



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:22 am BST

PDB ID : 2Q5O
Title : X-ray structure of phenylpyruvate decarboxylase in complex with 3-deaza-ThDP and phenylpyruvate
Authors : Versees, W.; Spaepen, S.; Wood, M.D.; Leeper, F.J.; Vanderleyden, J.; Steyaert, J.
Deposited on : 2007-06-01
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

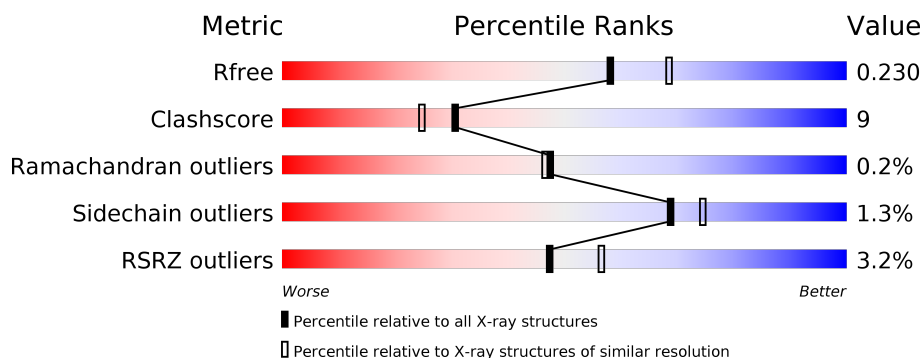
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	565	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>6%</div> </div> </div>
1	B	565	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8762 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 Phenylpyruvate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	1	0
			3944	2499	688	733	24			
1	B	531	Total	C	N	O	S	0	1	0
			3971	2514	699	735	23			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P51852
A	-18	GLY	-	EXPRESSION TAG	UNP P51852
A	-17	SER	-	EXPRESSION TAG	UNP P51852
A	-16	SER	-	EXPRESSION TAG	UNP P51852
A	-15	HIS	-	EXPRESSION TAG	UNP P51852
A	-14	HIS	-	EXPRESSION TAG	UNP P51852
A	-13	HIS	-	EXPRESSION TAG	UNP P51852
A	-12	HIS	-	EXPRESSION TAG	UNP P51852
A	-11	HIS	-	EXPRESSION TAG	UNP P51852
A	-10	HIS	-	EXPRESSION TAG	UNP P51852
A	-9	SER	-	EXPRESSION TAG	UNP P51852
A	-8	SER	-	EXPRESSION TAG	UNP P51852
A	-7	GLY	-	EXPRESSION TAG	UNP P51852
A	-6	LEU	-	EXPRESSION TAG	UNP P51852
A	-5	VAL	-	EXPRESSION TAG	UNP P51852
A	-4	PRO	-	EXPRESSION TAG	UNP P51852
A	-3	ARG	-	EXPRESSION TAG	UNP P51852
A	-2	GLY	-	EXPRESSION TAG	UNP P51852
A	-1	SER	-	EXPRESSION TAG	UNP P51852
A	0	HIS	-	EXPRESSION TAG	UNP P51852
A	155	GLN	LEU	EXPRESSION TAG	UNP P51852
A	327	ARG	GLY	SEE REMARK 999	UNP P51852
B	-19	MET	-	EXPRESSION TAG	UNP P51852
B	-18	GLY	-	EXPRESSION TAG	UNP P51852
B	-17	SER	-	EXPRESSION TAG	UNP P51852

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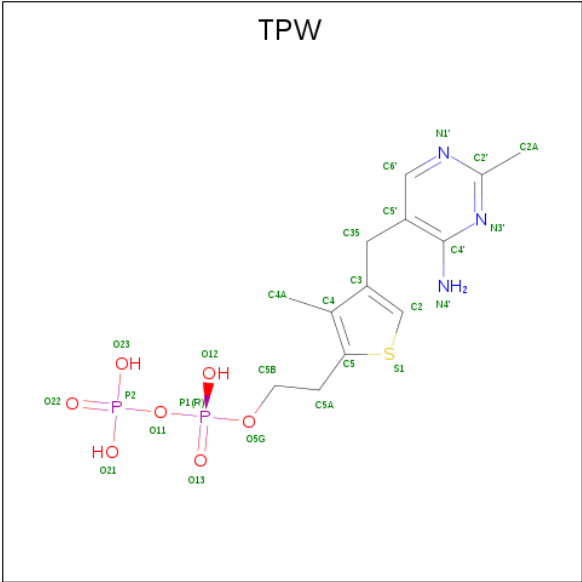
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP P51852
B	-15	HIS	-	EXPRESSION TAG	UNP P51852
B	-14	HIS	-	EXPRESSION TAG	UNP P51852
B	-13	HIS	-	EXPRESSION TAG	UNP P51852
B	-12	HIS	-	EXPRESSION TAG	UNP P51852
B	-11	HIS	-	EXPRESSION TAG	UNP P51852
B	-10	HIS	-	EXPRESSION TAG	UNP P51852
B	-9	SER	-	EXPRESSION TAG	UNP P51852
B	-8	SER	-	EXPRESSION TAG	UNP P51852
B	-7	GLY	-	EXPRESSION TAG	UNP P51852
B	-6	LEU	-	EXPRESSION TAG	UNP P51852
B	-5	VAL	-	EXPRESSION TAG	UNP P51852
B	-4	PRO	-	EXPRESSION TAG	UNP P51852
B	-3	ARG	-	EXPRESSION TAG	UNP P51852
B	-2	GLY	-	EXPRESSION TAG	UNP P51852
B	-1	SER	-	EXPRESSION TAG	UNP P51852
B	0	HIS	-	EXPRESSION TAG	UNP P51852
B	155	GLN	LEU	EXPRESSION TAG	UNP P51852
B	327	ARG	GLY	SEE REMARK 999	UNP P51852

