	0
4	B	112	0	0	2	0
All	All	6098	0	5570	295	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 26.

All (295) 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	1.27	0.95
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:30:TRP:HE1	1:A:356:MET:CE	1.96	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:A:30:TRP:NE1	1:A:356:MET:HE2	2.00	0.75
1:B:1337:ALA:HB3	1:B:1344:MET:HE1	1.67	0.74
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:6:LYS:NZ	1:A:356:MET:HE3	2.02	0.73
1:A:104:LYS:HE2	1:A:108:THR:OG1	1.89	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:B:1205:ALA:C	1:B:1215:ARG:HH22	1.99	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HZ1	1:A:356:MET:HE3	1.64	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:1116:LEU:C	1:B:1116:LEU:HD13	2.29	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:1097:LEU:HD23	1:B:1097:LEU:C	2.29	0.57
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:1199:ILE:C	1:B:1237[C]:VAL:HG13	2.29	0.57
1:B:1097:LEU:CD2	1:B:1101:GLN:HB2	2.33	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
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:B:1210:ILE:HD12	1:B:1281:MET:HE2	1.88	0.56
1:A:321:ARG:HD3	1:A:355:TYR:CZ	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:48:VAL:HA	1:A:49:PRO:C	2.30	0.55
1:B:1305:LEU:C	1:B:1305:LEU:HD23	2.32	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:1336:LYS:O	1:B:1337:ALA:C	2.50	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:6:LYS:HE2	1:A:356:MET:CE	2.38	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:1005:ASP:OD2	1:B:1008:PHE:HB2	2.08	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:A:215:ARG:HD3	1:A:215:ARG:C	2.34	0.52
1:B:1049:PRO:HG2	1:B:1204:TRP:CD2	2.44	0.52
1:A:179:ASN:O	1:A:186:HIS:HE1	1.92	0.52
1:A:6:LYS:CE	1:A:356:MET:HE3	2.39	0.52
1:B:1297:ASN:C	1:B:1299:PRO:HD3	2.34	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:267:ARG:HB2	1:A:269:GLU:CD	2.37	0.49
1:A:337:ALA:HB1	1:A:342:GLU:HG3	1.94	0.49
1:B:1074:LEU:HD12	1:B:1074:LEU:C	2.36	0.49
1:B:1234:TRP:CD1	1:B:1277:ILE:HD11	2.48	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:1032:THR:O	1:B:1033:GLU:C	2.55	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:HIS:HD2	1:A:188:VAL:N	1.99	0.47
1:A:182:ASN:HD22	1:A:186:HIS:HE1	1.60	0.47
1:B:1280:LYS:HZ3	1:B:1283:THR:HG21	1.79	0.47
1:B:1209:LEU:HD12	1:B:1209:LEU:C	2.39	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: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:27:LEU:HD23	1:A:89:MET:HE2	1.95	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: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:1256:ALA:O	1:B:1257:LYS:C	2.58	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: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: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
1:B:1180:PRO:C	1:B:1182:ASN:H	2.24	0.45
1:B:1335:HIS:O	1:B:1338:TRP:HB3	2.16	0.45
1:A:44:ASP:O	1:A:45:ALA:C	2.60	0.45
1:A:232:ARG:HB2	1:A:234:TRP:CZ2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1223:VAL:O	1:B:1292:LEU:N	2.30	0.44
1:B:1215:ARG:O	1:B:1216:SER:C	2.59	0.44
1:A:136:LYS:NZ	3:A:401:CTX: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:B:1334:TRP:O	1:B:1344:MET:HE2	2.18	0.44
1:A:151:GLU:HB3	1:A:152:PRO:HD2	2.00	0.44
1:A:179:ASN:O	1:A:180:PRO:C	2.61	0.44
1:B:1050:SER:OG	1:B:1053:GLU:HG2	2.17	0.44
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:A:161:ASN:CG	1:B:1172:ALA:HB2	2.44	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:A:310:SER:HB3	1:A:314:MET:HE2	1.99	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:1092:GLN:CD	1:B:1097:LEU:HD22	2.43	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
1:B:1276:PHE:HA	1:B:1279:ASP:OD2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:SER:OG	1:A:53:GLU:HG2	2.19	0.42
1:B:1007:ASN:HA	1:B:1010:GLN:CD	2.44	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:276:PHE:CD2	1:A:276:PHE:C	2.97	0.42
1:A:5:ASP:O	1:A:8:PHE:HB3	2.19	0.42
1:B:1276:PHE:CD2	1:B:1276:PHE:C	2.97	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:269:GLU:CD	1:A:269:GLU:H	2.28	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:1279:ASP:O	1:B:1280:LYS:C	2.63	0.41
1:B:1180:PRO:C	1:B:1182:ASN:N	2.79	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:1011:GLY:C	1:B:1037:ILE:HD12	2.45	0.41
1:B:1212:ASP:O	1:B:1213:ILE:C	2.63	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: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:1047:THR:C	1:B:1048:VAL:HG23	2.45	0.41
1:B:1054:ILE:HD13	1:B:1204:TRP:CZ3	2.56	0.41
1:B:1100:GLU:C	1:B:1101:GLN:NE2	2.79	0.41
1:B:1334:TRP:CE3	1:B:1334:TRP:C	2.98	0.41
1:B:1041:TYR:CD2	1:B:1041:TYR:C	2.99	0.40
1:B:1051:LEU:O	1:B:1052:PHE:C	2.61	0.40
1:B:1210:ILE:O	1:B:1211:PRO:C	2.63	0.40
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
1:A:178:PHE:C	1:A:186:HIS:CE1	3.00	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%)	21	11
1	B	346/359 (96%)	322 (93%)	23 (7%)	1 (0%)	36	25
All	All	695/718 (97%)	657 (94%)	35 (5%)	3 (0%)	30	19

