



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 02:09 AM EDT

PDB ID : 4TVA
Title : Universal Pathway for Post-Transfer Editing Reactions: Insight from Crystal structure of TthPheRS with Puromycine
Authors : Safro, M.; Klipcan, L.; Tworowski, D.; Peretz, M.
Deposited on : 2014-06-26
Resolution : 2.60 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 : 2.35.1
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) : 2.35.1

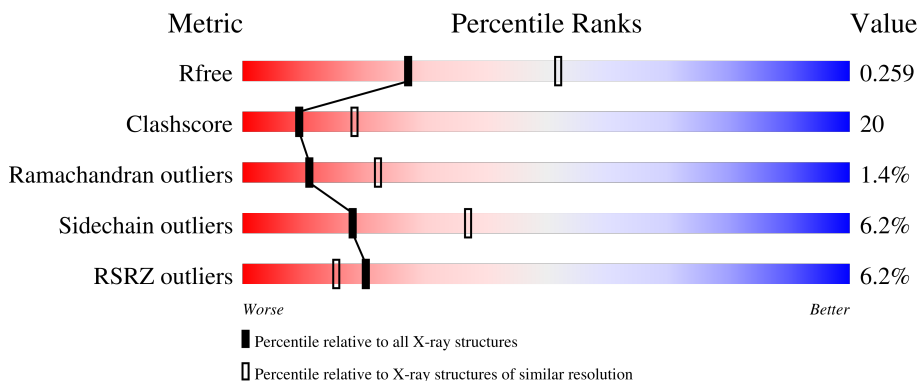
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	350	
2	B	785	

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
4	PUY	B	801	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8471 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.

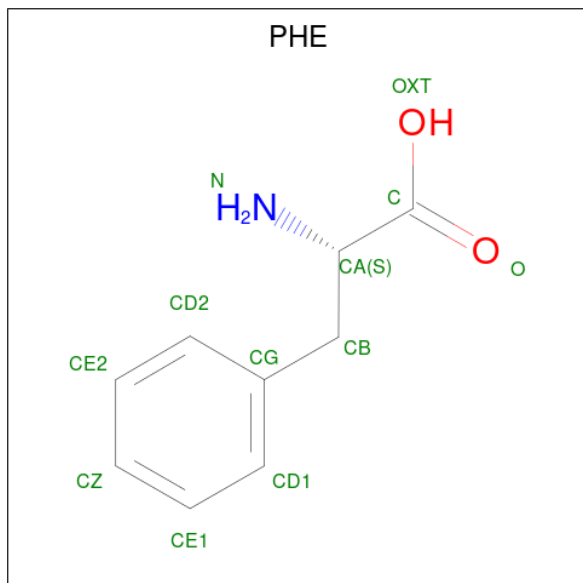
- Molecule 1 is a protein called Phenylalanine-tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2123	1388	363	365	7	0	0	0

- Molecule 2 is a protein called Phenylalanine-tRNA ligase beta subunit.

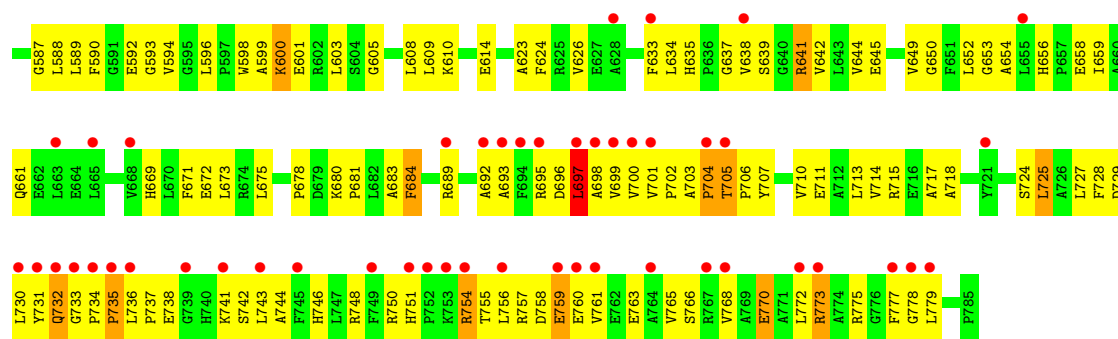
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	785	6127	3925	1091	1101	10	46	0	0

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	12	9	1	2	0	0

- Molecule 4 is PUROMYCIN (three-letter code: PUY) (formula: C₂₂H₂₉N₇O₅).



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.47Å 173.47Å 138.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.06 – 2.60 47.09 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (27.06-2.60) 78.8 (47.09-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.249 , 0.258 0.254 , 0.259	Depositor DCC
R_{free} test set	1997 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtrriage
Anisotropy	0.437	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8471	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: PUY

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	0.41	0/2191	0.62	0/2971
2	B	0.39	0/6280	0.66	4/8536 (0.0%)
All	All	0.39	0/8471	0.65	4/11507 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	VAL	N-CA-C	7.08	130.12	111.00
2	B	260	MET	O-C-N	-6.25	112.70	122.70
2	B	133	LEU	CA-CB-CG	5.40	127.71	115.30
2	B	69	GLY	N-CA-C	-5.32	99.79	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	260	MET	Mainchain

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	2123	0	2075	80	0
2	B	6127	0	6180	261	0
3	A	12	0	8	0	0
4	B	34	0	29	12	0
5	A	29	0	0	0	0
5	B	146	0	0	5	0
All	All	8471	0	8292	327	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 20.

