



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:31 PM UTC

PDB ID : 4FXJ / pdb_00004fxj
Title : Structure of M2 pyruvate kinase in complex with phenylalanine
Authors : Walkinshaw, M.D.; Morgan, H.P.
Deposited on : 2012-07-03
Resolution : 2.90 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

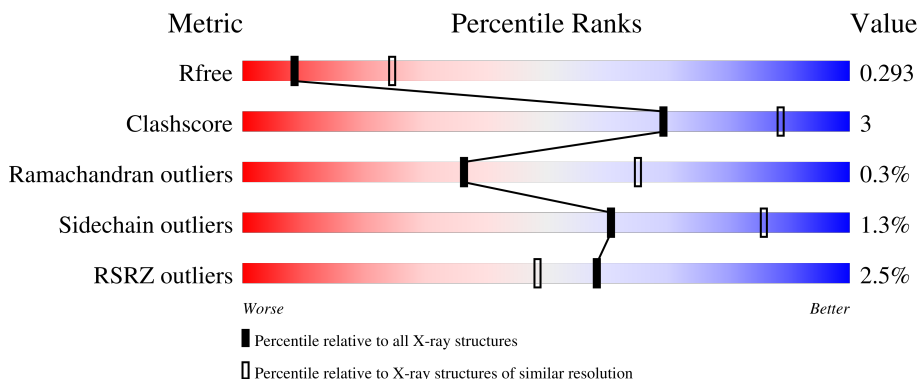
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	0.2% 82% 8% 10%
1	B	551	0.2% 66% 9% 25%
1	C	551	2% 83% 8% 9%
1	D	551	4% 79% 12% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14897 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 isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3810	2397	675	714	24			
1	B	413	Total	C	N	O	S	0	0	0
			3169	1991	567	590	21			
1	C	504	Total	C	N	O	S	0	0	0
			3860	2430	681	725	24			
1	D	508	Total	C	N	O	S	0	0	0
			3882	2442	685	731	24			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	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
A	379	ASN	HIS	SEE REMARK 999	UNP P14618

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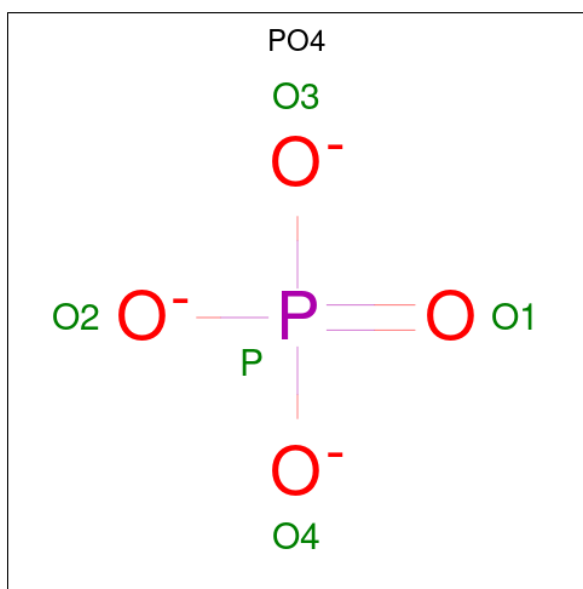
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP P14618
B	-18	GLY	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	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
B	379	ASN	HIS	SEE REMARK 999	UNP P14618
C	-19	MET	-	expression tag	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
C	379	ASN	HIS	SEE REMARK 999	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP P14618
D	-18	GLY	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618
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
D	379	ASN	HIS	SEE REMARK 999	UNP P14618