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%)	264 (87%)	40 (13%)	4	1
All	All	607/618 (98%)	541 (89%)	66 (11%)	6	1

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	54	ILE
1	A	73	LYS
1	A	75	ARG
1	A	80	GLU
1	A	82	LYS
1	A	84	GLU
1	A	92	GLN
1	A	127	LYS
1	A	182	ASN
1	A	206	LYS
1	A	222	GLN
1	A	226	ARG
1	A	277	ILE
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	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	1060	LEU
1	B	1065	ILE
1	B	1068	ILE
1	B	1089	MET
1	B	1092	GLN
1	B	1096	ARG
1	B	1100	GLU
1	B	1120	VAL
1	B	1127	LYS
1	B	1182	ASN
1	B	1207	ASP
1	B	1216	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1220	ASN
1	B	1222	GLN
1	B	1224	ILE
1	B	1226	ARG
1	B	1227	ASN
1	B	1231	ILE
1	B	1232	ARG
1	B	1257	LYS
1	B	1268	ASP
1	B	1274	VAL
1	B	1280	LYS
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 (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	150	ASN
1	A	182	ASN
1	A	186	HIS
1	A	197	ASN
1	A	219	ASN
1	A	227	ASN
1	A	313	ASN
1	B	1010	GLN
1	B	1058	ASN
1	B	1101	GLN
1	B	1131	ASN
1	B	1220	ASN
1	B	1222	GLN
1	B	1227	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1236	HIS
1	B	1303	HIS
1	B	1313	ASN
1	B	1315	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	39,39,39	1.03	4 (10%)	56,60,60	0.96	2 (3%)
3	CXY	A	401	-	35,36,36	1.67	5 (14%)	52,55,55	1.57	8 (15%)
2	APR	B	1400	-	39,39,39	1.26	4 (10%)	56,60,60	1.08	3 (5%)

