



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:20 PM UTC

PDB ID : 1NIU / pdb_00001niu
Title : ALANINE RACEMASE WITH BOUND INHIBITOR DERIVED FROM L-CYCLOSERINE
Authors : Fenn, T.D.; Stamper, G.F.; Morollo, A.A.; Ringe, D.
Deposited on : 2002-12-26
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	:	4-5-2 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

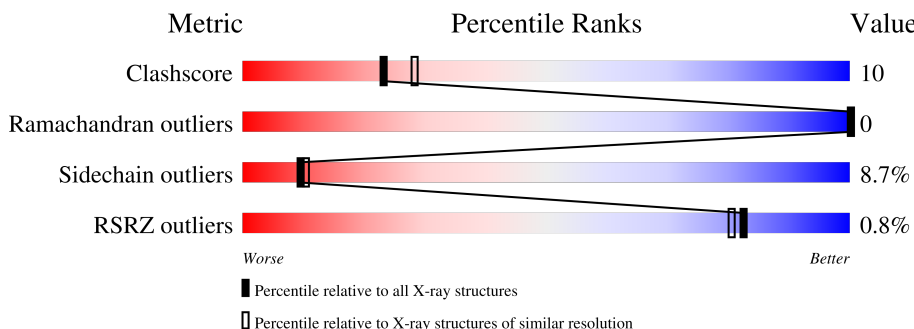
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	388	
1	B	388	

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
1	KCX	B	129	-	-	X	-
2	DCS	A	800	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DCS	B	900	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6387 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.

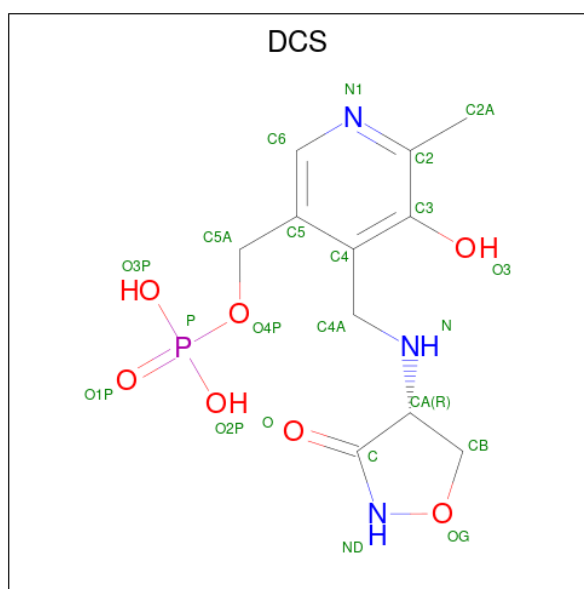
- Molecule 1 is a protein called Alanine Racemase.

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-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL]-N,O-CYCLOSERYLAMIDE (CCD ID: 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		

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

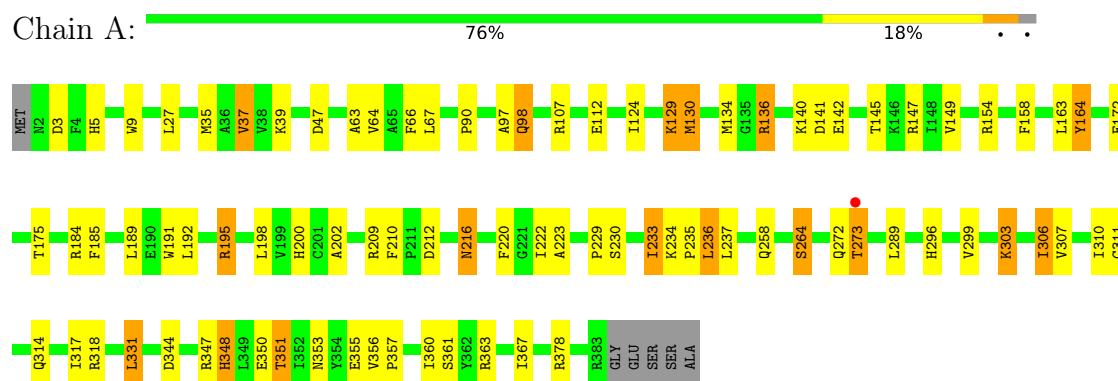
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total	O	0	0
			139	139		
3	B	147	Total	O	0	0
			147	147		

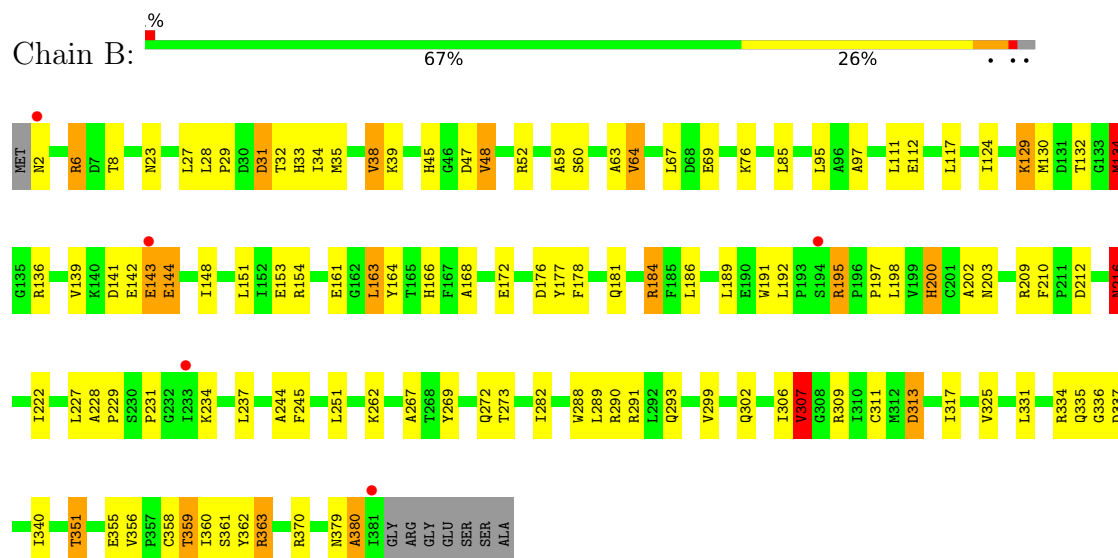
3 Residue-property plots [i](#)

