

Full wwPDB X-ray Structure Validation Report (i)

Apr 4, 2024 – 12:38 PM JST

PDB ID	:	8JWK
Title	:	The second purified state crystal structure of AKRtyl
Authors	:	Lin, S.; Dai, S.; Xiao, Z.
Deposited on	:	2023-06-29
Resolution	:	2.32 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 (i) 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 (1)) 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	:	2.36
buster-report	:	1.1.7(2018)
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.32 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5974(2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	$5855\ (2.34-2.30)$

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 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 <=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		051	6%		
	A	351	79%	5% •	16%
			8%		
1	В	351	81%	8%	• 11%
			9%		
1	С	351	75%	8%	17%
			7%		
1	D	351	81%	8%	11%
			6%		
1	\mathbf{E}	351	74%	10%	16%
			6%		
1	F	351	79%	9%	11%



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Mol	Chain	Length	Quality of chain		
			5%		
1	G	351	74% 10%		16%
			4%		20/0
1	Н	351	910/	6%	1 20/
-		001	5%	070 •	13./0
1	т	251			
1	1	- 391	80%	6%	15%
	-		5%		
1	J	351	83%	7%	• 9%
			5%		
1	K	351	74% 9%	1	.6%
			4%		
1	L	351	87%	6	% 7%
			4%		
1	Μ	351	75% 9%		16%
			3%		
1	Ν	351	81%	8% •	10%
			3%		
1	0	351	76% 8%		16%
			4%		
1	Р	351	89%		5% 6%



8JWK

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 40000 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	206	Total	С	Ν	0	S	0	0	0
	11	250	2309	1454	413	436	6	0	0	0
1	В	319	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
		012	2414	1522	429	455	8	0	0	0
1	C	292	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
		252	2272	1432	408	425	7	0	0	0
1	D	314	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
		011	2437	1537	435	457	8		Ŭ	
1	E	294	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
-			2288	1441	412	428	7	Ŭ		Ŭ
1	F	313	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
-	-	010	2433	1533	434	458	8	Ŭ		Ŭ
1	G	296	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
-	<u> </u>	200	2305	1451	412	436	6	Ŭ	0	0
1	Н	307	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
			2383	1502	425	448	8	Ŭ		Ŭ
1	T	300	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	-		2333	1469	417	440	7	Ŭ		Ŭ
1	J	321	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	, in the second		2480	1558	446	468	8	Ŭ		
1	K	295	Total	С	Ν	Ο	\mathbf{S}	0	0	0
			2295	1445	411	432	7	Ŭ		Ŭ
1	L	326	Total	С	Ν	Ο	\mathbf{S}	0	0	0
			2526	1585	457	476	8	Ŭ		Ŭ
1	М	295	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
		200	2298	1446	414	431	7	Ŭ	0	
1	N	315	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	1,	010	2446	1542	436	460	8	Ŭ		
1	0	295	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
		200	2295	1447	411	430	7			
1	Р	330	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	1	000	2552	1600	462	482	8		Ŭ	

• Molecule 1 is a protein called Aldo/keto reductase.



Chain	Residue	Modelled	Actual	Comment	Reference
А	-19	MET	-	initiating methionine	UNP A0A3R7J519
А	-18	GLY	-	expression tag	UNP A0A3R7J519
A	-17	SER	-	expression tag	UNP A0A3R7J519
А	-16	SER	-	expression tag	UNP A0A3R7J519
А	-15	HIS	-	expression tag	UNP A0A3R7J519
А	-14	HIS	-	expression tag	UNP A0A3R7J519
А	-13	HIS	-	expression tag	UNP A0A3R7J519
А	-12	HIS	-	expression tag	UNP A0A3R7J519
А	-11	HIS	-	expression tag	UNP A0A3R7J519
А	-10	HIS	-	expression tag	UNP A0A3R7J519
А	-9	SER	-	expression tag	UNP A0A3R7J519
А	-8	SER	-	expression tag	UNP A0A3R7J519
А	-7	GLY	-	expression tag	UNP A0A3R7J519
А	-6	LEU	-	expression tag	UNP A0A3R7J519
А	-5	VAL	-	expression tag	UNP A0A3R7J519
A	-4	PRO	-	expression tag	UNP A0A3R7J519
A	-3	ARG	-	expression tag	UNP A0A3R7J519
A	-2	GLY	-	expression tag	UNP A0A3R7J519
A	-1	SER	-	expression tag	UNP A0A3R7J519
A	0	HIS	-	expression tag	UNP A0A3R7J519
B	-19	MET	-	initiating methionine	UNP A0A3R7J519
В	-18	GLY	-	expression tag	UNP A0A3R7J519
B	-17	SER	-	expression tag	UNP A0A3R7J519
B	-16	SER	-	expression tag	UNP A0A3R7J519
B	-15	HIS	-	expression tag	UNP A0A3R7J519
B	-14	HIS	-	expression tag	UNP A0A3R7J519
B	-13	HIS	-	expression tag	UNP A0A3R7J519
B	-12	HIS	-	expression tag	UNP A0A3R7J519
B	-11	HIS	-	expression tag	UNP A0A3R7J519
B	-10	HIS	-	expression tag	UNP A0A3R7J519
B	-9	SER	-	expression tag	UNP A0A3R7J519
B	-8	SER	-	expression tag	UNP A0A3R7J519
B	-7	GLY	-	expression tag	UNP A0A3R7J519
B	-6	LEU	-	expression tag	UNP A0A3R7J519
B	-5	VAL	-	expression tag	UNP A0A3R7J519
<u> </u>	-4	PRO	-	expression tag	UNP A0A3R7J519
B	-3	ARG	-	expression tag	UNP A0A3R7J519
B	-2	GLY	-	expression tag	UNP A0A3R7J519
B	-1	SER	-	expression tag	UNP A0A3R7J519
B	0	HIS	-	expression tag	UNP A0A3R7J519
C	-19	MET	-	initiating methionine	UNP A0A3R7J519
C	-18	GLY	-	expression tag	UNP A0A3R7J519

There are 320 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
С	-17	SER	-	expression tag	UNP A0A3R7J519
C	-16	SER	-	expression tag	UNP A0A3R7J519
C	-15	HIS	-	expression tag	UNP A0A3R7J519
C	-14	HIS	-	expression tag	UNP A0A3R7J519
C	-13	HIS	-	expression tag	UNP A0A3R7J519
С	-12	HIS	-	expression tag	UNP A0A3R7J519
С	-11	HIS	_	expression tag	UNP A0A3R7J519
С	-10	HIS	_	expression tag	UNP A0A3R7J519
С	-9	SER	_	expression tag	UNP A0A3R7J519
С	-8	SER	-	expression tag	UNP A0A3R7J519
С	-7	GLY	-	expression tag	UNP A0A3R7J519
С	-6	LEU	-	expression tag	UNP A0A3R7J519
С	-5	VAL	-	expression tag	UNP A0A3R7J519
С	-4	PRO	-	expression tag	UNP A0A3R7J519
С	-3	ARG	-	expression tag	UNP A0A3R7J519
С	-2	GLY	-	expression tag	UNP A0A3R7J519
С	-1	SER	-	expression tag	UNP A0A3R7J519
С	0	HIS	-	expression tag	UNP A0A3R7J519
D	-19	MET	_	initiating methionine	UNP A0A3R7J519
D	-18	GLY	-	expression tag	UNP A0A3R7J519
D	-17	SER	-	expression tag	UNP A0A3R7J519
D	-16	SER	-	expression tag	UNP A0A3R7J519
D	-15	HIS	-	expression tag	UNP A0A3R7J519
D	-14	HIS	-	expression tag	UNP A0A3R7J519
D	-13	HIS	-	expression tag	UNP A0A3R7J519
D	-12	HIS	-	expression tag	UNP A0A3R7J519
D	-11	HIS	-	expression tag	UNP A0A3R7J519
D	-10	HIS	-	expression tag	UNP A0A3R7J519
D	-9	SER	-	expression tag	UNP A0A3R7J519
D	-8	SER	-	expression tag	UNP A0A3R7J519
D	-7	GLY	-	expression tag	UNP A0A3R7J519
D	-6	LEU	-	expression tag	UNP A0A3R7J519
D	-5	VAL	-	expression tag	UNP A0A3R7J519
D	-4	PRO	-	expression tag	UNP A0A3R7J519
D	-3	ARG	-	expression tag	UNP A0A3R7J519
D	-2	GLY	-	expression tag	UNP A0A3R7J519
D	-1	SER	-	expression tag	UNP A0A3R7J519
D	0	HIS	-	expression tag	UNP A0A3R7J519
E	-19	MET	-	initiating methionine	UNP A0A3R7J519
E	-18	GLY	-	expression tag	UNP A0A3R7J519
E	-17	SER	-	expression tag	UNP A0A3R7J519
E	-16	SER	-	expression tag	UNP A0A3R7J519



