WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 10:52 pm GMT

PDB ID	:	6XV5
Title	:	Crystal structure of penicillin-binding protein 2 from Yersinia pestis in complex with ertapenem
Authors	:	Pankov, G.; Hunter, W.N.; Dawson, A.
Deposited on	:	2020-01-21
Resolution	:	2.67 Å(reported)

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
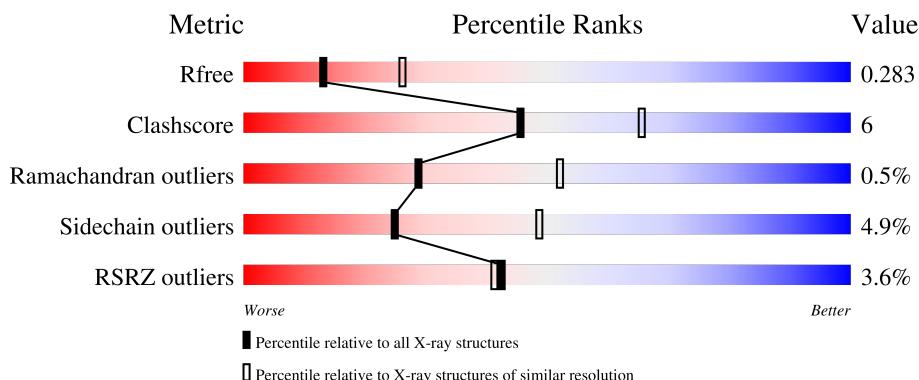
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
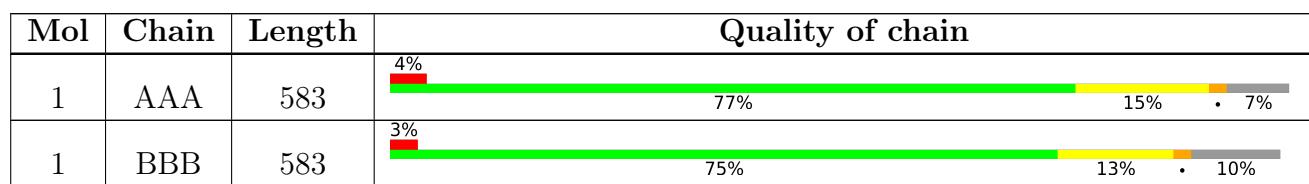
The reported resolution of this entry is 2.67 Å.

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	Percentile Ranks	Value
Rfree		0.283
Clashscore		6
Ramachandran outliers		0.5%
Sidechain outliers		4.9%
RSRZ outliers		3.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	AAA	583	4% / 77% 15% · 7%
1	BBB	583	3% / 75% 13% · 10%

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
1	O2E	AAA	331	X	-	-	-
1	O2E	BBB	331	X	-	-	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8700 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 Peptidoglycan D,D-transpeptidase MrdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	BBB	526	4205	2683	726	786	10	0	3	0
1	AAA	543	Total	C	N	O	S	0	1	0
			4336	2761	757	808	10			

