



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:46 PM UTC

PDB ID : 9I9T / pdb\_00009i9t  
Title : Room-temperature structure of PBP2a at EuXFEL  
Authors : Grieco, A.; Botha, S.; Martin-Garcia, J.M.  
Deposited on : 2025-02-07  
Resolution : 3.50 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

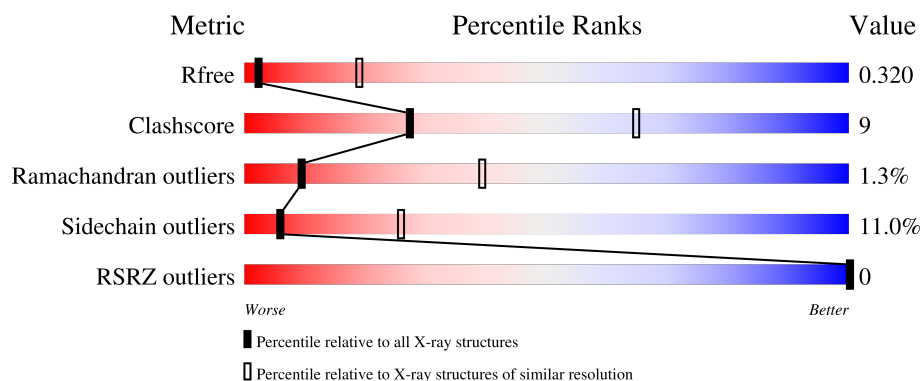
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 3.50 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))
$R_{free}$	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	643	 71% 24% .
1	B	643	 70% 27% ..

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	CL	B	704	-	-	X	-
3	CL	B	706	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10505 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 MecA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	3	0
			5183	3268	876	1023	16			
1	B	639	Total	C	N	O	S	0	4	0
			5175	3262	875	1023	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	GLU	GLY	conflict	UNP B3VQ68
A	664	TYR	-	expression tag	UNP B3VQ68
A	665	ASP	-	expression tag	UNP B3VQ68
A	666	ILE	-	expression tag	UNP B3VQ68
A	667	ASP	-	expression tag	UNP B3VQ68
A	668	GLU	-	expression tag	UNP B3VQ68
B	246	GLU	GLY	conflict	UNP B3VQ68
B	664	TYR	-	expression tag	UNP B3VQ68
B	665	ASP	-	expression tag	UNP B3VQ68
B	666	ILE	-	expression tag	UNP B3VQ68
B	667	ASP	-	expression tag	UNP B3VQ68
B	668	GLU	-	expression tag	UNP B3VQ68

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cd	0	0
			2	2		
2	B	3	Total	Cd	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

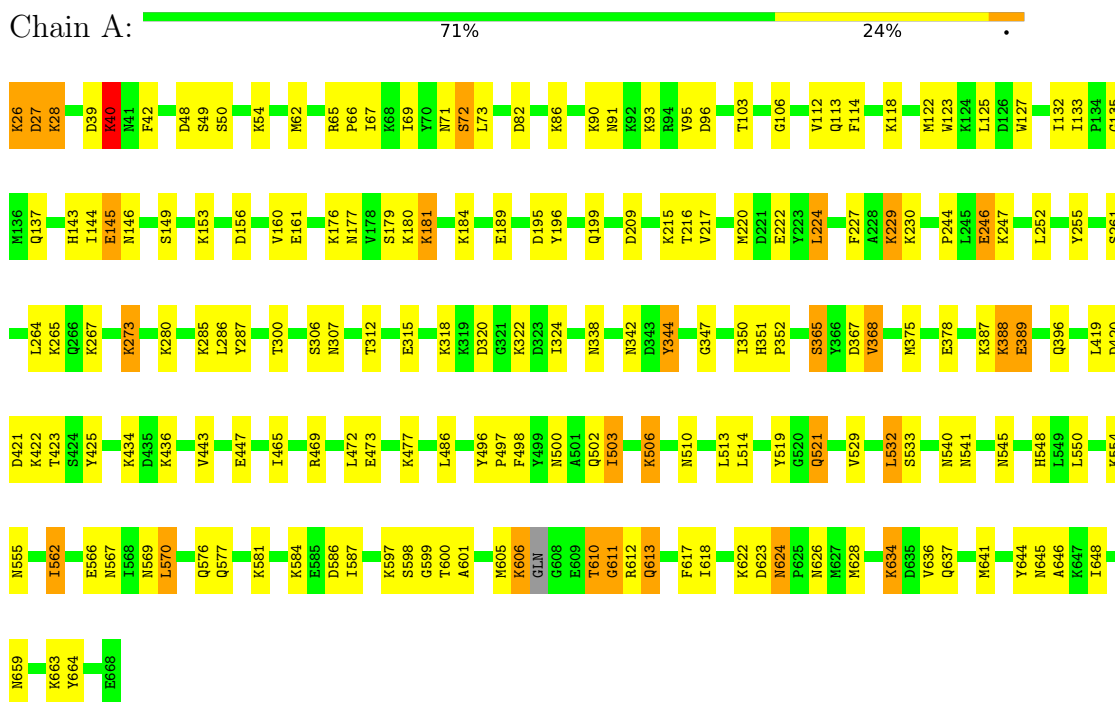
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	64	Total	O	0	0
			64	64		