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	-	-	4/22/54/54	0/4/4/4
3	CXY	A	401	-	-	5/21/54/54	0/3/3/3
2	APR	B	1400	-	-	6/22/54/54	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	CXY	PA-O3A	5.11	1.65	1.59
3	A	401	CXY	C4-N4	-4.47	1.23	1.33
2	B	1400	APR	PA-O3A	-4.29	1.54	1.59
3	A	401	CXY	PB-O3A	-4.18	1.55	1.59
2	B	1400	APR	PB-O3A	3.55	1.63	1.59
2	A	400	APR	PB-O3A	3.36	1.63	1.59
3	A	401	CXY	C4-N3	3.21	1.40	1.34
2	B	1400	APR	C2-N3	-2.33	1.29	1.33
3	A	401	CXY	O5'-C1'	2.30	1.46	1.41
2	B	1400	APR	O4D-C1D	-2.28	1.40	1.43
2	A	400	APR	O4D-C1D	-2.24	1.40	1.43
2	A	400	APR	O1D-C1D	2.08	1.46	1.39
2	A	400	APR	C2-N3	-2.04	1.30	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	CXY	C5-C4-N3	-4.57	113.63	121.32
3	A	401	CXY	O3A-PB-O1B	-4.47	97.24	110.70
3	A	401	CXY	C4-N3-C2	4.18	126.84	120.26
3	A	401	CXY	O2B-PB-O3A	3.26	116.08	107.27
3	A	401	CXY	C5-C4-N4	3.05	125.97	120.63
3	A	401	CXY	N1-C2-N3	-2.65	114.20	118.80
2	B	1400	APR	O1D-C1D-O4D	-2.55	107.87	111.12
2	B	1400	APR	C2'-C3'-C4'	-2.37	98.03	102.61
2	B	1400	APR	N6-C6-N1	2.36	123.63	118.38
3	A	401	CXY	C6-C5-C4	2.30	121.30	117.53
3	A	401	CXY	C2D-C3D-C4D	-2.27	98.23	102.61
2	A	400	APR	O2D-C2D-C3D	-2.09	105.11	111.82
2	A	400	APR	O3A-PA-O1A	-2.02	104.63	110.70

There are no chirality outliers.

All (15) torsion outliers are listed below:

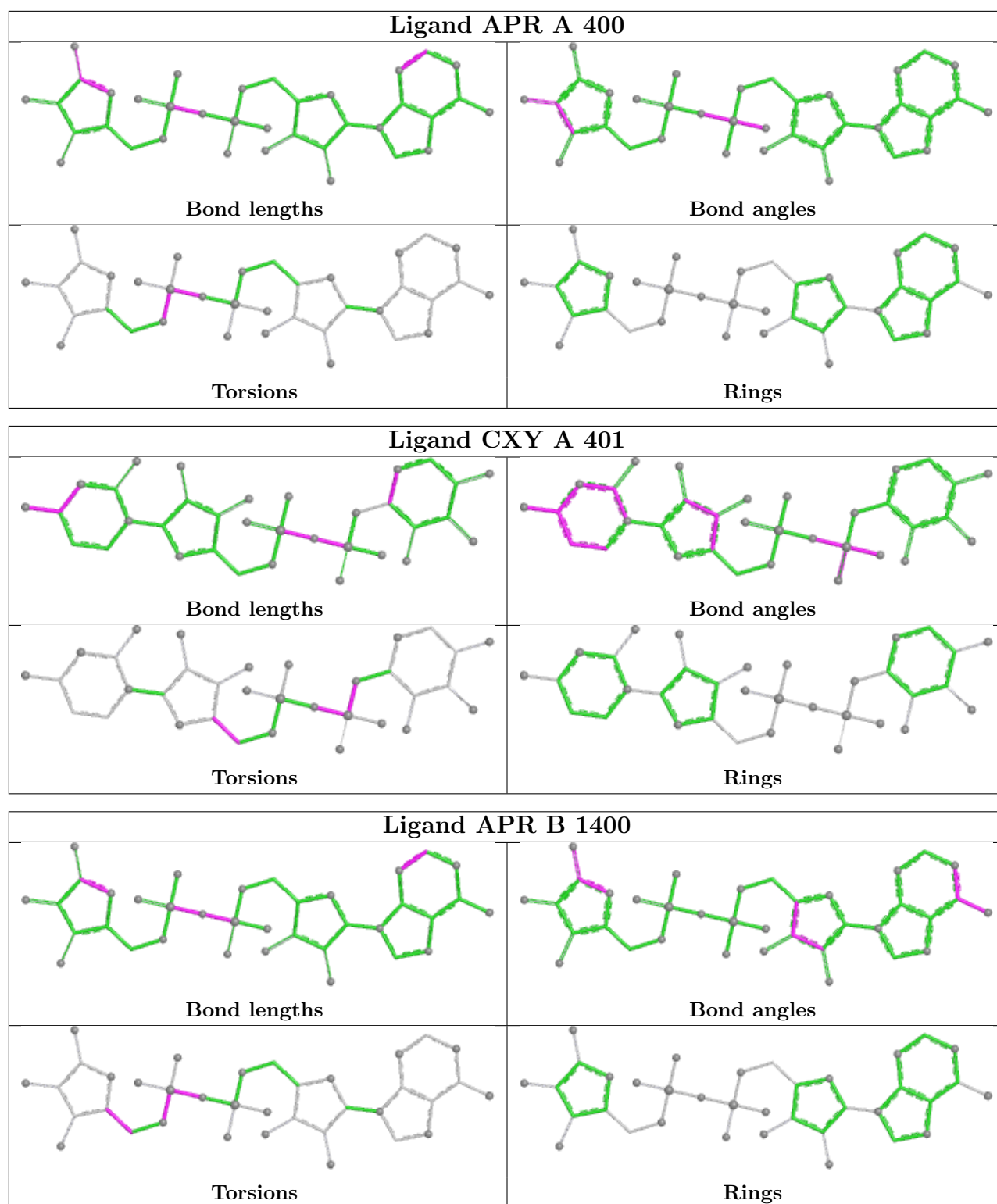
Mol	Chain	Res	Type	Atoms
2	A	400	APR	C5D-O5D-PB-O3A
2	A	400	APR	C5D-O5D-PB-O1B
2	A	400	APR	C5D-O5D-PB-O2B
2	B	1400	APR	C5D-O5D-PB-O3A
2	B	1400	APR	C5D-O5D-PB-O2B
2	B	1400	APR	O4D-C4D-C5D-O5D
3	A	401	CXY	C1'-O1'-PB-O3A
2	B	1400	APR	C3D-C4D-C5D-O5D
3	A	401	CXY	C1'-O1'-PB-O1B
2	B	1400	APR	C5D-O5D-PB-O1B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