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



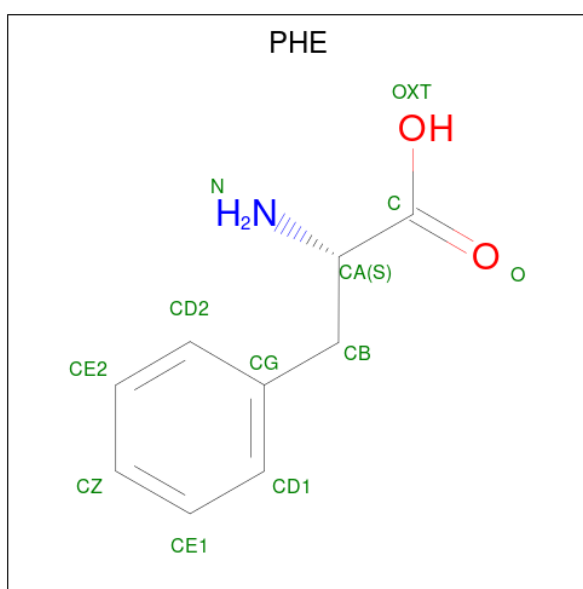
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		

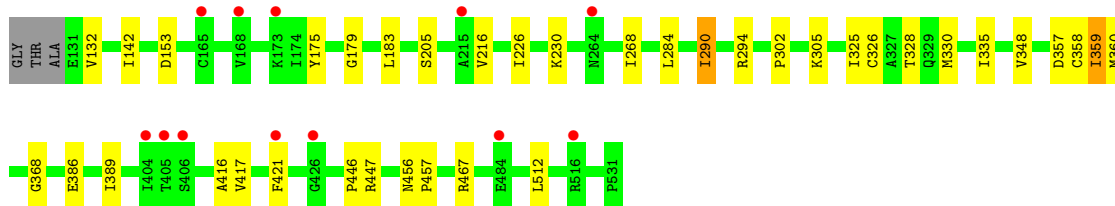
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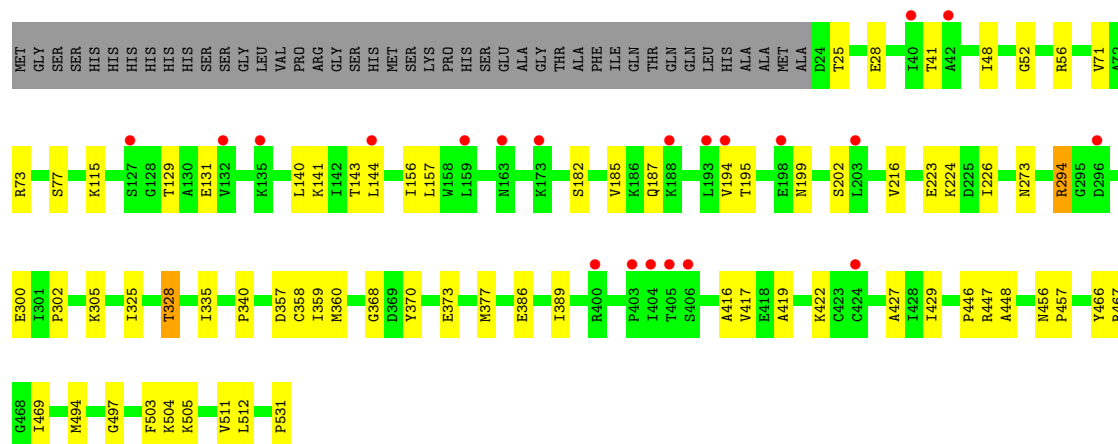
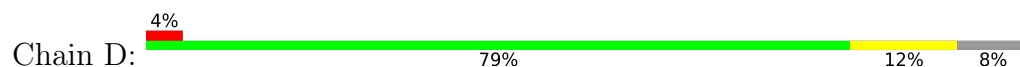
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	26	Total 26	O 26	0	0
4	C	16	Total 16	O 16	0	0
4	D	26	Total 26	O 26	0	0

- Molecule 1: Pyruvate kinase isozymes M1/M2





● Molecule 1: Pyruvate kinase isozymes M1/M2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.26Å 70.60Å 167.60Å 90.00° 105.72° 90.00°	Depositor
Resolution (Å)	56.14 – 2.90 56.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.4 (56.14-2.90) 89.4 (56.14-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.246 , 0.297 0.240 , 0.293	Depositor DCC
R_{free} test set	2477 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14897	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: 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	0.42	0/3869	0.76	0/5221
1	B	0.42	0/3223	0.80	0/4356
1	C	0.42	0/3921	0.76	0/5294
1	D	0.43	0/3944	0.80	0/5327
All	All	0.43	0/14957	0.78	0/20198

There are no bond length outliers.

