



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:20 PM UTC

PDB ID : 2TPL / pdb_00002tpl
Title : TYROSINE PHENOL-LYASE FROM CITROBACTER INTERMEDIUS
COMPLEX WITH 3-(4'-HYDROXYPHENYL)PROPIONIC ACID, PY
RIDOXAL-5'-PHOSPHATE AND CS⁺ 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

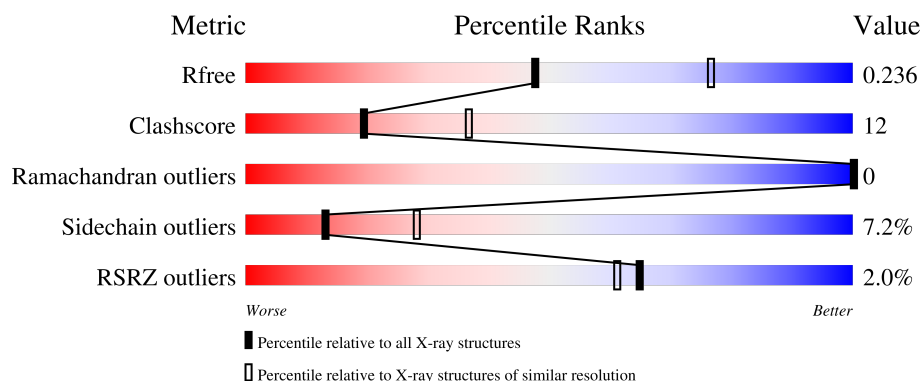
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	456	2% 62% 34% .
1	B	456	2% 65% 30% 5%

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			

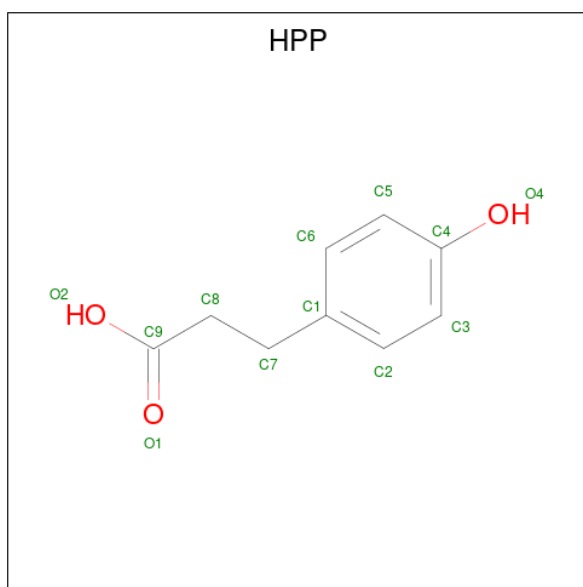
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: CS) (formula: Cs).

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

- Molecule 3 is HYDROXYPHENYL PROPIONIC ACID (CCD ID: HPP) (formula: C₉H₁₀O₃).