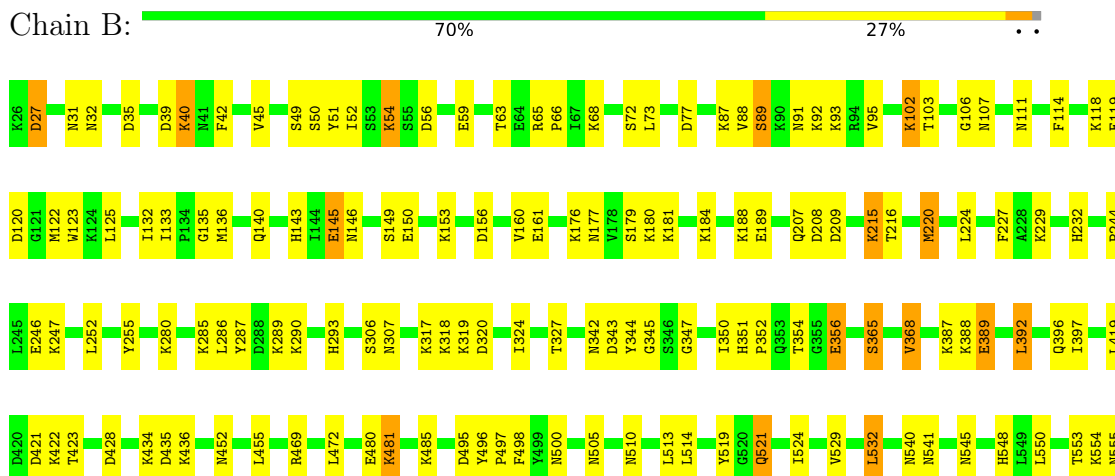
### 3 Residue-property plots

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: MecA



#### • Molecule 1: MecA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.70Å 106.60Å 186.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.39 – 3.50 25.39 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.39-3.50) 99.6 (25.39-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.46Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.245 , 0.316 0.251 , 0.320	Depositor DCC
$R_{free}$ test set	1032 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	102.6	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.32$ , $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CD

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	0.52	0/5268	1.04	4/7077 (0.1%)
1	B	0.51	0/5261	1.04	7/7072 (0.1%)
All	All	0.52	0/10529	1.04	11/14149 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ASP	CA-CB-CG	7.07	119.67	112.60
1	B	56	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	496	TYR	CB-CA-C	5.52	117.12	108.63
1	A	496	TYR	CB-CA-C	5.44	117.01	108.63
1	B	320	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	367	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	320	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	82	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	667	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	209	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	435	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5183	0	5193	94	0
1	B	5175	0	5169	97	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
3	A	3	0	0	1	0
3	B	4	0	0	6	0
4	A	71	0	0	16	0
4	B	64	0	0	9	0
All	All	10505	0	10362	189	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 9.

