



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:16 pm BST

PDB ID : 2TPL  
Title : TYROSINE PHENOL-LYASE FROM CITROBACTER INTERMEDIUS  
COMPLEX WITH 3-(4'-HYDROXYPHENYL)PROPIONIC ACID, PY  
RIDOXAL-5'-PHOSPHATE AND CS<sup>+</sup> ION  
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Deposited on : 1997-01-23  
Resolution : 2.50 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](mailto: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.

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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  
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

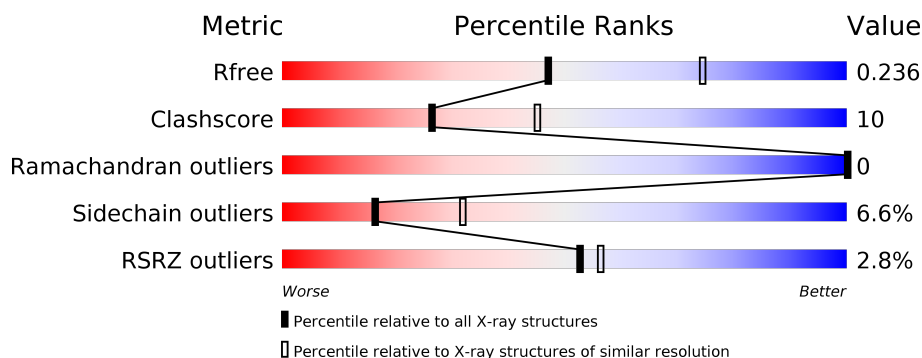
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	456	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>.</div> </div> </div>
1	B	456	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7504 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 TYROSINE PHENOL-LYASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	P	S	0	0	0
			3619	2289	625	679	1	25			
1	B	455	Total	C	N	O	P	S	0	0	0
			3619	2289	625	679	1	25			

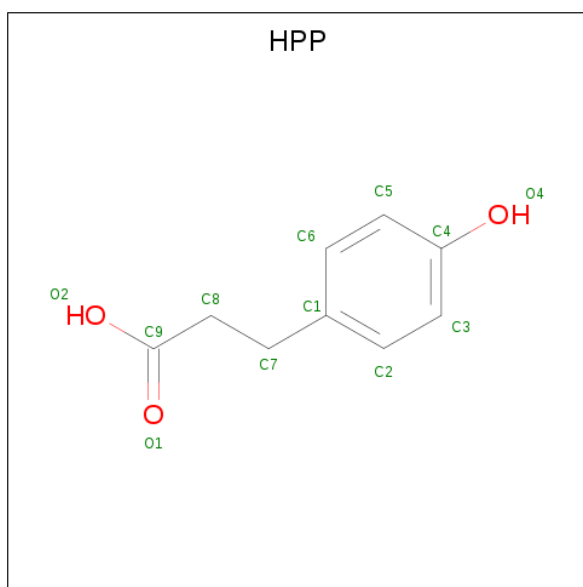
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	LLP	LYS	MODIFIED RESIDUE	UNP P31013
B	257	LLP	LYS	MODIFIED RESIDUE	UNP P31013

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cs	0	0
			1	1		
2	A	1	Total	Cs	0	0
			1	1		

- Molecule 3 is HYDROXYPHENYL PROPIONIC ACID (three-letter code: HPP) (formula: C<sub>9</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	9	3		

