



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:18 PM UTC

PDB ID : 4ZJZ / pdb_00004zjz
Title : Crystal structure of a benzoate coenzyme A ligase with Benzoyl-AMP
Authors : Strom, S.; Nosrati, M.; Thornburg, C.; Walker, K.D.; Geiger, J.H.
Deposited on : 2015-04-29
Resolution : 1.70 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

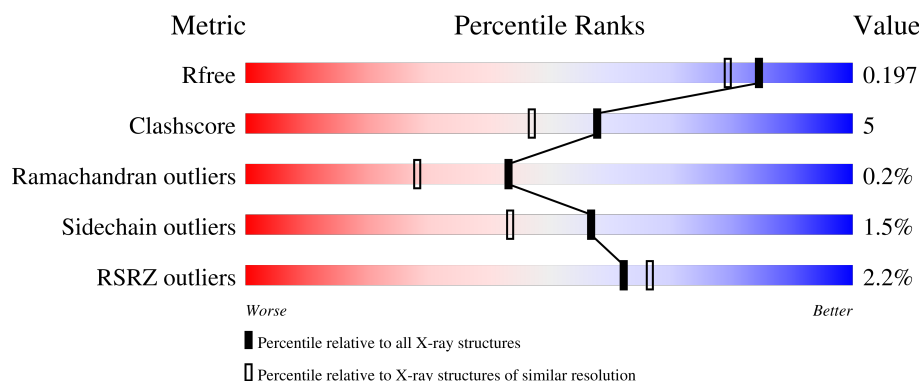
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	524	2% 85% 13% ..
1	B	524	2% 85% 13% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	604	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8658 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.

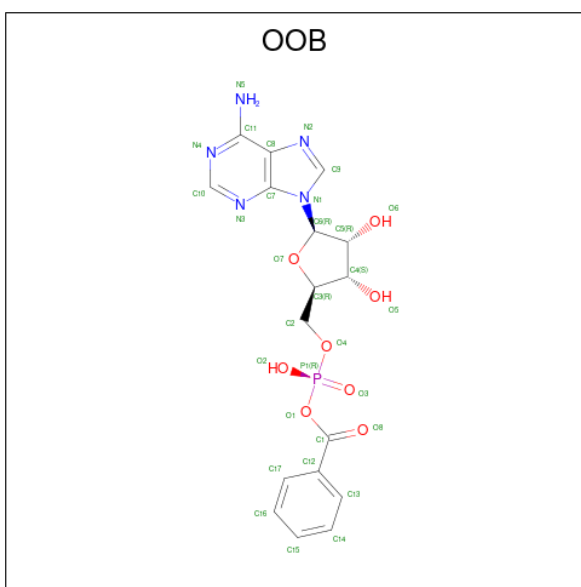
- Molecule 1 is a protein called Benzoate-coenzyme A ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	2	0
			3921	2511	678	722	10			
1	B	519	Total	C	N	O	S	0	5	0
			3950	2531	680	728	11			

There are 8 discrepancies between the modelled and reference sequences:

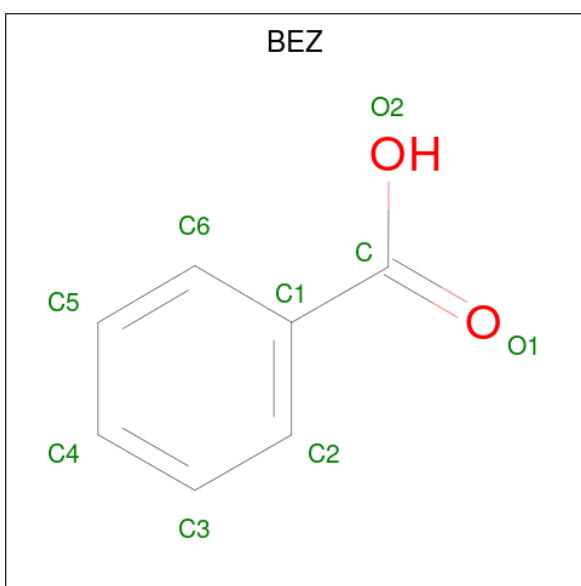
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q93TK0
A	83	ALA	THR	conflict	UNP Q93TK0
A	341	ASP	GLY	conflict	UNP Q93TK0
A	524	GLY	SER	conflict	UNP Q93TK0
B	1	MET	-	initiating methionine	UNP Q93TK0
B	83	ALA	THR	conflict	UNP Q93TK0
B	341	ASP	GLY	conflict	UNP Q93TK0
B	524	GLY	SER	conflict	UNP Q93TK0

- Molecule 2 is 5'-O-[(R)-(benzoyloxy)(hydroxy)phosphoryl]adenosine (CCD ID: OOB) (formula: C₁₇H₁₈N₅O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 17	N 5	O 8	P 1	0	0
2	B	1	Total 31	C 17	N 5	O 8	P 1	0	0

- Molecule 3 is BENZOIC ACID (CCD ID: BEZ) (formula: $\text{C}_7\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 7 2	0	0
3	B	1	Total C O 9 7 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	316	Total	O	0	0
			316	316		

Continued on next page...

