



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:59 am BST

PDB ID : 2I4M
Title : Rhodopseudomonas palustris prolyl-tRNA synthetase in complex with ProAMS
Authors : Crepin, T.; Yaremchuk, A.; Tukalo, M.; Cusack, S.
Deposited on : 2006-08-22
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

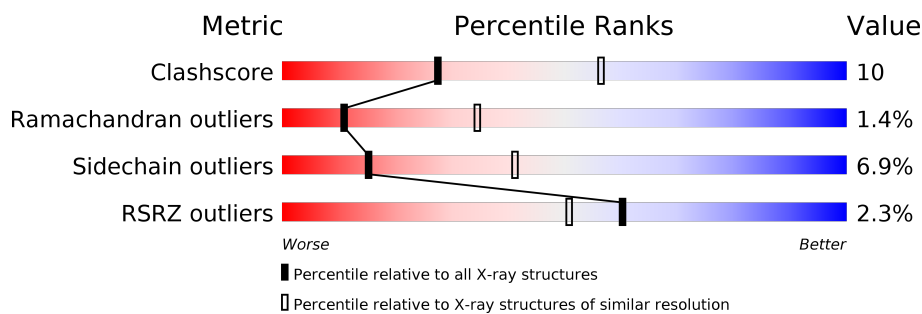
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	458	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	458	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>• •</div> </div> </div>
1	C	458	<div> <div></div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10682 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 Proline-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3479	2201	618	646	14			
1	B	441	Total	C	N	O	S	0	0	0
			3495	2211	620	650	14			
1	C	441	Total	C	N	O	S	0	13	0
			3586	2268	635	669	14			

There are 60 discrepancies between the modelled and reference sequences:

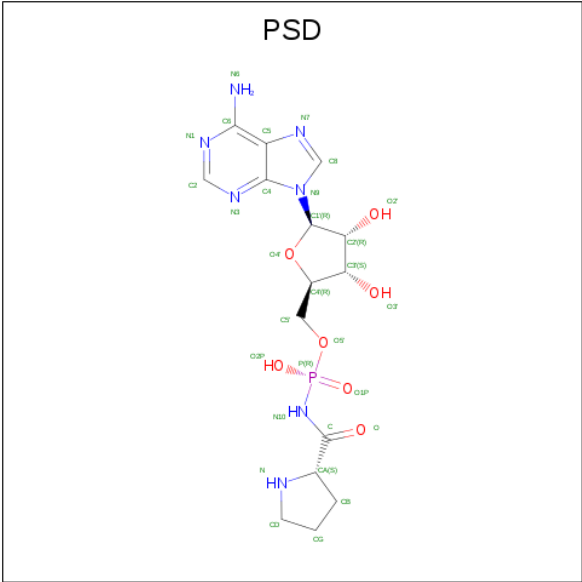
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q6N5P6
A	-18	GLY	-	EXPRESSION TAG	UNP Q6N5P6
A	-17	SER	-	EXPRESSION TAG	UNP Q6N5P6
A	-16	SER	-	EXPRESSION TAG	UNP Q6N5P6
A	-15	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-14	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-13	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-12	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-11	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-10	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-9	SER	-	EXPRESSION TAG	UNP Q6N5P6
A	-8	SER	-	EXPRESSION TAG	UNP Q6N5P6
A	-7	GLY	-	EXPRESSION TAG	UNP Q6N5P6
A	-6	LEU	-	EXPRESSION TAG	UNP Q6N5P6
A	-5	VAL	-	EXPRESSION TAG	UNP Q6N5P6
A	-4	PRO	-	EXPRESSION TAG	UNP Q6N5P6
A	-3	ARG	-	EXPRESSION TAG	UNP Q6N5P6
A	-2	GLY	-	EXPRESSION TAG	UNP Q6N5P6
A	-1	SER	-	EXPRESSION TAG	UNP Q6N5P6
A	0	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-19	MET	-	EXPRESSION TAG	UNP Q6N5P6
B	-18	GLY	-	EXPRESSION TAG	UNP Q6N5P6
B	-17	SER	-	EXPRESSION TAG	UNP Q6N5P6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP Q6N5P6
B	-15	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-14	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-13	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-12	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-11	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-10	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-9	SER	-	EXPRESSION TAG	UNP Q6N5P6
B	-8	SER	-	EXPRESSION TAG	UNP Q6N5P6
B	-7	GLY	-	EXPRESSION TAG	UNP Q6N5P6
B	-6	LEU	-	EXPRESSION TAG	UNP Q6N5P6
B	-5	VAL	-	EXPRESSION TAG	UNP Q6N5P6
B	-4	PRO	-	EXPRESSION TAG	UNP Q6N5P6
B	-3	ARG	-	EXPRESSION TAG	UNP Q6N5P6
B	-2	GLY	-	EXPRESSION TAG	UNP Q6N5P6
B	-1	SER	-	EXPRESSION TAG	UNP Q6N5P6
B	0	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-19	MET	-	EXPRESSION TAG	UNP Q6N5P6
C	-18	GLY	-	EXPRESSION TAG	UNP Q6N5P6
C	-17	SER	-	EXPRESSION TAG	UNP Q6N5P6
C	-16	SER	-	EXPRESSION TAG	UNP Q6N5P6
C	-15	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-14	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-13	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-12	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-11	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-10	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-9	SER	-	EXPRESSION TAG	UNP Q6N5P6
C	-8	SER	-	EXPRESSION TAG	UNP Q6N5P6
C	-7	GLY	-	EXPRESSION TAG	UNP Q6N5P6
C	-6	LEU	-	EXPRESSION TAG	UNP Q6N5P6
C	-5	VAL	-	EXPRESSION TAG	UNP Q6N5P6
C	-4	PRO	-	EXPRESSION TAG	UNP Q6N5P6
C	-3	ARG	-	EXPRESSION TAG	UNP Q6N5P6
C	-2	GLY	-	EXPRESSION TAG	UNP Q6N5P6
C	-1	SER	-	EXPRESSION TAG	UNP Q6N5P6
C	0	HIS	-	EXPRESSION TAG	UNP Q6N5P6

- Molecule 2 is 5'-O-[N-(PROLYL)-SULFAMOYL]ADENOSINE (three-letter code: PSD) (formula: C₁₅H₂₂N₇O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			30	15	7	7	1		
2	C	1	Total	C	N	O	P	0	0
			30	15	7	7	1		