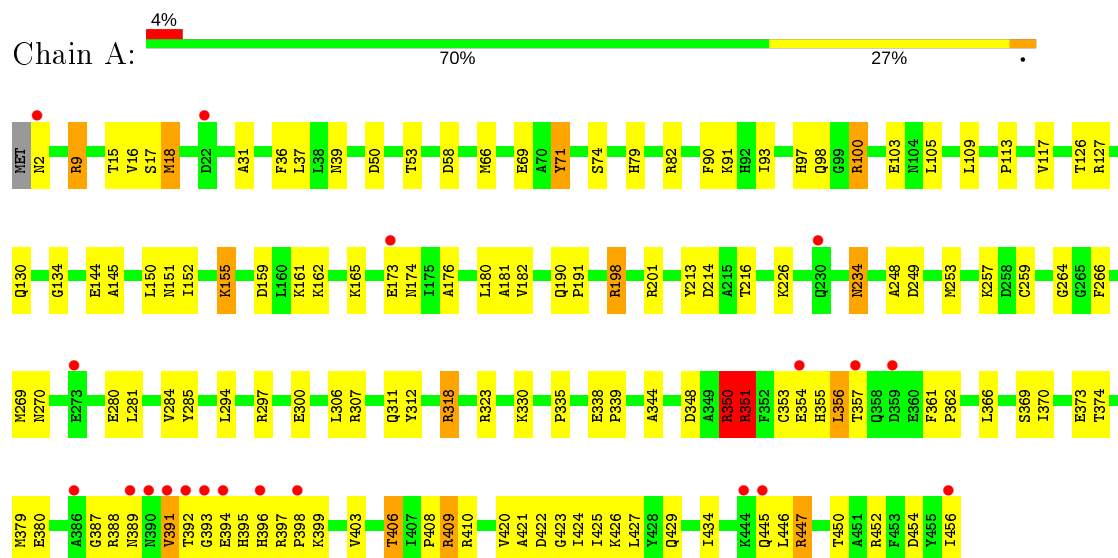
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total	O	0	0
			118	118		
4	B	134	Total	O	0	0
			134	134		

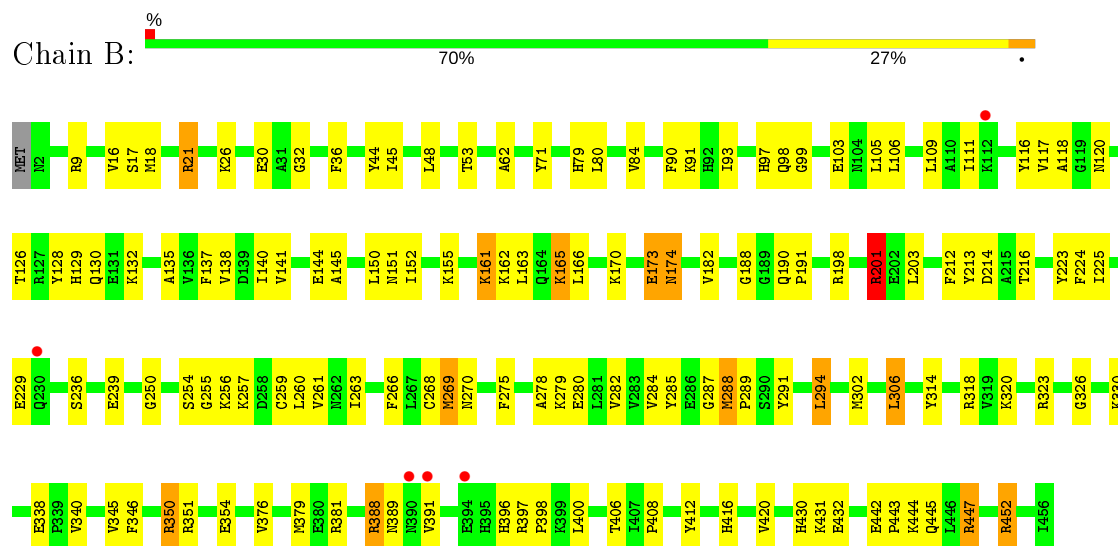
### 3 Residue-property plots

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: TYROSINE PHENOL-LYASE



#### • Molecule 1: TYROSINE PHENOL-LYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.07Å 143.91Å 59.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 14.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	78.5 (15.00-2.50) 80.9 (14.84-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.183 , 0.263 0.197 , 0.236	Depositor DCC
$R_{free}$ test set	957 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7504	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CS, HPP, LLP

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	0.42	0/3666	1.31	26/4937 (0.5%)
1	B	0.41	0/3666	1.18	18/4937 (0.4%)
All	All	0.42	0/7332	1.24	44/9874 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
All	All	0	7

