



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:28 PM GMT

PDB ID : 4XYK
Title : Crystal structure of human phosphofructokinase-1 in complex with ADP, Northeast Structural Genomics Consortium Target HR9275
Authors : Forouhar, F.; Webb, B.A.; Szu, F.-E.; Seetharaman, J.; Barber, D.L.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2015-02-02
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

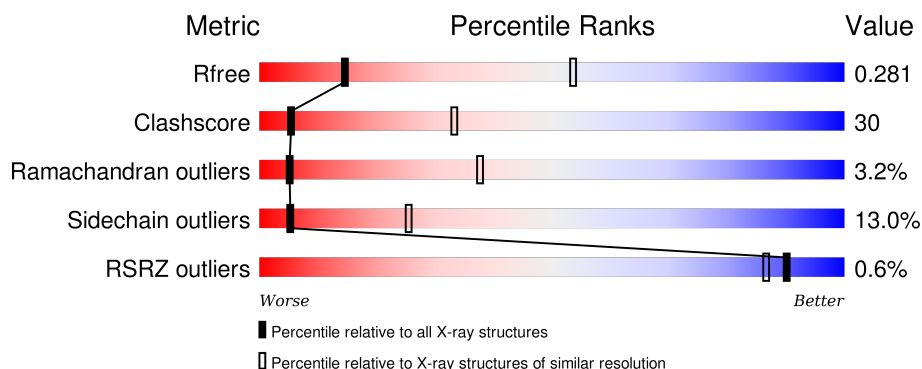
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	812	<div> <div>40%</div> <div>43%</div> <div>7% • 9%</div> </div>
1	B	812	<div> <div>41%</div> <div>43%</div> <div>7% • 8%</div> </div>
1	C	812	<div> <div>40%</div> <div>43%</div> <div>8% 8%</div> </div>
1	D	812	<div> <div>43%</div> <div>41%</div> <div>8% 8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	803	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22897 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 ATP-dependent 6-phosphofructokinase, platelet type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	0	0
			5640	3542	1000	1059	39			
1	B	749	Total	C	N	O	S	0	0	0
			5727	3595	1019	1074	39			
1	C	743	Total	C	N	O	S	0	0	0
			5681	3566	1008	1068	39			
1	D	743	Total	C	N	O	S	0	0	0
			5681	3566	1008	1068	39			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q01813
A	-26	SER	-	expression tag	UNP Q01813
A	-25	TYR	-	expression tag	UNP Q01813
A	-24	TYR	-	expression tag	UNP Q01813
A	-23	HIS	-	expression tag	UNP Q01813
A	-22	HIS	-	expression tag	UNP Q01813
A	-21	HIS	-	expression tag	UNP Q01813
A	-20	HIS	-	expression tag	UNP Q01813
A	-19	HIS	-	expression tag	UNP Q01813
A	-18	HIS	-	expression tag	UNP Q01813
A	-17	ASP	-	expression tag	UNP Q01813
A	-16	TYR	-	expression tag	UNP Q01813
A	-15	ASP	-	expression tag	UNP Q01813
A	-14	ILE	-	expression tag	UNP Q01813
A	-13	PRO	-	expression tag	UNP Q01813
A	-12	THR	-	expression tag	UNP Q01813
A	-11	THR	-	expression tag	UNP Q01813
A	-10	GLU	-	expression tag	UNP Q01813
A	-9	ASN	-	expression tag	UNP Q01813
A	-8	LEU	-	expression tag	UNP Q01813
A	-7	TYR	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	PHE	-	expression tag	UNP Q01813
A	-5	GLN	-	expression tag	UNP Q01813
A	-4	GLY	-	expression tag	UNP Q01813
A	-3	ALA	-	expression tag	UNP Q01813
A	-2	MET	-	expression tag	UNP Q01813
A	-1	ASP	-	expression tag	UNP Q01813
A	0	PRO	-	expression tag	UNP Q01813
B	-27	MET	-	initiating methionine	UNP Q01813
B	-26	SER	-	expression tag	UNP Q01813
B	-25	TYR	-	expression tag	UNP Q01813
B	-24	TYR	-	expression tag	UNP Q01813
B	-23	HIS	-	expression tag	UNP Q01813
B	-22	HIS	-	expression tag	UNP Q01813
B	-21	HIS	-	expression tag	UNP Q01813
B	-20	HIS	-	expression tag	UNP Q01813
B	-19	HIS	-	expression tag	UNP Q01813
B	-18	HIS	-	expression tag	UNP Q01813
B	-17	ASP	-	expression tag	UNP Q01813
B	-16	TYR	-	expression tag	UNP Q01813
B	-15	ASP	-	expression tag	UNP Q01813
B	-14	ILE	-	expression tag	UNP Q01813
B	-13	PRO	-	expression tag	UNP Q01813
B	-12	THR	-	expression tag	UNP Q01813
B	-11	THR	-	expression tag	UNP Q01813
B	-10	GLU	-	expression tag	UNP Q01813
B	-9	ASN	-	expression tag	UNP Q01813
B	-8	LEU	-	expression tag	UNP Q01813
B	-7	TYR	-	expression tag	UNP Q01813
B	-6	PHE	-	expression tag	UNP Q01813
B	-5	GLN	-	expression tag	UNP Q01813
B	-4	GLY	-	expression tag	UNP Q01813
B	-3	ALA	-	expression tag	UNP Q01813
B	-2	MET	-	expression tag	UNP Q01813
B	-1	ASP	-	expression tag	UNP Q01813
B	0	PRO	-	expression tag	UNP Q01813
C	-27	MET	-	initiating methionine	UNP Q01813
C	-26	SER	-	expression tag	UNP Q01813
C	-25	TYR	-	expression tag	UNP Q01813
C	-24	TYR	-	expression tag	UNP Q01813
C	-23	HIS	-	expression tag	UNP Q01813
C	-22	HIS	-	expression tag	UNP Q01813
C	-21	HIS	-	expression tag	UNP Q01813