All (189) 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:232:HIS:NE2	3:B:706:CL:CL	2.34	0.96
1:B:93:LYS:HD2	1:B:123:TRP:CZ2	2.08	0.88
1:A:229:LYS:NZ	4:A:802:HOH:O	2.07	0.86
1:A:217:VAL:HG21	4:A:815:HOH:O	1.76	0.84
1:B:215:LYS:HE2	4:B:807:HOH:O	1.78	0.82
1:B:548:HIS:CE1	3:B:704:CL:CL	2.75	0.76
1:B:587:ILE:HD12	1:B:617:PHE:CZ	2.20	0.76
1:A:217:VAL:CG2	4:A:815:HOH:O	2.33	0.76
1:A:375:MET:HA	4:A:806:HOH:O	1.87	0.74
1:B:587:ILE:HD12	1:B:617:PHE:CE1	2.22	0.74
3:A:703:CL:CL	1:B:207:GLN:HG3	2.24	0.74
1:A:224:LEU:HD21	4:A:815:HOH:O	1.88	0.73
1:B:51:TYR:CD2	4:B:837:HOH:O	2.42	0.73
1:A:338:ASN:CB	4:A:814:HOH:O	2.38	0.72
1:A:338:ASN:HB3	4:A:814:HOH:O	1.89	0.70
1:A:220:MET:HG2	4:A:815:HOH:O	1.92	0.70
1:B:180[B]:LYS:O	1:B:180[B]:LYS:HG3	1.93	0.69
1:B:51:TYR:HD2	4:B:837:HOH:O	1.77	0.67
1:B:180[B]:LYS:O	1:B:180[B]:LYS:CG	2.43	0.67
1:A:189:GLU:HG2	1:A:227:PHE:CE1	2.29	0.67
1:A:606:LYS:N	1:A:610:THR:HG21	2.10	0.66
1:A:71:ASN:OD1	1:A:72:SER:N	2.29	0.65
1:A:548:HIS:NE2	1:A:555:ASN:OD1	2.30	0.65
1:A:50:SER:O	1:A:54:LYS:HB2	1.95	0.65
1:B:50:SER:O	1:B:54:LYS:HB3	1.98	0.64
1:B:65:ARG:HA	1:B:68:LYS:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:HIS:CE1	3:B:706:CL:CL	2.88	0.63
1:A:548:HIS:CE1	1:A:555:ASN:OD1	2.53	0.61
1:A:315:GLU:HB3	4:A:827:HOH:O	2.01	0.60
1:A:486:LEU:HA	1:A:562:ILE:HD11	1.83	0.59
1:B:39:ASP:O	1:B:40:LYS:C	2.45	0.59
1:B:658:GLU:HA	4:B:833:HOH:O	2.03	0.58
1:A:519:TYR:CE2	1:A:521:GLN:HG3	2.38	0.58
1:A:135:GLY:C	4:A:801:HOH:O	2.40	0.57
1:A:184:LYS:NZ	4:A:804:HOH:O	2.37	0.57
1:B:519:TYR:CE2	1:B:521:GLN:HG3	2.39	0.57
1:A:39:ASP:O	1:A:40:LYS:C	2.47	0.57
1:B:189:GLU:HG2	1:B:227:PHE:CE1	2.39	0.56
1:A:286:LEU:HD21	1:A:497:PRO:HD3	1.88	0.55
1:A:215:LYS:NZ	4:A:806:HOH:O	2.40	0.55
1:B:553:THR:O	3:B:704:CL:CL	2.62	0.55
1:B:286:LEU:HD21	1:B:497:PRO:HD3	1.89	0.55
1:B:587:ILE:CD1	1:B:617:PHE:CE1	2.91	0.54
1:A:144:ILE:O	1:B:307[B]:ASN:ND2	2.40	0.54
1:B:153:LYS:HD2	1:B:161:GLU:OE2	2.08	0.54
1:A:605:MET:HE3	1:A:610:THR:HG23	1.89	0.54
1:B:554:LYS:C	3:B:704:CL:CL	2.88	0.54
1:A:622:LYS:HG2	4:A:830:HOH:O	2.07	0.53
1:A:606:LYS:H	1:A:610:THR:HG21	1.73	0.53
1:B:118:LYS:HD2	1:B:123:TRP:CZ2	2.43	0.53
1:B:452:ASN:ND2	4:B:804:HOH:O	2.42	0.52
1:B:102:LYS:HG3	1:B:107:ASN:OD1	2.09	0.52
1:A:26:LYS:O	1:A:28:LYS:HE2	2.09	0.52
1:B:589:ARG:NH1	1:B:654:ASP:OD1	2.43	0.52
1:B:180[B]:LYS:O	1:B:180[B]:LYS:HD2	2.09	0.52
1:A:598:SER:OG	1:A:599:GLY:N	2.42	0.52
1:B:103:THR:OG1	1:B:106:GLY:O	2.20	0.52
1:A:153:LYS:HD2	1:A:161:GLU:OE2	2.10	0.51
1:B:603:LEU:HD13	1:B:612[B]:ARG:HB2	1.93	0.51
1:A:95:VAL:HB	1:A:114:PHE:HB2	1.94	0.50
1:A:396:GLN:NE2	1:A:497:PRO:O	2.39	0.50
1:B:603:LEU:HD11	1:B:614:ILE:HG13	1.94	0.50
1:A:137:GLN:HG3	4:A:801:HOH:O	2.11	0.50