Chain	Residue	Modelled	Actual	Comment	Reference
Е	-15	HIS	-	expression tag	UNP A0A3R7J519
Е	-14	HIS	_	expression tag	UNP A0A3R7J519
Е	-13	HIS	-	expression tag	UNP A0A3R7J519
Е	-12	HIS	_	expression tag	UNP A0A3R7J519
Е	-11	HIS	-	expression tag	UNP A0A3R7J519
Е	-10	HIS	-	expression tag	UNP A0A3R7J519
Е	-9	SER	-	expression tag	UNP A0A3R7J519
Е	-8	SER	-	expression tag	UNP A0A3R7J519
Е	-7	GLY	-	expression tag	UNP A0A3R7J519
Е	-6	LEU	-	expression tag	UNP A0A3R7J519
Е	-5	VAL	-	expression tag	UNP A0A3R7J519
Е	-4	PRO	-	expression tag	UNP A0A3R7J519
Е	-3	ARG	-	expression tag	UNP A0A3R7J519
Е	-2	GLY	_	expression tag	UNP A0A3R7J519
Е	-1	SER	-	expression tag	UNP A0A3R7J519
Е	0	HIS	-	expression tag	UNP A0A3R7J519
F	-19	MET	-	initiating methionine	UNP A0A3R7J519
F	-18	GLY	-	expression tag	UNP A0A3R7J519
F	-17	SER	-	expression tag	UNP A0A3R7J519
F	-16	SER	-	expression tag	UNP A0A3R7J519
F	-15	HIS	-	expression tag	UNP A0A3R7J519
F	-14	HIS	-	expression tag	UNP A0A3R7J519
F	-13	HIS	-	expression tag	UNP A0A3R7J519
F	-12	HIS	-	expression tag	UNP A0A3R7J519
F	-11	HIS	-	expression tag	UNP A0A3R7J519
F	-10	HIS	-	expression tag	UNP A0A3R7J519
F	-9	SER	-	expression tag	UNP A0A3R7J519
F	-8	SER	-	expression tag	UNP A0A3R7J519
F	-7	GLY	-	expression tag	UNP A0A3R7J519
F	-6	LEU	-	expression tag	UNP A0A3R7J519
F	-5	VAL	-	expression tag	UNP A0A3R7J519
F	-4	PRO	-	expression tag	UNP A0A3R7J519
F	-3	ARG	-	expression tag	UNP A0A3R7J519
F	-2	GLY	-	expression tag	UNP A0A3R7J519
F	-1	SER	-	expression tag	UNP A0A3R7J519
F	0	HIS	-	expression tag	UNP A0A3R7J519
G	-19	MET	-	initiating methionine	UNP A0A3R7J519
G	-18	GLY	-	expression tag	UNP A0A3R7J519
G	-17	SER	-	expression tag	UNP A0A3R7J519
G	-16	SER	-	expression tag	UNP A0A3R7J519
G	-15	HIS	-	expression tag	UNP A0A3R7J519
G	-14	HIS	_	expression tag	UNP A0A3R7J519



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00	V V L	17

Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	expression tag	UNP A0A3R7J519
G	-12	HIS	-	expression tag	UNP A0A3R7J519
G	-11	HIS	_	expression tag	UNP A0A3R7J519
G	-10	HIS	-	expression tag	UNP A0A3R7J519
G	-9	SER	_	expression tag	UNP A0A3R7J519
G	-8	SER	_	expression tag	UNP A0A3R7J519
G	-7	GLY	_	expression tag	UNP A0A3R7J519
G	-6	LEU	-	expression tag	UNP A0A3R7J519
G	-5	VAL	-	expression tag	UNP A0A3R7J519
G	-4	PRO	-	expression tag	UNP A0A3R7J519
G	-3	ARG	-	expression tag	UNP A0A3R7J519
G	-2	GLY	-	expression tag	UNP A0A3R7J519
G	-1	SER	-	expression tag	UNP A0A3R7J519
G	0	HIS	-	expression tag	UNP A0A3R7J519
Н	-19	MET	-	initiating methionine	UNP A0A3R7J519
Н	-18	GLY	-	expression tag	UNP A0A3R7J519
Н	-17	SER	_	expression tag	UNP A0A3R7J519
Н	-16	SER	-	expression tag	UNP A0A3R7J519
Н	-15	HIS	_	expression tag	UNP A0A3R7J519
Н	-14	HIS	-	expression tag	UNP A0A3R7J519
Н	-13	HIS	-	expression tag	UNP A0A3R7J519
Н	-12	HIS	-	expression tag	UNP A0A3R7J519
Н	-11	HIS	-	expression tag	UNP A0A3R7J519
Н	-10	HIS	-	expression tag	UNP A0A3R7J519
Н	-9	SER	-	expression tag	UNP A0A3R7J519
Н	-8	SER	-	expression tag	UNP A0A3R7J519
Н	-7	GLY	-	expression tag	UNP A0A3R7J519
Н	-6	LEU	-	expression tag	UNP A0A3R7J519
Н	-5	VAL	-	expression tag	UNP A0A3R7J519
Н	-4	PRO	-	expression tag	UNP A0A3R7J519
Н	-3	ARG	-	expression tag	UNP A0A3R7J519
Н	-2	GLY	-	expression tag	UNP A0A3R7J519
Н	-1	SER	-	expression tag	UNP A0A3R7J519
Н	0	HIS	-	expression tag	UNP A0A3R7J519
Ι	-19	MET	-	initiating methionine	UNP A0A3R7J519
Ι	-18	GLY	-	expression tag	UNP A0A3R7J519
Ι	-17	SER	-	expression tag	UNP A0A3R7J519
Ι	-16	SER	-	expression tag	UNP A0A3R7J519
Ι	-15	HIS	-	expression tag	UNP A0A3R7J519
Ι	-14	HIS	-	expression tag	UNP A0A3R7J519
Ι	-13	HIS	-	expression tag	UNP A0A3R7J519
Ι	-12	HIS	-	expression tag	UNP A0A3R7J519



Chain	Residue	Modelled	Actual	Comment	Reference
Ι	-11	HIS	-	expression tag	UNP A0A3R7J519
Ι	-10	HIS	-	expression tag	UNP A0A3R7J519
Ι	-9	SER	-	expression tag	UNP A0A3R7J519
Ι	-8	SER	-	expression tag	UNP A0A3R7J519
Ι	-7	GLY	-	expression tag	UNP A0A3R7J519
Ι	-6	LEU	-	expression tag	UNP A0A3R7J519
Ι	-5	VAL	_	expression tag	UNP A0A3R7J519
Ι	-4	PRO	-	expression tag	UNP A0A3R7J519
Ι	-3	ARG	-	expression tag	UNP A0A3R7J519
Ι	-2	GLY	-	expression tag	UNP A0A3R7J519
Ι	-1	SER	-	expression tag	UNP A0A3R7J519
Ι	0	HIS	-	expression tag	UNP A0A3R7J519
J	-19	MET	-	initiating methionine	UNP A0A3R7J519
J	-18	GLY	-	expression tag	UNP A0A3R7J519
J	-17	SER	-	expression tag	UNP A0A3R7J519
J	-16	SER	-	expression tag	UNP A0A3R7J519
J	-15	HIS	-	expression tag	UNP A0A3R7J519
J	-14	HIS	-	expression tag	UNP A0A3R7J519
J	-13	HIS	-	expression tag	UNP A0A3R7J519
J	-12	HIS	-	expression tag	UNP A0A3R7J519
J	-11	HIS	-	expression tag	UNP A0A3R7J519
J	-10	HIS	-	expression tag	UNP A0A3R7J519
J	-9	SER	-	expression tag	UNP A0A3R7J519
J	-8	SER	-	expression tag	UNP A0A3R7J519
J	-7	GLY	-	expression tag	UNP A0A3R7J519
J	-6	LEU	-	expression tag	UNP A0A3R7J519
J	-5	VAL	-	expression tag	UNP A0A3R7J519
J	-4	PRO	-	expression tag	UNP A0A3R7J519
J	-3	ARG	-	expression tag	UNP A0A3R7J519
J	-2	GLY	-	expression tag	UNP A0A3R7J519
J	-1	SER	-	expression tag	UNP A0A3R7J519
J	0	HIS	-	expression tag	UNP A0A3R7J519
K	-19	MET	-	initiating methionine	UNP A0A3R7J519
K	-18	GLY	-	expression tag	UNP A0A3R7J519
K	-17	SER	-	expression tag	UNP A0A3R7J519
K	-16	SER	-	expression tag	UNP A0A3R7J519
K	-15	HIS	-	expression tag	UNP A0A3R7J519
K	-14	HIS	-	expression tag	UNP A0A3R7J519
K	-13	HIS	-	expression tag	UNP A0A3R7J519
K	-12	HIS	-	expression tag	UNP A0A3R7J519
K	-11	HIS	-	expression tag	UNP A0A3R7J519
K	-10	HIS	-	expression tag	UNP A0A3R7J519



Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	SER	-	expression tag	UNP A0A3R7J519
K	-8	SER	-	expression tag	UNP A0A3R7J519
K	-7	GLY	-	expression tag	UNP A0A3R7J519
K	-6	LEU	_	expression tag	UNP A0A3R7J519
K	-5	VAL	-	expression tag	UNP A0A3R7J519
K	-4	PRO	-	expression tag	UNP A0A3R7J519
K	-3	ARG	-	expression tag	UNP A0A3R7J519
K	-2	GLY	_	expression tag	UNP A0A3R7J519
K	-1	SER	_	expression tag	UNP A0A3R7J519
K	0	HIS	-	expression tag	UNP A0A3R7J519
L	-19	MET	-	initiating methionine	UNP A0A3R7J519
L	-18	GLY	-	expression tag	UNP A0A3R7J519
L	-17	SER	-	expression tag	UNP A0A3R7J519
L	-16	SER	-	expression tag	UNP A0A3R7J519
L	-15	HIS	-	expression tag	UNP A0A3R7J519
L	-14	HIS	-	expression tag	UNP A0A3R7J519
L	-13	HIS	-	expression tag	UNP A0A3R7J519
L	-12	HIS	-	expression tag	UNP A0A3R7J519
L	-11	HIS	_	expression tag	UNP A0A3R7J519
L	-10	HIS	-	expression tag	UNP A0A3R7J519
L	-9	SER	-	expression tag	UNP A0A3R7J519
L	-8	SER	-	expression tag	UNP A0A3R7J519
L	-7	GLY	-	expression tag	UNP A0A3R7J519
L	-6	LEU	-	expression tag	UNP A0A3R7J519
L	-5	VAL	-	expression tag	UNP A0A3R7J519
L	-4	PRO	-	expression tag	UNP A0A3R7J519
L	-3	ARG	-	expression tag	UNP A0A3R7J519
L	-2	GLY	-	expression tag	UNP A0A3R7J519
L	-1	SER	-	expression tag	UNP A0A3R7J519
L	0	HIS	-	expression tag	UNP A0A3R7J519
M	-19	MET	-	initiating methionine	UNP A0A3R7J519
M	-18	GLY	-	expression tag	UNP A0A3R7J519
M	-17	SER	-	expression tag	UNP A0A3R7J519
M	-16	SER	-	expression tag	UNP A0A3R7J519
M	-15	HIS	-	expression tag	UNP A0A3R7J519
M	-14	HIS	-	expression tag	UNP A0A3R7J519
M	-13	HIS	-	expression tag	UNP A0A3R7J519
М	-12	HIS	-	expression tag	UNP A0A3R7J519
M	-11	HIS	-	expression tag	UNP A0A3R7J519
M	-10	HIS	-	expression tag	UNP A0A3R7J519
M	-9	SER	-	expression tag	UNP A0A3R7J519
М	-8	SER	-	expression tag	UNP A0A3R7J519



Chain	Residue	Modelled	Actual	Comment	Reference
М	-7	GLY	-	expression tag	UNP A0A3R7J519
М	-6	LEU	-	expression tag	UNP A0A3R7J519
М	-5	VAL	-	expression tag	UNP A0A3R7J519
M	-4	PRO	-	expression tag	UNP A0A3R7J519
М	-3	ARG	-	expression tag	UNP A0A3R7J519
М	-2	GLY	-	expression tag	UNP A0A3R7J519
М	-1	SER	_	expression tag	UNP A0A3R7J519
М	0	HIS	_	expression tag	UNP A0A3R7J519
N	-19	MET	_	initiating methionine	UNP A0A3R7J519
N	-18	GLY	-	expression tag	UNP A0A3R7J519
N	-17	SER	-	expression tag	UNP A0A3R7J519
N	-16	SER	-	expression tag	UNP A0A3R7J519
N	-15	HIS	-	expression tag	UNP A0A3R7J519
N	-14	HIS	-	expression tag	UNP A0A3R7J519
N	-13	HIS	-	expression tag	UNP A0A3R7J519
N	-12	HIS	-	expression tag	UNP A0A3R7J519
N	-11	HIS	_	expression tag	UNP A0A3R7J519
N	-10	HIS	-	expression tag	UNP A0A3R7J519
N	-9	SER	-	expression tag	UNP A0A3R7J519
N	-8	SER	-	expression tag	UNP A0A3R7J519
N	-7	GLY	_	expression tag	UNP A0A3R7J519
N	-6	LEU	-	expression tag	UNP A0A3R7J519
N	-5	VAL	-	expression tag	UNP A0A3R7J519
N	-4	PRO	-	expression tag	UNP A0A3R7J519
N	-3	ARG	-	expression tag	UNP A0A3R7J519
N	-2	GLY	-	expression tag	UNP A0A3R7J519
N	-1	SER	-	expression tag	UNP A0A3R7J519
N	0	HIS	-	expression tag	UNP A0A3R7J519
0	-19	MET	-	initiating methionine	UNP A0A3R7J519
0	-18	GLY	-	expression tag	UNP A0A3R7J519
0	-17	SER	-	expression tag	UNP A0A3R7J519
0	-16	SER	-	expression tag	UNP A0A3R7J519
0	-15	HIS	-	expression tag	UNP A0A3R7J519
0	-14	HIS	-	expression tag	UNP A0A3R7J519
0	-13	HIS	-	expression tag	UNP A0A3R7J519
0	-12	HIS	-	expression tag	UNP A0A3R7J519
0	-11	HIS	-	expression tag	UNP A0A3R7J519
0	-10	HIS	-	expression tag	UNP A0A3R7J519
0	-9	SER	-	expression tag	UNP A0A3R7J519
0	-8	SER	-	expression tag	UNP A0A3R7J519
0	-7	GLY	-	expression tag	UNP A0A3R7J519
0	-6	LEU	-	expression tag	UNP A0A3R7J519



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Chain	Residue	Modelled	Actual	Comment	Reference
0	-5	VAL	-	expression tag	UNP A0A3R7J519
0	-4	PRO	-	expression tag	UNP A0A3R7J519
0	-3	ARG	-	expression tag	UNP A0A3R7J519
0	-2	GLY	-	expression tag	UNP A0A3R7J519
0	-1	SER	-	expression tag	UNP A0A3R7J519
0	0	HIS	-	expression tag	UNP A0A3R7J519
Р	-19	MET	-	initiating methionine	UNP A0A3R7J519
Р	-18	GLY	-	expression tag	UNP A0A3R7J519
Р	-17	SER	-	expression tag	UNP A0A3R7J519
Р	-16	SER	-	expression tag	UNP A0A3R7J519
Р	-15	HIS	-	expression tag	UNP A0A3R7J519
Р	-14	HIS	-	expression tag	UNP A0A3R7J519
Р	-13	HIS	-	expression tag	UNP A0A3R7J519
Р	-12	HIS	-	expression tag	UNP A0A3R7J519
Р	-11	HIS	-	expression tag	UNP A0A3R7J519
Р	-10	HIS	-	expression tag	UNP A0A3R7J519
Р	-9	SER	-	expression tag	UNP A0A3R7J519
Р	-8	SER	-	expression tag	UNP A0A3R7J519
Р	-7	GLY	-	expression tag	UNP A0A3R7J519
Р	-6	LEU	-	expression tag	UNP A0A3R7J519
Р	-5	VAL	-	expression tag	UNP A0A3R7J519
Р	-4	PRO	-	expression tag	UNP A0A3R7J519
Р	-3	ARG	-	expression tag	UNP A0A3R7J519
Р	-2	GLY	-	expression tag	UNP A0A3R7J519
Р	-1	SER	-	expression tag	UNP A0A3R7J519
Р	0	HIS	-	expression tag	UNP A0A3R7J519

• Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
9	Л	1	Total	С	Ν	Ο	Р	0	0	
	D	1	48	21	7	17	3	0	0	
0	Ц	1	Total	С	Ν	Ο	Р	0	0	
	11	1	48	21	7	17	3	0	0	
9	т	1	Total	С	Ν	Ο	Р	0	0	
	J	1	48	21	7	17	3	0	0	
9	т	1	Total	С	Ν	Ο	Р	0	0	
	L	1	48	21	7	17	3	0	0	
9	Ν	1	Total	С	Ν	Ο	Р	0	0	
	11	1	48	21	7	17	3	0	U	
9	P	1	Total	С	Ν	Ο	Р	0	0	
	1	1	48	21	7	17	3	0	0	

• Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	Ι	1	Total 8	С 4	N 1	O 3	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	69	Total O 69 69	0	0
4	В	70	Total O 70 70	0	0
4	С	55	$\begin{array}{cc} \text{Total} & \text{O} \\ 55 & 55 \end{array}$	0	0
4	D	110	Total O 110 110	0	0
4	Е	66	Total O 66 66	0	0
4	F	90	Total O 90 90	0	0
4	G	70	Total O 70 70	0	0
4	Н	97	Total O 97 97	0	0
4	Ι	114	Total O 114 114	0	0
4	J	144	Total O 144 144	0	0
4	К	96	Total O 96 96	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	152	Total O 152 152	0	0
4	М	100	Total O 100 100	0	0
4	Ν	140	Total O 140 140	0	0
4	О	99	Total O 99 99	0	0
4	Р	166	Total O 166 166	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Aldo/keto reductase













4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants	111.89Å 111.89Å 563.24Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	35.38 - 2.32	Depositor
Resolution (A)	37.77 - 2.32	EDS
% Data completeness	99.2 (35.38-2.32)	Depositor
(in resolution range)	99.4 (37.77-2.32)	EDS
R _{merge}	0.16	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.42 (at 2.31 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
D D.	0.181 , 0.217	Depositor
Λ, Λ_{free}	0.181 , 0.218	DCC
R_{free} test set	14758 reflections (4.98%)	wwPDB-VP
Wilson B-factor $(Å^2)$	37.2	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.34 , 46.4	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	40000	wwPDB-VP
Average B, all atoms $(Å^2)$	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 34.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1494e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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: TRS, NDP

