



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2025 – 10:13 AM JST

PDB ID : 9LFT / pdb\_00009lft  
Title : Biochemical and structural characterization of a novel 4-hydroxyphenylacetate 3-monooxygenase from *Geobacillus mahadii* Geo-05  
Authors : Che Husain, N.A.; Jamaluddin, H.; Jonet, M.A.; Padzil, A.M.; Taib, A.Z.M.; Zain, N.C.; Bakar, M.F.A.; Acharya, K.R.; Gregory, K.S.  
Deposited on : 2025-01-09  
Resolution : 2.40 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.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

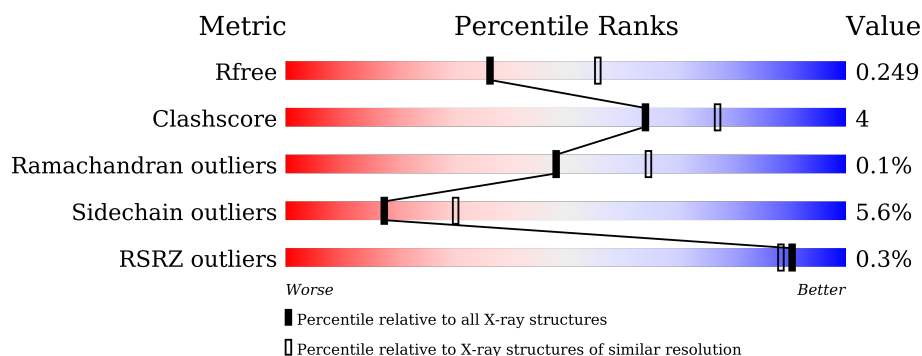
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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  $\geq 3$ , 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	518	
1	B	518	
1	C	518	
1	D	518	

## 2 Entry composition [i](#)

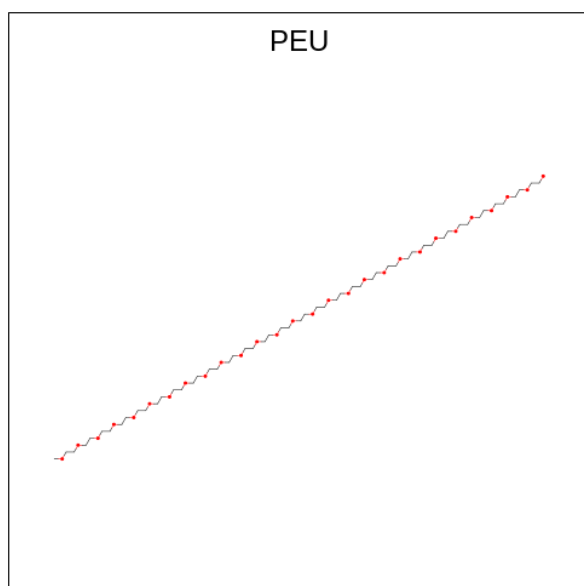
There are 3 unique types of molecules in this entry. The entry contains 15614 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-Hydroxyphenylacetate-3-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3844	2437	669	713	25			
1	B	485	Total	C	N	O	S	0	0	0
			3868	2454	672	717	25			
1	C	480	Total	C	N	O	S	0	0	0
			3839	2434	668	712	25			
1	D	484	Total	C	N	O	S	0	0	0
			3866	2451	673	717	25			

- Molecule 2 is 2,5,8,11,14,17,20,23,26,29,32,35,38,41,44,47,50,53,56,59,62,65,68,71,74,77,80-HEPTACOSAOXADOCTACONTAN-82-OL (CCD ID: PEU) (formula:  $C_{55}H_{112}O_{28}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			76	49	27		