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	A	9	ARG	NE-CZ-NH2	10.10	125.35	120.30
1	A	307	ARG	CD-NE-CZ	9.85	137.38	123.60
1	B	198	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	A	100	ARG	CD-NE-CZ	9.42	136.78	123.60
1	A	100	ARG	NE-CZ-NH2	-9.31	115.65	120.30
1	A	71	TYR	CB-CG-CD1	-8.52	115.89	121.00
1	B	71	TYR	CB-CG-CD1	-8.49	115.91	121.00
1	A	350	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	B	44	TYR	CB-CG-CD1	8.48	126.09	121.00
1	A	410	ARG	CD-NE-CZ	8.25	135.16	123.60
1	B	412	TYR	CB-CG-CD1	-8.07	116.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	ARG	NE-CZ-NH1	-8.03	116.29	120.30
1	A	58	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	71	TYR	CB-CG-CD2	7.59	125.55	121.00
1	B	71	TYR	CB-CG-CD2	7.45	125.47	121.00
1	B	412	TYR	CB-CG-CD2	7.38	125.42	121.00
1	A	318	ARG	NE-CZ-NH1	-7.27	116.67	120.30
1	A	297	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	44	TYR	CB-CG-CD2	-7.06	116.77	121.00
1	A	100	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	307	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	350	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	A	397	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	198	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	266	PHE	CB-CG-CD2	-6.03	116.58	120.80
1	B	21	ARG	CD-NE-CZ	5.96	131.95	123.60
1	A	409	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	18	MET	CA-CB-CG	5.86	123.27	113.30
1	A	69	GLU	OE1-CD-OE2	-5.76	116.39	123.30
1	B	9	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	213	TYR	CB-CG-CD1	5.67	124.40	121.00
1	B	388	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	9	ARG	CD-NE-CZ	-5.61	115.75	123.60
1	B	397	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	351	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	447	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	A	452	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	454	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	201	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	323	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	A	395	HIS	CA-CB-CG	5.11	122.29	113.60
1	A	422	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	447	ARG	NE-CZ-NH2	5.05	122.83	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	ASN	Mainchain
1	A	74	SER	Mainchain
1	B	161	LYS	Mainchain
1	B	288	MET	Mainchain
1	B	306	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	B	452	ARG	Mainchain
1	B	62	ALA	Mainchain