All (327) 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)
2:B:323:GLU:HB2	4:B:801:PUY:C2	1.88	1.02
2:B:323:GLU:CB	4:B:801:PUY:H2	1.89	1.02
2:B:260:MET:H	4:B:801:PUY:HN1	1.05	0.94
1:A:198:VAL:HG13	1:A:220:GLU:HB2	1.49	0.94
2:B:732:GLN:HB3	2:B:741:LYS:HB3	1.50	0.93
1:A:191:THR:HG22	2:B:484:ASP:OD2	1.70	0.92
2:B:323:GLU:HB2	4:B:801:PUY:H2	0.94	0.86
2:B:214:THR:HG22	2:B:394:GLU:HG3	1.64	0.79
1:A:251:VAL:HG12	1:A:269:VAL:HG12	1.64	0.79
1:A:179:THR:OG1	1:A:220:GLU:HG2	1.83	0.78
2:B:120:PRO:HG3	2:B:133:LEU:HD13	1.65	0.78
2:B:323:GLU:OE2	4:B:801:PUY:N1	2.17	0.77
2:B:757:ARG:HG3	2:B:759:GLU:HG3	1.65	0.77
2:B:773:ARG:HG2	2:B:777:PHE:O	1.84	0.77
1:A:108:ARG:O	1:A:112:GLU:HG2	1.85	0.76
2:B:533:LEU:O	2:B:536:PRO:HD3	1.86	0.76
2:B:596:LEU:HB2	2:B:599:ALA:HB3	1.68	0.75
2:B:260:MET:N	4:B:801:PUY:HD1	2.02	0.74
2:B:600:LYS:H	2:B:600:LYS:HD2	1.52	0.73
2:B:775:ARG:HH21	2:B:777:PHE:HZ	1.34	0.73
2:B:192:LYS:H	2:B:381:GLN:HE22	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:732:GLN:HB3	2:B:741:LYS:CB	2.20	0.72
2:B:255:GLU:OE2	2:B:375:ARG:HD2	1.90	0.71
2:B:404:ILE:HD12	2:B:454:ARG:O	1.88	0.71
2:B:730:LEU:HD21	2:B:743:LEU:HD23	1.71	0.71
2:B:701:VAL:HG23	2:B:777:PHE:CE1	2.26	0.71
1:A:348:GLY:C	1:A:350:LEU:H	1.94	0.70
1:A:290:VAL:O	1:A:294:VAL:HG23	1.92	0.69
2:B:407:ARG:HD3	2:B:456:GLU:OE2	1.94	0.68
2:B:362:ARG:HH11	2:B:362:ARG:HG2	1.58	0.67
2:B:434:ARG:HB3	2:B:445:THR:HG23	1.76	0.67
1:A:140:PRO:HD2	1:A:143:HIS:ND1	2.09	0.67
2:B:578:ARG:HG3	2:B:578:ARG:O	1.96	0.66
2:B:730:LEU:HD13	2:B:742:SER:O	1.95	0.66
2:B:286:LEU:HD22	4:B:801:PUY:C4	2.26	0.65
1:A:160:ARG:HH12	2:B:579:GLU:HB3	1.62	0.65
2:B:427:ILE:HD12	2:B:466:ILE:CG2	2.27	0.65
1:A:244:LEU:HD21	1:A:322:LEU:HD21	1.80	0.64
2:B:20:VAL:O	2:B:24:ARG:HG2	1.98	0.64
2:B:710:VAL:HG11	2:B:743:LEU:HD12	1.80	0.64
2:B:519:GLU:HB3	2:B:523:ARG:NH1	2.12	0.64
2:B:409:GLU:OE1	2:B:413:ARG:HD3	1.97	0.63
2:B:432:GLY:O	2:B:447:PRO:HG3	1.99	0.63
2:B:337:CYS:SG	5:B:961:HOH:O	2.56	0.63
2:B:203:LYS:HE3	2:B:205:GLU:OE2	1.98	0.63
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.80	0.63
2:B:530:ARG:HD2	2:B:579:GLU:H	1.63	0.62
2:B:696:ASP:O	2:B:697:LEU:HB3	1.99	0.62
2:B:609:LEU:HD22	2:B:652:LEU:HD11	1.79	0.62
1:A:141:GLU:HG2	1:A:142:HIS:ND1	2.14	0.62
2:B:423:GLU:O	2:B:427:ILE:HG12	1.99	0.62
2:B:256:ARG:NH2	2:B:375:ARG:HG3	2.14	0.62
1:A:128:GLU:OE2	1:A:185:ARG:HD2	1.99	0.62
2:B:710:VAL:O	2:B:714:VAL:HG23	2.00	0.61
2:B:656:HIS:HB3	2:B:659:ILE:HG12	1.82	0.61
2:B:179:ALA:HA	2:B:430:ARG:HB3	1.82	0.61
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.82	0.61
1:A:270:TRP:O	1:A:272:PRO:HD3	2.01	0.60
2:B:707:TYR:CE1	2:B:727:LEU:HD22	2.35	0.60
2:B:505:LEU:N	5:B:902:HOH:O	2.35	0.60
2:B:730:LEU:HD21	2:B:743:LEU:CD2	2.31	0.60
2:B:509:GLU:HB2	2:B:571:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD23	1:A:325:LEU:O	2.03	0.59
1:A:164:PRO:HG2	1:A:188:VAL:HG21	1.85	0.58
2:B:730:LEU:HD11	2:B:743:LEU:HD23	1.84	0.58
2:B:699:VAL:O	2:B:742:SER:HA	2.03	0.58
2:B:600:LYS:HD2	2:B:600:LYS:N	2.18	0.58
2:B:715:ARG:HH12	2:B:725:LEU:HB3	1.68	0.58
2:B:710:VAL:HG11	2:B:743:LEU:CD1	2.33	0.58
2:B:695:ARG:HG3	2:B:695:ARG:HH11	1.69	0.58
2:B:414:LEU:HD23	2:B:460:VAL:HG21	1.86	0.58
2:B:578:ARG:O	2:B:579:GLU:HB2	2.04	0.58
2:B:44:GLY:HA3	2:B:94:THR:OG1	2.04	0.57
2:B:99:LEU:HD12	2:B:100:GLY:N	2.19	0.57
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.86	0.57
2:B:600:LYS:HG2	2:B:601:GLU:OE1	2.04	0.57
2:B:626:VAL:HG21	2:B:652:LEU:HD23	1.87	0.57
2:B:693:ALA:O	2:B:748:ARG:HA	2.04	0.57
2:B:699:VAL:HG22	2:B:772:LEU:HD21	1.86	0.57
2:B:274:VAL:HG12	2:B:298:LEU:HD21	1.87	0.57
