



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:51 PM UTC

PDB ID : 6GG4 / pdb_00006gg4
Title : Crystal structure of M2 PYK in complex with Phenylalanine.
Authors : McNae, I.W.; Yuan, M.; Walkinshaw, M.D.
Deposited on : 2018-05-02
Resolution : 2.46 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

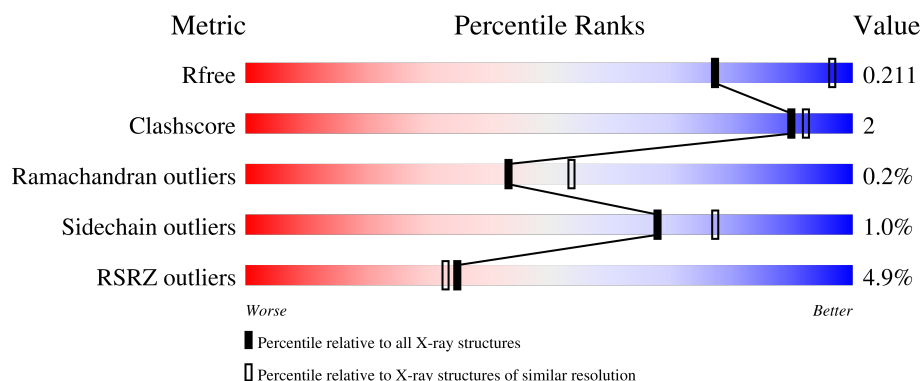
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	551	4% 89% • 8%
1	B	551	5% 89% • 8%
1	C	551	4% 71% • • 26%
1	D	551	3% 71% • 26%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14593 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 Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	2	0
			3912	2460	696	732	24			
1	B	509	Total	C	N	O	S	0	1	0
			3904	2455	693	732	24			
1	C	410	Total	C	N	O	S	0	2	0
			3169	1990	571	587	21			
1	D	410	Total	C	N	O	S	0	1	0
			3163	1986	571	585	21			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P14618
A	-18	GLY	-	expression tag	UNP P14618
A	-17	SER	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	HIS	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	SER	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	GLY	-	expression tag	UNP P14618
A	-6	LEU	-	expression tag	UNP P14618
A	-5	VAL	-	expression tag	UNP P14618
A	-4	PRO	-	expression tag	UNP P14618
A	-3	ARG	-	expression tag	UNP P14618
A	-2	GLY	-	expression tag	UNP P14618
A	-1	SER	-	expression tag	UNP P14618
A	0	HIS	-	expression tag	UNP P14618
B	-19	MET	-	initiating methionine	UNP P14618

Continued on next page...

Continued from previous page...