## 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	3619	0	3552	71	0
1	B	3619	0	3553	80	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	12	0	9	1	0
4	A	118	0	0	2	0
4	B	134	0	0	7	0
All	All	7504	0	7114	148	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 (148) 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:162:LYS:HA	1:B:165:LYS:HE2	1.45	0.94
1:A:53:THR:HG23	1:A:408:PRO:HB3	1.54	0.88
1:B:53:THR:HG23	1:B:408:PRO:HB3	1.54	0.87
1:A:162:LYS:HA	1:A:165:LYS:HE3	1.57	0.84
1:A:392:THR:HG22	1:A:394:GLU:HG3	1.69	0.74
1:B:430:HIS:HB2	4:B:645:HOH:O	1.89	0.73
1:A:373:GLU:HG3	1:A:427:LEU:HD21	1.68	0.73
1:A:214:ASP:OD1	1:A:216:THR:HG23	1.96	0.66
1:B:48:LEU:HD12	1:B:379:MET:HB2	1.77	0.66
1:A:103:GLU:OE2	1:A:257:LLP:H6	1.96	0.66
1:B:32:GLY:HA3	1:B:452:ARG:HB3	1.77	0.66
1:B:145:ALA:HA	1:B:155:LYS:HG2	1.79	0.65
1:B:236:SER:OG	1:B:239:GLU:HG3	1.97	0.64
1:A:284:VAL:HG11	1:B:128:TYR:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ASP:HB3	1:A:162:LYS:HG3	1.79	0.63
1:A:117:VAL:HG23	1:A:176:ALA:HB3	1.81	0.62
1:B:140:ILE:HD12	1:B:163:LEU:HD13	1.82	0.61
1:B:118:ALA:HB1	1:B:140:ILE:HD13	1.82	0.61
1:B:117:VAL:HG21	1:B:130:GLN:HG2	1.83	0.60
1:A:264:GLY:HA2	1:A:294:LEU:HD21	1.83	0.60
1:B:26:LYS:O	1:B:30:GLU:HG3	2.02	0.60
1:A:91:LYS:H	1:A:270:ASN:ND2	2.00	0.60
1:A:335:PRO:HB2	1:A:348:ASP:HB3	1.84	0.60
1:A:144:GLU:HB3	1:A:150:LEU:HD23	1.84	0.59
1:B:326:GLY:HA3	1:B:340:VAL:HG21	1.83	0.59
1:B:259:CYS:SG	1:B:306:LEU:HD13	2.43	0.59
1:A:257:LLP:NZ	1:A:257:LLP:O3	2.35	0.58
1:A:353:CYS:HB3	1:A:356:LEU:HD12	1.84	0.58
1:B:111:ILE:HD13	1:B:135:ALA:HB2	1.86	0.57
1:B:45:ILE:HB	1:B:376:VAL:HG22	1.85	0.57
1:B:116:TYR:CZ	1:B:170:LYS:HE3	2.40	0.57
1:B:396:HIS:O	1:B:398:PRO:HD3	2.04	0.57
1:A:91:LYS:H	1:A:270:ASN:HD22	1.51	0.56
1:A:17:SER:O	1:A:18:MET:HB2	2.05	0.56
1:B:99:GLY:O	1:B:103:GLU:HG3	2.07	0.55
1:B:284:VAL:HG23	1:B:285:TYR:CD2	2.41	0.55
1:B:106:LEU:HD21	1:B:212:PHE:CG	2.42	0.54
1:A:338:GLU:HB3	1:A:339:PRO:HA	1.90	0.54
1:A:113:PRO:HA	1:A:134:GLY:HA3	1.90	0.53
1:B:255:GLY:HA2	1:B:259:CYS:HB2	1.89	0.53
1:A:420:VAL:O	1:A:424:ILE:HG13	2.08	0.52
1:B:279:LYS:O	1:B:282:VAL:HG12	2.10	0.52
1:B:416:HIS:O	1:B:420:VAL:HG23	2.10	0.52
1:A:344:ALA:HB2	1:A:406:THR:HG23	1.91	0.52
1:B:161:LYS:HG2	4:B:674:HOH:O	2.10	0.51
1:B:269:MET:HE1	1:B:278:ALA:HB2	1.92	0.51
1:B:381:ARG:HA	1:B:381:ARG:HE	1.74	0.51
1:A:213:TYR:CE1	1:A:248:ALA:HB2	2.45	0.51
1:A:79:HIS:HB2	4:A:508:HOH:O	2.11	0.51
1:B:400:LEU:HG	4:B:718:HOH:O	2.09	0.51
1:A:389:ASN:O	1:A:393:GLY:N	2.42	0.50
1:B:330:LYS:HE3	1:B:338:GLU:OE1	2.12	0.50
1:A:281:LEU:HD11	1:A:285:TYR:HE2	1.77	0.50
1:A:445:GLN:HE21	1:A:446:LEU:H	1.59	0.50
1:A:145:ALA:HB2	1:A:155:LYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:CG2	1:A:176:ALA:HB3	2.42	0.49
1:A:105:LEU:O	1:A:109:LEU:HG	2.13	0.49
1:B:109:LEU:HD11	1:B:278:ALA:HA	1.95	0.49
1:A:17:SER:OG	1:A:18:MET:N	2.46	0.49
1:A:90:PHE:HA	1:A:270:ASN:HD21	1.77	0.49
1:B:255:GLY:CA	1:B:259:CYS:HB2	2.43	0.49
1:A:357:THR:HA	4:A:614:HOH:O	2.13	0.49
1:A:421:ALA:O	1:A:425:ILE:HG13	2.13	0.49
1:B:155:LYS:HE2	4:B:704:HOH:O	2.12	0.48
1:A:355:HIS:CD2	1:A:355:HIS:H	2.31	0.48
1:B:144:GLU:HB3	1:B:150:LEU:HD23	1.95	0.48
1:A:396:HIS:O	1:A:398:PRO:HD3	2.13	0.48
1:A:370:ILE:CD1	1:A:424:ILE:HG12	2.43	0.48
1:B:120:ASN:HB2	1:B:141:VAL:HG23	1.94	0.48
1:B:256:LYS:HE2	1:B:263:ILE:HD12	1.96	0.48
1:A:350:ARG:NH2	1:A:399:LYS:O	2.47	0.48
1:B:152:ILE:HD11	1:B:155:LYS:HG3	1.94	0.48
1:B:103:GLU:OE2	1:B:257:LLP:H6	2.13	0.48
1:A:335:PRO:HG3	1:A:351:ARG:HB3	1.95	0.48