2:B:730:LEU:CD2	2:B:743:LEU:HD23	2.35	0.56
2:B:729:ASP:HB3	2:B:744:ALA:CB	2.35	0.56
1:A:317:LEU:O	1:A:317:LEU:HD12	2.04	0.56
2:B:729:ASP:HB3	2:B:744:ALA:HB2	1.86	0.56
2:B:700:VAL:CG2	2:B:778:GLY:H	2.18	0.56
2:B:733:GLY:O	2:B:736:LEU:HB2	2.05	0.56
2:B:587:GLY:HA3	2:B:671:PHE:CE1	2.41	0.56
2:B:578:ARG:C	2:B:580:ARG:H	2.09	0.56
2:B:755:THR:HG22	2:B:756:LEU:N	2.21	0.56
1:A:94:SER:O	2:B:594:VAL:HG13	2.05	0.56
1:A:160:ARG:HG2	2:B:579:GLU:O	2.06	0.55
2:B:649:VAL:HG23	2:B:673:LEU:HD22	1.88	0.55
1:A:278:LEU:CD1	1:A:325:LEU:HD13	2.35	0.55
2:B:176:ASP:OD2	2:B:465:ARG:NH2	2.32	0.55
2:B:504:GLY:C	5:B:902:HOH:O	2.44	0.55
2:B:362:ARG:HG2	2:B:362:ARG:NH1	2.22	0.55
2:B:596:LEU:HB2	2:B:599:ALA:CB	2.38	0.54
1:A:271:TRP:CZ3	1:A:274:GLY:HA3	2.41	0.54
2:B:99:LEU:C	2:B:101:GLN:H	2.11	0.54
1:A:158:GLY:HA3	2:B:530:ARG:HE	1.72	0.54
2:B:260:MET:O	4:B:801:PUY:N	2.40	0.54
2:B:320:ALA:O	2:B:323:GLU:HG2	2.07	0.54
1:A:258:PHE:HB2	1:A:261:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:LYS:N	2:B:381:GLN:HE22	2.04	0.53
2:B:99:LEU:HD13	2:B:101:GLN:O	2.09	0.53
1:A:101:HIS:CG	1:A:102:PRO:HD2	2.43	0.53
1:A:237:ILE:HG22	1:A:251:VAL:HG11	1.90	0.53
2:B:293:LEU:HD13	2:B:299:VAL:HG21	1.90	0.53
2:B:427:ILE:HD12	2:B:466:ILE:HG21	1.90	0.53
2:B:731:TYR:O	2:B:732:GLN:HG3	2.09	0.53
1:A:165:LEU:HD12	1:A:301:LEU:CD2	2.38	0.53
2:B:188:GLU:HG3	2:B:188:GLU:O	2.09	0.53
1:A:210:ALA:HA	1:A:331:ASP:OD1	2.09	0.52
1:A:325:LEU:HD23	1:A:325:LEU:C	2.30	0.52
2:B:546:THR:HG23	2:B:547:HIS:ND1	2.24	0.52
2:B:277:ALA:O	2:B:295:PRO:HA	2.09	0.52
2:B:700:VAL:HA	2:B:741:LYS:O	2.09	0.52
2:B:751:HIS:HB2	2:B:756:LEU:HD21	1.91	0.52
2:B:692:ALA:HB2	2:B:750:ARG:HG3	1.92	0.52
2:B:701:VAL:CG2	2:B:702:PRO:HD2	2.40	0.52
2:B:697:LEU:HD13	2:B:697:LEU:O	2.10	0.52
1:A:143:HIS:HD2	1:A:144:PRO:HD2	1.75	0.52
2:B:440:PRO:HB2	5:B:1017:HOH:O	2.10	0.52
2:B:28:LEU:HD13	2:B:176:ASP:HB3	1.92	0.51
2:B:489:GLU:HG3	2:B:493:ARG:HD2	1.92	0.51
2:B:623:ALA:HB3	2:B:645:GLU:HA	1.92	0.51
2:B:727:LEU:HD11	2:B:730:LEU:CD2	2.41	0.51
2:B:259:PRO:C	4:B:801:PUY:HD1	2.30	0.51
2:B:563:ASP:C	2:B:565:PRO:HD3	2.31	0.51
2:B:596:LEU:HD13	2:B:598:TRP:CH2	2.45	0.51
2:B:519:GLU:HB3	2:B:523:ARG:HH12	1.75	0.51
1:A:288:PRO:O	1:A:292:GLN:HG3	2.11	0.51
2:B:697:LEU:HD22	2:B:697:LEU:C	2.30	0.51
1:A:127:VAL:HG23	2:B:577:PHE:CE2	2.46	0.51
1:A:191:THR:CG2	2:B:484:ASP:OD2	2.51	0.51
2:B:120:PRO:HG3	2:B:133:LEU:CD1	2.39	0.51
2:B:461:GLU:O	2:B:465:ARG:HG2	2.10	0.50
2:B:530:ARG:HB2	2:B:530:ARG:NH1	2.27	0.50
1:A:209:ASP:OD1	1:A:210:ALA:N	2.43	0.50
2:B:294:HIS:CE1	2:B:296:GLU:HB2	2.46	0.50
2:B:370:VAL:HB	2:B:371:PRO:HD3	1.93	0.50
2:B:728:PHE:CZ	2:B:744:ALA:HB1	2.46	0.50
2:B:610:LYS:O	2:B:614:GLU:HG3	2.11	0.50
1:A:250:LYS:HG3	1:A:270:TRP:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:GLY:C	1:A:350:LEU:N	2.64	0.50
2:B:768:VAL:O	2:B:772:LEU:HB2	2.11	0.50
1:A:201:ARG:NH1	1:A:336:PHE:HE1	2.10	0.49
2:B:70:ARG:HG2	2:B:70:ARG:HH11	1.76	0.49
1:A:201:ARG:NH1	1:A:336:PHE:CE1	2.81	0.49
1:A:252:ARG:HG2	1:A:268:ALA:HB3	1.94	0.49
2:B:425:ILE:HD11	2:B:442:TYR:CZ	2.48	0.49
2:B:635:HIS:O	2:B:639:SER:HB2	2.12	0.49
2:B:656:HIS:HB3	2:B:659:ILE:CG1	2.42	0.49
1:A:250:LYS:HG3	1:A:270:TRP:HB3	1.94	0.49
2:B:609:LEU:HD22	2:B:652:LEU:CD1	2.43	0.49
2:B:757:ARG:HE	2:B:760:GLU:HG3	1.78	0.49
2:B:729:ASP:N	2:B:744:ALA:HB3	2.27	0.48
1:A:278:LEU:HD12	1:A:325:LEU:HD13	1.95	0.48
1:A:128:GLU:OE1	1:A:132:PHE:HB2	2.14	0.48
1:A:165:LEU:HD11	1:A:303:LEU:HD11	1.95	0.48
2:B:409:GLU:OE2	2:B:413:ARG:NH1	2.43	0.48
2:B:656:HIS:ND1	2:B:658:GLU:HB2	2.28	0.48
2:B:697:LEU:O	2:B:697:LEU:HD22	2.14	0.48
2:B:530:ARG:HB2	2:B:530:ARG:HH11	1.78	0.48