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	APR	2	0
3	A	401	CXY	1	0
2	B	1400	APR	4	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.36	79 (22%) 2 2	15, 28, 62, 76	1 (0%)
1	B	350/359 (97%)	1.79	131 (37%) 1 0	13, 39, 72, 96	3 (0%)
All	All	702/718 (97%)	1.58	210 (29%) 1 1	13, 34, 67, 96	4 (0%)

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	GLY	5.5
1	B	1255	GLY	5.0
1	B	1223	VAL	5.0
1	B	1181	ALA	4.7
1	B	1233	PRO	4.3
1	B	1252	TYR	4.3
1	B	1217	PHE	4.2
1	A	358	ALA	4.1
1	B	1238	LEU	3.9
1	B	1315	GLN	3.9
1	A	289	ALA	3.8
1	B	1008	PHE	3.8
1	B	1287	ASP	3.7
1	A	291	TRP	3.7
1	B	1099	TYR	3.7
1	B	1064	HIS	3.7
1	B	1316	LEU	3.6
1	B	1010	GLN	3.6
1	B	1292	LEU	3.6
1	A	224	ILE	3.6
1	A	223	VAL	3.6
1	B	1097	LEU	3.6
1	B	1125	ASN	3.6
1	B	1256	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1048	VAL	3.5
1	B	1009	TRP	3.5
1	B	1182	ASN	3.5
1	B	1185	GLN	3.5
1	B	1156	TYR	3.4
1	A	332	VAL	3.4
1	A	294	ASP	3.4
1	B	1270	ASP	3.4
1	B	1081	PHE	3.4
1	A	287	ASP	3.3
1	B	1188	VAL	3.3
1	A	277	ILE	3.3
1	B	1300	HIS	3.3
1	A	220	ASN	3.2
1	A	285	TRP	3.2
1	A	303	HIS	3.2
1	A	213	ILE	3.2
1	B	1057	LEU	3.2
1	A	288	ASP	3.2
1	A	229	TYR	3.2
1	A	304	TYR	3.2
1	B	1284	LEU	3.2
1	A	331	ILE	3.1
1	B	1197	ASN	3.1
1	B	1041	TYR	3.1
1	B	1200	GLY	3.1
1	B	1285	TRP	3.1
1	A	271	ALA	3.1
1	B	1124	GLY	3.1
1	A	300	HIS	3.1
1	B	1353	SER	3.0
1	B	1224	ILE	3.0
1	B	1056	ARG	3.0
1	B	1095	VAL	3.0
1	B	1355	TYR	3.0
1	B	1291	TRP	3.0
1	B	1317	GLY	2.9
1	A	99	TYR	2.9
1	B	1254	GLU	2.9
1	A	204	TRP	2.9
1	A	292	LEU	2.9
1	A	339	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1004	ILE	2.9
1	A	278	VAL	2.8
1	A	347	CYS	2.8
1	B	1347	CYS	2.8
1	B	1346	ILE	2.8
1	B	1022	PHE	2.8
1	A	202	GLY	2.8
1	B	1065	ILE	2.8
1	B	1214	LEU	2.8
1	B	1357	SER	2.8
1	B	1074	LEU	2.8
1	B	1258	PHE	2.7
1	B	1189	GLY	2.7
1	B	1231	ILE	2.7
1	B	1180	PRO	2.7
1	B	1234	TRP	2.7
1	A	206	LYS	2.7
1	B	1006	LYS	2.7
1	B	1225	ILE	2.7
1	B	1247	VAL	2.7
1	B	1325	THR	2.7
1	B	1289	ALA	2.6
1	B	1229	TYR	2.6
1	A	321	ARG	2.6
1	A	290	SER	2.6
1	B	1349	LYS	2.6
1	B	1094	LEU	2.6
1	B	1298	HIS	2.6
1	A	44	ASP	2.6
1	A	327	THR	2.6
