



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:51 AM UTC

PDB ID : 1ELU / pdb_00001elu
Title : COMPLEX BETWEEN THE CYSTINE C-S LYASE C-DES AND ITS REACTION PRODUCT CYSTEINE PERSULFIDE.
Authors : Clausen, T.; Kaiser, J.T.; Steegborn, C.; Huber, R.; Kessler, D.
Deposited on : 2000-03-14
Resolution : 1.55 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

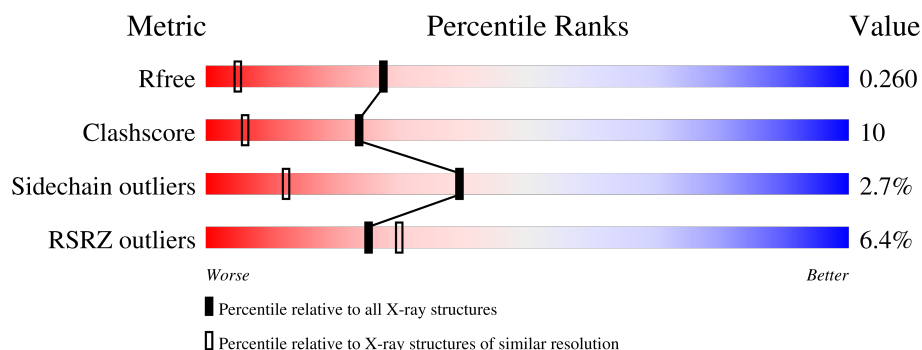
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	390	3% 79% 17% ..
1	B	390	10% 76% 20% ..

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
3	PDA	A	400	X	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PDA	B	400	X	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6680 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 L-CYSTEINE/L-CYSTINE C-S LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2943	1880	514	538	11			
1	B	381	Total	C	N	O	S	0	0	0
			2933	1875	510	537	11			

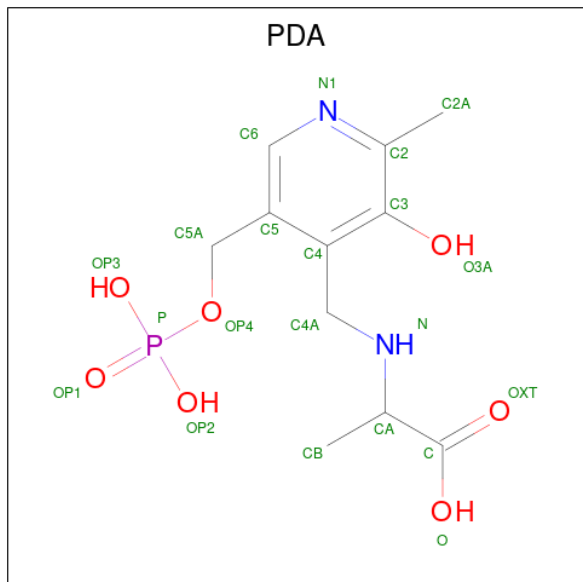
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	engineered mutation	UNP Q9ZHG9
A	5	THR	-	engineered mutation	UNP Q9ZHG9
A	6	MET	-	engineered mutation	UNP Q9ZHG9
A	7	ILE	-	engineered mutation	UNP Q9ZHG9
A	8	THR	-	engineered mutation	UNP Q9ZHG9
A	9	PRO	-	engineered mutation	UNP Q9ZHG9
A	10	SER	-	engineered mutation	UNP Q9ZHG9
A	11	LEU	-	engineered mutation	UNP Q9ZHG9
B	4	MET	-	engineered mutation	UNP Q9ZHG9
B	5	THR	-	engineered mutation	UNP Q9ZHG9
B	6	MET	-	engineered mutation	UNP Q9ZHG9
B	7	ILE	-	engineered mutation	UNP Q9ZHG9
B	8	THR	-	engineered mutation	UNP Q9ZHG9
B	9	PRO	-	engineered mutation	UNP Q9ZHG9
B	10	SER	-	engineered mutation	UNP Q9ZHG9
B	11	LEU	-	engineered mutation	UNP Q9ZHG9

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

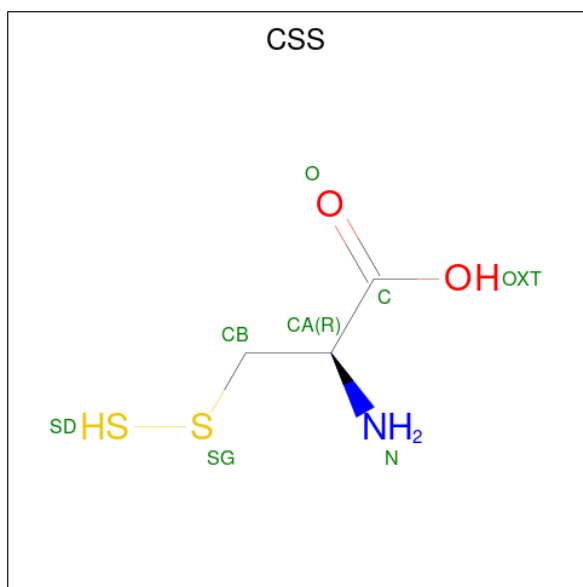
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-PROPIONIC ACID (CCD ID: PDA) (formula: $C_{11}H_{17}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 4 is S-MERCAPTOCYSTEINE (CCD ID: CSS) (formula: $C_3H_7NO_2S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			8	3	1	2	2		