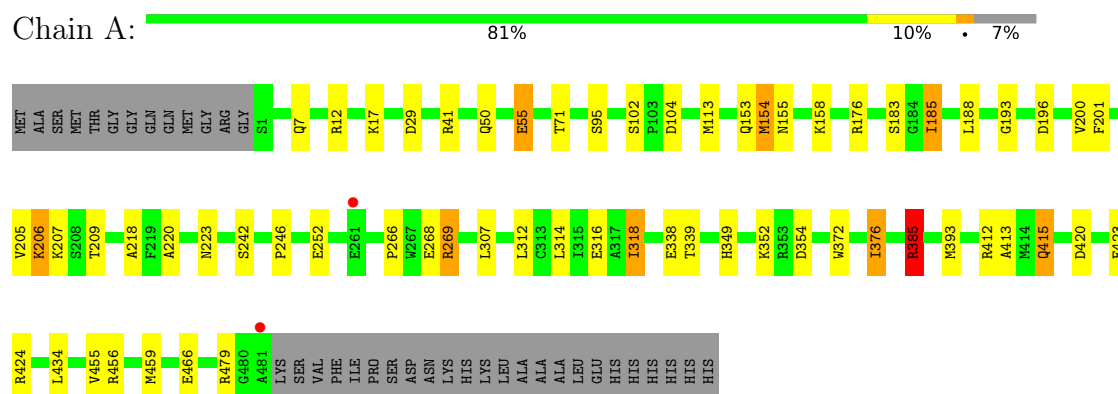
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total 36	O 36	0	0
3	B	22	Total 22	O 22	0	0
3	C	37	Total 37	O 37	0	0
3	D	26	Total 26	O 26	0	0

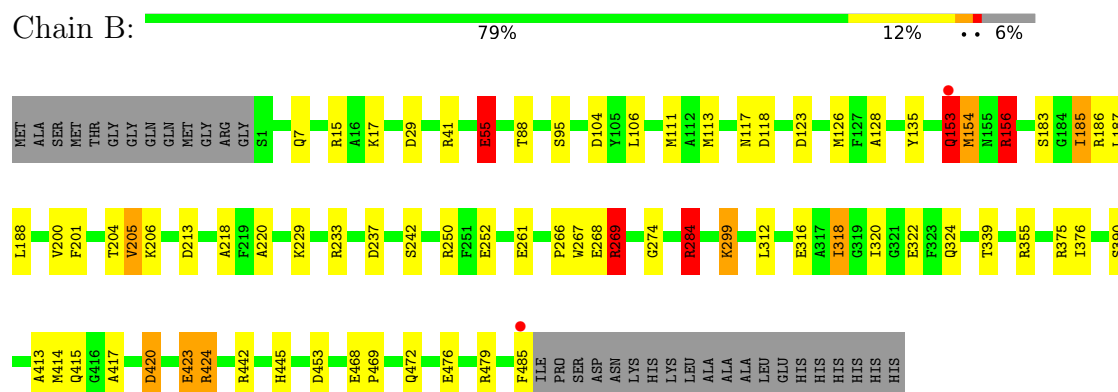
### 3 Residue-property plots

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.

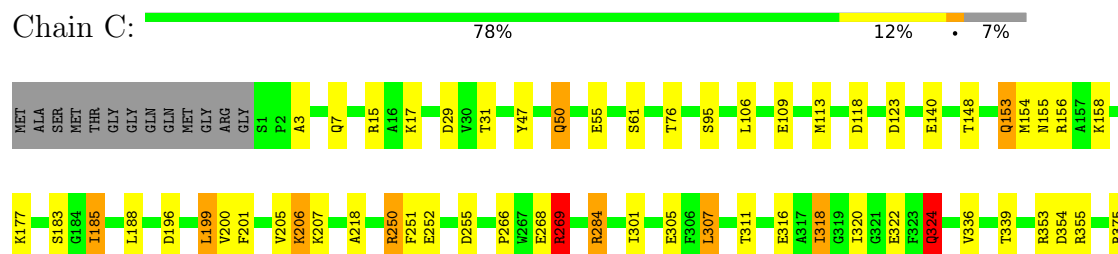
#### • Molecule 1: 4-Hydroxyphenylacetate-3-monooxygenase