1	B	1047	THR	2.6
1	A	217	PHE	2.6
1	B	1178	PHE	2.6
1	A	183	TYR	2.6
1	B	1031	LEU	2.6
1	B	1268	ASP	2.6
1	A	48	VAL	2.6
1	B	1051	LEU	2.5
1	B	1060	LEU	2.5
1	A	127	LYS	2.5
1	A	274	VAL	2.5
1	A	270	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	6	LYS	2.5
1	A	341	GLY	2.5
1	A	54	ILE	2.5
1	B	1329	SER	2.5
1	A	269	GLU	2.5
1	A	145	TRP	2.5
1	B	1322	TRP	2.5
1	B	1313	ASN	2.4
1	B	1027	LEU	2.4
1	B	1324	LEU	2.4
1	B	1275	GLU	2.4
1	B	1205	ALA	2.4
1	B	1271	ALA	2.4
1	B	1145	TRP	2.4
1	A	299	PRO	2.4
1	A	56	ARG	2.4
1	B	1267	ARG	2.4
1	B	1345	LEU	2.4
1	B	1073	LYS	2.4
1	B	1126	ILE	2.4
1	A	302	ALA	2.4
1	B	1208	ARG	2.4
1	B	1219	ASN	2.4
1	B	1003	SER	2.4
1	A	156	TYR	2.4
1	B	1013	ARG	2.4
1	B	1273	THR	2.4
1	B	1277	ILE	2.4
1	B	1079	ALA	2.4
1	B	1058	ASN	2.4
1	B	1187	GLY	2.4
1	B	1314	MET	2.4
1	B	1350	ARG	2.3
1	B	1186	HIS	2.3
1	B	1236	HIS	2.3
1	A	323	GLY	2.3
1	A	257	LYS	2.3
1	B	1055	VAL	2.3
1	B	1123	VAL	2.3
1	A	340	ARG	2.3
1	A	334	TRP	2.3
1	A	182	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	205	ALA	2.3
1	B	1312	ALA	2.3
1	A	100	GLU	2.3
1	B	1084	GLU	2.3
1	A	293	LEU	2.3
1	B	1226	ARG	2.3
1	A	214	LEU	2.3
1	B	1026	TRP	2.2
1	A	53	GLU	2.2
1	B	1246	VAL	2.2
1	A	219	ASN	2.2
1	A	283	THR	2.2
1	B	1323	GLY	2.2
1	B	1052	PHE	2.2
1	A	346	ILE	2.2
1	A	314	MET	2.2
1	B	1012	LYS	2.2
1	A	215	ARG	2.2
1	B	1120	VAL	2.2
1	A	97	LEU	2.2
1	B	1251	LEU	2.2
1	B	1293	LEU	2.2
1	A	3	SER	2.2
1	A	11	GLY	2.2
1	B	1152	PRO	2.2
1	A	68	ILE	2.2
1	A	280	LYS	2.2
1	A	59	ASP	2.2
1	B	1117	LEU	2.2
1	B	1286	GLY	2.2
1	A	121	LYS	2.2
1	A	133	THR	2.1
1	B	1032	THR	2.1
1	A	241	LEU	2.1
1	A	4	ILE	2.1
1	B	1331	ILE	2.1
1	B	1278	VAL	2.1
1	A	64	HIS	2.1
1	A	101	GLN	2.1
1	A	350	ARG	2.1
1	B	1096	ARG	2.1
1	B	1020	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	281	MET	2.1
1	B	1204	TRP	2.1
1	A	225	ILE	2.0
1	B	1257	LYS	2.0
1	B	1276	PHE	2.0
1	B	1019	HIS	2.0
1	B	1222	GLN	2.0
1	A	305	LEU	2.0
1	B	1090	ALA	2.0
1	B	1076	SER	2.0
1	B	1281	MET	2.0
1	B	1177	PHE	2.0
1	A	221	GLN	2.0
1	B	1007	ASN	2.0
1	B	1011	GLY	2.0
1	B	1021	GLY	2.0
1	B	1221	GLN	2.0
1	B	1193	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