There are 36 discrepancies between the modelled and reference sequences:
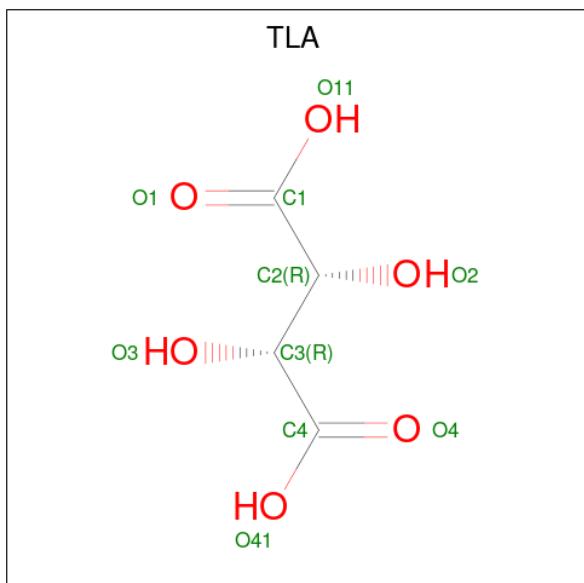
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	31	HIS	-	expression tag	UNP A0A384KFW3
BBB	32	HIS	-	expression tag	UNP A0A384KFW3
BBB	33	HIS	-	expression tag	UNP A0A384KFW3
BBB	34	HIS	-	expression tag	UNP A0A384KFW3
BBB	35	HIS	-	expression tag	UNP A0A384KFW3
BBB	36	HIS	-	expression tag	UNP A0A384KFW3
BBB	37	SER	-	expression tag	UNP A0A384KFW3
BBB	38	SER	-	expression tag	UNP A0A384KFW3
BBB	39	GLY	-	expression tag	UNP A0A384KFW3
BBB	40	GLU	-	expression tag	UNP A0A384KFW3
BBB	41	ASN	-	expression tag	UNP A0A384KFW3
BBB	42	LEU	-	expression tag	UNP A0A384KFW3
BBB	43	TYR	-	expression tag	UNP A0A384KFW3
BBB	44	PHE	-	expression tag	UNP A0A384KFW3
BBB	45	GLN	-	expression tag	UNP A0A384KFW3
BBB	46	GLY	-	expression tag	UNP A0A384KFW3
BBB	47	HIS	-	expression tag	UNP A0A384KFW3
BBB	48	MET	-	expression tag	UNP A0A384KFW3
AAA	31	HIS	-	expression tag	UNP A0A384KFW3
AAA	32	HIS	-	expression tag	UNP A0A384KFW3
AAA	33	HIS	-	expression tag	UNP A0A384KFW3
AAA	34	HIS	-	expression tag	UNP A0A384KFW3
AAA	35	HIS	-	expression tag	UNP A0A384KFW3
AAA	36	HIS	-	expression tag	UNP A0A384KFW3
AAA	37	SER	-	expression tag	UNP A0A384KFW3

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	38	SER	-	expression tag	UNP A0A384KFW3
AAA	39	GLY	-	expression tag	UNP A0A384KFW3
AAA	40	GLU	-	expression tag	UNP A0A384KFW3
AAA	41	ASN	-	expression tag	UNP A0A384KFW3
AAA	42	LEU	-	expression tag	UNP A0A384KFW3
AAA	43	TYR	-	expression tag	UNP A0A384KFW3
AAA	44	PHE	-	expression tag	UNP A0A384KFW3
AAA	45	GLN	-	expression tag	UNP A0A384KFW3
AAA	46	GLY	-	expression tag	UNP A0A384KFW3
AAA	47	HIS	-	expression tag	UNP A0A384KFW3
AAA	48	MET	-	expression tag	UNP A0A384KFW3

