



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:55 PM UTC

PDB ID : 4IZ6 / pdb_00004iz6
Title : Structure of EntE and EntB, an NRPS adenylation-PCP fusion protein with pseudo translational symmetry
Authors : Gulick, A.M.; Sundlov, J.A.
Deposited on : 2013-01-29
Resolution : 2.40 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

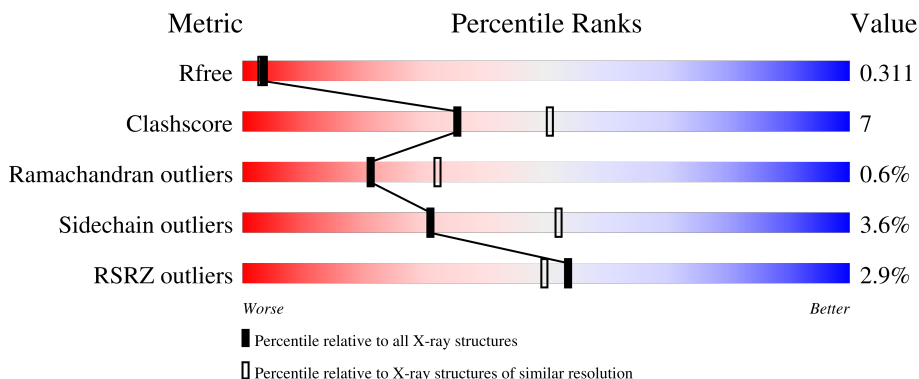
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	635	 3% 77% 18% . .
1	B	635	 3% 76% 20% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9564 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 Enterobactin synthase component E, Isochorismatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	1	0
			4644	2949	802	875	18			
1	B	612	Total	C	N	O	S	0	0	0
			4609	2936	790	865	18			

There are 48 discrepancies between the modelled and reference sequences:

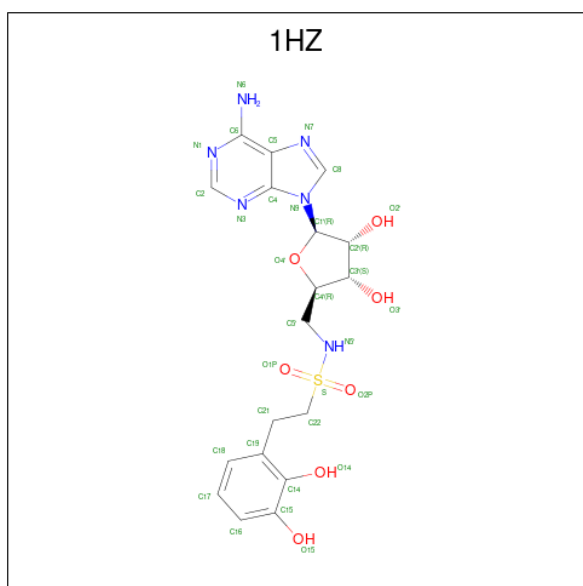
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P10378
A	-18	GLY	-	expression tag	UNP P10378
A	-17	SER	-	expression tag	UNP P10378
A	-16	SER	-	expression tag	UNP P10378
A	-15	HIS	-	expression tag	UNP P10378
A	-14	HIS	-	expression tag	UNP P10378
A	-13	HIS	-	expression tag	UNP P10378
A	-12	HIS	-	expression tag	UNP P10378
A	-11	HIS	-	expression tag	UNP P10378
A	-10	SER	-	expression tag	UNP P10378
A	-9	SER	-	expression tag	UNP P10378
A	-8	GLY	-	expression tag	UNP P10378
A	-7	GLU	-	expression tag	UNP P10378
A	-6	ASN	-	expression tag	UNP P10378
A	-5	LEU	-	expression tag	UNP P10378
A	-4	TYR	-	expression tag	UNP P10378
A	-3	PHE	-	expression tag	UNP P10378
A	-2	GLN	-	expression tag	UNP P10378
A	-1	GLY	-	expression tag	UNP P10378
A	0	HIS	-	expression tag	UNP P10378
A	537	GLY	-	linker	UNP P10378
A	538	ARG	-	linker	UNP P10378
A	539	ALA	-	linker	UNP P10378
A	540	SER	-	linker	UNP P10378
B	-19	MET	-	expression tag	UNP P10378

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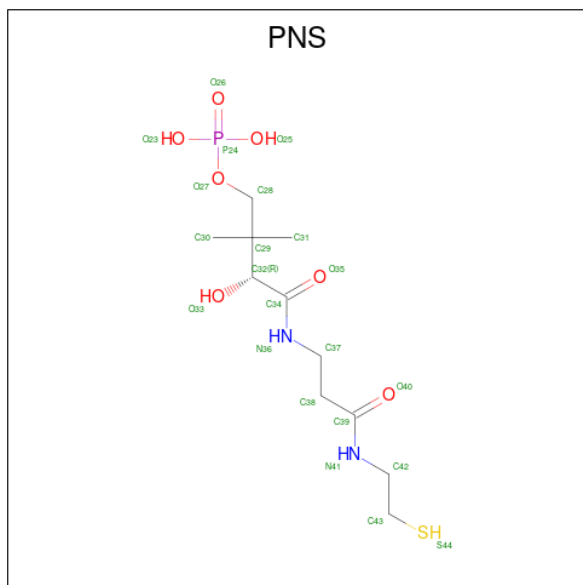
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P10378
B	-17	SER	-	expression tag	UNP P10378
B	-16	SER	-	expression tag	UNP P10378
B	-15	HIS	-	expression tag	UNP P10378
B	-14	HIS	-	expression tag	UNP P10378
B	-13	HIS	-	expression tag	UNP P10378
B	-12	HIS	-	expression tag	UNP P10378
B	-11	HIS	-	expression tag	UNP P10378
B	-10	SER	-	expression tag	UNP P10378
B	-9	SER	-	expression tag	UNP P10378
B	-8	GLY	-	expression tag	UNP P10378
B	-7	GLU	-	expression tag	UNP P10378
B	-6	ASN	-	expression tag	UNP P10378
B	-5	LEU	-	expression tag	UNP P10378
B	-4	TYR	-	expression tag	UNP P10378
B	-3	PHE	-	expression tag	UNP P10378
B	-2	GLN	-	expression tag	UNP P10378
B	-1	GLY	-	expression tag	UNP P10378
B	0	HIS	-	expression tag	UNP P10378
B	537	GLY	-	linker	UNP P10378
B	538	ARG	-	linker	UNP P10378
B	539	ALA	-	linker	UNP P10378
B	540	SER	-	linker	UNP P10378