1:B:170:LYS:HE2	4:B:733:HOH:O	2.14	0.48
1:A:351:ARG:O	1:A:354:GLU:HG3	2.13	0.48
1:B:129:HIS:HB2	4:B:671:HOH:O	2.14	0.48
1:B:17:SER:O	1:B:18:MET:HB2	2.14	0.48
1:B:432:GLU:CD	1:B:432:GLU:H	2.17	0.47
1:B:443:PRO:HG2	1:B:447:ARG:HA	1.96	0.47
1:B:275:PHE:CZ	1:B:279:LYS:HE2	2.50	0.47
1:B:223:TYR:OH	1:B:320:LYS:HE3	2.15	0.47
1:A:173:GLU:HG2	1:A:174:ASN:ND2	2.29	0.47
1:A:31:ALA:O	1:A:37:LEU:HD12	2.15	0.47
1:A:234:ASN:HD22	1:A:234:ASN:H	1.64	0.46
1:B:80:LEU:O	1:B:84:VAL:HG23	2.15	0.46
1:A:280:GLU:OE2	1:B:445:GLN:HG2	2.16	0.46
1:B:340:VAL:HG22	1:B:345:VAL:HG22	1.96	0.46
1:B:163:LEU:HG	1:B:203:LEU:HD23	1.97	0.46
1:B:97:HIS:CD2	1:B:98:GLN:HG2	2.51	0.46
1:A:71:TYR:CZ	3:B:600:HPP:H71	2.51	0.45
1:B:91:LYS:HB3	1:B:270:ASN:HA	1.98	0.45
1:A:127:ARG:HA	1:A:130:GLN:NE2	2.31	0.45
1:B:138:VAL:HG21	1:B:166:LEU:HD11	1.98	0.45
1:B:214:ASP:OD1	1:B:216:THR:HG23	2.17	0.45
1:A:97:HIS:CD2	1:A:98:GLN:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:GLY:HA2	1:B:346:PHE:CE1	2.53	0.44
1:B:16:VAL:HG23	1:B:18:MET:HG2	2.00	0.44
1:A:79:HIS:HD2	1:A:300:GLU:OE2	2.00	0.44
1:A:152:ILE:HG13	1:A:155:LYS:HG3	2.00	0.44
1:A:355:HIS:HE1	1:A:434:ILE:O	2.01	0.43
1:A:445:GLN:HA	1:A:445:GLN:NE2	2.33	0.43
1:B:105:LEU:O	1:B:109:LEU:HG	2.18	0.43
1:B:279:LYS:HG2	1:B:289:PRO:HB3	2.00	0.43
1:A:370:ILE:HD12	1:A:424:ILE:HG12	2.00	0.43
1:B:225:ILE:HG23	1:B:229:GLU:OE1	2.18	0.43
1:B:261:VAL:HG11	1:B:302:MET:HA	1.99	0.43
1:B:191:PRO:HG3	1:B:224:PHE:CG	2.54	0.43
1:B:442:GLU:HA	1:B:443:PRO:HD3	1.81	0.43
1:A:201:ARG:HH12	1:A:249:ASP:CG	2.21	0.43
1:A:388:ARG:HD3	1:A:393:GLY:O	2.18	0.43
1:A:50:ASP:OD2	1:A:409:ARG:NH2	2.49	0.43
1:B:170:LYS:O	1:B:174:ASN:ND2	2.46	0.43
1:A:253:MET:HG2	1:A:266:PHE:CZ	2.54	0.43
1:A:387:GLY:HA2	1:A:447:ARG:CD	2.49	0.43
1:B:260:LEU:HD21	1:B:314:TYR:OH	2.19	0.43
1:B:323:ARG:HA	1:B:340:VAL:HG11	2.01	0.43
1:B:79:HIS:HB2	4:B:675:HOH:O	2.19	0.42
1:B:201:ARG:HE	1:B:201:ARG:HA	1.83	0.42
1:A:366:LEU:HD23	1:A:403:VAL:HG21	2.01	0.42
1:B:190:GLN:HA	1:B:191:PRO:HD3	1.90	0.42
1:B:117:VAL:O	1:B:137:PHE:HA	2.19	0.42
1:B:389:ASN:OD1	1:B:391:VAL:HB	2.20	0.42
1:A:311:GLN:O	1:A:312:TYR:C	2.58	0.42
1:B:144:GLU:H	1:B:144:GLU:CD	2.23	0.42
1:B:350:ARG:HH11	1:B:350:ARG:HD2	1.50	0.42
1:A:214:ASP:OD2	1:A:257:LLP:N1	2.53	0.42
1:A:373:GLU:CG	1:A:427:LEU:HD21	2.45	0.42
1:A:97:HIS:NE2	1:A:98:GLN:HG2	2.35	0.42
1:B:106:LEU:HD11	1:B:212:PHE:CZ	2.54	0.41
1:A:259:CYS:SG	1:A:306:LEU:HD13	2.61	0.41
1:B:291:TYR:O	1:B:294:LEU:HB2	2.20	0.41
1:A:389:ASN:OD1	1:A:391:VAL:HG23	2.21	0.41
1:B:269:MET:HE1	1:B:278:ALA:CB	2.50	0.41
1:A:379:MET:HG2	1:A:380:GLU:O	2.21	0.41
1:A:198:ARG:HE	1:A:198:ARG:HB2	1.59	0.41
1:B:90:PHE:CE1	1:B:250:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PHE:N	1:A:362:PRO:CD	2.83	0.41
1:B:173:GLU:HG3	1:B:173:GLU:H	1.57	0.41
1:A:100:ARG:NH1	1:B:287:GLY:HA2	2.36	0.41
1:B:288:MET:HB3	1:B:289:PRO:HD2	2.02	0.41
1:A:182:VAL:O	1:A:182:VAL:HG23	2.21	0.41
1:A:180:LEU:HD23	1:A:181:ALA:N	2.36	0.40
1:B:99:GLY:HA3	1:B:254:SER:HB2	2.03	0.40
1:A:190:GLN:HA	1:A:191:PRO:HD3	1.90	0.40
1:A:374:THR:CG2	1:A:423:GLY:HA3	2.51	0.40
1:B:376:VAL:HG21	1:B:420:VAL:HG22	2.03	0.40
1:B:90:PHE:CB	1:B:268:CYS:HB3	2.51	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	452/456 (99%)	433 (96%)	19 (4%)	0	100	100
1	B	452/456 (99%)	437 (97%)	15 (3%)	0	100	100
All	All	904/912 (99%)	870 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	376/377 (100%)	347 (92%)	29 (8%)	13	25
1	B	376/377 (100%)	355 (94%)	21 (6%)	21	40
All	All	752/754 (100%)	702 (93%)	50 (7%)	16	32