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	AAA	1	10	4	6	0	0
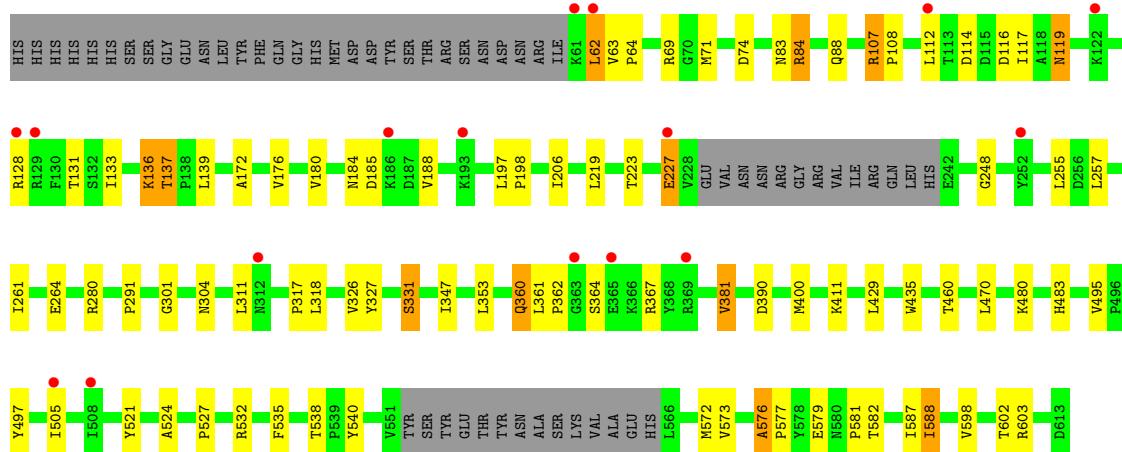
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	BBB	88	88	88	0	0
3	AAA	61	61	61	0	0
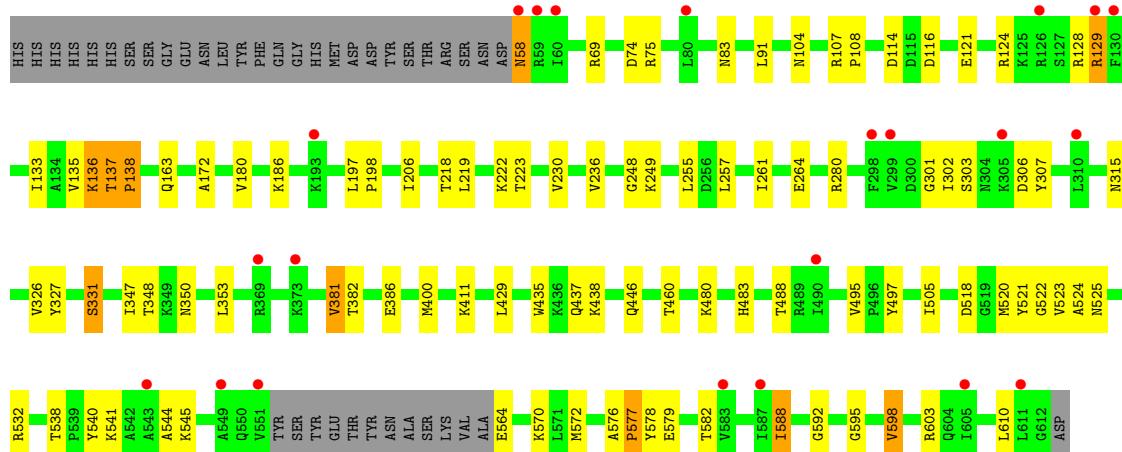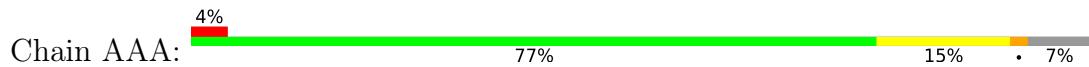
3 Residue-property plots ⓘ

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: Peptidoglycan D,D-transpeptidase MrdA

Chain BBB:

• Molecule 1: Peptidoglycan D,D-transpeptidase MrdA

Chain AAA:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.27Å 147.77Å 164.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.94 – 2.67 109.94 – 2.67	Depositor EDS
% Data completeness (in resolution range)	77.2 (109.94-2.67) 77.2 (109.94-2.67)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.69 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.213 , 0.285 0.216 , 0.283	Depositor DCC
R_{free} test set	1485 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	75.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.1	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8700	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: O2E, TLA

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	AAA	0.65	0/4396	0.75	0/5963
1	BBB	0.64	0/4266	0.75	0/5787
All	All	0.64	0/8662	0.75	0/11750

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	AAA	1	2
1	BBB	1	2
All	All	2	4

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	BBB	331	O2E	C11
1	AAA	331	O2E	C11

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	137	THR	Peptide
1	AAA	576	ALA	Peptide
1	BBB	137	THR	Peptide
1	BBB	576	ALA	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	AAA	4336	0	4295	53	0
1	BBB	4205	0	4159	57	0
2	AAA	10	0	4	0	0
3	AAA	61	0	0	0	0
3	BBB	88	0	0	2	0
All	All	8700	0	8458	109	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 6.