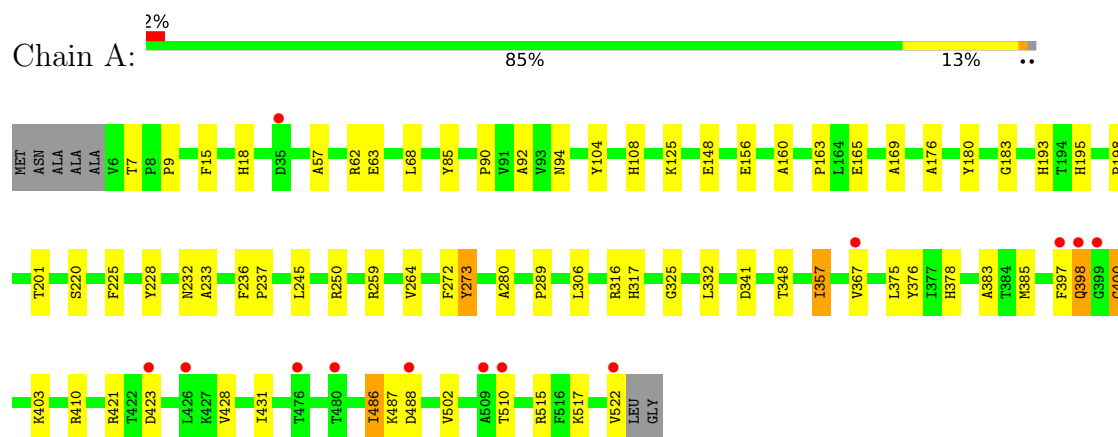
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	331	Total 331	O 331	0	0

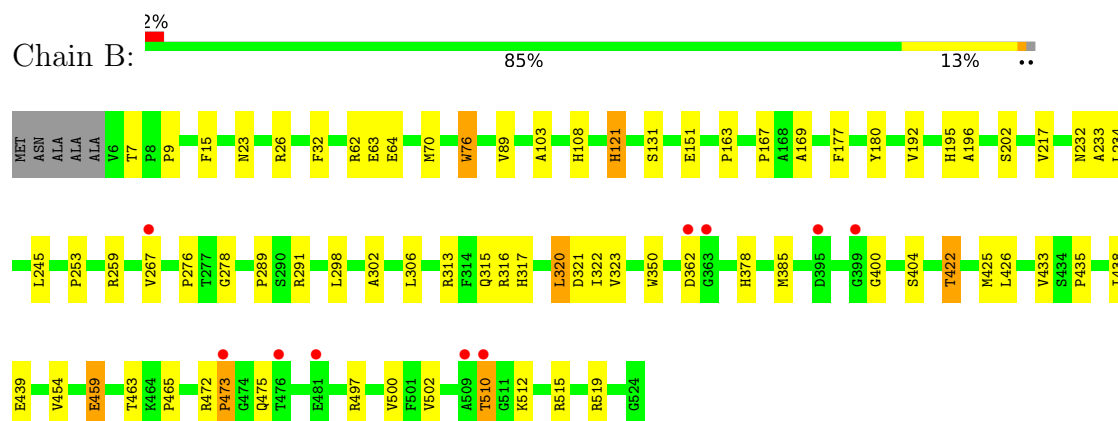
3 Residue-property plots

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: Benzoate-coenzyme A ligase



• Molecule 1: Benzoate-coenzyme A ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.62Å 95.61Å 95.71Å 90.00° 104.53° 90.00°	Depositor
Resolution (Å)	29.39 – 1.70 29.39 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.39-1.70) 96.7 (29.39-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.152 , 0.192 0.161 , 0.197	Depositor DCC
R_{free} test set	5437 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8658	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: GOL, BEZ, OOB

