

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 5, 2023 – 02:19 PM EST

PDB ID	:	8EHV
Title	:	Kelch domain of human KEAP1 bound to Nrf2 cyclic peptide, c[DhA-
		GDPET(bAla)E]
Authors	:	Muellers, S.N.; Allen, K.N.
Deposited on	:	2022-09-14
Resolution	:	2.29  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
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 2.29 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 <sub>free</sub>	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	А	336	7%	68%		17%	•	14%
1	В	336	23%	53%	28%			17%
2	Р	7	14%		86%			

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
2	B3A	Р	76	Х	Х	-	Х



#### 8EHV

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4608 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	200	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	A	289	2222	1381	404	421	16	0	0	0
1	В	270	Total	С	Ν	0	S	0	0	0
	D	219	2145	1337	388	405	15	0	0	U

• Molecule 1 is a protein called Kelch-like ECH-associated protein 1.

Chain	Residue	Modelled	Actual	Comment	Reference
А	289	MET	-	expression tag	UNP Q14145
А	290	GLY	-	expression tag	UNP Q14145
А	291	SER	-	expression tag	UNP Q14145
А	292	SER	-	expression tag	UNP Q14145
А	293	HIS	-	expression tag	UNP Q14145
А	294	HIS	-	expression tag	UNP Q14145
А	295	HIS	-	expression tag	UNP Q14145
А	296	HIS	-	expression tag	UNP Q14145
А	297	HIS	-	expression tag	UNP Q14145
А	298	HIS	-	expression tag	UNP Q14145
А	299	SER	-	expression tag	UNP Q14145
А	300	SER	-	expression tag	UNP Q14145
А	301	GLY	-	expression tag	UNP Q14145
А	302	GLY	-	expression tag	UNP Q14145
А	303	GLU	-	expression tag	UNP Q14145
А	304	ASN	-	expression tag	UNP Q14145
A	305	LEU	-	expression tag	UNP Q14145
А	306	TYR	-	expression tag	UNP Q14145
А	307	PHE	-	expression tag	UNP Q14145
A	308	GLN	-	expression tag	UNP Q14145
А	309	GLY	-	expression tag	UNP Q14145
A	310	HIS	-	expression tag	UNP Q14145
А	311	MET	-	expression tag	UNP Q14145
A	319	SER	CYS	conflict	UNP Q14145
A	540	ALA	GLU	engineered mutation	UNP Q14145

There are 58 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
А	542	ALA	GLU	engineered mutation	UNP Q14145
А	613	SER	CYS	engineered mutation	UNP Q14145
А	622	SER	CYS	conflict	UNP Q14145
А	624	SER	CYS	conflict	UNP Q14145
В	289	MET	-	expression tag	UNP Q14145
В	290	GLY	-	expression tag	UNP Q14145
В	291	SER	-	expression tag	UNP Q14145
В	292	SER	-	expression tag	UNP Q14145
В	293	HIS	-	expression tag	UNP Q14145
В	294	HIS	-	expression tag	UNP Q14145
В	295	HIS	-	expression tag	UNP Q14145
В	296	HIS	-	expression tag	UNP Q14145
В	297	HIS	-	expression tag	UNP Q14145
В	298	HIS	-	expression tag	UNP Q14145
В	299	SER	-	expression tag	UNP Q14145
В	300	SER	-	expression tag	UNP Q14145
В	301	GLY	-	expression tag	UNP Q14145
В	302	GLY	-	expression tag	UNP Q14145
В	303	GLU	-	expression tag	UNP Q14145
В	304	ASN	-	expression tag	UNP Q14145
В	305	LEU	-	expression tag	UNP Q14145
В	306	TYR	-	expression tag	UNP Q14145
В	307	PHE	-	expression tag	UNP Q14145
В	308	GLN	-	expression tag	UNP Q14145
В	309	GLY	-	expression tag	UNP Q14145
В	310	HIS	-	expression tag	UNP Q14145
В	311	MET	-	expression tag	UNP Q14145
В	319	SER	CYS	conflict	UNP Q14145
В	540	ALA	GLU	engineered mutation	UNP Q14145
В	542	ALA	GLU	engineered mutation	UNP Q14145
В	613	SER	CYS	engineered mutation	UNP Q14145
В	622	SER	CYS	conflict	UNP Q14145
В	624	SER	CYS	conflict	UNP Q14145