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

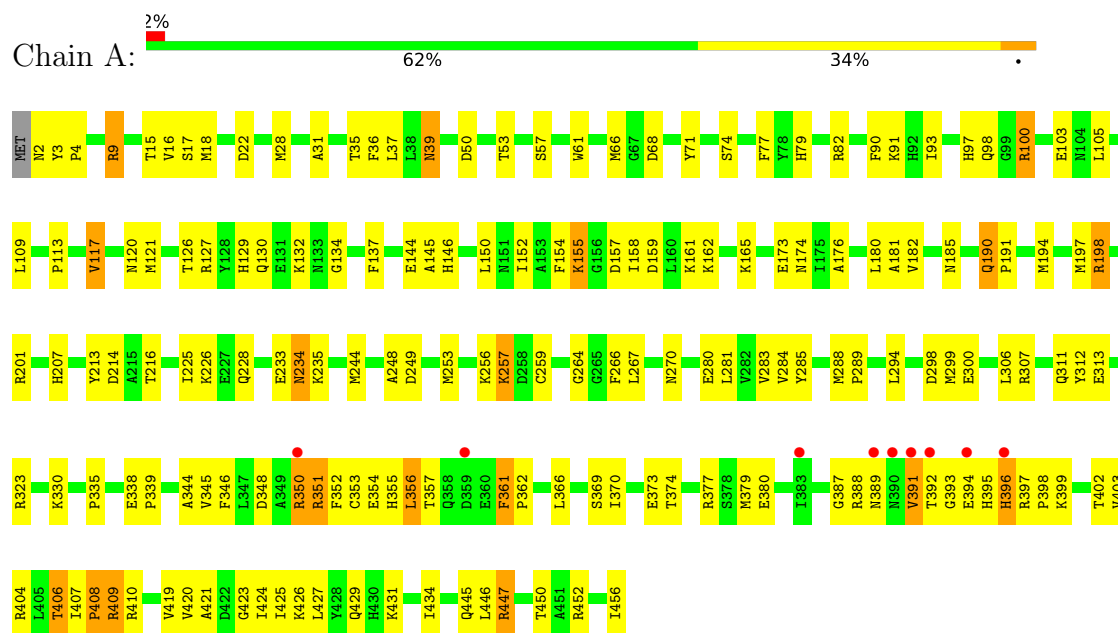
- Molecule 4 is water.

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

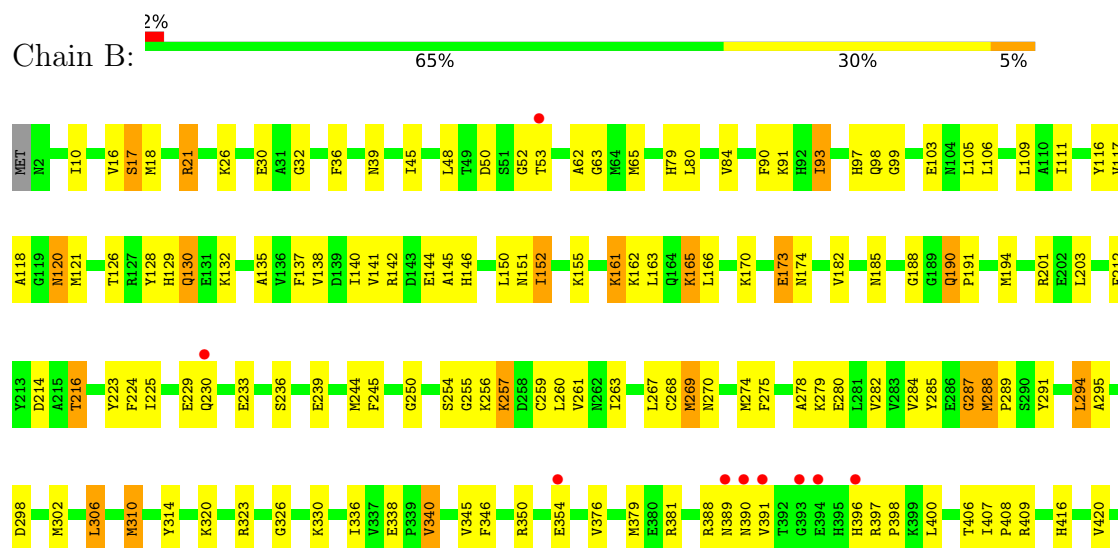
3 Residue-property plots

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

• Molecule 1: TYROSINE PHENOL-LYASE



• Molecule 1: TYROSINE PHENOL-LYASE



H430	K431	E432	K438	F439	E442	P443	K444	Q445	L446	R447	F448	F449	R452	L456
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.07Å 143.91Å 59.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	78.5 (15.00-2.50) 80.4 (15.00-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	22.7	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.3	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	0.92	EDS
Total number of atoms	7504	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, CS, HPP

