



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 03:08 PM EDT

PDB ID : 1EPV
Title : ALANINE RACEMASE WITH BOUND INHIBITOR DERIVED FROM D-CYCLOSERINE
Authors : Fenn, T.D.; Stamper, G.F.; Morollo, A.A.; Ringe, D.
Deposited on : 2000-03-29
Resolution : 2.20 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

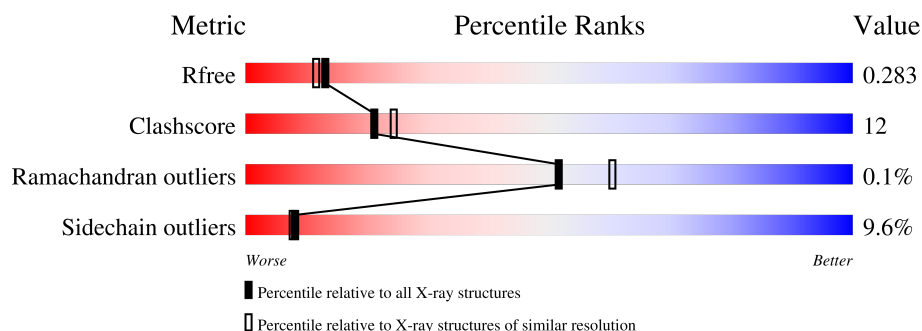
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	387	<div> <div style="width: 75%;"></div> <div style="width: 20%;"></div> <div style="width: 5%;"></div> </div> <div>75% 20% .</div>
1	B	387	<div> <div style="width: 72%;"></div> <div style="width: 19%;"></div> <div style="width: 7%;"></div> <div style="width: 2%;"></div> </div> <div>72% 19% 7% .</div>

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
2	DCS	A	1001	X	-	X	-
2	DCS	B	1002	X	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6356 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.

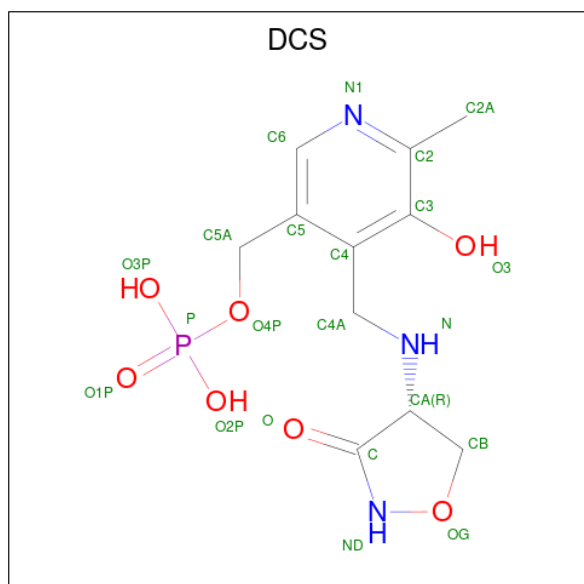
- Molecule 1 is a protein called ALANINE RACEMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3033	1941	538	541	13			
1	B	380	Total	C	N	O	S	0	0	0
			3024	1936	536	539	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	KCX	LYS	MODIFIED RESIDUE	UNP P10724
B	129	KCX	LYS	MODIFIED RESIDUE	UNP P10724

- Molecule 2 is D-[3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YLMETHYL]-N,O-CYCLOSERYLAMIDE (three-letter code: DCS) (formula: $C_{11}H_{16}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	3	7	1		

- Molecule 3 is water.

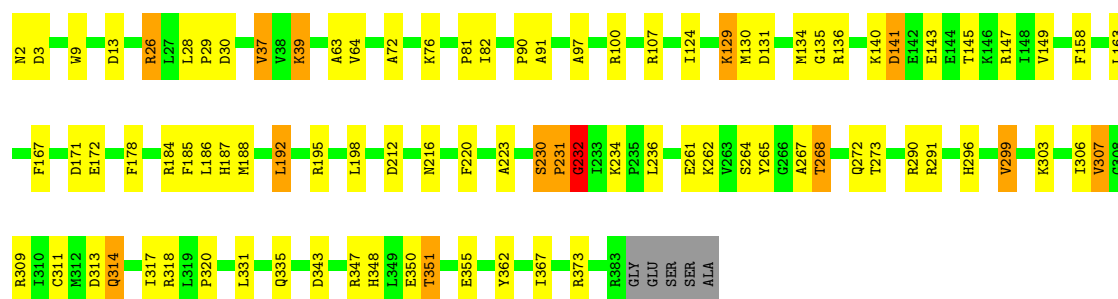
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		
3	B	128	Total	O	0	0
			128	128		

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. 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. 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.