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: Alanine Racemase



• Molecule 1: Alanine Racemase



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)	35.00 – 2.20 35.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.20) 86.8 (35.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.231 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6387	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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	0.56	0/3098	1.14	32/4211 (0.8%)
1	B	0.60	3/3089 (0.1%)	1.14	25/4199 (0.6%)
All	All	0.58	3/6187 (0.0%)	1.14	57/8410 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	CYS	C-O	10.97	1.37	1.24
1	B	359	THR	C-N	-6.81	1.26	1.33
1	B	359	THR	N-CA	5.45	1.53	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	SER	N-CA-C	14.27	127.96	110.41
1	A	361	SER	N-CA-C	10.58	123.42	110.41
1	B	47	ASP	N-CA-C	8.90	120.67	110.97
1	B	202	ALA	N-CA-C	8.79	123.74	109.76
1	A	47	ASP	N-CA-C	8.22	121.06	111.02
1	A	202	ALA	N-CA-C	7.56	121.47	110.28
1	A	210	PHE	CA-C-N	7.16	127.15	119.28
1	A	210	PHE	C-N-CA	7.16	127.15	119.28
1	A	216	ASN	N-CA-C	7.15	122.11	112.88
1	A	230	SER	CA-C-N	-7.13	112.36	119.56
1	A	230	SER	C-N-CA	-7.13	112.36	119.56
1	A	306	ILE	N-CA-C	-6.88	99.81	108.89
1	A	237	LEU	CA-C-N	6.84	126.64	119.05
1	A	237	LEU	C-N-CA	6.84	126.64	119.05
1	A	136	ARG	NE-CZ-NH1	-6.78	114.72	121.50
1	B	67	LEU	N-CA-C	6.75	119.50	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ARG	CA-C-N	-6.72	113.46	120.38
1	A	195	ARG	C-N-CA	-6.72	113.46	120.38
1	B	359	THR	CA-C-O	6.72	127.14	119.27
1	A	289	LEU	N-CA-C	6.67	118.91	110.24
1	A	67	LEU	N-CA-C	6.57	118.99	111.11
1	B	144	GLU	N-CA-C	-6.53	103.66	111.69
1	B	216	ASN	N-CA-C	6.49	120.51	112.59
1	A	136	ARG	NE-CZ-NH2	6.44	125.00	119.20
1	B	289	LEU	N-CA-C	6.26	118.38	110.24
1	A	5	HIS	N-CA-C	6.24	120.67	111.87
1	B	380	ALA	N-CA-C	6.06	118.68	111.71
1	B	340	ILE	N-CA-C	-6.06	98.91	107.75
1	A	112	GLU	N-CA-C	-5.96	104.69	111.07
1	B	32	THR	N-CA-C	5.89	118.27	109.25
1	A	27	LEU	N-CA-C	5.87	117.68	111.28
1	A	154	ARG	N-CA-C	5.87	118.62	111.82
1	B	306	ILE	N-CA-C	-5.79	99.97	108.54
1	B	28	LEU	CA-C-N	5.71	125.47	119.76
1	B	28	LEU	C-N-CA	5.71	125.47	119.76
1	A	360	ILE	N-CA-C	-5.67	100.52	108.12
1	A	356	VAL	CA-C-N	-5.65	113.07	119.28
1	A	356	VAL	C-N-CA	-5.65	113.07	119.28
1	A	185	PHE	N-CA-C	-5.61	105.07	111.07
1	A	233	ILE	N-CA-C	5.59	120.97	109.34
1	B	307	VAL	N-CA-CB	-5.30	104.05	111.25
1	B	244	ALA	N-CA-C	5.29	119.83	112.90
1	B	203	ASN	N-CA-C	-5.21	101.75	109.94
1	A	264	SER	N-CA-C	5.21	121.90	110.80
1	A	164	TYR	N-CA-C	5.20	116.71	108.96
1	A	175	THR	N-CA-C	5.20	118.76	112.93
1	B	356	VAL	CA-C-N	-5.19	114.27	119.56
1	B	356	VAL	C-N-CA	-5.19	114.27	119.56
1	B	134	MET	N-CA-C	-5.16	107.12	113.41
1	B	293	GLN	N-CA-C	5.14	118.33	111.75
1	A	273	THR	N-CA-C	-5.13	101.64	109.65
1	A	130	MET	N-CA-C	-5.13	96.64	111.00
1	A	258	GLN	N-CA-C	-5.09	102.76	110.50
1	B	176	ASP	N-CA-C	5.09	117.73	111.82
1	B	177	TYR	N-CA-C	-5.08	105.83	112.23
1	B	356	VAL	N-CA-C	5.03	119.74	108.88
1	B	234	LYS	N-CA-C	5.00	119.75	113.25

