



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:03 PM UTC

PDB ID : 2EZ2 / pdb_00002ez2
Title : Apo tyrosine phenol-lyase from *Citrobacter freundii* at pH 8.0
Authors : Milic, D.; Matkovic-Calogovic, D.; Demidkina, T.V.; Antson, A.A.
Deposited on : 2005-11-10
Resolution : 1.85 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

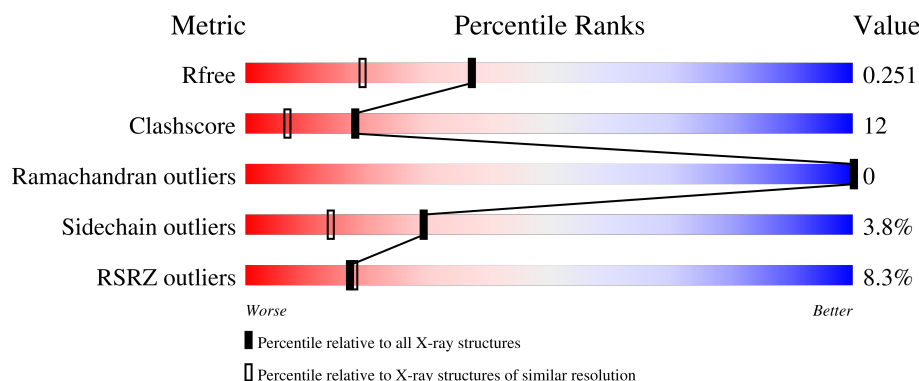
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	15% 76% 21% .
1	B	456	2% 90% 8% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8266 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	456	Total	C	N	O	S	0	1	0
			3614	2287	625	676	26			
1	B	456	Total	C	N	O	S	0	1	0
			3619	2290	628	675	26			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

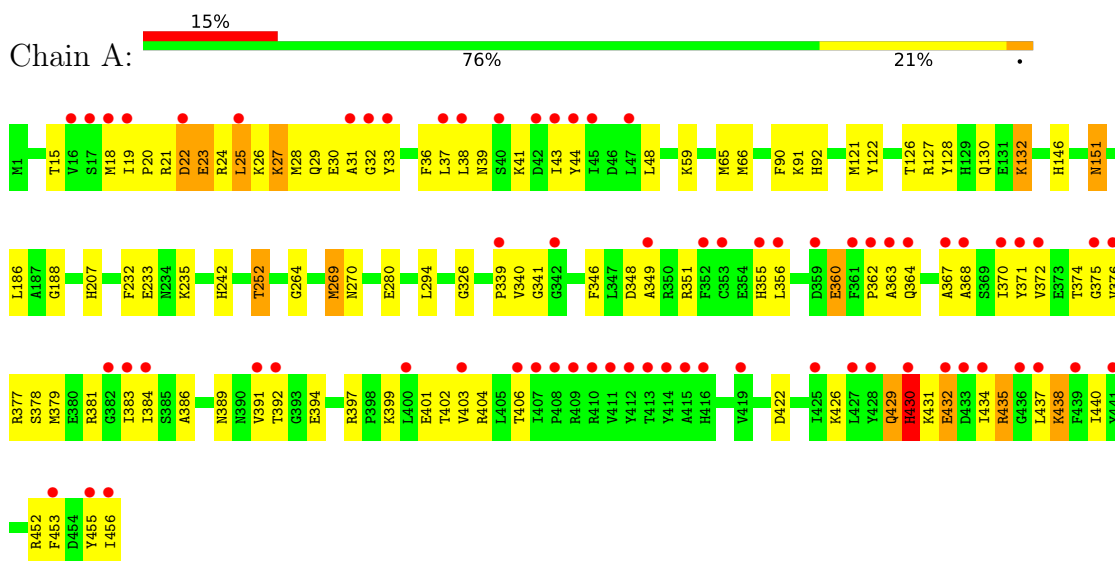
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	512	Total	O	0	0
			512	512		
4	B	509	Total	O	0	0
			509	509		