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

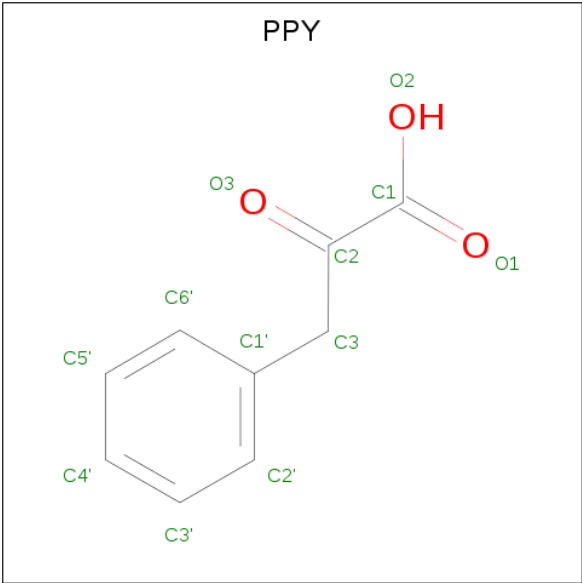
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYLTHIOPHEN-2-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: TPW) (formula: C₁₃H₁₉N₃O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		

- Molecule 4 is 3-PHENYLPYRUVIC ACID (three-letter code: PPY) (formula: C₉H₈O₃).



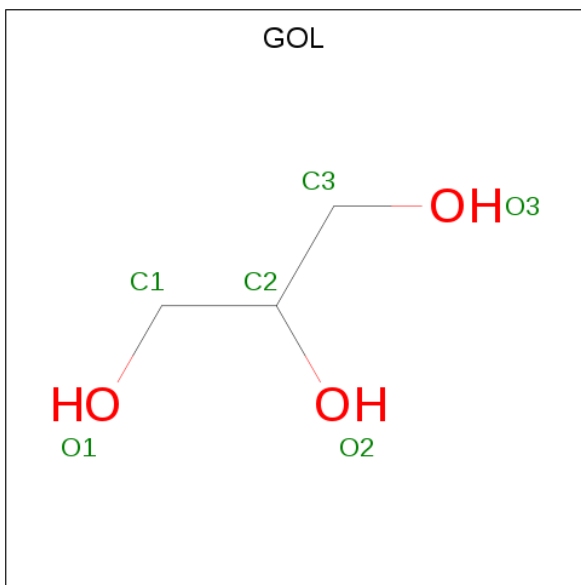
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	9	3		
4	A	1	Total	C	O	0	0
			12	9	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	9	3		
4	B	1	Total	C	O	0	0
			12	9	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

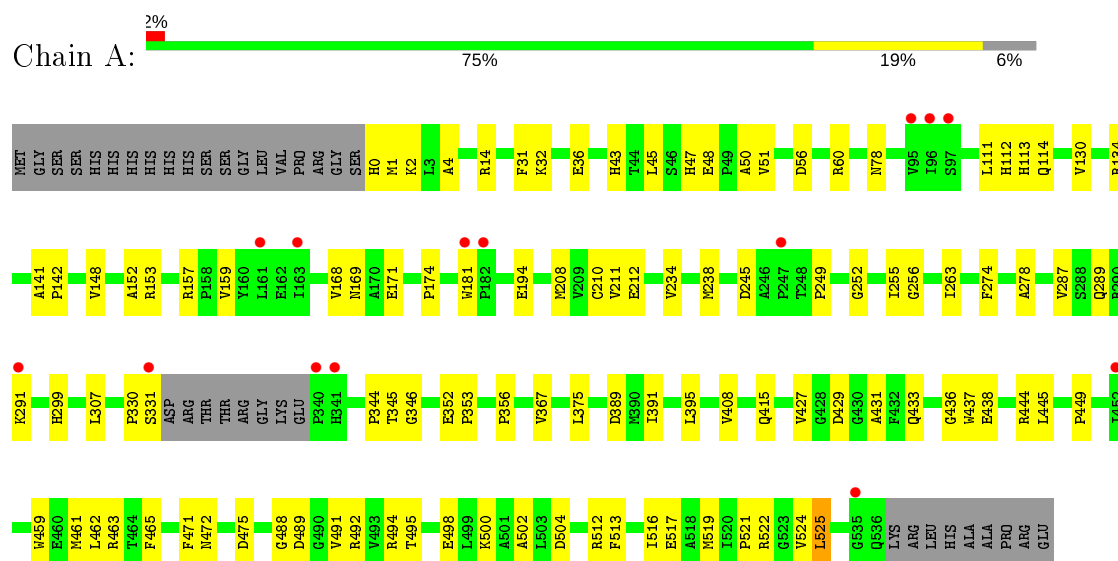
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	358	Total	O	0	0
			358	358		
6	B	381	Total	O	0	0
			381	381		