All (109) 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:BBB:84[B]:ARG:HH21	1:BBB:84[B]:ARG:HG2	1.11	1.12
1:BBB:62:LEU:HD21	1:BBB:227:GLU:OE1	1.46	1.12
1:BBB:84[B]:ARG:HH21	1:BBB:84[B]:ARG:CG	1.82	0.93
1:BBB:131:THR:O	1:BBB:133:ILE:HD12	1.68	0.92
1:BBB:62:LEU:HD21	1:BBB:227:GLU:CD	1.98	0.84
1:BBB:131:THR:O	1:BBB:133:ILE:CD1	2.25	0.83
1:BBB:62:LEU:CD2	1:BBB:227:GLU:CD	2.48	0.82
1:AAA:83:ASN:HB3	1:AAA:163:GLN:HE22	1.54	0.73
1:BBB:84[B]:ARG:HG2	1:BBB:84[B]:ARG:NH2	1.92	0.71
1:BBB:62:LEU:CD2	1:BBB:227:GLU:OE1	2.34	0.68
1:BBB:360:GLN:HG2	1:BBB:367:ARG:HG2	1.76	0.68
1:BBB:311:LEU:HD12	1:BBB:318:LEU:CD1	2.24	0.67
1:BBB:62:LEU:HD23	1:BBB:227:GLU:CD	2.21	0.60
1:BBB:331:O2E:N	1:BBB:331:O2E:O1	2.34	0.60
1:BBB:116:ASP:OD2	1:BBB:136:LYS:HE3	2.01	0.60
1:AAA:121:GLU:O	1:AAA:124:ARG:HG2	2.02	0.60
1:AAA:331:O2E:O1	1:AAA:331:O2E:N	2.35	0.60
1:AAA:577:PRO:HD3	1:AAA:610:LEU:CD1	2.32	0.60
1:AAA:58:ASN:N	1:AAA:230:VAL:O	2.35	0.59
1:BBB:71:MET:HE1	3:BBB:704:HOH:O	2.05	0.57
1:BBB:114:ASP:O	1:BBB:117:ILE:HG13	2.07	0.55
1:AAA:577:PRO:HD3	1:AAA:610:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:116:ASP:OD2	1:AAA:136:LYS:HE2	2.07	0.54
1:BBB:84[B]:ARG:CG	1:BBB:84[B]:ARG:NH2	2.52	0.53
1:AAA:129:ARG:N	1:AAA:129:ARG:HD3	2.24	0.53
1:AAA:521:TYR:CD1	1:AAA:525:ASN:ND2	2.76	0.53
1:BBB:527:PRO:HA	1:BBB:532:ARG:HD3	1.91	0.53
1:BBB:257:LEU:O	1:BBB:261:ILE:HG12	2.09	0.52
1:AAA:347:ILE:HD12	1:AAA:381:VAL:HG13	1.90	0.52
1:AAA:257:LEU:O	1:AAA:261:ILE:HG12	2.09	0.51
1:AAA:524:ALA:O	1:AAA:532:ARG:HA	2.10	0.51
1:AAA:538:THR:HG22	1:AAA:603:ARG:CZ	2.40	0.51
1:BBB:347:ILE:HD12	1:BBB:381:VAL:HG13	1.92	0.51
1:BBB:524:ALA:O	1:BBB:532:ARG:HA	2.11	0.50
1:BBB:107:ARG:HG3	1:BBB:112:LEU:O	2.11	0.49
1:AAA:302:ILE:HG13	1:AAA:307:TYR:HB2	1.93	0.49
1:BBB:572:MET:HE2	1:BBB:602:THR:HG21	1.94	0.49
1:AAA:520:MET:HA	1:AAA:523:VAL:HG12	1.93	0.49
1:BBB:326:VAL:HG13	1:BBB:460:THR:HB	1.95	0.49
1:AAA:429:LEU:HD21	1:AAA:435:TRP:CZ2	2.48	0.49
1:AAA:197:LEU:N	1:AAA:198:PRO:HD2	2.27	0.49
1:AAA:197:LEU:N	1:AAA:198:PRO:CD	2.76	0.48
1:AAA:572:MET:HB3	1:AAA:598:VAL:CG2	2.43	0.48
1:AAA:521:TYR:CE1	1:AAA:525:ASN:ND2	2.82	0.48
1:BBB:304:ASN:OD1	1:AAA:564:GLU:N	2.47	0.47
1:BBB:197:LEU:N	1:BBB:198:PRO:CD	2.77	0.47
1:BBB:116:ASP:OD2	1:BBB:136:LYS:CE	2.62	0.47
1:BBB:347:ILE:HD12	1:BBB:381:VAL:CG1	2.44	0.47
1:BBB:197:LEU:N	1:BBB:198:PRO:HD2	2.30	0.47
1:BBB:411:LYS:HB3	1:BBB:505:ILE:HD12	1.96	0.47
1:AAA:523:VAL:CG1	1:AAA:544:ALA:O	2.62	0.47
1:BBB:291:PRO:HG2	1:BBB:317:PRO:HB3	1.97	0.47
1:BBB:136:LYS:HG2	1:BBB:139:LEU:CD2	2.45	0.47
1:AAA:348:THR:OG1	1:AAA:350:ASN:OD1	2.33	0.47
1:BBB:69:ARG:O	1:BBB:83:ASN:ND2	2.48	0.46
1:AAA:230:VAL:HG12	1:AAA:236:VAL:HA	1.98	0.46
1:BBB:172:ALA:HA	1:BBB:264:GLU:OE2	2.16	0.46
1:AAA:570:LYS:HG2	1:AAA:592:GLY:HA2	1.97	0.46
1:AAA:218:THR:O	1:AAA:249:LYS:HG2	2.15	0.46
1:AAA:538:THR:OG1	1:AAA:540:TYR:O	2.22	0.46