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	0.50	0/3666	1.63	54/4937 (1.1%)
1	B	0.49	0/3666	1.48	31/4937 (0.6%)
All	All	0.50	0/7332	1.56	85/9874 (0.9%)

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 (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	CD-NE-CZ	9.28	137.38	124.40
1	A	100	ARG	CD-NE-CZ	8.85	136.78	124.40
1	B	439	PHE	CA-CB-CG	8.51	122.31	113.80
1	A	395	HIS	CA-CB-CG	8.49	122.29	113.80
1	A	397	ARG	CA-C-O	8.09	124.55	119.29
1	A	207	HIS	CA-CB-CG	-7.94	105.86	113.80
1	A	410	ARG	CD-NE-CZ	7.68	135.16	124.40
1	A	396	HIS	CA-CB-CG	7.67	121.47	113.80
1	A	68	ASP	CA-CB-CG	7.25	119.85	112.60
1	B	267	LEU	CA-C-O	-7.04	112.76	120.36
1	A	9	ARG	NE-CZ-NH2	6.83	125.35	119.20
1	A	129	HIS	CA-CB-CG	-6.75	107.05	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	PHE	CA-CB-CG	-6.69	107.11	113.80
1	A	117	VAL	N-CA-CB	6.66	120.30	111.64
1	A	57	SER	CA-C-O	6.59	129.51	121.94
1	B	430	HIS	CA-CB-CG	6.46	120.26	113.80
1	B	120	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	345	VAL	CA-C-O	-6.42	113.68	120.48
1	A	313	GLU	CA-C-O	-6.41	113.71	120.63
1	A	402	THR	CA-C-O	6.41	128.96	121.46
1	B	336	ILE	CA-C-O	-6.40	115.14	121.67
1	A	185	ASN	OD1-CG-ND2	6.34	128.94	122.60
1	B	230	GLN	CB-CG-CD	6.29	123.30	112.60
1	A	299	MET	N-CA-C	-6.29	104.50	111.36
1	A	267	LEU	CA-C-O	-6.23	113.88	120.80
1	A	9	ARG	CD-NE-CZ	-6.18	115.75	124.40
1	B	390	ASN	CA-C-N	6.17	128.25	120.72
1	B	390	ASN	C-N-CA	6.17	128.25	120.72
1	A	407	ILE	N-CA-C	6.16	114.19	107.60
1	A	361	PHE	CA-C-N	6.10	125.32	118.97
1	A	361	PHE	C-N-CA	6.10	125.32	118.97
1	A	397	ARG	CB-CA-C	6.04	117.03	110.08
1	B	442	GLU	CA-C-O	5.98	124.25	119.59
1	B	39	ASN	OD1-CG-ND2	5.93	128.53	122.60
1	A	298	ASP	CA-CB-CG	-5.78	106.82	112.60
1	A	154	PHE	CA-CB-CG	-5.75	108.05	113.80
1	B	52	GLY	O-C-N	-5.74	114.72	122.35
1	A	397	ARG	CA-C-N	5.62	126.06	119.99
1	A	397	ARG	C-N-CA	5.62	126.06	119.99
1	A	228	GLN	N-CA-C	5.57	121.49	114.31