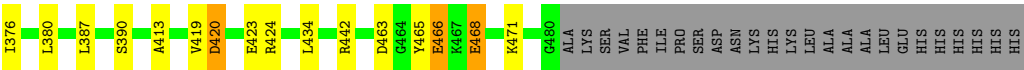


#### • Molecule 1: 4-Hydroxyphenylacetate-3-monooxygenase



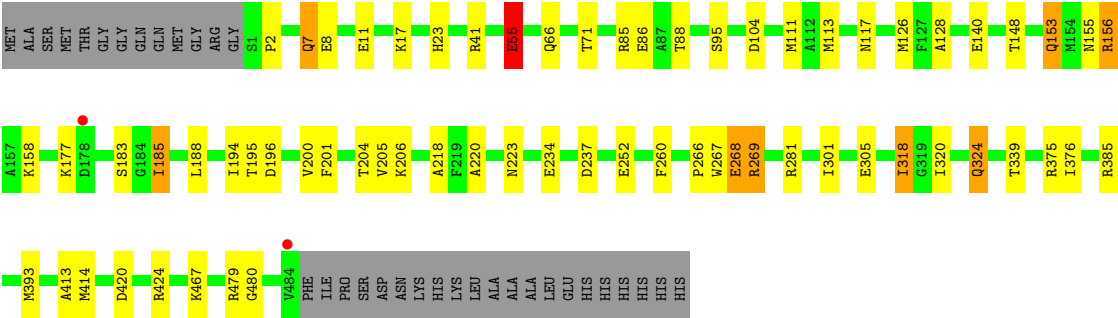
#### • Molecule 1: 4-Hydroxyphenylacetate-3-monooxygenase





● Molecule 1: 4-Hydroxyphenylacetate-3-monooxygenase

Chain D: 81% 11% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.57Å 108.20Å 99.06Å 90.00° 99.46° 90.00°	Depositor
Resolution (Å)	97.90 – 2.40 97.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (97.90-2.40) 99.9 (97.71-2.40)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.184 , 0.250 0.189 , 0.249	Depositor DCC
$R_{free}$ test set	3637 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: PEU

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	0.60	0/3935	1.16	14/5324 (0.3%)
1	B	0.60	0/3960	1.20	20/5360 (0.4%)
1	C	0.62	0/3930	1.17	14/5317 (0.3%)
1	D	0.59	0/3957	1.14	13/5353 (0.2%)
All	All	0.60	0/15782	1.17	61/21354 (0.3%)

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	8
1	B	0	8
1	C	0	5
1	D	0	4
All	All	0	25

