



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 04:54 am GMT

PDB ID : 6FMQ  
Title : Keap1 - peptide complex  
Authors : Talapatra, S.K.; Kozielski, F.; Wells, G.; Georgakopoulos, N.D.  
Deposited on : 2018-02-02  
Resolution : 2.10 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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

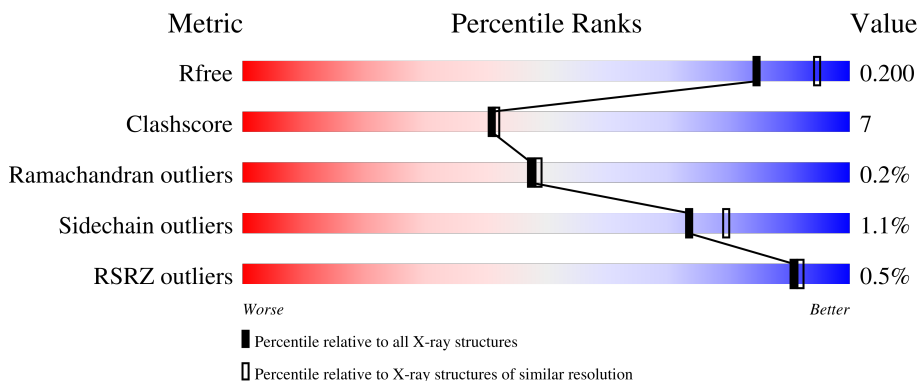
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	414	
1	B	414	
2	D	7	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	702	-	-	X	-
4	ACT	A	704	-	-	X	-
4	ACT	A	706	-	-	X	-
5	NA	B	708	-	-	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 4983 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2279	1408	422	432	17	0	11	0
1	B	285	2241	1387	408	430	16	1	7	0

There are 250 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	MET	-	initiating methionine	UNP Q14145
A	197	ALA	-	expression tag	UNP Q14145
A	198	MET	-	expression tag	UNP Q14145
A	199	GLY	-	expression tag	UNP Q14145
A	200	SER	-	expression tag	UNP Q14145
A	201	SER	-	expression tag	UNP Q14145
A	202	HIS	-	expression tag	UNP Q14145
A	203	HIS	-	expression tag	UNP Q14145
A	204	HIS	-	expression tag	UNP Q14145
A	205	HIS	-	expression tag	UNP Q14145
A	206	HIS	-	expression tag	UNP Q14145
A	207	HIS	-	expression tag	UNP Q14145
A	208	HIS	-	expression tag	UNP Q14145
A	209	HIS	-	expression tag	UNP Q14145
A	210	SER	-	expression tag	UNP Q14145
A	211	SER	-	expression tag	UNP Q14145
A	212	GLY	-	expression tag	UNP Q14145
A	213	LEU	-	expression tag	UNP Q14145
A	214	VAL	-	expression tag	UNP Q14145
A	215	PRO	-	expression tag	UNP Q14145
A	216	ARG	-	expression tag	UNP Q14145
A	217	GLY	-	expression tag	UNP Q14145
A	218	SER	-	expression tag	UNP Q14145
A	219	HIS	-	expression tag	UNP Q14145
A	220	MET	-	expression tag	UNP Q14145