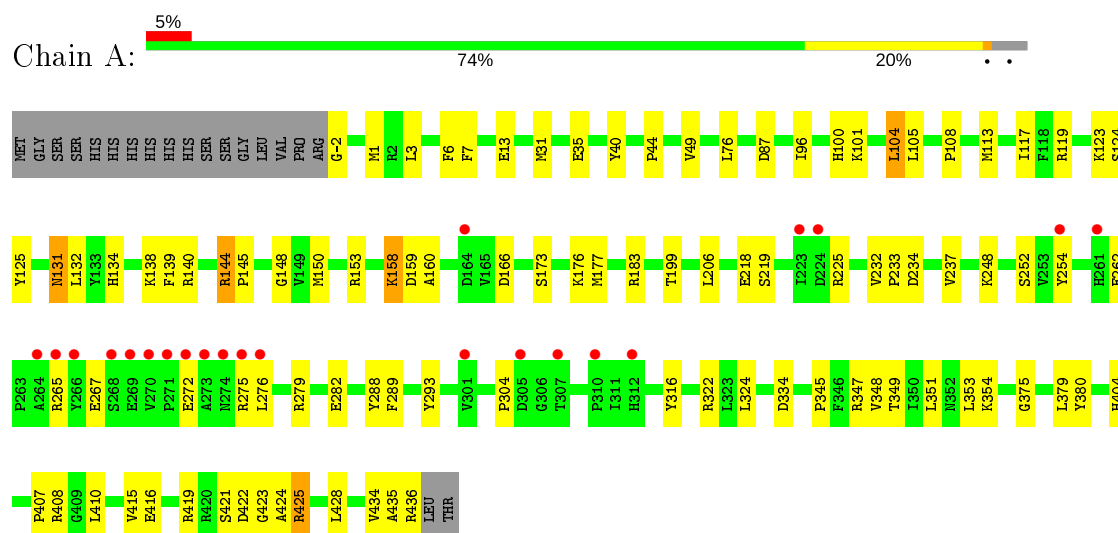
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	22	Total	O	0	0
			22	22		
3	C	20	Total	O	0	0
			20	20		

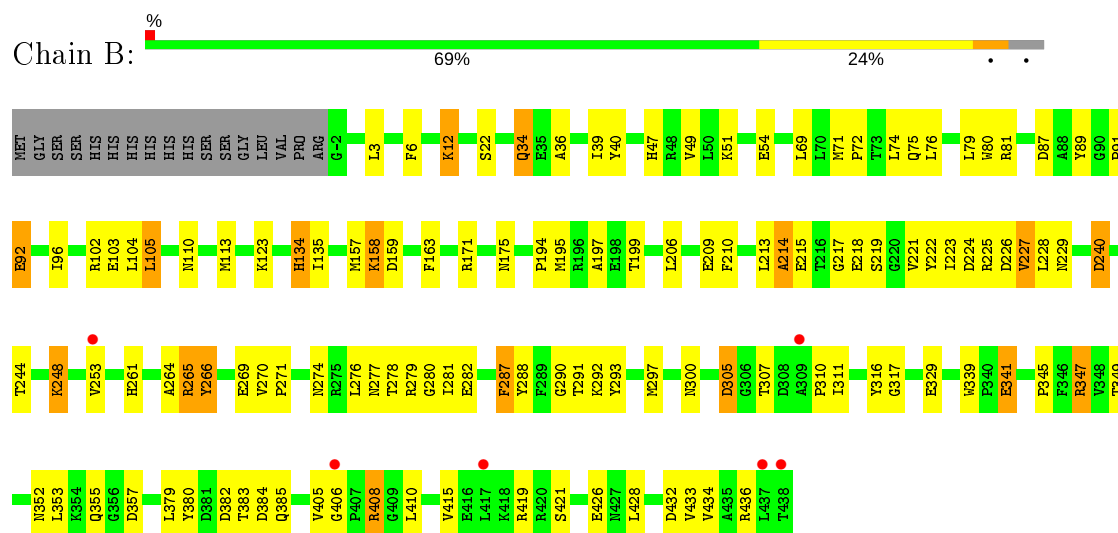
3 Residue-property plots

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

• Molecule 1: Proline-tRNA ligase

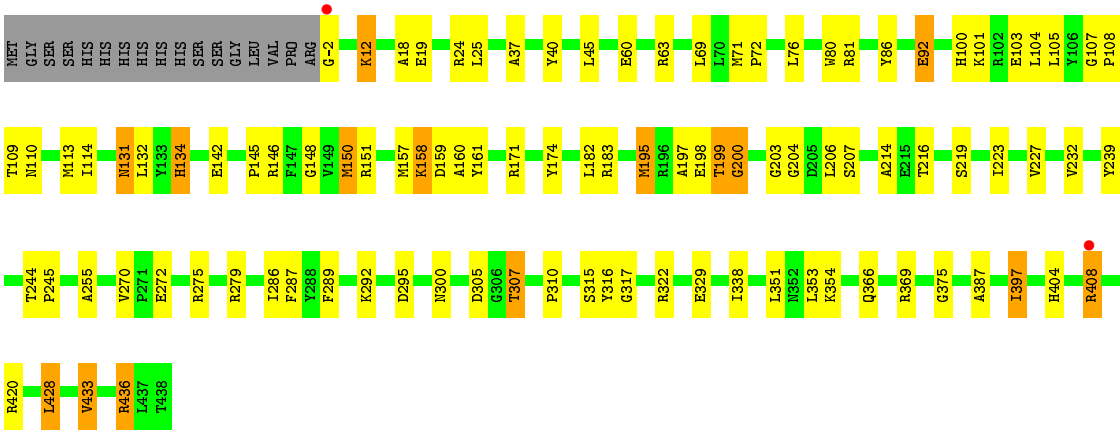


• Molecule 1: Proline-tRNA ligase



• Molecule 1: Proline-tRNA ligase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	110.36Å 211.90Å 150.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80 45.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 ((Not available)-2.80) 98.7 (45.27-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.269 0.201 , (Not available)	Depositor DCC
R_{free} test set	2416 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	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	0.94	EDS
Total number of atoms	10682	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PSD

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	0/3554	0.66	0/4807
1	B	0.59	0/3570	0.70	0/4828
1	C	0.60	0/3664	0.72	1/4956 (0.0%)
All	All	0.59	0/10788	0.69	1/14591 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	428	LEU	CA-CB-CG	5.47	127.89	115.30

