



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:36 PM UTC

PDB ID : 6M9G / pdb_00006m9g
Title : BbvCI B2 dimer with Ta6Br14 clusters
Authors : Shen, B.W.; Stoddard, B.L.
Deposited on : 2018-08-23
Resolution : 2.35 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

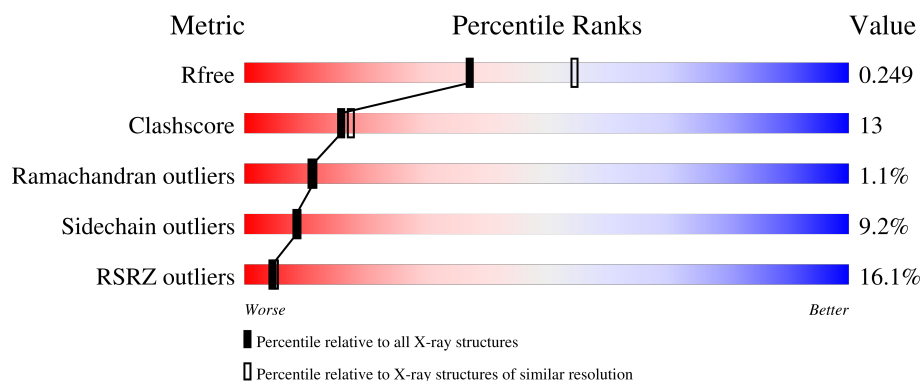
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 $\leq 5\%$. 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	285	17% 71% 22% 5% ..
1	B	285	14% 68% 22% .. 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
2	TBR	A	302	-	-	X	-
2	TBR	A	305	-	-	X	-
4	EDO	A	311	-	-	X	-

2 Entry composition [i](#)

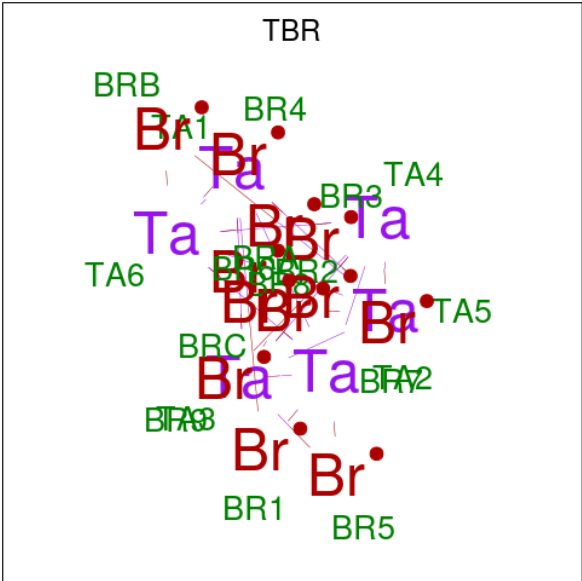
There are 7 unique types of molecules in this entry. The entry contains 4629 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BbvCI endonuclease subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2252	1438	384	422	8			
1	B	266	Total	C	N	O	S	0	0	0
			2140	1364	363	405	8			

- Molecule 2 is HEXATANTALUM DODECABROMIDE (CCD ID: TBR) (formula: Br₁₂Ta₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Br	Ta	0	1
			36	24	12		
2	A	1	Total	Br	Ta	0	0
			18	12	6		
2	A	1	Total	Br	Ta	0	0
			18	12	6		
2	A	1	Total	Br	Ta	0	0
			18	12	6		

Continued on next page...

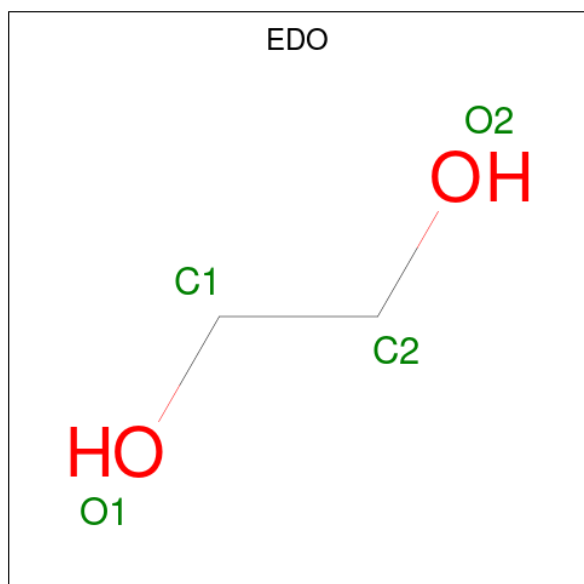
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Br	Ta	0	0
			18	12	6		
2	A	1	Total	Br	Ta	0	0
			18	12	6		
2	A	1	Total	Br	Ta	0	0
			18	12	6		
2	B	1	Total	Br	Ta	0	0
			18	12	6		
2	B	1	Total	Br	Ta	0	0
			18	12	6		
2	B	1	Total	Br	Ta	0	0
			12	6	6		

