



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 07:51 PM EDT

PDB ID : 4FXJ
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

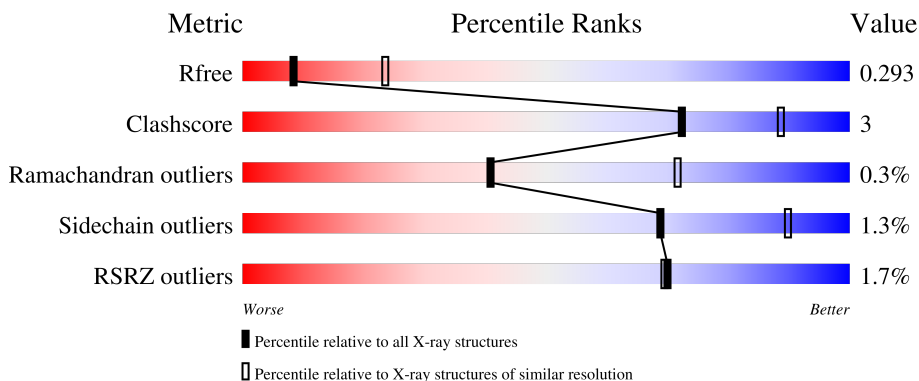
1 Overall quality at a glance

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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	 82% 8% 10%
1	B	551	 0% 66% 9% 25%
1	C	551	 0% 84% 8% 9%
1	D	551	 4% 80% 12% 8%

2 Entry composition i

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

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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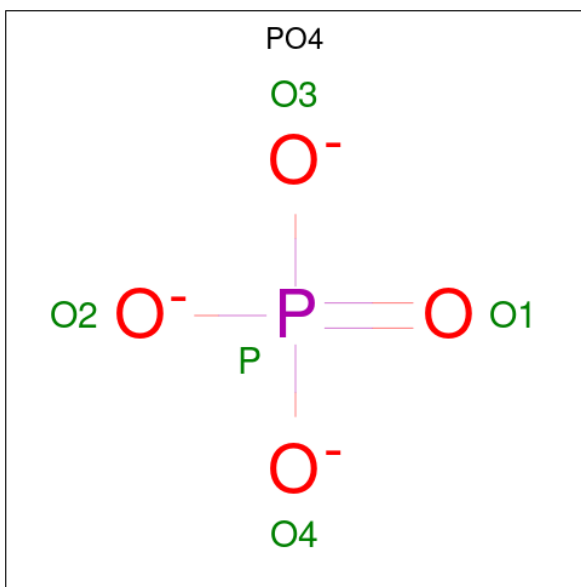
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP P14618
B	-18	GLY	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	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 (three-letter code: PO4) (formula: O₄P).



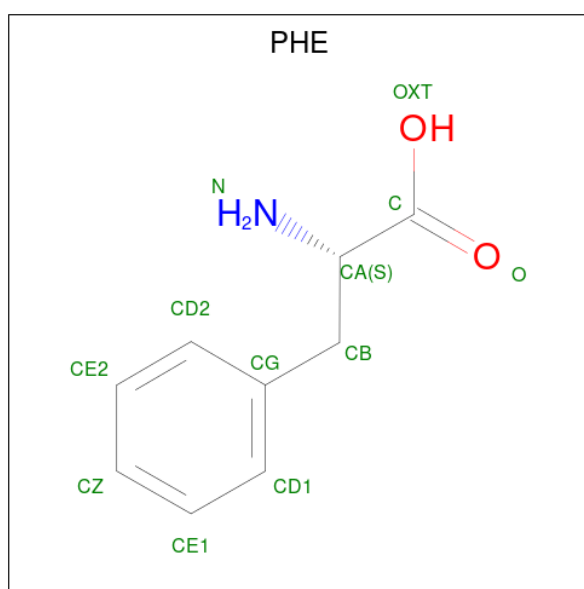
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

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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 (three-letter code: PHE) (formula: C₉H₁₁NO₂).