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	1.57	25/4032 (0.6%)	1.32	11/5500 (0.2%)
1	B	1.55	22/4070 (0.5%)	1.28	8/5552 (0.1%)
All	All	1.56	47/8102 (0.6%)	1.30	19/11052 (0.2%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	ALA	CA-CB	7.96	1.63	1.52
1	A	273	TYR	C-O	-7.50	1.15	1.23
1	B	169	ALA	CA-CB	7.28	1.62	1.52
1	B	463	THR	N-CA	6.95	1.54	1.46
1	B	233	ALA	CA-CB	6.78	1.64	1.53
1	A	325	GLY	N-CA	6.77	1.52	1.45
1	A	183	GLY	N-CA	6.56	1.49	1.44
1	A	9	PRO	CA-C	6.51	1.58	1.52
1	A	163	PRO	C-O	6.45	1.31	1.23
1	B	234	LEU	N-CA	6.45	1.54	1.46
1	B	302	ALA	CA-CB	6.43	1.63	1.53
1	B	350	TRP	N-CA	6.35	1.52	1.45
1	B	426	LEU	C-O	-6.35	1.16	1.23
1	B	192	VAL	CA-CB	6.33	1.61	1.54
1	A	280	ALA	N-CA	6.32	1.54	1.46
1	B	322	ILE	C-O	6.19	1.31	1.24
1	B	76	TRP	C-O	-5.91	1.18	1.24
1	B	202	SER	C-O	-5.79	1.16	1.24
1	A	488	ASP	CA-C	5.70	1.60	1.52
1	A	233	ALA	CA-CB	5.65	1.62	1.53
1	A	57	ALA	CA-CB	-5.64	1.44	1.53
1	B	167	PRO	C-O	5.61	1.30	1.23
1	B	385	MET	C-O	5.54	1.29	1.23
1	A	264	VAL	CA-CB	5.54	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	ALA	CA-CB	5.53	1.62	1.53
1	B	459	GLU	N-CA	5.48	1.53	1.46
1	B	350	TRP	CA-CB	5.43	1.60	1.54
1	A	198	PRO	N-CA	5.41	1.54	1.47
1	B	121	HIS	C-O	-5.39	1.19	1.24
1	A	160	ALA	CA-CB	5.38	1.62	1.53
1	B	306	LEU	CA-C	5.33	1.58	1.52
1	B	32	PHE	N-CA	5.28	1.52	1.46
1	A	104	TYR	C-O	-5.28	1.18	1.24
1	B	362	ASP	N-CA	5.22	1.52	1.46
1	B	64	GLU	N-CA	5.20	1.52	1.45
1	A	431	ILE	N-CA	5.19	1.52	1.46
1	A	502	VAL	C-O	5.19	1.29	1.23
1	A	92	ALA	C-O	5.17	1.30	1.24
1	A	85	TYR	N-CA	5.17	1.52	1.46
1	A	228	TYR	N-CA	5.16	1.52	1.46
1	A	18	HIS	CA-C	5.15	1.59	1.52
1	A	165	GLU	CA-C	-5.15	1.45	1.52
1	A	316	ARG	N-CA	5.13	1.52	1.46
1	B	9	PRO	CA-C	5.10	1.55	1.52
1	A	250	ARG	C-O	5.10	1.30	1.24
1	A	341	ASP	C-O	-5.02	1.17	1.24
1	A	183	GLY	C-O	5.00	1.28	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TYR	O-C-N	-15.31	104.68	123.36
1	A	272	PHE	CA-C-N	-7.80	109.23	122.33
1	A	272	PHE	C-N-CA	-7.80	109.23	122.33
1	A	272	PHE	O-C-N	7.19	132.54	123.19
1	B	425	MET	O-C-N	7.01	131.13	122.86
1	A	428	VAL	N-CA-C	-6.43	99.11	108.11
1	B	422	THR	N-CA-CB	-6.06	100.95	110.46
1	A	306	LEU	CA-C-N	-5.73	113.86	119.76
1	A	306	LEU	C-N-CA	-5.73	113.86	119.76
1	B	232	ASN	N-CA-C	5.68	117.47	111.28
1	B	7	THR	CA-C-N	-5.60	115.63	119.66
1	B	7	THR	C-N-CA	-5.60	115.63	119.66
1	B	422	THR	OG1-CB-CG2	5.43	120.16	109.30
1	A	400	GLY	N-CA-C	-5.42	108.63	115.08
1	A	486	ILE	N-CA-C	5.40	118.68	111.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	THR	N-CA-C	-5.34	105.53	111.36
1	B	404	SER	CA-C-N	-5.17	112.70	122.05
1	B	404	SER	C-N-CA	-5.17	112.70	122.05
1	A	410	ARG	CB-CG-CD	-5.08	99.61	111.30

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	3921	0	3847	34	0
1	B	3950	0	3884	38	0
2	A	31	0	17	0	0
2	B	31	0	17	0	0
3	A	9	0	5	0	0
3	B	9	0	5	1	0
4	A	24	0	32	0	0
4	B	36	0	48	5	0
5	A	316	0	0	2	0
5	B	331	0	0	4	0
All	All	8658	0	7855	72	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 5.