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	3033	0	3016	50	0
1	B	3024	0	3011	79	0
2	A	22	0	12	5	0
2	B	22	0	13	6	0
3	A	139	0	0	6	0
3	B	147	0	0	10	0
All	All	6387	0	6052	125	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 (125) 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:351:THR:HG21	1:B:355:GLU:OE1	1.59	1.00
1:B:141:ASP:OD1	1:B:144:GLU:HB2	1.62	1.00
1:B:52:ARG:HD2	3:B:655:HOH:O	1.66	0.94
1:B:129:KCX:C	1:B:130:MET:N	2.31	0.94
1:A:351:THR:HG21	1:A:355:GLU:OE1	1.69	0.93
1:A:163:LEU:HD21	1:A:189:LEU:HD22	1.52	0.91
1:A:163:LEU:HD21	1:A:189:LEU:CD2	2.10	0.82
1:B:129:KCX:OQ2	1:B:136:ARG:NH2	2.12	0.81
1:B:195:ARG:HG3	1:B:195:ARG:HH11	1.47	0.79
1:B:39:LYS:CE	2:B:900:DCS:H4A1	2.13	0.78
1:B:85:LEU:HD22	2:B:900:DCS:H2A3	1.65	0.78
1:A:136:ARG:NH1	2:A:800:DCS:O	2.17	0.77
1:B:198:LEU:HD21	3:B:669:HOH:O	1.84	0.76
1:B:195:ARG:HH11	1:B:195:ARG:CG	1.98	0.75
1:B:163:LEU:HD13	1:B:192:LEU:HD11	1.68	0.74
1:A:39:LYS:HE2	1:B:313:ASP:OD2	1.87	0.73
1:A:198:LEU:HA	1:A:216:ASN:HD21	1.52	0.73
1:B:132:THR:O	1:B:181:GLN:HG2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:GLU:HA	1:B:143:GLU:OE1	1.88	0.72
1:A:129:KCX:OQ2	1:A:136:ARG:HB3	1.92	0.69
1:A:129:KCX:C	1:A:130:MET:N	2.55	0.68
1:B:309:ARG:NH1	3:B:679:HOH:O	2.25	0.68
1:B:195:ARG:HG3	1:B:195:ARG:NH1	2.05	0.68
1:A:348:HIS:CE1	3:A:544:HOH:O	2.48	0.67
1:A:130:MET:N	1:A:164:TYR:O	2.28	0.67
1:B:33:HIS:HD2	1:B:60:SER:OG	1.79	0.66
1:B:33:HIS:CE1	3:B:669:HOH:O	2.49	0.66
1:A:39:LYS:HZ2	2:A:800:DCS:H4A1	1.61	0.65
1:B:38:VAL:HG13	1:B:38:VAL:O	1.95	0.65
1:B:262:LYS:HD3	1:B:267:ALA:HB1	1.79	0.64
1:B:136:ARG:NH1	2:B:900:DCS:O	2.30	0.64
1:B:129:KCX:CX	1:B:136:ARG:HH21	2.11	0.63
1:B:134:MET:HB2	3:B:616:HOH:O	1.98	0.63
1:B:334:ARG:NH1	1:B:336:GLY:O	2.32	0.63
1:B:130:MET:N	1:B:164:TYR:O	2.33	0.62
1:A:378:ARG:NH2	3:A:665:HOH:O	2.33	0.61
1:B:39:LYS:HE3	2:B:900:DCS:H4A1	1.82	0.61
1:B:134:MET:HB3	3:B:604:HOH:O	2.02	0.60
1:A:163:LEU:HD22	1:A:192:LEU:HD11	1.86	0.58
1:B:198:LEU:HA	1:B:216:ASN:HD21	1.69	0.58
1:B:39:LYS:NZ	2:B:900:DCS:H4A1	2.18	0.57
1:A:97:ALA:HB2	1:A:124:ILE:HG12	1.87	0.57
1:A:350:GLU:HB2	1:B:291:ARG:HH22	1.70	0.56
1:A:163:LEU:CD2	1:A:189:LEU:HD22	2.31	0.55
1:B:129:KCX:OQ2	1:B:166:HIS:CB	2.55	0.55
1:B:6:ARG:HD3	1:B:8:THR:HB	1.89	0.54
1:A:314:GLN:HG3	1:B:136:ARG:HD2	1.90	0.53
1:A:66:PHE:HZ	1:B:363:ARG:HG2	1.73	0.53
1:A:348:HIS:HE1	3:A:544:HOH:O	1.90	0.52
1:B:38:VAL:O	1:B:38:VAL:CG1	2.57	0.52
1:A:209:ARG:HH11	1:A:236:LEU:HD12	1.74	0.52
1:A:124:ILE:HD12	1:A:158:PHE:CE1	2.45	0.51
1:A:220:PHE:CE1	1:A:223:ALA:HB3	2.45	0.51
1:A:163:LEU:HD22	1:A:192:LEU:CD1	2.41	0.51
1:A:311:CYS:HB2	1:A:314:GLN:O	2.11	0.51
1:B:97:ALA:HB2	1:B:124:ILE:HG12	1.92	0.50
1:A:134:MET:HB3	3:A:494:HOH:O	2.10	0.50
1:A:311:CYS:HB3	2:B:900:DCS:O	2.12	0.50
1:B:33:HIS:CD2	1:B:60:SER:OG	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:KCX:OQ2	1:B:166:HIS:CG	2.65	0.49
1:B:48:VAL:HG11	1:B:76:LYS:HB3	1.94	0.49
1:A:234:LYS:N	1:A:235:PRO:HD2	2.28	0.49
1:B:186:LEU:HA	1:B:189:LEU:HD12	1.95	0.48