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		

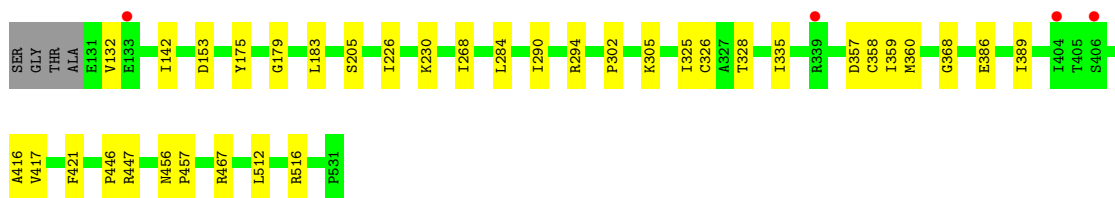
- Molecule 4 is water.

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

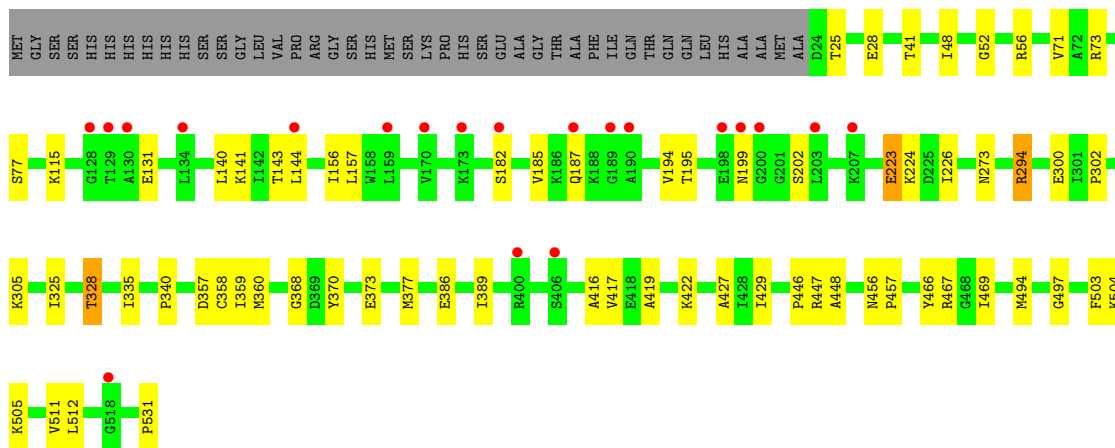
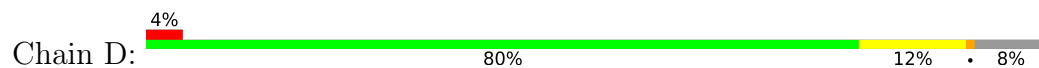
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	26	Total 26	O 26	0	0
4	C	16	Total 16	O 16	0	0
4	D	26	Total 26	O 26	0	0



● Molecule 1: Pyruvate kinase isozymes M1/M2



4 Data and refinement statistics i

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)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.246 , 0.297 0.240 , 0.293	Depositor DCC
R_{free} test set	2209 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtrriage
Anisotropy	0.480	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtrriage
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

Xtrriage'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	0.30	0/3869	0.44	0/5221
1	B	0.30	0/3223	0.44	0/4356
1	C	0.30	0/3921	0.43	0/5294
1	D	0.30	0/3944	0.44	0/5327
All	All	0.30	0/14957	0.44	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	21	0
1	B	3169	0	3221	28	0
1	C	3860	0	3943	20	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	100	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 (100) 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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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%)	47	78
1	B	409/551 (74%)	398 (97%)	9 (2%)	2 (0%)	29	61
1	C	500/551 (91%)	478 (96%)	20 (4%)	2 (0%)	34	66
1	D	506/551 (92%)	488 (96%)	18 (4%)	0	100	100
All	All	1907/2204 (86%)	1840 (96%)	62 (3%)	5 (0%)	41	71

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 [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	409/453 (90%)	404 (99%)	5 (1%)	71	91
1	B	340/453 (75%)	336 (99%)	4 (1%)	71	91
1	C	416/453 (92%)	413 (99%)	3 (1%)	84	95
1	D	418/453 (92%)	410 (98%)	8 (2%)	57	84
All	All	1583/1812 (87%)	1563 (99%)	20 (1%)	69	90

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	VAL
1	A	261	LYS
1	A	319	ARG
1	A	342	ARG
1	A	494	MET
1	B	45	THR
1	B	318	ASN
1	B	342	ARG
1	B	467	ARG
1	C	41	THR
1	C	294	ARG
1	C	516	ARG
1	D	143	THR
1	D	144	LEU
1	D	185	VAL
1	D	195	THR
1	D	223	GLU
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	274	HIS
1	B	393	GLN
1	C	393	GLN
1	D	252	HIS