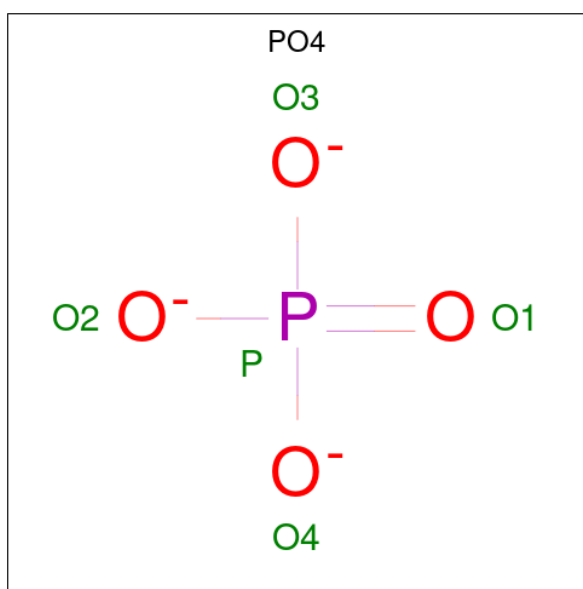
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	SER	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	GLY	-	expression tag	UNP P14618
B	-6	LEU	-	expression tag	UNP P14618
B	-5	VAL	-	expression tag	UNP P14618
B	-4	PRO	-	expression tag	UNP P14618
B	-3	ARG	-	expression tag	UNP P14618
B	-2	GLY	-	expression tag	UNP P14618
B	-1	SER	-	expression tag	UNP P14618
B	0	HIS	-	expression tag	UNP P14618
C	-19	MET	-	initiating methionine	UNP P14618
C	-18	GLY	-	expression tag	UNP P14618
C	-17	SER	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	HIS	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	SER	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	GLY	-	expression tag	UNP P14618
C	-6	LEU	-	expression tag	UNP P14618
C	-5	VAL	-	expression tag	UNP P14618
C	-4	PRO	-	expression tag	UNP P14618
C	-3	ARG	-	expression tag	UNP P14618
C	-2	GLY	-	expression tag	UNP P14618
C	-1	SER	-	expression tag	UNP P14618
C	0	HIS	-	expression tag	UNP P14618
D	-19	MET	-	initiating methionine	UNP P14618
D	-18	GLY	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P14618
D	-15	HIS	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	SER	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	GLY	-	expression tag	UNP P14618
D	-6	LEU	-	expression tag	UNP P14618
D	-5	VAL	-	expression tag	UNP P14618
D	-4	PRO	-	expression tag	UNP P14618
D	-3	ARG	-	expression tag	UNP P14618
D	-2	GLY	-	expression tag	UNP P14618
D	-1	SER	-	expression tag	UNP P14618
D	0	HIS	-	expression tag	UNP P14618

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



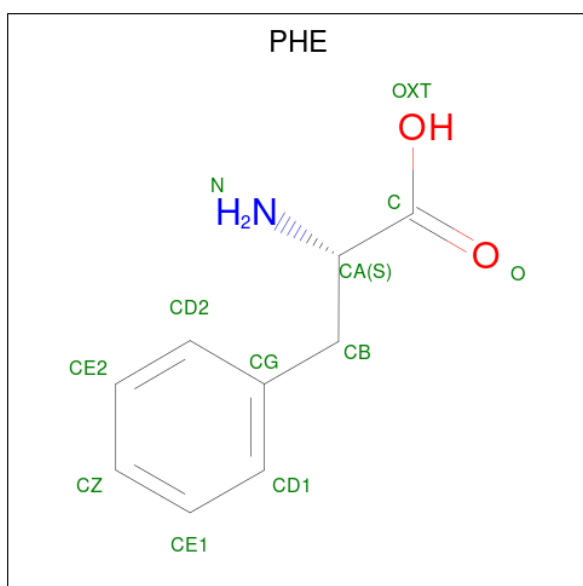
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



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

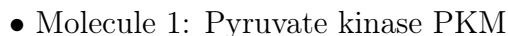
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

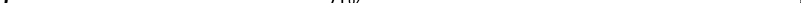
- Molecule 5 is water.

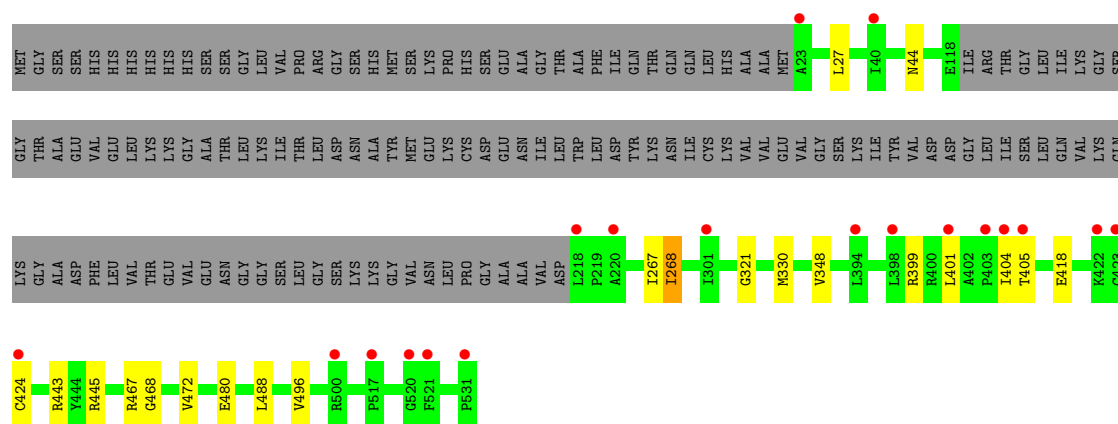
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	106	Total O 106 106	0	0
5	B	92	Total O 92 92	0	0
5	C	99	Total O 99 99	0	0
5	D	56	Total O 56 56	0	0