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Chain	Residue	Modelled	Actual	Comment	Reference
A	221	ALA	-	expression tag	UNP Q14145
A	222	SER	-	expression tag	UNP Q14145
A	223	MET	-	expression tag	UNP Q14145
A	224	SER	-	expression tag	UNP Q14145
A	225	ASP	-	expression tag	UNP Q14145
A	226	SER	-	expression tag	UNP Q14145
A	227	GLU	-	expression tag	UNP Q14145
A	228	VAL	-	expression tag	UNP Q14145
A	229	ASN	-	expression tag	UNP Q14145
A	230	GLN	-	expression tag	UNP Q14145
A	231	GLU	-	expression tag	UNP Q14145
A	232	ALA	-	expression tag	UNP Q14145
A	233	LYS	-	expression tag	UNP Q14145
A	234	PRO	-	expression tag	UNP Q14145
A	235	GLU	-	expression tag	UNP Q14145
A	236	VAL	-	expression tag	UNP Q14145
A	237	LYS	-	expression tag	UNP Q14145
A	238	PRO	-	expression tag	UNP Q14145
A	239	GLU	-	expression tag	UNP Q14145
A	240	VAL	-	expression tag	UNP Q14145
A	241	LYS	-	expression tag	UNP Q14145
A	242	PRO	-	expression tag	UNP Q14145
A	243	GLU	-	expression tag	UNP Q14145
A	244	THR	-	expression tag	UNP Q14145
A	245	HIS	-	expression tag	UNP Q14145
A	246	ILE	-	expression tag	UNP Q14145
A	247	ASN	-	expression tag	UNP Q14145
A	248	LEU	-	expression tag	UNP Q14145
A	249	LYS	-	expression tag	UNP Q14145
A	250	VAL	-	expression tag	UNP Q14145
A	251	SER	-	expression tag	UNP Q14145
A	252	ASP	-	expression tag	UNP Q14145
A	253	GLY	-	expression tag	UNP Q14145
A	254	SER	-	expression tag	UNP Q14145
A	255	SER	-	expression tag	UNP Q14145
A	256	GLU	-	expression tag	UNP Q14145
A	257	ILE	-	expression tag	UNP Q14145
A	258	PHE	-	expression tag	UNP Q14145
A	259	PHE	-	expression tag	UNP Q14145
A	260	LYS	-	expression tag	UNP Q14145
A	261	ILE	-	expression tag	UNP Q14145
A	262	LYS	-	expression tag	UNP Q14145

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Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LYS	-	expression tag	UNP Q14145
A	264	THR	-	expression tag	UNP Q14145
A	265	THR	-	expression tag	UNP Q14145
A	266	PRO	-	expression tag	UNP Q14145
A	267	LEU	-	expression tag	UNP Q14145
A	268	ARG	-	expression tag	UNP Q14145
A	269	ARG	-	expression tag	UNP Q14145
A	270	LEU	-	expression tag	UNP Q14145
A	271	MET	-	expression tag	UNP Q14145
A	272	GLU	-	expression tag	UNP Q14145
A	273	ALA	-	expression tag	UNP Q14145
A	274	PHE	-	expression tag	UNP Q14145
A	275	ALA	-	expression tag	UNP Q14145
A	276	LYS	-	expression tag	UNP Q14145
A	277	ARG	-	expression tag	UNP Q14145
A	278	GLN	-	expression tag	UNP Q14145
A	279	GLY	-	expression tag	UNP Q14145
A	280	LYS	-	expression tag	UNP Q14145
A	281	GLU	-	expression tag	UNP Q14145
A	282	MET	-	expression tag	UNP Q14145
A	283	ASP	-	expression tag	UNP Q14145
A	284	SER	-	expression tag	UNP Q14145
A	285	LEU	-	expression tag	UNP Q14145
A	286	ARG	-	expression tag	UNP Q14145
A	287	PHE	-	expression tag	UNP Q14145
A	288	LEU	-	expression tag	UNP Q14145
A	289	TYR	-	expression tag	UNP Q14145
A	290	ASP	-	expression tag	UNP Q14145
A	291	GLY	-	expression tag	UNP Q14145
A	292	ILE	-	expression tag	UNP Q14145
A	293	ARG	-	expression tag	UNP Q14145
A	294	ILE	-	expression tag	UNP Q14145
A	295	GLN	-	expression tag	UNP Q14145
A	296	ALA	-	expression tag	UNP Q14145
A	297	ASP	-	expression tag	UNP Q14145
A	298	GLN	-	expression tag	UNP Q14145
A	299	THR	-	expression tag	UNP Q14145
A	300	PRO	-	expression tag	UNP Q14145
A	301	GLU	-	expression tag	UNP Q14145
A	302	ASP	-	expression tag	UNP Q14145
A	303	LEU	-	expression tag	UNP Q14145
A	304	ASP	-	expression tag	UNP Q14145