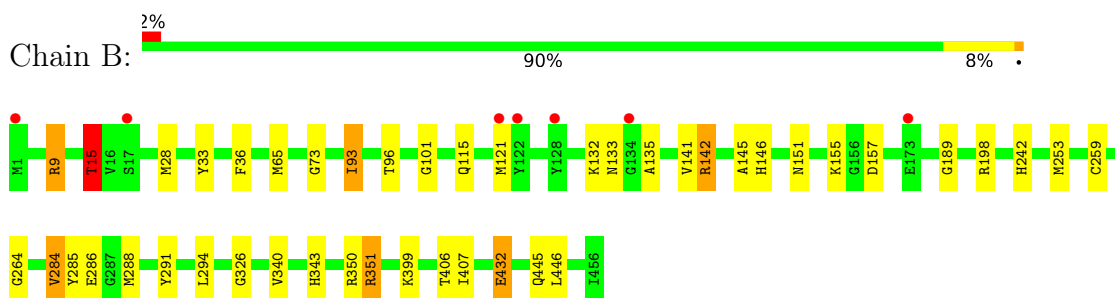
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.64Å 143.74Å 59.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.74 – 1.85 16.74 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (16.74-1.85) 92.7 (16.74-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.174 , 0.206 (Not available) , 0.251	Depositor DCC
R_{free} test set	939 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8266	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: K, PO4

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	0.89	1/3690 (0.0%)	0.98	4/4969 (0.1%)
1	B	0.82	1/3695 (0.0%)	0.87	1/4975 (0.0%)
All	All	0.85	2/7385 (0.0%)	0.92	5/9944 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	THR	N-CA	6.11	1.53	1.46
1	B	15	THR	CA-CB	5.10	1.61	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	HIS	N-CA-C	8.71	121.47	109.54
1	A	15	THR	N-CA-C	5.74	118.16	110.35
1	B	407	ILE	N-CA-C	5.25	112.75	107.55
1	A	23	GLU	CA-C-N	5.20	127.50	120.38
1	A	23	GLU	C-N-CA	5.20	127.50	120.38

There are no chirality outliers.

There are no planarity outliers.

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	3614	0	3559	147	0
1	B	3619	0	3567	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	512	0	0	70	1
4	B	509	0	0	11	1
All	All	8266	0	7126	176	1