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• Molecule 2 is a protein called cyclic peptide c[DhA-GDPET(bAla)E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Р	7	Total 51	C 30	N 7	0 14	0	0	0

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	137	Total O 137 137	0	0
3	В	53	Total O 53 53	0	0



Chain P:

14%

# 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: Kelch-like ECH-associated protein 1



86%





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	162.35Å $68.85$ Å $77.22$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $117.63^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	29.58 - 2.29	Depositor
Resolution (A)	29.59 - 2.29	EDS
% Data completeness	99.3 (29.58-2.29)	Depositor
(in resolution range)	99.3 (29.59-2.29)	EDS
R <sub>merge</sub>	0.15	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.58 (at 2.29 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
D D.	0.203 , $0.253$	Depositor
$\Pi, \Pi_{free}$	0.203 , $0.252$	DCC
$R_{free}$ test set	1996 reflections $(5.85\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	37.7	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.34 , $45.6$	EDS
L-test for $twinning^2$	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.012 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4608	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: B3A, BAL

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		Bo	nd lengths	Bond angles		
MOI	Moi Chain		# Z  > 5	RMSZ	# Z  > 5	
1	А	0.94	5/2276~(0.2%)	0.89	1/3099~(0.0%)	
1	В	0.74	0/2196	0.87	4/2990~(0.1%)	
2	Р	1.52	0/39	1.18	0/51	
All	All	0.86	$5/4511 \ (0.1\%)$	0.88	5/6140 (0.1%)	

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	А	0	1
2	Р	1	1
All	All	1	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	391	SER	CB-OG	7.13	1.51	1.42
1	А	535	GLU	CG-CD	6.05	1.61	1.51
1	А	395	CYS	CB-SG	-5.97	1.72	1.81
1	А	349	ASP	CB-CG	-5.61	1.40	1.51
1	А	525	TYR	CD2-CE2	5.21	1.47	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	380	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	В	538	ASP	CB-CG-OD1	6.02	123.72	118.30
1	В	422	ASP	CB-CG-OD1	5.98	123.68	118.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	483	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	В	494	ARG	NE-CZ-NH1	-5.03	117.78	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	Р	76	B3A	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	609	THR	Mainchain
2	Р	80	THR	Peptide

### 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	2222	0	2119	41	3
1	В	2145	0	2046	90	3
2	Р	51	0	33	3	0
3	А	137	0	0	4	0
3	В	53	0	0	8	0
All	All	4608	0	4198	133	3

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 15.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:HD12	1:B:450:TRP:HZ2	1.09	1.14
1:B:441:GLU:HB3	1:B:452:LEU:HD23	1.39	1.03
1:B:393:LEU:HD12	1:B:450:TRP:CZ2	1.94	1.03
1:B:346:ASN:HD22	1:B:351:THR:HG22	1.26	1.00
1:B:441:GLU:HB3	1:B:452:LEU:CD2	1.92	1.00