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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.48	0/2353	0.62	0/3189	
1	В	0.44	0/2467	0.63	0/3349	
1	С	0.43	0/2316	0.63	0/3136	
1	D	0.43	0/2490	0.65	0/3379	
1	Е	0.43	0/2333	0.61	0/3163	
1	F	0.43	0/2487	0.63	0/3376	
1	G	0.43	0/2350	0.64	0/3187	
1	Н	0.47	0/2434	0.67	0/3301	
1	Ι	0.44	0/2380	0.67	0/3227	
1	J	0.47	0/2534	0.65	0/3439	
1	К	0.45	0/2339	0.63	0/3168	
1	L	0.48	0/2578	0.67	0/3495	
1	М	0.45	0/2343	0.65	0/3175	
1	N	0.45	0/2501	0.65	0/3397	
1	0	0.46	0/2342	0.66	0/3176	
1	Р	0.46	0/2607	0.67	0/3538	
All	All	0.45	0/38854	0.65	0/52695	

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	А	2309	0	2260	11	0
1	В	2414	0	2352	16	0
1	С	2272	0	2230	13	0
1	D	2437	0	2383	16	0
1	Е	2288	0	2254	23	0
1	F	2433	0	2374	18	0
1	G	2305	0	2253	18	0
1	Н	2383	0	2321	16	0
1	Ι	2333	0	2287	11	0
1	J	2480	0	2411	19	0
1	Κ	2295	0	2250	21	0
1	L	2526	0	2462	21	0
1	М	2298	0	2262	17	0
1	Ν	2446	0	2391	18	0
1	0	2295	0	2248	19	0
1	Р	2552	0	2490	14	0
2	D	48	0	26	1	0
2	Н	48	0	26	4	0
2	J	48	0	26	2	0
2	L	48	0	26	7	0
2	Ν	48	0	26	1	0
2	Р	48	0	26	4	0
3	Ι	8	0	12	0	0
4	А	69	0	0	0	0
4	В	70	0	0	0	0
4	С	55	0	0	0	0
4	D	110	0	0	0	0
4	Ε	66	0	0	0	0
4	F	90	0	0	1	0
4	G	70	0	0	0	0
4	H	97	0	0	0	0
4	Ι	114	0	0	1	0
4	J	144	0	0	1	0
4	K	96	0	0	0	0
4	L	152	0	0	2	0
4	М	100	0	0	1	0
4	N	140	0	0	0	0
4	0	99	0	0	1	0
4	Р	166	0	0	2	0
All	All	40000	0	37396	245	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.



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:112:VAL:HG22	1:C:127:TYR:CZ	2.20	0.76
1:L:214:TRP:CE3	2:L:401:NDP:H41N	2.24	0.71
1:B:152:GLY:O	1:H:109:ARG:NH1	2.24	0.70
1:B:268:GLU:O	1:B:272:VAL:HG23	1.93	0.68
1:G:17:VAL:HG13	1:G:287:ILE:HA	1.74	0.68
1:L:327:GLU:OE2	1:O:134:ARG:NH1	2.26	0.68
1:F:262:LEU:HD11	1:F:272:VAL:HG11	1.78	0.66
1:M:50:ALA:HB2	1:M:85:LYS:NZ	2.11	0.65
1:O:108:ILE:O	1:O:112:VAL:HG23	1.98	0.63
1:J:12:LYS:HD2	1:P:98:PRO:HB3	1.80	0.62
1:G:291:ARG:HH21	1:G:295:GLN:HE22	1.48	0.61
1:O:112:VAL:HG22	1:0:127:TYR:CZ	2.36	0.61
1:E:229:GLU:OE1	1:E:252:ARG:NH2	2.33	0.60
1:A:152:GLY:O	1:E:109:ARG:NH1	2.34	0.60
1:E:225:ALA:HA	1:E:228:LYS:HG3	1.83	0.60
1:H:212:ILE:HG22	1:H:287:ILE:CG1	2.31	0.59
1:J:246:LEU:C	1:J:248:ASP:N	2.56	0.59
1:E:205:ARG:HH21	1:E:205:ARG:HG2	1.66	0.59
1:G:148:LEU:HD13	1:G:154:ILE:HD12	1.85	0.58
1:F:262:LEU:CD1	1:F:272:VAL:HG11	2.34	0.58
1:K:20:THR:HG21	1:K:62:THR:OG1	2.03	0.58
1:L:205:ARG:HD2	1:L:282:GLY:HA3	1.84	0.58
1:M:228:LYS:NZ	4:M:402:HOH:O	2.36	0.58
1:I:205:ARG:HG2	1:I:205:ARG:HH21	1.69	0.57
1:H:252:ARG:HA	1:H:255:ILE:HD12	1.87	0.57
1:L:214:TRP:CZ3	2:L:401:NDP:H41N	2.39	0.57
1:K:61:ARG:NH1	1:K:64:GLU:OE1	2.35	0.57
1:I:152:GLY:O	1:M:109:ARG:NH1	2.37	0.57
1:I:326:PRO:HG3	1:P:161:ASN:O	2.05	0.56
1:M:32:SER:O	1:M:36:MET:HG3	2.05	0.56
1:J:226:ILE:C	1:J:228:LYS:H	2.09	0.56
1:L:287:ILE:HG22	2:L:401:NDP:H4D	1.87	0.56
1:O:52:VAL:HG21	1:O:289:GLY:HA3	1.87	0.56
1:E:150:ARG:HH12	1:G:150:ARG:HD2	1.70	0.56
1:C:112:VAL:HG22	1:C:127:TYR:CE2	2.41	0.56
1:L:327:GLU:CD	1:O:134:ARG:HH12	2.10	0.55
1:M:205:ARG:HH21	1:M:205:ARG:HG2	1.71	0.55
1:M:249:PRO:HD2	1:M:251:GLN:HB2	1.88	0.55
1:L:295:GLN:HE22	2:L:401:NDP:H2B	1.72	0.55
1:N:250:GLN:O	1:N:253:GLU:OE1	2.23	0.55

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:176:ARG:NH1	4:F:402:HOH:O	2.35	0.55
1:E:151:GLN:OE1	1:E:153:LYS:HE3	2.06	0.55
1:H:314:ALA:O	1:H:318:ILE:HG12	2.07	0.55
1:K:148:LEU:HD13	1:K:154:ILE:HD12	1.89	0.55
1:P:151:GLN:OE1	1:P:153:LYS:HE2	2.07	0.55
1:L:212:ILE:HG22	1:L:287:ILE:CG1	2.37	0.54
1:L:214:TRP:CE3	1:L:215:SER:HB3	2.42	0.54
1:B:109:ARG:NH1	1:F:152:GLY:O	2.40	0.54
1:C:326:PRO:HG3	1:F:161:ASN:O	2.08	0.54
1:B:59:LYS:HE3	1:B:91:GLY:O	2.07	0.54
1:N:186:GLN:OE1	2:N:401:NDP:H2N	2.07	0.54
1:C:245:ALA:C	1:C:247:LYS:N	2.61	0.54
1:N:62:THR:O	1:N:66:LEU:HD12	2.07	0.54
1:0:15:ARG:HD2	1:O:284:THR:O	2.06	0.54
1:M:15:ARG:HD2	1:M:284:THR:O	2.06	0.54
1:F:216:PRO:HG3	1:F:287:ILE:O	2.08	0.54
1:C:148:LEU:HB3	1:C:154:ILE:HD12	1.90	0.53
1:D:194:ARG:NH1	1:D:319:PHE:O	2.39	0.53
1:E:221:LEU:HD11	1:E:255:ILE:HG13	1.89	0.53
1:M:50:ALA:HB2	1:M:85:LYS:HZ3	1.72	0.53
1:O:271:GLU:OE1	1:O:301:ARG:NH1	2.41	0.53
1:H:186:GLN:OE1	2:H:401:NDP:H2N	2.08	0.53
1:K:86:VAL:O	1:K:87:TYR:HB2	2.08	0.53
1:I:102:LYS:HE3	4:I:542:HOH:O	2.09	0.53
1:B:291:ARG:HH11	1:B:291:ARG:HG2	1.73	0.53
1:D:161:ASN:O	1:G:326:PRO:HG3	2.09	0.53
1:H:212:ILE:HG22	1:H:287:ILE:HG12	1.91	0.52
1:K:326:PRO:HG3	1:N:161:ASN:O	2.10	0.52
1:N:246:LEU:HD23	1:N:246:LEU:N	2.25	0.52
1:M:102:LYS:HB3	1:M:133:ASP:OD2	2.10	0.52
1:B:326:PRO:HG3	1:E:161:ASN:O	2.10	0.52
1:D:155:LEU:HD21	1:F:109:ARG:HD2	1.93	0.51
1:J:212:ILE:HG22	1:J:287:ILE:HG12	1.90	0.51
1:L:1:MET:N	4:L:504:HOH:O	2.44	0.51
1:P:214:TRP:CE3	2:P:401:NDP:H41N	2.45	0.51
1:C:224:GLY:O	1:C:228:LYS:HG3	2.10	0.51
1:K:205:ARG:HG2	1:K:205:ARG:HH21	1.76	0.51
1:G:224:GLY:O	1:G:228:LYS:HG3	2.11	0.51
1:E:4:THR:HB	1:E:15:ARG:HD3	1.92	0.51
1:G:262:LEU:CD1	1:G:269:PRO:HA	2.41	0.50
1:D:186:GLN:OE1	2:D:401:NDP:H2N	2.13	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:31:GLU:O	1:I:35:ILE:HD12	2.12	0.49
1:J:212:ILE:HG22	1:J:287:ILE:CG1	2.43	0.49
1:E:20:THR:HB	1:E:62:THR:HG21	1.93	0.49
1:B:313:THR:O	1:B:317:GLU:HG2	2.13	0.48
1:N:83:ALA:HA	1:N:126:LEU:O	2.13	0.48
1:O:191:LEU:HD22	1:O:319:PHE:CD2	2.48	0.48
1:A:85:LYS:HG3	1:A:128:GLN:HB2	1.94	0.48
1:D:109:ARG:NH1	1:H:152:GLY:O	2.44	0.48
1:K:227:ARG:HH22	1:K:263:ASP:CG	2.17	0.48
1:C:229:GLU:O	1:C:230:GLN:HG2	2.14	0.48
1:F:86:VAL:O	1:F:87:TYR:HB2	2.13	0.48
1:F:269:PRO:HA	1:F:272:VAL:HG12	1.95	0.48
2:H:401:NDP:H3B	2:H:401:NDP:H8A	1.95	0.48
1:G:15:ARG:HD2	1:G:284:THR:O	2.13	0.48
1:D:15:ARG:HD2	1:D:284:THR:O	2.14	0.48
1:E:308:THR:OG1	1:E:311:VAL:HG23	2.14	0.48
1:F:86:VAL:O	1:F:87:TYR:CB	2.62	0.48
1:D:59:LYS:HE3	1:D:89:ASN:O	2.13	0.47
1:C:35:ILE:H	1:C:35:ILE:HG13	1.50	0.47
1:J:186:GLN:OE1	2:J:401:NDP:H2N	2.14	0.47
1:I:148:LEU:HD13	1:I:154:ILE:HD12	1.97	0.47
1:K:12:LYS:HD2	1:O:98:PRO:HB3	1.97	0.47
1:K:227:ARG:NH1	1:K:263:ASP:OD1	2.36	0.47
1:0:102:LYS:HB3	1:0:133:ASP:OD2	2.14	0.47
1:P:124:ILE:O	1:P:154:ILE:HA	2.14	0.46
1:D:138:TRP:CZ2	1:D:170:ALA:HB2	2.51	0.46
1:E:51:ASN:HD22	1:E:51:ASN:HA	1.52	0.46
1:J:264:LYS:HE3	1:J:265:HIS:CE1	2.51	0.46
1:L:214:TRP:CE3	2:L:401:NDP:C4N	2.98	0.46
1:L:287:ILE:CG2	2:L:401:NDP:H4D	2.46	0.46
1:A:148:LEU:HB3	1:A:154:ILE:HD12	1.98	0.45
1:E:256:GLN:HE21	1:E:260:ASP:CG	2.20	0.45
1:F:226:ILE:HB	1:F:259:GLU:OE2	2.16	0.45
1:L:212:ILE:HG22	1:L:287:ILE:HG12	1.97	0.45
1:N:124:ILE:O	1:N:154:ILE:HA	2.16	0.45
1:B:103:LEU:O	1:B:136:THR:HG21	2.15	0.45
1:F:145:MET:HE2	1:F:157:VAL:HG22	1.98	0.45
1:P:186:GLN:OE1	2:P:401:NDP:H2N	2.17	0.45
1:E:36:MET:HE3	1:E:69:TRP:CD1	2.52	0.45
1:L:118:ARG:HD3	4:L:555:HOH:O	2.16	0.45
1:H:212:ILE:CG2	1:H:287:ILE:HG12	2.47	0.45