1:B:141:ASP:OD1	1:B:141:ASP:C	2.55	0.48
1:B:143:GLU:OE1	1:B:143:GLU:CA	2.60	0.48
1:B:172:GLU:O	1:B:209:ARG:NH2	2.47	0.48
1:B:45:HIS:NE2	1:B:245:PHE:HB2	2.30	0.47
1:B:129:KCX:C	1:B:130:MET:CA	2.92	0.47
1:B:134:MET:HG2	1:B:168:ALA:HB2	1.96	0.47
1:B:370:ARG:NH2	3:B:424:HOH:O	2.46	0.47
1:B:134:MET:HE2	1:B:168:ALA:CB	2.45	0.47
1:A:140:LYS:HE3	3:B:641:HOH:O	2.15	0.46
1:A:351:THR:HG22	1:B:290:ARG:HE	1.81	0.46
1:A:90:PRO:HG2	3:A:418:HOH:O	2.14	0.46
1:B:222:ILE:HG13	1:B:227:LEU:HB2	1.98	0.46
1:B:64:VAL:HG13	1:B:69:GLU:HB2	1.98	0.46
1:B:129:KCX:CX	1:B:166:HIS:HB3	2.46	0.46
1:B:35:MET:SD	1:B:63:ALA:HB2	2.56	0.45
2:A:800:DCS:O3	2:A:800:DCS:N	2.46	0.45
1:A:37:VAL:HB	1:A:63:ALA:HB3	1.98	0.45
1:B:331:LEU:HD12	1:B:331:LEU:N	2.31	0.45
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.81	0.45
1:B:379:ASN:C	1:B:379:ASN:HD22	2.25	0.45
1:A:129:KCX:C	1:A:130:MET:CA	2.94	0.45
2:A:800:DCS:HND	1:B:311:CYS:HB3	1.82	0.45
1:B:29:PRO:HB2	1:B:31:ASP:OD1	2.17	0.45
1:B:151:LEU:CD2	1:B:154:ARG:HH21	2.30	0.44
1:A:331:LEU:N	1:A:331:LEU:CD2	2.81	0.44
1:A:331:LEU:N	1:A:331:LEU:HD22	2.32	0.44
1:B:362:TYR:O	1:B:380:ALA:HB3	2.16	0.44
1:A:9:TRP:CD1	1:A:367:ILE:HD12	2.52	0.44
1:A:145:THR:O	1:A:149:VAL:HG23	2.18	0.44
1:B:151:LEU:HD23	1:B:154:ARG:HH21	1.83	0.44
1:A:296:HIS:NE2	1:A:303:LYS:HD2	2.32	0.43
1:A:347:ARG:NH1	3:A:544:HOH:O	2.49	0.43
1:B:6:ARG:HD2	3:B:575:HOH:O	2.18	0.43
1:A:353:ASN:O	1:A:357:PRO:HD2	2.19	0.43
1:B:178:PHE:CE2	1:B:210:PHE:CE2	3.07	0.43
1:B:251:LEU:HD21	1:B:317:ILE:HD11	2.01	0.43
1:A:35:MET:SD	1:A:63:ALA:HB2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ILE:HA	1:A:317:ILE:HG22	2.01	0.43
1:B:269:TYR:CE1	1:B:307:VAL:HG22	2.53	0.42
1:B:282:ILE:HG21	1:B:331:LEU:HD21	2.00	0.42
1:A:229:PRO:HB2	1:A:233:ILE:HD11	2.02	0.42
1:B:34:ILE:HB	1:B:59:ALA:HA	2.02	0.42
1:B:111:LEU:HD11	1:B:148:ILE:HG23	2.01	0.42
1:A:198:LEU:HA	1:A:216:ASN:ND2	2.28	0.41
1:B:288:TRP:CE2	1:B:331:LEU:HD23	2.55	0.41
1:B:228:ALA:HA	1:B:229:PRO:HD3	1.95	0.41
1:B:142:GLU:HA	1:B:191:TRP:CE3	2.55	0.41
1:B:161:GLU:O	1:B:197:PRO:HG2	2.20	0.41
1:B:134:MET:CE	1:B:168:ALA:HA	2.49	0.41
1:A:98:GLN:HE21	1:A:98:GLN:HB2	1.52	0.41
1:A:147:ARG:HG3	1:A:147:ARG:NH1	2.36	0.41
1:B:189:LEU:HB3	1:B:195:ARG:HH12	1.84	0.41
1:A:164:TYR:HB3	1:A:200:HIS:CE1	2.56	0.41
1:B:112:GLU:HG3	1:B:151:LEU:HD11	2.03	0.41
1:B:163:LEU:HD11	1:B:189:LEU:HD23	2.02	0.40
1:A:222:ILE:N	2:A:800:DCS:O1P	2.41	0.40
1:B:200:HIS:CD2	1:B:200:HIS:N	2.89	0.40
1:A:142:GLU:HG3	1:A:191:TRP:CG	2.57	0.40
1:A:344:ASP:OD1	1:A:347:ARG:NH2	2.55	0.40
1:B:23:ASN:HD22	1:B:23:ASN:HA	1.70	0.40
1:B:359:THR:O	1:B:360:ILE:C	2.59	0.40
1:B:184:ARG:NH2	3:B:678:HOH:O	2.53	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	378/388 (97%)	364 (96%)	14 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	376/388 (97%)	362 (96%)	14 (4%)	0	100	100
All	All	754/776 (97%)	726 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	317/322 (98%)	294 (93%)	23 (7%)	13	15
1	B	317/322 (98%)	285 (90%)	32 (10%)	7	7
All	All	634/644 (98%)	579 (91%)	55 (9%)	9	10