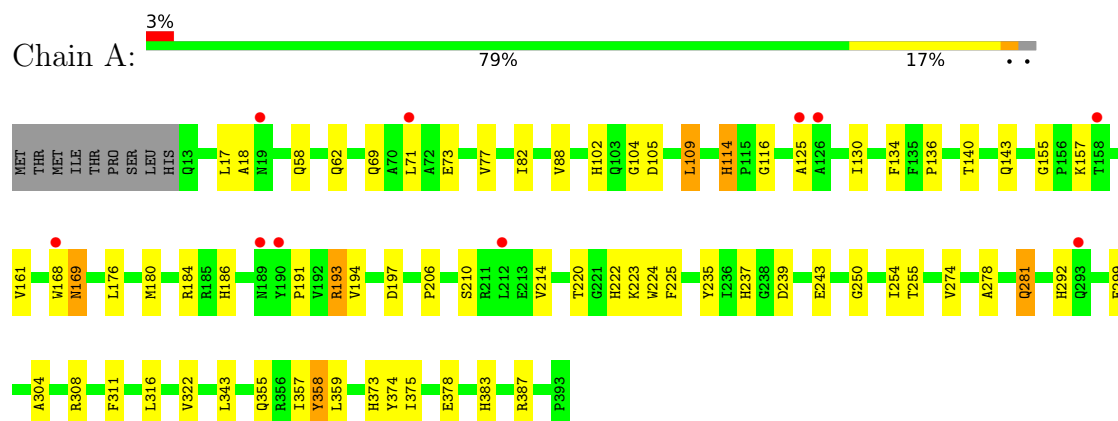
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	377	Total	O	0	0
			377	377		
5	B	375	Total	O	0	0
			375	375		

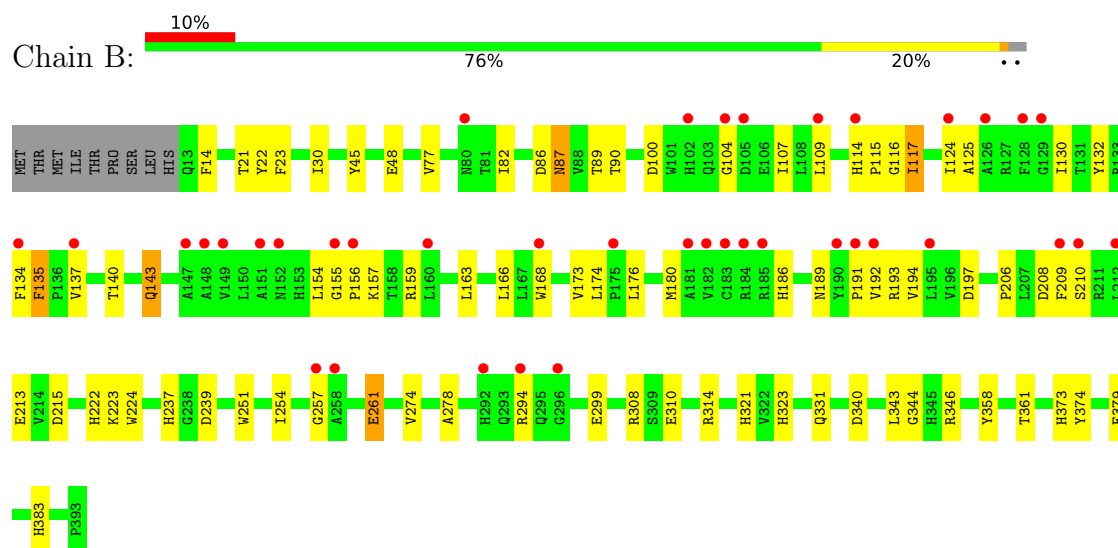
3 Residue-property plots

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: L-CYSTEINE/L-CYSTINE C-S LYASE



• Molecule 1: L-CYSTEINE/L-CYSTINE C-S LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.45Å 65.39Å 170.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.55 25.00 – 1.55	Depositor EDS
% Data completeness (in resolution range)	93.7 (25.00-1.55) 93.7 (25.00-1.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.55Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.259 0.214 , 0.260	Depositor DCC
R_{free} test set	4786 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6680	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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: CSS, PDA, K

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	0.65	0/3019	1.02	13/4120 (0.3%)
1	B	0.64	0/3009	1.03	18/4108 (0.4%)
All	All	0.64	0/6028	1.03	31/8228 (0.4%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	LEU	N-CA-C	10.39	122.69	111.36
1	A	18	ALA	N-CA-C	9.46	122.56	111.02
1	B	343	LEU	N-CA-C	8.59	120.64	111.28
1	A	254	ILE	N-CA-C	8.03	120.69	109.29
1	B	191	PRO	N-CA-C	-7.65	98.49	110.50
1	B	14	PHE	CA-C-N	7.43	127.79	119.32
1	B	14	PHE	C-N-CA	7.43	127.79	119.32
1	A	255	THR	N-CA-C	-7.06	99.47	110.42
1	A	191	PRO	N-CA-C	-7.00	99.51	110.50
1	A	210	SER	N-CA-C	-6.33	102.93	112.04
1	A	176	LEU	N-CA-C	6.32	118.70	111.11
1	B	22	TYR	N-CA-C	6.14	118.72	108.96
1	B	135	PHE	N-CA-C	-6.13	101.06	110.32
1	B	210	SER	N-CA-C	-6.13	105.93	113.41
1	A	358	TYR	N-CA-C	6.06	118.72	107.99
1	A	82	ILE	N-CA-C	6.05	116.64	108.17
1	B	254	ILE	N-CA-C	5.97	117.44	108.96
1	A	222	HIS	N-CA-C	5.87	120.43	113.16
1	A	274	VAL	N-CA-C	5.83	121.46	109.34
1	B	358	TYR	N-CA-C	5.74	118.15	107.99
1	B	274	VAL	N-CA-C	5.74	121.27	109.34
1	B	206	PRO	N-CA-C	-5.58	102.37	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	VAL	N-CA-C	5.57	116.20	108.84
1	B	82	ILE	N-CA-C	5.35	115.66	108.17
1	B	48	GLU	N-CA-C	5.32	117.16	111.36
1	A	136	PRO	N-CA-C	5.29	118.81	110.50
1	A	206	PRO	N-CA-C	-5.26	101.59	110.21
1	B	294	ARG	N-CA-C	-5.23	105.76	111.82
1	B	344	GLY	N-CA-C	-5.15	106.25	112.48
1	B	222	HIS	N-CA-C	5.05	119.42	113.16
1	B	194	VAL	N-CA-C	5.01	115.07	107.75