There are no bond angle outliers.

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	3810	0	3893	22	0
1	B	3169	0	3221	30	0
1	C	3860	0	3943	21	0
1	D	3882	0	3964	32	0
2	A	10	0	0	0	0
2	B	5	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	8	0	0
3	C	12	0	8	0	0
3	D	12	0	8	0	0
4	A	35	0	0	0	0
4	B	26	0	0	0	0
4	C	16	0	0	0	0
4	D	26	0	0	0	0
All	All	14897	0	15053	104	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 3.

All (104) 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:405:THR:CB	1:B:406:SER:HA	1.79	1.12
1:B:405:THR:HB	1:B:406:SER:CA	1.88	1.02
1:B:405:THR:HB	1:B:406:SER:HA	0.97	0.96
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.75	0.67
1:A:423:CYS:HB3	1:B:405:THR:HG21	1.80	0.64
1:B:330:MET:HE2	1:B:359:ILE:HG23	1.81	0.60
1:B:389:ILE:HD13	1:B:467:ARG:HH22	1.68	0.59
1:B:357:ASP:HA	1:B:467:ARG:HB2	1.85	0.57
1:A:330:MET:HE3	1:A:348:VAL:HG22	1.85	0.57
1:D:417:VAL:HG13	1:D:446:PRO:HB3	1.88	0.56
1:D:325:ILE:HG12	1:D:358:CYS:HB2	1.88	0.56
1:D:504:LYS:HG3	1:D:505:LYS:H	1.71	0.54
1:B:330:MET:HE3	1:B:348:VAL:HG22	1.88	0.54
1:A:117:PRO:HD2	1:A:244:PHE:HB2	1.89	0.54
1:C:73:ARG:HD3	1:C:360:MET:SD	2.48	0.53
1:B:417:VAL:HG13	1:B:446:PRO:HB3	1.91	0.53
1:A:268:ILE:HG21	1:A:325:ILE:HD12	1.91	0.53
1:C:357:ASP:HA	1:C:467:ARG:HB2	1.91	0.53
1:A:417:VAL:HG13	1:A:446:PRO:HB3	1.89	0.53
1:B:405:THR:CB	1:B:406:SER:CA	2.66	0.53
1:A:472:VAL:HG21	1:A:496:VAL:HG21	1.91	0.52
1:C:330:MET:HE3	1:C:348:VAL:HG22	1.91	0.52
1:B:106:ARG:NH1	1:B:471:PRO:O	2.43	0.52
1:D:357:ASP:HA	1:D:467:ARG:HB2	1.91	0.52
1:A:357:ASP:HA	1:A:467:ARG:HB2	1.92	0.52
1:D:77:SER:HA	1:D:115:LYS:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD11	1:A:88:ILE:HG13	1.91	0.51
1:B:482:TRP:HB2	1:B:517:PRO:HG3	1.92	0.51
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.91	0.51
1:C:302:PRO:HG2	1:C:305:LYS:HD2	1.93	0.51
1:C:417:VAL:HG13	1:C:446:PRO:HB3	1.92	0.50
1:A:361:LEU:HD11	1:A:378:GLN:HG3	1.92	0.50
1:D:370:TYR:HB3	1:D:373:GLU:HB2	1.93	0.50
1:D:73:ARG:HD2	1:D:360:MET:SD	2.52	0.49
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.94	0.49
1:A:48:ILE:HG12	1:A:71:VAL:HB	1.93	0.49
1:A:187:GLN:HB2	1:A:194:VAL:HB	1.95	0.49
1:D:182:SER:H	1:D:199:ASN:HB2	1.78	0.48
1:D:48:ILE:HG12	1:D:71:VAL:HB	1.94	0.47
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.95	0.47
1:D:340:PRO:HG3	1:D:377:MET:HG2	1.96	0.47
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.97	0.47
1:D:494:MET:HG2	1:D:531:PRO:HD2	1.97	0.47
1:A:325:ILE:HG12	1:A:358:CYS:HB2	1.96	0.47
1:D:386:GLU:HA	1:D:389:ILE:HD12	1.97	0.47
1:B:48:ILE:HG12	1:B:71:VAL:HB	1.97	0.46
1:D:427:ALA:HA	1:D:448:ALA:HB1	1.96	0.46
1:C:123:LEU:HD23	1:C:205:SER:HB3	1.96	0.46
1:D:429:ILE:HB	1:D:511:VAL:HG22	1.98	0.46
1:B:386:GLU:HA	1:B:389:ILE:HD12	1.97	0.46