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	3479	0	3448	53	0
1	B	3495	0	3466	83	0
1	C	3586	0	3545	84	0
2	B	30	0	21	4	0
2	C	30	0	21	7	0
3	A	20	0	0	0	0
3	B	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	20	0	0	1	0
All	All	10682	0	10501	212	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 (212) 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:C:199[A]:THR:HG21	1:C:203[A]:GLY:O	1.59	1.03
1:B:347:ARG:HG2	1:B:347:ARG:HH11	1.24	1.01
1:C:12:LYS:HE3	1:C:12:LYS:H	1.25	1.00
1:C:199[A]:THR:CG2	1:C:203[A]:GLY:O	2.20	0.90
1:B:408:ARG:HH11	1:B:408:ARG:HG2	1.37	0.89
1:C:199[B]:THR:O	1:C:200[B]:GLY:O	1.93	0.85
1:C:199[B]:THR:O	1:C:200[B]:GLY:C	2.14	0.85
1:A:101:LYS:NZ	1:C:199[A]:THR:HB	1.92	0.84
1:A:173:SER:HA	1:A:176:LYS:HE3	1.61	0.83
1:C:199[A]:THR:HG21	1:C:203[A]:GLY:C	2.00	0.82
1:B:406:GLY:O	1:B:410:LEU:HB2	1.81	0.80
1:B:380:TYR:CE2	1:B:382:ASP:HB3	2.19	0.77
1:A:101:LYS:HZ3	1:C:199[A]:THR:HB	1.49	0.77
1:C:131:ASN:HD22	1:C:131:ASN:C	1.90	0.74
1:B:419:ARG:HG2	1:B:421:SER:HB3	1.72	0.72
1:C:244:THR:HB	1:C:245:PRO:HD3	1.72	0.72
1:B:197:ALA:HB2	1:B:209:GLU:HG3	1.72	0.71
1:C:131:ASN:HD21	1:C:160:ALA:HB1	1.56	0.71
1:C:71:MET:H	1:C:134:HIS:HD2	1.37	0.71
1:B:282:GLU:OE2	2:B:439:PSD:O3'	2.09	0.70
1:B:199:THR:HG22	1:B:287:PHE:HD2	1.58	0.69
1:C:131:ASN:HD22	1:C:132:LEU:N	1.90	0.69
1:A:131:ASN:C	1:A:131:ASN:HD22	1.97	0.68
1:B:347:ARG:NH1	1:B:347:ARG:HG2	1.99	0.66
1:C:287[B]:PHE:HE1	2:C:439:PSD:HCB1	1.61	0.66
1:C:351:LEU:HD12	1:C:404:HIS:CD2	2.31	0.66
1:B:408:ARG:HH11	1:B:408:ARG:CG	2.08	0.65
1:C:195:MET:HB3	1:C:255:ALA:HB1	1.78	0.65
1:C:199[A]:THR:HG23	3:C:443:HOH:O	1.95	0.65
1:B:248:LYS:NZ	1:B:248:LYS:HB3	2.11	0.65
1:C:71:MET:H	1:C:134:HIS:CD2	2.14	0.64
1:B:271:PRO:HG2	1:B:274:ASN:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199[B]:THR:HG21	1:C:203[B]:GLY:O	1.99	0.63
1:B:22:SER:HB3	1:B:329:GLU:HG2	1.81	0.63
1:B:199:THR:HG22	1:B:287:PHE:CD2	2.34	0.62
1:B:282:GLU:OE2	2:B:439:PSD:C3'	2.47	0.62
1:B:71:MET:H	1:B:134:HIS:CD2	2.17	0.61
1:B:197:ALA:CB	1:B:209:GLU:HG3	2.29	0.61
1:B:282:GLU:OE2	2:B:439:PSD:HC'3	1.99	0.61
1:C:272:GLU:N	1:C:275:ARG:HH21	1.97	0.61
1:A:349:THR:HA	1:A:379:LEU:O	2.00	0.61
1:A:434:VAL:C	1:A:436:ARG:H	2.03	0.61
1:B:277:ASN:O	1:B:278:THR:HB	2.00	0.60
1:B:76:LEU:HD23	1:B:104:LEU:HD23	1.82	0.60
1:B:71:MET:H	1:B:134:HIS:HD2	1.48	0.60
1:A:96:ILE:HG12	1:B:96:ILE:HG12	1.84	0.59
1:B:12:LYS:H	1:B:12:LYS:CE	2.15	0.59
1:B:300:ASN:HD22	1:B:310:PRO:HA	1.68	0.59
1:B:158:LYS:O	1:B:317:GLY:HA2	2.02	0.59
1:C:223:ILE:HG22	1:C:255:ALA:HA	1.85	0.59
1:B:265:ARG:O	1:B:266:TYR:C	2.40	0.58
1:C:305:ASP:OD1	1:C:307:THR:HB	2.03	0.58
1:C:338:ILE:HG22	1:C:338:ILE:O	2.02	0.58
1:C:287[B]:PHE:CE1	2:C:439:PSD:HCB1	2.37	0.58
1:C:214:ALA:O	1:C:279:ARG:HB2	2.03	0.58
1:B:433:VAL:HG13	1:B:434:VAL:H	1.68	0.58
1:B:225:ARG:HG3	1:B:228:LEU:HD12	1.86	0.57
1:C:199[B]:THR:CG2	1:C:203[B]:GLY:O	2.53	0.57
1:C:12:LYS:N	1:C:12:LYS:HE3	2.08	0.56
1:C:40:TYR:OH	1:C:148:GLY:HA2	2.04	0.56
1:B:408:ARG:HG2	1:B:408:ARG:NH1	2.10	0.56
1:A:101:LYS:HZ1	1:C:199[A]:THR:HB	1.69	0.56
1:C:157:MET:SD	2:C:439:PSD:H5'1	2.45	0.56
1:A:254:TYR:HE1	1:A:265:ARG:HD3	1.71	0.55
1:B:224:ASP:C	1:B:224:ASP:OD1	2.45	0.55
1:B:226:ASP:O	1:B:228:LEU:N	2.40	0.55
1:C:244:THR:HB	1:C:245:PRO:CD	2.37	0.55