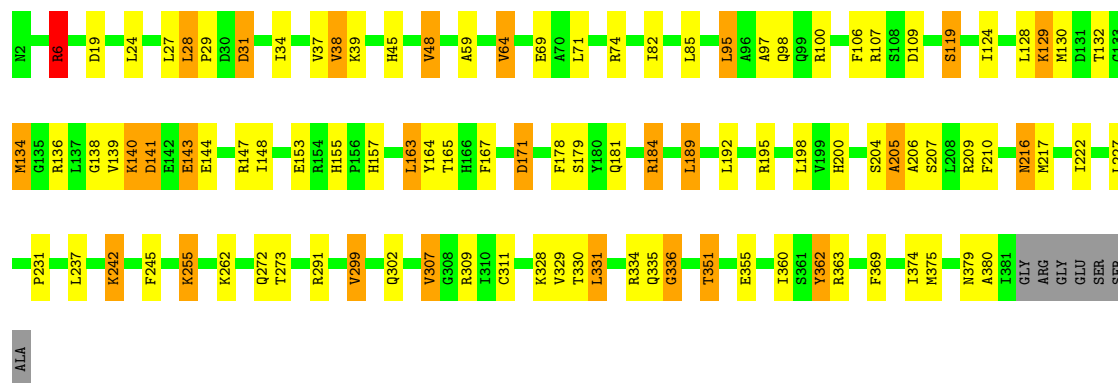
• Molecule 1: ALANINE RACEMASE

Chain A: 



• Molecule 1: ALANINE RACEMASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.16Å 90.24Å 85.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.79 – 2.20 29.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	86.8 (28.79-2.20) 85.3 (29.58-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.226 0.286 , 0.283	Depositor DCC
R_{free} test set	2234 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.8	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	0.89	EDS
Total number of atoms	6356	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 4.50% 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: DCS, KCX

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	1.11	11/3098 (0.4%)	1.29	26/4211 (0.6%)
1	B	0.82	1/3089 (0.0%)	1.21	18/4199 (0.4%)
All	All	0.97	12/6187 (0.2%)	1.25	44/8410 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	SER	C-N	29.05	1.89	1.34
1	A	231	PRO	C-N	27.49	1.82	1.33
1	B	205	ALA	C-N	14.79	1.68	1.34
1	A	81	PRO	C-N	11.85	1.61	1.34
1	A	30	ASP	C-N	9.67	1.56	1.34
1	A	91	ALA	C-N	8.95	1.54	1.34
1	A	29	PRO	C-N	7.53	1.51	1.34
1	A	82	ILE	C-N	6.99	1.50	1.34
1	A	90	PRO	C-N	6.45	1.48	1.34
1	A	187	HIS	C-N	5.92	1.47	1.34
1	A	186	LEU	C-N	5.79	1.47	1.34
1	A	143	GLU	CG-CD	5.45	1.60	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	GLY	O-C-N	-16.95	95.58	122.70
1	A	232	GLY	CA-C-N	11.92	143.43	117.20
1	A	30	ASP	O-C-N	-11.61	104.12	122.70
1	A	232	GLY	C-N-CA	10.83	148.78	121.70
1	A	230	SER	C-N-CD	9.79	148.95	128.40
1	A	230	SER	O-C-N	8.46	137.16	121.10
1	A	29	PRO	O-C-N	8.10	135.65	122.70
1	A	82	ILE	O-C-N	7.96	135.43	122.70
1	A	347	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	30	ASP	CA-C-N	7.70	134.14	117.20
1	B	27	LEU	CA-CB-CG	7.50	132.54	115.30
1	A	192	LEU	CA-CB-CG	7.30	132.10	115.30
1	A	347	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	30	ASP	C-N-CA	6.94	139.04	121.70
1	B	307	VAL	N-CA-CB	-6.77	96.60	111.50
1	B	171	ASP	CB-CG-OD1	6.76	124.39	118.30
1	B	98	GLN	CA-CB-CG	6.66	128.06	113.40
1	B	6	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	81	PRO	O-C-N	6.54	133.16	122.70
1	B	209	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	141	ASP	CB-CA-C	-6.31	97.79	110.40
1	B	6	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	109	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	230	SER	CA-C-N	-5.87	100.68	117.10
1	A	29	PRO	CA-C-N	-5.84	104.35	117.20
1	A	82	ILE	CA-C-N	-5.84	104.35	117.20
1	B	209	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	307	VAL	CB-CA-C	5.68	122.20	111.40
1	A	13	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	100	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	363	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	143	GLU	CA-CB-CG	5.39	125.26	113.40
1	A	230	SER	C-N-CA	-5.31	99.72	122.00
1	B	38	VAL	N-CA-CB	-5.28	99.89	111.50
1	A	307	VAL	N-CA-CB	-5.23	99.99	111.50
1	B	307	VAL	CG1-CB-CG2	5.22	119.25	110.90
1	B	360	ILE	N-CA-C	-5.17	97.03	111.00
1	A	29	PRO	C-N-CA	-5.17	108.79	121.70
1	A	81	PRO	CA-C-N	-5.13	105.90	117.20
1	B	184	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	373	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	48	VAL	CB-CA-C	-5.09	101.72	111.40
1	B	28	LEU	CA-CB-CG	5.02	126.84	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	GLY	Mainchain
1	A	362	TYR	Sidechain
1	B	204	SER	Mainchain
1	B	362	TYR	Sidechain