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:M:124:ILE:O	1:M:154:ILE:HA	2.16	0.45	
1:N:308:THR:OG1	1:N:311:VAL:HG23	2.17	0.45	
1:D:83:ALA:HA	1:D:126:LEU:O	2.17	0.45	
1:G:262:LEU:HD13	1:G:269:PRO:HA	1.98	0.45	
1:J:287:ILE:HG22	2:J:401:NDP:H4D	1.97	0.45	
1:P:287:ILE:O	2:P:401:NDP:H51N	2.17	0.45	
1:P:79:LYS:NZ	4:P:511:HOH:O	2.50	0.45	
1:A:326:PRO:HG3	1:H:161:ASN:O	2.17	0.44	
1:C:124:ILE:O	1:C:154:ILE:HA	2.16	0.44	
1:J:176:ARG:HD3	1:M:176:ARG:HG2	1.98	0.44	
1:J:226:ILE:O	1:J:228:LYS:N	2.49	0.44	
1:N:212:ILE:HG22	1:N:287:ILE:CG1	2.46	0.44	
1:G:102:LYS:HB3	1:G:133:ASP:OD2	2.17	0.44	
1:L:212:ILE:CG2	1:L:287:ILE:HG12	2.47	0.44	
1:E:256:GLN:NE2	1:E:260:ASP:OD1	2.50	0.44	
1:G:2:GLU:OE1	1:G:303:ALA:HB1	2.17	0.44	
1:I:109:ARG:NH1	1:0:152:GLY:0	2.51	0.44	
1:E:262:LEU:HD22	1:E:272:VAL:HG21	2.00	0.44	
2:H:401:NDP:O5D	2:H:401:NDP:H6N	2.18	0.44	
1:O:35:ILE:HD12	1:O:35:ILE:HA	1.66	0.44	
1:K:28:ASP:HB3	1:K:31:GLU:HG2	1.99	0.44	
1:A:32:SER:HA	1:A:35:ILE:HG22	2.00	0.43	
1:0:87:TYR:0	1:O:88:GLY:C	2.57	0.43	
1:J:212:ILE:CG2	1:J:287:ILE:HG12	2.48	0.43	
1:M:20:THR:OG1	1:M:62:THR:HG21	2.18	0.43	
1:N:212:ILE:CG2	1:N:287:ILE:HG12	2.49	0.43	
1:F:128:GLN:HA	1:F:158:GLY:O	2.19	0.43	
1:F:257:ARG:NH1	1:F:317:GLU:OE2	2.51	0.43	
1:K:36:MET:HE3	1:K:69:TRP:CD1	2.53	0.43	
1:K:148:LEU:HD13	1:K:154:ILE:CD1	2.48	0.43	
1:E:15:ARG:O	1:E:285:GLY:HA3	2.19	0.43	
1:H:17:VAL:HG21	1:H:212:ILE:HG23	1.99	0.43	
1:N:142:TRP:O	1:N:146:ASP:HB2	2.19	0.43	
1:A:148:LEU:HD13	1:A:154:ILE:HD12	2.01	0.43	
1:E:15:ARG:HD2	1:E:284:THR:O	2.19	0.43	
1:G:141:ILE:O	1:G:145:MET:HG2	2.19	0.43	
1:K:161:ASN:O	1:N:326:PRO:HG3	2.19	0.43	
1:A:309:ASP:O	1:A:313:THR:OG1	2.30	0.43	
1:F:314:ALA:O	1:F:318:ILE:HG13	2.18	0.43	
1:O:112:VAL:HG22	1:0:127:TYR:CE2	2.53	0.43	
1:C:192:CYS:SG	1:C:222:LEU:HD21	2.59	0.43	