1:A:617:PHE:CE2	1:A:646:ALA:HB2	2.47	0.50
1:B:42:PHE:CE1	1:B:66:PRO:HB3	2.47	0.50
1:B:598:SER:OG	1:B:599:GLY:N	2.43	0.49
1:A:143:HIS:HB3	1:A:145:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:MET:HA	1:B:220:MET:HE2	1.93	0.49
1:B:180[B]:LYS:O	1:B:180[B]:LYS:CD	2.60	0.49
1:B:626:ASN:ND2	1:B:664:TYR:O	2.45	0.49
1:B:327:THR:CG2	1:B:356:GLU:HG3	2.42	0.49
1:A:626:ASN:ND2	1:A:664:TYR:O	2.45	0.49
1:B:387:LYS:NZ	4:B:806:HOH:O	2.44	0.49
1:A:569:ASN:HD22	1:A:569:ASN:N	2.11	0.48
1:B:617:PHE:CE2	1:B:646:ALA:HB2	2.48	0.48
1:B:255:TYR:HB3	1:B:368:VAL:HG12	1.95	0.48
1:A:255:TYR:HB3	1:A:368:VAL:HG12	1.96	0.48
1:A:605:MET:HB3	1:A:610:THR:HG23	1.96	0.48
1:B:95:VAL:HB	1:B:114:PHE:HB2	1.96	0.48
1:A:425:TYR:OH	1:A:473:GLU:HG3	2.13	0.47
1:B:455:LEU:HD23	1:B:570:LEU:HD22	1.96	0.47
1:A:422:LYS:O	1:A:423:THR:C	2.57	0.47
1:A:196:TYR:O	1:A:199:GLN:HG2	2.15	0.47
1:B:396:GLN:NE2	1:B:497:PRO:O	2.39	0.47
1:B:422:LYS:O	1:B:423:THR:C	2.59	0.46
1:A:27:ASP:CG	1:A:93:LYS:HZ3	2.24	0.46
1:B:327:THR:HG21	1:B:356:GLU:HG3	1.97	0.46
1:B:625:PRO:HG3	4:B:808:HOH:O	2.15	0.46
1:A:352:PRO:HG3	1:A:628:MET:HE3	1.98	0.46
1:B:627:MET:CE	1:B:629:MET:HB2	2.46	0.46
1:B:32:ASN:HA	4:B:830:HOH:O	2.16	0.46
1:B:600:THR:O	1:B:601:ALA:HB2	2.16	0.46
1:A:264:LEU:HD21	1:A:273:LYS:O	2.16	0.46
1:B:573:ASP:O	1:B:576:GLN:HB3	2.15	0.46
1:A:91:ASN:ND2	1:A:118:LYS:HB2	2.30	0.46
1:A:247:LYS:O	1:A:365:SER:OG	2.27	0.45
1:A:306:SER:O	1:A:307:ASN:C	2.59	0.45
1:A:351:HIS:HA	1:A:626:ASN:O	2.17	0.45
1:A:195:ASP:O	1:A:199:GLN:OE1	2.34	0.45
1:A:577:GLN:NE2	1:A:581:LYS:HE2	2.32	0.45
1:A:156:ASP:OD1	1:A:160:VAL:N	2.45	0.45
1:B:161:GLU:O	1:B:244:PRO:HG2	2.16	0.45
1:B:498:PHE:CE1	1:B:529:VAL:HG21	2.52	0.45
1:B:587:ILE:CD1	1:B:617:PHE:CZ	2.96	0.45
1:B:247:LYS:O	1:B:365:SER:OG	2.29	0.45
1:A:663[A]:LYS:HZ2	1:A:663[A]:LYS:HG2	1.22	0.44
1:B:481:LYS:CD	1:B:481:LYS:O	2.65	0.44
1:A:600:THR:O	1:A:601:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ASN:HB3	1:B:118:LYS:HB2	1.99	0.44
1:B:280:LYS:O	1:B:285:LYS:HD2	2.18	0.44
1:B:388:LYS:O	1:B:389:GLU:C	2.60	0.44
1:A:540:ASN:O	1:A:541:ASN:C	2.61	0.44
1:B:521:GLN:NE2	1:B:602:GLU:O	2.50	0.44
1:A:42:PHE:CZ	1:A:67:ILE:HD11	2.51	0.44
1:A:161:GLU:O	1:A:244:PRO:HG2	2.17	0.44
1:A:498:PHE:CE1	1:A:529:VAL:HG21	2.53	0.44
1:A:506:LYS:O	1:A:506:LYS:HD2	2.17	0.44
1:A:65:ARG:N	1:A:66:PRO:HD2	2.33	0.44
1:A:287:TYR:CZ	1:A:550:LEU:HD11	2.53	0.44
1:A:388:LYS:O	1:A:389:GLU:C	2.60	0.44
1:A:659:ASN:OD1	1:A:659:ASN:N	2.51	0.44
1:A:605:MET:HB3	1:A:610:THR:CG2	2.47	0.44
1:A:179:SER:C	1:A:181:LYS:H	2.26	0.44
1:B:352:PRO:HG3	1:B:628:MET:HE3	2.00	0.44
1:B:306:SER:O	1:B:307[A]:ASN:C	2.61	0.43
1:A:644:TYR:CE2	1:A:648:ILE:HD11	2.54	0.43
1:A:577:GLN:HE21	1:A:581:LYS:HE2	1.83	0.43