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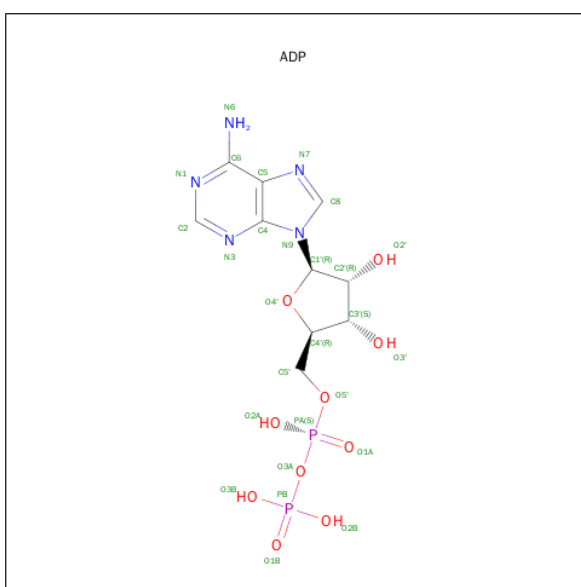
Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP Q01813
C	-19	HIS	-	expression tag	UNP Q01813
C	-18	HIS	-	expression tag	UNP Q01813
C	-17	ASP	-	expression tag	UNP Q01813
C	-16	TYR	-	expression tag	UNP Q01813
C	-15	ASP	-	expression tag	UNP Q01813
C	-14	ILE	-	expression tag	UNP Q01813
C	-13	PRO	-	expression tag	UNP Q01813
C	-12	THR	-	expression tag	UNP Q01813
C	-11	THR	-	expression tag	UNP Q01813
C	-10	GLU	-	expression tag	UNP Q01813
C	-9	ASN	-	expression tag	UNP Q01813
C	-8	LEU	-	expression tag	UNP Q01813
C	-7	TYR	-	expression tag	UNP Q01813
C	-6	PHE	-	expression tag	UNP Q01813
C	-5	GLN	-	expression tag	UNP Q01813
C	-4	GLY	-	expression tag	UNP Q01813
C	-3	ALA	-	expression tag	UNP Q01813
C	-2	MET	-	expression tag	UNP Q01813
C	-1	ASP	-	expression tag	UNP Q01813
C	0	PRO	-	expression tag	UNP Q01813
D	-27	MET	-	initiating methionine	UNP Q01813
D	-26	SER	-	expression tag	UNP Q01813
D	-25	TYR	-	expression tag	UNP Q01813
D	-24	TYR	-	expression tag	UNP Q01813
D	-23	HIS	-	expression tag	UNP Q01813
D	-22	HIS	-	expression tag	UNP Q01813
D	-21	HIS	-	expression tag	UNP Q01813
D	-20	HIS	-	expression tag	UNP Q01813
D	-19	HIS	-	expression tag	UNP Q01813
D	-18	HIS	-	expression tag	UNP Q01813
D	-17	ASP	-	expression tag	UNP Q01813
D	-16	TYR	-	expression tag	UNP Q01813
D	-15	ASP	-	expression tag	UNP Q01813
D	-14	ILE	-	expression tag	UNP Q01813
D	-13	PRO	-	expression tag	UNP Q01813
D	-12	THR	-	expression tag	UNP Q01813
D	-11	THR	-	expression tag	UNP Q01813
D	-10	GLU	-	expression tag	UNP Q01813
D	-9	ASN	-	expression tag	UNP Q01813
D	-8	LEU	-	expression tag	UNP Q01813
D	-7	TYR	-	expression tag	UNP Q01813