- Molecule 1: Pyruvate kinase PKM



- Molecule 1: Pyruvate kinase PKM

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.37Å 70.34Å 168.64Å 90.00° 106.06° 90.00°	Depositor
Resolution (Å)	162.06 – 2.46 162.06 – 2.46	Depositor EDS
% Data completeness (in resolution range)	98.6 (162.06-2.46) 98.6 (162.06-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.197 , 0.225 (Not available) , 0.211	Depositor DCC
R_{free} test set	3904 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14593	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, PO4, CSO

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	0.63	0/3973	0.82	0/5363
1	B	0.61	0/3962	0.81	0/5349
1	C	0.63	0/3222	0.83	2/4351 (0.0%)
1	D	0.62	0/3213	0.83	0/4339
All	All	0.62	0/14370	0.82	2/19402 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	515	TRP	N-CA-C	5.23	119.56	112.04
1	C	515	TRP	CB-CA-C	5.22	120.11	110.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3912	0	4006	17	0
1	B	3904	0	3993	11	0
1	C	3169	0	3227	15	0
1	D	3163	0	3222	14	0
2	A	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	12	0	8	0	0
3	B	12	0	8	0	0
3	C	12	0	8	0	0
3	D	12	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	106	0	0	0	0
5	B	92	0	0	1	0
5	C	99	0	0	1	0
5	D	56	0	0	0	0
All	All	14593	0	14480	51	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 2.