1	B	185	ASN	CA-CB-CG	-5.51	107.09	112.60
1	A	22	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	346	PHE	CA-C-O	-5.47	114.31	120.32
1	A	3	TYR	CA-C-N	5.44	125.39	119.78
1	A	3	TYR	C-N-CA	5.44	125.39	119.78
1	B	245	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	408	PRO	N-CA-CB	5.43	108.14	103.31
1	A	409	ARG	CA-C-O	5.42	127.05	120.81
1	B	190	GLN	CA-C-N	5.41	125.88	120.14
1	B	190	GLN	C-N-CA	5.41	125.88	120.14
1	B	21	ARG	CD-NE-CZ	5.39	131.95	124.40
1	A	452	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	A	289	PRO	N-CA-CB	5.39	108.47	103.41
1	B	287	GLY	CA-C-O	-5.36	116.28	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	GLY	N-CA-C	-5.33	105.95	112.77
1	B	50	ASP	N-CA-C	-5.29	106.42	112.92
1	A	323	ARG	CD-NE-CZ	-5.27	117.03	124.40
1	A	235	LYS	CB-CA-C	5.26	119.03	109.83
1	B	10	ILE	CA-C-O	-5.25	114.87	120.85
1	A	77	PHE	N-CA-C	-5.23	105.66	111.36
1	B	407	ILE	N-CA-C	5.23	112.73	107.55
1	B	409	ARG	O-C-N	-5.22	117.27	123.22
1	A	323	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	B	216	THR	N-CA-CB	5.18	117.84	110.06
1	B	298	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	157	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	377	ARG	CA-C-O	-5.12	115.12	120.80
1	A	345	VAL	CA-C-N	-5.12	115.88	123.05
1	A	345	VAL	C-N-CA	-5.12	115.88	123.05
1	B	397	ARG	CA-C-O	5.12	122.62	119.29
1	B	295	ALA	CA-C-N	5.12	125.77	119.99
1	B	295	ALA	C-N-CA	5.12	125.77	119.99
1	B	216	THR	CA-CB-OG1	5.11	117.26	109.60
1	B	39	ASN	CA-CB-CG	-5.11	107.50	112.60
1	A	407	ILE	CA-C-N	5.10	125.01	119.76
1	A	407	ILE	C-N-CA	5.10	125.01	119.76
1	A	404	ARG	CA-C-O	5.07	125.95	120.43
1	A	4	PRO	N-CA-CB	5.05	107.74	103.35
1	A	120	ASN	CA-CB-CG	5.04	117.64	112.60
1	B	17	SER	CA-C-O	-5.04	115.08	120.42
1	B	407	ILE	N-CA-CB	-5.04	105.36	111.31
1	A	39	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	A	419	VAL	CA-C-O	-5.03	116.18	121.41
1	A	190	GLN	CA-C-N	5.02	125.23	120.31
1	A	190	GLN	C-N-CA	5.02	125.23	120.31