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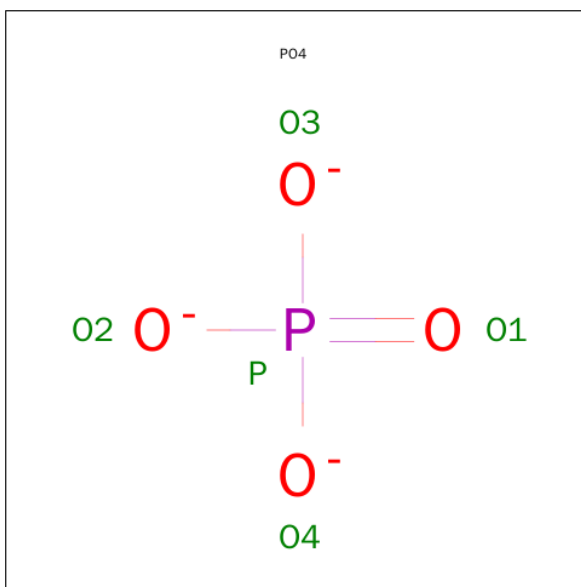
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	PHE	-	expression tag	UNP Q01813
D	-5	GLN	-	expression tag	UNP Q01813
D	-4	GLY	-	expression tag	UNP Q01813
D	-3	ALA	-	expression tag	UNP Q01813
D	-2	MET	-	expression tag	UNP Q01813
D	-1	ASP	-	expression tag	UNP Q01813
D	0	PRO	-	expression tag	UNP Q01813