All (51) 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:500[B]:ARG:HG3	1:A:500[B]:ARG:HH11	1.29	0.97
1:A:330:MET:HE2	1:A:348:VAL:HG22	1.59	0.84
1:D:330:MET:HE2	1:D:348:VAL:HG22	1.60	0.82
1:A:500[B]:ARG:HH11	1:A:500[B]:ARG:CG	1.93	0.81
1:A:330:MET:CE	1:A:348:VAL:HG22	2.16	0.76
1:D:330:MET:CE	1:D:348:VAL:HG22	2.17	0.74
1:C:482:TRP:CH2	1:C:515:TRP:O	2.51	0.62
1:A:500[B]:ARG:CG	1:A:500[B]:ARG:NH1	2.62	0.60
1:A:399:ARG:NH1	1:A:418:GLU:OE1	2.36	0.59
1:B:399:ARG:NH1	1:B:418:GLU:OE1	2.36	0.58
1:C:399:ARG:NH1	1:C:418:GLU:OE1	2.37	0.58
1:D:399:ARG:NH1	1:D:418:GLU:OE1	2.37	0.57
1:C:326:CYS:HB3	1:C:330:MET:HE1	1.86	0.56
1:B:27:LEU:HD23	1:C:401:LEU:HD12	1.88	0.56
1:A:525:MET:HE2	1:C:525:MET:HE3	1.90	0.54
1:D:321:GLY:HA3	1:D:443:ARG:HD2	1.92	0.52
1:C:268:ILE:HD12	1:C:268:ILE:N	2.25	0.52
1:B:326:CYS:HB3	1:B:330:MET:HE1	1.90	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.92	0.51
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.92	0.51
1:A:27:LEU:HD23	1:D:401:LEU:HD12	1.93	0.51
1:C:107:PRO:O	1:C:464:HIS:HE1	1.92	0.51
1:D:268:ILE:HD12	1:D:268:ILE:N	2.26	0.51
1:A:401:LEU:HD12	1:D:27:LEU:HD23	1.93	0.50
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.94	0.50
1:B:401:LEU:HD12	1:C:27:LEU:HD23	1.94	0.49
1:B:157:LEU:HD13	1:B:203:LEU:HD21	1.94	0.49
1:B:234:GLU:OE1	5:B:701:HOH:O	2.20	0.48
1:C:482:TRP:CZ3	1:C:515:TRP:O	2.67	0.48
1:B:210:ASN:ND2	1:B:299:ILE:HD13	2.29	0.48
1:A:157:LEU:HD13	1:A:203:LEU:HD21	1.96	0.48
1:B:44:ASN:HD22	1:B:468:GLY:HA2	1.80	0.46
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.98	0.46
1:D:445[B]:ARG:NE	1:D:467:ARG:HD3	2.31	0.45
1:D:44:ASN:HD22	1:D:468:GLY:HA2	1.81	0.45
1:A:330:MET:HE3	1:A:330:MET:HA	1.98	0.45
1:C:488:LEU:C	1:C:488:LEU:HD23	2.42	0.44
1:D:488:LEU:C	1:D:488:LEU:HD23	2.42	0.44
1:A:500[B]:ARG:HG3	1:A:500[B]:ARG:NH1	2.10	0.43
1:A:508:VAL:HG21	1:C:406:SER:HB2	2.00	0.43
1:C:107:PRO:O	1:C:464:HIS:CE1	2.70	0.43
1:A:431:LEU:HD12	1:A:513:THR:HG22	2.00	0.43
1:C:268:ILE:N	1:C:268:ILE:CD1	2.82	0.42
1:D:268:ILE:N	1:D:268:ILE:CD1	2.82	0.42
1:D:330:MET:HE3	1:D:330:MET:HA	2.02	0.42
1:B:121:THR:HB	1:B:157:LEU:HD11	2.01	0.41
1:A:121:THR:HB	1:A:157:LEU:HD11	2.01	0.41
1:D:267:ILE:C	1:D:268:ILE:HD12	2.46	0.41
1:C:267:ILE:C	1:C:268:ILE:HD12	2.46	0.40
1:B:401:LEU:HD21	5:C:710:HOH:O	2.20	0.40
1:A:330:MET:HE1	1:A:348:VAL:HA	2.02	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	508/551 (92%)	496 (98%)	11 (2%)	1 (0%)	43	54
1	B	507/551 (92%)	494 (97%)	12 (2%)	1 (0%)	43	54
1	C	407/551 (74%)	400 (98%)	6 (2%)	1 (0%)	43	54
1	D	406/551 (74%)	400 (98%)	5 (1%)	1 (0%)	43	54
All	All	1828/2204 (83%)	1790 (98%)	34 (2%)	4 (0%)	43	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	CYS
1	B	424	CYS
1	C	424	CYS
1	D	424	CYS

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	420/452 (93%)	416 (99%)	4 (1%)	68	77
1	B	419/452 (93%)	416 (99%)	3 (1%)	76	84
1	C	339/452 (75%)	335 (99%)	4 (1%)	63	74
1	D	338/452 (75%)	334 (99%)	4 (1%)	63	74
All	All	1516/1808 (84%)	1501 (99%)	15 (1%)	68	77