1:C:436:ARG:HH11	1:C:436:ARG:HB3	1.70	0.55
1:C:287[B]:PHE:CE1	2:C:439:PSD:CB	2.90	0.55
1:B:352:ASN:HB3	1:B:355:GLN:OE1	2.07	0.54
1:A:233:PRO:HB3	1:A:237:VAL:HG21	1.90	0.54
1:A:100:HIS:ND1	1:C:198[A]:GLU:OE1	2.29	0.54
1:C:300:ASN:HD22	1:C:310:PRO:N	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:LEU:O	1:C:134:HIS:HB3	2.08	0.54
1:B:248:LYS:HZ1	1:B:248:LYS:HB3	1.71	0.53
1:A:138:LYS:HE3	1:A:159:ASP:OD1	2.09	0.53
1:B:225:ARG:O	1:B:228:LEU:HB2	2.08	0.53
1:C:204[B]:GLY:HA3	1:C:289:PHE:HA	1.90	0.53
1:A:76:LEU:HD23	1:A:104:LEU:HD23	1.90	0.53
1:C:351:LEU:HD12	1:C:404:HIS:HD2	1.73	0.52
1:C:12:LYS:CE	1:C:12:LYS:H	2.10	0.52
1:C:408:ARG:CG	1:C:408:ARG:HH11	2.22	0.52
1:C:216:THR:OG1	1:C:329:GLU:OE1	2.28	0.52
1:A:233:PRO:CB	1:A:237:VAL:HG21	2.40	0.52
1:B:287:PHE:N	1:B:287:PHE:CD1	2.79	0.51
1:B:349:THR:HA	1:B:379:LEU:O	2.11	0.51
1:B:194:PRO:HB3	1:B:210:PHE:CE1	2.46	0.51
1:B:12:LYS:H	1:B:12:LYS:NZ	2.10	0.50
1:C:109:THR:OG1	1:C:110:ASN:N	2.44	0.50
1:C:69:LEU:O	1:C:134:HIS:CB	2.60	0.50
1:C:159:ASP:CB	2:C:439:PSD:HCD2	2.41	0.50
1:B:353:LEU:HG	1:B:405:VAL:O	2.12	0.49
1:A:351:LEU:HD12	1:A:404:HIS:CD2	2.48	0.49
1:A:267:GLU:HG2	1:A:275:ARG:HH12	1.77	0.49
1:B:433:VAL:HG13	1:B:434:VAL:N	2.27	0.49
1:A:131:ASN:ND2	1:A:131:ASN:C	2.65	0.49
1:A:262:GLU:HB2	1:A:265:ARG:HB3	1.95	0.49
1:B:199:THR:CG2	1:B:287:PHE:HD2	2.25	0.48
1:C:131:ASN:C	1:C:131:ASN:ND2	2.61	0.48
1:C:114:ILE:HG21	1:C:161:TYR:CG	2.49	0.48
1:B:47:HIS:CE1	1:B:51:LYS:HD2	2.49	0.47
1:C:76:LEU:HD23	1:C:104:LEU:HD23	1.96	0.47
1:B:213:LEU:O	1:B:214:ALA:HB2	2.15	0.47
1:A:234:ASP:O	1:A:237:VAL:HG23	2.15	0.47
1:A:434:VAL:O	1:A:436:ARG:N	2.47	0.47
1:B:159:ASP:HA	1:B:316:TYR:O	2.15	0.47
1:A:-2:GLY:HA3	1:A:375:GLY:HA2	1.95	0.47
1:C:159:ASP:HB3	2:C:439:PSD:HCD2	1.95	0.47
1:A:248:LYS:O	1:A:252:SER:HB3	2.15	0.47
1:A:354:LYS:HD2	1:A:407:PRO:HG2	1.97	0.47
1:B:219:SER:HB2	1:B:280:GLY:O	2.15	0.47
1:B:91:PRO:HD2	1:B:92:GLU:OE2	2.15	0.47
1:C:171:ARG:HG2	1:C:206[A]:LEU:HD11	1.96	0.47
1:C:287[B]:PHE:HE1	2:C:439:PSD:HN01	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:HIS:HB2	1:A:416:GLU:HB3	1.95	0.46
1:B:222:TYR:CD1	1:B:261:HIS:CE1	3.03	0.46
1:B:36:ALA:HB3	1:B:39:ILE:HB	1.96	0.46
1:A:139:PHE:HA	1:A:153:ARG:O	2.15	0.46
1:B:293:TYR:O	1:B:297:MET:HB2	2.15	0.46
1:C:81:ARG:NH2	1:C:103:GLU:OE1	2.39	0.46
1:C:100:HIS:O	1:C:101:LYS:HB2	2.15	0.46
1:A:353:LEU:HD11	1:A:404:HIS:HB3	1.98	0.46
1:A:40:TYR:OH	1:A:148:GLY:HA2	2.16	0.46
1:B:76:LEU:O	1:B:79:LEU:HB3	2.16	0.46
1:A:289:PHE:CE1	1:A:293:TYR:HD2	2.34	0.46
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.78	0.46
1:B:300:ASN:HD22	1:B:310:PRO:CA	2.28	0.46
1:C:428:LEU:HD11	1:C:433:VAL:HG23	1.96	0.46
1:B:224:ASP:HB3	1:B:253:VAL:HG12	1.98	0.45
1:B:240:ASP:N	1:B:240:ASP:OD1	2.48	0.45
1:C:142:GLU:HG2	1:C:151:ARG:HD3	1.98	0.45
1:A:419:ARG:NH2	1:A:422:ASP:OD2	2.39	0.45
1:B:226:ASP:C	1:B:228:LEU:H	2.20	0.45
1:C:289:PHE:HE2	1:C:315:SER:HB3	1.81	0.45
1:C:19:GLU:OE1	1:C:146:ARG:NH2	2.38	0.45
1:A:139:PHE:CE1	1:B:74:LEU:HD12	2.52	0.45
1:B:405:VAL:HG22	1:B:415:VAL:HG11	1.98	0.45
1:B:12:LYS:H	1:B:12:LYS:HE3	1.81	0.45
1:B:34:GLN:HG3	1:B:40:TYR:CE1	2.52	0.45
1:A:35:GLU:OE1	1:B:113:MET:HE2	2.17	0.44
1:B:221:VAL:HG22	1:B:278:THR:O	2.18	0.44
1:A:347:ARG:HH12	1:A:436:ARG:HG2	1.82	0.44