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	3033	0	3015	75	1
1	B	3024	0	3011	79	0
2	A	22	0	12	14	0
2	B	22	0	12	11	0
3	A	127	0	0	10	0
3	B	128	0	0	12	0
All	All	6356	0	6050	143	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (143) 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:205:ALA:C	1:B:206:ALA:N	1.68	1.46
1:A:231:PRO:C	1:A:232:GLY:N	1.82	1.32
1:A:230:SER:C	1:A:231:PRO:N	1.89	1.25
1:A:147:ARG:NH2	3:A:419:HOH:O	1.64	1.24
1:A:39:LYS:NZ	2:A:1001:DCS:H4A1	1.53	1.22
1:A:163:LEU:CD2	1:A:192:LEU:HD11	1.68	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LYS:NZ	2:B:1002:DCS:H4A1	1.56	1.19
1:A:39:LYS:CE	2:A:1001:DCS:H4A1	1.77	1.13
1:B:141:ASP:OD2	1:B:144:GLU:HB2	1.52	1.07
1:A:163:LEU:HD21	1:A:192:LEU:HD11	1.40	1.03
1:B:39:LYS:HZ1	2:B:1002:DCS:H4A1	0.87	1.01
1:A:39:LYS:HE3	2:A:1001:DCS:H4A1	1.42	1.00
1:A:163:LEU:HD22	1:A:192:LEU:HD11	1.38	0.99
1:A:39:LYS:NZ	2:A:1001:DCS:C4A	2.27	0.98
1:B:39:LYS:HZ1	2:B:1002:DCS:C4A	1.77	0.97
1:B:351:THR:HG21	1:B:355:GLU:OE1	1.67	0.94
1:A:39:LYS:HZ1	2:A:1001:DCS:H4A1	1.14	0.94
1:B:39:LYS:NZ	2:B:1002:DCS:C4A	2.32	0.92
1:A:163:LEU:CD2	1:A:192:LEU:CD1	2.50	0.89
1:A:291:ARG:HH21	1:B:291:ARG:NE	1.69	0.89
1:B:309:ARG:NH1	3:B:653:HOH:O	2.07	0.86
1:A:39:LYS:HZ1	2:A:1001:DCS:C4A	1.85	0.84
1:A:39:LYS:CE	2:A:1001:DCS:C4A	2.57	0.83
1:B:331:LEU:N	1:B:331:LEU:HD23	1.91	0.83
1:A:299:VAL:CG1	1:A:299:VAL:O	2.27	0.83
1:A:2:ASN:N	3:A:440:HOH:O	2.14	0.81
1:A:311:CYS:HB3	2:B:1002:DCS:O	1.81	0.80
1:A:39:LYS:HE3	2:A:1001:DCS:C4A	2.12	0.78
1:A:351:THR:HG21	1:A:355:GLU:OE1	1.83	0.78
1:B:19:ASP:OD2	1:B:242:LYS:HE2	1.84	0.76
1:B:132:THR:O	1:B:181:GLN:HG2	1.87	0.75
1:A:265:TYR:O	3:A:546:HOH:O	2.05	0.74
1:B:178:PHE:CE2	1:B:210:PHE:CE2	2.75	0.73
1:B:328:LYS:NZ	3:B:434:HOH:O	2.21	0.73
1:A:163:LEU:HD21	1:A:192:LEU:CD1	2.15	0.73
1:A:230:SER:C	1:A:231:PRO:CA	2.57	0.72
1:B:141:ASP:OD2	1:B:144:GLU:CB	2.35	0.71
1:A:163:LEU:HD22	1:A:192:LEU:CD1	2.17	0.71
1:B:155:HIS:O	3:B:565:HOH:O	2.07	0.71
1:B:129:KCX:C	1:B:130:MET:CA	2.66	0.70
1:B:299:VAL:HG12	1:B:329:VAL:HG22	1.73	0.70
1:A:100:ARG:O	3:A:427:HOH:O	2.09	0.69
1:B:334:ARG:NH1	1:B:336:GLY:O	2.25	0.69
1:A:350:GLU:HB2	1:B:291:ARG:HH22	1.59	0.68
1:A:299:VAL:O	1:A:299:VAL:HG13	1.94	0.68
1:B:31:ASP:OD2	3:B:447:HOH:O	2.12	0.67
1:A:198:LEU:HA	1:A:216:ASN:HD21	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:HZ3	2:A:1001:DCS:CA	2.08	0.67
1:A:268:THR:HB	3:A:546:HOH:O	1.94	0.67
1:A:291:ARG:NH2	1:B:291:ARG:NE	2.43	0.66
1:B:198:LEU:HA	1:B:216:ASN:HD21	1.60	0.65
1:B:143:GLU:OE2	3:B:633:HOH:O	2.15	0.64
1:A:130:MET:HE3	1:A:185:PHE:CE1	2.33	0.63
1:B:24:LEU:HD23	1:B:34:ILE:HD13	1.81	0.63
1:A:299:VAL:O	1:A:299:VAL:HG12	1.99	0.63
1:A:130:MET:HE3	1:A:185:PHE:CD1	2.34	0.62
1:B:134:MET:HB2	3:B:600:HOH:O	2.00	0.62
1:B:328:LYS:CE	3:B:434:HOH:O	2.49	0.61
1:B:163:LEU:HD13	1:B:192:LEU:HD11	1.82	0.60
1:A:230:SER:CA	1:A:231:PRO:N	2.64	0.60
1:A:291:ARG:HG3	1:A:291:ARG:HH11	1.66	0.60
1:B:129:KCX:CA	1:B:130:MET:N	2.63	0.60
1:B:328:LYS:HE3	3:B:434:HOH:O	2.01	0.60
1:B:71:LEU:HD21	1:B:95:LEU:CD1	2.32	0.59
1:B:299:VAL:O	1:B:299:VAL:HG23	2.03	0.59
1:B:167:PHE:CE2	1:B:178:PHE:HE1	2.21	0.59
1:A:130:MET:CE	1:A:185:PHE:CE1	2.87	0.58
1:B:129:KCX:HG2	1:B:138:GLY:HA2	1.86	0.58
1:A:39:LYS:NZ	2:A:1001:DCS:N	2.52	0.58