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 monosaccharides 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
3	PHE	A	603	-	11,12,12	0.74	1 (9%)	14,15,15	0.98	2 (14%)
2	PO4	A	602	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PHE	B	602	-	11,12,12	0.74	1 (9%)	14,15,15	0.97	2 (14%)
3	PHE	C	602	-	11,12,12	0.74	1 (9%)	14,15,15	0.98	2 (14%)
3	PHE	D	602	-	11,12,12	0.74	1 (9%)	14,15,15	1.00	2 (14%)
2	PO4	B	601	-	4,4,4	0.91	0	6,6,6	0.44	0
2	PO4	D	601	-	4,4,4	0.91	0	6,6,6	0.43	0
2	PO4	C	601	-	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	A	601	-	4,4,4	0.91	0	6,6,6	0.41	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	B	602	-	-	0/8/8/8	0/1/1/1
3	PHE	D	602	-	-	1/8/8/8	0/1/1/1
3	PHE	C	602	-	-	0/8/8/8	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	-2.14	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	PHE	OXT-C	-2.13	1.23	1.30
3	A	603	PHE	OXT-C	-2.12	1.23	1.30
3	D	602	PHE	OXT-C	-2.12	1.23	1.30

All (8) 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	124.09
3	C	602	PHE	OXT-C-O	-2.82	117.68	124.09
3	A	603	PHE	OXT-C-O	-2.77	117.81	124.09
3	B	602	PHE	OXT-C-O	-2.75	117.84	124.09
3	A	603	PHE	OXT-C-CA	2.30	121.22	113.38
3	D	602	PHE	OXT-C-CA	2.30	121.22	113.38
3	B	602	PHE	OXT-C-CA	2.29	121.19	113.38
3	C	602	PHE	OXT-C-CA	2.24	121.01	113.38

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%)	0.02	1 (0%) 95 95	25, 37, 57, 69	0
1	B	413/551 (74%)	0.03	6 (1%) 73 73	23, 33, 57, 107	0
1	C	504/551 (91%)	0.08	6 (1%) 79 79	28, 44, 73, 82	1 (0%)
1	D	508/551 (92%)	0.22	20 (3%) 39 35	28, 41, 85, 94	0
All	All	1923/2204 (87%)	0.09	33 (1%) 70 69	23, 39, 77, 107	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	406	SER	4.9
1	D	199	ASN	4.4
1	D	182	SER	3.6
1	B	219	PRO	3.6
1	D	134	LEU	3.5
1	D	159	LEU	3.5
1	D	173	LYS	3.1
1	C	125	LYS	3.0
1	D	203	LEU	3.0
1	D	200	GLY	2.9
1	D	130	ALA	2.9
1	C	133	GLU	2.7
1	D	207	LYS	2.6
1	B	531	PRO	2.6
1	B	221	VAL	2.6
1	D	198	GLU	2.6
1	C	123	LEU	2.6
1	D	406	SER	2.6
1	D	128	GLY	2.6
1	D	187	GLN	2.5
1	D	190	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	189	GLY	2.4
1	A	518	GLY	2.3
1	D	129	THR	2.3
1	D	170	VAL	2.3
1	B	217	ASP	2.3
1	D	400	ARG	2.3
1	B	114	THR	2.2
1	D	144	LEU	2.2
1	B	216	VAL	2.2
1	C	339	ARG	2.2
1	C	404	ILE	2.1
1	D	518	GLY	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 monosaccharides 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
3	PHE	C	602	12/12	0.87	0.36	96,96,96,96	0
3	PHE	D	602	12/12	0.88	0.40	104,104,104,104	0
2	PO4	A	602	5/5	0.91	0.20	87,87,87,87	0
3	PHE	A	603	12/12	0.91	0.32	80,80,81,81	0
3	PHE	B	602	12/12	0.92	0.23	50,50,50,50	0
2	PO4	B	601	5/5	0.94	0.17	69,69,69,69	0
2	PO4	C	601	5/5	0.94	0.29	87,87,87,87	0
2	PO4	A	601	5/5	0.95	0.16	35,35,35,35	0
2	PO4	D	601	5/5	0.95	0.16	55,55,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.