1:C:300:ASN:HD22	1:C:310:PRO:CA	2.30	0.44
1:A:206:LEU:HB3	1:A:288:TYR:HB3	1.99	0.44
1:A:423:GLY:O	1:A:425:ARG:HG2	2.17	0.44
1:B:214:ALA:HB3	1:B:281:ILE:HD12	1.99	0.44
1:B:288:TYR:CE1	1:B:290:GLY:HA2	2.53	0.44
1:B:49:VAL:HG22	1:B:345:PRO:HD3	1.99	0.44
1:C:71:MET:SD	1:C:113:MET:HG2	2.58	0.44
1:C:197[A]:ALA:O	1:C:207[A]:SER:HB3	2.18	0.44
1:A:7:PHE:HB3	1:A:44:PRO:HG2	2.00	0.44
1:C:158:LYS:O	1:C:317:GLY:HA2	2.18	0.44
1:C:270:VAL:CG1	1:C:275:ARG:HG3	2.48	0.44
1:A:108:PRO:O	1:A:140:ARG:NH2	2.51	0.44
1:C:199[B]:THR:C	1:C:200[B]:GLY:O	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199[A]:THR:HG21	1:C:203[A]:GLY:CA	2.47	0.44
1:B:158:LYS:C	1:B:158:LYS:HD2	2.37	0.44
1:B:305:ASP:N	1:B:305:ASP:OD1	2.42	0.44
1:B:225:ARG:O	1:B:226:ASP:C	2.57	0.43
1:C:366:GLN:HA	1:C:369:ARG:NH2	2.33	0.43
1:A:232:VAL:HA	1:A:233:PRO:HD2	1.79	0.43
1:A:1:MET:HG2	1:A:6:PHE:CD1	2.53	0.43
1:A:31:MET:HB3	1:A:31:MET:HE2	1.87	0.43
1:B:80:TRP:CD1	1:B:105:LEU:HD21	2.53	0.43
1:A:144:ARG:O	1:A:145:PRO:C	2.55	0.43
1:B:171:ARG:O	1:B:175:ASN:ND2	2.51	0.43
1:A:225:ARG:HH12	1:A:276:LEU:HD13	1.84	0.43
1:B:81:ARG:NH2	1:B:103:GLU:OE2	2.50	0.42
1:A:49:VAL:HG22	1:A:345:PRO:HD3	2.00	0.42
1:B:163:PHE:HD1	1:B:311:ILE:HD13	1.85	0.42
1:C:92:GLU:H	1:C:92:GLU:HG2	1.47	0.42
1:A:434:VAL:C	1:A:436:ARG:N	2.70	0.42
1:A:177:MET:HG3	1:A:316:TYR:CD2	2.55	0.42
1:B:54:GLU:HG3	1:B:135:ILE:HG21	2.02	0.42
1:C:182:LEU:HB3	1:C:232:VAL:HG13	2.02	0.42
1:C:353:LEU:HD22	1:C:387:ALA:HB1	2.01	0.42
1:B:157:MET:SD	2:B:439:PSD:HCG2	2.60	0.42
1:C:80:TRP:CD1	1:C:105:LEU:HD21	2.54	0.42
1:C:60:GLU:OE2	1:C:63:ARG:NH2	2.48	0.42
1:A:132:LEU:HD23	1:A:132:LEU:HA	1.80	0.42
1:B:339:TRP:CD1	1:B:345:PRO:HD2	2.54	0.42
1:A:158:LYS:HD2	1:A:158:LYS:C	2.39	0.42
1:C:203[B]:GLY:HA3	1:C:292:LYS:HD2	2.02	0.42
1:C:107:GLY:HA2	1:C:108:PRO:HD2	1.83	0.41
1:C:72:PRO:HD2	1:C:113:MET:SD	2.60	0.41
1:B:157:MET:HG2	1:B:158:LYS:N	2.35	0.41
1:B:75:GLN:NE2	1:B:110:ASN:ND2	2.68	0.41
1:B:383:THR:C	1:B:385:GLN:H	2.23	0.41
1:C:63:ARG:HG2	1:C:239:TYR:HE2	1.85	0.41
1:A:113:MET:O	1:A:117:ILE:HG13	2.20	0.41
1:B:134:HIS:HE1	1:B:159:ASP:OD2	2.04	0.41
1:B:291:THR:O	1:B:292:LYS:C	2.59	0.41
1:C:174:TYR:CZ	1:C:206[B]:LEU:HD22	2.56	0.41
1:C:286:ILE:HG22	1:C:316:TYR:HD1	1.86	0.41
1:C:150:MET:HG3	1:C:322:ARG:HG3	2.03	0.41
1:A:108:PRO:HB2	1:A:140:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-2:GLY:HA3	1:C:375:GLY:HA2	2.02	0.41
1:C:71:MET:HB2	1:C:134:HIS:CD2	2.56	0.41
1:A:125:TYR:CE1	1:A:304:PRO:HB3	2.56	0.41
1:A:419:ARG:HB3	1:A:424:ALA:HB3	2.03	0.41
1:B:270:VAL:HG13	1:B:271:PRO:HD2	2.03	0.41
1:C:45:LEU:HD21	1:C:397:ILE:HB	2.02	0.41
1:B:72:PRO:HD2	1:B:113:MET:SD	2.61	0.41
1:C:18:ALA:O	1:C:24:ARG:NH2	2.54	0.41
1:C:338:ILE:HG12	1:C:420:ARG:HG3	2.03	0.41
1:B:436:ARG:O	1:B:436:ARG:HG2	2.21	0.40
1:A:101:LYS:HZ1	1:C:199[A]:THR:CB	2.34	0.40
1:C:37:ALA:HB1	1:C:145:PRO:HG2	2.03	0.40
1:A:158:LYS:HZ3	1:A:160:ALA:HB2	1.87	0.40
1:B:341:GLU:HG2	1:B:347:ARG:NE	2.36	0.40
1:A:123:LYS:HA	1:A:123:LYS:HD3	1.80	0.40
1:B:217:GLY:O	1:B:279:ARG:HD3	2.21	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	437/458 (95%)	401 (92%)	33 (8%)	3 (1%)	22	53
1	B	439/458 (96%)	388 (88%)	39 (9%)	12 (3%)	5	17
1	C	452/458 (99%)	421 (93%)	27 (6%)	4 (1%)	17	46
All	All	1328/1374 (97%)	1210 (91%)	99 (8%)	19 (1%)	11	34