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

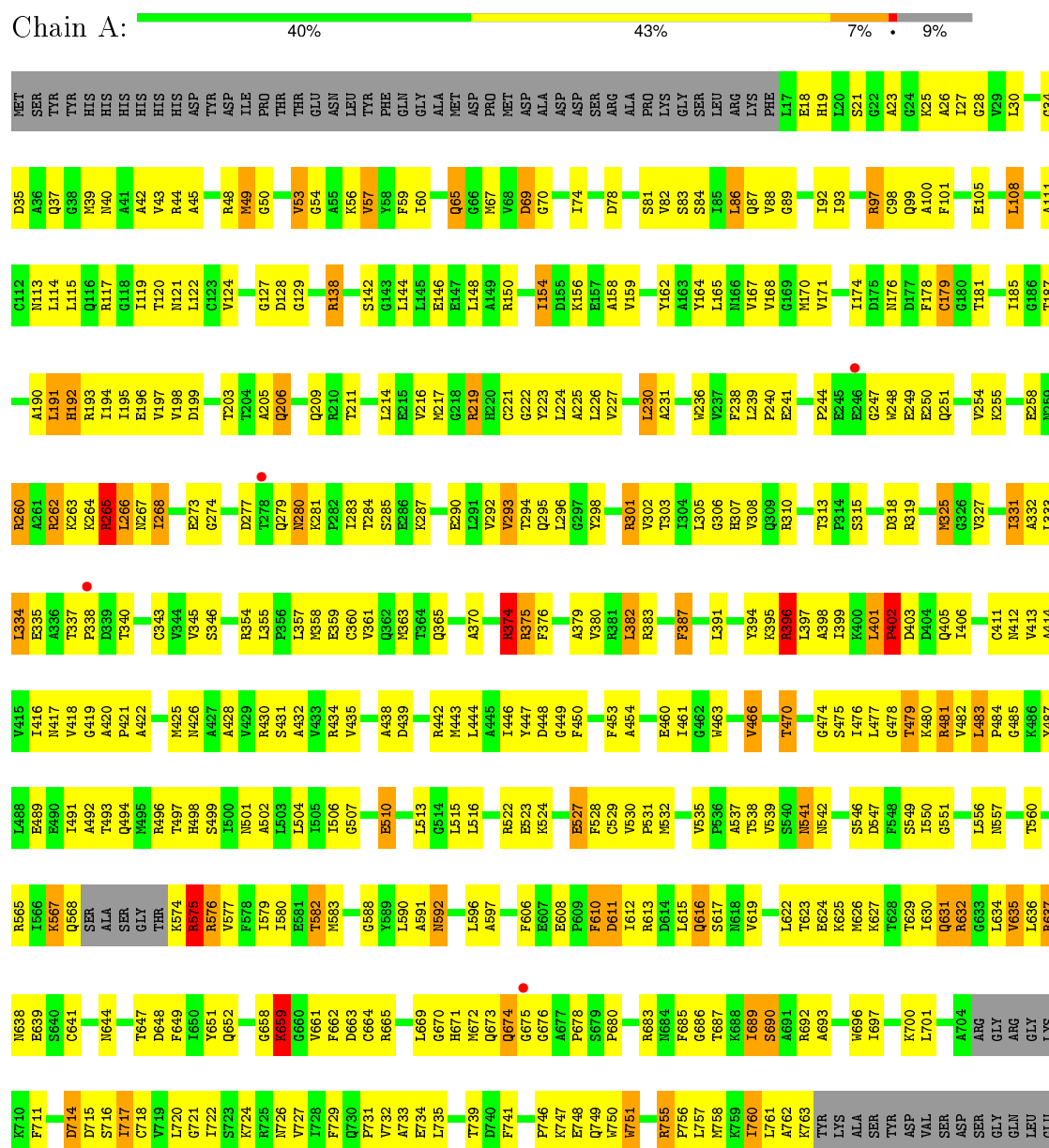


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ATP-dependent 6-phosphofructokinase, platelet type