All (72) 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:510:THR:HG21	5:B:964:HOH:O	1.42	1.16
1:A:385:MET:HA	1:A:397:PHE:CE2	2.06	0.90
1:B:121:HIS:HE1	1:B:151:GLU:OE2	1.56	0.88
1:A:15:PHE:H	1:A:195:HIS:HD2	1.23	0.84
1:B:15:PHE:H	1:B:195:HIS:HD2	1.27	0.83
1:A:62:ARG:O	1:A:63:GLU:HB2	1.84	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:MET:CA	1:A:397:PHE:CE2	2.72	0.72
1:A:245:LEU:HD21	1:A:259:ARG:HG2	1.72	0.71
1:B:321:ASP:HB2	4:B:604:GOL:H31	1.74	0.70
1:A:398:GLN:CB	5:A:1386:HOH:O	2.40	0.69
1:A:108:HIS:HD2	1:A:180:TYR:OH	1.76	0.68
1:B:298:LEU:HD12	4:B:604:GOL:H12	1.75	0.68
1:B:62:ARG:O	1:B:63:GLU:HB2	1.94	0.67
1:B:108:HIS:HD2	1:B:180:TYR:OH	1.79	0.66
1:B:15:PHE:H	1:B:195:HIS:CD2	2.14	0.66
1:B:435:PRO:O	1:B:439:GLU:HG3	1.97	0.65
1:B:163:PRO:HG3	5:B:921:HOH:O	1.97	0.63
1:A:515:ARG:HH11	1:A:515:ARG:HG2	1.62	0.63
1:A:289:PRO:O	1:A:317:HIS:HE1	1.81	0.63
1:B:454:VAL:HB	1:B:519:ARG:HG3	1.84	0.59
1:A:15:PHE:H	1:A:195:HIS:CD2	2.12	0.59
1:B:23:ASN:HD22	1:B:26:ARG:HH11	1.50	0.59
1:A:195:HIS:HE1	5:A:1311:HOH:O	1.85	0.59
1:B:121:HIS:HD2	5:B:1012:HOH:O	1.86	0.58
1:B:378:HIS:HD2	1:B:400:GLY:O	1.87	0.58
1:A:385:MET:HA	1:A:397:PHE:HE2	1.69	0.57
1:B:217:VAL:HG21	1:B:267:VAL:CG2	2.34	0.56
1:B:289:PRO:O	1:B:317:HIS:HE1	1.87	0.56
1:A:62:ARG:O	1:A:63:GLU:CB	2.53	0.54
1:B:23:ASN:ND2	1:B:26:ARG:HH11	2.06	0.54
1:B:313:ARG:HG2	1:B:316:ARG:NH2	2.24	0.53
1:A:421:ARG:NH2	1:A:423:ASP:OD2	2.34	0.52
1:B:323:VAL:HG23	4:B:604:GOL:H11	1.90	0.52
1:B:195:HIS:HE1	5:B:902:HOH:O	1.92	0.52
1:B:439:GLU:OE2	1:B:515:ARG:NH1	2.37	0.52
1:B:298:LEU:CD1	4:B:604:GOL:H12	2.38	0.52
1:B:62:ARG:O	1:B:63:GLU:CB	2.56	0.52
1:A:383:ALA:O	1:A:397:PHE:CE1	2.63	0.51
1:B:459:GLU:H	1:B:459:GLU:CD	2.18	0.51
1:B:245:LEU:HD21	1:B:259:ARG:HG2	1.93	0.51
1:B:465:PRO:HD2	1:B:497:ARG:HD3	1.95	0.48
1:A:125:LYS:HE3	1:A:148:GLU:OE2	2.13	0.48
1:A:515:ARG:HG2	1:A:515:ARG:NH1	2.26	0.48
1:B:472:ARG:O	1:B:473:PRO:C	2.57	0.48
1:B:323:VAL:CG2	4:B:604:GOL:H11	2.45	0.47
1:B:510:THR:HG22	1:B:512:LYS:H	1.80	0.47
1:A:357:ILE:HG23	1:A:375:LEU:CD1	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:LYS:HB3	1:A:522:VAL:HG11	1.95	0.46
1:B:103:ALA:HB1	1:B:131:SER:HB3	1.98	0.46
1:B:121:HIS:CE1	1:B:151:GLU:OE2	2.49	0.46
1:A:193:HIS:CE1	1:A:332:LEU:HB2	2.50	0.46
1:A:236:PHE:HB2	1:A:237:PRO:CD	2.46	0.46
1:A:68:LEU:C	1:A:68:LEU:HD23	2.41	0.45
1:A:220:SER:HA	1:A:273:TYR:HB2	1.98	0.45
1:A:385:MET:CA	1:A:397:PHE:HE2	2.25	0.44
1:B:439:GLU:CD	1:B:515:ARG:HH12	2.25	0.44
1:A:378:HIS:HD2	1:A:400:GLY:O	2.00	0.44
1:A:397:PHE:O	1:A:398:GLN:C	2.61	0.43
1:A:232:ASN:HB3	1:A:273:TYR:CD2	2.53	0.43
1:A:90:PRO:HD2	1:A:176:ALA:O	2.18	0.43
1:A:357:ILE:HG23	1:A:375:LEU:HD11	2.00	0.43
1:A:421:ARG:HE	1:A:423:ASP:CG	2.26	0.42
1:B:500:VAL:HG12	1:B:502:VAL:HG13	2.01	0.42
1:B:89:VAL:HG13	1:B:177:PHE:HA	2.02	0.42
1:B:278:GLY:HA3	3:B:601:BEZ:C6	2.51	0.41
1:A:486:ILE:HG13	1:A:487:LYS:N	2.35	0.41
1:A:376:TYR:CE1	1:A:403:LYS:HB2	2.55	0.41
1:B:315:GLN:HA	1:B:320:LEU:O	2.20	0.41
1:A:94:ASN:HA	1:A:225:PHE:CE1	2.55	0.41
1:B:70[B]:MET:HB3	1:B:76:TRP:CD1	2.55	0.41
1:A:367:VAL:O	1:A:367:VAL:HG23	2.21	0.40
1:B:433:VAL:CG1	1:B:438:ILE:HD11	2.52	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	517/524 (99%)	504 (98%)	12 (2%)	1 (0%)	43 28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	522/524 (100%)	516 (99%)	5 (1%)	1 (0%)	43	28
All	All	1039/1048 (99%)	1020 (98%)	17 (2%)	2 (0%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	GLN
1	B	473	PRO