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	GLN	CB-CA-C	8.56	123.79	109.84
1	C	420	ASP	CA-CB-CG	7.87	120.47	112.60
1	A	50	GLN	N-CA-CB	7.32	120.89	110.12
1	D	148	THR	CA-CB-OG1	-7.19	98.81	109.60
1	C	322	GLU	CB-CG-CD	7.06	124.60	112.60
1	B	17	LYS	CB-CA-C	-6.96	102.54	111.86
1	C	148	THR	CA-CB-OG1	-6.86	99.32	109.60
1	B	206	LYS	CB-CA-C	6.84	120.52	110.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	17	LYS	CB-CA-C	-6.77	102.79	111.86
1	A	17	LYS	CB-CA-C	-6.54	103.10	111.86
1	B	55	GLU	CB-CG-CD	6.44	123.55	112.60
1	C	50	GLN	N-CA-CB	-6.33	100.46	110.22
1	A	420	ASP	CA-CB-CG	6.27	118.87	112.60
1	D	177	LYS	CB-CA-C	-6.24	101.09	110.88
1	A	154	MET	N-CA-C	-6.22	104.76	112.72
1	C	354	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	322	GLU	CB-CG-CD	6.10	122.97	112.60
1	A	354	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	7	GLN	CB-CA-C	6.07	122.32	110.67
1	D	55	GLU	CB-CG-CD	5.99	122.78	112.60
1	A	415	GLN	N-CA-CB	-5.99	99.68	109.56
1	A	206	LYS	CB-CA-C	5.96	119.72	110.67
1	B	453	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	420	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	55	GLU	CB-CG-CD	5.89	122.62	112.60
1	A	385	ARG	N-CA-CB	-5.88	101.49	110.01
1	D	11	GLU	CB-CG-CD	5.87	122.58	112.60
1	D	268	GLU	N-CA-CB	5.86	120.12	110.39
1	C	196	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	385	ARG	CB-CA-C	5.78	119.96	110.88
1	C	153	GLN	N-CA-CB	5.76	118.51	109.69
1	D	420	ASP	CA-CB-CG	5.76	118.36	112.60
1	D	324	GLN	N-CA-CB	5.68	119.08	110.28
1	B	154	MET	N-CA-C	-5.66	104.38	112.13
1	B	237	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	196	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	50	GLN	CB-CA-C	-5.59	101.51	110.79
1	A	196	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	104	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	206	LYS	CB-CA-C	5.50	118.50	110.26
1	C	466	GLU	CB-CG-CD	5.48	121.91	112.60
1	D	177	LYS	N-CA-CB	5.48	117.95	110.01
1	C	269	ARG	CB-CA-C	-5.44	101.52	110.72
1	D	234	GLU	N-CA-CB	5.43	118.02	109.83
1	D	237	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	29	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	316	GLU	CB-CA-C	-5.37	102.22	110.81
1	B	485	PHE	CA-CB-CG	5.33	119.13	113.80
1	B	123	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	205	VAL	N-CA-CB	5.31	117.25	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	29	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	415	GLN	CB-CA-C	-5.21	100.41	109.64
1	B	205	VAL	CB-CA-C	-5.10	106.60	111.44
1	B	324	GLN	N-CA-CB	5.09	117.70	110.16
1	C	463	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	284	ARG	N-CA-CB	5.07	117.64	110.13
1	C	324	GLN	N-CA-CB	5.02	117.59	110.16
1	B	269	ARG	CB-CA-C	-5.02	102.08	110.56
1	C	468	GLU	CB-CG-CD	5.00	121.10	112.60
1	D	260	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	ARG	Sidechain
1	A	176	ARG	Sidechain
1	A	269	ARG	Sidechain
1	A	385	ARG	Sidechain
1	A	41	ARG	Sidechain
1	A	424	ARG	Sidechain
1	A	456	ARG	Sidechain
1	A	479	ARG	Sidechain
1	B	156	ARG	Sidechain
1	B	186	ARG	Peptide
1	B	233	ARG	Sidechain
1	B	250	ARG	Sidechain
1	B	269	ARG	Sidechain
1	B	284	ARG	Sidechain
1	B	41	ARG	Sidechain
1	B	424	ARG	Sidechain
1	C	15	ARG	Sidechain
1	C	250	ARG	Sidechain
1	C	269	ARG	Sidechain
1	C	284	ARG	Sidechain
1	C	424	ARG	Sidechain
1	D	269	ARG	Sidechain
1	D	281	ARG	Sidechain
1	D	385	ARG	Sidechain
1	D	41	ARG	Sidechain

## 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	3844	0	3752	31	0
1	B	3868	0	3763	37	0
1	C	3839	0	3747	34	0
1	D	3866	0	3779	34	0
2	B	76	0	95	10	0
3	A	36	0	0	4	0
3	B	22	0	0	0	0
3	C	37	0	0	0	0
3	D	26	0	0	1	0
All	All	15614	0	15136	115	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 4.