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	37	VAL
1	A	64	VAL
1	A	98	GLN
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	272	GLN
1	A	273	THR
1	A	299	VAL
1	A	303	LYS
1	A	307	VAL
1	A	310	ILE

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Mol	Chain	Res	Type
1	A	318	ARG
1	A	331	LEU
1	A	348	HIS
1	A	351	THR
1	A	363	ARG
1	B	2	ASN
1	B	6	ARG
1	B	27	LEU
1	B	31	ASP
1	B	38	VAL
1	B	48	VAL
1	B	64	VAL
1	B	95	LEU
1	B	117	LEU
1	B	134	MET
1	B	139	VAL
1	B	143	GLU
1	B	153	GLU
1	B	163	LEU
1	B	184	ARG
1	B	195	ARG
1	B	200	HIS
1	B	212	ASP
1	B	216	ASN
1	B	231	PRO
1	B	237	LEU
1	B	272	GLN
1	B	273	THR
1	B	299	VAL
1	B	302	GLN
1	B	307	VAL
1	B	313	ASP
1	B	325	VAL
1	B	335	GLN
1	B	337	ASP
1	B	351	THR
1	B	363	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN

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Mol	Chain	Res	Type
1	A	216	ASN
1	A	272	GLN
1	A	314	GLN
1	B	2	ASN
1	B	5	HIS
1	B	23	ASN
1	B	33	HIS
1	B	216	ASN
1	B	258	GLN
1	B	294	HIS
1	B	296	HIS
1	B	348	HIS
1	B	371	HIS
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	B	129	1	10,11,12	1.50	2 (20%)	6,12,14	2.23	1 (16%)
1	KCX	A	129	1	10,11,12	1.50	2 (20%)	6,12,14	1.65	2 (33%)

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	B	129	1	-	2/9/10/12	-
1	KCX	A	129	1	-	2/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	KCX	OQ1-CX	2.68	1.26	1.21
1	A	129	KCX	O-C	2.64	1.30	1.20
1	A	129	KCX	OQ1-CX	2.56	1.26	1.21
1	B	129	KCX	O-C	2.35	1.28	1.20

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	KCX	OQ1-CX-NZ	-4.90	117.48	124.92
1	A	129	KCX	CD-CE-NZ	2.20	118.36	112.20
1	A	129	KCX	CE-NZ-CX	2.16	125.64	121.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	129	KCX	7	0
1	A	129	KCX	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	800	-	22,23,23	5.31	12 (54%)	27,33,33	1.69	7 (25%)
2	DCS	B	900	-	22,23,23	4.99	12 (54%)	27,33,33	1.57	5 (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
2	DCS	A	800	-	1/1/3/5	3/11/21/21	0/2/2/2
2	DCS	B	900	-	1/1/3/5	3/11/21/21	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	DCS	CA-C	-17.18	1.39	1.52
2	B	900	DCS	CA-C	-14.96	1.41	1.52
2	B	900	DCS	P-O1P	8.35	1.76	1.50
2	A	800	DCS	P-O1P	8.20	1.76	1.50
2	B	900	DCS	P-O2P	7.43	1.82	1.54
2	A	800	DCS	P-O2P	7.11	1.81	1.54
2	B	900	DCS	O-C	6.94	1.36	1.23
2	A	800	DCS	P-O3P	6.48	1.78	1.54
2	B	900	DCS	P-O3P	6.36	1.78	1.54
2	A	800	DCS	C-ND	-6.07	1.27	1.34
2	A	800	DCS	CB-CA	-6.00	1.39	1.53
2	B	900	DCS	CB-CA	-5.78	1.39	1.53
2	A	800	DCS	O-C	5.43	1.33	1.23
2	B	900	DCS	C-ND	-4.55	1.29	1.34
2	A	800	DCS	C5-C4	4.28	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	DCS	C5-C4	4.22	1.46	1.40
2	B	900	DCS	CA-N	-3.50	1.38	1.46
2	A	800	DCS	CA-N	-3.33	1.39	1.46
2	A	800	DCS	OG-CB	-3.15	1.37	1.44
2	B	900	DCS	OG-CB	-3.10	1.37	1.44
2	A	800	DCS	C4A-C4	-2.57	1.48	1.52
2	B	900	DCS	C2A-C2	2.40	1.54	1.50
2	A	800	DCS	C3-C2	-2.24	1.38	1.41
2	B	900	DCS	C6-C5	2.19	1.42	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	DCS	C4A-N-CA	4.38	122.05	113.84
2	A	800	DCS	CA-C-ND	4.31	110.28	107.63
2	A	800	DCS	C4A-N-CA	3.74	120.87	113.84
2	B	900	DCS	C6-C5-C4	-2.64	116.06	118.06
2	B	900	DCS	CA-C-ND	2.55	109.19	107.63
2	A	800	DCS	O4P-C5A-C5	2.55	114.14	109.36
2	A	800	DCS	C6-N1-C2	2.36	123.47	119.20
2	B	900	DCS	C6-N1-C2	2.16	123.12	119.20
2	A	800	DCS	C6-C5-C4	-2.12	116.46	118.06
2	A	800	DCS	C5-C6-N1	-2.10	120.42	123.83
2	B	900	DCS	CB-OG-ND	2.10	109.57	105.92
2	A	800	DCS	O-C-CA	-2.07	124.70	126.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	800	DCS	CA
2	B	900	DCS	CA