V732	R665	I580	L503	R430	L355	T278
A733	I669	E581	L504	S431	M358	Q279
E734	I670	M583	I505	R434	K281	N280
L735	H671	Y586	G507	V435	C360	K281
K736	M672	C587	E510	D439	K363	P282
Q738	Q673	G588	A511	R442	T364	L283
I739	Q674	Y512	Y512	M443	Q365	T284
D740	A591	N592	L515	L444	A370	S285
H743	M592	L516	L516	Y447	R374	E286
P746	L596	E517	L518	D448	R375	K287
K747	A597	S519	S519	F450	F376	E290
E748	F606	A521	A521	F453	A379	V292
Q749	F610	H525	H525	A454	V380	V293
W750	L615	E526	E526	I458	R381	T294
W751	V619	F528	F528	K459	R382	Q295
L752	H621	E620	C529	E460	R383	L296
R755	L622	P531	P531	I461	S386	Q297
P756	T623	H532	H532	M463	G462	Y298
L757	E624	V533	V533	T464	T387	R301
W758	K625	M534	M534	D465	M390	R302
K759	M626	V535	V535	V466	Y394	T303
I760	K627	P536	P536	T470	R396	T304
L761	I630	T538	T538	G474	L397	L305
L762	Q631	V539	V539	I476	A398	G306
A763	R632	S540	S540	I477	K400	H307
K763	L634	M541	M541	L477	L401	R310
T764	V635	P544	P544	G478	P402	S315
L765	L636	G545	G545	T479	D403	D318
L766	R637	S546	S546	K480	P494	R319
L767	M638	D547	D547	R481	Q405	I320
L768	E639	F548	F548	V482	G325	M325
L769	S640	S549	S549	L483	V327	G326
L770	C641	I550	I550	P484	C411	V327
T771	M644	N557	N557	G485	N412	I331
L772	T647	T560	T560	K486	V413	A332
L773	Q652	R565	R565	Y487	A414	L333
L774	S655	K567	K567	L488	V415	L334
L775	E656	Q568	Q568	E489	I416	T337
L776	E657	G572	G572	E490	N417	P338
L777	G658	K659	K659	I491	V418	D339
L778	K660	R575	R575	A492	G419	T340
L779	V661	A576	A576	M495	A420	C343
L780	F662	F577	F577	R496	P421	V344
L781	D663	D663	D663	T497	A423	V345
L782	C664	C664	C664	H498	G424	S346
L783				S499	M425	H351
L784				I500	N501	R354
L785				A502	V429	
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.34Å 168.37Å 133.27Å 90.00° 103.78° 90.00°	Depositor
Resolution (Å)	45.37 – 3.40 45.37 – 3.40	Depositor EDS
% Data completeness (in resolution range)	74.2 (45.37-3.40) 84.5 (45.37-3.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.40Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.256 , 0.290 0.269 , 0.281	Depositor DCC
R_{free} test set	3943 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 14.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 39429 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22897	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, ADP

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	0.57	1/5730 (0.0%)	0.75	15/7735 (0.2%)
1	B	0.55	0/5819	0.85	18/7854 (0.2%)
1	C	0.54	1/5773 (0.0%)	0.81	16/7795 (0.2%)
1	D	0.53	0/5773	0.89	16/7795 (0.2%)
All	All	0.55	2/23095 (0.0%)	0.83	65/31179 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	4
1	D	0	2
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	664	CYS	CB-SG	-6.17	1.71	1.82
1	A	360	CYS	CB-SG	-5.68	1.72	1.81

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	ARG	NE-CZ-NH2	-22.12	109.24	120.30
1	D	374	ARG	NE-CZ-NH1	-21.17	109.71	120.30
1	D	374	ARG	NE-CZ-NH2	21.17	130.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	665	ARG	NE-CZ-NH1	-20.40	110.10	120.30
1	C	97	ARG	NE-CZ-NH1	19.91	130.25	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	ARG	Sidechain
1	A	262	ARG	Sidechain
1	A	301	ARG	Sidechain
1	A	632	ARG	Sidechain
1	A	692	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5640	0	5674	340	0
1	B	5727	0	5764	340	0
1	C	5681	0	5709	358	0
1	D	5681	0	5709	376	0
2	A	27	0	12	2	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	0	0
3	A	15	0	0	2	0
3	B	10	0	0	0	0
3	C	20	0	0	1	0
3	D	15	0	0	1	0
All	All	22897	0	22904	1376	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 30.