All (115) 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:414:MET:O	1:B:424:ARG:HD2	1.72	0.90
1:B:126:MET:HE1	1:B:267:TRP:HB3	1.65	0.77
1:B:375:ARG:HD3	2:B:601:PEU:HAI2	1.68	0.76
1:B:420:ASP:OD1	1:B:423:GLU:HG2	1.85	0.76
1:C:76:THR:O	1:C:353:ARG:NH1	2.20	0.74
1:D:23:HIS:HD2	3:D:626:HOH:O	1.70	0.72
1:B:476:GLU:HG2	1:B:479:ARG:HH12	1.54	0.71
1:A:307:LEU:HD22	1:A:434:LEU:HD21	1.73	0.70
1:C:156:ARG:HD2	1:D:318:ILE:HG23	1.76	0.67
1:D:126:MET:HE1	1:D:267:TRP:HB3	1.78	0.65
1:C:318:ILE:HG22	1:C:320:ILE:HG23	1.79	0.65
1:C:413:ALA:HB2	1:D:185:ILE:HD13	1.80	0.64
1:B:318:ILE:HG22	1:B:320:ILE:HG23	1.81	0.62
1:A:349:HIS:HE1	3:A:634:HOH:O	1.82	0.62
1:B:420:ASP:OD1	1:B:423:GLU:CG	2.48	0.61
1:A:193:GLY:HA2	1:A:223:ASN:HD22	1.66	0.61
1:B:318:ILE:CG2	1:B:320:ILE:HG23	2.31	0.61
1:A:185:ILE:HD13	1:B:413:ALA:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ILE:HG12	2:B:601:PEU:HBF2	1.85	0.58
1:B:266:PRO:HG2	1:B:269:ARG:HG2	1.85	0.58
1:C:199:LEU:HD23	1:C:201:PHE:CE1	2.38	0.58
1:A:412:ARG:HD2	3:A:602:HOH:O	2.04	0.57
1:D:266:PRO:HG2	1:D:269:ARG:HG2	1.87	0.57
1:D:318:ILE:HG22	1:D:320:ILE:HG12	1.87	0.56
1:B:118:ASP:OD2	1:B:355:ARG:NH2	2.40	0.55
1:C:318:ILE:CG2	1:C:320:ILE:HG23	2.36	0.55
1:C:307:LEU:HD22	1:C:434:LEU:HD21	1.88	0.55
1:C:109:GLU:O	1:C:113:MET:HG2	2.07	0.54
1:C:419:VAL:HB	1:C:423:GLU:HG3	1.89	0.54
1:A:314:LEU:O	1:A:318:ILE:HG13	2.07	0.54
1:A:200:VAL:O	1:A:218:ALA:HA	2.08	0.54
1:B:113:MET:SD	1:B:201:PHE:HE2	2.31	0.53
1:C:199:LEU:HD23	1:C:201:PHE:CD1	2.44	0.52
1:B:55:GLU:H	1:B:55:GLU:CD	2.17	0.52
1:A:372:TRP:CD1	2:B:601:PEU:HBL1	2.45	0.52
1:A:349:HIS:HD2	3:A:635:HOH:O	1.92	0.52
1:B:375:ARG:HH11	2:B:601:PEU:HAI2	1.75	0.51
1:B:229:LYS:HE3	1:B:261:GLU:OE1	2.11	0.51
1:B:113:MET:SD	1:B:201:PHE:CE2	3.04	0.51
1:B:339:THR:HG23	1:D:339:THR:HG23	1.93	0.50
1:C:200:VAL:O	1:C:218:ALA:HA	2.11	0.50
1:A:71:THR:HG21	1:A:104:ASP:HB3	1.93	0.50
1:A:113:MET:SD	1:A:201:PHE:CE2	3.05	0.50
1:A:412:ARG:CD	3:A:602:HOH:O	2.60	0.50
1:A:113:MET:HE1	1:A:201:PHE:CE2	2.47	0.50
1:C:318:ILE:HG23	1:D:156:ARG:HD2	1.93	0.50
1:A:459:MET:SD	1:C:324:GLN:HB2	2.52	0.50
1:A:312:LEU:HB3	1:C:471:LYS:HD3	1.93	0.49
1:B:220:ALA:O	1:B:269:ARG:HB3	2.12	0.49
1:C:255:ASP:OD2	1:C:442:ARG:NH1	2.45	0.49
1:C:266:PRO:HG2	1:C:269:ARG:HG2	1.93	0.49
1:A:413:ALA:HB2	1:B:185:ILE:HD13	1.96	0.48
1:B:318:ILE:HG22	1:B:320:ILE:HG12	1.94	0.48
1:C:47:TYR:O	1:C:50:GLN:HB3	2.13	0.48
1:C:442:ARG:HG3	1:D:393:MET:SD	2.54	0.48
1:A:415:GLN:HG2	1:B:154:MET:HE3	1.95	0.47
1:D:55:GLU:H	1:D:55:GLU:CD	2.21	0.47
1:A:155:ASN:ND2	1:A:158:LYS:HE2	2.31	0.46
1:D:200:VAL:O	1:D:218:ALA:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:MET:SD	1:D:201:PHE:CE2	3.08	0.46