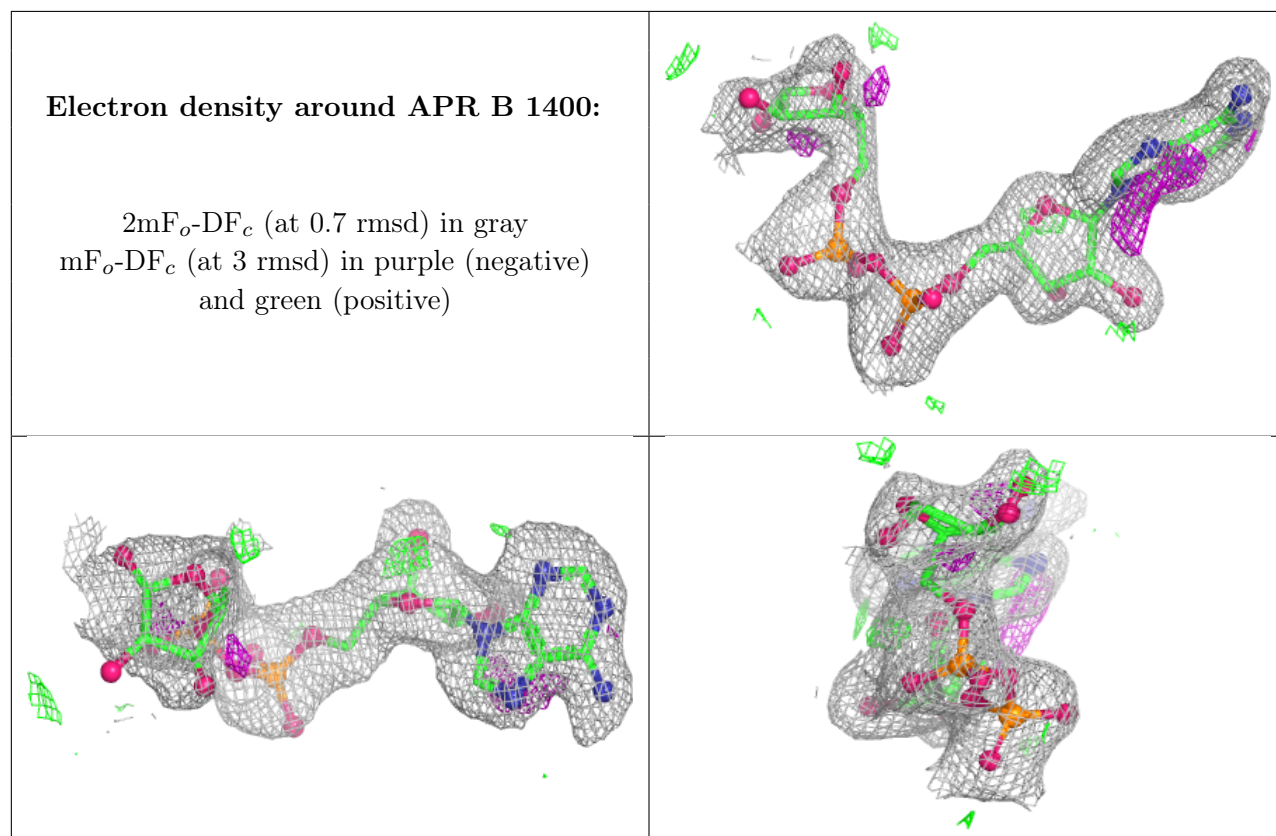
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	APR	B	1400	36/36	0.90	0.15	17,33,100,100	0
3	CXY	A	401	34/34	0.91	0.11	17,26,35,41	0
2	APR	A	400	36/36	0.93	0.10	11,23,40,80	0