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Chain	Residue	Modelled	Actual	Comment	Reference
A	305	MET	-	expression tag	UNP Q14145
A	306	GLU	-	expression tag	UNP Q14145
A	307	ASP	-	expression tag	UNP Q14145
A	308	ASN	-	expression tag	UNP Q14145
A	309	ASP	-	expression tag	UNP Q14145
A	310	ILE	-	expression tag	UNP Q14145
A	311	ILE	-	expression tag	UNP Q14145
A	312	GLU	-	expression tag	UNP Q14145
A	313	ALA	-	expression tag	UNP Q14145
A	314	HIS	-	expression tag	UNP Q14145
A	315	ARG	-	expression tag	UNP Q14145
A	316	GLU	-	expression tag	UNP Q14145
A	317	GLN	-	expression tag	UNP Q14145
A	318	ILE	-	expression tag	UNP Q14145
A	319	GLY	-	expression tag	UNP Q14145
A	320	GLY	-	expression tag	UNP Q14145
B	196	MET	-	initiating methionine	UNP Q14145
B	197	ALA	-	expression tag	UNP Q14145
B	198	MET	-	expression tag	UNP Q14145
B	199	GLY	-	expression tag	UNP Q14145
B	200	SER	-	expression tag	UNP Q14145
B	201	SER	-	expression tag	UNP Q14145
B	202	HIS	-	expression tag	UNP Q14145
B	203	HIS	-	expression tag	UNP Q14145
B	204	HIS	-	expression tag	UNP Q14145
B	205	HIS	-	expression tag	UNP Q14145
B	206	HIS	-	expression tag	UNP Q14145
B	207	HIS	-	expression tag	UNP Q14145
B	208	HIS	-	expression tag	UNP Q14145
B	209	HIS	-	expression tag	UNP Q14145
B	210	SER	-	expression tag	UNP Q14145
B	211	SER	-	expression tag	UNP Q14145
B	212	GLY	-	expression tag	UNP Q14145
B	213	LEU	-	expression tag	UNP Q14145
B	214	VAL	-	expression tag	UNP Q14145
B	215	PRO	-	expression tag	UNP Q14145
B	216	ARG	-	expression tag	UNP Q14145
B	217	GLY	-	expression tag	UNP Q14145
B	218	SER	-	expression tag	UNP Q14145
B	219	HIS	-	expression tag	UNP Q14145
B	220	MET	-	expression tag	UNP Q14145
B	221	ALA	-	expression tag	UNP Q14145

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Chain	Residue	Modelled	Actual	Comment	Reference
B	222	SER	-	expression tag	UNP Q14145
B	223	MET	-	expression tag	UNP Q14145
B	224	SER	-	expression tag	UNP Q14145
B	225	ASP	-	expression tag	UNP Q14145
B	226	SER	-	expression tag	UNP Q14145
B	227	GLU	-	expression tag	UNP Q14145
B	228	VAL	-	expression tag	UNP Q14145
B	229	ASN	-	expression tag	UNP Q14145
B	230	GLN	-	expression tag	UNP Q14145
B	231	GLU	-	expression tag	UNP Q14145
B	232	ALA	-	expression tag	UNP Q14145
B	233	LYS	-	expression tag	UNP Q14145
B	234	PRO	-	expression tag	UNP Q14145
B	235	GLU	-	expression tag	UNP Q14145
B	236	VAL	-	expression tag	UNP Q14145
B	237	LYS	-	expression tag	UNP Q14145
B	238	PRO	-	expression tag	UNP Q14145
B	239	GLU	-	expression tag	UNP Q14145
B	240	VAL	-	expression tag	UNP Q14145
B	241	LYS	-	expression tag	UNP Q14145
B	242	PRO	-	expression tag	UNP Q14145
B	243	GLU	-	expression tag	UNP Q14145
B	244	THR	-	expression tag	UNP Q14145
B	245	HIS	-	expression tag	UNP Q14145
B	246	ILE	-	expression tag	UNP Q14145
B	247	ASN	-	expression tag	UNP Q14145
B	248	LEU	-	expression tag	UNP Q14145
B	249	LYS	-	expression tag	UNP Q14145
B	250	VAL	-	expression tag	UNP Q14145
B	251	SER	-	expression tag	UNP Q14145
B	252	ASP	-	expression tag	UNP Q14145
B	253	GLY	-	expression tag	UNP Q14145
B	254	SER	-	expression tag	UNP Q14145
B	255	SER	-	expression tag	UNP Q14145
B	256	GLU	-	expression tag	UNP Q14145
B	257	ILE	-	expression tag	UNP Q14145
B	258	PHE	-	expression tag	UNP Q14145
B	259	PHE	-	expression tag	UNP Q14145
B	260	LYS	-	expression tag	UNP Q14145
B	261	ILE	-	expression tag	UNP Q14145
B	262	LYS	-	expression tag	UNP Q14145
B	263	LYS	-	expression tag	UNP Q14145