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	2943	0	2869	67	0
1	B	2933	0	2852	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	21	0	12	6	0
3	B	21	0	12	3	0
4	A	8	0	7	3	0
5	A	377	0	0	8	0
5	B	375	0	0	6	0
All	All	6680	0	5752	118	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 10.

All (118) 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:125:ALA:HA	1:B:130:ILE:HG13	1.43	0.97
1:A:355:GLN:HE22	1:A:387:ARG:HE	1.03	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLN:NE2	1:A:387:ARG:HE	1.64	0.94
1:B:237:HIS:HD2	1:B:239:ASP:H	1.18	0.92
1:A:169:ASN:H	1:A:169:ASN:HD22	1.29	0.81
1:A:114:HIS:ND1	4:A:2001:CSS:SD	2.54	0.81
1:A:180:MET:HE1	1:A:194:VAL:HG21	1.61	0.81
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.47	0.79
1:A:278:ALA:HB1	1:A:281:GLN:NE2	1.97	0.79
1:A:278:ALA:HB3	5:A:2138:HOH:O	1.84	0.76
1:A:17:LEU:HD11	1:A:375:ILE:HD12	1.66	0.76
1:A:125:ALA:HA	1:A:130:ILE:HG13	1.67	0.74
1:A:225:PHE:O	1:A:292:HIS:HE1	1.71	0.74
1:A:355:GLN:HE22	1:A:387:ARG:NE	1.84	0.72
1:A:373:HIS:CD2	1:A:374:TYR:H	2.08	0.71
1:B:299:GLU:HG2	5:B:1170:HOH:O	1.89	0.71
1:B:323:HIS:HE1	1:B:340:ASP:OD1	1.75	0.70
1:A:180:MET:HE1	1:A:194:VAL:CB	2.22	0.70
1:B:379:GLU:HG2	5:B:1209:HOH:O	1.92	0.70
1:A:180:MET:HE1	1:A:194:VAL:CG2	2.21	0.69
1:A:237:HIS:HD2	1:A:239:ASP:H	1.40	0.68
1:B:237:HIS:CD2	1:B:239:ASP:H	2.07	0.68
1:B:87:ASN:ND2	1:B:90:THR:H	1.92	0.68
1:A:373:HIS:HD2	1:A:374:TYR:H	1.40	0.67
1:A:223:LYS:HE3	3:A:400:PDA:H4A1	1.76	0.67
1:A:237:HIS:CD2	1:A:239:ASP:H	2.13	0.67
1:A:180:MET:HA	1:A:180:MET:HE2	1.79	0.65
1:A:105:ASP:HB2	1:A:130:ILE:HG22	1.79	0.64
1:A:355:GLN:NE2	1:A:387:ARG:NE	2.40	0.64
1:A:223:LYS:NZ	3:A:400:PDA:H4A1	2.14	0.63
1:B:310:GLU:HG2	1:B:314:ARG:HH11	1.64	0.62
1:B:223:LYS:NZ	3:B:400:PDA:H4A1	2.15	0.62
1:A:223:LYS:CE	3:A:400:PDA:H4A1	2.30	0.62
1:A:114:HIS:NE2	1:A:168:TRP:CE3	2.68	0.61
1:A:193:ARG:HH11	1:A:193:ARG:HG3	1.65	0.60
1:B:278:ALA:HB3	5:B:1288:HOH:O	2.01	0.59
1:A:114:HIS:NE2	1:A:168:TRP:CD2	2.70	0.59
1:A:278:ALA:HB1	1:A:281:GLN:HE21	1.68	0.58
1:A:197:ASP:OD1	3:A:400:PDA:N1	2.36	0.58
1:B:223:LYS:HZ1	3:B:400:PDA:H4A1	1.69	0.58
1:A:292:HIS:HD2	1:A:374:TYR:OH	1.87	0.57
1:A:180:MET:CE	1:A:194:VAL:HG21	2.34	0.56
1:B:193:ARG:HG2	1:B:193:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLY:O	1:B:157:LYS:HE2	2.06	0.55
1:B:373:HIS:CD2	1:B:374:TYR:H	2.23	0.55
1:A:357:ILE:CD1	1:A:387:ARG:HG3	2.37	0.55
1:A:169:ASN:H	1:A:169:ASN:ND2	2.01	0.54
1:A:169:ASN:HD22	1:A:169:ASN:N	1.99	0.54
1:A:223:LYS:HZ1	3:A:400:PDA:HB3	1.73	0.54
1:A:102:HIS:HE1	5:A:2076:HOH:O	1.91	0.53
1:B:180:MET:HE2	1:B:213:GLU:O	2.08	0.53
1:A:184:ARG:HG2	1:A:184:ARG:NH1	2.20	0.52
1:A:387:ARG:NH1	5:A:2238:HOH:O	2.43	0.52
1:A:304:ALA:O	1:A:308:ARG:HG2	2.09	0.51
1:B:310:GLU:HG2	1:B:314:ARG:NH1	2.25	0.51
1:A:383:HIS:O	1:A:387:ARG:HG2	2.10	0.51