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
1	B	452	ARG	Mainchain

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Mol	Chain	Res	Type	Group
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	84	0
1	B	3619	0	3553	91	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	3	0
4	B	134	0	0	7	0
All	All	7504	0	7114	167	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 12.

All (167) 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
1:A:159:ASP:HB3	1:A:162:LYS:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:HG23	1:A:176:ALA:HB3	1.81	0.62
1:A:121:MET:HE2	1:A:146:HIS:CE1	2.34	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:310:MET:HA	1:B:310:MET:HE2	1.83	0.60
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:A:288:MET:HE3	1:B:449:PHE:CD1	2.37	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:O3	1:A:257:LLP:NZ	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:B:269:MET:HE3	1:B:274:MET:HE2	1.89	0.54
1:A:194:MET:HE2	1:A:225:ILE:HD13	1.90	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:B:432:GLU:H	1:B:432:GLU:CD	2.17	0.53
1:A:420:VAL:O	1:A:424:ILE:HG13	2.08	0.52
1:A:288:MET:HE1	1:B:448:PHE:HE2	1.75	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:288:MET:HE1	1:B:448:PHE:CE2	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:HG	4:B:718:HOH:O	2.09	0.51
1:A:194:MET:HE1	1:A:244:MET:HG3	1.93	0.50
1:B:36:PHE:CZ	1:B:379:MET:HE2	2.46	0.50
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
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:28:MET:HE1	1:A:35:THR:HA	1.95	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:201:ARG:HH12	1:A:249:ASP:CG	2.21	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: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:311:GLN:O	1:A:312:TYR:C	2.58	0.47
1:B:144:GLU:H	1:B:144:GLU:CD	2.23	0.47
1:A:234:ASN:H	1:A:234:ASN:HD22	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:HIS:CD2	1:B:98:GLN:HG2	2.51	0.46
1:B:163:LEU:HG	1:B:203:LEU:HD23	1.97	0.46
1:B:194:MET:HE1	1:B:244:MET:HG3	1.98	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:269:MET:HE1	1:B:278:ALA:HB2	1.99	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
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:197:MET:HE1	1:A:244:MET:HG2	1.99	0.44
1:A:152:ILE:HG13	1:A:155:LYS:HG3	2.00	0.44
1:A:180:LEU:C	1:A:180:LEU:HD23	2.43	0.43
1:A:355:HIS:HE1	1:A:434:ILE:O	2.01	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:121:MET:HE3	1:B:146:HIS:CE1	2.53	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:50:ASP:OD2	1:A:409:ARG:NH2	2.49	0.43
1:A:388:ARG:HD3	1:A:393:GLY:O	2.18	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:A:351:ARG:O	1:A:352:PHE:C	2.62	0.43
1:A:445:GLN:NE2	1:A:445:GLN:HA	2.33	0.43
1:B:79:HIS:HB2	4:B:675:HOH:O	2.19	0.42
1:B:201:ARG:HA	1:B:201:ARG:HE	1.83	0.42
1:A:61:TRP:CZ3	1:B:65:MET:HE1	2.54	0.42
1:A:256:LYS:NZ	4:A:539:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:97:HIS:NE2	1:A:98:GLN:HG2	2.35	0.42
1:A:373:GLU:CG	1:A:427:LEU:HD21	2.45	0.42
1:B:93:ILE:C	1:B:93:ILE:HD13	2.46	0.41
1:B:106:LEU:HD11	1:B:212:PHE:CZ	2.54	0.41
1:B:269:MET:HE3	1:B:274:MET:CE	2.51	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:A:379:MET:HG2	1:A:380:GLU:O	2.21	0.41
1:A:100:ARG:NH1	1:B:287:GLY:HA2	2.36	0.41
1:A:198:ARG:HE	1:A:198:ARG:HB2	1.59	0.41
1:A:361:PHE:N	1:A:362:PRO:CD	2.83	0.41
1:B:90:PHE:CE1	1:B:250:GLY:HA2	2.55	0.41
1:B:173:GLU:H	1:B:173:GLU:HG3	1.57	0.41
1:B:288:MET:HB3	1:B:289:PRO:HD2	2.02	0.41
1:A:182:VAL:HG23	1:A:182:VAL:O	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:280:GLU:CD	1:B:445:GLN:HG2	2.46	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	345 (92%)	31 (8%)	10	23
1	B	376/377 (100%)	353 (94%)	23 (6%)	17	35
All	All	752/754 (100%)	698 (93%)	54 (7%)	13	28

All (54) 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	132	LYS
1	A	155	LYS
1	A	158	ILE
1	A	161	LYS
1	A	198	ARG
1	A	226	LYS
1	A	233	GLU
1	A	234	ASN
1	A	283	VAL

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Mol	Chain	Res	Type
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	431	LYS
1	A	447	ARG
1	A	450	THR
1	A	456	ILE
1	B	21	ARG
1	B	93	ILE
1	B	126	THR
1	B	130	GLN
1	B	132	LYS
1	B	142	ARG
1	B	151	ASN
1	B	152	ILE
1	B	165	LYS
1	B	173	GLU
1	B	182	VAL
1	B	233	GLU
1	B	269	MET
1	B	280	GLU
1	B	294	LEU
1	B	310	MET
1	B	340	VAL
1	B	354	GLU
1	B	388	ARG
1	B	406	THR
1	B	438	LYS
1	B	444	LYS
1	B	446	LEU