1:A:287:HIS:HB3	1:A:290:VAL:HG23	1.95	0.48
2:B:554:ARG:O	2:B:558:GLU:HG2	2.13	0.48
1:A:140:PRO:O	1:A:143:HIS:HB2	2.13	0.48
1:A:182:MET:HE3	1:A:185:ARG:HB2	1.96	0.48
2:B:730:LEU:CD1	2:B:743:LEU:HD23	2.44	0.48
1:A:256:VAL:HG12	1:A:265:ALA:C	2.33	0.48
2:B:22:GLU:OE1	2:B:35:ILE:HD11	2.14	0.48
2:B:530:ARG:NH1	2:B:579:GLU:HG3	2.28	0.48
2:B:198:LEU:HD23	2:B:198:LEU:N	2.28	0.48
2:B:278:ARG:NH2	2:B:308:SER:OG	2.47	0.48
2:B:296:GLU:HB3	2:B:349:ARG:NH1	2.29	0.47
1:A:271:TRP:CE3	1:A:274:GLY:HA3	2.49	0.47
2:B:731:TYR:C	2:B:732:GLN:HG3	2.34	0.47
1:A:165:LEU:HD12	1:A:301:LEU:HD23	1.95	0.47
1:A:274:GLY:O	1:A:276:LYS:HG3	2.15	0.47
2:B:195:ALA:HA	2:B:390:GLU:HG2	1.97	0.47
2:B:605:GLY:HA2	2:B:669:HIS:CD2	2.49	0.47
2:B:779:LEU:N	2:B:779:LEU:HD12	2.30	0.47
1:A:182:MET:HE3	1:A:182:MET:O	2.14	0.47
1:A:343:LEU:HD13	2:B:509:GLU:O	2.14	0.47
2:B:695:ARG:HD2	2:B:761:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:696:ASP:OD2	2:B:746:HIS:HD2	1.97	0.47
2:B:778:GLY:C	2:B:779:LEU:HD12	2.34	0.47
2:B:683:ALA:O	2:B:684:PHE:C	2.53	0.47
2:B:717:ALA:C	2:B:768:VAL:HG22	2.35	0.47
2:B:755:THR:HG22	2:B:756:LEU:H	1.80	0.47
2:B:260:MET:N	4:B:801:PUY:HN1	1.89	0.47
2:B:589:LEU:CB	2:B:609:LEU:HD12	2.45	0.47
2:B:285:THR:HB	2:B:317:MET:SD	2.55	0.46
2:B:296:GLU:HB3	2:B:349:ARG:HH12	1.80	0.46
2:B:98:GLY:O	2:B:100:GLY:N	2.48	0.46
2:B:552:LEU:O	2:B:555:VAL:HG22	2.16	0.46
2:B:567:ARG:O	2:B:568:ALA:HB2	2.15	0.46
2:B:700:VAL:HG23	2:B:778:GLY:H	1.81	0.46
2:B:729:ASP:O	2:B:730:LEU:HD22	2.16	0.46
2:B:196:LEU:HB2	2:B:197:PRO:HD2	1.96	0.46
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.45	0.46
2:B:321:GLU:O	2:B:325:ARG:NH2	2.37	0.46
2:B:323:GLU:OE2	4:B:801:PUY:C2	2.62	0.46
2:B:549:PHE:CG	2:B:550:PRO:HD3	2.49	0.46
1:A:210:ALA:O	1:A:332:ILE:HG22	2.16	0.46
2:B:70:ARG:HG2	2:B:70:ARG:NH1	2.31	0.46
2:B:701:VAL:HG21	2:B:705:THR:HG21	1.98	0.46
2:B:703:ALA:N	2:B:704:PRO:CD	2.79	0.46
2:B:728:PHE:CE1	2:B:744:ALA:HB1	2.51	0.46
2:B:652:LEU:HD12	2:B:653:GLY:H	1.81	0.46
2:B:259:PRO:HB2	2:B:360:PHE:CE2	2.51	0.46
2:B:736:LEU:O	2:B:738:GLU:N	2.48	0.46
1:A:160:ARG:NH1	2:B:579:GLU:HB3	2.29	0.46
2:B:717:ALA:HB3	2:B:768:VAL:HG13	1.97	0.46
1:A:98:GLY:HA3	2:B:503:SER:O	2.16	0.46
2:B:638:VAL:HB	2:B:654:ALA:HB3	1.98	0.45
2:B:644:VAL:HG11	2:B:678:PRO:HD2	1.98	0.45
2:B:730:LEU:HD11	2:B:743:LEU:CD2	2.46	0.45
2:B:732:GLN:HA	2:B:741:LYS:HA	1.96	0.45
1:A:182:MET:CE	1:A:185:ARG:HB2	2.46	0.45
1:A:190:HIS:HD2	2:B:484:ASP:O	2.00	0.45
2:B:206:ASP:OD2	2:B:276:ARG:HD3	2.16	0.45
2:B:583:THR:HG22	2:B:675:LEU:HD12	1.98	0.45
2:B:641:ARG:HG3	2:B:641:ARG:HH11	1.82	0.45
2:B:656:HIS:CE1	2:B:658:GLU:HB2	2.52	0.45
2:B:766:SER:O	2:B:770:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:VAL:HG13	2:B:444:VAL:HG22	1.99	0.45
2:B:348:ARG:NH1	2:B:361:GLU:OE1	2.47	0.44
2:B:549:PHE:CD1	2:B:549:PHE:C	2.90	0.44
2:B:427:ILE:HD12	2:B:466:ILE:HG22	1.99	0.44
1:A:178:HIS:HB2	1:A:218:GLN:HE22	1.82	0.44
1:A:94:SER:C	2:B:594:VAL:HG13	2.37	0.44
2:B:467:GLN:OE1	2:B:467:GLN:HA	2.17	0.44
2:B:635:HIS:ND1	2:B:637:GLY:N	2.54	0.44
2:B:650:GLY:HA3	2:B:672:GLU:O	2.18	0.44
2:B:751:HIS:HB3	2:B:754:ARG:O	2.18	0.44
2:B:556:LEU:O	2:B:560:LEU:HG	2.18	0.44
2:B:589:LEU:CD2	2:B:609:LEU:HB2	2.48	0.44
1:A:160:ARG:HG3	2:B:580:ARG:NE	2.33	0.44
1:A:348:GLY:O	1:A:350:LEU:N	2.48	0.44
2:B:99:LEU:O	2:B:101:GLN:N	2.51	0.43
2:B:734:PRO:HA	2:B:735:PRO:HA	1.81	0.43
2:B:698:ALA:HA	2:B:743:LEU:O	2.18	0.43
2:B:775:ARG:HB3	2:B:777:PHE:CE2	2.53	0.43
1:A:162:GLU:O	1:A:185:ARG:NH2	2.51	0.43
1:A:260:PHE:C	1:A:287:HIS:HB2	2.38	0.43
2:B:624:PHE:HE1	2:B:642:VAL:HG13	1.83	0.43
2:B:652:LEU:HD13	2:B:671:PHE:HB3	1.99	0.43