1:A:193:ARG:HG3	5:A:2298:HOH:O	2.11	0.51
1:A:223:LYS:NZ	3:A:400:PDA:HB3	2.26	0.51
1:B:173:VAL:H	1:B:331:GLN:NE2	2.09	0.50
1:A:88:VAL:HG23	1:A:220:THR:HB	1.93	0.49
1:A:225:PHE:O	1:A:292:HIS:CE1	2.60	0.49
1:A:77:VAL:HG11	1:A:235:TYR:CE2	2.48	0.49
1:A:180:MET:HE1	1:A:194:VAL:HG11	1.94	0.49
5:A:2151:HOH:O	1:B:30:ILE:HD12	2.11	0.49
1:B:237:HIS:HD2	1:B:239:ASP:N	1.99	0.49
1:B:100:ASP:O	1:B:159:ARG:NH1	2.46	0.49
1:A:193:ARG:NH1	1:A:243:GLU:OE1	2.46	0.48
1:B:193:ARG:HD2	1:B:215:ASP:CG	2.38	0.48
1:B:116:GLY:HA3	5:B:1079:HOH:O	2.12	0.48
1:B:321:HIS:HD2	5:B:1165:HOH:O	1.95	0.48
1:A:155:GLY:O	1:A:186:HIS:HE1	1.97	0.48
1:A:357:ILE:HD11	1:A:387:ARG:HG3	1.96	0.48
1:B:21:THR:OG1	1:B:383:HIS:HD2	1.96	0.48
1:A:316:LEU:HD22	1:A:322:VAL:HG11	1.96	0.47
1:A:224:TRP:O	1:A:373:HIS:HE1	1.96	0.47
1:A:104:GLY:O	1:A:157:LYS:HD3	2.15	0.47
1:B:137:VAL:HG11	1:B:174:LEU:HD21	1.96	0.47
1:B:163:LEU:HD12	1:B:163:LEU:C	2.39	0.47
1:B:168:TRP:CD1	1:B:168:TRP:H	2.33	0.47
1:A:114:HIS:CE1	4:A:2001:CSS:HD	2.22	0.47
1:B:107:ILE:O	1:B:132:TYR:HA	2.15	0.47
1:B:109:LEU:O	1:B:134:PHE:HA	2.16	0.46
4:A:2001:CSS:SD	1:B:251:TRP:HB3	2.56	0.45
1:A:180:MET:HE1	1:A:194:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:THR:HA	1:B:143:GLN:O	2.17	0.45
1:A:109:LEU:O	1:A:134:PHE:HA	2.17	0.44
1:B:197:ASP:OD1	3:B:400:PDA:N1	2.50	0.44
1:B:21:THR:HG22	1:B:23:PHE:HE1	1.83	0.44
5:A:2151:HOH:O	1:B:30:ILE:CD1	2.65	0.44
1:A:161:VAL:HB	1:A:194:VAL:HG22	1.99	0.44
1:B:346:ARG:HA	1:B:361:THR:HG21	1.99	0.44
1:A:250:GLY:HA3	1:B:89:THR:HG21	2.00	0.43
1:A:180:MET:HE1	1:A:194:VAL:HB	1.97	0.43
1:A:58:GLN:O	1:A:62:GLN:HG3	2.18	0.43
1:B:176:LEU:O	1:B:180:MET:HG2	2.18	0.43
1:A:358:TYR:C	1:A:359:LEU:HD12	2.43	0.43
1:B:86:ASP:CG	5:B:1216:HOH:O	2.61	0.43
1:B:224:TRP:O	1:B:373:HIS:HE1	2.01	0.43
1:B:156:PRO:O	1:B:189:ASN:HB2	2.19	0.43
1:A:281:GLN:NE2	1:A:281:GLN:H	2.16	0.43
1:A:373:HIS:CD2	1:A:374:TYR:N	2.83	0.42
1:B:114:HIS:CG	1:B:115:PRO:HD2	2.54	0.42
1:B:45:TYR:CD1	1:B:45:TYR:C	2.98	0.42
1:B:373:HIS:HD2	1:B:374:TYR:H	1.65	0.42
1:A:116:GLY:HA3	5:A:2283:HOH:O	2.18	0.42
1:A:69:GLN:HE21	1:A:73:GLU:CG	2.33	0.42
1:B:77:VAL:CG1	1:B:209:PHE:HB2	2.50	0.42
1:B:208:ASP:OD2	1:B:208:ASP:C	2.63	0.42
1:B:124:ILE:HG22	1:B:130:ILE:HG12	2.01	0.41
1:B:117:ILE:N	1:B:117:ILE:HD13	2.36	0.41
1:A:69:GLN:HE21	1:A:73:GLU:HG3	1.85	0.41
1:A:311:PHE:CE1	1:A:378:GLU:HG2	2.55	0.41
1:A:140:THR:HA	1:A:143:GLN:O	2.21	0.41
1:B:155:GLY:O	1:B:186:HIS:CE1	2.74	0.41
5:A:2195:HOH:O	1:B:261:GLU:HA	2.20	0.40
1:B:87:ASN:HD21	1:B:90:THR:H	1.69	0.40
1:B:257:GLY:HA3	1:B:261:GLU:OE1	2.20	0.40
1:B:87:ASN:HD22	1:B:90:THR:H	1.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	300/311 (96%)	292 (97%)	8 (3%)	39	12
1	B	298/311 (96%)	290 (97%)	8 (3%)	39	12
All	All	598/622 (96%)	582 (97%)	16 (3%)	39	12