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	ALA

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Mol	Chain	Res	Type
1	B	215	GLU
1	B	218	GLU
1	B	227	VAL
1	A	272	GLU
1	B	266	TYR
1	B	384	ASP
1	C	200[A]	GLY
1	C	200[B]	GLY
1	B	214	ALA
1	B	265	ARG
1	B	432	ASP
1	C	86	TYR
1	B	264	ALA
1	C	295	ASP
1	A	408	ARG
1	B	305	ASP
1	B	269	GLU
1	B	426	GLU

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	359/376 (96%)	330 (92%)	29 (8%)	11	33
1	B	361/376 (96%)	332 (92%)	29 (8%)	12	34
1	C	370/376 (98%)	352 (95%)	18 (5%)	25	57
All	All	1090/1128 (97%)	1014 (93%)	76 (7%)	15	40

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	13	GLU
1	A	87	ASP
1	A	104	LEU

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Mol	Chain	Res	Type
1	A	105	LEU
1	A	119	ARG
1	A	124	SER
1	A	131	ASN
1	A	134	HIS
1	A	144	ARG
1	A	150	MET
1	A	158	LYS
1	A	166	ASP
1	A	183	ARG
1	A	199	THR
1	A	218	GLU
1	A	219	SER
1	A	279	ARG
1	A	282	GLU
1	A	322	ARG
1	A	324	LEU
1	A	334	ASP
1	A	348	VAL
1	A	380	TYR
1	A	410	LEU
1	A	415	VAL
1	A	421	SER
1	A	425	ARG
1	A	428	LEU
1	B	3	LEU
1	B	6	PHE
1	B	12	LYS
1	B	34	GLN
1	B	69	LEU
1	B	87	ASP
1	B	89	TYR
1	B	92	GLU
1	B	102	ARG
1	B	105	LEU
1	B	123	LYS
1	B	134	HIS
1	B	158	LYS
1	B	195	MET
1	B	206	LEU
1	B	223	ILE
1	B	227	VAL

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Mol	Chain	Res	Type
1	B	229	ASN
1	B	240	ASP
1	B	244	THR
1	B	248	LYS
1	B	276	LEU
1	B	287	PHE
1	B	307	THR
1	B	341	GLU
1	B	347	ARG
1	B	357	ASP
1	B	408	ARG
1	B	428	LEU
1	C	12	LYS
1	C	92	GLU
1	C	131	ASN
1	C	134	HIS
1	C	150	MET
1	C	158	LYS
1	C	183	ARG
1	C	195	MET
1	C	199[A]	THR
1	C	199[B]	THR
1	C	219	SER
1	C	227	VAL
1	C	307	THR
1	C	354	LYS
1	C	397	ILE
1	C	408	ARG
1	C	433	VAL
1	C	436	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	131	ASN
1	A	229	ASN
1	A	335	ASN
1	B	0	HIS
1	B	34	GLN
1	B	47	HIS
1	B	75	GLN

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Mol	Chain	Res	Type
1	B	110	ASN
1	B	134	HIS
1	B	285	GLN
1	B	300	ASN
1	B	332	HIS
1	B	335	ASN
1	B	366	GLN
1	C	131	ASN
1	C	134	HIS
1	C	285	GLN
1	C	300	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	PSD	B	439	-	29,33,33	1.22	3 (10%)	32,49,49	1.69	6 (18%)
2	PSD	C	439	-	29,33,33	1.17	4 (13%)	32,49,49	1.71	6 (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	PSD	B	439	-	-	3/13/42/42	0/4/4/4
2	PSD	C	439	-	-	2/13/42/42	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	439	PSD	P-O1P	3.41	1.51	1.46
2	C	439	PSD	P-O1P	3.31	1.51	1.46
2	C	439	PSD	O4'-C1'	2.76	1.44	1.41
2	B	439	PSD	O4'-C1'	2.56	1.44	1.41
2	B	439	PSD	C2-N3	2.32	1.35	1.32
2	C	439	PSD	C2-N3	2.06	1.35	1.32
2	C	439	PSD	P-O2P	-2.00	1.51	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	439	PSD	O2P-P-O1P	5.14	120.71	109.92
2	C	439	PSD	O2P-P-O1P	4.74	119.86	109.92
2	B	439	PSD	N3-C2-N1	-4.48	121.68	128.68
2	C	439	PSD	N3-C2-N1	-4.25	122.03	128.68
2	B	439	PSD	CB-CA-C	-4.15	104.79	111.16
2	C	439	PSD	O1P-P-N10	-3.19	105.00	111.17
2	C	439	PSD	C4-C5-N7	-3.06	106.21	109.40
2	C	439	PSD	CB-CA-C	-2.87	106.76	111.16
2	C	439	PSD	C3'-C2'-C1'	2.67	105.00	100.98
2	B	439	PSD	C3'-C2'-C1'	2.12	104.16	100.98
2	B	439	PSD	O1P-P-N10	-2.11	107.08	111.17
2	B	439	PSD	C4-C5-N7	-2.11	107.20	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	439	PSD	O-C-CA-CB
2	B	439	PSD	N10-C-CA-CB
2	C	439	PSD	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	C	439	PSD	N10-C-CA-CB
2	B	439	PSD	C-N10-P-O5'

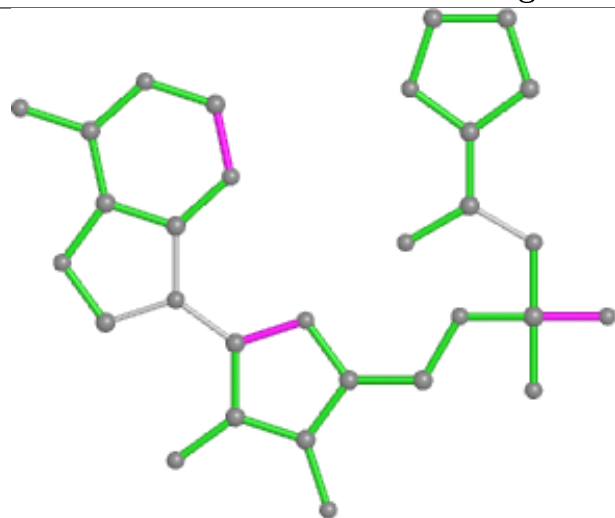
There are no ring outliers.