2:B:367:LEU:HD21	2:B:398:PRO:HB2	2.01	0.43
2:B:560:LEU:HD21	2:B:590:PHE:CE2	2.54	0.43
2:B:701:VAL:HG23	2:B:702:PRO:HD2	1.99	0.43
1:A:101:HIS:HE1	1:A:103:ILE:HG12	1.82	0.43
2:B:264:ASP:OD2	2:B:266:ARG:HD3	2.19	0.43
1:A:143:HIS:CE1	1:A:145:ALA:HB3	2.52	0.43
2:B:51:LEU:HD11	2:B:67:ASP:HB2	2.01	0.43
2:B:559:ASN:O	2:B:563:ASP:O	2.37	0.43
2:B:578:ARG:O	2:B:579:GLU:CB	2.67	0.43
2:B:641:ARG:HG3	2:B:641:ARG:NH1	2.33	0.43
2:B:184:LEU:HD22	2:B:186:GLU:HG3	2.00	0.43
2:B:589:LEU:HB2	2:B:609:LEU:HD12	2.00	0.43
2:B:724:SER:O	2:B:725:LEU:HB2	2.17	0.43
2:B:408:PRO:HG2	2:B:421:GLU:HG3	2.00	0.43
2:B:497:ARG:HG3	2:B:497:ARG:HH11	1.84	0.43
2:B:556:LEU:HD22	2:B:588:LEU:HD21	1.99	0.43
2:B:592:GLU:HG3	2:B:593:GLY:N	2.33	0.43
2:B:90:ALA:HB2	2:B:118:LEU:HD11	2.01	0.42
2:B:701:VAL:O	2:B:741:LYS:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ARG:HG3	1:A:85:ARG:HH11	1.84	0.42
1:A:260:PHE:CD1	1:A:260:PHE:N	2.86	0.42
2:B:695:ARG:HG3	2:B:695:ARG:NH1	2.33	0.42
2:B:705:THR:HA	2:B:706:PRO:HD3	1.79	0.42
2:B:732:GLN:O	2:B:732:GLN:CD	2.57	0.42
1:A:179:THR:C	1:A:181:PRO:HD2	2.39	0.42
1:A:221:GLY:HA3	1:A:315:PHE:CZ	2.54	0.42
1:A:159:PHE:N	2:B:530:ARG:HD3	2.34	0.42
2:B:555:VAL:O	2:B:559:ASN:HB2	2.20	0.42
1:A:109:GLU:O	1:A:113:ILE:HG13	2.19	0.42
2:B:696:ASP:OD2	2:B:746:HIS:CD2	2.73	0.42
1:A:339:ARG:O	1:A:342:PHE:HB3	2.20	0.42
2:B:158:LEU:HD12	2:B:173:LEU:HD21	2.01	0.42
2:B:407:ARG:NH1	2:B:456:GLU:OE1	2.52	0.42
2:B:497:ARG:HG3	2:B:497:ARG:NH1	2.35	0.42
2:B:417:THR:HG22	2:B:473:PRO:HD3	2.02	0.42
2:B:32:THR:HG21	2:B:156:LEU:HD23	2.01	0.41
2:B:184:LEU:HD23	2:B:185:VAL:N	2.34	0.41
2:B:431:LEU:HD13	2:B:462:GLU:OE1	2.20	0.41
2:B:689:ARG:HB3	2:B:689:ARG:NH1	2.35	0.41
1:A:203:PHE:CD1	1:A:203:PHE:N	2.88	0.41
1:A:280:LEU:CD2	1:A:322:LEU:HD13	2.51	0.41
2:B:75:VAL:HG23	2:B:111:VAL:HG22	2.02	0.41
1:A:107:GLU:O	1:A:111:VAL:HG23	2.21	0.41
1:A:228:ILE:HG21	1:A:312:GLY:HA2	2.02	0.41
2:B:49:ARG:HG3	2:B:137:GLU:CG	2.50	0.41
2:B:549:PHE:N	2:B:550:PRO:CD	2.83	0.41
2:B:603:LEU:O	2:B:608:LEU:HD22	2.21	0.41
2:B:153:GLU:HG3	2:B:154:VAL:N	2.36	0.41
2:B:704:PRO:O	2:B:705:THR:C	2.59	0.41
2:B:707:TYR:CD1	2:B:727:LEU:HD22	2.55	0.41
2:B:718:ALA:HA	2:B:768:VAL:HG21	2.02	0.41
2:B:633:PHE:CD1	2:B:634:LEU:HG	2.55	0.41
2:B:692:ALA:HB2	2:B:750:ARG:NH1	2.36	0.41
2:B:140:LEU:HD21	2:B:149:ALA:HB2	2.01	0.41
2:B:2:ARG:NH1	2:B:236:ALA:O	2.53	0.41
2:B:92:PRO:HG2	2:B:114:PHE:CE1	2.55	0.41
2:B:268:VAL:HG13	2:B:272:ILE:HG13	2.02	0.41
1:A:331:ASP:HB3	1:A:334:TYR:CE2	2.56	0.41
2:B:275:ARG:HG3	2:B:275:ARG:HH11	1.86	0.41
2:B:695:ARG:HD2	2:B:761:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:486:ARG:NH2	5:B:903:HOH:O	2.53	0.41
2:B:624:PHE:CE1	2:B:642:VAL:HG13	2.56	0.41
2:B:701:VAL:CG2	2:B:702:PRO:CD	2.99	0.41
1:A:180:SER:N	1:A:181:PRO:HD2	2.35	0.40
2:B:759:GLU:O	2:B:763:GLU:HB3	2.21	0.40
1:A:198:VAL:HA	1:A:199:PRO:HD2	1.96	0.40
1:A:199:PRO:HB3	1:A:219:LEU:HD12	2.03	0.40
2:B:297:ASP:OD2	2:B:350:HIS:HE1	2.03	0.40
2:B:680:LYS:HA	2:B:681:PRO:HD3	1.93	0.40
1:A:197:VAL:HA	1:A:220:GLU:O	2.21	0.40
2:B:179:ALA:HB2	2:B:431:LEU:HD23	2.02	0.40
2:B:507:PHE:HB3	2:B:571:PHE:HB3	2.04	0.40
2:B:588:LEU:HD23	2:B:588:LEU:C	2.42	0.40
2:B:751:HIS:HB2	2:B:756:LEU:CD2	2.51	0.40
1:A:132:PHE:CD2	1:A:185:ARG:NH1	2.90	0.40
2:B:472:ILE:HA	2:B:473:PRO:HD3	1.96	0.40
2:B:592:GLU:HG3	2:B:593:GLY:H	1.86	0.40
2:B:761:VAL:O	2:B:765:VAL:HG12	2.21	0.40
2:B:286:LEU:HD22	4:B:801:PUY:N3	2.36	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	264/350 (75%)	251 (95%)	12 (4%)	1 (0%)	34	57
2	B	783/785 (100%)	713 (91%)	56 (7%)	14 (2%)	8	16
All	All	1047/1135 (92%)	964 (92%)	68 (6%)	15 (1%)	11	22