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	399/414 (96%)	394 (99%)	5 (1%)	61	48
1	B	404/414 (98%)	397 (98%)	7 (2%)	53	38
All	All	803/828 (97%)	791 (98%)	12 (2%)	57	43

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	156	GLU
1	A	348	THR
1	A	357	ILE
1	A	510	THR
1	B	253	PRO
1	B	276	PRO
1	B	291	ARG
1	B	320	LEU
1	B	422	THR
1	B	475	GLN
1	B	510	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	112	GLN
1	A	195	HIS
1	A	317	HIS
1	A	378	HIS
1	B	23	ASN
1	B	108	HIS
1	B	112	GLN
1	B	121	HIS
1	B	195	HIS
1	B	317	HIS
1	B	378	HIS
1	B	444	GLN
1	B	475	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](#)

14 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	OOB	B	603	-	34,34,34	2.23	8 (23%)	50,50,50	2.00	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	604	-	5,5,5	0.52	0	5,5,5	1.84	2 (40%)
4	GOL	B	608	-	5,5,5	0.56	0	5,5,5	1.60	1 (20%)
2	OOB	A	1000	-	34,34,34	2.20	9 (26%)	50,50,50	1.96	14 (28%)
4	GOL	A	1003	-	5,5,5	0.20	0	5,5,5	0.82	0
4	GOL	B	607	-	5,5,5	0.35	0	5,5,5	1.42	1 (20%)
4	GOL	B	602	-	5,5,5	0.45	0	5,5,5	2.00	2 (40%)
4	GOL	B	606	-	5,5,5	0.58	0	5,5,5	1.14	1 (20%)
4	GOL	A	1004	-	5,5,5	0.77	0	5,5,5	1.86	2 (40%)
4	GOL	B	605	-	5,5,5	0.66	0	5,5,5	0.66	0
3	BEZ	B	601	-	9,9,9	1.93	5 (55%)	11,11,11	1.65	2 (18%)
4	GOL	A	1005	-	5,5,5	0.41	0	5,5,5	1.27	1 (20%)
4	GOL	A	1002	-	5,5,5	0.95	0	5,5,5	1.43	1 (20%)
3	BEZ	A	1001	-	9,9,9	1.69	2 (22%)	11,11,11	1.80	4 (36%)