1:B:143:GLU:CD	3:B:633:HOH:O	2.42	0.58
1:B:39:LYS:HZ3	2:B:1002:DCS:C4A	2.17	0.57
1:A:291:ARG:HH21	1:B:291:ARG:CD	2.18	0.57
1:A:234:LYS:NZ	1:A:343:ASP:OD2	2.37	0.57
1:B:37:VAL:HG12	1:B:39:LYS:HG2	1.88	0.56
1:B:299:VAL:CG1	1:B:329:VAL:HG22	2.34	0.56
1:A:131:ASP:HB3	1:A:140:LYS:HG3	1.87	0.56
1:A:136:ARG:NH1	2:A:1001:DCS:O	2.39	0.55
1:B:85:LEU:HD22	2:B:1002:DCS:H2A3	1.89	0.55
1:A:130:MET:CE	1:A:185:PHE:HE1	2.20	0.54
1:B:129:KCX:OQ1	1:B:136:ARG:NH2	2.25	0.54
1:B:143:GLU:CG	3:B:633:HOH:O	2.55	0.54
1:A:265:TYR:HE2	1:A:311:CYS:HG	1.49	0.54
1:B:132:THR:HG23	1:B:165:THR:OG1	2.08	0.54
1:B:167:PHE:CD2	1:B:178:PHE:HE1	2.27	0.53
1:A:39:LYS:HE3	2:A:1001:DCS:C4	2.38	0.53
1:A:309:ARG:O	3:A:468:HOH:O	2.19	0.53
1:B:134:MET:HB3	3:B:588:HOH:O	2.09	0.53
1:A:220:PHE:CE1	1:A:223:ALA:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:MET:SD	1:A:188:MET:HB3	2.50	0.52
1:B:178:PHE:HE2	1:B:210:PHE:CE2	2.25	0.52
1:A:291:ARG:HG3	1:A:291:ARG:NH1	2.23	0.52
1:A:311:CYS:HA	2:B:1002:DCS:HND	1.74	0.52
1:A:129:KCX:OQ2	1:A:136:ARG:HB3	2.10	0.51
1:A:171:ASP:OD1	3:A:449:HOH:O	2.19	0.51
1:B:119:SER:O	1:B:157:HIS:CE1	2.64	0.51
1:A:290:ARG:HH11	1:B:351:THR:HG22	1.76	0.51
1:B:74:ARG:CZ	1:B:82:ILE:HD12	2.41	0.51
1:A:291:ARG:HH21	1:B:291:ARG:HE	1.55	0.49
1:B:200:HIS:HB3	1:B:217:MET:HB3	1.95	0.49
1:B:129:KCX:HG2	1:B:138:GLY:CA	2.43	0.49
1:B:178:PHE:CE2	1:B:210:PHE:CD2	3.01	0.49
1:A:37:VAL:HB	1:A:63:ALA:HB3	1.94	0.49
1:B:39:LYS:CE	2:B:1002:DCS:H4A1	2.40	0.48
1:B:39:LYS:NZ	2:B:1002:DCS:N	2.59	0.48
2:A:1001:DCS:O	1:B:311:CYS:HB3	2.14	0.47
1:A:97:ALA:HB2	1:A:124:ILE:HG12	1.96	0.47
1:A:311:CYS:HB3	2:B:1002:DCS:C	2.46	0.46
3:A:517:HOH:O	1:B:262:LYS:HB3	2.13	0.46
1:B:163:LEU:HD11	1:B:189:LEU:CD1	2.45	0.46
1:B:334:ARG:CZ	1:B:336:GLY:O	2.62	0.46
1:A:314:GLN:HG3	1:B:136:ARG:HD2	1.98	0.46
1:A:296:HIS:CD2	1:A:303:LYS:HD2	2.50	0.46
1:A:311:CYS:HB2	1:A:314:GLN:O	2.15	0.46
1:B:45:HIS:NE2	1:B:245:PHE:HB2	2.31	0.45
1:B:330:THR:C	1:B:331:LEU:HD23	2.36	0.45
1:B:34:ILE:HB	1:B:59:ALA:HA	1.99	0.45
1:B:128:LEU:HD13	1:B:148:ILE:HG21	1.99	0.45
1:A:135:GLY:O	1:B:255:LYS:HE2	2.17	0.45
1:B:362:TYR:O	1:B:380:ALA:HB3	2.16	0.45
1:A:320:PRO:HD3	3:A:514:HOH:O	2.15	0.44
1:B:222:ILE:HG13	1:B:227:LEU:HB2	1.99	0.44
1:A:72:ALA:O	1:A:76:LYS:HE2	2.18	0.44
1:A:145:THR:O	1:A:149:VAL:HG23	2.18	0.43
1:A:350:GLU:HB2	1:B:291:ARG:NH2	2.28	0.43
1:A:291:ARG:NH2	1:B:291:ARG:HE	2.11	0.43
1:A:262:LYS:HB3	1:A:267:ALA:HB1	2.02	0.42
1:B:64:VAL:HG13	1:B:69:GLU:HB2	2.01	0.42
1:B:97:ALA:HB2	1:B:124:ILE:HG12	2.01	0.42
1:A:291:ARG:HH11	1:A:291:ARG:CG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:TYR:HB2	1:B:200:HIS:O	2.20	0.42
1:A:39:LYS:NZ	2:A:1001:DCS:HB1	2.35	0.42
1:A:124:ILE:HD12	1:A:158:PHE:CE1	2.55	0.42
1:B:334:ARG:HG2	1:B:334:ARG:HH11	1.85	0.42
1:A:306:ILE:HA	1:A:317:ILE:HG22	2.02	0.41
1:A:134:MET:HB3	3:A:482:HOH:O	2.19	0.41
1:A:167:PHE:CD2	1:A:178:PHE:HE1	2.37	0.41
1:A:261:GLU:OE2	1:B:140:LYS:NZ	2.52	0.41
1:B:6:ARG:HD2	3:B:560:HOH:O	2.20	0.41
1:A:9:TRP:CD1	1:A:367:ILE:HD12	2.56	0.41
1:B:29:PRO:HB2	1:B:31:ASP:OD1	2.21	0.41
1:B:369:PHE:CE2	1:B:374:ILE:HG12	2.56	0.41
1:B:28:LEU:HA	1:B:29:PRO:HD2	1.91	0.40
1:B:106:PHE:CD2	1:B:107:ARG:HG3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:NH2	1:A:320:PRO:O[3_546]	1.72	0.48