1:AAA:315:ASN:N	1:AAA:315:ASN:HD22	2.13	0.46
1:AAA:411:LYS:HB3	1:AAA:505:ILE:HD12	1.96	0.46
1:AAA:197:LEU:O	1:AAA:197:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:326:VAL:HG13	1:AAA:460:THR:HB	1.98	0.46
1:AAA:347:ILE:HD12	1:AAA:381:VAL:CG1	2.45	0.45
1:BBB:119:ASN:HD22	1:BBB:119:ASN:C	2.20	0.45
1:AAA:172:ALA:HA	1:AAA:264:GLU:OE2	2.17	0.45
1:AAA:280:ARG:O	1:AAA:480:LYS:HE3	2.17	0.45
1:BBB:587:ILE:HG12	1:BBB:598:VAL:HG23	1.98	0.45
1:BBB:88:GLN:HE21	1:BBB:137:THR:HB	1.82	0.44
1:BBB:180:VAL:HA	1:BBB:206:ILE:O	2.17	0.44
1:BBB:579:GLU:OE1	3:BBB:701:HOH:O	2.21	0.44
1:AAA:327:TYR:CD1	1:AAA:588:ILE:HD11	2.53	0.44
1:BBB:361:LEU:HD12	1:BBB:362:PRO:HD2	1.98	0.43
1:BBB:219:LEU:O	1:BBB:248:GLY:HA3	2.18	0.43
1:AAA:91:LEU:HD23	1:AAA:135:VAL:HG21	1.99	0.43
1:AAA:137:THR:HA	1:AAA:138:PRO:HA	1.79	0.43
1:AAA:303:SER:OG	1:AAA:306:ASP:OD1	2.34	0.43
1:BBB:107:ARG:N	1:BBB:108:PRO:HD2	2.33	0.43
1:AAA:129:ARG:N	1:AAA:129:ARG:CD	2.81	0.43
1:AAA:219:LEU:O	1:AAA:248:GLY:HA3	2.19	0.43
1:BBB:280:ARG:O	1:BBB:480:LYS:HE3	2.18	0.43
1:BBB:429:LEU:HD21	1:BBB:435:TRP:CZ2	2.54	0.43
1:AAA:107:ARG:N	1:AAA:108:PRO:HD2	2.33	0.43
1:AAA:541:LYS:O	1:AAA:578:TYR:HB2	2.19	0.43
1:BBB:63:VAL:HB	1:BBB:64:PRO:HD2	2.00	0.42
1:AAA:107:ARG:HB2	1:AAA:108:PRO:HD3	2.01	0.42
1:AAA:180:VAL:HA	1:AAA:206:ILE:O	2.20	0.42
1:BBB:74:ASP:HB2	1:BBB:255:LEU:O	2.20	0.42
1:AAA:538:THR:HG22	1:AAA:603:ARG:NH2	2.34	0.42
1:AAA:483:HIS:CE1	1:AAA:497:TYR:CD2	3.08	0.42
1:BBB:576:ALA:O	1:BBB:581:PRO:HA	2.20	0.42
1:AAA:572:MET:HB3	1:AAA:598:VAL:HG22	2.01	0.42
1:BBB:331:O2E:O4	1:BBB:390:ASP:OD1	2.38	0.42
1:AAA:69:ARG:O	1:AAA:83:ASN:ND2	2.51	0.42
1:AAA:386:GLU:HG2	1:AAA:522:GLY:HA3	2.01	0.41
1:BBB:483:HIS:CE1	1:BBB:497:TYR:CD2	3.07	0.41
1:BBB:327:TYR:CD1	1:BBB:588:ILE:HD11	2.55	0.41
1:BBB:470:LEU:HD22	1:BBB:573:VAL:HB	2.03	0.41
1:AAA:74:ASP:HB2	1:AAA:255:LEU:O	2.20	0.41
1:BBB:535:PHE:HZ	1:BBB:572:MET:CE	2.33	0.41
1:AAA:124:ARG:HB3	1:AAA:133:ILE:CD1	2.50	0.41
1:BBB:521:TYR:C	1:BBB:521:TYR:CD1	2.93	0.41
1:AAA:518:ASP:O	1:AAA:521:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:104:ASN:OD1	1:AAA:107:ARG:HD2	2.20	0.41
1:BBB:538:THR:CG2	1:BBB:540[A]:TYR:CE2	3.04	0.40
1:BBB:538:THR:CG2	1:BBB:540[B]:TYR:CE2	3.04	0.40
1:BBB:188:VAL:HG23	1:BBB:197:LEU:HD11	2.04	0.40
1:BBB:331:O2E:O1	1:BBB:331:O2E:CA	2.68	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	AAA	539/583 (92%)	514 (95%)	22 (4%)	3 (1%)	25	47
1	BBB	522/583 (90%)	499 (96%)	21 (4%)	2 (0%)	34	58
All	All	1061/1166 (91%)	1013 (96%)	43 (4%)	5 (0%)	29	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	301	GLY
1	BBB	577	PRO
1	AAA	577	PRO
1	AAA	301	GLY
1	AAA	595	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	AAA	458/493 (93%)	434 (95%)	24 (5%)	23	46
1	BBB	444/493 (90%)	423 (95%)	21 (5%)	26	50
All	All	902/986 (92%)	857 (95%)	45 (5%)	25	47