- Molecule 2 is 5'-deoxy-5'-([2-(2,3-dihydroxyphenyl)ethyl]sulfonyl)amino)adenosine (CCD ID: 1HZ) (formula: C₁₈H₂₂N₆O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	18	6	7	1		
2	B	1	Total	C	N	O	S	0	0
			32	18	6	7	1		

- Molecule 3 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
3	B	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

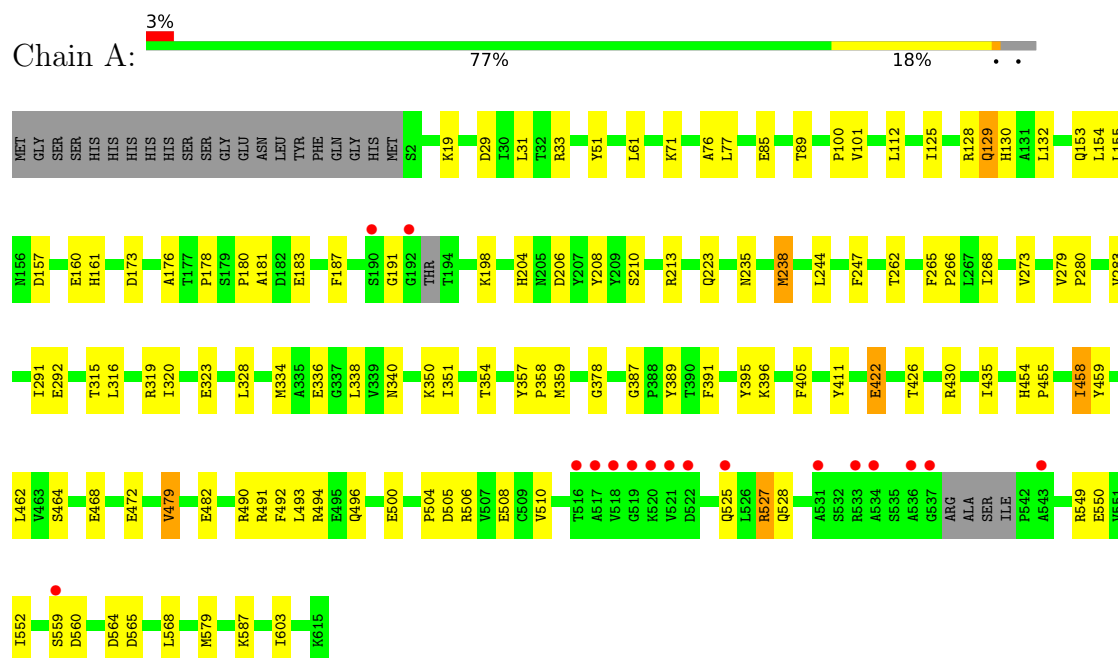
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total	O	0	0
			99	99		
4	B	106	Total	O	0	0
			106	106		

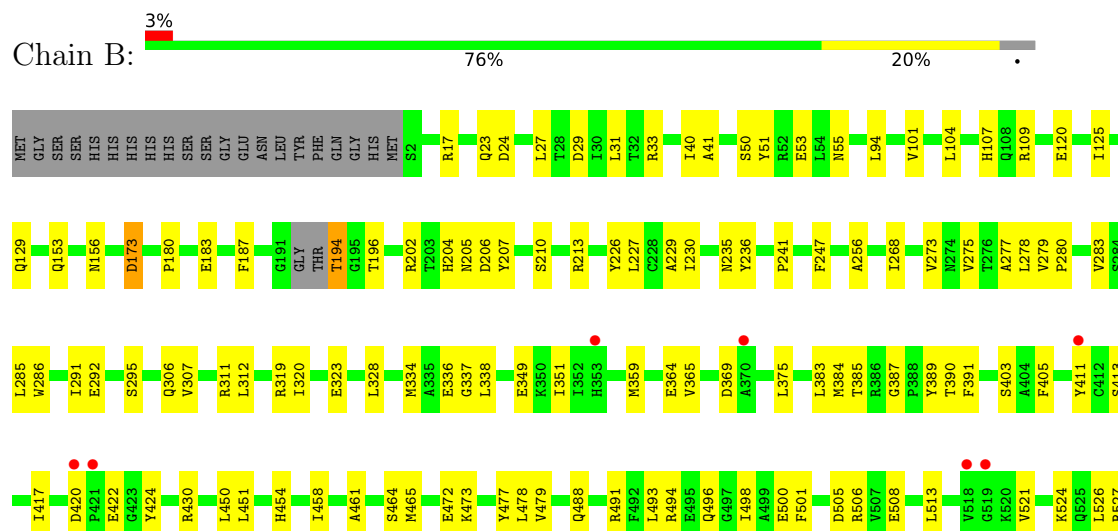
3 Residue-property plots

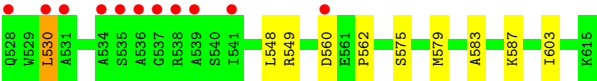
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Enterobactin synthase component E, Isochorismatase



- Molecule 1: Enterobactin synthase component E, Isochorismatase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.99Å 119.11Å 99.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 2.40 48.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.50-2.40) 97.7 (48.50-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_837)	Depositor
R, R_{free}	0.250 , 0.313 0.247 , 0.311	Depositor DCC
R_{free} test set	2659 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.0	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	0.93	EDS
Total number of atoms	9564	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7283e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PNS, 1HZ