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:518:CYS:SG	1:B:536:ARG:HD2	2.09	0.92
1:A:466:ALA:HB1	1:A:514:VAL:HG23	1.51	0.90
1:B:455:PRO:O	1:B:497:TRP:CD1	2.25	0.90
1:A:614:ARG:HH21	1:A:614:ARG:HG3	1.38	0.86
1:A:515:LEU:HD22	1:A:566:ILE:HG13	1.61	0.82
1:B:327:LEU:HB3	1:B:329:TYR:CE1	2.15	0.81
1:B:550:MET:CE	1:B:568:VAL:HG11	2.12	0.80
1:B:393:LEU:CD1	1:B:450:TRP:HZ2	1.93	0.80
1:B:397:ASN:HB3	1:B:400:THR:HB	1.65	0.79
1:B:567:TYR:HE1	1:B:594:VAL:HG11	1.47	0.78
1:B:329:TYR:CE2	1:B:344:ALA:HB2	2.19	0.78
1:B:327:LEU:HB3	1:B:329:TYR:HE1	1.50	0.77
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.67	0.76
1:B:396:TYR:OH	1:B:401:ASN:ND2	2.18	0.74
1:A:515:LEU:HB3	1:A:520:TYR:CE1	2.22	0.74
1:B:380:ARG:NH2	1:B:387:ASN:HD21	1.86	0.74
1:B:518:CYS:HB3	1:B:536:ARG:HB2	1.70	0.74
1:B:550:MET:HE1	1:B:568:VAL:HG11	1.70	0.73
1:B:373:LEU:HB3	3:B:722:HOH:O	1.88	0.73
1:B:327:LEU:HD22	1:B:329:TYR:OH	1.89	0.72
1:B:327:LEU:HB2	1:B:609:THR:O	1.88	0.72
1:B:515:LEU:HD21	1:B:586:PRO:HG3	1.69	0.72
1:B:424:HIS:ND1	3:B:701:HOH:O	2.23	0.71
1:B:338:SER:OG	1:B:381:ASN:HA	1.90	0.71
1:B:395:CYS:SG	3:B:722:HOH:O	2.49	0.70
1:B:425:ILE:HB	1:B:443:TYR:HB3	1.74	0.69
1:B:422:ASP:O	3:B:701:HOH:O	2.11	0.68
1:B:346:ASN:ND2	1:B:351:THR:HG22	2.06	0.68
1:B:490:TYR:OH	1:B:495:ASN:OD1	2.10	0.68
1:B:567:TYR:CE1	1:B:594:VAL:HG11	2.28	0.67
1:B:393:LEU:CD1	1:B:450:TRP:CZ2	2.74	0.67
1:A:498:ARG:NE	3:A:703:HOH:O	2.28	0.66
1:A:614:ARG:HG3	1:A:614:ARG:NH2	2.10	0.64
1:B:518:CYS:SG	1:B:536:ARG:CD	2.87	0.63
1:A:335:PHE:HD2	3:A:819:HOH:O	1.81	0.63
1:B:410:SER:HB3	1:B:441:GLU:OE2	1.99	0.63
1:B:561:VAL:HG12	1:B:566:ILE:HG12	1.82	0.62
1:B:518:CYS:CB	1:B:536:ARG:HD2	2.29	0.62
1:B:373:LEU:HD22	1:B:397:ASN:HA	1.80	0.62
1:A:551:LYS:HE2	1:A:591:TRP:O	1.99	0.61
1:B:359:GLN:HG3	1:B:360:VAL:HG23	1.82	0.61