All (6) torsion outliers are listed below:

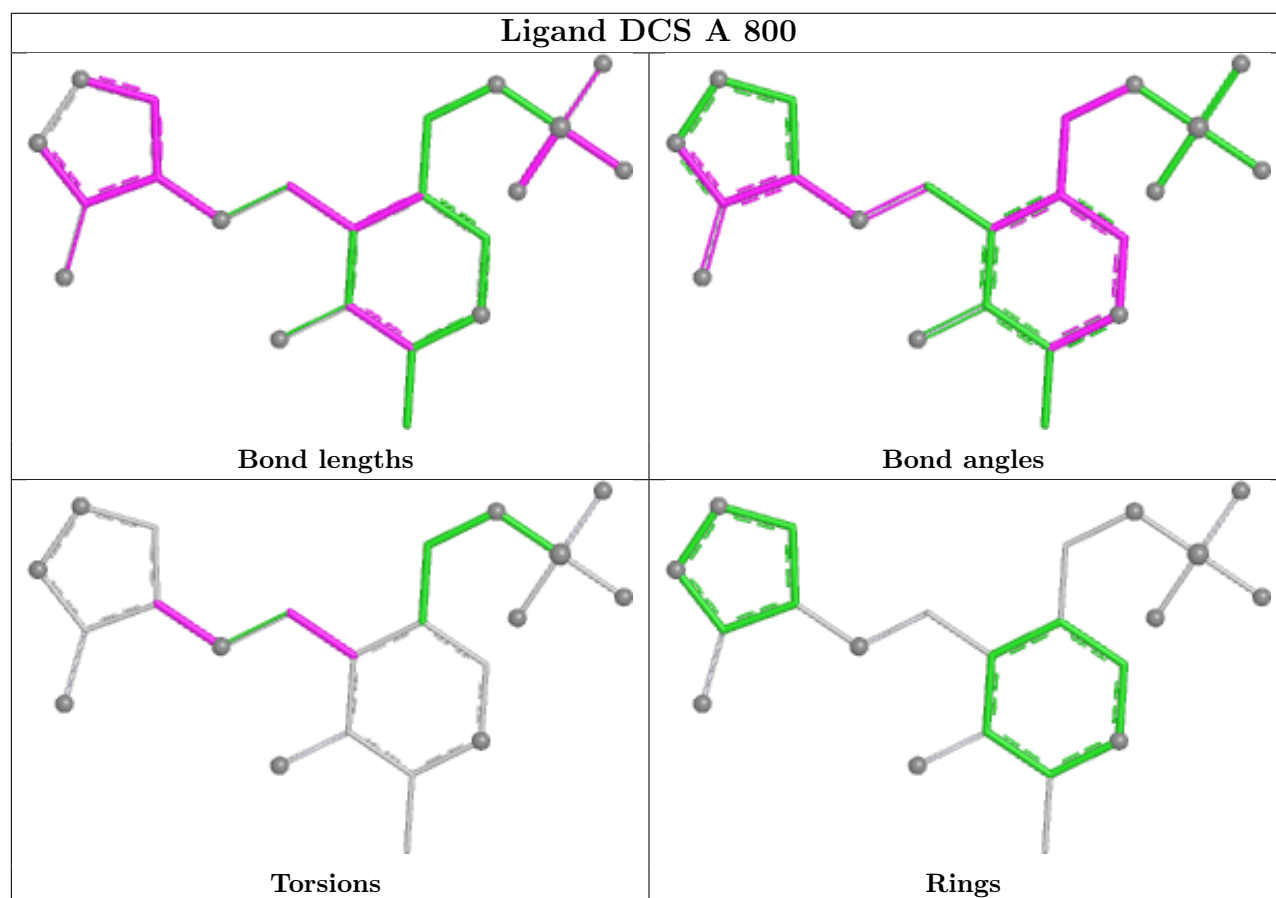
Mol	Chain	Res	Type	Atoms
2	A	800	DCS	C3-C4-C4A-N
2	A	800	DCS	C5-C4-C4A-N
2	A	800	DCS	CB-CA-N-C4A
2	B	900	DCS	CB-CA-N-C4A
2	B	900	DCS	C5-C4-C4A-N
2	B	900	DCS	C3-C4-C4A-N