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 (176) 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:A:375:GLY:HA2	4:A:2042:HOH:O	1.23	1.36
1:A:363:ALA:HB1	4:A:2098:HOH:O	1.58	1.04
1:A:349:ALA:HB2	4:A:2081:HOH:O	1.55	1.04
1:A:252:THR:HG23	4:A:1679:HOH:O	1.60	1.01
1:A:27:LYS:HA	1:A:30:GLU:OE1	1.61	0.99
1:A:364:GLN:HG3	4:A:2070:HOH:O	1.62	0.98
1:A:24:ARG:HD2	4:A:2042:HOH:O	1.63	0.98
1:A:92:HIS:HB2	1:A:269:MET:HE3	1.50	0.91
1:A:363:ALA:CB	4:A:2098:HOH:O	2.14	0.89
1:A:434:ILE:HG21	4:A:2060:HOH:O	1.77	0.84
1:A:24:ARG:NH2	4:A:2107:HOH:O	1.71	0.84
1:B:15:THR:HB	4:B:6098:HOH:O	1.78	0.83
1:A:422:ASP:OD1	4:A:2089:HOH:O	1.96	0.82
1:A:38:LEU:HG	4:A:2068:HOH:O	1.80	0.81
1:A:25:LEU:HD23	4:A:1921:HOH:O	1.81	0.80
1:A:44:TYR:CD2	4:A:2097:HOH:O	2.35	0.79
1:A:374:THR:HB	4:A:1733:HOH:O	1.83	0.78
1:A:367:ALA:HB2	4:A:2029:HOH:O	1.84	0.77
1:A:384:ILE:HD13	1:A:453:PHE:CZ	2.21	0.75
1:A:92:HIS:CB	1:A:269:MET:HE3	2.17	0.74
1:A:372:VAL:HG22	4:A:2080:HOH:O	1.88	0.73
1:B:142:ARG:HG2	1:B:157:ASP:O	1.89	0.73
1:B:189:GLY:HA3	4:B:6093:HOH:O	1.87	0.73
1:A:351:ARG:O	4:A:2092:HOH:O	2.08	0.72
1:A:92:HIS:HB2	1:A:269:MET:CE	2.20	0.72
1:B:351:ARG:HD2	4:B:5941:HOH:O	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLY:HA3	1:A:452:ARG:CD	2.20	0.71
1:A:435:ARG:HG2	4:A:1848:HOH:O	1.91	0.70
1:A:429:GLN:HG3	4:A:1846:HOH:O	1.89	0.70
1:A:402:THR:O	4:A:2098:HOH:O	2.10	0.70
1:A:32:GLY:HA3	1:A:452:ARG:HD3	1.74	0.69
1:A:18:MET:O	4:A:2096:HOH:O	2.11	0.69
1:A:356:LEU:HD22	1:A:360:GLU:HG2	1.73	0.69
1:A:37:LEU:HD13	1:A:452:ARG:HE	1.58	0.68
1:A:367:ALA:CB	4:A:2029:HOH:O	2.40	0.67
1:A:426:LYS:HG3	4:A:1758:HOH:O	1.95	0.67
1:A:188:GLY:O	1:A:341:GLY:HA3	1.95	0.67
1:A:39:ASN:HB2	4:A:2077:HOH:O	1.95	0.66
1:A:364:GLN:NE2	1:A:437:LEU:HD13	2.10	0.66
1:A:59:LYS:HE3	4:A:1971:HOH:O	1.94	0.66
1:A:392:THR:HG23	1:A:394:GLU:H	1.59	0.65
1:A:33:TYR:O	4:A:2099:HOH:O	2.13	0.65
1:A:440:ILE:HG22	4:A:2100:HOH:O	1.95	0.65
1:A:452:ARG:HD2	4:A:2105:HOH:O	1.96	0.65
1:A:39:ASN:HA	1:B:73:GLY:HA3	1.79	0.65
1:A:364:GLN:NE2	1:A:453:PHE:CD1	2.65	0.65
1:A:20:PRO:O	1:A:24:ARG:HG3	1.97	0.64
1:A:28:MET:SD	4:A:2068:HOH:O	2.54	0.64
1:B:101:GLY:HA3	1:B:286:GLU:OE1	1.98	0.64
1:B:350:ARG:NH1	1:B:399:LYS:O	2.21	0.63
1:A:32:GLY:HA3	1:A:452:ARG:CG	2.27	0.63
1:A:41:LYS:O	4:A:2087:HOH:O	2.15	0.63
1:A:364:GLN:HB2	1:A:384:ILE:HD12	1.80	0.63
1:A:48:LEU:HB2	1:A:377:ARG:HG2	1.80	0.62
1:A:355:HIS:CD2	4:A:1711:HOH:O	2.52	0.62
1:B:9[A]:ARG:NH2	4:B:6102:HOH:O	2.13	0.62
1:A:379:MET:C	4:A:1726:HOH:O	2.43	0.62
1:A:378:SER:CB	4:A:2104:HOH:O	2.48	0.62