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	0.57	0/4748	0.92	7/6470 (0.1%)
1	B	0.57	0/4711	0.91	6/6431 (0.1%)
All	All	0.57	0/9459	0.91	13/12901 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	GLY	CA-C-N	6.92	127.06	119.87
1	B	387	GLY	C-N-CA	6.92	127.06	119.87
1	A	387	GLY	CA-C-N	6.07	126.86	120.12
1	A	387	GLY	C-N-CA	6.07	126.86	120.12
1	A	280	PRO	N-CA-C	5.98	118.00	110.70
1	B	230	ILE	CA-C-N	-5.80	113.09	120.23
1	B	230	ILE	C-N-CA	-5.80	113.09	120.23
1	A	525	GLN	N-CA-C	-5.57	107.13	114.31
1	A	71	LYS	CA-C-N	-5.47	114.06	119.92
1	A	71	LYS	C-N-CA	-5.47	114.06	119.92
1	B	205	ASN	N-CA-C	5.41	117.60	111.11
1	A	552	ILE	N-CA-C	5.35	115.55	110.42
1	B	280	PRO	N-CA-C	5.06	116.88	110.70

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	4644	0	4499	67	0
1	B	4609	0	4431	74	0
2	A	32	0	20	1	0
2	B	32	0	20	1	0
3	A	21	0	20	1	0
3	B	21	0	20	1	0
4	A	99	0	0	3	0
4	B	106	0	0	4	0
All	All	9564	0	9010	136	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 7.