2 monomers are involved in 11 short contacts:

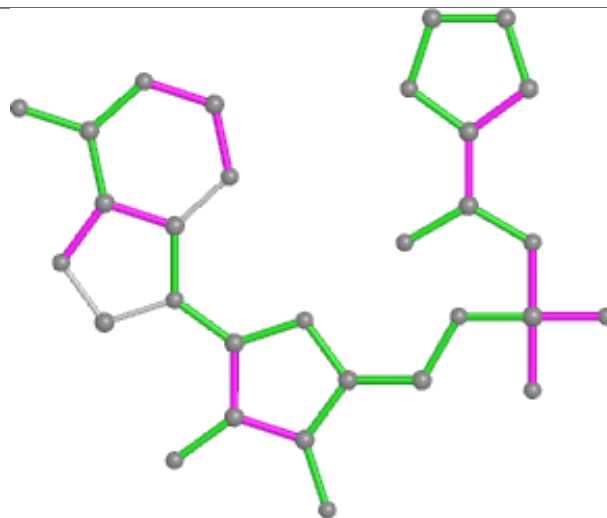
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	439	PSD	4	0
2	C	439	PSD	7	0

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.

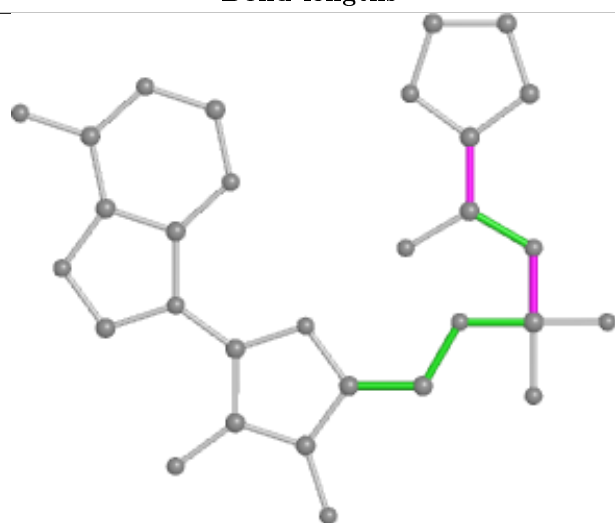
Ligand PSD B 439



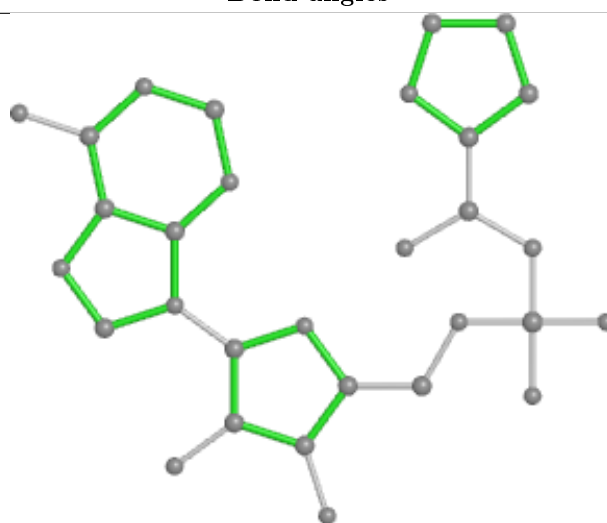
Bond lengths



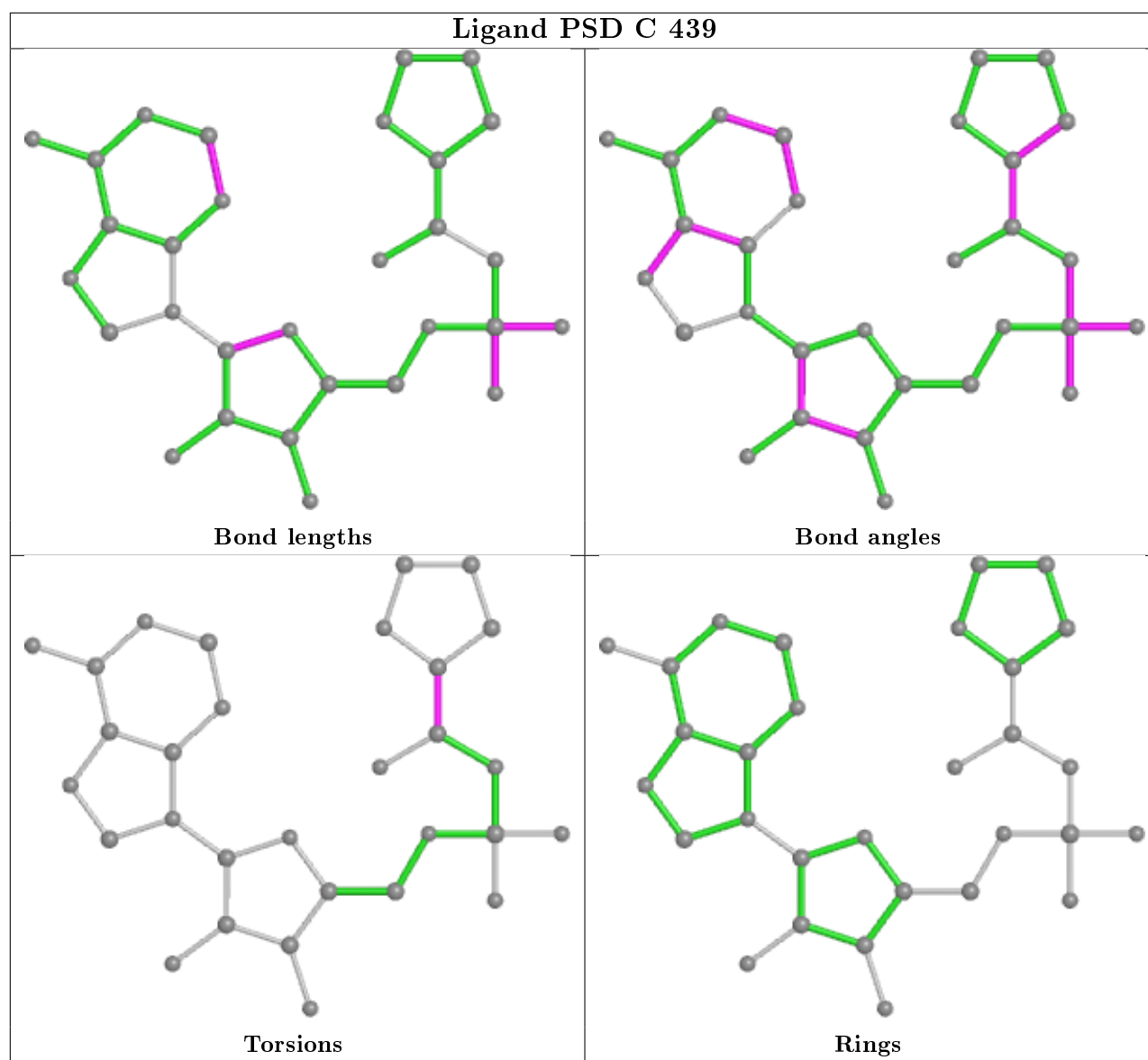
Bond angles



Torsions



Rings



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	439/458 (95%)	0.19	22 (5%)	28 19	30, 49, 74, 84	0
1	B	441/458 (96%)	-0.01	6 (1%)	75 70	27, 44, 69, 83	0
1	C	441/458 (96%)	-0.18	2 (0%)	91 88	20, 38, 55, 63	0
All	All	1321/1374 (96%)	-0.00	30 (2%)	60 51	20, 43, 69, 84	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	GLU	3.5
1	A	268	SER	3.3
1	A	224	ASP	3.2
1	A	276	LEU	2.8
1	A	274	ASN	2.8
1	A	305	ASP	2.8
1	A	312	HIS	2.8
1	A	223	ILE	2.7
1	A	264	ALA	2.5
1	A	270	VAL	2.4
1	A	273	ALA	2.4
1	A	265	ARG	2.4
1	A	266	TYR	2.4
1	B	437	LEU	2.3