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:565:ARG:NH2	1:B:585:ASP:HB2	2.18	0.59
1:B:588:THR:OG1	1:B:590:THR:HG22	2.03	0.58
1:A:565:ARG:HD2	3:A:813:HOH:O	2.03	0.58
1:B:535:GLU:HB3	1:B:546:PHE:CD1	2.40	0.56
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.85	0.56
1:B:530:GLN:NE2	2:P:78:PRO:O	2.39	0.56
1:B:455:PRO:O	1:B:497:TRP:HD1	1.85	0.55
1:B:581:VAL:HB	1:B:595:THR:CG2	2.36	0.55
1:B:469:ASN:C	1:B:470:ARG:HE	2.10	0.55
1:A:466:ALA:HB1	1:A:514:VAL:CG2	2.30	0.55
1:B:399:MET:HE1	3:B:752:HOH:O	2.06	0.54
1:B:442:ARG:NH2	1:B:451:HIS:HB2	2.22	0.54
1:B:504:ASN:HB2	1:B:546:PHE:CZ	2.43	0.54
1:B:581:VAL:HB	1:B:595:THR:HG23	1.90	0.54
1:B:518:CYS:HB2	1:B:520:TYR:CE1	2.42	0.54
1:B:472:LEU:HB3	1:B:490:TYR:HB3	1.88	0.53
1:B:483:ARG:HB3	1:B:506:ILE:CG2	2.38	0.53
1:B:443:TYR:HB2	1:B:450:TRP:CH2	2.44	0.52
1:A:490:TYR:CE2	1:A:492:PRO:HA	2.45	0.51
1:B:338:SER:HB2	1:B:381:ASN:OD1	2.09	0.51
1:B:469:ASN:O	1:B:471:LEU:HD22	2.10	0.51
1:B:353:LEU:HD23	1:B:355:LEU:HD11	1.93	0.51
1:A:421:ILE:HD11	1:A:472:LEU:HB2	1.93	0.50
1:B:492:PRO:HD2	3:B:709:HOH:O	2.10	0.50
1:A:614:ARG:NH2	1:A:614:ARG:CG	2.73	0.50
1:B:424:HIS:CE1	3:B:701:HOH:O	2.64	0.49
1:A:467:VAL:O	1:A:514:VAL:HG21	2.12	0.49
1:A:515:LEU:HB3	1:A:520:TYR:HE1	1.72	0.48
1:B:532:ASN:HB2	1:B:550:MET:O	2.14	0.48
1:A:557:LEU:HD23	1:A:557:LEU:H	1.78	0.48
1:B:422:ASP:HB3	3:B:701:HOH:O	2.14	0.48
1:B:395:CYS:O	1:B:403:TRP:HA	2.14	0.47
1:A:515:LEU:HD22	1:A:566:ILE:CG1	2.40	0.47
1:A:409:MET:SD	1:A:413:ARG:HD2	2.55	0.47
1:A:566:ILE:HB	1:A:584:TYR:HB3	1.97	0.46
1:B:362:ARG:HA	1:B:380:ARG:O	2.15	0.46
1:B:443:TYR:CE2	1:B:445:PRO:HA	2.51	0.46
1:B:490:TYR:HB2	1:B:497:TRP:CH2	2.50	0.46
1:A:347:PRO:HG2	1:A:562:HIS:CE1	2.51	0.46
1:A:512:VAL:HA	1:A:520:TYR:O	2.16	0.45
1:A:345:TYR:HB2	1:A:352:TRP:CH2	2.52	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:470:ABG:CZ	1:A:470:ABG:H	2.29	0.45
1:A:472:LEU:HB3	1:A:490:TYR:HB3	1.97	0.45
1:A:430:GLY:O	1:A:461:ILE:HG22	2.17	0.45
1:B:550:MET:HE3	1:B:568:VAL:HG11	1.98	0.45
1:B:498:ARG:NH1	1:B:498:ARG:HB3	2.33	0.45
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.77	0.44
1:A:430:GLY:C	1:A:461:ILE:HG22	2.37	0.44
1:A:519:ILE:O	1:A:536:ARG:HA	2.17	0.44
1:B:534:VAL:HB	1:B:547:VAL:HG23	1.99	0.44
1:B:467:VAL:HA	1:B:471:LEU:O	2.17	0.44
1:A:388:THR:HG22	1:A:389:ASP:O	2.19	0.43
1:B:369:VAL:HA	1:B:373:LEU:O	2.18	0.43
1:B:554:ARG:HG3	1:B:557:LEU:HD22	2.01	0.43
1:A:494:ARG:HA	1:A:494:ARG:HD3	1.81	0.43
1:B:604:VAL:HG23	1:B:606:VAL:HG23	2.01	0.43
1:B:431:SER:HB3	1:B:461:ILE:HG21	2.01	0.42
1:A:596:ARG:NH1	3:A:705:HOH:O	2.30	0.42
1:A:425:ILE:HB	1:A:443:TYB:HB3	2.01	0.42
1:A:504:ASN:HB3	1:A:546:PHE:CE2	2.54	0.42
1:B:356:ALA:HB2	1:B:401:ASN:OD1	2.19	0.42
2:P:77:ASP:HA	2:P:78:PRO:HD2	1.90	0.42
1:A:515:LEU:HD12	1:A:516:HIS:H	1.85	0.42
1:B:338:SER:HB3	1:B:361:PRO:HB2	2.01	0.42
1:B:585:ASP:HB3	1:B:588:THR:OG1	2.20	0.42
1:B:468:LEU:HD11	1:B:517:ASN:HD22	1.85	0.42
1:A:327:LEU:HG	1:A:611:GLU:HB3	2.02	0.41
1:B:413:ARG:HB2	1:B:416:ILE:HD12	2.00	0.41
1:B:519:ILE:O	1:B:536:ARG:HA	2.18	0.41
1:B:338:SER:HG	1:B:362:ARG:HA	1.84	0.41
1:B:498:ARG:CB	1:B:498:ARG:HH11	2.33	0.41
1:A:361:PRO:C	1:A:362:ARG:HG3	2.41	0.41
1:A:534:VAL:O	1:A:547:VAL:HG22	2.20	0.41
1:B:344:ALA:O	1:B:352:TRP:CE3	2.73	0.41
1:B:345:TYR:HB2	1:B:352:TRP:CZ3	2.55	0.41
1:A:504:ASN:CB	1:A:546:PHE:CE2	3.03	0.41
1:A:345:TYR:HB2	1:A:352:TRP:CZ3	2.56	0.41
1:A:470:ARG:NE	1:A:470:ARG:N	2.69	0.41
1:B:519:ILE:HB	1:B:537:TYR:HB3	2.03	0.41
1:B:355:LEU:HD23	1:B:396:TYR:OH	2.21	0.41
1:B:421:ILE:HG13	1:B:426:TYR:HE1	1.86	0.41
2:P:77:ASP:OD2	2:P:79:GLU:N	2.48	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1.A.330.THB.O	1.A.330.THB.HC23	2.21	0.40
1 D 222 CLV O	1 D 262 CED 11D2	2.21	0.40
1:B:333:GLY:O	1:B:363:SER:HB3	2.21	0.40
1:B:346:ASN:HB3	1:B:351:THR:N	2.36	0.40
1:B:536:ARG:HH11	1:B:536:ARG:HD3	1.71	0.40
1:B:561:VAL:CG1	1:B:566:ILE:HG12	2.50	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ASN:OD1	1:B:470:ARG:NH1[2_555]	0.37	1.83
1:A:517:ASN:CG	1:B:470:ARG:NH1[2_555]	1.54	0.66
1:A:517:ASN:OD1	1:B:470:ARG:CZ[2_555]	1.55	0.65