1:A:509:VAL:HG23	1:A:528:VAL:HG13	1.98	0.45
1:D:140:LEU:HD21	1:D:157:LEU:HD13	1.98	0.45
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.99	0.45
1:D:25:THR:HB	1:D:28:GLU:HB2	1.99	0.45
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.97	0.45
1:D:41:THR:HG22	1:D:447:ARG:HH22	1.81	0.45
1:A:416:ALA:HB2	1:A:512:LEU:HD21	1.99	0.45
1:D:187:GLN:HB2	1:D:194:VAL:CG1	2.47	0.45
1:A:274:HIS:CD2	1:A:278:ARG:HE	2.34	0.44
1:B:241:PHE:HB3	1:B:270:LYS:HD2	1.98	0.44
1:C:268:ILE:HG21	1:C:325:ILE:HD12	1.99	0.44
1:A:402:ALA:HA	1:A:403:PRO:HD3	1.88	0.44
1:B:241:PHE:HD1	1:B:268:ILE:HB	1.82	0.44
1:D:115:LYS:HD2	1:D:224:LYS:HD3	2.00	0.44
1:B:268:ILE:HG21	1:B:325:ILE:HD12	1.99	0.44
1:B:113:ASP:HA	1:B:241:PHE:HB2	2.00	0.43
1:B:25:THR:HG22	1:B:27:LEU:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLU:HG2	1:B:422:LYS:HE2	2.01	0.43
1:D:294:ARG:NH1	1:D:328:THR:O	2.51	0.43
1:C:226:ILE:HG22	1:C:230:LYS:HE2	2.00	0.43
1:C:335:ILE:HG23	1:C:368:GLY:HA2	2.01	0.43
1:D:131:GLU:HG2	1:D:202:SER:HB3	2.00	0.43
1:D:141:LYS:HB3	1:D:156:ILE:HD12	2.00	0.43
1:D:273:ASN:HA	1:D:300:GLU:HG3	2.01	0.43
1:D:419:ALA:HA	1:D:422:LYS:HB3	2.01	0.43
1:A:125:LYS:HB3	1:A:151:LYS:HA	2.00	0.42
1:B:515:TRP:CD1	1:B:516:ARG:HG3	2.55	0.42
1:C:284:LEU:HA	1:C:290:ILE:HD11	2.02	0.42
1:A:528:VAL:HA	1:A:529:PRO:HD3	1.90	0.42
1:C:132:VAL:HG11	1:C:153:ASP:HA	2.02	0.41
1:A:37:SER:HA	1:A:38:PRO:HD3	1.93	0.41
1:D:335:ILE:HG23	1:D:368:GLY:HA2	2.00	0.41
1:A:335:ILE:HG23	1:A:368:GLY:HA2	2.02	0.41
1:C:71:VAL:HG22	1:C:109:ALA:HB3	2.02	0.41
1:B:229:LEU:HD21	1:B:240:VAL:HG11	2.03	0.41
1:C:142:ILE:HD11	1:C:183:LEU:HD13	2.01	0.41
1:D:52:GLY:O	1:D:56:ARG:HG3	2.21	0.41
1:A:243:SER:HA	1:A:270:LYS:HD3	2.03	0.41
1:C:416:ALA:HB2	1:C:512:LEU:HD21	2.02	0.41
1:B:429:ILE:HB	1:B:511:VAL:HG22	2.03	0.41
1:D:223:GLU:HA	1:D:226:ILE:HD12	2.02	0.41
1:C:421:PHE:HE2	1:C:447:ARG:HG3	1.85	0.41
1:C:326:CYS:HB2	1:C:359:ILE:HG22	2.03	0.41
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.55	0.41
1:D:302:PRO:HG2	1:D:305:LYS:HD2	2.03	0.41
1:C:175:TYR:HB3	1:C:179:GLY:HA2	2.03	0.40
1:D:456:ASN:HA	1:D:457:PRO:HD3	1.95	0.40
1:B:73:ARG:HD2	1:B:360:MET:SD	2.62	0.40
1:B:294:ARG:NH2	1:B:330:MET:SD	2.94	0.40
1:B:528:VAL:HA	1:B:529:PRO:HD3	1.94	0.40
1:C:325:ILE:HG12	1:C:358:CYS:HB2	2.04	0.40
1:B:334:MET:HA	1:B:337:LYS:O	2.21	0.40
1:C:386:GLU:HA	1:C:389:ILE:HD12	2.03	0.40
1:C:456:ASN:HA	1:C:457:PRO:HD3	1.89	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	492/551 (89%)	476 (97%)	15 (3%)	1 (0%)	43	72
1	B	409/551 (74%)	398 (97%)	9 (2%)	2 (0%)	24	54
1	C	500/551 (91%)	478 (96%)	20 (4%)	2 (0%)	30	59
1	D	506/551 (92%)	488 (96%)	18 (4%)	0	100	100
All	All	1907/2204 (86%)	1840 (96%)	62 (3%)	5 (0%)	36	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	C	328	THR
1	B	328	THR
1	B	404	ILE
1	C	40	ILE