All (136) 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:213:ARG:HB3	1:B:359:MET:HE3	1.50	0.92
1:B:210:SER:HA	1:B:359:MET:HE1	1.55	0.85
1:A:292:GLU:O	1:B:587:LYS:NZ	2.18	0.75
1:A:206:ASP:HB2	1:A:389:TYR:HA	1.69	0.75
1:B:180:PRO:HB2	1:B:183:GLU:HG3	1.71	0.72
3:A:702:PNS:H371	1:B:279:VAL:HG11	1.74	0.69
1:A:129:GLN:OE1	4:A:892:HOH:O	2.08	0.69
1:A:29:ASP:OD2	1:A:33:ARG:NH2	2.27	0.68
1:A:180:PRO:HB2	1:A:183:GLU:HG3	1.76	0.68
1:B:206:ASP:HB2	1:B:389:TYR:HA	1.76	0.67
1:B:129:GLN:HG3	1:B:156:ASN:ND2	2.11	0.66
1:B:194:THR:HG23	1:B:196:THR:H	1.60	0.66
1:A:587:LYS:NZ	1:B:292:GLU:O	2.30	0.65
1:A:549:ARG:NH2	1:A:564:ASP:OD2	2.30	0.61
1:B:27:LEU:HB2	1:B:94:LEU:HD13	1.84	0.60
1:B:268:ILE:HG23	1:B:273:VAL:HB	1.84	0.59
1:A:279:VAL:HG11	3:B:702:PNS:H371	1.85	0.58
1:B:125:ILE:HG12	1:B:153:GLN:HB2	1.85	0.58
1:B:210:SER:CA	1:B:359:MET:HE1	2.31	0.58
1:A:336:GLU:HG2	1:A:411:TYR:CZ	2.39	0.58
1:B:210:SER:HA	1:B:359:MET:CE	2.28	0.58
1:B:336:GLU:HG2	1:B:411:TYR:CZ	2.39	0.57
1:A:268:ILE:HG23	1:A:273:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:SER:HB2	1:B:53:GLU:H	1.70	0.57
1:B:501:PHE:O	4:B:828:HOH:O	2.17	0.57
1:B:505:ASP:O	1:B:506:ARG:NH1	2.36	0.57
1:A:210:SER:O	1:A:359:MET:HE1	2.05	0.56
1:B:227:LEU:HB2	1:B:273:VAL:HG21	1.87	0.56
1:B:575:SER:O	1:B:579:MET:HG3	2.06	0.55
1:A:315:THR:O	1:A:319:ARG:HG3	2.07	0.55
1:A:61:LEU:HD23	1:A:89:THR:HA	1.88	0.55
1:B:27:LEU:HG	1:B:204:HIS:ND1	2.21	0.55
1:B:29:ASP:OD2	1:B:33:ARG:NH2	2.39	0.55
1:B:549:ARG:NH2	1:B:562:PRO:O	2.22	0.54
1:B:364:GLU:O	1:B:385:THR:HA	2.08	0.54
1:B:454:HIS:O	4:B:826:HOH:O	2.18	0.54
1:A:459:TYR:HB2	1:A:479:VAL:HG13	1.89	0.54
1:A:494:ARG:HH12	1:A:500:GLU:HG2	1.74	0.53
1:B:337:GLY:HA3	1:B:390:THR:HA	1.91	0.52
1:A:336:GLU:N	1:A:336:GLU:OE1	2.43	0.52
1:A:265:PHE:HB2	1:A:266:PRO:HD3	1.91	0.51
1:A:125:ILE:HG12	1:A:153:GLN:HB2	1.91	0.51
1:A:458:ILE:HG12	1:A:479:VAL:O	2.11	0.51
1:B:51:TYR:OH	1:B:247:PHE:HA	2.11	0.51
1:B:320:ILE:HD13	1:B:328:LEU:HD13	1.94	0.50
1:A:430:ARG:NH1	1:A:472:GLU:OE2	2.32	0.50
1:A:603:ILE:H	1:A:603:ILE:HD12	1.77	0.50
1:A:454:HIS:CG	1:A:455:PRO:HD2	2.46	0.50
1:B:405:PHE:CE2	1:B:411:TYR:HB2	2.47	0.49
1:B:526:LEU:O	1:B:530:LEU:HB2	2.12	0.49
1:A:154:LEU:HD12	1:A:161:HIS:HB2	1.95	0.49
1:B:235:ASN:HB3	2:B:701:1HZ:O14	2.13	0.49
1:A:426:THR:OG1	4:A:872:HOH:O	2.19	0.49
1:B:213:ARG:CB	1:B:359:MET:HE3	2.35	0.49
1:A:176:ALA:HB1	1:A:178:PRO:HD3	1.94	0.48
1:B:17:ARG:NH1	1:B:24:ASP:OD1	2.47	0.48
1:A:334:MET:HG3	1:A:336:GLU:HB2	1.96	0.48
1:A:378:GLY:O	1:B:349:GLU:HB2	2.12	0.48
1:A:568:LEU:HD21	1:A:603:ILE:HD11	1.94	0.48
1:A:395:TYR:CZ	1:A:396:LYS:HE3	2.49	0.48
1:B:319:ARG:O	1:B:323:GLU:HB2	2.14	0.47
1:B:311:ARG:HA	4:B:820:HOH:O	2.14	0.47
1:B:549:ARG:HG2	1:B:603:ILE:HD13	1.97	0.47
1:B:101:VAL:HG22	1:B:187:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASP:O	1:B:33:ARG:HD2	2.15	0.47
1:A:77:LEU:HD21	1:A:112:LEU:HD22	1.97	0.46
1:B:31:LEU:HD21	1:B:55:ASN:HA	1.96	0.46
1:B:461:ALA:HB2	1:B:521:VAL:HG11	1.97	0.46
1:A:191:GLY:HA3	4:A:828:HOH:O	2.16	0.46
1:A:128:ARG:NE	1:A:157:ASP:OD1	2.41	0.46
1:A:430:ARG:HH12	1:A:472:GLU:CD	2.21	0.45
1:A:493:LEU:HD23	1:A:493:LEU:HA	1.68	0.45
1:A:181:ALA:HA	1:A:204:HIS:HB2	1.97	0.45
1:B:548:LEU:HD23	1:B:603:ILE:HG23	1.98	0.45
1:A:130:HIS:HE1	1:A:132:LEU:HG	1.82	0.45
1:A:505:ASP:O	1:A:506:ARG:NH1	2.49	0.45
1:B:307:VAL:HG11	1:B:312:LEU:HD22	1.98	0.45
1:A:235:ASN:HB3	2:A:701:1HZ:O14	2.15	0.45
1:A:435:ILE:HD12	1:A:464:SER:HB3	1.99	0.45
1:B:241:PRO:HD3	1:B:306:GLN:HE22	1.81	0.45
1:B:365:VAL:HA	1:B:384:MET:O	2.17	0.44
1:B:479:VAL:HG23	1:B:513:LEU:HD12	1.98	0.44
1:A:213:ARG:HB3	1:A:359:MET:CE	2.47	0.44
1:B:336:GLU:N	1:B:336:GLU:OE1	2.51	0.44
1:B:420:ASP:HB3	1:B:422:GLU:H	1.83	0.44
1:A:238:MET:O	1:A:244:LEU:HG	2.17	0.44
1:A:283:VAL:HG11	1:A:320:ILE:HD11	2.00	0.44
1:A:357:TYR:HB2	1:A:358:PRO:HD2	2.00	0.43
1:A:492:PHE:O	1:A:496:GLN:HG2	2.18	0.43
1:B:369:ASP:HB3	1:B:375:LEU:HD21	2.00	0.43
1:A:198:LYS:HA	1:A:198:LYS:HD3	1.81	0.43
1:B:451:LEU:HD13	1:B:478:LEU:HD21	2.00	0.43
1:B:477:TYR:CD1	1:B:508:GLU:HB3	2.54	0.43
1:A:160:GLU:OE1	1:A:160:GLU:N	2.41	0.43
1:A:405:PHE:CE2	1:A:411:TYR:HB2	2.53	0.43
1:B:411:TYR:HE1	4:B:849:HOH:O	2.02	0.43
1:B:494:ARG:NH2	1:B:500:GLU:OE2	2.47	0.43
1:A:33:ARG:NH2	1:A:208:TYR:OH	2.51	0.42
1:B:328:LEU:HD23	1:B:351:ILE:HG22	2.01	0.42
1:A:319:ARG:NH2	1:A:323:GLU:OE1	2.49	0.42
1:A:350:LYS:O	1:A:354:THR:OG1	2.34	0.42
1:B:278:LEU:HD11	1:B:286:TRP:CZ3	2.55	0.42
1:B:424:TYR:N	1:B:424:TYR:CD2	2.87	0.42
1:B:210:SER:O	1:B:359:MET:HE1	2.20	0.42
1:B:226:TYR:HA	1:B:275:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ALA:HB2	1:B:51:TYR:CD1	2.55	0.42
1:B:383:LEU:HD22	1:B:413:SER:OG	2.20	0.42
1:A:490:ARG:HD3	1:A:504:PRO:O	2.20	0.42
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.89	0.42
1:A:579:MET:HB2	1:B:285:LEU:HD21	2.01	0.42
1:B:229:ALA:HB2	1:B:256:ALA:HB3	2.02	0.42
1:B:493:LEU:HA	1:B:496:GLN:HG2	2.02	0.42
1:A:334:MET:HE2	1:A:334:MET:HB3	1.69	0.41
1:A:101:VAL:HG22	1:A:187:PHE:HB2	2.01	0.41
1:B:383:LEU:HD12	1:B:417:ILE:HD13	2.01	0.41
1:B:430:ARG:NH1	1:B:472:GLU:OE2	2.54	0.41
1:A:130:HIS:CE1	1:A:132:LEU:HG	2.55	0.41
1:B:104:LEU:HD12	1:B:107:HIS:NE2	2.36	0.41
1:B:334:MET:HE2	1:B:334:MET:HB3	1.74	0.41
1:A:85:GLU:HG2	1:A:155:LEU:HD13	2.03	0.41
1:A:262:THR:HG21	1:B:583:ALA:HA	2.03	0.41
1:A:494:ARG:HH12	1:A:500:GLU:CG	2.33	0.41
1:B:40:ILE:N	1:B:40:ILE:HD12	2.35	0.41
1:B:450:LEU:HD13	1:B:498:ILE:HG21	2.02	0.41
1:B:202:ARG:CZ	1:B:207:TYR:HD1	2.34	0.41
1:A:19:LYS:HE2	1:A:19:LYS:HB3	1.96	0.41
1:A:51:TYR:OH	1:A:247:PHE:HA	2.20	0.41
1:A:76:ALA:O	1:A:100:PRO:HA	2.21	0.41
1:A:350:LYS:HE3	1:A:422:GLU:OE2	2.20	0.40
1:B:236:TYR:CE2	1:B:277:ALA:HB1	2.56	0.40
1:A:328:LEU:HD23	1:A:351:ILE:HG22	2.04	0.40
1:A:565:ASP:OD1	1:A:565:ASP:N	2.53	0.40
1:A:506:ARG:HA	1:A:506:ARG:HD3	1.74	0.40
1:B:464:SER:HA	1:B:473:LYS:O	2.21	0.40
1:A:527:ARG:HH21	1:A:528:GLN:HB3	1.87	0.40
1:B:283:VAL:HG11	1:B:320:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