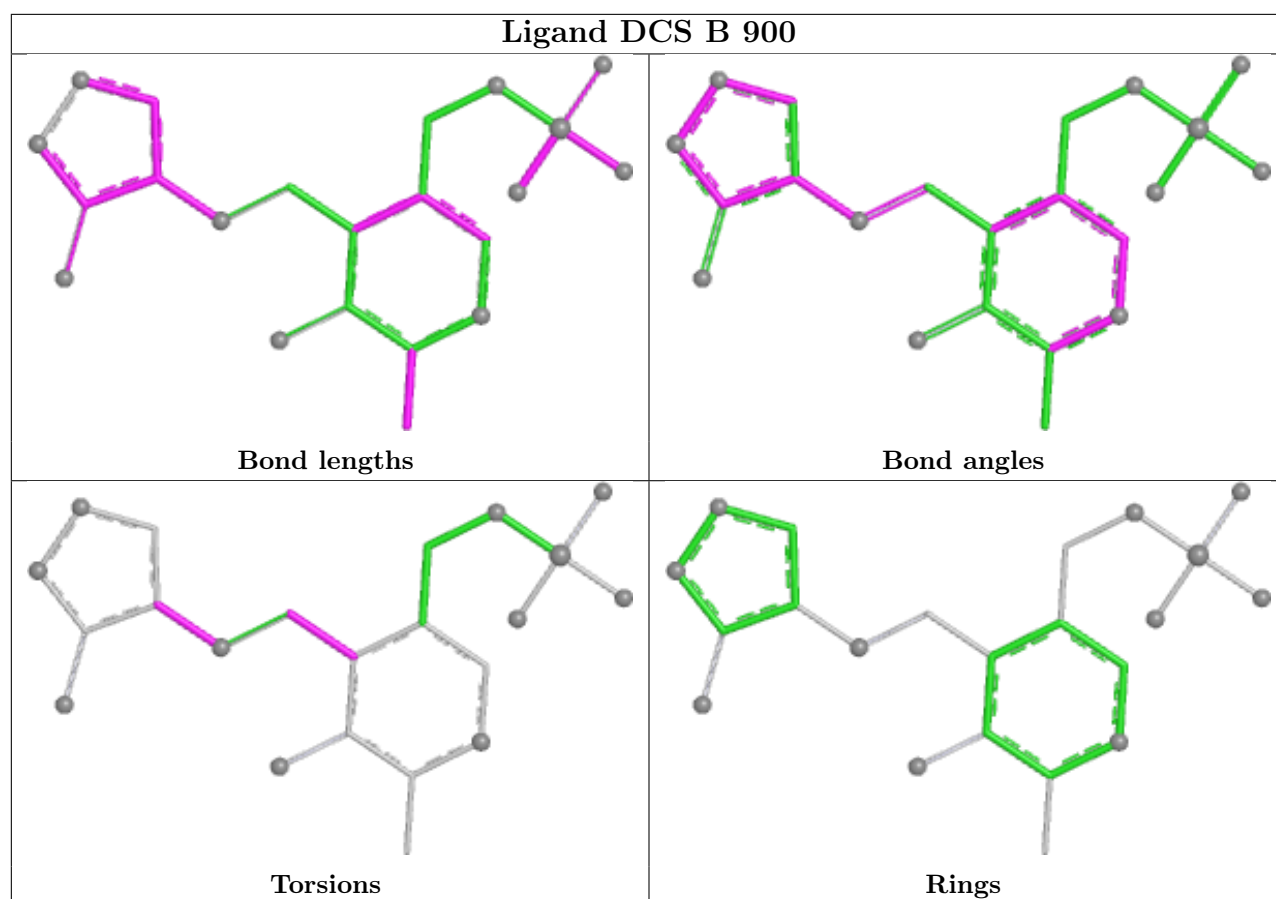
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	DCS	5	0
2	B	900	DCS	6	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	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	129:KCX	C	130:MET	N	2.55
1	B	129:KCX	C	130:MET	N	2.31

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	381/388 (98%)	-0.05	1 (0%) 90 88	11, 23, 45, 53	0
1	B	379/388 (97%)	0.02	5 (1%) 75 73	13, 24, 45, 57	0
All	All	760/776 (97%)	-0.01	6 (0%) 82 80	11, 24, 45, 57	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	GLU	3.3
1	B	381	ILE	2.8
1	B	2	ASN	2.7
1	B	233	ILE	2.4
1	B	194	SER	2.2
1	A	273	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	B	129	12/13	0.71	0.20	20,26,53,58	0
1	KCX	A	129	12/13	0.84	0.12	19,22,27,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