1:A:37:LEU:HD13	1:A:452:ARG:NE	2.15	0.62
1:A:403:VAL:HG13	4:A:1726:HOH:O	2.00	0.62
1:A:151:ASN:HD22	1:A:151:ASN:C	2.08	0.61
1:A:65:MET:HE1	1:B:65:MET:HE1	1.83	0.61
1:A:27:LYS:HE3	4:A:1820:HOH:O	2.00	0.60
1:A:378:SER:OG	4:A:2104:HOH:O	2.15	0.60
1:A:33:TYR:OH	4:A:2048:HOH:O	2.17	0.59
1:A:426:LYS:O	1:A:429:GLN:HB2	2.03	0.59
1:A:422:ASP:HB3	4:A:1861:HOH:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LYS:CA	1:A:30:GLU:OE1	2.45	0.58
1:B:284:VAL:HG22	1:B:285:TYR:CD1	2.38	0.58
1:A:242:HIS:HD2	4:A:1712:HOH:O	1.87	0.58
1:A:21:ARG:HD2	4:A:2038:HOH:O	2.04	0.58
1:A:18:MET:HE2	1:A:24:ARG:HH12	1.69	0.58
1:A:25:LEU:HB2	4:A:2082:HOH:O	2.04	0.57
1:A:430:HIS:CE1	1:A:432:GLU:HG2	2.39	0.57
1:B:253:MET:HE3	1:B:259:CYS:SG	2.45	0.57
1:A:280:GLU:CG	1:B:445:GLN:HG3	2.34	0.57
1:A:43:ILE:HD13	1:A:377:ARG:CZ	2.35	0.57
1:A:151:ASN:ND2	1:A:339:PRO:HG3	2.20	0.56
1:A:32:GLY:HA3	1:A:452:ARG:HG2	1.87	0.56
1:A:39:ASN:CB	4:A:2077:HOH:O	2.52	0.55
1:A:378:SER:HB3	4:A:2104:HOH:O	2.05	0.55
1:A:18:MET:HB3	4:A:2096:HOH:O	2.06	0.55
1:A:26:LYS:O	1:A:29:GLN:HG2	2.08	0.54
1:A:207:HIS:HD2	4:A:1923:HOH:O	1.90	0.54
1:A:368:ALA:HB2	4:A:2099:HOH:O	2.08	0.53
1:A:32:GLY:CA	1:A:452:ARG:HD3	2.38	0.53
1:A:44:TYR:HD2	4:A:2097:HOH:O	1.82	0.53
1:A:44:TYR:CE2	4:A:2097:HOH:O	2.60	0.53
1:A:364:GLN:CD	1:A:437:LEU:HD13	2.32	0.53
1:A:18:MET:HE2	1:A:24:ARG:NH1	2.24	0.52
1:A:374:THR:O	4:A:2078:HOH:O	2.19	0.52
1:A:438:LYS:HG3	1:A:456:ILE:HG12	1.92	0.51
1:A:128:TYR:O	1:A:132:LYS:HB3	2.10	0.51
1:A:429:GLN:HE21	1:A:429:GLN:CA	2.24	0.51
1:A:389:ASN:CG	1:A:392:THR:HG22	2.36	0.50
1:A:399:LYS:HA	4:A:1841:HOH:O	2.11	0.50
1:B:121:MET:HE2	1:B:146:HIS:CE1	2.46	0.50
1:A:127:ARG:HA	1:A:130:GLN:NE2	2.27	0.50
1:A:121:MET:HE2	1:A:146:HIS:CE1	2.47	0.50
1:B:242:HIS:HE1	4:B:5740:HOH:O	1.94	0.50
1:B:284:VAL:HG22	1:B:285:TYR:CE1	2.47	0.50
1:A:90:PHE:HA	1:A:270:ASN:HD21	1.76	0.50
1:A:186:LEU:CD2	1:A:381:ARG:HD3	2.42	0.50
1:A:348:ASP:OD2	1:A:351:ARG:HD3	2.12	0.49
1:A:36:PHE:CZ	1:A:379:MET:HE2	2.47	0.49
1:A:435:ARG:HG3	1:A:455:TYR:CE1	2.47	0.49
1:A:378:SER:HB2	1:A:404:ARG:O	2.13	0.49
1:A:19:ILE:O	1:A:24:ARG:NH1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HA	4:A:2080:HOH:O	2.12	0.49
1:B:242:HIS:HD2	4:B:5677:HOH:O	1.94	0.49
1:A:24:ARG:CD	4:A:2042:HOH:O	2.40	0.49
1:A:383:ILE:HD12	4:A:2095:HOH:O	2.11	0.49
1:A:403:VAL:HG23	4:A:2081:HOH:O	2.13	0.48
1:A:31:ALA:C	1:A:452:ARG:HD3	2.38	0.48
1:A:384:ILE:HD13	1:A:453:PHE:HZ	1.78	0.48
1:A:389:ASN:HB3	1:A:392:THR:HG22	1.95	0.48
1:A:91:LYS:H	1:A:270:ASN:HD22	1.61	0.47
1:B:28:MET:HE2	1:B:33:TYR:HA	1.96	0.47