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	604/635 (95%)	584 (97%)	17 (3%)	3 (0%)	24	37
1	B	608/635 (96%)	581 (96%)	23 (4%)	4 (1%)	18	28
All	All	1212/1270 (95%)	1165 (96%)	40 (3%)	7 (1%)	21	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	GLU
1	A	338	LEU
1	B	173	ASP
1	B	524	LYS
1	B	527	ARG
1	A	559	SER
1	B	338	LEU

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	475/525 (90%)	456 (96%)	19 (4%)	28	47
1	B	462/525 (88%)	447 (97%)	15 (3%)	34	56
All	All	937/1050 (89%)	903 (96%)	34 (4%)	31	52

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	129	GLN
1	A	173	ASP
1	A	223	GLN
1	A	238	MET
1	A	291	ILE

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Mol	Chain	Res	Type
1	A	340	ASN
1	A	391	PHE
1	A	458	ILE
1	A	462	LEU
1	A	468	GLU
1	A	479	VAL
1	A	482	GLU
1	A	491	ARG
1	A	508	GLU
1	A	510	VAL
1	A	527	ARG
1	A	550	GLU
1	A	560	ASP
1	B	23	GLN
1	B	109	ARG
1	B	120	GLU
1	B	173	ASP
1	B	194	THR
1	B	291	ILE
1	B	295	SER
1	B	391	PHE
1	B	403	SER
1	B	458	ILE
1	B	465	MET
1	B	488	GLN
1	B	491	ARG
1	B	530	LEU
1	B	560	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	113	ASN
1	A	146	HIS
1	A	327	GLN
1	B	55	ASN
1	B	56	GLN
1	B	108	GLN
1	B	156	ASN
1	B	400	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
3	PNS	B	702	1,2	15,20,21	0.52	0	18,26,29	1.62	4 (22%)
2	1HZ	B	701	3	35,35,35	0.93	2 (5%)	48,52,52	1.81	9 (18%)
3	PNS	A	702	2,1	15,20,21	0.39	0	18,26,29	1.83	4 (22%)
2	1HZ	A	701	3	35,35,35	1.03	4 (11%)	48,52,52	1.88	9 (18%)

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	PNS	B	702	1,2	-	0/24/26/27	-
2	1HZ	B	701	3	-	0/16/32/32	0/4/4/4
3	PNS	A	702	2,1	-	0/24/26/27	-
2	1HZ	A	701	3	-	1/16/32/32	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	1HZ	C22-S	-3.03	1.68	1.78
2	B	701	1HZ	C22-S	-2.72	1.69	1.78
2	A	701	1HZ	C8-N9	-2.20	1.33	1.37
2	A	701	1HZ	C8-N7	2.17	1.35	1.31
2	A	701	1HZ	C5-N7	-2.15	1.35	1.39
2	B	701	1HZ	C4-N9	-2.06	1.33	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	1HZ	O2P-S-O1P	-5.26	111.98	119.34
2	B	701	1HZ	N3-C2-N1	-5.22	120.68	128.58
3	A	702	PNS	C43-C42-N41	-4.82	101.36	112.31
2	B	701	1HZ	O2P-S-O1P	-4.79	112.64	119.34
2	A	701	1HZ	C5-C4-N3	-4.76	120.17	126.72
2	A	701	1HZ	N3-C2-N1	-4.54	121.70	128.58
2	B	701	1HZ	C5-C4-N3	-4.51	120.51	126.72
2	A	701	1HZ	N9-C8-N7	-3.86	108.46	113.94
3	A	702	PNS	C38-C37-N36	-3.63	104.27	112.00
2	B	701	1HZ	N9-C8-N7	-3.53	108.93	113.94
2	B	701	1HZ	C4-N9-C8	3.45	109.36	105.74
3	B	702	PNS	C43-C42-N41	-3.42	104.55	112.31
2	B	701	1HZ	C2-N3-C4	3.41	120.16	111.83
2	B	701	1HZ	N3-C4-N9	3.39	132.93	127.17
2	A	701	1HZ	C4-N9-C8	3.25	109.15	105.74
2	A	701	1HZ	C4-C5-N7	-3.20	106.92	110.58
2	A	701	1HZ	N3-C4-N9	3.18	132.58	127.17
2	A	701	1HZ	C2-N3-C4	3.10	119.40	111.83
2	A	701	1HZ	C5-N7-C8	3.03	108.21	103.45
3	B	702	PNS	C38-C37-N36	-2.79	106.06	112.00
3	A	702	PNS	C37-C38-C39	-2.78	107.77	112.39
3	B	702	PNS	C42-N41-C39	2.68	127.80	122.82
3	B	702	PNS	C37-C38-C39	-2.25	108.64	112.39
2	B	701	1HZ	C5-N7-C8	2.18	106.87	103.45
3	A	702	PNS	C30-C29-C32	2.16	112.46	108.77
2	B	701	1HZ	C4-C5-N7	-2.02	108.27	110.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