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	379/387 (98%)	363 (96%)	16 (4%)	0	100	100
1	B	377/387 (97%)	364 (97%)	12 (3%)	1 (0%)	41	46
All	All	756/774 (98%)	727 (96%)	28 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	336	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	317/321 (99%)	292 (92%)	25 (8%)	12	12
1	B	317/321 (99%)	281 (89%)	36 (11%)	5	5
All	All	634/642 (99%)	573 (90%)	61 (10%)	8	8

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	26	ARG
1	A	37	VAL
1	A	39	LYS
1	A	64	VAL
1	A	107	ARG
1	A	141	ASP
1	A	172	GLU
1	A	184	ARG
1	A	195	ARG
1	A	212	ASP
1	A	236	LEU
1	A	264	SER
1	A	268	THR
1	A	272	GLN
1	A	273	THR
1	A	299	VAL
1	A	307	VAL
1	A	313	ASP
1	A	314	GLN
1	A	318	ARG
1	A	331	LEU
1	A	335	GLN

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Mol	Chain	Res	Type
1	A	348	HIS
1	A	351	THR
1	B	6	ARG
1	B	31	ASP
1	B	38	VAL
1	B	48	VAL
1	B	64	VAL
1	B	95	LEU
1	B	119	SER
1	B	134	MET
1	B	139	VAL
1	B	140	LYS
1	B	141	ASP
1	B	143	GLU
1	B	147	ARG
1	B	153	GLU
1	B	163	LEU
1	B	171	ASP
1	B	179	SER
1	B	184	ARG
1	B	189	LEU
1	B	195	ARG
1	B	207	SER
1	B	216	ASN
1	B	231	PRO
1	B	237	LEU
1	B	242	LYS
1	B	255	LYS
1	B	272	GLN
1	B	273	THR
1	B	299	VAL
1	B	302	GLN
1	B	307	VAL
1	B	331	LEU
1	B	335	GLN
1	B	351	THR
1	B	375	MET
1	B	379	ASN

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	216	ASN
1	A	253	HIS
1	A	272	GLN
1	A	293	GLN
1	A	314	GLN
1	B	216	ASN
1	B	258	GLN
1	B	314	GLN
1	B	379	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	KCX	A	129	1	9,11,12	1.25	2 (22%)	5,12,14	3.03	2 (40%)
1	KCX	B	129	1	9,11,12	1.11	1 (11%)	5,12,14	2.18	2 (40%)

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
1	KCX	A	129	1	-	3/9/10/12	-
1	KCX	B	129	1	-	4/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	KCX	OQ1-CX	2.55	1.26	1.21
1	B	129	KCX	OQ1-CX	2.38	1.26	1.21
1	A	129	KCX	CX-NZ	-2.17	1.31	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	KCX	OQ1-CX-NZ	-6.30	115.19	124.96
1	B	129	KCX	OQ1-CX-NZ	-3.40	119.69	124.96
1	B	129	KCX	CE-NZ-CX	3.06	126.81	121.89
1	A	129	KCX	CE-NZ-CX	-2.02	118.65	121.89