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	LEU
2	B	754	ARG
1	A	349	VAL
2	B	102	LYS
2	B	697	LEU
2	B	725	LEU
2	B	578	ARG
2	B	684	PHE
2	B	704	PRO
2	B	732	GLN
2	B	737	PRO
2	B	568	ALA
2	B	705	THR
2	B	100	GLY
2	B	735	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	214/277 (77%)	201 (94%)	13 (6%)	18	38
2	B	630/630 (100%)	591 (94%)	39 (6%)	18	37
All	All	844/907 (93%)	792 (94%)	52 (6%)	18	37

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	170	GLU
1	A	178	HIS
1	A	179	THR
1	A	191	THR
1	A	197	VAL
1	A	198	VAL
1	A	213	GLU
1	A	219	LEU

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Mol	Chain	Res	Type
1	A	260	PHE
1	A	278	LEU
1	A	321	ARG
1	A	350	LEU
2	B	32	THR
2	B	89	LEU
2	B	111	VAL
2	B	158	LEU
2	B	170	LEU
2	B	171	LEU
2	B	173	LEU
2	B	180	LEU
2	B	208	GLU
2	B	276	ARG
2	B	298	LEU
2	B	313	LEU
2	B	329	GLU
2	B	333	LEU
2	B	334	GLU
2	B	353	ARG
2	B	362	ARG
2	B	375	ARG
2	B	393	LEU
2	B	441	THR
2	B	445	THR
2	B	459	LEU
2	B	460	VAL
2	B	496	GLN
2	B	497	ARG
2	B	505	LEU
2	B	549	PHE
2	B	571	PHE
2	B	575	ARG
2	B	600	LYS
2	B	641	ARG
2	B	661	GLN
2	B	697	LEU
2	B	711	GLU
2	B	713	LEU
2	B	758	ASP
2	B	759	GLU
2	B	770	GLU