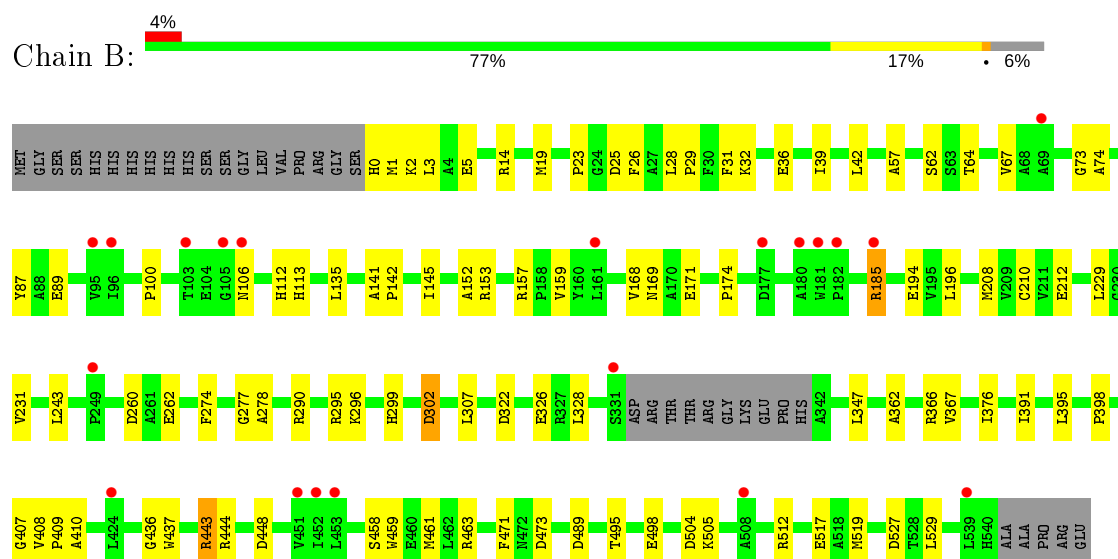
3 Residue-property plots

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

• Molecule 1: Phenylpyruvate decarboxylase



• Molecule 1: Phenylpyruvate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	74.90Å 145.58Å 194.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.10 – 2.15 28.10 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.8 (28.10-2.15) 93.5 (28.10-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.71 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.182 , 0.240 0.175 , 0.230	Depositor DCC
R_{free} test set	2754 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8762	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: TPW, GOL, MG, PPY

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	0.42	0/4026	0.66	0/5472
1	B	0.42	0/4052	0.64	1/5506 (0.0%)
All	All	0.42	0/8078	0.65	1/10978 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	TRP	N-CA-C	-6.11	94.49	111.00

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	3944	0	3941	79	0
1	B	3971	0	3979	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	1	0
4	A	24	0	14	0	0
4	B	24	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	8	1	0
6	A	358	0	0	9	0
6	B	381	0	0	11	0
All	All	8762	0	7988	148	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 9.