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Chain	Residue	Modelled	Actual	Comment	Reference
B	264	THR	-	expression tag	UNP Q14145
B	265	THR	-	expression tag	UNP Q14145
B	266	PRO	-	expression tag	UNP Q14145
B	267	LEU	-	expression tag	UNP Q14145
B	268	ARG	-	expression tag	UNP Q14145
B	269	ARG	-	expression tag	UNP Q14145
B	270	LEU	-	expression tag	UNP Q14145
B	271	MET	-	expression tag	UNP Q14145
B	272	GLU	-	expression tag	UNP Q14145
B	273	ALA	-	expression tag	UNP Q14145
B	274	PHE	-	expression tag	UNP Q14145
B	275	ALA	-	expression tag	UNP Q14145
B	276	LYS	-	expression tag	UNP Q14145
B	277	ARG	-	expression tag	UNP Q14145
B	278	GLN	-	expression tag	UNP Q14145
B	279	GLY	-	expression tag	UNP Q14145
B	280	LYS	-	expression tag	UNP Q14145
B	281	GLU	-	expression tag	UNP Q14145
B	282	MET	-	expression tag	UNP Q14145
B	283	ASP	-	expression tag	UNP Q14145
B	284	SER	-	expression tag	UNP Q14145
B	285	LEU	-	expression tag	UNP Q14145
B	286	ARG	-	expression tag	UNP Q14145
B	287	PHE	-	expression tag	UNP Q14145
B	288	LEU	-	expression tag	UNP Q14145
B	289	TYR	-	expression tag	UNP Q14145
B	290	ASP	-	expression tag	UNP Q14145
B	291	GLY	-	expression tag	UNP Q14145
B	292	ILE	-	expression tag	UNP Q14145
B	293	ARG	-	expression tag	UNP Q14145
B	294	ILE	-	expression tag	UNP Q14145
B	295	GLN	-	expression tag	UNP Q14145
B	296	ALA	-	expression tag	UNP Q14145
B	297	ASP	-	expression tag	UNP Q14145
B	298	GLN	-	expression tag	UNP Q14145
B	299	THR	-	expression tag	UNP Q14145
B	300	PRO	-	expression tag	UNP Q14145
B	301	GLU	-	expression tag	UNP Q14145
B	302	ASP	-	expression tag	UNP Q14145
B	303	LEU	-	expression tag	UNP Q14145
B	304	ASP	-	expression tag	UNP Q14145
B	305	MET	-	expression tag	UNP Q14145

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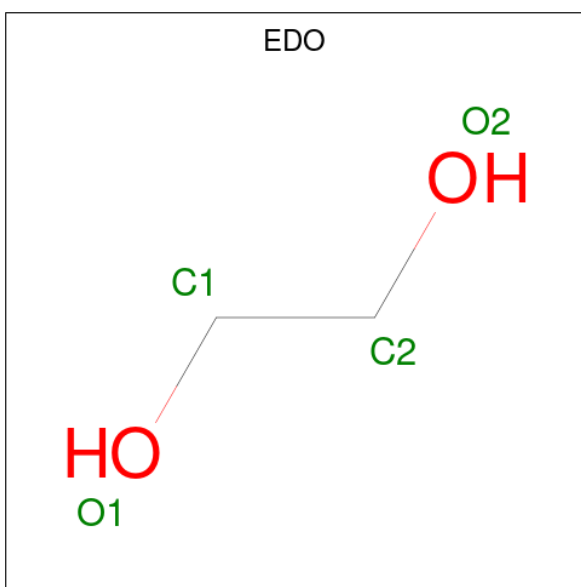
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Chain	Residue	Modelled	Actual	Comment	Reference
B	306	GLU	-	expression tag	UNP Q14145
B	307	ASP	-	expression tag	UNP Q14145
B	308	ASN	-	expression tag	UNP Q14145
B	309	ASP	-	expression tag	UNP Q14145
B	310	ILE	-	expression tag	UNP Q14145
B	311	ILE	-	expression tag	UNP Q14145
B	312	GLU	-	expression tag	UNP Q14145
B	313	ALA	-	expression tag	UNP Q14145
B	314	HIS	-	expression tag	UNP Q14145
B	315	ARG	-	expression tag	UNP Q14145
B	316	GLU	-	expression tag	UNP Q14145
B	317	GLN	-	expression tag	UNP Q14145
B	318	ILE	-	expression tag	UNP Q14145
B	319	GLY	-	expression tag	UNP Q14145
B	320	GLY	-	expression tag	UNP Q14145

- Molecule 2 is a protein called ACY-SC1-GLU-THR-GLY-GLU-LEU.