1	A	301	VAL	2.3
1	A	272	GLU	2.3
1	B	309	ALA	2.3
1	A	261	HIS	2.3
1	B	253	VAL	2.2
1	B	438	THR	2.2
1	A	271	PRO	2.2
1	A	164	ASP	2.2
1	A	310	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	406	GLY	2.1
1	A	275	ARG	2.1
1	A	254	TYR	2.1
1	A	307	THR	2.1
1	C	408	ARG	2.1
1	B	417	LEU	2.0
1	C	-2	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

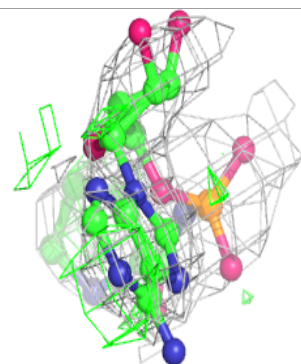
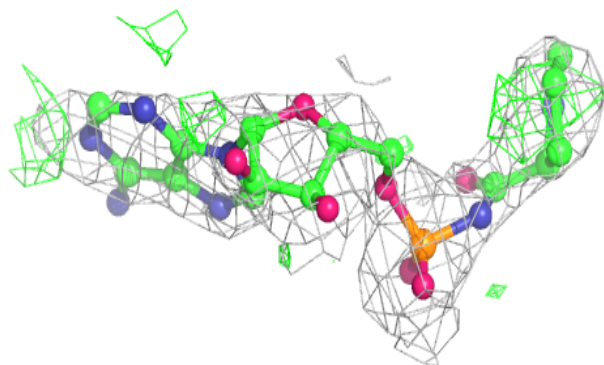
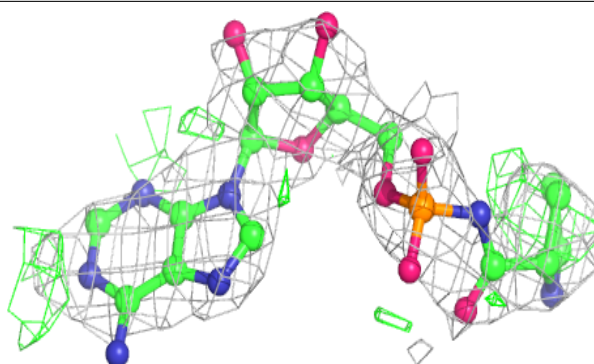
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PSD	C	439	30/30	0.90	0.33	22,25,28,28	30
2	PSD	B	439	30/30	0.92	0.19	59,60,61,61	0

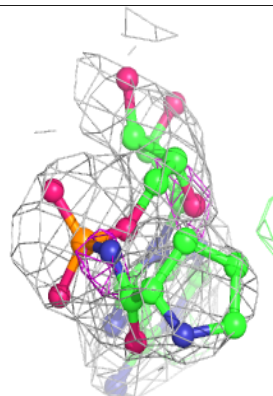
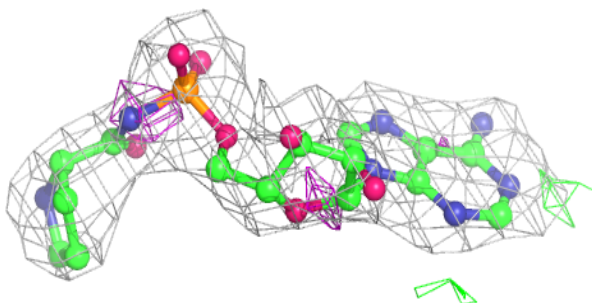
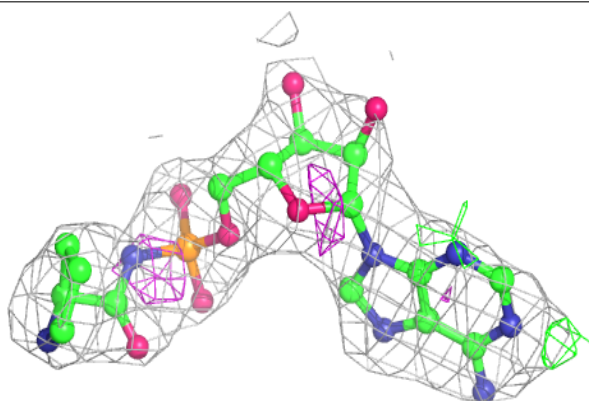
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PSD C 439:

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

**Electron density around PSD B 439:**

$2mF_o-DF_c$ (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.