All (148) 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:2:LYS:HD2	1:A:169:ASN:HD22	1.24	1.01
1:A:111:LEU:H	1:A:114:GLN:HE21	1.04	0.91
1:A:463:ARG:HH12	1:A:522:ARG:HD3	1.39	0.87
1:B:517:GLU:HG2	1:B:519:MET:HE1	1.61	0.82
1:B:2:LYS:HD2	1:B:169:ASN:HD22	1.46	0.80
1:B:517:GLU:HG2	1:B:519:MET:CE	2.10	0.80
1:A:2:LYS:HD2	1:A:169:ASN:ND2	1.97	0.80
1:A:463:ARG:NH1	1:A:522:ARG:HD3	1.99	0.78
1:A:111:LEU:H	1:A:114:GLN:NE2	1.82	0.74
1:B:295:ARG:HD2	6:B:5061:HOH:O	1.90	0.71
1:A:517:GLU:HG2	1:A:519[A]:MET:CE	2.20	0.71
1:A:463:ARG:HH12	1:A:522:ARG:CD	2.03	0.71
1:B:290:ARG:HB2	6:B:5052:HOH:O	1.91	0.69
1:A:32:LYS:O	1:A:36:GLU:HG3	1.93	0.69
1:A:492:ARG:NE	1:A:519[A]:MET:HE3	2.09	0.68
1:B:463:ARG:NH2	1:B:473:ASP:OD1	2.27	0.68
1:B:443:ARG:HB3	1:B:443:ARG:HH11	1.59	0.66
1:B:32:LYS:O	1:B:36:GLU:HG3	1.96	0.65
1:A:210:CYS:HB3	1:A:278:ALA:HA	1.79	0.65
1:B:194:GLU:HG2	1:B:307:LEU:HD11	1.79	0.64
1:B:443:ARG:HH12	1:B:444:ARG:HB2	1.61	0.64
1:B:278:ALA:O	1:B:299:HIS:HE1	1.81	0.64
1:B:112:HIS:O	1:B:113:HIS:HB2	1.98	0.63
1:B:210:CYS:HB3	1:B:278:ALA:HA	1.80	0.63
1:B:106:ASN:HA	6:B:5113:HOH:O	1.98	0.63
1:B:135:LEU:HD11	1:B:145:ILE:HD11	1.80	0.62
1:B:135:LEU:CD1	1:B:145:ILE:HD11	2.30	0.62
1:A:111:LEU:O	1:A:114:GLN:HG2	2.00	0.61
1:A:494:ARG:NH1	6:A:5355:HOH:O	2.34	0.59
1:B:2:LYS:HD2	1:B:169:ASN:ND2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:NH1	6:A:5301:HOH:O	2.36	0.58
1:A:134:ARG:HD3	6:A:5299:HOH:O	2.04	0.58
1:A:444:ARG:HD2	6:A:5069:HOH:O	2.04	0.58
1:A:495:THR:OG1	1:A:498:GLU:HG3	2.04	0.57
1:B:347:LEU:HD22	1:B:362:ALA:HB2	1.85	0.57
1:B:25:ASP:HA	1:B:28:LEU:HD12	1.87	0.56
1:A:395:LEU:C	1:A:395:LEU:HD23	2.25	0.56
1:B:527:ASP:HB2	6:B:5385:HOH:O	2.06	0.56
1:B:1:MET:CE	1:B:174:PRO:HB3	2.35	0.55
1:A:517:GLU:HG2	1:A:519[A]:MET:HE1	1.87	0.55
1:B:196:LEU:HD11	1:B:328:LEU:HD21	1.89	0.55
1:B:495:THR:OG1	1:B:498:GLU:HG3	2.07	0.55
1:B:152:ALA:HB2	1:B:159:VAL:CG1	2.37	0.55
1:A:291:LYS:O	1:A:291:LYS:HG3	2.08	0.54
1:A:521:PRO:HG2	6:A:5260:HOH:O	2.07	0.54
1:A:500:LYS:HD3	1:A:504:ASP:OD2	2.08	0.53
1:A:249:PRO:HB3	6:A:5191:HOH:O	2.08	0.53
1:B:262:GLU:HG2	6:B:5273:HOH:O	2.08	0.53
1:B:14:ARG:HD3	1:B:153:ARG:HD2	1.91	0.52
3:A:2002:TPW:H2A2	1:B:74:ALA:O	2.10	0.52
1:A:289:GLN:HG2	6:A:5104:HOH:O	2.09	0.52
1:A:112:HIS:O	1:A:113:HIS:HB2	2.10	0.52
1:B:19:MET:HE1	1:B:42:LEU:HD13	1.92	0.52
1:A:352:GLU:HB3	1:A:353:PRO:HD2	1.92	0.51
1:A:427:VAL:HG23	1:A:431:ALA:HB3	1.91	0.51
1:B:408:VAL:HB	1:B:409:PRO:HD3	1.93	0.51
1:A:252:GLY:HA3	1:A:263:ILE:CD1	2.40	0.51
1:B:443:ARG:NH1	1:B:444:ARG:N	2.59	0.51
1:A:31:PHE:HB3	1:B:471:PHE:CE2	2.46	0.50
1:A:210:CYS:CB	1:A:278:ALA:HA	2.41	0.50
1:A:208:MET:HA	1:A:234:VAL:O	2.12	0.50
1:A:4:ALA:HB2	1:A:168:VAL:HG13	1.94	0.50
1:B:505:LYS:HE3	6:B:5129:HOH:O	2.12	0.50
1:A:408:VAL:HG21	1:A:436:GLY:HA2	1.94	0.49
1:A:463:ARG:HH12	1:A:522:ARG:CG	2.24	0.49
1:A:130:VAL:HG11	1:A:157:ARG:HD2	1.93	0.49
1:A:459:TRP:HE3	1:A:472:ASN:HD22	1.60	0.49
1:B:141:ALA:HB3	1:B:142:PRO:HD3	1.94	0.48
1:B:210:CYS:CB	1:B:278:ALA:HA	2.42	0.48
1:B:322:ASP:O	1:B:326:GLU:HG3	2.12	0.48
1:A:255:ILE:HG22	1:A:255:ILE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ASP:OD2	1:B:262:GLU:HB2	2.13	0.48
1:A:502:ALA:HB1	1:A:516:ILE:HD12	1.96	0.48
1:B:461:MET:HG3	1:B:529:LEU:HD11	1.96	0.48
1:B:19:MET:HG3	1:B:67:VAL:HG12	1.96	0.48