1:A:19:ILE:HD12	1:A:23:GLU:HB3	1.96	0.47
1:A:362:PRO:HD2	1:A:401:GLU:OE1	2.14	0.47
1:A:376:VAL:HG23	4:A:1733:HOH:O	2.14	0.47
1:A:430:HIS:CE1	1:A:432:GLU:CG	2.98	0.47
1:A:402:THR:C	4:A:2081:HOH:O	2.58	0.47
1:B:132:LYS:NZ	1:B:133:ASN:HD21	2.12	0.47
1:B:432:GLU:H	1:B:432:GLU:CD	2.21	0.47
1:B:432:GLU:HG2	4:B:6108:HOH:O	2.15	0.47
1:A:355:HIS:CD2	4:A:1682:HOH:O	2.68	0.47
1:A:375:GLY:C	4:A:1722:HOH:O	2.58	0.46
1:A:371:TYR:CD2	4:A:2080:HOH:O	2.56	0.46
1:A:31:ALA:HB1	1:A:37:LEU:HB2	1.98	0.46
1:A:232:PHE:HA	1:A:235:LYS:HD2	1.98	0.46
1:A:326:GLY:HA3	1:A:340:VAL:HG21	1.97	0.46
1:A:19:ILE:HG13	1:A:24:ARG:HG2	1.97	0.45
1:A:188:GLY:HA2	1:A:346:PHE:CE1	2.51	0.45
1:A:431:LYS:O	1:A:434:ILE:HD12	2.16	0.45
1:B:264:GLY:HA2	1:B:294:LEU:HD21	1.97	0.45
1:A:18:MET:HG3	4:A:2078:HOH:O	2.17	0.45
1:A:43:ILE:CD1	1:A:377:ARG:CZ	2.95	0.45
1:A:20:PRO:HA	4:A:1728:HOH:O	2.17	0.45
1:A:429:GLN:HB3	4:A:1879:HOH:O	2.16	0.45
1:A:38:LEU:CG	4:A:2068:HOH:O	2.51	0.45
1:A:383:ILE:CD1	4:A:2095:HOH:O	2.65	0.44
1:A:264:GLY:HA2	1:A:294:LEU:HD21	2.00	0.44
1:A:360:GLU:HG3	1:A:456:ILE:HD12	2.00	0.44
1:A:370:ILE:O	1:A:374:THR:OG1	2.30	0.44
1:A:28:MET:HE1	1:A:38:LEU:HD11	2.00	0.43
1:A:429:GLN:HE21	1:A:429:GLN:N	2.15	0.43
1:A:438:LYS:CG	1:A:456:ILE:HG12	2.48	0.43
1:A:22:ASP:HB3	4:A:1778:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ARG:HG3	1:A:455:TYR:CD1	2.52	0.43
1:B:96:THR:HB	1:B:286:GLU:OE1	2.17	0.43
1:A:364:GLN:CB	1:A:384:ILE:HD12	2.48	0.43
1:A:32:GLY:N	1:A:452:ARG:HD3	2.34	0.43
1:B:115:GLN:O	1:B:135:ALA:HA	2.18	0.43
1:A:18:MET:HE2	4:A:2107:HOH:O	2.19	0.43
1:B:445:GLN:HB3	4:B:5922:HOH:O	2.19	0.42
1:A:397:ARG:NH2	4:A:2095:HOH:O	2.51	0.42
1:B:28:MET:HE3	1:B:28:MET:HA	2.01	0.42
1:B:145:ALA:HA	1:B:155:LYS:HG2	2.02	0.42
1:A:280:GLU:HG2	1:B:445:GLN:HG3	2.02	0.42
1:B:198:ARG:NH2	4:B:5994:HOH:O	2.53	0.41
1:A:403:VAL:N	4:A:2081:HOH:O	2.53	0.41
1:A:430:HIS:ND1	1:A:432:GLU:HG2	2.35	0.41
1:A:122:TYR:OH	1:A:386:ALA:HA	2.20	0.41
1:A:28:MET:HE3	1:A:368:ALA:HA	2.03	0.41
1:A:355:HIS:CE1	1:A:356:LEU:HG	2.55	0.41
1:B:93:ILE:HB	4:B:6106:HOH:O	2.21	0.41
1:A:28:MET:HE2	1:A:371:TYR:CD2	2.55	0.41
1:A:355:HIS:ND1	1:A:355:HIS:C	2.78	0.41
1:A:402:THR:HA	4:A:2081:HOH:O	2.21	0.41
1:B:121:MET:HG3	1:B:141:VAL:HG11	2.03	0.41
1:B:343:HIS:CE1	4:B:6093:HOH:O	2.73	0.41
1:B:288:MET:HB2	1:B:291:TYR:CD1	2.57	0.40
1:B:326:GLY:HA3	1:B:340:VAL:HG21	2.03	0.40
1:A:437:LEU:HD22	1:A:453:PHE:HB2	2.03	0.40
1:A:438:LYS:NZ	4:A:2044:HOH:O	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1750:HOH:O	4:B:6098:HOH:O[2_565]	2.02	0.18