The worst 5 of 1376 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:D:480:LYS:HB3	1:D:482:VAL:HG23	1.29	1.05
1:B:522:ARG:HH12	1:B:529:CYS:HA	1.25	1.00
1:D:532:MET:HB2	1:D:717:ILE:HG22	1.41	1.00
1:A:539:VAL:HG11	1:A:674:GLN:HB3	1.43	0.99
1:A:121:ASN:HB3	1:A:333:LEU:HD22	1.46	0.97

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	731/812 (90%)	610 (83%)	95 (13%)	26 (4%)	4	34
1	B	745/812 (92%)	631 (85%)	87 (12%)	27 (4%)	4	34
1	C	739/812 (91%)	620 (84%)	97 (13%)	22 (3%)	5	39
1	D	739/812 (91%)	618 (84%)	101 (14%)	20 (3%)	6	41
All	All	2954/3248 (91%)	2479 (84%)	380 (13%)	95 (3%)	5	38

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ASP
1	A	724	LYS
1	B	724	LYS
1	C	19	HIS
1	C	724	LYS

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	594/658 (90%)	516 (87%)	78 (13%)	5	25
1	B	602/658 (92%)	529 (88%)	73 (12%)	6	28
1	C	598/658 (91%)	518 (87%)	80 (13%)	5	24
1	D	598/658 (91%)	517 (86%)	81 (14%)	5	24
All	All	2392/2632 (91%)	2080 (87%)	312 (13%)	5	25

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	671	HIS
1	C	230	LEU
1	D	519	SER
1	B	702	LYS
1	C	59	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	65	GLN
1	C	295	GLN
1	D	541	ASN
1	C	73	ASN
1	C	116	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 carbohydrates in this entry.