1:B:376:ILE:O	1:B:395:LEU:HA	2.13	0.47
1:A:475:ASP:OD2	1:B:443:ARG:NH1	2.48	0.47
1:B:152:ALA:HB2	1:B:159:VAL:HG11	1.95	0.47
1:A:56:ASP:O	1:A:60:ARG:HG3	2.14	0.47
1:A:429:ASP:O	1:A:433:GLN:HG3	2.14	0.47
1:A:524:VAL:C	1:A:525:LEU:HD23	2.35	0.47
1:B:367:VAL:HG11	1:B:391:ILE:HG21	1.96	0.47
1:A:148:VAL:CG1	1:A:159:VAL:HB	2.45	0.47
1:B:489:ASP:OD1	1:B:512:ARG:NH1	2.48	0.47
1:B:3:LEU:HD23	1:B:3:LEU:C	2.35	0.46
1:B:0:HIS:HB3	1:B:171:GLU:CG	2.45	0.46
1:B:87:TYR:O	1:B:157:ARG:NH1	2.49	0.46
1:B:62:SER:HB2	1:B:64:THR:HG22	1.97	0.46
1:B:505:LYS:HD3	6:B:5227:HOH:O	2.15	0.46
1:B:229:LEU:HB3	1:B:231:VAL:HG13	1.98	0.46
1:B:212:GLU:HB2	1:B:277:GLY:HA3	1.97	0.45
1:A:491:VAL:HG13	1:A:491:VAL:O	2.16	0.45
1:A:181:TRP:HB3	6:A:5250:HOH:O	2.17	0.45
1:B:5:GLU:HG3	1:B:39:ILE:HD11	1.99	0.45
1:A:141:ALA:HB3	1:A:142:PRO:HD3	1.97	0.45
1:A:0:HIS:HB3	1:A:171:GLU:CG	2.47	0.45
1:B:29:PRO:HB2	1:B:168:VAL:HG21	1.99	0.45
1:B:458:SER:OG	1:B:463:ARG:NH1	2.50	0.45
1:A:367:VAL:HG11	1:A:391:ILE:HG21	1.99	0.45
1:A:211:VAL:HG23	1:A:212:GLU:H	1.83	0.44
1:A:356:PRO:HD3	1:A:524:VAL:HG12	1.99	0.44
1:B:243:LEU:N	1:B:243:LEU:HD12	2.32	0.44
1:A:1:MET:CE	1:A:174:PRO:HG3	2.47	0.44
1:A:211:VAL:HG23	1:A:212:GLU:N	2.33	0.43
1:A:415:GLN:HE22	1:A:449:PRO:HA	1.83	0.43
1:A:50:ALA:HB2	1:A:438:GLU:HG3	2.00	0.43
1:A:278:ALA:O	1:A:299:HIS:HE1	2.00	0.43
1:B:302:ASP:HA	6:B:5279:HOH:O	2.17	0.43
1:A:492:ARG:HG3	1:A:519[A]:MET:HE3	2.00	0.43
1:B:141:ALA:O	1:B:145:ILE:HG12	2.18	0.43
1:B:57:ALA:HB2	1:B:410:ALA:HA	2.00	0.43
1:A:345:THR:OG1	1:A:346:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:0:HIS:HB3	1:B:171:GLU:HG2	2.00	0.43
1:A:256:GLY:HA3	1:A:287:VAL:HG13	2.00	0.43
1:A:32:LYS:HE2	6:A:5225:HOH:O	2.18	0.43
1:B:2:LYS:HB2	1:B:2:LYS:HE3	1.80	0.43
1:A:437:TRP:CD1	1:B:437:TRP:CD1	3.06	0.43
1:B:1:MET:HE3	1:B:174:PRO:HB3	2.00	0.43
1:A:488:GLY:HA3	1:A:513:PHE:CE2	2.55	0.42
1:B:19:MET:CE	1:B:42:LEU:HD13	2.48	0.42
1:A:14:ARG:HD3	1:A:153:ARG:HD2	2.02	0.42
1:B:296:LYS:HD2	6:B:5116:HOH:O	2.19	0.42
1:A:489:ASP:OD1	1:A:512:ARG:HD2	2.20	0.42
1:A:492:ARG:HG3	1:A:519[A]:MET:CE	2.49	0.42
1:A:148:VAL:HG13	1:A:159:VAL:HB	2.02	0.42
1:A:287:VAL:HG22	1:A:287:VAL:O	2.19	0.42
1:A:330:PRO:O	1:A:331:SER:C	2.57	0.42
1:A:344:PRO:HG3	1:A:389:ASP:HB3	2.02	0.42
1:A:47:HIS:CD2	1:A:78:ASN:HD21	2.38	0.42
1:A:471:PHE:CE2	1:B:31:PHE:HB3	2.54	0.42
1:B:112:HIS:O	1:B:113:HIS:CB	2.66	0.42
1:A:48:GLU:OE2	3:B:2001:TPW:N1'	2.52	0.42
1:A:211:VAL:HG13	1:A:238:MET:HG3	2.02	0.41
1:B:448:ASP:HB2	1:B:512:ARG:O	2.20	0.41
1:A:194:GLU:HG2	1:A:307:LEU:HD11	2.03	0.41
1:A:43:HIS:HB3	1:A:445:LEU:CD2	2.50	0.41
1:B:89:GLU:OE1	1:B:398:PRO:HA	2.20	0.41
1:B:366:ARG:NH1	1:B:504:ASP:OD1	2.49	0.41
1:A:152:ALA:HB2	1:A:159:VAL:CG1	2.51	0.41
1:B:26:PHE:CE1	1:B:100:PRO:HA	2.56	0.41
1:A:427:VAL:CG2	1:A:431:ALA:HB3	2.51	0.41
1:A:462:LEU:CD1	1:B:23:PRO:HG2	2.50	0.41
5:B:5005:GOL:H32	6:B:5069:HOH:O	2.21	0.41
1:B:185:ARG:HG3	6:B:5361:HOH:O	2.19	0.40
1:A:252:GLY:HA3	1:A:263:ILE:HD11	2.04	0.40
1:A:45:LEU:HD12	1:A:51:VAL:HA	2.03	0.40
1:B:408:VAL:HG21	1:B:436:GLY:HA2	2.03	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	526/565 (93%)	515 (98%)	11 (2%)	0	100	100
1	B	528/565 (94%)	512 (97%)	14 (3%)	2 (0%)	34	29
All	All	1054/1130 (93%)	1027 (97%)	25 (2%)	2 (0%)	47	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73	GLY
1	B	407	GLY