	A + 0	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:D:228:LYS:HD2	1:D:228:LYS:HA	1.81	0.43	
1:G:128:GLN:HA	1:G:158:GLY:O	2.19	0.43	
1:N:97:TRP:CD2	1:N:98:PRO:HD2	2.53	0.43	
1:P:231:GLU:H	1:P:231:GLU:HG2	1.60	0.43	
1:B:86:VAL:O	1:B:87:TYR:CB	2.67	0.43	
1:J:124:ILE:O	1:J:154:ILE:HA	2.19	0.43	
1:J:217:LEU:HD22	1:J:273:ALA:HB3	2.01	0.43	
1:F:61:ARG:HA	1:F:61:ARG:HD2	1.87	0.42	
1:H:201:VAL:O	1:H:205:ARG:HG3	2.20	0.42	
1:L:15:ARG:O	1:L:285:GLY:HA3	2.20	0.42	
1:A:215:SER:O	1:A:215:SER:OG	2.35	0.42	
1:D:221:LEU:HD12	1:D:221:LEU:HA	1.90	0.42	
1:L:23:PHE:HB2	1:L:62:THR:HG23	2.00	0.42	
1:C:226:ILE:O	1:C:229:GLU:HB2	2.19	0.42	
1:E:83:ALA:HA	1:E:126:LEU:O	2.20	0.42	
1:I:6:LEU:O	1:I:9:ILE:HG12	2.18	0.42	
1:J:268:GLU:O	1:J:272:VAL:HG23	2.19	0.42	
1:N:29:GLU:OE2	1:N:61:ARG:NH2	2.52	0.42	
1:N:59:LYS:NZ	1:N:93:ASP:OD1	2.50	0.42	
1:C:256:GLN:NE2	1:C:260:ASP:OD1	2.50	0.42	
1:K:308:THR:OG1	1:K:311:VAL:HG23	2.20	0.42	
1:L:83:ALA:HA	1:L:126:LEU:O	2.18	0.42	
1:L:327:GLU:HG3	1:L:331:TRP:O	2.19	0.42	
1:K:36:MET:HE3	1:K:69:TRP:CG	2.54	0.42	
1:N:218:HIS:HD2	1:N:221:LEU:HD23	1.85	0.42	
1:G:195:ARG:HA	1:G:322:PRO:HG3	2.01	0.42	
1:L:212:ILE:HG22	1:L:287:ILE:HG13	2.01	0.42	
1:A:109:ARG:HG3	1:A:109:ARG:HH11	1.84	0.42	
1:B:136:THR:HG22	1:B:141:ILE:HG13	2.01	0.42	
1:E:189:TYR:OH	1:E:197:GLU:OE2	2.28	0.42	
1:G:314:ALA:O	1:G:318:ILE:HG13	2.20	0.42	
1:H:87:TYR:HB3	1:H:130:HIS:HB3	2.02	0.42	
1:N:198:MET:HA	1:N:324:PRO:HA	2.02	0.42	
1:A:116:LEU:CD1	1:A:153:LYS:HD3	2.50	0.41	
1:A:176:ARG:HG3	1:H:176:ARG:NE	2.35	0.41	
1:J:83:ALA:HA	1:J:126:LEU:O	2.20	0.41	
1:J:161:ASN:O	1:M:326:PRO:HG3	2.19	0.41	
1:F:6:LEU:O	1:F:9:ILE:HG12	2.20	0.41	
1:G:107:ASN:HA	1:G:110:ARG:HG2	2.01	0.41	
1:I:50:ALA:HB2	1:I:85:LYS:HZ3	1.84	0.41	
1:P:228:LYS:HB3	1:P:228:LYS:HE2	1.88	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:I:37:ASP:CG	1:I:76:ARG:HH11	2.24	0.41	
1:K:124:ILE:O	1:K:154:ILE:HA	2.20	0.41	
1:P:255:ILE:O	1:P:259:GLU:HG3	2.20	0.41	
1:O:136:THR:HG22	1:O:141:ILE:HG13	2.02	0.41	
1:H:287:ILE:HG22	2:H:401:NDP:H4D	2.02	0.41	
1:O:301:ARG:HG3	4:O:432:HOH:O	2.20	0.41	
1:B:29:GLU:OE2	1:B:61:ARG:NH2	2.54	0.41	
1:D:150:ARG:HH21	1:H:150:ARG:HG2	1.86	0.41	
1:G:87:TYR:OH	1:G:118:ARG:NE	2.49	0.41	
1:I:83:ALA:HA	1:I:126:LEU:O	2.20	0.41	
1:D:205:ARG:HD2	1:D:282:GLY:HA3	2.03	0.41	
1:D:215:SER:O	1:D:215:SER:OG	2.29	0.41	
1:K:152:GLY:O	1:O:109:ARG:NH1	2.53	0.41	
1:L:214:TRP:CD2	2:L:401:NDP:H41N	2.55	0.41	
1:E:258:TYR:CE1	1:E:262:LEU:HD11	2.56	0.41	
1:J:226:ILE:C	1:J:228:LYS:N	2.75	0.41	
1:P:241:ARG:HD2	4:P:557:HOH:O	2.20	0.41	
1:B:107:ASN:HA	1:B:110:ARG:HG2	2.03	0.40	
1:D:205:ARG:HG2	1:D:205:ARG:HH21	1.86	0.40	
1:K:150:ARG:NH2	1:M:150:ARG:HH11	2.18	0.40	
1:M:191:LEU:HD22	1:M:319:PHE:CD2	2.55	0.40	
1:P:287:ILE:HG22	2:P:401:NDP:H4D	2.03	0.40	
1:G:262:LEU:HD22	1:G:272:VAL:HG21	2.02	0.40	
1:J:79:LYS:NZ	4:J:515:HOH:O	2.53	0.40	
1:K:189:TYR:OH	1:K:197:GLU:OE2	2.25	0.40	
1:K:248:ASP:C	1:K:250:GLN:N	2.75	0.40	
1:M:128:GLN:HA	1:M:158:GLY:O	2.21	0.40	
1:B:249:PRO:HB2	1:B:250:GLN:H	1.57	0.40	
1:H:212:ILE:HG22	1:H:287:ILE:HG13	2.02	0.40	
1:J:86:VAL:O	1:J:87:TYR:HB2	2.22	0.40	
1:K:314:ALA:O	1:K:318:ILE:HG13	2.22	0.40	
1:M:280:ARG:HA	1:M:281:PRO:HD3	1.97	0.40	
1:N:97:TRP:CG	1:N:98:PRO:HD2	2.56	0.40	
1:O:88:GLY:HA2	1:O:101:ASP:HA	2.03	0.40	
1:P:292:THR:OG1	1:P:295:GLN:HG3	2.21	0.40	
1:B:124:ILE:O	1:B:154:ILE:HA	2.21	0.40	
1:B:161:ASN:O	1:E:326:PRO:HG3	2.20	0.40	
1:B:221:LEU:HD23	1:B:221:LEU:HA	1.91	0.40	
1:C:98:PRO:HB3	1:E:12:LYS:HD2	2.04	0.40	
1:D:150:ARG:HH11	1:F:150:ARG:HB3	1.87	0.40	
1:O:52:VAL:H	1:O:52:VAL:HG23	1.64	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	Perce	entiles
1	А	283/351~(81%)	274 (97%)	9~(3%)	0	100	100
1	В	304/351~(87%)	289~(95%)	13 (4%)	2(1%)	22	26
1	С	278/351~(79%)	269~(97%)	8 (3%)	1 (0%)	34	41
1	D	306/351~(87%)	294 (96%)	9(3%)	3(1%)	15	17
1	Е	284/351~(81%)	276 (97%)	7 (2%)	1 (0%)	34	41
1	F	307/351~(88%)	294 (96%)	11 (4%)	2 (1%)	22	26
1	G	284/351 (81%)	274 (96%)	10 (4%)	0	100	100
1	Н	297/351~(85%)	287 (97%)	8 (3%)	2 (1%)	22	26
1	Ι	290/351~(83%)	282 (97%)	8 (3%)	0	100	100
1	J	313/351~(89%)	300 (96%)	11 (4%)	2 (1%)	25	30
1	K	283/351~(81%)	276 (98%)	7 (2%)	0	100	100
1	L	316/351~(90%)	305 (96%)	10 (3%)	1 (0%)	41	50
1	М	285/351~(81%)	276 (97%)	7 (2%)	2(1%)	22	26
1	N	311/351~(89%)	296 (95%)	13 (4%)	2 (1%)	25	30
1	Ο	285/351 (81%)	277 (97%)	8 (3%)	0	100	100
1	Р	326/351~(93%)	315 (97%)	10 (3%)	1 (0%)	41	50
All	All	4752/5616 (85%)	4584 (96%)	149 (3%)	19 (0%)	34	41

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ε	249	PRO
1	J	227	ARG
1	М	249	PRO



Mol	Chain	Res	Type
1	В	87	TYR
1	D	87	TYR
1	F	87	TYR
1	Н	87	TYR
1	J	87	TYR
1	L	87	TYR
1	Ν	87	TYR
1	Р	87	TYR
1	F	55	TRP
1	Н	56	GLY
1	М	21	MET
1	С	87	TYR
1	В	55	TRP
1	N	55	TRP
1	D	55	TRP
1	D	102	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	А	237/275~(86%)	231 (98%)	6(2%)	47 64
1	В	246/275~(90%)	242 (98%)	4 (2%)	62 77
1	С	232/275~(84%)	222 (96%)	10 (4%)	29 40
1	D	249/275~(90%)	244 (98%)	5(2%)	55 71
1	Ε	235/275~(86%)	233~(99%)	2(1%)	78 89
1	F	249/275~(90%)	241 (97%)	8(3%)	39 53
1	G	236/275~(86%)	232~(98%)	4 (2%)	60 75
1	Η	243/275~(88%)	237~(98%)	6 (2%)	47 64
1	Ι	239/275~(87%)	236~(99%)	3~(1%)	69 81
1	J	252/275~(92%)	247 (98%)	5 (2%)	55 71
1	K	$23\overline{4/275}~(85\%)$	228 (97%)	6(3%)	46 62



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	256/275~(93%)	251~(98%)	5(2%)	55 71
1	М	236/275~(86%)	232~(98%)	4 (2%)	60 75
1	Ν	250/275~(91%)	247~(99%)	3~(1%)	71 83
1	Ο	234/275~(85%)	227~(97%)	7 (3%)	41 56
1	Р	258/275~(94%)	257~(100%)	1 (0%)	91 96
All	All	3886/4400 (88%)	3807 (98%)	79(2%)	55 71

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All (79) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	2	GLU
1	А	46	PHE
1	А	85	LYS
1	А	176	ARG
1	А	252	ARG
1	А	257	ARG
1	В	227	ARG
1	В	250	GLN
1	В	257	ARG
1	В	292	THR
1	С	21	MET
1	С	31	GLU
1	С	32	SER
1	С	35	ILE
1	С	46	PHE
1	С	68	SER
1	С	250	GLN
1	С	261	LEU
1	С	268	GLU
1	С	308	THR
1	D	226	ILE
1	D	227	ARG
1	D	247	LYS
1	D	261	LEU
1	D	264	LYS
1	Е	46	PHE
1	Е	51	ASN
1	F	21	MET
1	F	93	ASP
1	F	100	HIS



Mol	Chain	Res	Type
1	F	127	TYR
1	F	188	LEU
1	F	228	LYS
1	F	294	ASP
1	F	309	ASP
1	G	20	THR
1	G	61	ARG
1	G	130	HIS
1	G	251	GLN
1	Н	57	GLU
1	Н	93	ASP
1	Н	127	TYR
1	Н	251	GLN
1	Н	252	ARG
1	Н	253	GLU
1	Ι	46	PHE
1	Ι	230	GLN
1	Ι	291	ARG
1	J	28	ASP
1	J	93	ASP
1	J	239	SER
1	J	246	LEU
1	J	251	GLN
1	Κ	46	PHE
1	Κ	176	ARG
1	Κ	244	ASP
1	Κ	247	LYS
1	K	250	GLN
1	K	251	GLN
1	L	92	LEU
1	L	215	SER
1	L	234	ASN
1	L	239	SER
1	L	252	ARG
1	М	22	ASN
1	М	247	LYS
1	М	250	GLN
1	М	291	ARG
1	N	57	GLU
1	N	66	LEU
1	Ν	246	LEU
1	0	21	MET



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Mol	Chain	Res	Type
1	0	35	ILE
1	0	46	PHE
1	0	176	ARG
1	0	230	GLN
1	0	250	GLN
1	0	325	SER
1	Р	231	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such side chains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	251	GLN
1	Е	22	ASN
1	Ε	51	ASN
1	F	254	GLN
1	Κ	186	GLN
1	М	22	ASN
1	0	72	GLN
1	0	177	HIS
1	Р	234	ASN

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)

7 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).