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	455/456 (100%)	445 (98%)	10 (2%)	0	100	100
1	B	455/456 (100%)	446 (98%)	9 (2%)	0	100	100
All	All	910/912 (100%)	891 (98%)	19 (2%)	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	379/379 (100%)	361 (95%)	18 (5%)	23	9
1	B	379/379 (100%)	367 (97%)	12 (3%)	34	19
All	All	758/758 (100%)	728 (96%)	30 (4%)	29	13

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	25	LEU
1	A	27	LYS
1	A	66	MET
1	A	126	THR
1	A	132	LYS
1	A	151	ASN
1	A	233	GLU
1	A	252	THR
1	A	269	MET
1	A	360	GLU
1	A	391	VAL
1	A	406	THR
1	A	429	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	430	HIS
1	A	432	GLU
1	A	435	ARG
1	A	438	LYS
1	B	9[A]	ARG
1	B	9[B]	ARG
1	B	15	THR
1	B	36	PHE
1	B	93	ILE
1	B	142	ARG
1	B	151	ASN
1	B	284	VAL
1	B	351	ARG
1	B	406	THR
1	B	432	GLU
1	B	446	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) 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	185	ASN
1	A	207	HIS
1	A	228	GLN
1	A	242	HIS
1	A	270	ASN
1	A	311	GLN
1	A	321	GLN
1	A	355	HIS
1	A	364	GLN
1	A	396	HIS
1	A	429	GLN
1	A	430	HIS
1	B	130	GLN
1	B	133	ASN
1	B	151	ASN
1	B	190	GLN
1	B	242	HIS
1	B	321	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	PO4	A	1600	-	4,4,4	0.98	0	6,6,6	0.64	0
3	PO4	B	5600	-	4,4,4	0.84	0	6,6,6	1.25	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5600	PO4	O3-P-O2	2.75	116.48	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	456/456 (100%)	0.82	69 (15%) 5 5	11, 23, 37, 42	1 (0%)
1	B	456/456 (100%)	0.06	7 (1%) 72 76	10, 21, 36, 50	1 (0%)
All	All	912/912 (100%)	0.44	76 (8%) 17 18	10, 22, 36, 50	2 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	ALA	6.0
1	A	31	ALA	5.7
1	A	364	GLN	5.3
1	A	434	ILE	5.2
1	A	19	ILE	5.0
1	A	433	ASP	4.4
1	A	383	ILE	4.2
1	A	371	TYR	4.1
1	A	411	VAL	4.0
1	A	437	LEU	4.0
1	A	352	PHE	3.9
1	A	410	ARG	3.9
1	A	372	VAL	3.9
1	A	33	TYR	3.7
1	A	44	TYR	3.6
1	A	391	VAL	3.6
1	A	22	ASP	3.5
1	A	408	PRO	3.5
1	A	356	LEU	3.4
1	A	436	GLY	3.4
1	A	428	TYR	3.3
1	A	375	GLY	3.3
1	A	453	PHE	3.3
1	A	17[A]	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	407	ILE	3.3
1	A	368	ALA	3.2
1	A	38	LEU	3.2
1	A	430	HIS	3.2
1	A	456	ILE	3.2
1	A	355	HIS	3.1
1	A	414	TYR	3.1
1	A	409	ARG	3.1
1	A	392	THR	3.0
1	A	353	CYS	3.0
1	A	25	LEU	3.0
1	A	400	LEU	2.9
1	A	384	ILE	2.9
1	A	16	VAL	2.9
1	A	361	PHE	2.8
1	A	403	VAL	2.8
1	A	362	PRO	2.8
1	A	413	THR	2.7
1	A	427	LEU	2.7
1	B	173	GLU	2.7
1	A	43	ILE	2.7
1	A	419	VAL	2.7
1	B	121	MET	2.7
1	A	370	ILE	2.6
1	A	47	LEU	2.6
1	A	425	ILE	2.5
1	A	32	GLY	2.4
1	B	122	TYR	2.4
1	A	18	MET	2.4
1	A	339	PRO	2.4
1	A	455	TYR	2.4
1	A	406	THR	2.4
1	A	415	ALA	2.4
1	A	367	ALA	2.4
1	A	441	TYR	2.3
1	A	382	GLY	2.3
1	B	134	GLY	2.3
1	A	359	ASP	2.3
1	A	40	SER	2.3
1	B	17	SER	2.3
1	A	416	HIS	2.3
1	B	1	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	37	LEU	2.2
1	A	342	GLY	2.2
1	A	349	ALA	2.2
1	A	376	VAL	2.1
1	A	432	GLU	2.1
1	A	439	PHE	2.1
1	A	412	TYR	2.1
1	B	128	TYR	2.1
1	A	45	ILE	2.1
1	A	42	ASP	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, 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	PO4	B	5600	5/5	0.98	0.11	19,22,23,25	0
3	PO4	A	1600	5/5	0.99	0.10	21,22,27,27	0
2	K	B	5500	1/1	0.99	0.10	17,17,17,17	0
2	K	A	1500	1/1	1.00	0.11	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.