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	395/426 (93%)	389 (98%)	6 (2%)	65	69
1	B	398/426 (93%)	394 (99%)	4 (1%)	76	81
All	All	793/852 (93%)	783 (99%)	10 (1%)	69	74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	ASP
1	A	274	PHE
1	A	375	LEU
1	A	461	MET

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Mol	Chain	Res	Type
1	A	465	PHE
1	A	525	LEU
1	B	185	ARG
1	B	274	PHE
1	B	302	ASP
1	B	443	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	169	ASN
1	A	289	GLN
1	A	299	HIS
1	A	415	GLN
1	A	466	GLN
1	A	472	ASN
1	A	536	GLN
1	B	169	ASN
1	B	299	HIS
1	B	415	GLN
1	B	472	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GOL	B	5005	-	5,5,5	0.60	0	5,5,5	0.75	0
3	TPW	B	2001	2	23,27,27	2.72	6 (26%)	30,40,40	2.40	9 (30%)
4	PPY	B	5002	-	9,12,12	1.16	0	10,15,15	0.57	0
4	PPY	A	5003	-	9,12,12	1.09	0	10,15,15	0.55	0
4	PPY	A	5001	-	9,12,12	1.23	0	10,15,15	0.71	0
4	PPY	B	5004	-	9,12,12	1.17	0	10,15,15	0.49	0
3	TPW	A	2002	2	23,27,27	2.10	5 (21%)	30,40,40	2.35	9 (30%)

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
5	GOL	B	5005	-	-	0/4/4/4	-
3	TPW	B	2001	2	-	1/16/17/17	0/2/2/2
4	PPY	B	5002	-	-	2/4/8/8	0/1/1/1
4	PPY	A	5003	-	-	2/4/8/8	0/1/1/1
4	PPY	A	5001	-	-	2/4/8/8	0/1/1/1
4	PPY	B	5004	-	-	2/4/8/8	0/1/1/1
3	TPW	A	2002	2	-	1/16/17/17	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	TPW	C5A-C5	-8.86	1.47	1.50
3	A	2002	TPW	C2-C3	-7.23	1.32	1.37
3	B	2001	TPW	C2-C3	-5.72	1.33	1.37
3	B	2001	TPW	C2-S1	3.16	1.75	1.70
3	B	2001	TPW	C35-C3	3.12	1.58	1.52
3	A	2002	TPW	P1-O13	3.01	1.61	1.50
3	B	2001	TPW	C5'-C4'	2.82	1.47	1.42
3	A	2002	TPW	C35-C3	2.80	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	TPW	P1-O13	2.62	1.60	1.50
3	A	2002	TPW	C35-C5'	2.54	1.57	1.52
3	A	2002	TPW	C5'-C4'	2.49	1.47	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	TPW	C3-C2-S1	-8.33	103.39	112.26
3	A	2002	TPW	C3-C2-S1	-7.68	104.08	112.26
3	A	2002	TPW	P1-O11-P2	-5.54	113.81	132.83
3	B	2001	TPW	P1-O11-P2	-5.20	115.00	132.83
3	B	2001	TPW	C6'-N1'-C2'	3.42	121.78	115.96
3	A	2002	TPW	C2-C3-C4	3.34	118.92	110.34
3	A	2002	TPW	C6'-N1'-C2'	3.34	121.64	115.96
3	B	2001	TPW	C2-C3-C4	3.24	118.65	110.34
3	A	2002	TPW	P1-O5G-C5B	-2.46	109.48	121.59
3	A	2002	TPW	N1'-C2'-N3'	-2.44	121.34	125.54
3	B	2001	TPW	N1'-C2'-N3'	-2.43	121.36	125.54
3	B	2001	TPW	O21-P2-O11	2.38	112.61	104.64
3	B	2001	TPW	C5'-C6'-N1'	-2.27	120.04	123.82
3	B	2001	TPW	P1-O5G-C5B	-2.26	110.46	121.59
3	B	2001	TPW	C35-C3-C4	-2.08	122.77	126.49
3	A	2002	TPW	C2'-N3'-C4'	2.07	121.31	118.08
3	A	2002	TPW	O21-P2-O11	2.06	111.54	104.64
3	A	2002	TPW	C5'-C6'-N1'	-2.04	120.42	123.82

There are no chirality outliers.