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	VAL
1	A	342	ARG
1	A	480	GLU
1	A	488	LEU
1	B	40	ILE
1	B	123	LEU
1	B	168	VAL
1	C	261	LYS
1	C	268	ILE
1	C	418	GLU
1	C	443	ARG
1	D	268	ILE
1	D	404	ILE
1	D	405	THR
1	D	480	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	458	GLN
1	B	44	ASN
1	B	184	GLN
1	B	210	ASN
1	B	440	GLN
1	B	458	GLN
1	C	75	ASN
1	C	227	GLN
1	C	440	GLN
1	C	464	HIS
1	D	44	ASN
1	D	227	GLN
1	D	391	HIS
1	D	440	GLN
1	D	458	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	CSO	C	474	1	3,6,7	0.56	0	1,6,8	0.74	0
1	CSO	B	474	1	3,6,7	0.64	0	1,6,8	0.64	0
1	CSO	D	474	1	3,6,7	0.66	0	1,6,8	0.66	0
1	CSO	A	474	1	3,6,7	0.55	0	1,6,8	0.73	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
1	CSO	C	474	1	-	0/1/5/7	-
1	CSO	B	474	1	-	0/1/5/7	-
1	CSO	D	474	1	-	0/1/5/7	-
1	CSO	A	474	1	-	0/1/5/7	-

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.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
2	PO4	A	604	-	4,4,4	0.73	0	6,6,6	0.66	0
2	PO4	B	602	-	4,4,4	0.85	0	6,6,6	0.59	0
3	PHE	B	603	-	11,12,12	0.66	0	11,15,15	0.59	0
3	PHE	A	603	-	11,12,12	0.79	0	11,15,15	0.56	0
2	PO4	A	601	-	4,4,4	1.06	0	6,6,6	0.99	0
3	PHE	C	602	-	11,12,12	0.63	0	11,15,15	0.72	1 (9%)
2	PO4	B	604	-	4,4,4	0.94	0	6,6,6	0.47	0
2	PO4	D	601	-	4,4,4	0.82	0	6,6,6	0.79	0
2	PO4	A	602	-	4,4,4	0.92	0	6,6,6	0.74	0
2	PO4	C	601	-	4,4,4	0.84	0	6,6,6	0.84	0
3	PHE	D	602	-	11,12,12	0.80	0	11,15,15	0.64	0
2	PO4	B	601	-	4,4,4	0.85	0	6,6,6	0.83	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	PHE	A	603	-	-	0/8/8/8	0/1/1/1
3	PHE	B	603	-	-	0/8/8/8	0/1/1/1
3	PHE	D	602	-	-	0/8/8/8	0/1/1/1
3	PHE	C	602	-	-	0/8/8/8	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	C	602	PHE	OXT-C-O	-2.29	118.89	124.08