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Mol	Chain	Res	Type
2	B	773	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	190	HIS
1	A	218	GLN
2	B	54	HIS
2	B	101	GLN
2	B	178	HIS
2	B	250	ASN
2	B	350	HIS
2	B	381	GLN
2	B	746	HIS

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 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
4	PUY	B	801	-	32,37,37	2.62	10 (31%)	33,53,53	2.44	12 (36%)
3	PHE	A	401	-	11,12,12	0.74	0	14,15,15	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PUY	B	801	-	-	9/20/40/40	0/4/4/4
3	PHE	A	401	-	-	0/8/8/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	PUY	C6-N1	8.28	1.45	1.33
4	B	801	PUY	C4-N3	7.56	1.46	1.35
4	B	801	PUY	C2-N1	4.56	1.42	1.33
4	B	801	PUY	C2-N3	4.22	1.38	1.32
4	B	801	PUY	CE2-CZ	2.71	1.44	1.38
4	B	801	PUY	C5-C4	2.42	1.47	1.40
4	B	801	PUY	CE1-CD1	2.39	1.43	1.38
4	B	801	PUY	C8-N7	2.38	1.38	1.34
4	B	801	PUY	CE1-CZ	2.24	1.43	1.38
4	B	801	PUY	C-N3'	2.21	1.38	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	PUY	CB-CA-C	6.49	124.17	108.97
4	B	801	PUY	CD2-CG-CD1	5.07	126.14	118.17
4	B	801	PUY	N3-C2-N1	-4.73	121.28	128.68
4	B	801	PUY	CMZ-OM-CZ	4.23	126.70	117.51
4	B	801	PUY	C3'-N3'-C	-4.14	116.97	123.21
4	B	801	PUY	CB-CG-CD2	-3.47	114.02	120.91
4	B	801	PUY	CA-C-N3'	3.24	120.65	116.15
4	B	801	PUY	CG-CB-CA	2.89	120.15	114.13
4	B	801	PUY	CE1-CD1-CG	-2.55	117.51	121.03
4	B	801	PUY	CE2-CD2-CG	-2.49	117.61	121.03
4	B	801	PUY	N1-C6-N6	2.38	119.56	117.06
4	B	801	PUY	C1'-N9-C4	2.08	130.29	126.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

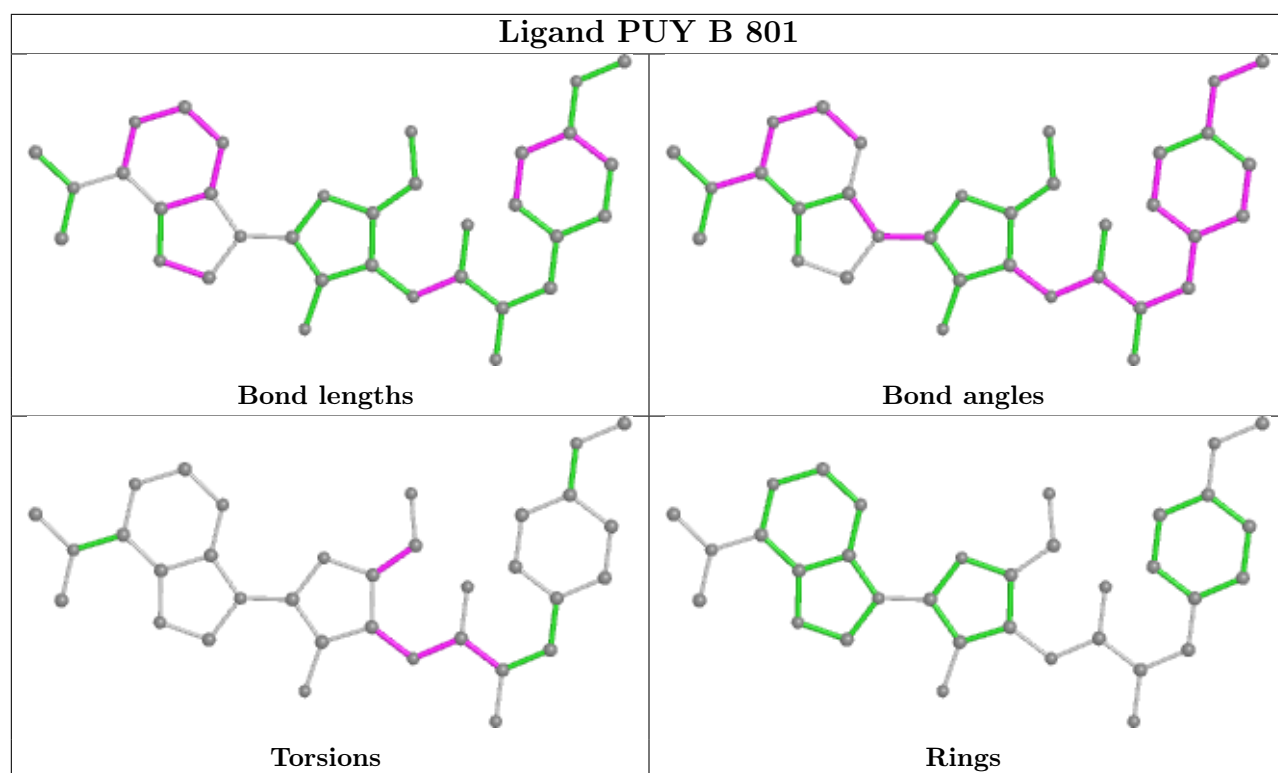
Mol	Chain	Res	Type	Atoms
4	B	801	PUY	O-C-CA-N
4	B	801	PUY	O-C-CA-CB
4	B	801	PUY	N3'-C-CA-CB
4	B	801	PUY	CA-C-N3'-C3'
4	B	801	PUY	O4'-C4'-C5'-O5'
4	B	801	PUY	C3'-C4'-C5'-O5'
4	B	801	PUY	C4'-C3'-N3'-C
4	B	801	PUY	O-C-N3'-C3'
4	B	801	PUY	N3'-C-CA-N