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	62	LEU
1	BBB	84[A]	ARG
1	BBB	84[B]	ARG
1	BBB	107	ARG
1	BBB	119	ASN
1	BBB	128	ARG
1	BBB	136	LYS
1	BBB	176	VAL
1	BBB	184	ASN
1	BBB	185	ASP
1	BBB	223	THR
1	BBB	227	GLU
1	BBB	353	LEU
1	BBB	360	GLN
1	BBB	364	SER
1	BBB	381	VAL
1	BBB	400	MET
1	BBB	495	VAL
1	BBB	582	THR
1	BBB	588	ILE
1	BBB	603	ARG
1	AAA	58	ASN
1	AAA	75	ARG
1	AAA	114	ASP
1	AAA	128	ARG
1	AAA	129	ARG
1	AAA	136	LYS
1	AAA	138	PRO
1	AAA	186	LYS
1	AAA	222	LYS
1	AAA	223	THR
1	AAA	353	LEU
1	AAA	381	VAL
1	AAA	382	THR

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Mol	Chain	Res	Type
1	AAA	400	MET
1	AAA	437	GLN
1	AAA	438	LYS
1	AAA	446	GLN
1	AAA	488	THR
1	AAA	495	VAL
1	AAA	545	LYS
1	AAA	579	GLU
1	AAA	582	THR
1	AAA	588	ILE
1	AAA	598	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	O2E	BBB	331	1	36,41,41	1.85	6 (16%)	31,58,58	1.14	4 (12%)
1	O2E	AAA	331	1	36,41,41	1.81	6 (16%)	31,58,58	1.16	4 (12%)