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

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

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	508/551 (92%)	0.31	23 (4%) 38 37	34, 57, 91, 124	2 (0%)
1	B	508/551 (92%)	0.47	27 (5%) 32 30	35, 62, 100, 120	1 (0%)
1	C	409/551 (74%)	0.25	21 (5%) 33 31	30, 55, 85, 123	2 (0%)
1	D	409/551 (74%)	0.39	19 (4%) 37 36	34, 60, 96, 134	1 (0%)
All	All	1834/2204 (83%)	0.36	90 (4%) 35 33	30, 59, 97, 134	6 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	GLY	5.6
1	A	423	CYS	4.7
1	C	404	ILE	4.4
1	B	404	ILE	4.3
1	B	216	VAL	4.0
1	C	516[A]	ARG	3.9
1	C	405	THR	3.5
1	A	404	ILE	3.4
1	B	40	ILE	3.4
1	D	405	THR	3.3
1	D	404	ILE	3.3
1	A	424	CYS	3.2
1	D	40	ILE	3.2
1	D	521	PHE	3.2
1	C	402	ALA	3.1
1	A	519	SER	3.1
1	B	215	ALA	3.1
1	B	403	PRO	3.1
1	A	521	PHE	3.1
1	C	218	LEU	3.0
1	B	130	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	218	LEU	3.0
1	C	406	SER	3.0
1	D	23	ALA	3.0
1	C	403	PRO	3.0
1	A	190	ALA	2.9
1	D	401	LEU	2.9
1	A	394	LEU	2.8
1	C	40	ILE	2.8
1	C	392	LEU	2.8
1	B	424	CYS	2.8
1	D	517	PRO	2.7
1	A	129	THR	2.7
1	D	422	LYS	2.7
1	A	127	SER	2.7
1	D	424	CYS	2.7
1	B	531	PRO	2.6
1	D	394	LEU	2.6
1	C	480	GLU	2.6
1	A	128	GLY	2.6
1	B	521	PHE	2.6
1	B	127	SER	2.6
1	B	406	SER	2.6
1	A	479	GLN	2.6
1	A	40	ILE	2.6
1	D	301	ILE	2.5
1	C	394	LEU	2.5
1	B	190	ALA	2.5
1	D	220	ALA	2.5
1	D	423	CYS	2.5
1	A	244	PHE	2.5
1	D	398	LEU	2.4
1	A	518	GLY	2.4
1	B	520	GLY	2.4
1	B	405	THR	2.4
1	A	477	PRO	2.4
1	B	156	ILE	2.4
1	A	401	LEU	2.4
1	C	423	CYS	2.4
1	C	118	GLU	2.4
1	A	520	GLY	2.3
1	B	164	ILE	2.3
1	A	480	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	299	ILE	2.3
1	A	41	THR	2.3
1	A	422	LYS	2.3
1	B	41	THR	2.3
1	B	398	LEU	2.3
1	B	129	THR	2.2
1	B	301	ILE	2.2
1	B	303	ALA	2.2
1	B	423	CYS	2.2
1	C	424	CYS	2.2
1	C	300	GLU	2.2
1	B	482	TRP	2.2
1	D	531	PRO	2.1
1	B	192	PHE	2.1
1	B	422	LYS	2.1
1	C	475	LYS	2.1
1	A	517	PRO	2.1
1	C	77	SER	2.1
1	A	303	ALA	2.1
1	C	219	PRO	2.1
1	D	403	PRO	2.1
1	C	78	HIS	2.1
1	A	405	THR	2.0
1	D	500	ARG	2.0
1	C	520	GLY	2.0
1	D	520	GLY	2.0
1	B	161	TYR	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(Å ²)	Q<0.9
1	CSO	A	474	7/8	0.92	0.11	60,63,65,65	0
1	CSO	B	474	7/8	0.94	0.08	69,75,79,83	0
1	CSO	D	474	7/8	0.94	0.11	62,68,72,75	0
1	CSO	C	474	7/8	0.96	0.08	55,58,62,64	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
2	PO4	A	602	5/5	0.80	0.11	83,90,90,91	0
2	PO4	B	602	5/5	0.80	0.11	86,87,93,93	0
4	K	C	603	1/1	0.82	0.15	90,90,90,90	0
2	PO4	B	604	5/5	0.89	0.10	84,85,88,89	0
2	PO4	A	604	5/5	0.92	0.09	72,76,78,80	0
3	PHE	A	603	12/12	0.94	0.09	48,49,52,52	0
4	K	D	603	1/1	0.94	0.17	81,81,81,81	0
3	PHE	B	603	12/12	0.95	0.09	50,52,53,54	0
3	PHE	D	602	12/12	0.95	0.08	49,50,54,58	0
3	PHE	C	602	12/12	0.96	0.08	44,45,49,50	0
2	PO4	D	601	5/5	0.96	0.06	53,54,57,57	0
2	PO4	B	601	5/5	0.97	0.07	52,52,54,55	0
4	K	B	605	1/1	0.97	0.08	61,61,61,61	0
4	K	A	605	1/1	0.98	0.04	57,57,57,57	0
2	PO4	A	601	5/5	0.98	0.05	52,55,56,57	0
2	PO4	C	601	5/5	0.99	0.04	49,49,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.