1:A:605:MET:HG3	4:A:847:HOH:O	2.18	0.43
1:A:613:GLN:HB3	1:A:636:VAL:HG22	2.01	0.43
1:A:118:LYS:HE2	1:A:123:TRP:CZ2	2.53	0.43
1:B:31:ASN:O	1:B:35:ASP:N	2.39	0.43
1:B:45:VAL:O	1:B:49:SER:OG	2.31	0.43
1:B:392:LEU:HD21	1:B:397:ILE:HG21	2.00	0.43
1:B:627:MET:HE3	1:B:627:MET:HB2	1.94	0.43
1:A:132:ILE:HG22	1:A:133:ILE:HG12	2.01	0.43
1:B:287:TYR:CZ	1:B:550:LEU:HD11	2.54	0.43
1:A:623:ASP:O	1:A:624:ASN:HB2	2.18	0.43
1:B:351:HIS:HA	1:B:626:ASN:O	2.19	0.43
1:A:469:ARG:O	1:A:472:LEU:N	2.52	0.43
1:B:469:ARG:O	1:B:472:LEU:N	2.51	0.43
1:A:645:ASN:HD22	1:A:645:ASN:H	1.66	0.42
1:B:156:ASP:OD1	1:B:160:VAL:N	2.46	0.42
1:A:49:SER:O	1:A:54:LYS:NZ	2.35	0.42
1:B:176:LYS:HG3	1:B:208:ASP:O	2.19	0.42
1:B:625:PRO:CG	4:B:808:HOH:O	2.67	0.42
1:B:343:ASP:OD1	1:B:639:LYS:NZ	2.49	0.42
1:A:612:ARG:O	1:A:613:GLN:NE2	2.52	0.42
1:A:350:ILE:HG22	1:A:532:LEU:HD22	2.02	0.42
1:A:567:ASN:HA	1:A:570:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:MET:HE3	1:B:140:GLN:O	2.20	0.42
1:A:443:VAL:O	1:A:465:ILE:CD1	2.67	0.42
1:B:65:ARG:N	1:B:66:PRO:HD2	2.34	0.42
1:B:354:THR:OG1	1:B:356:GLU:HB2	2.19	0.42
1:A:338:ASN:CG	4:A:814:HOH:O	2.62	0.42
1:B:540:ASN:O	1:B:541:ASN:C	2.63	0.42
1:B:644:TYR:CE2	1:B:648:ILE:HD11	2.55	0.42
1:A:584:LYS:C	1:A:586:ASP:H	2.28	0.42
1:B:555:ASN:N	3:B:704:CL:CL	2.89	0.42
1:A:610:THR:O	1:A:611:GLY:C	2.62	0.42
1:B:132:ILE:HG22	1:B:133:ILE:HG12	2.01	0.41
1:B:88:VAL:O	1:B:89:SER:C	2.63	0.41
1:B:119:GLU:O	1:B:120:ASP:HB2	2.21	0.41
1:B:481:LYS:O	1:B:481:LYS:HD3	2.19	0.41
1:A:350:ILE:CG2	1:A:532:LEU:HD22	2.51	0.41
1:B:59:GLU:O	1:B:63:THR:OG1	2.39	0.41
1:B:584:LYS:C	1:B:586:ASP:H	2.27	0.41
1:A:420:ASP:O	1:A:421:ASP:C	2.63	0.41
1:B:637:GLN:HA	1:B:641:MET:SD	2.61	0.41
1:A:209:ASP:OD2	1:B:135:GLY:HA2	2.21	0.41
1:A:118:LYS:HA	1:A:122:MET:O	2.21	0.40
1:A:180:LYS:O	1:A:180:LYS:CG	2.68	0.40
1:B:143:HIS:HB3	1:B:145:GLU:OE1	2.20	0.40
1:B:421:ASP:N	1:B:421:ASP:OD1	2.54	0.40
1:A:103:THR:OG1	1:A:106:GLY:O	2.18	0.40
1:A:62:MET:HG3	1:A:127:TRP:CE2	2.57	0.40
1:A:280:LYS:O	1:A:285:LYS:HD2	2.21	0.40
1:B:150:GLU:O	1:B:293:HIS:HB3	2.22	0.40
1:B:287:TYR:OH	1:B:495:ASP:O	2.33	0.40
1:A:261:SER:O	1:A:265:LYS:HG2	2.20	0.40
1:A:300:THR:HG22	1:A:312:THR:HA	2.02	0.40
1:B:345:GLY:HA3	1:B:632:ASN:O	2.22	0.40
1:B:350:ILE:CG2	1:B:532:LEU:HD22	2.51	0.40
1:B:623:ASP:O	1:B:624:ASN:HB2	2.21	0.40
1:A:96:ASP:HA	1:A:112:VAL:O	2.21	0.40
1:A:344:TYR:CE1	1:A:634:LYS:HE3	2.57	0.40
1:A:637:GLN:HA	1:A:641:MET:SD	2.60	0.40
1:B:603:LEU:HG	1:B:614:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	641/643 (100%)	570 (89%)	63 (10%)	8 (1%)	10	41
1	B	639/643 (99%)	563 (88%)	68 (11%)	8 (1%)	9	39
All	All	1280/1286 (100%)	1133 (88%)	131 (10%)	16 (1%)	9	39