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
1	O2E	BBB	331	1	1/1/13/16	28/35/64/64	0/3/3/3
1	O2E	AAA	331	1	1/1/13/16	26/35/64/64	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	331	O2E	C11-C24	-7.15	1.50	1.55
1	BBB	331	O2E	C11-C24	-6.85	1.50	1.55
1	BBB	331	O2E	C9-N2	5.71	1.33	1.28
1	AAA	331	O2E	C9-N2	4.60	1.32	1.28
1	BBB	331	O2E	C11-S1	-4.07	1.74	1.84
1	AAA	331	O2E	C11-S1	-3.88	1.75	1.84
1	AAA	331	O2E	O7-C19	2.95	1.31	1.22
1	BBB	331	O2E	O7-C19	2.92	1.31	1.22
1	AAA	331	O2E	O6-C10	-2.92	1.22	1.30
1	BBB	331	O2E	O8-C19	-2.56	1.22	1.30
1	BBB	331	O2E	O6-C10	-2.55	1.23	1.30
1	AAA	331	O2E	O8-C19	-2.52	1.22	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	331	O2E	C23-C14-N3	-2.99	100.40	106.22
1	BBB	331	O2E	O8-C19-C18	2.74	121.97	114.85
1	AAA	331	O2E	O8-C19-C18	2.74	121.97	114.85
1	AAA	331	O2E	O2-C1-C5	2.67	114.30	111.08
1	AAA	331	O2E	O7-C19-C18	-2.55	114.66	121.45
1	BBB	331	O2E	O7-C19-C18	-2.51	114.76	121.45
1	BBB	331	O2E	C25-C24-C11	-2.32	109.24	113.35
1	AAA	331	O2E	C7-C6-C5	2.18	115.14	112.15

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	BBB	331	O2E	C11
1	AAA	331	O2E	C11

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BBB	331	O2E	C24-C11-S1-C12
1	BBB	331	O2E	CA-C2-O2-C1

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Mol	Chain	Res	Type	Atoms
1	BBB	331	O2E	O2-C2-CA-C
1	BBB	331	O2E	N3-C14-C15-O9
1	BBB	331	O2E	N3-C14-C15-N4
1	BBB	331	O2E	C14-C15-N4-C16
1	BBB	331	O2E	O9-C15-N4-C16
1	BBB	331	O2E	C13-C12-S1-C11
1	BBB	331	O2E	O6-C10-C9-C11
1	BBB	331	O2E	O6-C10-C9-N2
1	BBB	331	O2E	O5-C10-C9-C11
1	BBB	331	O2E	O5-C10-C9-N2
1	AAA	331	O2E	CA-C2-O2-C1
1	AAA	331	O2E	O2-C2-CA-C
1	AAA	331	O2E	N3-C14-C15-O9
1	AAA	331	O2E	C23-C14-C15-O9
1	AAA	331	O2E	N3-C14-C15-N4
1	AAA	331	O2E	C14-C15-N4-C16
1	AAA	331	O2E	O9-C15-N4-C16
1	AAA	331	O2E	C13-C12-S1-C11
1	AAA	331	O2E	C23-C12-S1-C11
1	AAA	331	O2E	O6-C10-C9-C11
1	AAA	331	O2E	O6-C10-C9-N2
1	AAA	331	O2E	O5-C10-C9-C11
1	AAA	331	O2E	O5-C10-C9-N2
1	BBB	331	O2E	C5-C1-O2-C2
1	BBB	331	O2E	O1-C1-O2-C2
1	AAA	331	O2E	C5-C1-O2-C2
1	AAA	331	O2E	O1-C1-O2-C2
1	AAA	331	O2E	C20-C18-C19-O8
1	AAA	331	O2E	C20-C18-C19-O7
1	AAA	331	O2E	C17-C18-C19-O7
1	AAA	331	O2E	C17-C18-C19-O8
1	BBB	331	O2E	C20-C18-C19-O8
1	BBB	331	O2E	C20-C18-C19-O7
1	BBB	331	O2E	C17-C18-C19-O8
1	BBB	331	O2E	C17-C18-C19-O7
1	BBB	331	O2E	C23-C14-C15-O9
1	AAA	331	O2E	C23-C14-C15-N4
1	BBB	331	O2E	C22-C16-N4-C15
1	AAA	331	O2E	C8-C5-C6-C7
1	BBB	331	O2E	C1-C5-C6-C7
1	BBB	331	O2E	C1-C5-C8-C24
1	AAA	331	O2E	C1-C5-C8-C24