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	409/453 (90%)	404 (99%)	5 (1%)	63	86
1	B	340/453 (75%)	338 (99%)	2 (1%)	78	93
1	C	416/453 (92%)	411 (99%)	5 (1%)	63	86
1	D	418/453 (92%)	409 (98%)	9 (2%)	45	77
All	All	1583/1812 (87%)	1562 (99%)	21 (1%)	61	86

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	VAL
1	A	319	ARG
1	A	342	ARG
1	A	494	MET
1	A	528	VAL
1	B	45	THR
1	B	342	ARG
1	C	41	THR
1	C	216	VAL
1	C	290	ILE
1	C	294	ARG
1	C	359	ILE
1	D	129	THR
1	D	143	THR
1	D	144	LEU
1	D	185	VAL
1	D	195	THR
1	D	216	VAL
1	D	294	ARG
1	D	328	THR
1	D	359	ILE

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	90	ASN
1	A	273	ASN
1	A	274	HIS
1	A	462	GLN
1	B	44	ASN
1	B	227	GLN
1	C	44	ASN
1	C	146	ASN
1	C	318	ASN
1	C	440	GLN
1	D	75	ASN
1	D	187	GLN
1	D	199	ASN
1	D	391	HIS
1	D	479	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](#)

9 ligands 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$
2	PO4	B	601	-	4,4,4	0.96	0	6,6,6	0.47	0
2	PO4	A	601	-	4,4,4	0.96	0	6,6,6	0.44	0
2	PO4	A	602	-	4,4,4	0.97	0	6,6,6	0.46	0
2	PO4	D	601	-	4,4,4	0.96	0	6,6,6	0.46	0
3	PHE	C	602	-	11,12,12	0.78	1 (9%)	11,15,15	0.87	1 (9%)
2	PO4	C	601	-	4,4,4	0.97	0	6,6,6	0.46	0
3	PHE	D	602	-	11,12,12	0.77	1 (9%)	11,15,15	0.89	1 (9%)
3	PHE	A	603	-	11,12,12	0.77	1 (9%)	11,15,15	0.85	1 (9%)
3	PHE	B	602	-	11,12,12	0.77	1 (9%)	11,15,15	0.85	1 (9%)