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	109	LEU
1	A	114	HIS
1	A	169	ASN
1	A	193	ARG
1	A	214	VAL
1	A	281	GLN
1	A	299	GLU
1	B	87	ASN
1	B	117	ILE
1	B	135	PHE
1	B	143	GLN
1	B	154	LEU
1	B	166	LEU
1	B	261	GLU
1	B	308	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	80	ASN
1	A	102	HIS
1	A	103	GLN
1	A	143	GLN
1	A	152	ASN
1	A	169	ASN
1	A	172	GLN
1	A	186	HIS
1	A	187	GLN
1	A	237	HIS
1	A	281	GLN
1	A	292	HIS
1	A	321	HIS
1	A	350	GLN
1	A	355	GLN
1	A	373	HIS
1	B	58	GLN
1	B	87	ASN
1	B	103	GLN
1	B	122	GLN
1	B	143	GLN
1	B	186	HIS
1	B	237	HIS
1	B	292	HIS
1	B	303	GLN
1	B	307	GLN
1	B	321	HIS
1	B	323	HIS
1	B	331	GLN
1	B	350	GLN
1	B	373	HIS
1	B	383	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PDA	B	400	-	20,21,21	4.24	14 (70%)	26,30,30	2.04	11 (42%)
3	PDA	A	400	-	20,21,21	4.73	12 (60%)	26,30,30	2.26	11 (42%)
4	CSS	A	2001	-	5,7,7	3.42	2 (40%)	3,8,8	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PDA	B	400	-	1/1/3/4	8/15/15/15	0/1/1/1
3	PDA	A	400	-	1/1/3/4	9/15/15/15	0/1/1/1
4	CSS	A	2001	-	-	2/6/7/7	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	PDA	C4A-C4	-9.70	1.37	1.52
3	B	400	PDA	C3-C2	8.71	1.50	1.41
3	A	400	PDA	C3-C2	8.65	1.49	1.41
3	B	400	PDA	C4A-C4	-8.44	1.39	1.52
3	A	400	PDA	CA-C	-8.10	1.40	1.52
3	A	400	PDA	C3-C4	7.53	1.51	1.40
4	A	2001	CSS	O-C	6.87	1.42	1.22
3	B	400	PDA	C5-C4	6.32	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	PDA	CA-C	-6.22	1.43	1.52
3	A	400	PDA	C5-C4	5.99	1.48	1.40
3	A	400	PDA	C2-N1	5.63	1.43	1.33
3	B	400	PDA	C3-C4	5.26	1.47	1.40
3	A	400	PDA	CB-CA	-5.26	1.39	1.52
3	B	400	PDA	C6-C5	5.03	1.47	1.37
3	B	400	PDA	C2-N1	5.00	1.42	1.33
3	A	400	PDA	C6-C5	4.04	1.45	1.37
3	A	400	PDA	C4A-N	-3.67	1.36	1.46
3	B	400	PDA	CB-CA	-3.44	1.43	1.52
4	A	2001	CSS	OXT-C	3.20	1.40	1.30
3	A	400	PDA	OXT-C	3.16	1.31	1.22
3	B	400	PDA	OXT-C	2.98	1.30	1.22
3	A	400	PDA	C2A-C2	2.69	1.54	1.50
3	A	400	PDA	C6-N1	2.63	1.39	1.34
3	B	400	PDA	P-OP3	-2.62	1.45	1.54
3	B	400	PDA	C6-N1	2.59	1.39	1.34
3	B	400	PDA	C4A-N	-2.47	1.39	1.46
3	B	400	PDA	C5A-C5	2.43	1.57	1.50
3	B	400	PDA	O3A-C3	-2.07	1.32	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	PDA	C2A-C2-C3	5.93	127.74	120.80
3	B	400	PDA	C2A-C2-C3	4.93	126.57	120.80
3	A	400	PDA	CB-CA-C	4.78	120.70	110.23
3	B	400	PDA	CB-CA-C	4.38	119.83	110.23
3	A	400	PDA	C6-C5-C4	3.37	120.61	118.06
3	B	400	PDA	C6-C5-C4	3.01	120.34	118.06
3	A	400	PDA	C6-N1-C2	2.69	124.07	119.20
3	A	400	PDA	C5-C6-N1	-2.47	119.82	123.83
3	B	400	PDA	C5-C6-N1	-2.40	119.92	123.83
3	A	400	PDA	O-C-CA	2.38	121.69	113.84
3	B	400	PDA	OP4-C5A-C5	2.31	113.69	109.36
3	A	400	PDA	OP2-P-OP4	2.30	112.66	106.67
3	A	400	PDA	C5A-C5-C6	-2.27	115.65	119.36
3	A	400	PDA	C2A-C2-N1	-2.27	113.36	117.64
3	A	400	PDA	OP4-C5A-C5	2.27	113.61	109.36
3	B	400	PDA	OP4-P-OP1	2.27	112.56	106.44
3	B	400	PDA	O-C-CA	2.27	121.31	113.84
3	A	400	PDA	OP3-P-OP4	-2.24	100.84	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	PDA	OP3-P-OP4	-2.23	100.86	106.67
3	B	400	PDA	C4A-C4-C5	2.18	122.12	119.75
3	B	400	PDA	C2A-C2-N1	-2.11	113.66	117.64
3	B	400	PDA	C6-N1-C2	2.02	122.86	119.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	400	PDA	CA
3	B	400	PDA	CA

All (19) torsion outliers are listed below:

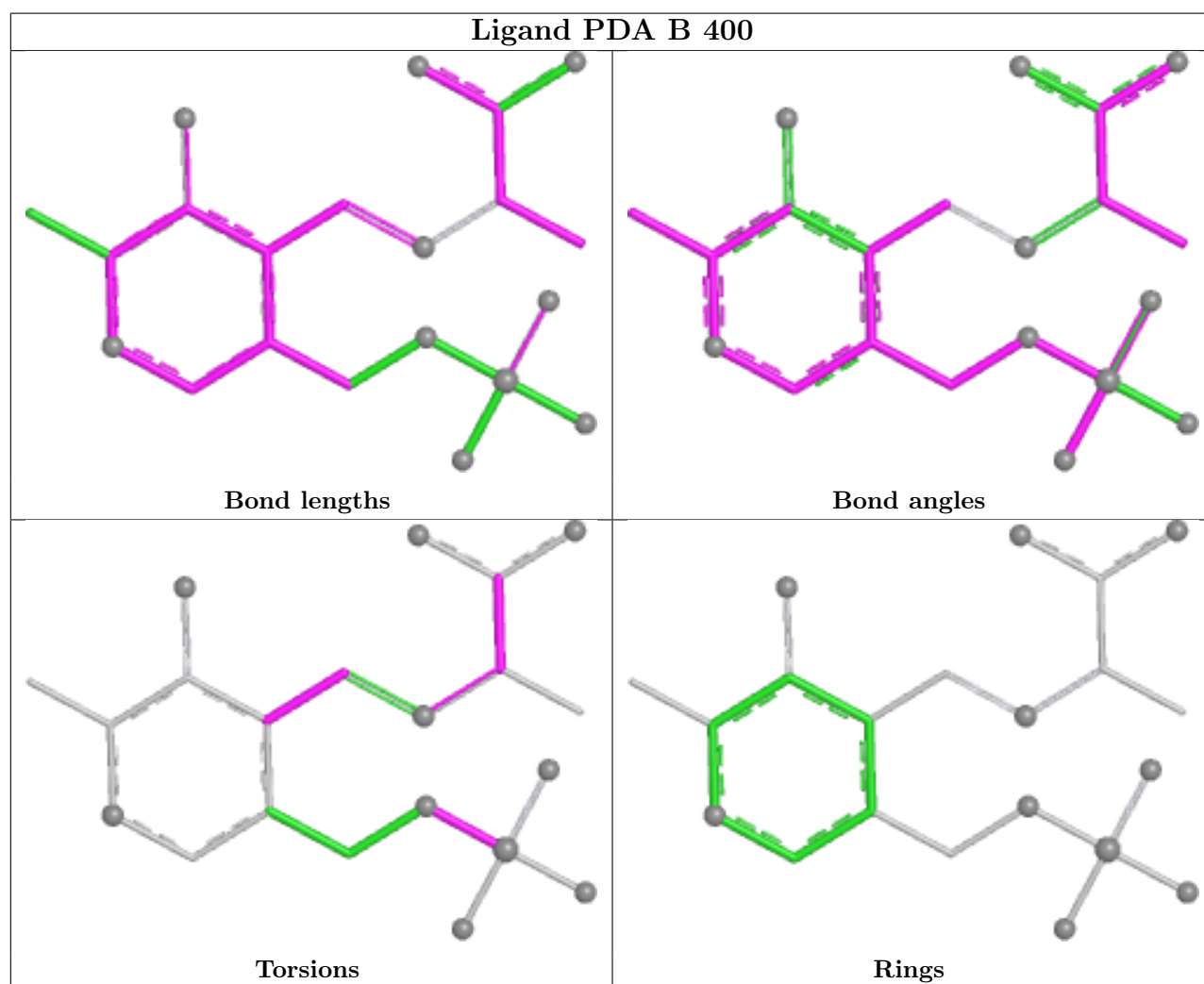
Mol	Chain	Res	Type	Atoms
3	A	400	PDA	CB-CA-N-C4A
3	A	400	PDA	C-CA-N-C4A
3	A	400	PDA	C5A-OP4-P-OP3
3	B	400	PDA	CB-CA-N-C4A
3	B	400	PDA	C-CA-N-C4A
3	B	400	PDA	C5-C4-C4A-N
3	A	400	PDA	C5-C4-C4A-N
3	B	400	PDA	OXT-C-CA-CB
4	A	2001	CSS	OXT-C-CA-N
3	A	400	PDA	O-C-CA-CB
3	B	400	PDA	O-C-CA-CB
3	A	400	PDA	C5A-OP4-P-OP1
3	B	400	PDA	C5A-OP4-P-OP1
3	A	400	PDA	C3-C4-C4A-N
4	A	2001	CSS	O-C-CA-N
3	B	400	PDA	C3-C4-C4A-N
3	A	400	PDA	OXT-C-CA-CB
3	A	400	PDA	C5A-OP4-P-OP2
3	B	400	PDA	C5A-OP4-P-OP3