1:C:61:SER:OG	1:C:140:GLU:OE1	2.31	0.46
1:D:414:MET:CE	1:D:424:ARG:NH1	2.78	0.46
1:A:339:THR:HG23	1:C:339:THR:HG23	1.98	0.46
1:C:413:ALA:CB	1:D:185:ILE:HD13	2.45	0.46
1:D:71:THR:HG21	1:D:104:ASP:HB3	1.96	0.46
1:C:336:VAL:HG21	1:C:380:LEU:HD21	1.98	0.45
1:D:318:ILE:HG22	1:D:320:ILE:HG23	1.96	0.45
1:A:155:ASN:HA	1:B:417:ALA:HB2	1.99	0.45
1:B:111:MET:HA	1:B:135:TYR:CD1	2.52	0.45
1:D:318:ILE:CG2	1:D:320:ILE:HG23	2.47	0.45
2:B:601:PEU:HBA1	1:D:375:ARG:HH11	1.81	0.45
1:C:419:VAL:HB	1:C:423:GLU:CG	2.47	0.45
1:A:385:ARG:HD3	1:B:445:HIS:ND1	2.32	0.44
1:C:29:ASP:OD1	1:C:31:THR:OG1	2.32	0.44
1:C:113:MET:CE	1:C:201:PHE:CE2	3.00	0.44
1:A:385:ARG:CD	1:B:445:HIS:ND1	2.80	0.44
1:B:375:ARG:NH1	2:B:601:PEU:HAG1	2.32	0.44
2:B:601:PEU:HAX1	1:D:375:ARG:HD3	2.00	0.44
1:C:466:GLU:O	1:C:466:GLU:HG2	2.17	0.44
1:B:468:GLU:HB2	1:B:469:PRO:HD3	1.99	0.44
1:C:95:SER:HA	1:C:251:PHE:CZ	2.52	0.44
1:A:266:PRO:HG2	1:A:269:ARG:HG2	2.00	0.43
1:B:126:MET:CE	1:B:267:TRP:HB3	2.42	0.43
2:B:601:PEU:HBA1	1:D:375:ARG:NH1	2.34	0.43
1:B:153:GLN:HB2	1:B:156:ARG:NE	2.33	0.43
1:C:301:ILE:O	1:C:305:GLU:HG3	2.19	0.43
1:A:455:VAL:HG22	2:B:601:PEU:HBW2	1.99	0.43
1:D:220:ALA:O	1:D:269:ARG:HB3	2.18	0.43
1:D:117:ASN:OD1	1:D:128:ALA:HB1	2.19	0.43
1:B:200:VAL:O	1:B:218:ALA:HA	2.19	0.43
1:C:118:ASP:OD2	1:C:355:ARG:NH2	2.51	0.43
1:D:7:GLN:HG3	1:D:8:GLU:N	2.33	0.43
1:D:85:ARG:HD2	1:D:85:ARG:C	2.44	0.42
2:B:601:PEU:HCL2	1:C:375:ARG:HH11	1.84	0.42
1:C:155:ASN:ND2	1:C:158:LYS:HE2	2.35	0.42
1:D:301:ILE:O	1:D:305:GLU:HG3	2.19	0.42
1:B:117:ASN:OD1	1:B:128:ALA:HB1	2.19	0.42
1:D:111:MET:C	1:D:111:MET:SD	3.02	0.42
1:A:185:ILE:CD1	1:B:413:ALA:HB2	2.50	0.42
1:B:299:LYS:HE3	1:B:299:LYS:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ILE:HD13	1:D:413:ALA:HB2	2.02	0.41
1:D:155:ASN:ND2	1:D:158:LYS:HE2	2.35	0.41
1:D:113:MET:SD	1:D:201:PHE:HE2	2.43	0.41
1:C:311:THR:HG23	1:C:387:LEU:HD12	2.02	0.41
1:D:195:THR:O	1:D:223:ASN:ND2	2.54	0.41
1:D:479:ARG:O	1:D:480:GLY:C	2.63	0.41
1:A:220:ALA:O	1:A:269:ARG:HB3	2.20	0.41
1:A:338:GLU:OE1	1:C:465:TYR:OH	2.32	0.41
1:B:312:LEU:HD22	1:D:467:LYS:HD2	2.03	0.41
1:A:185:ILE:HD13	1:B:413:ALA:CB	2.50	0.40
1:D:153:GLN:HB2	1:D:156:ARG:HE	1.87	0.40
1:A:242:SER:O	1:A:246:PRO:HA	2.22	0.40
1:D:2:PRO:HB2	1:D:140:GLU:O	2.21	0.40
1:A:393:MET:SD	1:B:442:ARG:HG3	2.60	0.40
1:B:213:ASP:O	1:B:274:GLY:HA2	2.21	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	479/518 (92%)	467 (98%)	12 (2%)	0	100	100
1	B	483/518 (93%)	475 (98%)	8 (2%)	0	100	100
1	C	478/518 (92%)	464 (97%)	13 (3%)	1 (0%)	44	59
1	D	482/518 (93%)	473 (98%)	9 (2%)	0	100	100
All	All	1922/2072 (93%)	1879 (98%)	42 (2%)	1 (0%)	48	65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	ALA