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	129	KCX	OQ1-CX-NZ-CE
1	B	129	KCX	OQ2-CX-NZ-CE
1	B	129	KCX	CG-CD-CE-NZ
1	B	129	KCX	CE-CD-CG-CB
1	A	129	KCX	CG-CD-CE-NZ
1	A	129	KCX	CA-CB-CG-CD
1	A	129	KCX	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	129	KCX	1	0
1	B	129	KCX	5	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	DCS	A	1001	1	22,23,23	4.72	11 (50%)	25,33,33	1.70	4 (16%)
2	DCS	B	1002	1	22,23,23	4.93	10 (45%)	25,33,33	1.45	2 (8%)

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	DCS	A	1001	1	1/1/3/5	6/10/21/21	0/2/2/2
2	DCS	B	1002	1	1/1/3/5	6/10/21/21	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	DCS	CA-C	-15.71	1.41	1.52
2	A	1001	DCS	CA-C	-13.72	1.42	1.52
2	B	1002	DCS	P-O1P	9.02	1.79	1.50
2	A	1001	DCS	P-O1P	8.44	1.77	1.50
2	A	1001	DCS	CB-CA	-7.49	1.37	1.54
2	B	1002	DCS	CB-CA	-7.32	1.37	1.54
2	A	1001	DCS	O-C	6.45	1.36	1.23
2	A	1001	DCS	P-O3P	6.18	1.78	1.54
2	B	1002	DCS	P-O2P	6.14	1.78	1.54
2	A	1001	DCS	P-O2P	5.85	1.77	1.54
2	B	1002	DCS	P-O3P	5.85	1.77	1.54
2	B	1002	DCS	O-C	5.40	1.34	1.23
2	B	1002	DCS	OG-CB	-4.44	1.35	1.44
2	A	1001	DCS	OG-CB	-4.23	1.35	1.44
2	B	1002	DCS	CA-N	-3.21	1.39	1.46
2	A	1001	DCS	C5-C4	3.12	1.44	1.40
2	B	1002	DCS	C-ND	-3.08	1.30	1.34
2	A	1001	DCS	CA-N	-3.07	1.39	1.46
2	A	1001	DCS	C-ND	-2.92	1.31	1.34
2	A	1001	DCS	C4A-C4	-2.50	1.48	1.51
2	B	1002	DCS	C5-C4	2.49	1.43	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	DCS	C4A-C4-C3	5.58	126.02	120.04
2	B	1002	DCS	C4A-N-CA	3.85	121.22	113.92
2	B	1002	DCS	C4A-C4-C3	3.75	124.06	120.04
2	A	1001	DCS	C4A-C4-C5	-3.34	116.00	119.71
2	A	1001	DCS	C4A-N-CA	2.40	118.46	113.92
2	A	1001	DCS	CB-OG-ND	2.12	108.95	105.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	DCS	CA
2	B	1002	DCS	CA

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	DCS	C5A-O4P-P-O1P
2	A	1001	DCS	C5A-O4P-P-O2P
2	A	1001	DCS	C5A-O4P-P-O3P
2	A	1001	DCS	CB-CA-N-C4A
2	B	1002	DCS	C5A-O4P-P-O1P
2	B	1002	DCS	C5A-O4P-P-O2P
2	B	1002	DCS	C5A-O4P-P-O3P
2	B	1002	DCS	CB-CA-N-C4A
2	A	1001	DCS	C5-C4-C4A-N
2	B	1002	DCS	C5-C4-C4A-N
2	B	1002	DCS	C3-C4-C4A-N
2	A	1001	DCS	C3-C4-C4A-N