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Mol	Chain	Res	Type	Atoms
1	BBB	331	O2E	O2-C1-C5-C8
1	AAA	331	O2E	O2-C1-C5-C8
1	BBB	331	O2E	C17-C16-N4-C15
1	BBB	331	O2E	C23-C14-C15-N4
1	AAA	331	O2E	C24-C11-S1-C12
1	BBB	331	O2E	C6-C5-C8-C24
1	AAA	331	O2E	C6-C5-C8-C24
1	BBB	331	O2E	O2-C2-CA-N
1	BBB	331	O2E	C6-C5-C8-N2
1	AAA	331	O2E	C6-C5-C8-N2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BBB	331	O2E	3	0
1	AAA	331	O2E	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	TLA	AAA	701	-	9,9,9	1.10	0	12,12,12	1.00	1 (8%)

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	TLA	AAA	701	-	-	10/12/12/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	701	TLA	O11-C1-C2	2.10	118.95	113.27

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	701	TLA	C1-C2-C3-O3
2	AAA	701	TLA	C1-C2-C3-C4
2	AAA	701	TLA	O2-C2-C3-O3
2	AAA	701	TLA	O2-C2-C3-C4
2	AAA	701	TLA	O3-C3-C4-O4
2	AAA	701	TLA	O3-C3-C4-O41
2	AAA	701	TLA	O1-C1-C2-C3
2	AAA	701	TLA	O1-C1-C2-O2
2	AAA	701	TLA	O11-C1-C2-C3
2	AAA	701	TLA	O11-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	542/583 (92%)	0.41	22 (4%)	37	35	47, 85, 126, 151	0
1	BBB	525/583 (90%)	0.40	16 (3%)	50	49	42, 73, 124, 148	0
All	All	1067/1166 (91%)	0.40	38 (3%)	42	41	42, 79, 126, 151	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	312	ASN	4.6
1	BBB	61	LYS	4.5
1	BBB	193	LYS	4.3
1	AAA	373	LYS	3.7
1	AAA	130	PHE	3.6
1	AAA	299	VAL	3.5
1	BBB	186	LYS	3.5
1	BBB	62	LEU	3.5
1	AAA	551	VAL	3.2
1	AAA	59	ARG	2.9
1	BBB	112	LEU	2.9
1	BBB	365	GLU	2.8
1	AAA	543	ALA	2.6
1	AAA	129	ARG	2.6
1	AAA	583	VAL	2.5
1	AAA	369	ARG	2.5
1	AAA	605	ILE	2.4
1	AAA	60	ILE	2.4
1	AAA	298	PHE	2.4
1	BBB	129	ARG	2.4
1	BBB	227	GLU	2.4
1	AAA	611	LEU	2.4
1	AAA	310	LEU	2.4
1	AAA	58	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	587	ILE	2.3
1	AAA	490	ILE	2.3
1	AAA	126	ARG	2.2
1	BBB	508	ILE	2.2
1	AAA	305	LYS	2.2
1	BBB	505	ILE	2.2
1	BBB	122	LYS	2.1
1	AAA	193	LYS	2.1
1	BBB	128	ARG	2.1
1	BBB	369	ARG	2.1
1	BBB	363	GLY	2.1
1	AAA	80	LEU	2.1
1	BBB	252	TYR	2.0
1	AAA	549	ALA	2.0

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	O2E	BBB	331	39/39	0.88	0.25	56,99,136,138	0
1	O2E	AAA	331	39/39	0.93	0.22	56,96,164,165	0

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TLA	AAA	701	10/10	0.80	0.27	111,122,126,127	0

6.5 Other polymers (i)

There are no such residues in this entry.