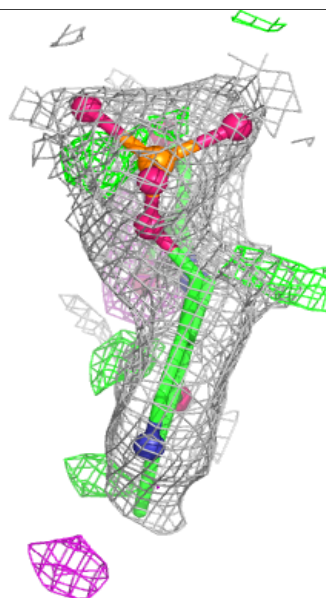
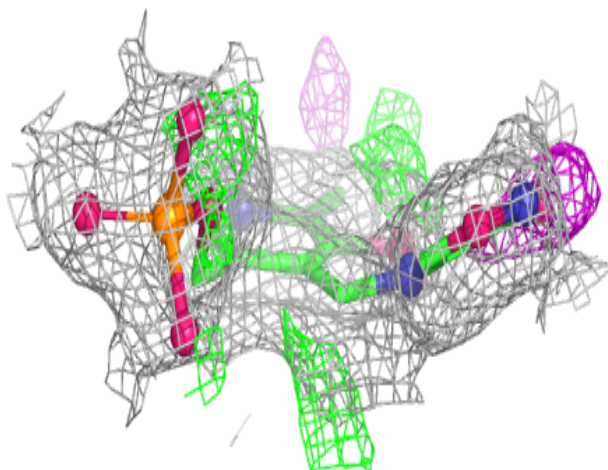
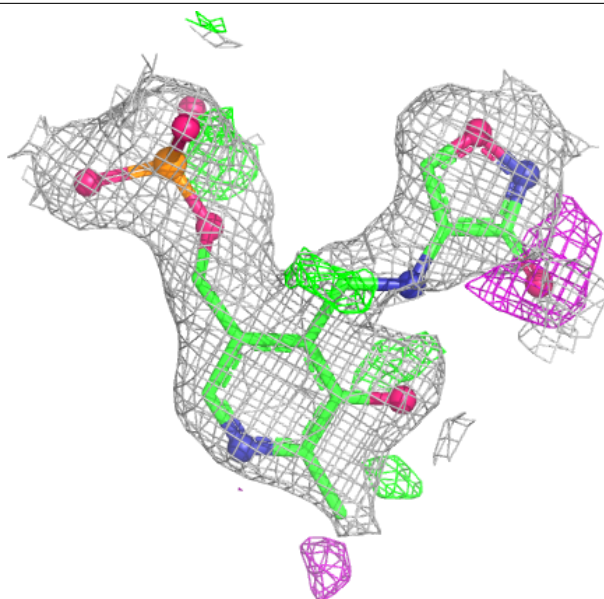
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DCS	A	800	22/22	0.91	0.12	13,21,30,43	0
2	DCS	B	900	22/22	0.92	0.12	18,26,33,37	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.

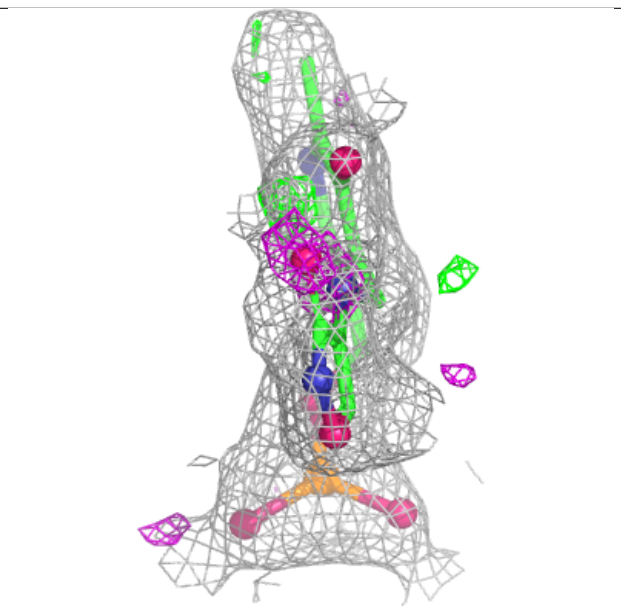
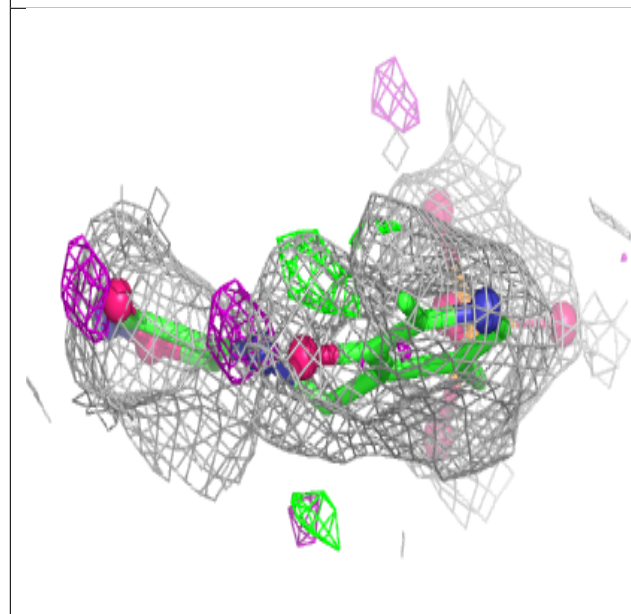
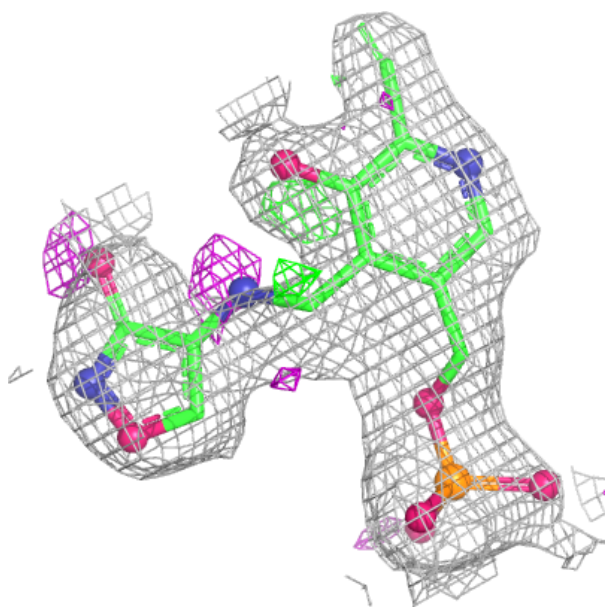
Electron density around DCS A 800:

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



Electron density around DCS B 900:

$2mF_o-DF_c$ (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.