## 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	А	287/336~(85%)	274 (96%)	12~(4%)	1 (0%)	41 50
1	В	275/336 (82%)	263~(96%)	11 (4%)	1 (0%)	34 42
2	Р	4/7~(57%)	3(75%)	1 (25%)	0	100 100
All	All	566/679~(83%)	540 (95%)	24 (4%)	2(0%)	34 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	516	HIS
1	В	453	VAL



#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	234/275~(85%)	228~(97%)	6 (3%)	46	63
1	В	225/275~(82%)	218 (97%)	7 (3%)	40	55
2	Р	5/5~(100%)	5 (100%)	0	100	100
All	All	464/555~(84%)	451 (97%)	13 (3%)	43	60

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	326	ARG
1	А	337	GLN
1	А	385	ASP
1	А	551	LYS
1	А	557	LEU
1	А	613	SER
1	В	336	ARG
1	В	424	HIS
1	В	447	ARG
1	В	452	LEU
1	В	470	ARG
1	В	494	ARG
1	В	557	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	В	346	ASN
1	В	387	ASN
1	В	401	ASN
1	В	517	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)

2 non-standard protein/DNA/RNA residues 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	True	Chain	Dec	Tinle	B	ond leng	$\mathbf{gths}$	E	Bond ang	gles
	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	B3A	Р	76	2	$5,\!5,\!6$	9.75	4 (80%)	$5,\!5,\!7$	7.78	3 (60%)
2	BAL	Р	81	2	4,4,5	1.98	1 (25%)	$3,\!3,\!5$	14.05	1 (33%)

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	B3A	Р	76	2	1/1/1/2	0/3/3/4	-
2	BAL	Р	81	2	-	0/1/2/3	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	Р	76	B3A	CB-CA	-20.98	1.25	1.53
2	Р	76	B3A	CA-N	-5.02	1.35	1.49
2	Р	81	BAL	CB-CA	-3.58	1.35	1.51
2	Р	76	B3A	O-C	2.41	1.33	1.19
2	Р	76	B3A	CB-C	-2.14	1.44	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
2	Р	81	BAL	CB-CA-C	24.32	147.54	111.42
2	Р	76	B3A	CA-CB-C	16.83	146.96	113.37



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Р	76	B3A	CB-CA-N	-3.09	102.28	110.72
2	Р	76	B3A	CG-CA-N	2.00	117.39	108.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	Р	76	B3A	CA

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	Р	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Р	81:BAL	С	82:GLU	N	1.16