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	OOB	B	603	-	-	1/19/35/35	0/4/4/4
4	GOL	B	604	-	-	2/4/4/4	-
4	GOL	B	608	-	-	4/4/4/4	-
2	OOB	A	1000	-	-	1/19/35/35	0/4/4/4
4	GOL	A	1003	-	-	2/4/4/4	-
4	GOL	B	607	-	-	0/4/4/4	-
4	GOL	B	602	-	-	2/4/4/4	-
4	GOL	B	606	-	-	4/4/4/4	-
4	GOL	A	1004	-	-	2/4/4/4	-
4	GOL	B	605	-	-	0/4/4/4	-
3	BEZ	B	601	-	-	0/4/4/4	0/1/1/1
4	GOL	A	1005	-	-	1/4/4/4	-
4	GOL	A	1002	-	-	0/4/4/4	-
3	BEZ	A	1001	-	-	0/4/4/4	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	603	OOB	O1-C1	9.28	1.47	1.37
2	A	1000	OOB	O1-C1	8.13	1.45	1.37
2	B	603	OOB	C9-N2	5.29	1.41	1.31
2	A	1000	OOB	C7-N3	4.09	1.42	1.34
2	A	1000	OOB	C8-C7	3.80	1.45	1.39
3	A	1001	BEZ	C6-C1	3.67	1.45	1.39
2	A	1000	OOB	P1-O1	3.19	1.66	1.60
2	A	1000	OOB	C9-N2	3.10	1.37	1.31
2	B	603	OOB	C8-C7	2.92	1.44	1.39
3	B	601	BEZ	O2-C	-2.86	1.22	1.30
2	A	1000	OOB	P1-O2	-2.84	1.42	1.55
3	B	601	BEZ	C3-C2	2.71	1.43	1.38
2	A	1000	OOB	C16-C15	2.60	1.44	1.38
2	A	1000	OOB	C8-C11	2.49	1.47	1.41
2	B	603	OOB	C7-N1	-2.49	1.32	1.37
2	A	1000	OOB	C7-N1	-2.43	1.32	1.37
3	B	601	BEZ	C5-C6	2.18	1.42	1.38
3	A	1001	BEZ	C3-C2	2.15	1.42	1.38
2	B	603	OOB	P1-O1	2.12	1.64	1.60
2	B	603	OOB	C16-C15	2.12	1.42	1.38
3	B	601	BEZ	C2-C1	2.12	1.42	1.39
2	B	603	OOB	C13-C12	2.10	1.42	1.39
3	B	601	BEZ	C5-C4	2.10	1.42	1.38
2	B	603	OOB	C10-N3	2.06	1.37	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	603	OOB	C7-N1-C9	5.70	111.72	105.74
2	B	603	OOB	N1-C9-N2	-5.15	106.63	113.94
2	A	1000	OOB	C8-C7-N3	-4.78	120.13	126.72
2	A	1000	OOB	N3-C7-N1	4.70	135.16	127.17
2	B	603	OOB	C16-C17-C12	-4.38	116.06	120.36
2	A	1000	OOB	C7-N1-C9	3.95	109.88	105.74
2	A	1000	OOB	C14-C13-C12	-3.74	116.69	120.36
2	A	1000	OOB	C17-C12-C13	3.64	123.19	118.57
2	B	603	OOB	N4-C10-N3	-3.45	123.35	128.58
2	B	603	OOB	C17-C12-C13	3.38	122.86	118.57
3	B	601	BEZ	O2-C-O1	-3.35	116.16	123.35
2	A	1000	OOB	C5-C4-C3	-3.16	96.51	102.61
2	A	1000	OOB	O2-P1-O3	3.12	126.95	112.44
2	B	603	OOB	C7-N1-C6	-2.85	119.96	126.63
2	A	1000	OOB	C7-N1-C6	-2.82	120.04	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	603	OOB	C8-C7-N3	-2.80	122.86	126.72
4	B	602	GOL	O2-C2-C3	2.79	120.71	109.18
4	B	604	GOL	O2-C2-C3	2.75	120.58	109.18
3	A	1001	BEZ	O2-C-O1	-2.75	117.44	123.35
4	B	602	GOL	C3-C2-C1	-2.75	101.71	111.80
2	A	1000	OOB	P1-O1-C1	2.75	128.99	123.01
2	A	1000	OOB	O1-P1-O3	-2.68	101.33	109.95
2	A	1000	OOB	C8-C11-N5	-2.67	116.67	123.29
2	A	1000	OOB	O1-C1-C12	2.65	115.21	112.39
2	B	603	OOB	N5-C11-N4	2.61	124.19	118.38
2	B	603	OOB	C7-C8-N2	-2.59	107.62	110.58
4	A	1004	GOL	O2-C2-C3	2.52	119.61	109.18
3	A	1001	BEZ	O2-C-C1	2.52	121.30	114.84
3	B	601	BEZ	O2-C-C1	2.52	121.29	114.84
4	B	608	GOL	O1-C1-C2	-2.48	99.19	110.38
2	A	1000	OOB	C10-N3-C7	2.47	117.86	111.83
2	B	603	OOB	C8-N2-C9	2.40	107.22	103.45
2	B	603	OOB	O6-C5-C6	-2.38	101.89	110.10
3	A	1001	BEZ	C5-C4-C3	2.35	123.09	119.87
2	B	603	OOB	C15-C16-C17	2.30	123.07	120.24
4	B	604	GOL	O3-C3-C2	2.29	120.71	110.38
4	B	607	GOL	O2-C2-C3	2.25	118.50	109.18
2	B	603	OOB	C10-N4-C11	2.25	122.42	118.73
4	A	1004	GOL	O1-C1-C2	-2.20	100.47	110.38
4	B	606	GOL	O1-C1-C2	-2.20	100.49	110.38
4	A	1005	GOL	O1-C1-C2	-2.19	100.52	110.38
4	A	1002	GOL	O1-C1-C2	2.15	120.06	110.38
3	A	1001	BEZ	C6-C1-C2	2.04	121.16	118.57
2	A	1000	OOB	C15-C16-C17	-2.00	117.77	120.24

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	GOL	C1-C2-C3-O3
4	B	608	GOL	O1-C1-C2-C3
4	B	606	GOL	O1-C1-C2-O2
4	A	1004	GOL	O1-C1-C2-C3
4	B	602	GOL	C1-C2-C3-O3
4	B	604	GOL	C1-C2-C3-O3
4	B	606	GOL	O1-C1-C2-C3
4	B	606	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