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	9	ARG
1	A	15	THR
1	A	16	VAL
1	A	36	PHE
1	A	66	MET
1	A	82	ARG
1	A	93	ILE
1	A	126	THR
1	A	151	ASN
1	A	155	LYS
1	A	161	LYS
1	A	198	ARG
1	A	226	LYS
1	A	234	ASN
1	A	269	MET
1	A	318	ARG
1	A	330	LYS
1	A	350	ARG
1	A	351	ARG
1	A	356	LEU
1	A	369	SER
1	A	391	VAL
1	A	406	THR
1	A	426	LYS
1	A	429	GLN
1	A	447	ARG
1	A	450	THR
1	A	456	ILE
1	B	21	ARG
1	B	36	PHE
1	B	93	ILE
1	B	126	THR
1	B	132	LYS
1	B	151	ASN

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Mol	Chain	Res	Type
1	B	165	LYS
1	B	173	GLU
1	B	174	ASN
1	B	182	VAL
1	B	201	ARG
1	B	269	MET
1	B	280	GLU
1	B	294	LEU
1	B	318	ARG
1	B	351	ARG
1	B	354	GLU
1	B	388	ARG
1	B	406	THR
1	B	431	LYS
1	B	444	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	79	HIS
1	A	130	GLN
1	A	151	ASN
1	A	174	ASN
1	A	234	ASN
1	A	270	ASN
1	A	311	GLN
1	A	355	HIS
1	A	358	GLN
1	A	429	GLN
1	A	445	GLN
1	B	130	GLN
1	B	151	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	LLP	A	257	1	23,24,25	1.14	1 (4%)	25,32,34	2.01	7 (28%)
1	LLP	B	257	1	23,24,25	1.20	1 (4%)	25,32,34	2.13	9 (36%)