### 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	403/432 (93%)	383 (95%)	20 (5%)	20	36
1	B	404/432 (94%)	380 (94%)	24 (6%)	16	28
1	C	403/432 (93%)	377 (94%)	26 (6%)	14	24
1	D	406/432 (94%)	386 (95%)	20 (5%)	21	36
All	All	1616/1728 (94%)	1526 (94%)	90 (6%)	17	30

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	95	SER
1	A	102	SER
1	A	153	GLN
1	A	154	MET
1	A	183	SER
1	A	185	ILE
1	A	188	LEU
1	A	205	VAL
1	A	206	LYS
1	A	207	LYS
1	A	209	THR
1	A	252	GLU
1	A	268	GLU
1	A	316	GLU
1	A	318	ILE
1	A	352	LYS
1	A	376	ILE
1	A	423	GLU
1	A	466	GLU
1	B	7	GLN

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Mol	Chain	Res	Type
1	B	15	ARG
1	B	55	GLU
1	B	88	THR
1	B	95	SER
1	B	106	LEU
1	B	153	GLN
1	B	156	ARG
1	B	183	SER
1	B	185	ILE
1	B	187	LEU
1	B	188	LEU
1	B	204	THR
1	B	205	VAL
1	B	242	SER
1	B	252	GLU
1	B	268	GLU
1	B	284	ARG
1	B	299	LYS
1	B	318	ILE
1	B	376	ILE
1	B	390	SER
1	B	423	GLU
1	B	472	GLN
1	C	7	GLN
1	C	17	LYS
1	C	55	GLU
1	C	106	LEU
1	C	153	GLN
1	C	154	MET
1	C	177	LYS
1	C	183	SER
1	C	185	ILE
1	C	188	LEU
1	C	199	LEU
1	C	205	VAL
1	C	206	LYS
1	C	207	LYS
1	C	250	ARG
1	C	252	GLU
1	C	268	GLU
1	C	284	ARG
1	C	307	LEU

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Mol	Chain	Res	Type
1	C	316	GLU
1	C	318	ILE
1	C	324	GLN
1	C	376	ILE
1	C	390	SER
1	C	420	ASP
1	C	468	GLU
1	D	7	GLN
1	D	55	GLU
1	D	66	GLN
1	D	86	GLU
1	D	88	THR
1	D	95	SER
1	D	153	GLN
1	D	156	ARG
1	D	183	SER
1	D	185	ILE
1	D	188	LEU
1	D	194	ILE
1	D	204	THR
1	D	205	VAL
1	D	206	LYS
1	D	252	GLU
1	D	268	GLU
1	D	318	ILE
1	D	324	GLN
1	D	376	ILE

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

Mol	Chain	Res	Type
1	A	23	HIS
1	A	153	GLN
1	A	161	HIS
1	A	223	ASN
1	A	349	HIS
1	A	415	GLN
1	B	7	GLN
1	B	153	GLN
1	B	324	GLN
1	C	23	HIS
1	C	66	GLN