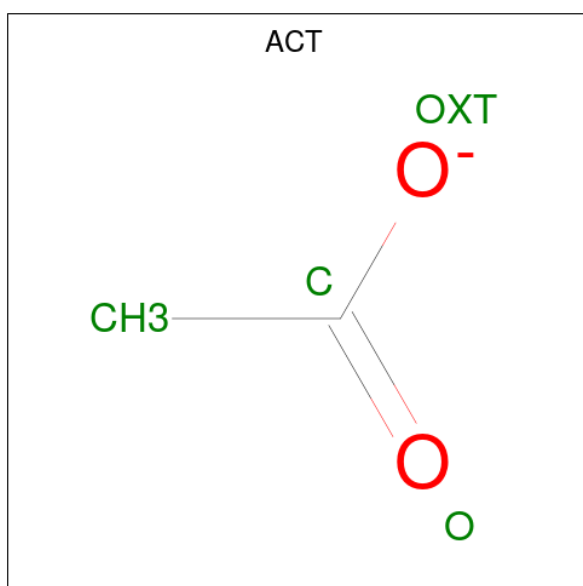
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	7	56	33	7	16	0	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	Na 3	0	0
5	B	4	Total 4	Na 4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	178	Total 178	O 178	0	0
6	B	174	Total 174	O 174	0	0
6	D	4	Total 4	O 4	0	0



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.65Å 76.13Å 211.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.84 – 2.10 47.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.84-2.10) 99.3 (47.84-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.165 , 0.200 0.166 , 0.200	Depositor DCC
$R_{free}$ test set	3641 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.9	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.032 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4983	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DYW, ACE, EDO, ACT, NA

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	0.59	0/2336	0.76	3/3174 (0.1%)
1	B	0.59	1/2298 (0.0%)	0.71	0/3127
2	D	2.42	4/37 (10.8%)	1.58	0/47
All	All	0.62	5/4671 (0.1%)	0.75	3/6348 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	THR	C-N	7.39	1.46	1.33
2	D	5	GLY	C-N	5.93	1.47	1.34
1	B	489	CYS	CB-SG	-5.82	1.72	1.81
2	D	6	GLU	C-N	5.47	1.46	1.34
2	D	3	GLU	C-N	5.02	1.45	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	380	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	494	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	2279	0	2159	42	0
1	B	2241	0	2115	26	0
2	D	56	0	35	1	0
3	A	8	0	12	2	0
3	B	8	0	12	4	0
4	A	20	0	15	9	0
4	B	8	0	6	0	0
5	A	3	0	0	0	0
5	B	4	0	0	0	0
6	A	178	0	0	2	0
6	B	174	0	0	0	0
6	D	4	0	0	0	0
All	All	4983	0	4354	64	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 7.