All (10) torsion outliers are listed below:

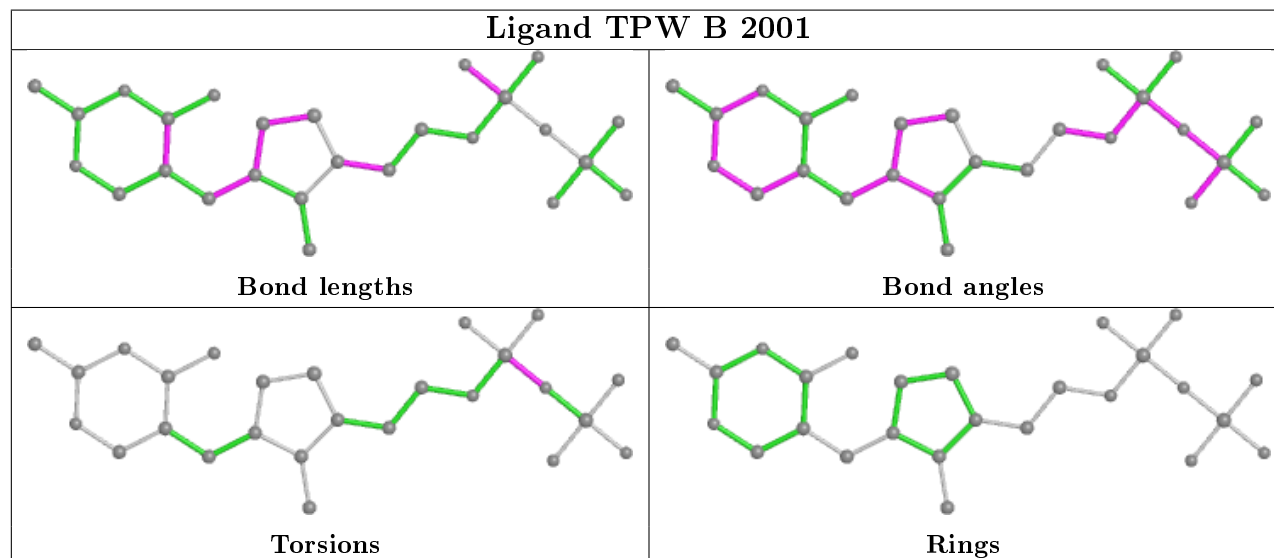
Mol	Chain	Res	Type	Atoms
4	A	5003	PPY	C1-C2-C3-C1'
4	A	5003	PPY	O3-C2-C3-C1'
4	A	5001	PPY	C1-C2-C3-C1'
4	B	5004	PPY	C1-C2-C3-C1'
3	B	2001	TPW	P2-O11-P1-O5G
3	A	2002	TPW	P2-O11-P1-O5G
4	B	5002	PPY	C1-C2-C3-C1'
4	B	5002	PPY	O3-C2-C3-C1'
4	A	5001	PPY	O3-C2-C3-C1'
4	B	5004	PPY	O3-C2-C3-C1'

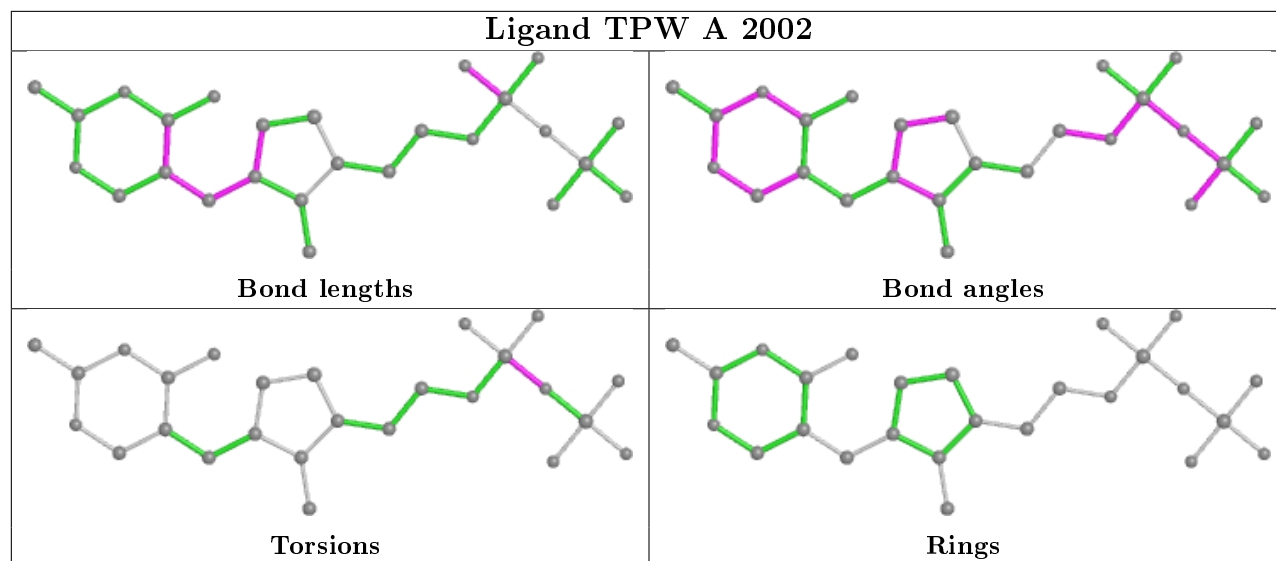
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5005	GOL	1	0
3	B	2001	TPW	1	0
3	A	2002	TPW	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	529/565 (93%)	-0.11	14 (2%) 56 64	23, 36, 56, 80	0
1	B	531/565 (93%)	-0.09	20 (3%) 40 49	25, 37, 56, 78	0
All	All	1060/1130 (93%)	-0.10	34 (3%) 47 56	23, 37, 56, 80	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	HIS	4.9
1	A	181	TRP	4.7
1	A	340	PRO	4.1
1	B	181	TRP	4.1
1	B	96	ILE	4.1
1	A	182	PRO	3.7
1	B	182	PRO	3.6
1	B	106	ASN	3.6
1	A	96	ILE	3.3
1	B	95	VAL	3.3
1	B	331	SER	3.2
1	A	163	ILE	3.0
1	A	161	LEU	2.9
1	B	180	ALA	2.8
1	B	161	LEU	2.7
1	A	291	LYS	2.7
1	B	103	THR	2.7
1	A	95	VAL	2.6
1	B	452	ILE	2.6
1	B	177	ASP	2.5
1	A	247	PRO	2.5
1	B	539	LEU	2.5
1	B	508	ALA	2.3
1	A	331	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	451	VAL	2.2
1	A	535	GLY	2.2
1	B	453	LEU	2.2
1	B	105	GLY	2.2
1	B	185	ARG	2.2
1	B	249	PRO	2.2
1	B	424	LEU	2.1
1	A	97	SER	2.1
1	B	69	ALA	2.1
1	A	452	ILE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