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	B	40	LYS
1	A	246	GLU
1	B	27	ASP
1	B	89	SER
1	B	246	GLU
1	A	389	GLU
1	A	611	GLY
1	A	624	ASN
1	B	389	GLU
1	B	624	ASN
1	A	610	THR
1	A	347	GLY
1	A	503	ILE
1	B	611	GLY
1	B	347	GLY

### 5.3.2 Protein sidechains

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	576/574 (100%)	512 (89%)	64 (11%)	6	25
1	B	575/574 (100%)	513 (89%)	62 (11%)	6	26
All	All	1151/1148 (100%)	1025 (89%)	126 (11%)	6	26

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	27	ASP
1	A	28	LYS
1	A	40	LYS
1	A	48	ASP
1	A	69	ILE
1	A	72	SER
1	A	73	LEU
1	A	86	LYS
1	A	90	LYS
1	A	113	GLN
1	A	125	LEU
1	A	145	GLU
1	A	146	ASN
1	A	149	SER
1	A	176	LYS
1	A	177	ASN
1	A	181	LYS
1	A	216	THR
1	A	222	GLU
1	A	224	LEU
1	A	229	LYS
1	A	230	LYS
1	A	246	GLU
1	A	252	LEU
1	A	267	LYS
1	A	273	LYS
1	A	318	LYS
1	A	322	LYS
1	A	324	ILE
1	A	342	ASN
1	A	344	TYR
1	A	365	SER
1	A	368	VAL
1	A	378	GLU