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Mol	Chain	Res	Type
1	C	349	HIS
1	C	415	GLN
1	D	23	HIS
1	D	74	GLN
1	D	223	ASN
1	D	262	ASN
1	D	415	GLN
1	D	472	GLN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

1 ligand is 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	PEU	B	601	-	71,71,82	0.58	0	70,70,81	0.42	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
2	PEU	B	601	-	-	39/69/69/80	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	PEU	OAT-CAU-CAV-OAW
2	B	601	PEU	OBS-CBT-CBU-OBV
2	B	601	PEU	OBZ-CBZ-CCA-OCB
2	B	601	PEU	OBJ-CBK-CBL-OBM
2	B	601	PEU	OCE-CCF-CCG-OBC
2	B	601	PEU	OCP-CCQ-CCR-OCS
2	B	601	PEU	OCJ-CCK-CCL-OCM
2	B	601	PEU	OCB-CCC-CCD-OCE
2	B	601	PEU	OCM-CCN-CCO-OCP
2	B	601	PEU	OAQ-CAR-CAS-OAT
2	B	601	PEU	OAZ-CBA-CBB-OBC
2	B	601	PEU	OAE-CAF-CAG-OAH
2	B	601	PEU	CBX-CBW-OBV-CBU
2	B	601	PEU	CCI-CCH-OB-DBE
2	B	601	PEU	CCH-CCI-OCJ-CCK
2	B	601	PEU	CCO-CCN-OCM-CCL
2	B	601	PEU	CBI-CBH-OBG-CBF
2	B	601	PEU	CCR-CCQ-OCP-CCO
2	B	601	PEU	CAM-CAL-OAK-CAJ
2	B	601	PEU	CAI-CAJ-OAK-CAL
2	B	601	PEU	CAC-CAD-OAE-CAF
2	B	601	PEU	CBZ-CCA-OCB-CCC
2	B	601	PEU	CCQ-CCR-OCS-CCT
2	B	601	PEU	OBM-CBN-CBO-OBP
2	B	601	PEU	CAJ-CAI-OAH-CAG
2	B	601	PEU	CBQ-CBR-OBS-CBT
2	B	601	PEU	OBP-CBQ-CBR-OBS
2	B	601	PEU	CBB-CBA-OAZ-CAY
2	B	601	PEU	OBV-CBW-CBX-OBZ
2	B	601	PEU	OAH-CAI-CAJ-OAK
2	B	601	PEU	CCK-CCL-OCM-CCN
2	B	601	PEU	CAV-CAU-OAT-CAS
2	B	601	PEU	CBT-CBU-OBV-CBW
2	B	601	PEU	CAR-CAS-OAT-CAU

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Mol	Chain	Res	Type	Atoms
2	B	601	PEU	CCG-CCF-OCE-CCD
2	B	601	PEU	OAB-CAC-CAD-OAE
2	B	601	PEU	CBK-CBL-OBM-CBN
2	B	601	PEU	OBD-CCH-CCI-OCJ
2	B	601	PEU	OAK-CAL-CAM-OAN

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	PEU	10	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 PEU B 601	
	
<b>Bond lengths</b>	<b>Bond angles</b>
	
<b>Torsions</b>	<b>Rings</b>

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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	481/518 (92%)	-0.40	2 (0%) 89 87	21, 36, 60, 75	0
1	B	485/518 (93%)	-0.41	2 (0%) 89 87	23, 35, 52, 87	0
1	C	480/518 (92%)	-0.47	0 100 100	22, 32, 53, 69	0
1	D	484/518 (93%)	-0.34	2 (0%) 89 87	22, 38, 61, 82	0
All	All	1930/2072 (93%)	-0.41	6 (0%) 90 88	21, 35, 57, 87	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	485	PHE	4.0
1	D	484	VAL	3.3
1	A	481	ALA	3.3
1	D	178	ASP	2.5
1	A	261	GLU	2.4
1	B	153	GLN	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 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, 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( $\text{\AA}^2$ )	Q<0.9
2	PEU	B	601	76/83	0.87	0.12	38,44,52,999	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.