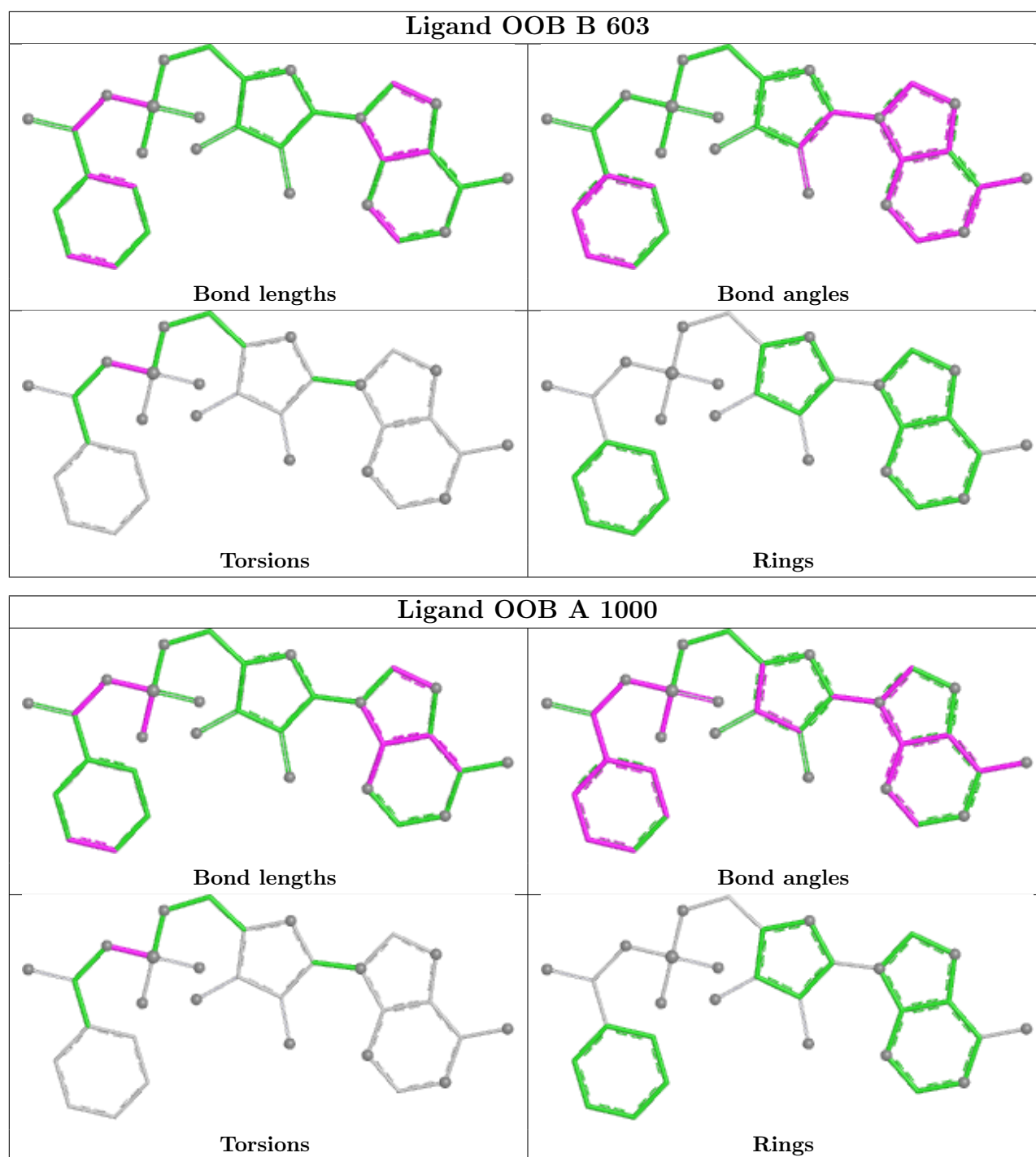
Mol	Chain	Res	Type	Atoms
4	B	608	GOL	C1-C2-C3-O3
4	A	1003	GOL	O2-C2-C3-O3
4	B	608	GOL	O1-C1-C2-O2
4	B	608	GOL	O2-C2-C3-O3
4	B	604	GOL	O2-C2-C3-O3
4	A	1004	GOL	O1-C1-C2-O2
4	B	602	GOL	O2-C2-C3-O3
4	B	606	GOL	O2-C2-C3-O3
4	A	1005	GOL	O2-C2-C3-O3
2	A	1000	OOB	C1-O1-P1-O4
2	B	603	OOB	C1-O1-P1-O4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	GOL	5	0
3	B	601	BEZ	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	517/524 (98%)	-0.37	13 (2%)	58 62	7, 16, 32, 43	2 (0%)
1	B	519/524 (99%)	-0.38	10 (1%)	66 71	6, 17, 31, 51	5 (0%)
All	All	1036/1048 (98%)	-0.37	23 (2%)	62 66	6, 16, 32, 51	7 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	397	PHE	9.5
1	A	398	GLN	4.9
1	A	426	LEU	4.6
1	B	476	THR	3.9
1	A	399	GLY	3.7
1	A	35	ASP	3.5
1	A	522	VAL	3.4
1	A	476	THR	3.2
1	B	473	PRO	3.1
1	A	423	ASP	3.1
1	A	509	ALA	3.0
1	B	267	VAL	2.9
1	B	362	ASP	2.6
1	B	399	GLY	2.4
1	A	488	ASP	2.2
1	A	367	VAL	2.1
1	B	481	GLU	2.1
1	B	363	GLY	2.1
1	A	510	THR	2.1
1	B	395	ASP	2.1
1	B	509	ALA	2.1
1	A	480	THR	2.0
1	B	510	THR	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](#)