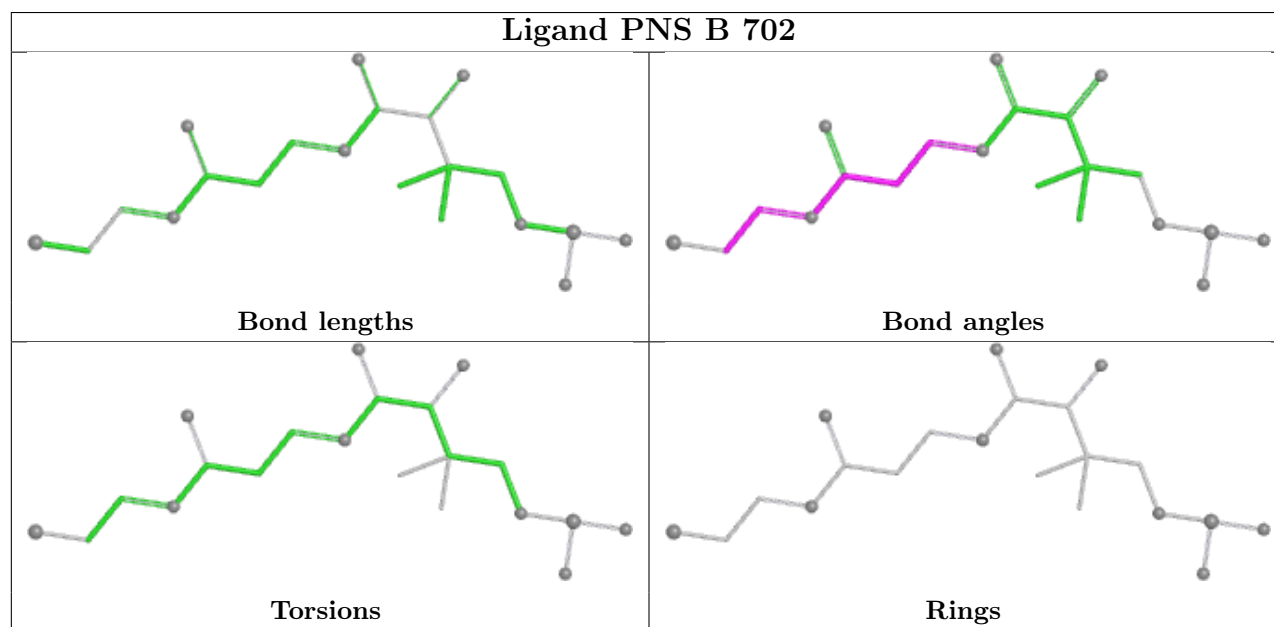
Mol	Chain	Res	Type	Atoms
2	A	701	1HZ	C19-C21-C22-S

There are no ring outliers.

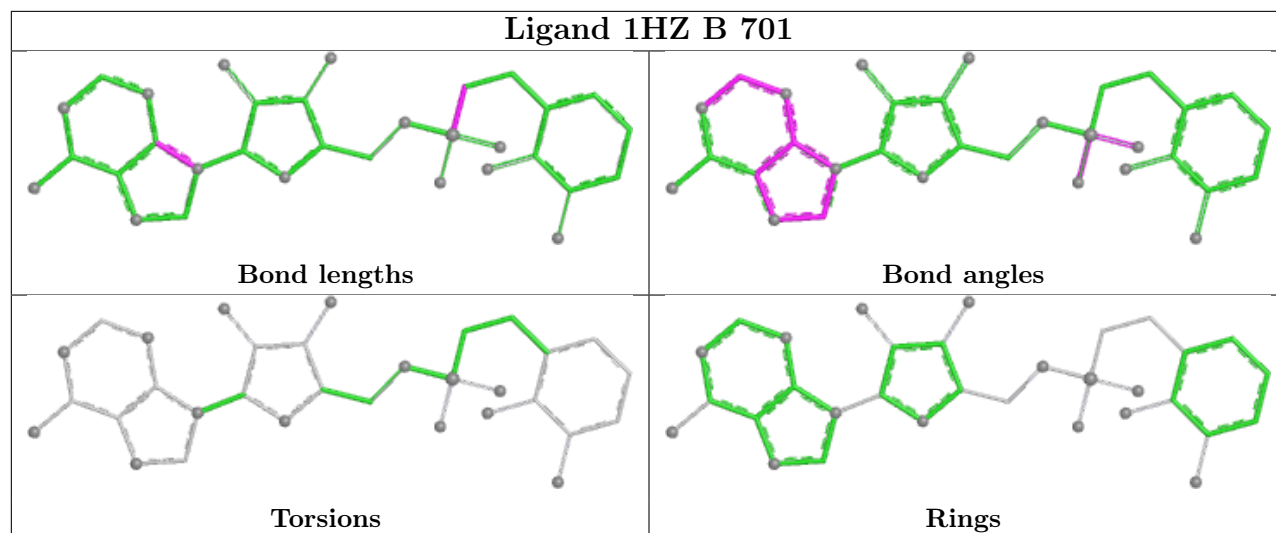
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	PNS	1	0
2	B	701	1HZ	1	0
3	A	702	PNS	1	0
2	A	701	1HZ	1	0