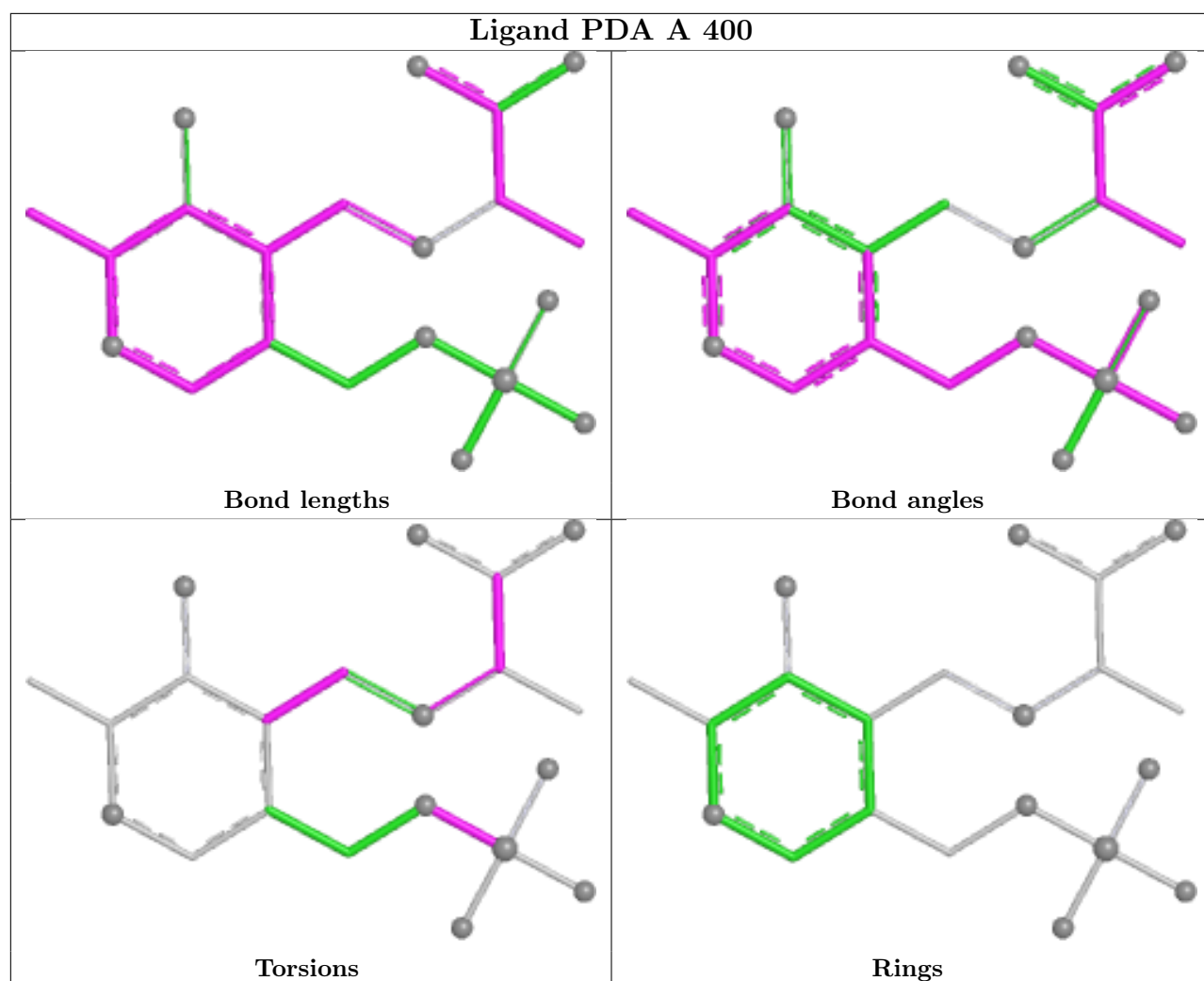
There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	PDA	3	0
3	A	400	PDA	6	0
4	A	2001	CSS	3	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	381/390 (97%)	0.39	10 (2%) 57 65	13, 23, 36, 43	0
1	B	381/390 (97%)	0.57	39 (10%) 12 14	13, 23, 39, 48	0
All	All	762/780 (97%)	0.48	49 (6%) 25 30	13, 23, 38, 48	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	ARG	4.1
1	B	129	GLY	3.9
1	A	190	TYR	3.9
1	B	126	ALA	3.8
1	B	134	PHE	3.7
1	B	156	PRO	3.7
1	B	148	ALA	3.7
1	B	128	PHE	3.4
1	B	104	GLY	3.4
1	B	155	GLY	3.4
1	B	151	ALA	2.9
1	B	182	VAL	2.9
1	B	192	VAL	2.9
1	A	212	LEU	2.9
1	B	152	ASN	2.8
1	B	258	ALA	2.8
1	A	293	GLN	2.7
1	B	181	ALA	2.7
1	B	296	GLY	2.7
1	A	126	ALA	2.6
1	B	184	ARG	2.6
1	B	102	HIS	2.6
1	A	168	TRP	2.5
1	A	125	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	124	ILE	2.5
1	A	189	ASN	2.5
1	B	212	LEU	2.4
1	B	168	TRP	2.4
1	A	158	THR	2.4
1	B	105	ASP	2.3
1	B	183	CYS	2.3
1	B	191	PRO	2.3
1	B	137	VAL	2.3
1	B	149	VAL	2.3
1	B	292	HIS	2.2
1	B	175	PRO	2.2
1	B	109	LEU	2.2
1	B	190	TYR	2.2
1	A	19	ASN	2.2
1	A	71	LEU	2.1
1	B	114	HIS	2.1
1	B	80	ASN	2.1
1	B	257	GLY	2.1
1	B	210	SER	2.1
1	B	294	ARG	2.0
1	B	195	LEU	2.0
1	B	147	ALA	2.0
1	B	209	PHE	2.0
1	B	160	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