5.6 Ligand geometry

16 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	ADP	A	801	-	22,29,29	1.41	2 (9%)	27,45,45	1.21	4 (14%)
3	PO4	A	802	-	4,4,4	1.11	0	6,6,6	0.27	0
3	PO4	A	803	-	4,4,4	0.89	0	6,6,6	0.27	0
3	PO4	A	804	-	4,4,4	1.11	0	6,6,6	0.27	0
2	ADP	B	801	-	22,29,29	1.67	3 (13%)	27,45,45	1.20	2 (7%)
3	PO4	B	802	-	4,4,4	1.01	0	6,6,6	0.27	0
3	PO4	B	803	-	4,4,4	1.01	0	6,6,6	0.27	0
2	ADP	C	801	-	22,29,29	1.58	3 (13%)	27,45,45	1.09	3 (11%)
3	PO4	C	802	-	4,4,4	1.11	0	6,6,6	0.27	0
3	PO4	C	803	-	4,4,4	1.06	0	6,6,6	0.28	0
3	PO4	C	804	-	4,4,4	0.97	0	6,6,6	0.27	0
3	PO4	C	805	-	4,4,4	1.04	0	6,6,6	0.27	0
3	PO4	D	801	-	4,4,4	1.03	0	6,6,6	0.27	0
2	ADP	D	802	-	22,29,29	1.85	4 (18%)	27,45,45	1.38	4 (14%)
3	PO4	D	803	-	4,4,4	1.08	0	6,6,6	0.27	0
3	PO4	D	804	-	4,4,4	1.05	0	6,6,6	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	801	-	-	0/12/32/32	0/3/3/3
3	PO4	A	802	-	-	0/0/0/0	0/0/0/0
3	PO4	A	803	-	-	0/0/0/0	0/0/0/0
3	PO4	A	804	-	-	0/0/0/0	0/0/0/0
2	ADP	B	801	-	-	0/12/32/32	0/3/3/3
3	PO4	B	802	-	-	0/0/0/0	0/0/0/0
3	PO4	B	803	-	-	0/0/0/0	0/0/0/0
2	ADP	C	801	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	C	802	-	-	0/0/0/0	0/0/0/0
3	PO4	C	803	-	-	0/0/0/0	0/0/0/0
3	PO4	C	804	-	-	0/0/0/0	0/0/0/0
3	PO4	C	805	-	-	0/0/0/0	0/0/0/0
3	PO4	D	801	-	-	0/0/0/0	0/0/0/0
2	ADP	D	802	-	-	0/12/32/32	0/3/3/3
3	PO4	D	803	-	-	0/0/0/0	0/0/0/0
3	PO4	D	804	-	-	0/0/0/0	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	ADP	PB-O2B	-2.13	1.47	1.54
2	D	802	ADP	C4-N3	2.15	1.38	1.35
2	B	801	ADP	O4'-C1'	2.52	1.44	1.41
2	B	801	ADP	C4-N3	2.53	1.39	1.35
2	C	801	ADP	O4'-C1'	2.77	1.44	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	802	ADP	O2B-PB-O1B	-2.51	102.49	110.58
2	D	802	ADP	C1'-N9-C4	-2.36	123.38	126.94
2	C	801	ADP	C1'-N9-C4	-2.11	123.75	126.94
2	B	801	ADP	O3A-PA-O5'	2.02	108.30	102.94
2	C	801	ADP	O3A-PA-O5'	2.05	108.38	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ADP	2	0
3	A	803	PO4	2	0
2	B	801	ADP	1	0
2	C	801	ADP	1	0
3	C	805	PO4	1	0
3	D	801	PO4	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	737/812 (90%)	-0.14	4 (0%) 91 89	27, 73, 113, 162	0
1	B	749/812 (92%)	-0.09	7 (0%) 85 81	25, 75, 114, 162	0
1	C	743/812 (91%)	-0.14	3 (0%) 93 91	26, 73, 112, 161	0
1	D	743/812 (91%)	-0.12	4 (0%) 91 89	29, 74, 113, 162	0
All	All	2972/3248 (91%)	-0.12	18 (0%) 90 86	25, 74, 113, 162	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	PRO	3.3
1	D	343	CYS	3.0
1	B	205	ALA	2.9
1	B	59	PHE	2.9
1	C	347	LEU	2.6

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ADP	C	801	27/27	0.93	0.18	-0.20	35,98,135,151	0
3	PO4	C	804	5/5	0.90	0.19	-0.24	6,89,105,127	0
2	ADP	A	801	27/27	0.94	0.19	-0.30	1,73,118,137	0
2	ADP	B	801	27/27	0.91	0.17	-0.40	21,98,154,163	0
2	ADP	D	802	27/27	0.94	0.21	-0.63	1,91,129,134	0
3	PO4	B	803	5/5	0.95	0.16	-1.02	7,34,89,107	0
3	PO4	A	803	5/5	0.91	0.17	-1.13	17,29,126,144	0
3	PO4	D	801	5/5	0.96	0.14	-1.15	14,27,57,97	0
3	PO4	A	804	5/5	0.99	0.13	-1.35	4,10,57,70	0
3	PO4	C	802	5/5	0.97	0.12	-1.38	1,66,70,97	0
3	PO4	A	802	5/5	0.97	0.13	-1.41	1,67,103,108	0
3	PO4	B	802	5/5	0.95	0.12	-1.62	16,71,134,135	0
3	PO4	D	804	5/5	0.98	0.13	-1.64	18,41,68,78	0
3	PO4	C	803	5/5	0.94	0.15	-1.73	1,20,85,87	0
3	PO4	D	803	5/5	0.97	0.10	-2.43	31,32,74,82	0
3	PO4	C	805	5/5	0.91	0.12	-2.51	65,81,155,163	0

6.5 Other polymers [i](#)

There are no such residues in this entry.