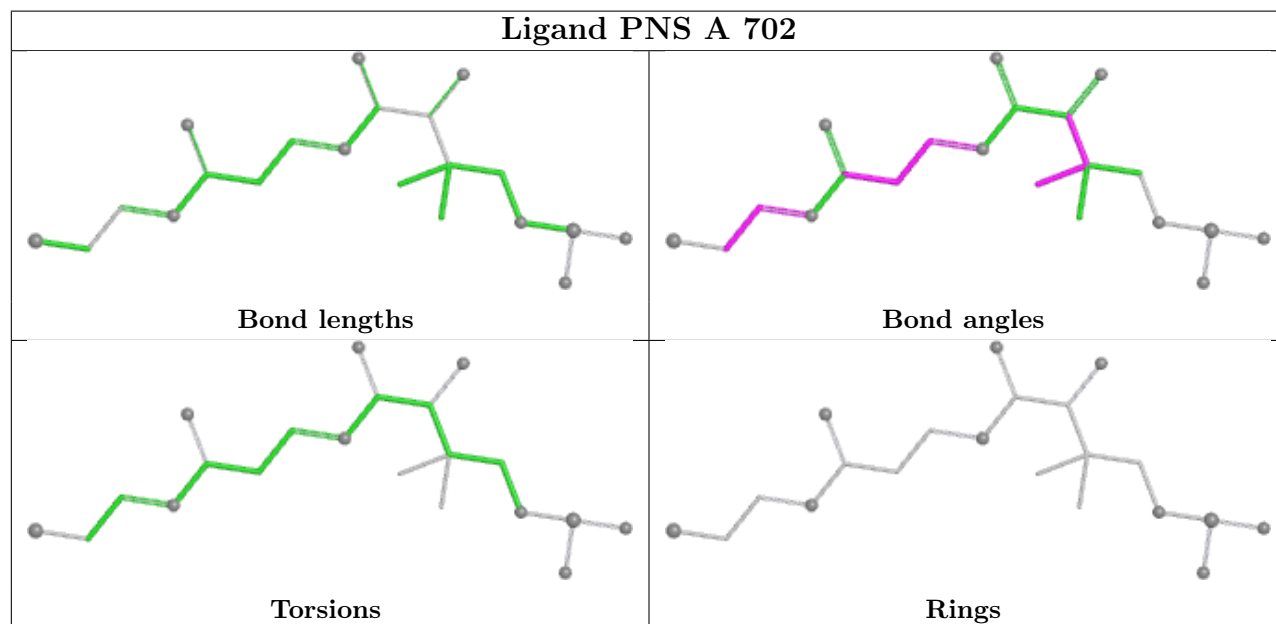
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



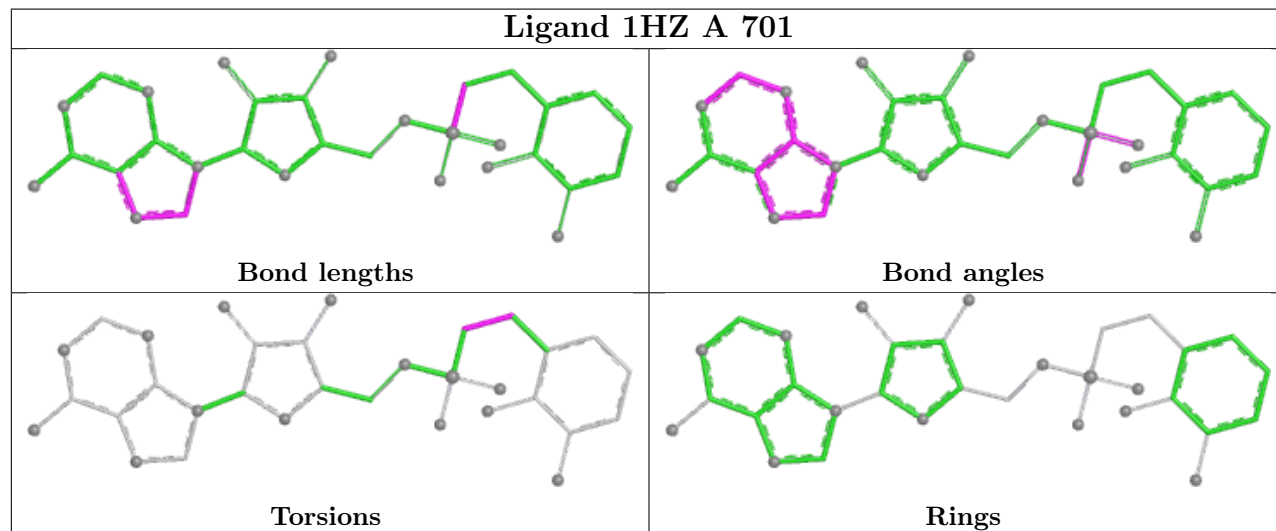
Ligand 1HZ B 701



Ligand PNS A 702



Ligand 1HZ A 701



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	609/635 (95%)	0.21	17 (2%) 55 51	9, 24, 48, 67	1 (0%)
1	B	612/635 (96%)	0.14	18 (2%) 53 50	11, 23, 43, 68	0
All	All	1221/1270 (96%)	0.17	35 (2%) 53 50	9, 24, 45, 68	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	ALA	5.3
1	A	519	GLY	5.0
1	A	518	VAL	3.8
1	A	520	LYS	3.6
1	B	536	ALA	3.6
1	A	536	ALA	3.6
1	B	539	ALA	3.5
1	A	516	THR	3.0
1	A	559	SER	2.9
1	B	534	ALA	2.9
1	B	519	GLY	2.9
1	A	531	ALA	2.8
1	A	192	GLY	2.8
1	B	353	HIS	2.8
1	A	543	ALA	2.7
1	A	525	GLN	2.6
1	B	541	ILE	2.5
1	B	528	GLN	2.5
1	B	421	PRO	2.5
1	B	535	SER	2.5
1	B	531	ALA	2.4
1	B	530	LEU	2.4
1	B	538	ARG	2.3
1	B	537	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	370	ALA	2.2
1	B	560	ASP	2.2
1	A	521	VAL	2.2
1	A	533	ARG	2.2
1	B	420	ASP	2.1
1	B	518	VAL	2.1
1	A	534	ALA	2.1
1	A	537	GLY	2.1
1	A	190	SER	2.1
1	A	522	ASP	2.1
1	B	411	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