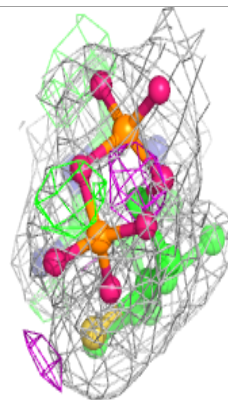
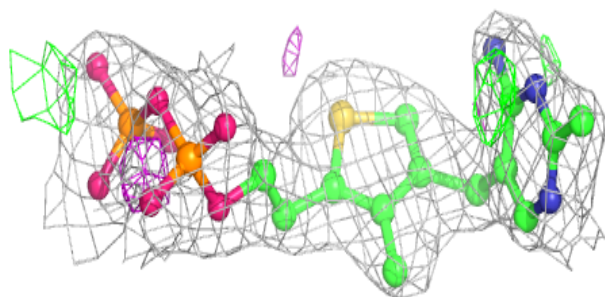
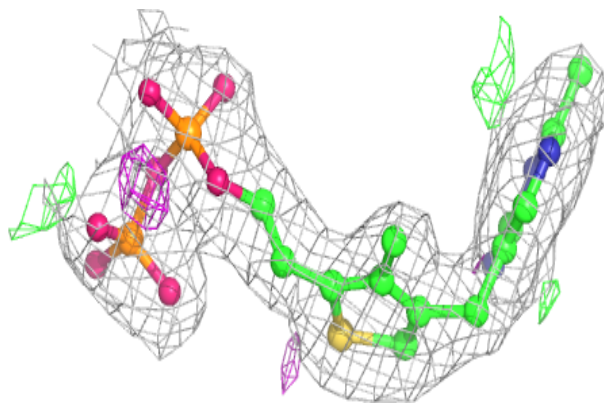
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PPY	B	5004	12/12	0.85	0.16	45,51,61,63	0
5	GOL	B	5005	6/6	0.87	0.20	52,60,64,65	0
4	PPY	B	5002	12/12	0.87	0.18	60,66,72,74	0
4	PPY	A	5003	12/12	0.88	0.13	45,53,64,68	0
4	PPY	A	5001	12/12	0.94	0.12	32,40,47,48	0
2	MG	B	4001	1/1	0.95	0.06	32,32,32,32	0
2	MG	A	4002	1/1	0.95	0.04	33,33,33,33	0
3	TPW	A	2002	26/26	0.97	0.12	29,36,43,48	0
3	TPW	B	2001	26/26	0.98	0.10	25,29,33,35	0

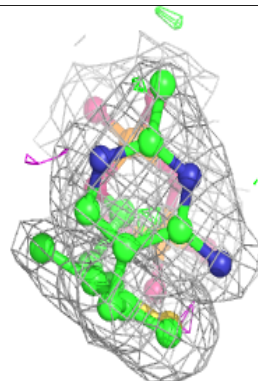
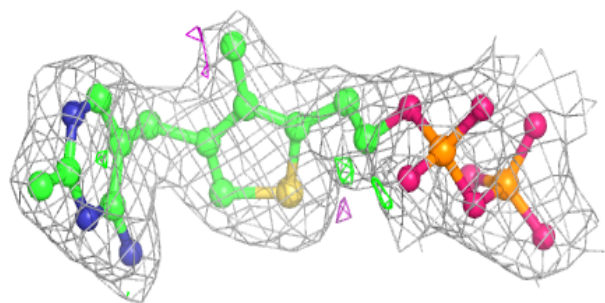
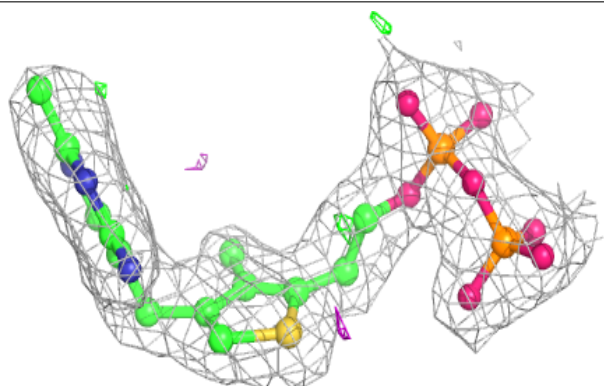
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPW A 2002:

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

**Electron density around TPW B 2001:**

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



6.5 Other polymers

There are no such residues in this entry.