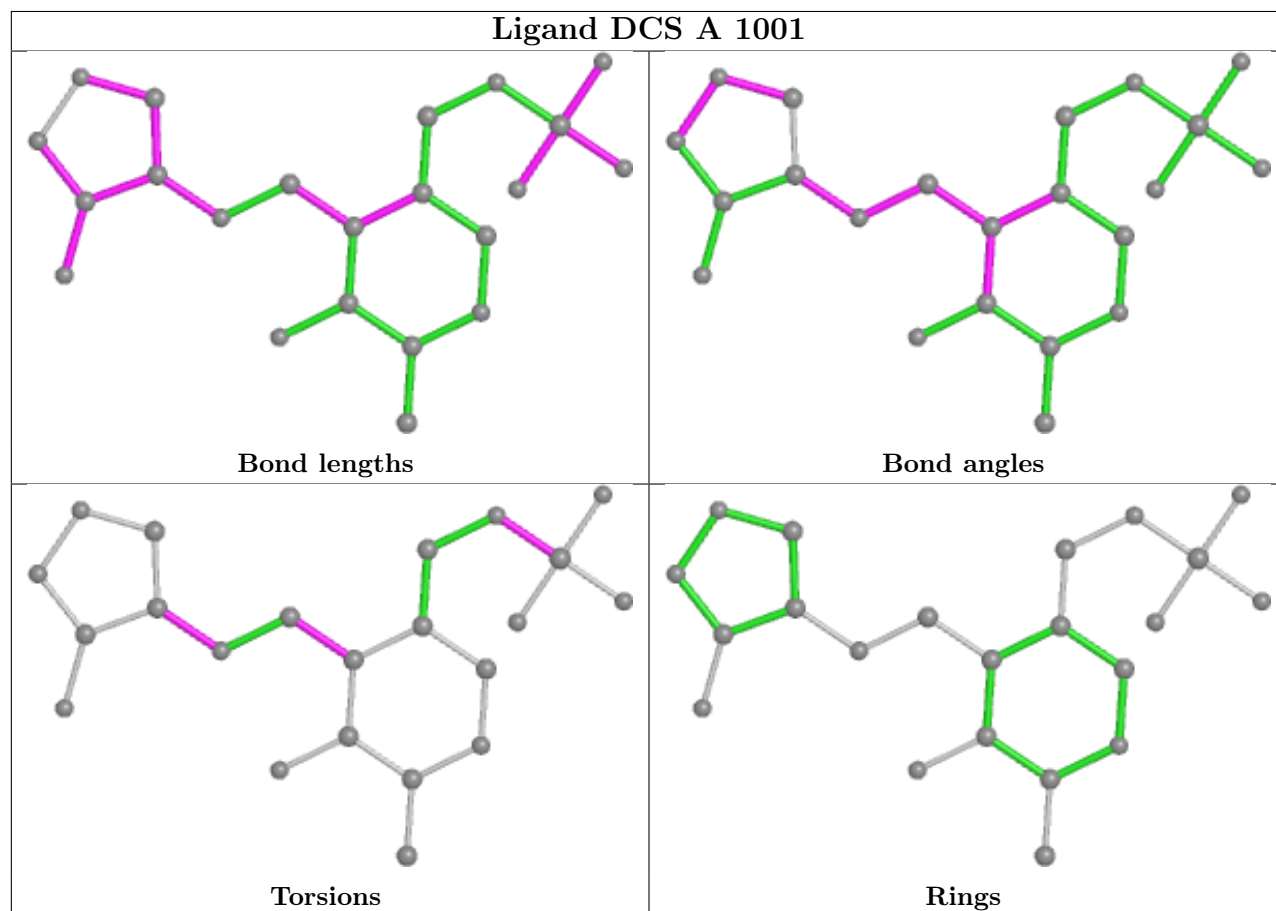
There are no ring outliers.

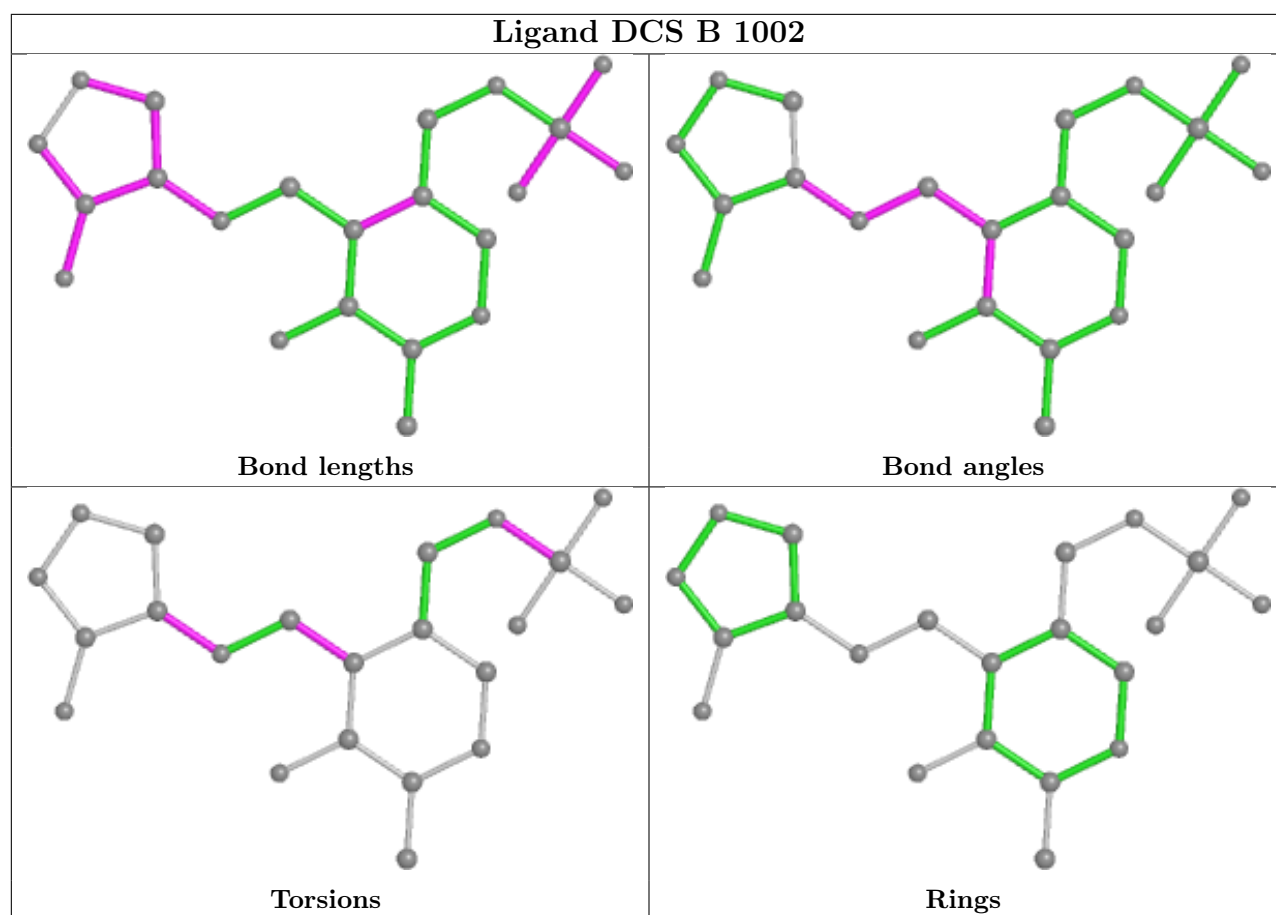
2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	DCS	14	0
2	B	1002	DCS	11	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	230:SER	C	231:PRO	N	1.89
1	A	231:PRO	C	232:GLY	N	1.82
1	B	129:KCX	C	130:MET	N	1.72
1	B	205:ALA	C	206:ALA	N	1.68
1	A	81:PRO	C	82:ILE	N	1.61