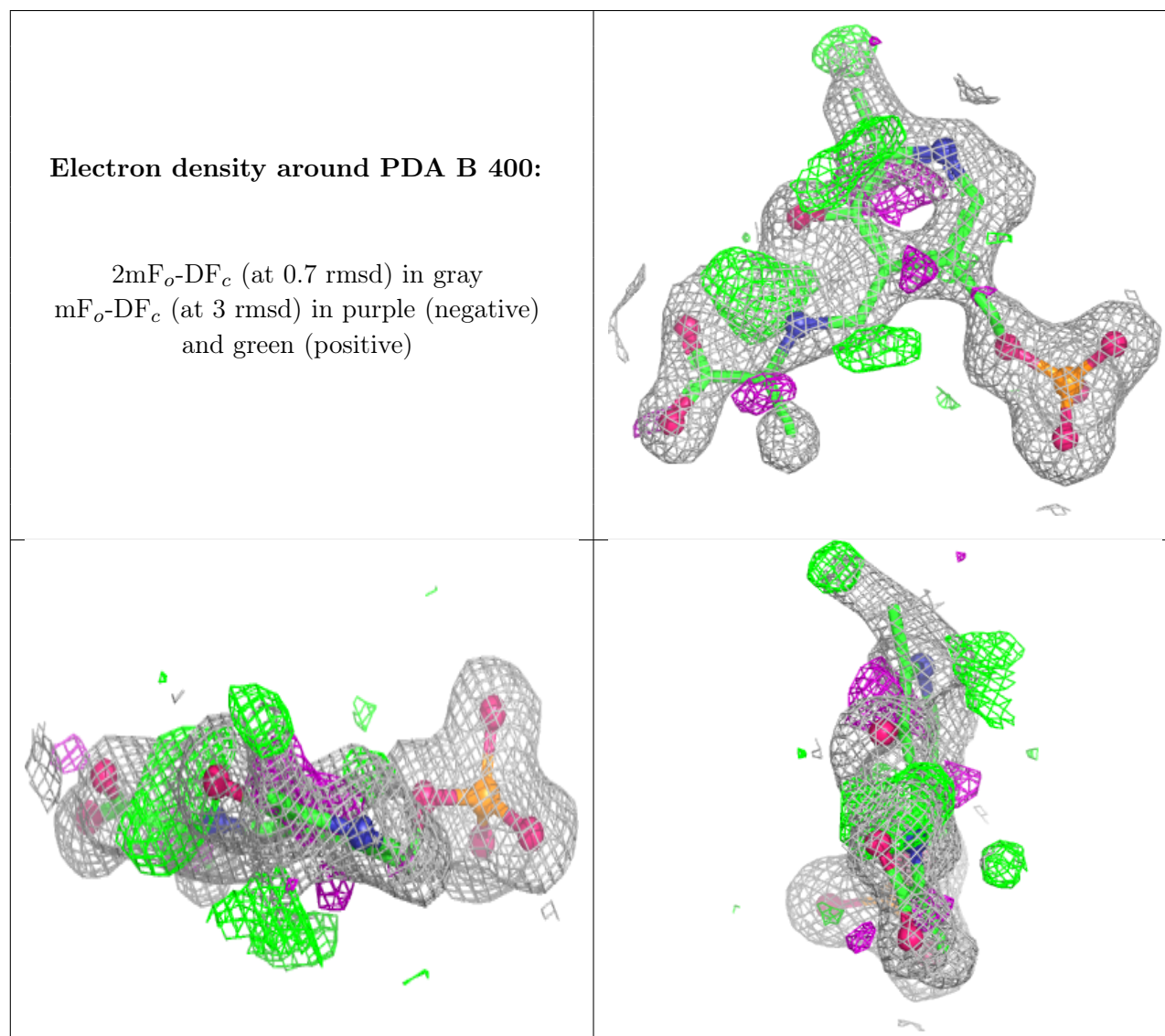
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

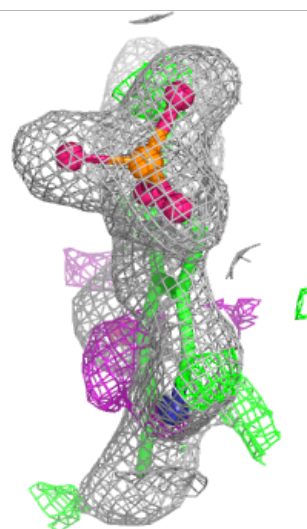
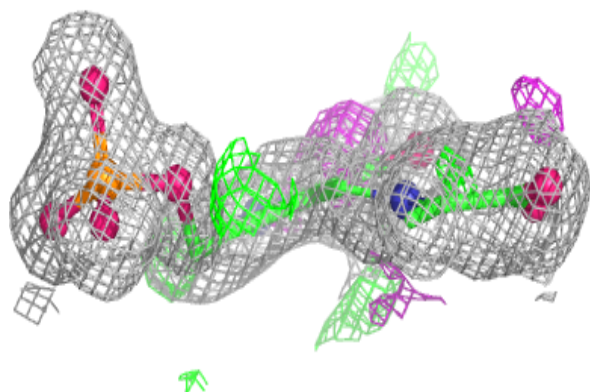
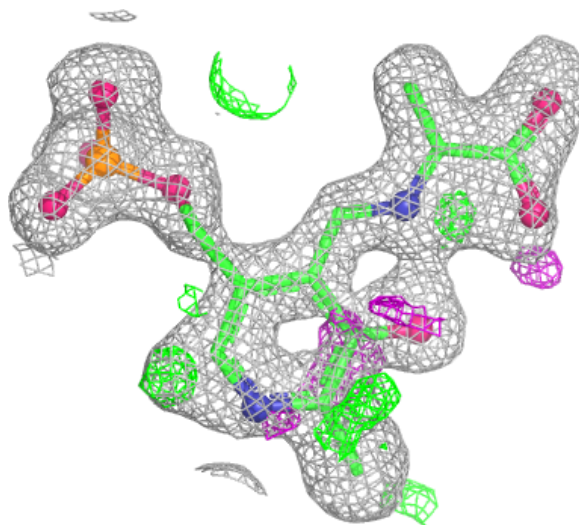
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CSS	A	2001	8/8	0.75	0.12	48,52,59,63	0
3	PDA	B	400	21/21	0.93	0.12	16,29,35,40	0
3	PDA	A	400	21/21	0.94	0.11	16,28,31,38	0
2	K	A	1001	1/1	0.97	0.06	25,25,25,25	0
2	K	B	1002	1/1	0.98	0.07	27,27,27,27	0

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 PDA 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 ⓘ

There are no such residues in this entry.