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	PUY	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	266/350 (76%)	0.28	9 (3%) 45 38	36, 56, 91, 122	0
2	B	779/785 (99%)	0.29	56 (7%) 15 11	31, 57, 119, 129	0
All	All	1045/1135 (92%)	0.29	65 (6%) 20 15	31, 57, 116, 129	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	ARG	9.5
1	A	350	LEU	7.6
2	B	731	TYR	5.9
2	B	698	ALA	5.8
2	B	697	LEU	5.4
2	B	778	GLY	5.2
2	B	736	LEU	5.2
2	B	694	PHE	4.8
2	B	761	VAL	4.7
2	B	779	LEU	4.5
2	B	756	LEU	4.3
2	B	699	VAL	4.3
2	B	732	GLN	4.1
1	A	143	HIS	4.0
2	B	704	PRO	4.0
2	B	692	ALA	4.0
2	B	752	PRO	3.7
2	B	100	GLY	3.6
2	B	745	PHE	3.6
2	B	700	VAL	3.5
2	B	768	VAL	3.4
2	B	705	THR	3.4
2	B	749	PHE	3.4
2	B	743	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	721	TYR	3.2
2	B	764	ALA	3.1
1	A	271	TRP	3.1
2	B	693	ALA	3.1
2	B	638	VAL	3.1
2	B	739	GLY	3.0
2	B	733	GLY	3.0
2	B	772	LEU	2.9
2	B	99	LEU	2.9
2	B	701	VAL	2.8
2	B	773	ARG	2.8
2	B	633	PHE	2.6
2	B	734	PRO	2.6
2	B	689	ARG	2.6
1	A	86	VAL	2.5
2	B	741	LYS	2.5
2	B	777	PHE	2.4
2	B	294	HIS	2.4
2	B	753	LYS	2.4
1	A	210	ALA	2.4
2	B	628	ALA	2.3
2	B	751	HIS	2.3
2	B	280	GLY	2.3
1	A	160	ARG	2.3
2	B	695	ARG	2.3
2	B	43	ARG	2.3
2	B	98	GLY	2.2
2	B	564	ARG	2.2
2	B	730	LEU	2.2
2	B	668	VAL	2.2
2	B	759	GLU	2.2
2	B	760	GLU	2.2
1	A	95	LEU	2.2
1	A	207	GLN	2.2
2	B	735	PRO	2.2
2	B	754	ARG	2.2
2	B	101	GLN	2.2
2	B	665	LEU	2.2
2	B	767	ARG	2.1
2	B	663	LEU	2.1
2	B	655	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

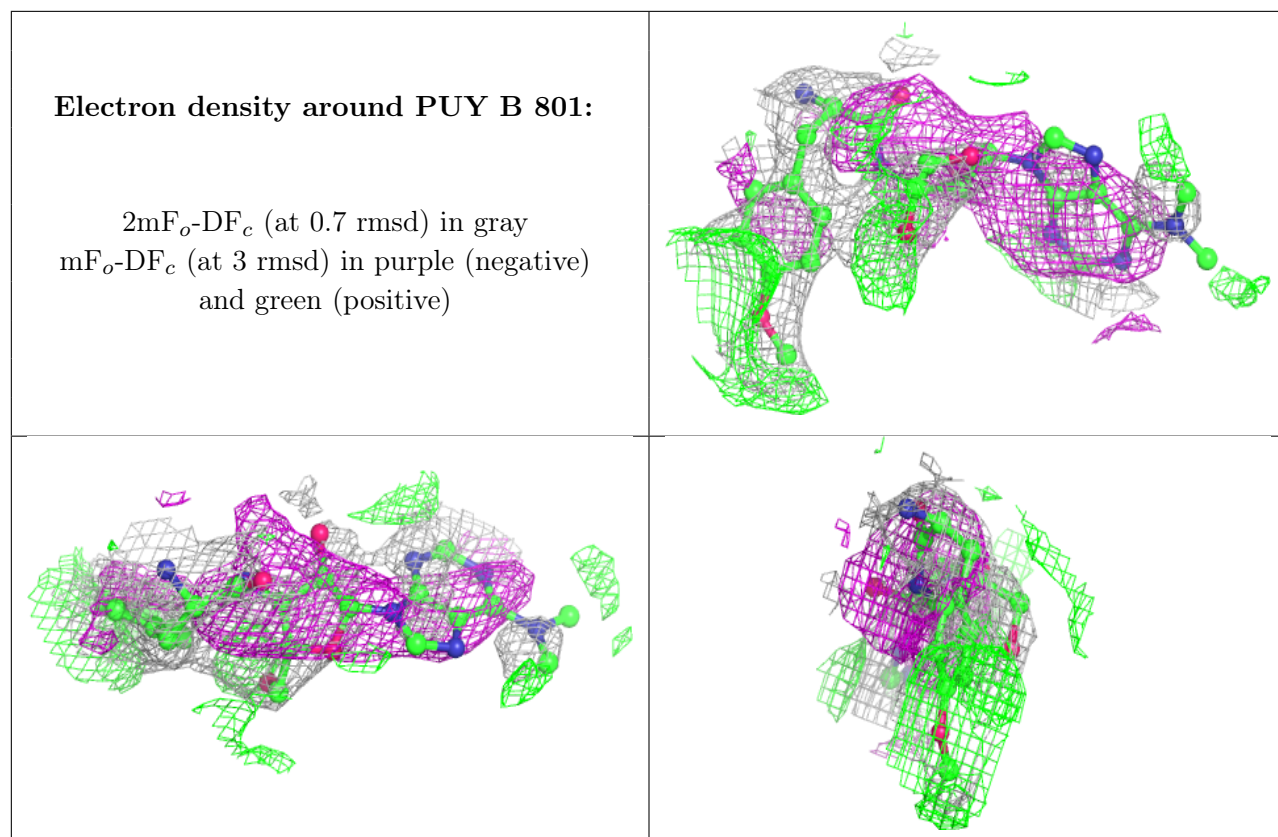
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PUY	B	801	34/34	0.48	0.50	75,90,100,100	0
3	PHE	A	401	12/12	0.93	0.18	59,61,67,68	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.