All (64) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483[A]:ARG:HE	4:A:706:ACT:H1	1.16	1.06
1:B:415:ARG:HE	3:B:702:EDO:H11	1.22	1.01
1:A:483[B]:ARG:HE	4:A:706:ACT:H1	1.39	0.87
1:B:415:ARG:HH21	3:B:702:EDO:H21	1.46	0.80
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.73	0.70
1:B:496:GLU:OE2	1:B:498[B]:ARG:NH2	2.24	0.70
1:A:466:ALA:HB1	1:A:514:VAL:HG23	1.73	0.69
1:A:496:GLU:OE2	1:A:498[B]:ARG:NH2	2.27	0.68
1:B:515:LEU:HD21	1:B:586:PRO:HG3	1.76	0.67
1:A:483[A]:ARG:NE	4:A:706:ACT:H1	2.00	0.67
1:A:442[A]:ARG:NH1	6:A:804:HOH:O	2.33	0.62
1:B:596:ARG:HG3	1:B:596:ARG:HH11	1.66	0.60
1:A:483[B]:ARG:NE	4:A:706:ACT:H1	2.15	0.58
1:A:491:TYR:CE1	1:A:498[B]:ARG:HG3	2.39	0.58
1:A:530:GLN:NE2	1:B:385[A]:ASP:OD2	2.35	0.57
1:A:582:GLU:HG2	1:A:593:GLU:HG2	1.85	0.57
1:A:483[B]:ARG:HE	4:A:706:ACT:CH3	2.15	0.55
1:B:415:ARG:HE	3:B:702:EDO:C1	2.07	0.55
1:B:491:TYR:CE1	1:B:498[B]:ARG:HG3	2.42	0.55
1:A:415:ARG:NH2	4:A:706:ACT:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ARG:NE	3:B:702:EDO:H11	2.06	0.54
1:A:357:ASP:H	3:A:702:EDO:C1	2.20	0.54
1:B:362:ARG:NH1	1:B:394:ASP:OD2	2.41	0.54
1:A:471:LEU:HD21	4:A:704:ACT:H2	1.90	0.53
1:A:483[B]:ARG:NH2	1:B:385[B]:ASP:OD1	2.40	0.53
1:B:557:LEU:H	1:B:557:LEU:HD23	1.74	0.53
1:A:557:LEU:HD23	1:A:557:LEU:H	1.74	0.53
1:B:395:CYS:HB2	1:B:406:CYS:SG	2.50	0.51
1:B:491:TYR:HE1	1:B:498[B]:ARG:HG3	1.76	0.51
1:A:494:ARG:HH21	4:A:704:ACT:H1	1.74	0.51
1:A:585:ASP:HB3	1:A:588:THR:HG22	1.92	0.51
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.92	0.50
1:A:483[B]:ARG:HB3	1:A:506:ILE:CG2	2.41	0.50
1:A:526:ASP:HB3	1:A:531:LEU:HD11	1.94	0.50
1:A:442[B]:ARG:HD3	6:A:833:HOH:O	2.11	0.50
1:B:369:VAL:HG21	1:B:609:THR:HB	1.94	0.50
1:A:357:ASP:H	3:A:702:EDO:H11	1.78	0.49
1:A:491:TYR:HE1	1:A:498[B]:ARG:HG3	1.78	0.49
1:A:416:ILE:HD11	1:A:427:ALA:HB1	1.94	0.49
1:A:326[B]:ARG:NH2	1:A:563:GLN:H	2.10	0.48
1:A:483[B]:ARG:HH11	1:A:527:GLY:HA2	1.78	0.48
1:A:525:TYR:CG	1:B:385[B]:ASP:OD2	2.67	0.48
1:A:365:LEU:HD23	1:A:365:LEU:H	1.78	0.48
1:A:483[B]:ARG:NH1	1:A:527:GLY:HA2	2.30	0.47
1:A:555:SER:OG	1:B:385[A]:ASP:OD1	2.25	0.47
1:A:478:PHE:HB2	4:A:706:ACT:H3	1.98	0.46
1:A:486:SER:HB2	1:A:499:MET:HE1	1.97	0.46
2:D:2:DYW:O51	2:D:2:DYW:C02	2.64	0.45
1:A:326[B]:ARG:HH22	1:A:563:GLN:H	1.65	0.45
1:A:552:HIS:HB2	1:A:554:ARG:HH21	1.82	0.44
1:B:472:LEU:HB3	1:B:490:TYR:HB3	2.00	0.44
1:A:369:VAL:HG21	1:A:609:THR:HB	1.98	0.44
1:A:431:SER:HB3	1:A:461:ILE:HG21	2.00	0.44
1:A:515:LEU:HD22	1:A:566:ILE:HG13	1.99	0.43
1:B:365:LEU:H	1:B:365:LEU:HD23	1.84	0.43
1:B:566:ILE:HB	1:B:584:TYR:HB3	2.01	0.42
1:B:369:VAL:HG23	1:B:607:ALA:HB1	2.01	0.42
1:A:336[A]:ARG:HD3	1:B:336:ARG:CZ	2.50	0.41
1:B:519:ILE:O	1:B:536:ARG:HA	2.20	0.41
1:A:365:LEU:H	1:A:365:LEU:CD2	2.34	0.41
1:A:373:LEU:HB3	1:A:395[A]:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LEU:HD13	1:B:395:CYS:SG	2.61	0.40
1:A:362:ARG:NH1	1:A:394:ASP:OD2	2.51	0.40
1:A:373:LEU:HD13	1:A:395[A]:CYS:SG	2.62	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	294/414 (71%)	287 (98%)	7 (2%)	0	100	100
1	B	290/414 (70%)	282 (97%)	6 (2%)	2 (1%)	22	18
2	D	3/7 (43%)	3 (100%)	0	0	100	100
All	All	587/835 (70%)	572 (97%)	13 (2%)	2 (0%)	47	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	385[A]	ASP
1	B	385[B]	ASP