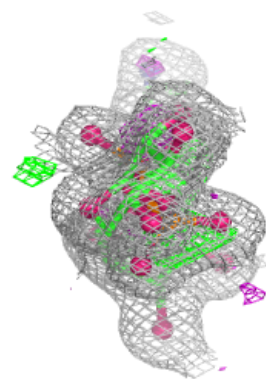
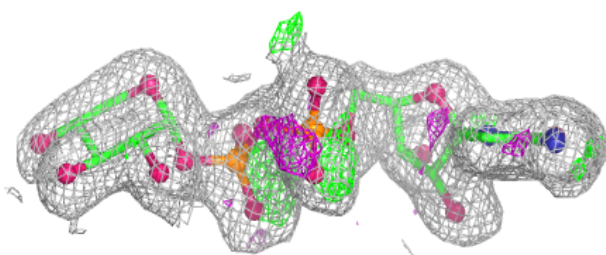
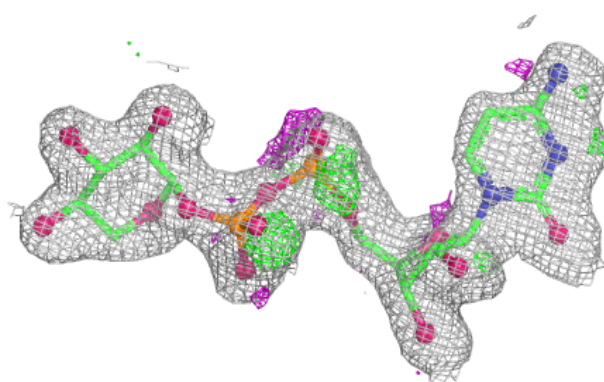
The following is a graphical depiction of the model fit to experimental electron density of all

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.

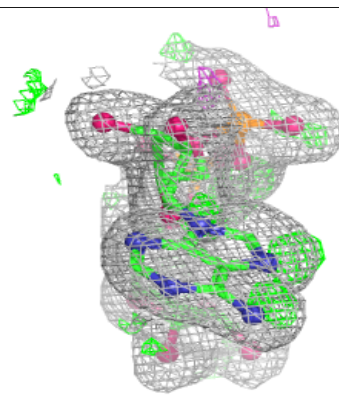
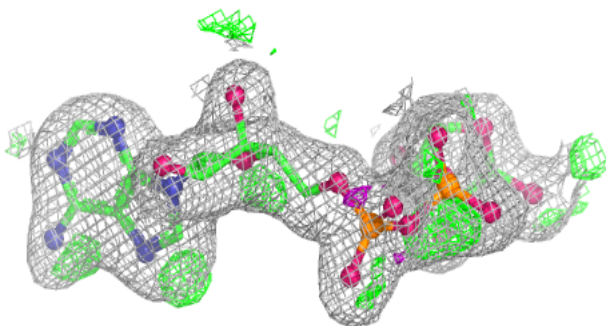
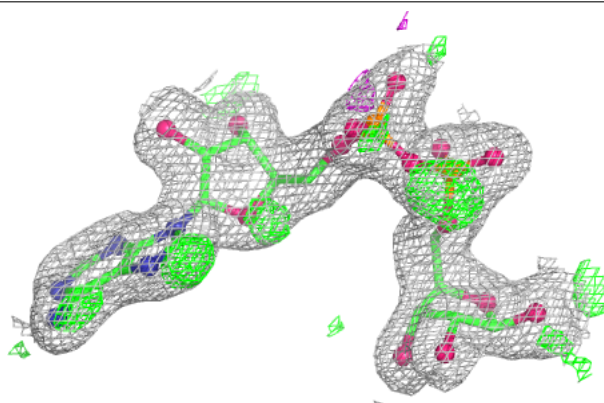


Electron density around CXY A 401:

$2mF_o-DF_c$ (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.