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	LLP	A	257	1	-	5/16/17/19	0/1/1/1
1	LLP	B	257	1	-	10/16/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	LLP	O3-C3	-3.03	1.29	1.37
1	A	257	LLP	O3-C3	-2.93	1.30	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	LLP	C3-C2-N1	-4.92	114.41	120.77
1	B	257	LLP	CE-NZ-C4'	4.29	132.08	118.90
1	B	257	LLP	C6-N1-C2	4.07	126.71	119.17
1	A	257	LLP	C6-N1-C2	3.98	126.54	119.17
1	B	257	LLP	C5-C6-N1	-3.59	117.84	123.82
1	B	257	LLP	OP4-C5'-C5	3.52	116.05	109.35
1	B	257	LLP	O3-C3-C2	3.41	124.93	117.49
1	A	257	LLP	C2'-C2-C3	3.26	124.91	120.89
1	A	257	LLP	C4-C3-C2	3.18	122.16	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	LLP	C3-C2-N1	-3.00	116.89	120.77
1	B	257	LLP	C2'-C2-C3	2.92	124.49	120.89
1	A	257	LLP	CE-NZ-C4'	2.88	127.76	118.90
1	A	257	LLP	C4-C4'-NZ	-2.72	111.82	124.31
1	B	257	LLP	C4-C4'-NZ	-2.36	113.46	124.31
1	B	257	LLP	C3-C4-C5	2.24	119.98	118.26
1	A	257	LLP	C5-C6-N1	-2.02	120.46	123.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	257	LLP	O-C-CA-CB
1	A	257	LLP	CG-CD-CE-NZ
1	B	257	LLP	C4-C5-C5'-OP4
1	B	257	LLP	C6-C5-C5'-OP4
1	B	257	LLP	C5'-OP4-P-OP2
1	B	257	LLP	C5'-OP4-P-OP3
1	B	257	LLP	O-C-CA-CB
1	A	257	LLP	CA-CB-CG-CD
1	B	257	LLP	C5'-OP4-P-OP1
1	A	257	LLP	CE-CD-CG-CB
1	A	257	LLP	C-CA-CB-CG
1	B	257	LLP	C3-C4-C4'-NZ
1	B	257	LLP	C-CA-CB-CG
1	B	257	LLP	CG-CD-CE-NZ
1	B	257	LLP	C5-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	257	LLP	3	0
1	B	257	LLP	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	HPP	B	600	-	9,12,12	0.34	0	12,15,15	0.58	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
3	HPP	B	600	-	-	0/3/5/5	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	600	HPP	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	454/456 (99%)	-0.36	20 (4%) 34 37	4, 22, 53, 88	0
1	B	454/456 (99%)	-0.51	5 (1%) 80 82	3, 22, 52, 86	0
All	All	908/912 (99%)	-0.43	25 (2%) 53 56	3, 22, 53, 88	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	VAL	8.1
1	A	390	ASN	6.8
1	B	390	ASN	5.6
1	A	392	THR	4.6
1	A	389	ASN	3.6
1	A	445	GLN	3.3
1	A	393	GLY	2.7
1	A	394	GLU	2.6
1	A	357	THR	2.5
1	A	2	ASN	2.5
1	A	230	GLN	2.4
1	B	112	LYS	2.3
1	A	359	ASP	2.3
1	A	444	LYS	2.3
1	B	230	GLN	2.3
1	A	273	GLU	2.3
1	A	398	PRO	2.2
1	A	173	GLU	2.2
1	B	394	GLU	2.2
1	A	386	ALA	2.1
1	A	396	HIS	2.1
1	A	22	ASP	2.1
1	A	456	ILE	2.1
1	A	354	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	391	VAL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	LLP	B	257	24/25	0.97	0.11	13,23,26,27	0
1	LLP	A	257	24/25	0.98	0.09	10,13,17,19	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	HPP	B	600	12/12	0.78	0.29	39,42,45,46	0
2	CS	A	500	1/1	0.97	0.41	2,2,2,2	0
2	CS	B	500	1/1	0.97	0.43	2,2,2,2	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.