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	B	ond ang	gles
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	Ν	401	-	45,52,52	0.77	0	53,80,80	0.90	2 (3%)
2	NDP	Р	401	-	45,52,52	0.67	0	53,80,80	1.02	3 (5%)
2	NDP	J	401	-	45,52,52	0.68	0	53,80,80	0.98	2 (3%)
3	TRS	Ι	401	-	7,7,7	0.41	0	9,9,9	0.59	0
2	NDP	D	401	-	45,52,52	0.70	0	53,80,80	0.84	1 (1%)
2	NDP	Н	401	-	45,52,52	0.69	0	53,80,80	0.86	0
2	NDP	L	401	-	45,52,52	0.75	1 (2%)	53,80,80	0.88	1 (1%)

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	NDP	Ν	401	-	-	3/30/77/77	0/5/5/5
2	NDP	Р	401	-	-	2/30/77/77	0/5/5/5
2	NDP	J	401	-	-	5/30/77/77	0/5/5/5
3	TRS	Ι	401	-	-	9/9/9/9	-
2	NDP	D	401	-	-	5/30/77/77	0/5/5/5
2	NDP	Н	401	-	-	3/30/77/77	0/5/5/5
2	NDP	L	401	-	-	3/30/77/77	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	L	401	NDP	P2B-O2B	2.45	1.63	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Р	401	NDP	O3B-C3B-C2B	3.01	119.71	111.17
2	N	401	NDP	C5A-C6A-N6A	2.68	124.43	120.35
2	J	401	NDP	C5A-C6A-N6A	2.65	124.38	120.35



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	J	401	NDP	O2B-P2B-O1X	-2.63	99.22	109.39
2	Р	401	NDP	C5A-C6A-N6A	2.40	124.00	120.35
2	Р	401	NDP	O2B-P2B-O1X	-2.37	100.23	109.39
2	Ν	401	NDP	O2A-PA-O1A	2.11	122.69	112.24
2	L	401	NDP	C5A-C6A-N6A	2.07	123.49	120.35
2	D	401	NDP	O2A-PA-O1A	2.03	122.30	112.24

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	D	401	NDP	C2B-O2B-P2B-O1X
2	Н	401	NDP	C5B-O5B-PA-O2A
2	J	401	NDP	C2B-O2B-P2B-O1X
2	L	401	NDP	C2B-O2B-P2B-O2X
2	Ν	401	NDP	C2B-O2B-P2B-O1X
3	Ι	401	TRS	C1-C-C2-O2
3	Ι	401	TRS	C3-C-C2-O2
3	Ι	401	TRS	N-C-C2-O2
2	L	401	NDP	O4D-C1D-N1N-C2N
2	Р	401	NDP	O4D-C1D-N1N-C2N
2	J	401	NDP	O4D-C1D-N1N-C2N
2	D	401	NDP	PN-O3-PA-O5B
2	Н	401	NDP	PN-O3-PA-O5B
2	J	401	NDP	PN-O3-PA-O5B
2	L	401	NDP	PN-O3-PA-O5B
2	Ν	401	NDP	PN-O3-PA-O5B
2	Р	401	NDP	PN-O3-PA-O5B
2	D	401	NDP	C2B-O2B-P2B-O2X
3	Ι	401	TRS	C2-C-C1-O1
3	Ι	401	TRS	N-C-C1-O1
3	Ι	401	TRS	C1-C-C3-O3
2	D	401	NDP	O4D-C1D-N1N-C2N
2	Н	401	NDP	O4D-C1D-N1N-C2N
2	Ν	401	NDP	O4D-C1D-N1N-C2N
3	Ι	401	TRS	C3-C-C1-O1
3	Ι	401	TRS	C2-C-C3-O3
2	J	401	NDP	C2B-O2B-P2B-O2X
2	D	401	NDP	PN-O3-PA-O2A
3	Ι	401	TRS	N-C-C3-O3
2	J	401	NDP	C2N-C3N-C7N-N7N

All (30) torsion outliers are listed below:



There are no ring outliers.

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Ν	401	NDP	1	0
2	Р	401	NDP	4	0
2	J	401	NDP	2	0
2	D	401	NDP	1	0
2	Н	401	NDP	4	0
2	L	401	NDP	7	0

6 monomers are involved in 19 short contacts:

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.































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, 95^{th} 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>	$\cdot 2$	$OWAB(Å^2)$	Q<0.9
1	А	296/351~(84%)	0.09	21 (7%) 16	21	28, 50, 91, 116	0
1	В	312/351~(88%)	0.28	27 (8%) 10	14	28, 49, 89, 116	0
1	С	292/351~(83%)	0.30	30 (10%) 6	9	29, 53, 88, 115	0
1	D	314/351~(89%)	0.10	23 (7%) 15	20	25, 41, 85, 127	0
1	Ε	294/351~(83%)	0.14	21 (7%) 16	21	30, 50, 87, 109	0
1	F	313/351~(89%)	0.18	22 (7%) 16	22	28, 48, 85, 111	0
1	G	296/351~(84%)	0.14	17 (5%) 23	30	28, 47, 82, 113	0
1	Η	307/351~(87%)	-0.02	13 (4%) 36	43	26, 41, 80, 114	0
1	Ι	300/351~(85%)	0.06	17 (5%) 23	30	23, 40, 80, 99	0
1	J	321/351~(91%)	-0.00	16 (4%) 28	36	22, 35, 76, 112	0
1	Κ	295/351~(84%)	-0.00	17 (5%) 23	29	24, 43, 76, 105	0
1	L	326/351~(92%)	-0.05	13 (3%) 38	45	22, 36, 71, 92	0
1	М	295/351~(84%)	-0.01	14 (4%) 31	38	24, 42, 81, 126	0
1	Ν	315/351~(89%)	-0.13	11 (3%) 44	51	24, 36, 70, 106	0
1	Ο	$29\overline{5}/351~(84\%)$	0.05	10 (3%) 45	52	25, 41, 74, 101	0
1	Р	330/351~(94%)	-0.04	14 (4%) 36	43	23, 33, 69, 93	0
All	All	4901/5616 (87%)	0.07	286 (5%) 23	29	22, 42, 82, 127	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	92	LEU	5.0
1	L	237	ALA	5.0
1	D	249	PRO	4.9
1	F	95	PRO	4.9
1	Ι	87	TYR	4.9



Mol	Chain	Res	Type	RSRZ
1	Р	92	LEU	4.9
1	В	226	ILE	4.8
1	L	95	PRO	4.8
1	Ν	249	PRO	4.8
1	В	224	GLY	4.6
1	С	87	TYR	4.6
1	М	260	ASP	4.6
1	L	230	GLN	4.5
1	В	230	GLN	4.5
1	G	256	GLN	4.5
1	Р	93	ASP	4.5
1	J	0	HIS	4.4
1	D	247	LYS	4.4
1	G	87	TYR	4.4
1	Е	71	ALA	4.4
1	С	225	ALA	4.4
1	J	-1	SER	4.4
1	Р	230	GLN	4.3
1	D	221	LEU	4.3
1	А	249	PRO	4.3
1	В	225	ALA	4.3
1	Р	242	ALA	4.3
1	М	60	GLY	4.3
1	В	92	LEU	4.2
1	А	260	ASP	4.2
1	С	256	GLN	4.2
1	Ι	60	GLY	4.2
1	K	87	TYR	4.2
1	J	245	ALA	4.2
1	0	53	TYR	4.2
1	F	93	ASP	4.1
1	Ι	95	PRO	3.9
1	D	331	TRP	3.9
1	F	226	ILE	3.9
1	0	96	ALA	3.9
1	F	260	ASP	3.9
1	C	224	GLY	3.9
1	М	225	ALA	3.9
1	М	226	ILE	3.9
1	D	95	PRO	3.9
1	М	256	GLN	3.8
1	K	246	LEU	3.8