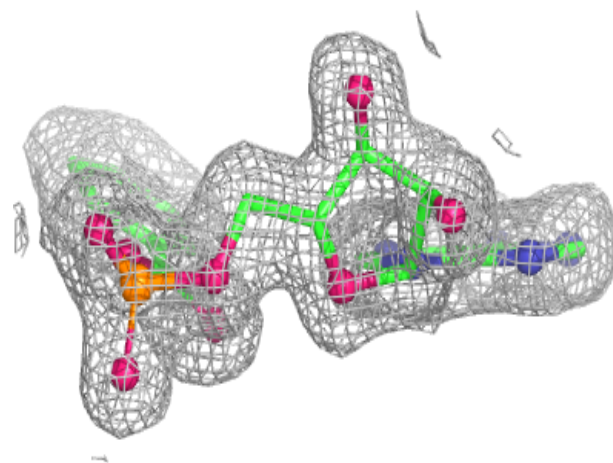
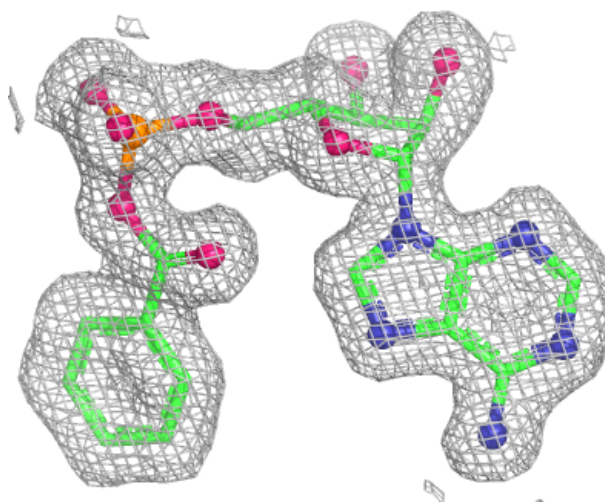
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	GOL	A	1004	6/6	0.83	0.13	36,37,41,42	0
4	GOL	B	606	6/6	0.85	0.14	27,37,41,46	0
3	BEZ	B	601	9/9	0.90	0.09	21,28,31,32	0
4	GOL	A	1005	6/6	0.91	0.11	22,33,43,51	0
3	BEZ	A	1001	9/9	0.91	0.09	20,26,28,28	0
4	GOL	B	604	6/6	0.93	0.16	13,24,38,38	0
4	GOL	A	1003	6/6	0.93	0.09	31,38,41,42	0
4	GOL	B	608	6/6	0.93	0.11	24,38,40,46	0
4	GOL	B	602	6/6	0.94	0.09	19,26,32,37	0
4	GOL	B	605	6/6	0.94	0.12	19,23,24,24	0
4	GOL	B	607	6/6	0.96	0.06	19,26,31,36	0
4	GOL	A	1002	6/6	0.97	0.09	14,20,24,26	0
2	OOB	B	603	31/31	0.97	0.05	7,13,17,20	0
2	OOB	A	1000	31/31	0.98	0.04	8,13,19,19	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.

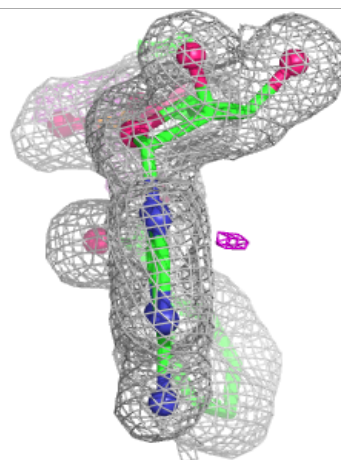
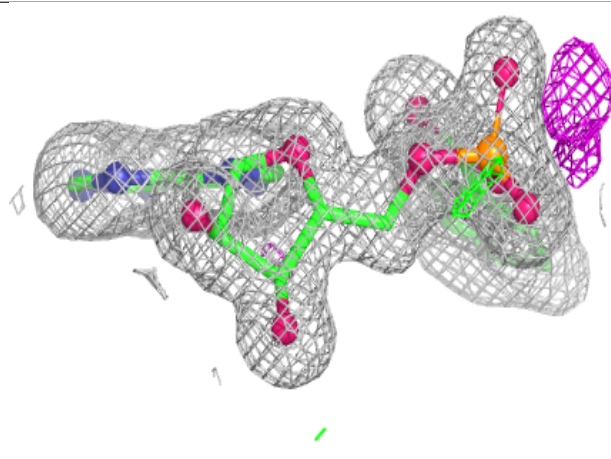
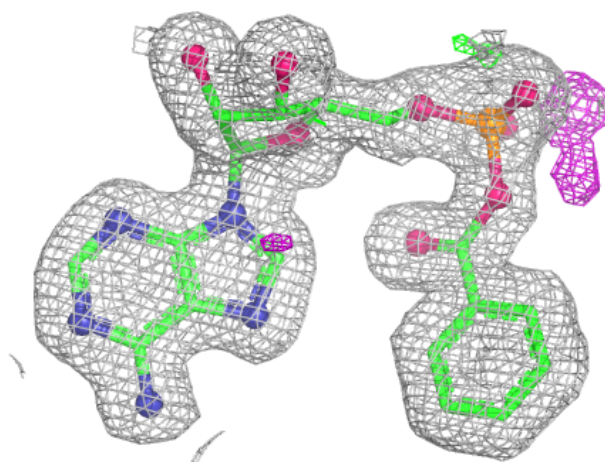
Electron density around OOB B 603:

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



Electron density around OOB A 1000:

$2mF_o-DF_c$ (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.