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Mol	Chain	Res	Type
1	A	387	LYS
1	A	388	LYS
1	A	419	LEU
1	A	434	LYS
1	A	436	LYS
1	A	447	GLU
1	A	477	LYS
1	A	500	ASN
1	A	502	GLN
1	A	503	ILE
1	A	506	LYS
1	A	510	ASN
1	A	513	LEU
1	A	514	LEU
1	A	521	GLN
1	A	532	LEU
1	A	533	SER
1	A	545	ASN
1	A	554	LYS
1	A	562	ILE
1	A	566	GLU
1	A	570	LEU
1	A	576	GLN
1	A	587	ILE
1	A	597	LYS
1	A	606	LYS
1	A	613	GLN
1	A	618	ILE
1	A	634	LYS
1	B	27	ASP
1	B	52	ILE
1	B	54	LYS
1	B	72	SER
1	B	73	LEU
1	B	87	LYS
1	B	92	LYS
1	B	102	LYS
1	B	111	ASN
1	B	122	MET
1	B	125	LEU
1	B	145	GLU
1	B	146	ASN

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Mol	Chain	Res	Type
1	B	149	SER
1	B	177	ASN
1	B	181	LYS
1	B	184	LYS
1	B	188	LYS
1	B	215	LYS
1	B	216	THR
1	B	220	MET
1	B	224	LEU
1	B	229	LYS
1	B	252	LEU
1	B	289	LYS
1	B	290	LYS
1	B	317	LYS
1	B	318	LYS
1	B	319	LYS
1	B	324	ILE
1	B	342	ASN
1	B	344	TYR
1	B	356	GLU
1	B	365	SER
1	B	368	VAL
1	B	392	LEU
1	B	419	LEU
1	B	428	ASP
1	B	434	LYS
1	B	436	LYS
1	B	480	GLU
1	B	481	LYS
1	B	485	LYS
1	B	500	ASN
1	B	505	ASN
1	B	510	ASN
1	B	513	LEU
1	B	514	LEU
1	B	521	GLN
1	B	524	ILE
1	B	532	LEU
1	B	545	ASN
1	B	559	LYS
1	B	570	LEU
1	B	581	LYS

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Mol	Chain	Res	Type
1	B	593	ASN
1	B	595	ILE
1	B	604	LYS
1	B	609	GLU
1	B	618	ILE
1	B	622	LYS
1	B	651	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	44	GLN
1	A	91	ASN
1	A	113	GLN
1	A	199	GLN
1	A	200	GLN
1	A	251	HIS
1	A	307	ASN
1	A	342	ASN
1	A	351	HIS
1	A	353	GLN
1	A	377	ASN
1	A	393	ASN
1	A	442	ASN
1	A	505	ASN
1	A	530	GLN
1	A	569	ASN
1	A	576	GLN
1	A	577	GLN
1	A	580	ASN
1	A	583	HIS
1	A	593	ASN
1	A	613	GLN
1	A	645	ASN
1	B	32	ASN
1	B	44	GLN
1	B	159	ASN
1	B	200	GLN
1	B	251	HIS
1	B	266	GLN
1	B	342	ASN

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Mol	Chain	Res	Type
1	B	353	GLN
1	B	393	ASN
1	B	500	ASN
1	B	502	GLN
1	B	530	GLN
1	B	569	ASN
1	B	593	ASN
1	B	613	GLN
1	B	645	ASN
1	B	659	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	642/643 (99%)	-0.66	0 100 100	35, 98, 146, 200	3 (0%)
1	B	639/643 (99%)	-0.65	0 100 100	39, 98, 142, 181	4 (0%)
All	All	1281/1286 (99%)	-0.66	0 100 100	35, 98, 144, 200	7 (0%)

There are no RSRZ outliers to report.

### 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 oligosaccharides 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	B	704	1/1	0.82	0.11	254,254,254,254	0
3	CL	B	706	1/1	0.87	0.07	97,97,97,97	0
2	CD	B	701	1/1	0.94	0.08	229,229,229,229	0
3	CL	B	707	1/1	0.94	0.03	85,85,85,85	0
3	CL	A	705	1/1	0.98	0.03	76,76,76,76	0
3	CL	A	703	1/1	0.98	0.05	32,32,32,32	0
3	CL	A	704	1/1	0.99	0.11	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	B	705	1/1	0.99	0.04	77,77,77,77	0
2	CD	B	703	1/1	1.00	0.01	102,102,102,102	0
2	CD	A	702	1/1	1.00	0.02	76,76,76,76	0
2	CD	A	701	1/1	1.00	0.02	87,87,87,87	0
2	CD	B	702	1/1	1.00	0.02	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.