### 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	241/344 (70%)	239 (99%)	2 (1%)	81	86
1	B	237/344 (69%)	234 (99%)	3 (1%)	69	75
2	D	4/4 (100%)	4 (100%)	0	100	100
All	All	482/692 (70%)	477 (99%)	5 (1%)	73	82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	ARG
1	A	557	LEU
1	B	362	ARG
1	B	553	ARG
1	B	557	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	B	528	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	702	-	3,3,3	0.51	0	2,2,2	0.81	0
4	ACT	B	704	-	3,3,3	1.22	0	3,3,3	0.89	0
3	EDO	B	701	-	3,3,3	0.51	0	2,2,2	0.25	0
4	ACT	A	706	-	3,3,3	1.00	0	3,3,3	0.41	0
4	ACT	A	703	-	3,3,3	1.01	0	3,3,3	0.86	0
3	EDO	A	701	-	3,3,3	0.45	0	2,2,2	0.61	0
3	EDO	B	702	-	3,3,3	0.60	0	2,2,2	0.44	0
4	ACT	A	707	-	3,3,3	0.87	0	3,3,3	1.14	0
4	ACT	A	705	-	3,3,3	1.00	0	3,3,3	1.59	1 (33%)
4	ACT	A	704	-	3,3,3	1.00	0	3,3,3	0.67	0
4	ACT	B	703	-	3,3,3	0.96	0	3,3,3	0.85	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	EDO	A	702	-	-	1/1/1/1	-
3	EDO	A	701	-	-	0/1/1/1	-
3	EDO	B	702	-	-	1/1/1/1	-
3	EDO	B	701	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	705	ACT	OXT-C-CH3	2.19	124.23	115.18

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	EDO	O1-C1-C2-O2
3	B	702	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	EDO	2	0
4	A	706	ACT	7	0
3	B	702	EDO	4	0
4	A	704	ACT	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	285/414 (68%)	-0.27	3 (1%) 80   84	32, 43, 63, 86	0
1	B	285/414 (68%)	-0.38	0 100   100	32, 43, 62, 76	0
2	D	5/7 (71%)	-0.35	0 100   100	38, 42, 50, 59	0
All	All	575/835 (68%)	-0.33	3 (0%) 91   92	32, 43, 63, 86	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	GLN	2.8
1	A	588	THR	2.4
1	A	349	ASP	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, 95<sup>th</sup> 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NA	B	708	1/1	0.75	0.46	61,61,61,61	0
3	EDO	A	702	4/4	0.81	0.16	53,55,59,64	0
4	ACT	A	707	4/4	0.82	0.26	74,76,88,90	0
4	ACT	B	704	4/4	0.85	0.14	49,54,58,69	0
5	NA	A	708	1/1	0.89	0.18	66,66,66,66	0
3	EDO	B	701	4/4	0.89	0.13	55,65,66,70	0
4	ACT	A	705	4/4	0.91	0.14	49,53,62,66	0
5	NA	B	706	1/1	0.92	0.21	76,76,76,76	0
4	ACT	A	706	4/4	0.93	0.15	37,47,48,60	4
5	NA	A	710	1/1	0.93	0.19	71,71,71,71	0
5	NA	A	709	1/1	0.94	0.08	64,64,64,64	0
3	EDO	A	701	4/4	0.94	0.13	55,64,68,71	0
3	EDO	B	702	4/4	0.97	0.16	51,51,60,71	0
5	NA	B	705	1/1	0.97	0.07	67,67,67,67	0
5	NA	B	707	1/1	0.98	0.05	56,56,56,56	0
4	ACT	A	703	4/4	0.98	0.20	56,58,60,66	0
4	ACT	A	704	4/4	0.99	0.11	42,42,45,46	0
4	ACT	B	703	4/4	0.99	0.10	40,45,48,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.