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

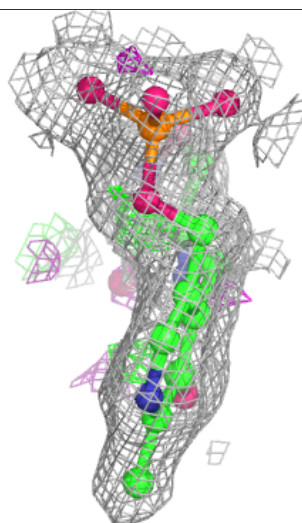
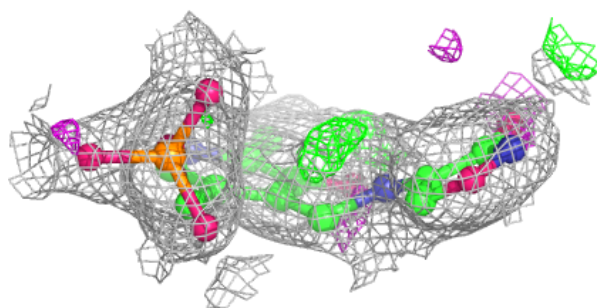
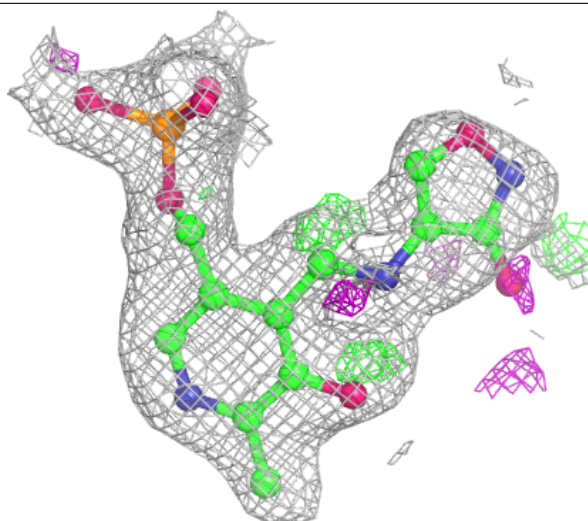
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

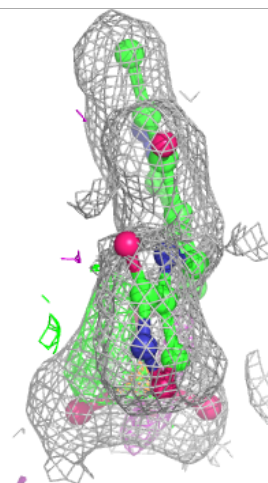
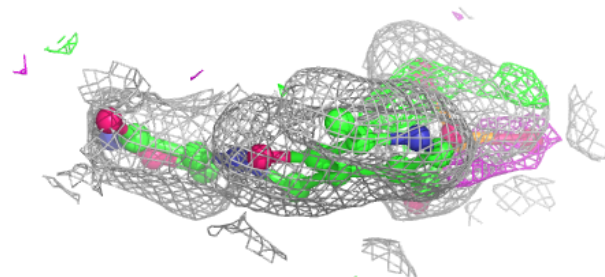
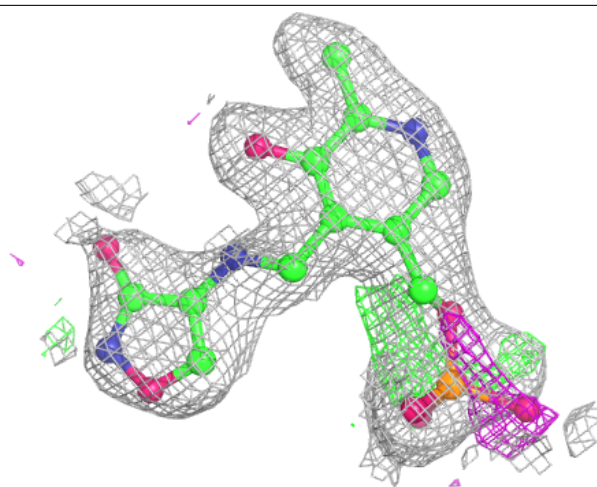
Electron density around DCS A 1001:

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



Electron density around DCS B 1002:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.