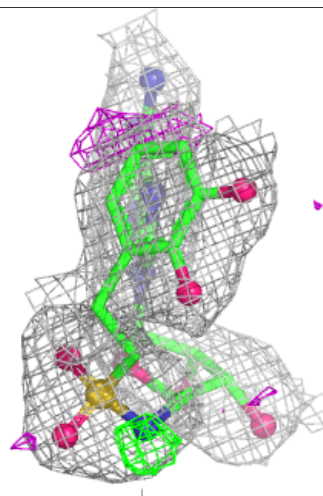
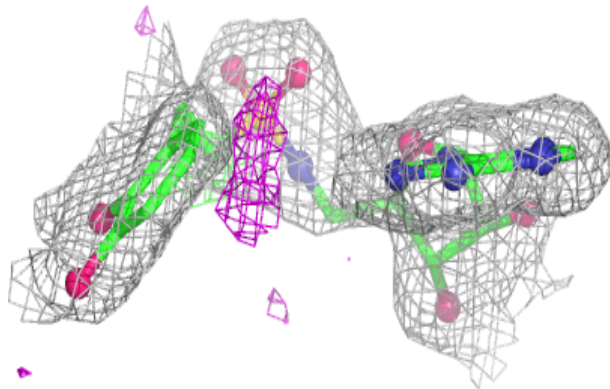
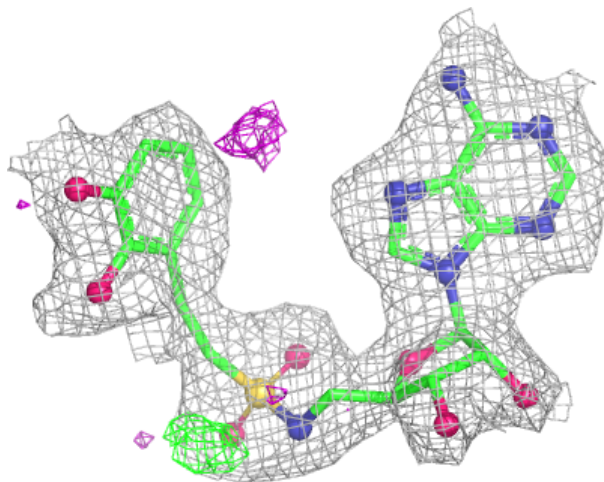
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	1HZ	B	701	32/32	0.93	0.09	12,21,29,31	0
2	1HZ	A	701	32/32	0.94	0.09	15,22,29,31	0
3	PNS	A	702	21/22	0.95	0.08	12,17,22,22	0
3	PNS	B	702	21/22	0.97	0.06	14,16,22,24	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.

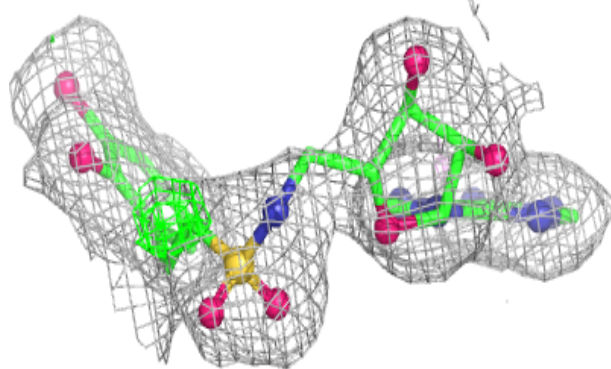
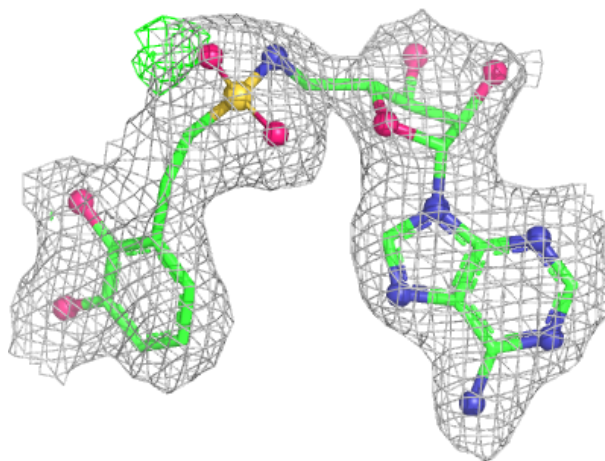
Electron density around 1HZ B 701:

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



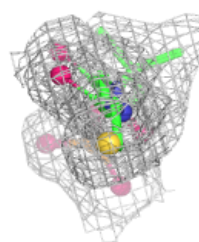
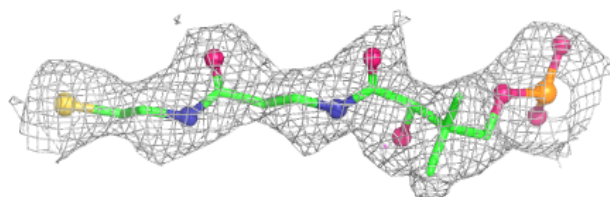
Electron density around 1HZ A 701:

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

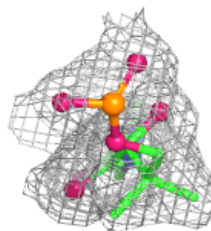
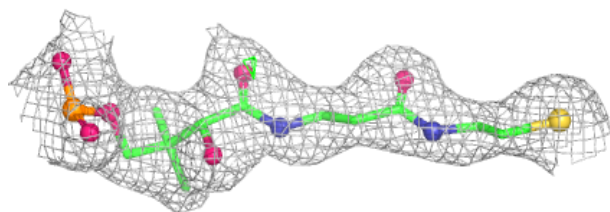
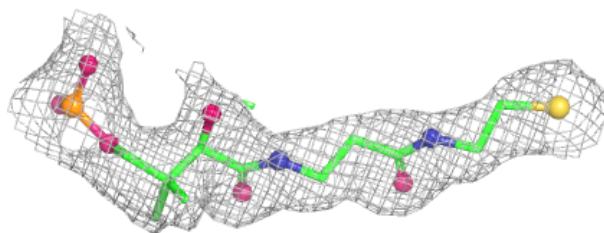


Electron density around PNS A 702:

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

**Electron density around PNS B 702:**

$2mF_o-DF_c$ (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.