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	C	602	-	-	0/8/8/8	0/1/1/1
3	PHE	B	602	-	-	0/8/8/8	0/1/1/1
3	PHE	D	602	-	-	1/8/8/8	0/1/1/1
3	PHE	A	603	-	-	1/8/8/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	PHE	OXT-C	-2.23	1.23	1.30
3	B	602	PHE	OXT-C	-2.22	1.23	1.30
3	A	603	PHE	OXT-C	-2.21	1.23	1.30
3	D	602	PHE	OXT-C	-2.21	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	PHE	OXT-C-O	-2.88	117.54	124.08
3	C	602	PHE	OXT-C-O	-2.82	117.68	124.08
3	A	603	PHE	OXT-C-O	-2.76	117.81	124.08
3	B	602	PHE	OXT-C-O	-2.75	117.84	124.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	602	PHE	O-C-CA-N
3	A	603	PHE	OXT-C-CA-N

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	498/551 (90%)	0.17	8 (1%) 70 62	25, 37, 57, 69	0
1	B	413/551 (74%)	0.13	7 (1%) 69 61	23, 33, 57, 107	0
1	C	504/551 (91%)	0.43	12 (2%) 59 50	28, 44, 73, 82	1 (0%)
1	D	508/551 (92%)	0.46	21 (4%) 41 33	28, 41, 85, 94	0
All	All	1923/2204 (87%)	0.30	48 (2%) 58 48	23, 39, 77, 107	1 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	ILE	5.2
1	B	114	THR	4.6
1	C	406	SER	3.6
1	C	404	ILE	3.2
1	D	127	SER	3.2
1	D	193	LEU	3.1
1	C	165	CYS	3.1
1	D	163	ASN	2.9
1	D	404	ILE	2.8
1	A	402	ALA	2.8
1	D	406	SER	2.7
1	D	296	ASP	2.7
1	D	400	ARG	2.7
1	D	203	LEU	2.6
1	D	144	LEU	2.6
1	D	42	ALA	2.6
1	A	403	PRO	2.6
1	D	159	LEU	2.6
1	C	484	GLU	2.6
1	A	126	GLY	2.5
1	A	130	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	215	ALA	2.5
1	D	424	CYS	2.5
1	B	117	PRO	2.5
1	D	188	LYS	2.4
1	C	421	PHE	2.4
1	C	405	THR	2.4
1	A	28	GLU	2.4
1	B	115	LYS	2.3
1	C	168	VAL	2.3
1	B	392	LEU	2.2
1	B	404	ILE	2.2
1	D	40	ILE	2.2
1	C	516	ARG	2.2
1	D	135	LYS	2.2
1	D	405	THR	2.1
1	A	244	PHE	2.1
1	D	198	GLU	2.1
1	A	29	HIS	2.1
1	C	264	ASN	2.1
1	D	173	LYS	2.1
1	D	403	PRO	2.1
1	C	426	GLY	2.1
1	A	144	LEU	2.1
1	B	297	LEU	2.1
1	D	132	VAL	2.0
1	C	173	LYS	2.0
1	D	194	VAL	2.0

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(Å ²)	Q<0.9
2	PO4	A	602	5/5	0.75	0.19	87,87,87,87	0
2	PO4	B	601	5/5	0.85	0.13	69,69,69,69	0
2	PO4	C	601	5/5	0.88	0.16	87,87,87,87	0
3	PHE	C	602	12/12	0.88	0.28	96,96,96,96	0
3	PHE	A	603	12/12	0.89	0.27	80,80,81,81	0
2	PO4	D	601	5/5	0.89	0.12	55,55,56,56	0
2	PO4	A	601	5/5	0.91	0.13	35,35,35,35	0
3	PHE	D	602	12/12	0.91	0.32	104,104,104,104	0
3	PHE	B	602	12/12	0.93	0.17	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.