# 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>2	$OWAB(Å^2)$	Q<0.9
1	А	289/336~(86%)	0.35	23 (7%) 12 16	22, 34, 56, 79	0
1	В	279/336~(83%)	1.30	78~(27%) 0 0	28, 63, 108, 132	0
2	Р	5/7~(71%)	0.90	1 (20%) 1 1	55, 56, 68, 79	0
All	All	573/679~(84%)	0.82	102 (17%) 1 1	22, 43, 102, 132	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	351	THR	6.3
1	А	613	SER	6.1
1	В	567	TYR	5.6
1	А	614	ARG	5.5
1	В	399	MET	5.3
1	В	447	ARG	5.1
1	В	366	ALA	5.0
1	А	335	PHE	5.0
1	В	416	ILE	4.9
1	В	329	TYR	4.9
1	В	353	LEU	4.9
1	В	590	THR	4.8
1	В	562	HIS	4.8
1	В	446	GLU	4.8
1	В	516	HIS	4.8
1	В	557	LEU	4.7
1	В	559	ILE	4.7
1	В	594	VAL	4.6
1	В	402	GLN	4.6
1	В	494	ARG	4.6
1	В	604	VAL	4.5
1	В	338	SER	4.2
1	В	561	VAL	4.2



Mol	Chain	Res	Type	RSRZ
1	В	418	VAL	4.1
1	В	371	GLY	4.1
1	В	327	LEU	4.0
1	В	563	GLN	3.9
1	В	352	TRP	3.9
1	В	588	THR	3.8
1	А	385	ASP	3.7
1	В	558	GLY	3.6
1	В	365	LEU	3.6
1	В	400	THR	3.6
1	В	422	ASP	3.6
1	А	610	MET	3.5
1	В	346	ASN	3.5
1	В	564	GLY	3.5
1	В	423	GLY	3.5
1	А	399	MET	3.5
1	В	608	VAL	3.4
1	В	444	GLU	3.3
1	В	452	LEU	3.3
1	В	377	VAL	3.3
1	А	605	GLY	3.2
1	В	397	ASN	3.2
1	А	366	ALA	3.2
1	В	331	ALA	3.2
1	В	575	HIS	3.1
1	В	495	ASN	3.1
1	В	421	ILE	3.1
1	А	383	SER	3.0
1	В	493	GLU	3.0
1	В	605	GLY	3.0
1	В	595	THR	2.9
1	В	589	ASP	2.9
1	В	344	ALA	2.9
1	В	367	GLY	2.9
1	A	416	ILE	2.9
1	В	470	ARG	2.9
1	A	606	VAL	2.9
1	В	510	ALA	2.8
1	А	465	VAL	2.8
1	A	365	LEU	2.8
1	В	498	ARG	2.8
1	В	373	LEU	2.7



Mol	Chain	Res	Type	RSRZ
1	A	336	ARG	2.7
1	В	449	GLU	2.6
1	А	512	VAL	2.6
1	В	405	PRO	2.6
1	В	552	HIS	2.6
1	В	556	ALA	2.6
1	В	565	ARG	2.6
1	В	417	GLY	2.6
1	В	398	PRO	2.6
1	А	604	VAL	2.6
1	В	448	ASP	2.6
1	А	612	PRO	2.5
1	В	550	MET	2.5
1	А	447	ARG	2.5
1	В	465	VAL	2.4
1	В	475	VAL	2.4
1	В	425	ILE	2.4
1	В	596	ARG	2.4
1	В	598	THR	2.4
1	В	345	TYR	2.4
1	В	463	VAL	2.4
1	В	592	SER	2.4
1	А	326	ARG	2.3
1	В	603	GLY	2.3
2	Р	78	PRO	2.3
1	В	368	CYS	2.3
1	В	442	ARG	2.2
1	В	375	TYR	2.2
1	В	609	THR	2.1
1	А	587	ASP	2.1
1	A	452	LEU	2.1
1	В	591	TRP	2.1
1	В	491	TYR	2.1
1	В	464	GLY	2.1
1	А	417	GLY	2.1
1	В	512	VAL	2.1
1	А	384	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains (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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
2	B3A	Р	76	6/7	0.71	0.50	$76,\!77,\!80,\!83$	0
2	BAL	Р	81	5/6	0.85	0.18	68,68,75,75	0

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.

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

There are no ligands in this entry.

### 6.5 Other polymers (i)

There are no such residues in this entry.