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

Mol	Chain	Res	Type
1	A	2	ASN
1	A	79	HIS

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Mol	Chain	Res	Type
1	A	130	GLN
1	A	151	ASN
1	A	185	ASN
1	A	234	ASN
1	A	270	ASN
1	A	355	HIS
1	A	358	GLN
1	A	429	GLN
1	A	430	HIS
1	A	445	GLN
1	B	130	GLN
1	B	146	HIS
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	2.08	7 (28%)
1	LLP	B	257	1	23,24,25	1.19	1 (4%)	25,32,34	2.17	10 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	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	-3.04	1.29	1.36
1	A	257	LLP	O3-C3	-2.94	1.30	1.36

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	LLP	C3-C2-N1	-5.19	114.41	120.96
1	B	257	LLP	CE-NZ-C4'	4.17	132.08	118.72
1	B	257	LLP	C6-N1-C2	4.14	126.71	119.20
1	A	257	LLP	C6-N1-C2	4.05	126.54	119.20
1	B	257	LLP	C5-C6-N1	-3.68	117.84	123.83
1	A	257	LLP	C4-C3-C2	3.58	122.16	120.14
1	B	257	LLP	OP4-C5'-C5	3.57	116.05	109.36
1	B	257	LLP	O3-C3-C2	3.54	124.93	117.58
1	A	257	LLP	C2'-C2-C3	3.52	124.91	120.80
1	B	257	LLP	C3-C2-N1	-3.23	116.89	120.96
1	B	257	LLP	C2'-C2-C3	3.15	124.49	120.80
1	A	257	LLP	CE-NZ-C4'	2.82	127.76	118.72
1	A	257	LLP	C4-C4'-NZ	-2.65	111.82	124.04
1	B	257	LLP	C4-C4'-NZ	-2.29	113.46	124.04
1	B	257	LLP	C3-C4-C5	2.12	119.98	118.28
1	A	257	LLP	C5-C6-N1	-2.07	120.46	123.83
1	B	257	LLP	OP2-P-OP4	2.06	112.03	106.67

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

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Mol	Chain	Res	Type	Atoms
1	B	257	LLP	C5'-OP4-P-OP1
1	A	257	LLP	C-CA-CB-CG
1	B	257	LLP	C-CA-CB-CG
1	B	257	LLP	C3-C4-C4'-NZ
1	A	257	LLP	CE-CD-CG-CB
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 [i](#)

There are no oligosaccharides 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	-	12,12,12	0.71	0	15,15,15	0.93	1 (6%)

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	-	-	2/5/5/5	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	HPP	O2-C9-C8	2.06	120.51	114.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	600	HPP	C7-C8-C9-O2
3	B	600	HPP	C7-C8-C9-O1

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	454/456 (99%)	-0.16	9 (1%) 65 61	4, 22, 53, 88	0
1	B	454/456 (99%)	-0.28	9 (1%) 65 61	3, 22, 52, 86	0
All	All	908/912 (99%)	-0.22	18 (1%) 65 61	3, 22, 53, 88	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	VAL	5.9
1	B	390	ASN	4.3
1	A	389	ASN	4.0
1	A	392	THR	3.4
1	A	390	ASN	3.2
1	B	391	VAL	3.2
1	A	396	HIS	3.0
1	B	53	THR	2.9
1	B	354	GLU	2.9
1	A	394	GLU	2.8
1	B	394	GLU	2.5
1	A	383	ILE	2.4
1	A	359	ASP	2.3
1	B	230	GLN	2.3
1	B	393	GLY	2.3
1	B	396	HIS	2.2
1	B	389	ASN	2.1
1	A	350	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	A	257	24/25	0.97	0.06	10,13,17,19	0
1	LLP	B	257	24/25	0.97	0.07	13,23,26,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	HPP	B	600	12/12	0.76	0.17	39,42,45,46	0
2	CS	B	500	1/1	0.86	0.51	2,2,2,2	0
2	CS	A	500	1/1	0.93	0.49	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.