Mol	Chain	Res	Type	RSRZ
1	С	88	GLY	3.8
1	В	227	ARG	3.8
1	С	247	LYS	3.8
1	J	252	ARG	3.8
1	В	91	GLY	3.7
1	Ι	61	ARG	3.7
1	М	248	ASP	3.7
1	М	65	ILE	3.7
1	А	230	GLN	3.7
1	J	253	GLU	3.6
1	С	117	LYS	3.6
1	Р	234	ASN	3.5
1	J	249	PRO	3.5
1	Р	94	GLY	3.5
1	В	331	TRP	3.5
1	Н	227	ARG	3.5
1	В	57	GLU	3.5
1	G	96	ALA	3.5
1	J	250	GLN	3.5
1	Н	331	TRP	3.4
1	Е	262	LEU	3.4
1	G	61	ARG	3.4
1	Е	51	ASN	3.4
1	В	245	ALA	3.4
1	А	246	LEU	3.4
1	А	87	TYR	3.4
1	D	93	ASP	3.4
1	В	246	LEU	3.4
1	0	230	GLN	3.4
1	Е	264	LYS	3.3
1	Р	245	ALA	3.3
1	Ι	246	LEU	3.3
1	Е	227	ARG	3.3
1	Ν	93	ASP	3.3
1	С	96	ALA	3.3
1	В	221	LEU	3.3
1	J	244	ASP	3.3
1	N	252	ARG	3.3
1	Ι	51	ASN	3.3
1	N	248	ASP	3.2
1	G	255	ILE	3.2
1	N	225	ALA	3.2



Mol	Chain	Res	Type	RSRZ
1	В	256	GLN	3.2
1	Е	62	THR	3.2
1	J	240	GLY	3.2
1	А	61	ARG	3.2
1	С	32	SER	3.2
1	K	29	GLU	3.2
1	В	95	PRO	3.2
1	В	55	TRP	3.1
1	L	96	ALA	3.1
1	Р	247	LYS	3.1
1	Н	226	ILE	3.1
1	0	87	TYR	3.1
1	А	264	LYS	3.1
1	Ι	247	LYS	3.1
1	G	52	VAL	3.1
1	N	251	GLN	3.1
1	F	331	TRP	3.1
1	Е	256	GLN	3.1
1	G	252	ARG	3.1
1	L	238	ALA	3.1
1	L	92	LEU	3.0
1	D	253	GLU	3.0
1	F	258	TYR	3.0
1	N	95	PRO	3.0
1	G	246	LEU	3.0
1	Н	262	LEU	3.0
1	G	251	GLN	3.0
1	0	231	GLU	3.0
1	В	260	ASP	3.0
1	D	248	ASP	3.0
1	L	244	ASP	3.0
1	D	92	LEU	2.9
1	Н	260	ASP	2.9
1	А	252	ARG	2.9
1	L	234	ASN	2.9
1	F	256	GLN	2.9
1	N	92	LEU	2.9
1	G	254	GLN	2.9
1	Е	261	LEU	2.9
1	D	251	GLN	2.9
1	Ι	231	GLU	2.9
1	С	252	ARG	2.9



Mol	Chain	Res	Type	RSRZ	
1	D	254	54 GLN 2.		
1	А	226	6 ILE 2.8		
1	Н	255	ILE	2.8	
1	J	254	GLN	2.8	
1	0	256	GLN	2.8	
1	G	231	GLU	2.8	
1	K	28	ASP	2.8	
1	Κ	225	ALA	2.8	
1	Е	230	GLN	2.8	
1	С	68	SER	2.8	
1	Е	229	GLU	2.8	
1	F	55	TRP	2.8	
1	Е	260	ASP	2.8	
1	0	226	ILE	2.8	
1	А	253	GLU	2.8	
1	Е	61	ARG	2.8	
1	Ι	256	GLN	2.7	
1	В	323	GLY	2.7	
1	L	94	GLY	2.7	
1	С	251	GLN	2.7	
1	D	55	TRP	2.7	
1	F	227	ARG	2.7	
1	В	261	LEU	2.7	
1	F	262	LEU	2.7	
1	Н	221	LEU	2.7	
1	В	244	ASP	2.7	
1	G	71	ALA	2.7	
1	0	21	MET	2.7	
1	Ι	260	ASP	2.7	
1	Κ	253	GLU	2.7	
1	С	254	GLN	2.6	
1	J	251	GLN	2.6	
1	С	255	ILE	2.6	
1	С	318	ILE	2.6	
1	А	221	LEU	2.6	
1	В	314	ALA	2.6	
1	В	258	TYR	2.6	
1	D	311	VAL	2.6	
1	М	262	LEU	2.6	
1	F	229	GLU	2.6	
1	Ι	253	GLU	2.6	
1	Р	244	ASP	2.6	



Mol	Chain	Res	Type	RSRZ
1	D	262	LEU	2.6
1	А	258	TYR	2.6
1	А	225	ALA	2.6
1	А	28	ASP	2.6
1	D	294	ASP	2.6
1	А	227	ARG	2.6
1	Κ	227	ARG	2.6
1	F	252	ARG	2.5
1	В	320	PRO	2.5
1	Н	224	GLY	2.5
1	М	253	GLU	2.5
1	В	263	ASP	2.5
1	F	221	LEU	2.5
1	С	310	GLU	2.5
1	Κ	261	LEU	2.5
1	С	31	GLU	2.5
1	Ν	256	GLN	2.5
1	С	248	ASP	2.5
1	С	64	GLU	2.5
1	Ι	52	VAL	2.5
1	D	94	GLY	2.5
1	F	263	ASP	2.5
1	F	57	GLU	2.5
1	Ε	21	MET	2.4
1	J	243	ALA	2.4
1	С	226	ILE	2.4
1	F	254	GLN	2.4
1	I	227	ARG	2.4
1	С	308	THR	2.4
1	Н	57	GLU	2.4
1	K	61	ARG	2.4
1	K	226	ILE	2.4
1	Н	254	GLN	2.4
1	K	245	ALA	2.4
1	Е	310	GLU	2.4
1	Н	229	GLU	2.4
1	G	227	ARG	2.4
1	Н	253	GLU	2.4
1	А	244	ASP	2.4
1	С	227	ARG	2.4
1	Ν	126	LEU	2.4
1	L	235	ARG	2.3



Mol	Chain	Res	Type	RSRZ
1	F	248	ASP	2.3
1	Е	265	HIS	2.3
1	D	256	GLN	2.3
1	Е	258	TYR	2.3
1	С	21	MET	2.3
1	Е	101	ASP	2.3
1	М	28	ASP	2.3
1	F	330	ALA	2.3
1	С	262	LEU	2.3
1	С	312	LEU	2.3
1	J	93	ASP	2.3
1	Е	228	LYS	2.3
1	Ι	96	ALA	2.3
1	A	262	LEU	2.3
1	G	120	GLY	2.3
1	K	260	ASP	2.3
1	F	249	PRO	2.3
1	Ι	245	ALA	2.3
1	D	313	THR	2.2
1	Ι	262	LEU	2.2
1	А	247	LYS	2.2
1	В	228	LYS	2.2
1	В	262	LEU	2.2
1	L	246	LEU	2.2
1	K	96	ALA	2.2
1	D	246	LEU	2.2
1	Ι	248	ASP	2.2
1	Н	95	PRO	2.2
1	М	61	ARG	2.2
1	F	318	ILE	2.2
1	0	51	ASN	2.2
1	G	312	LEU	2.2
1	Р	246	LEU	2.2
1	М	59	LYS	2.2
1	K	229	GLU	2.2
1	Р	229	GLU	2.2
1	E	96	ALA	2.2
1	Р	249	PRO	2.2
1	D	228	LYS	2.2
1	D	226	ILE	2.2
1	L	287	ILE	2.2
1	J	239	SER	2.2



Mol	Chain	Res	Type	RSRZ
1	С	314	ALA	2.1
1	Р	294	ASP	2.1
1	K	32	SER	2.1
1	Е	252	ARG	2.1
1	J	57	GLU	2.1
1	K	71	ALA	2.1
1	А	263	ASP	2.1
1	F	294	ASP	2.1
1	J	248	ASP	2.1
1	С	61	ARG	2.1
1	С	331	TRP	2.1
1	В	250	GLN	2.1
1	Е	68	SER	2.1
1	Р	126	LEU	2.1
1	Ν	94	GLY	2.1
1	D	314	ALA	2.1
1	М	21	MET	2.1
1	D	96	ALA	2.1
1	С	69	TRP	2.1
1	G	253	GLU	2.0
1	А	251	GLN	2.0
1	А	51	ASN	2.0
1	G	67	GLY	2.0
1	0	88	GLY	2.0
1	М	252	ARG	2.0
1	В	126	LEU	2.0
1	L	231	GLU	2.0
1	С	291	ARG	2.0
1	K	68	SER	2.0

Continued from previous page...

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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
3	TRS	Ι	401	8/8	0.74	0.29	56,64,67,70	0
2	NDP	N	401	48/48	0.83	0.22	37,62,81,84	48
2	NDP	Н	401	48/48	0.85	0.21	43,71,83,86	48
2	NDP	J	401	48/48	0.88	0.20	31,53,66,72	48
2	NDP	D	401	48/48	0.89	0.17	37,66,78,80	48
2	NDP	L	401	48/48	0.92	0.15	31,48,59,65	48
2	NDP	Р	401	48/48	0.93	0.16	27,43,55,59	48

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



















6.5 Other polymers (i)

There are no such residues in this entry.