- Molecule 3 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Br	0	0
			3	3		
3	B	3	Total	Br	0	0
			3	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



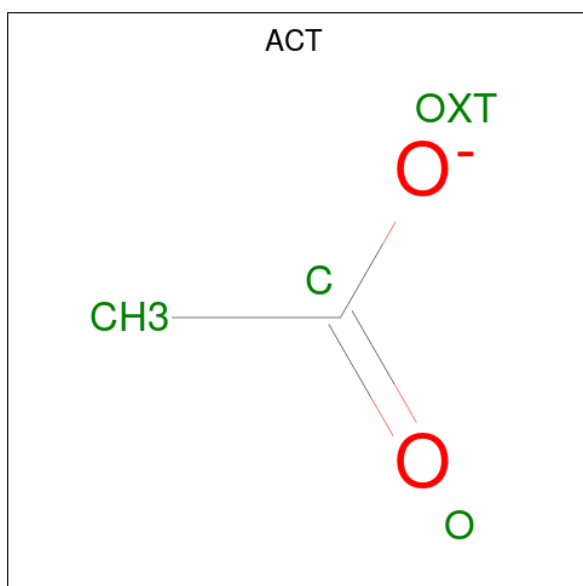
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

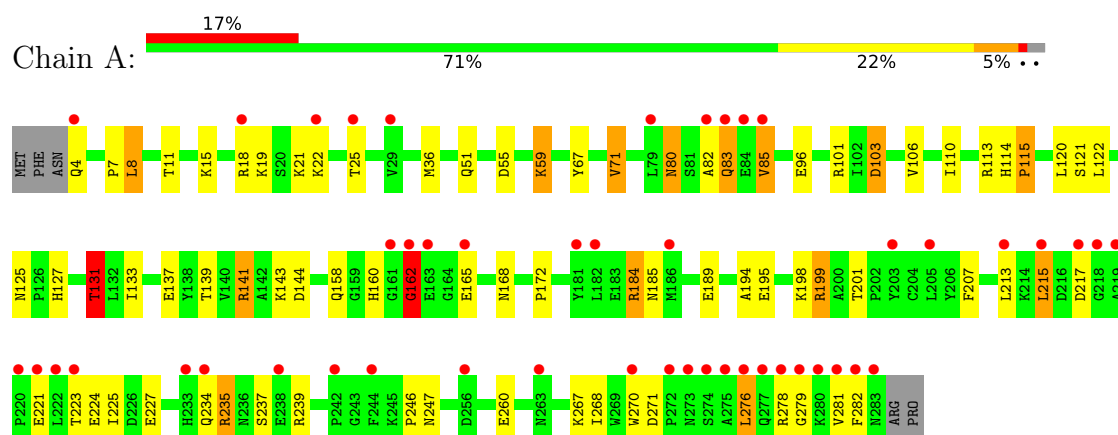
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total	O	0	0
			12	12		
7	B	9	Total	O	0	0
			9	9		

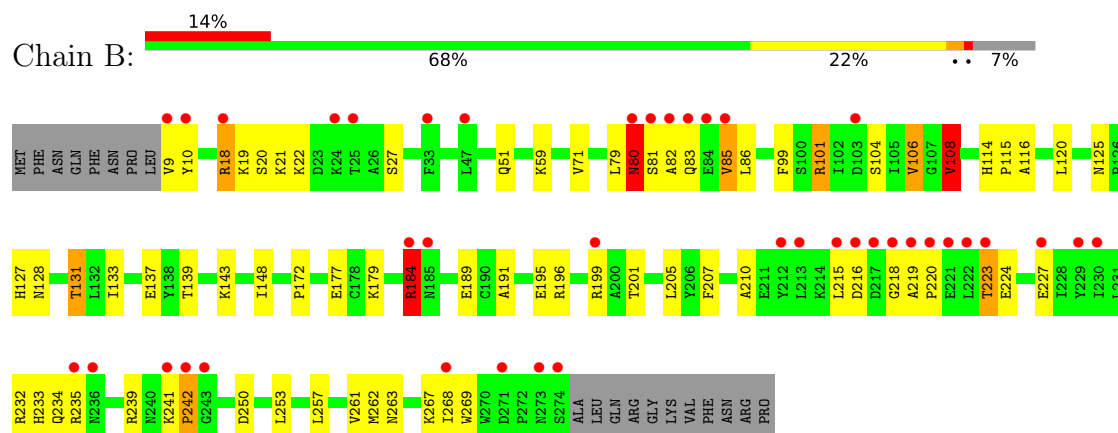
3 Residue-property plots [i](#)

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: BbvCI endonuclease subunit 2



• Molecule 1: BbvCI endonuclease subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	86.11Å 173.30Å 107.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.97 – 2.35 47.97 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.97-2.35) 98.9 (47.97-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.198 , 0.239 0.209 , 0.249	Depositor DCC
R_{free} test set	1702 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4629	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, TBR, ACT, BR, SO4

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	0.70	0/2304	1.31	17/3119 (0.5%)
1	B	0.67	0/2189	1.29	6/2964 (0.2%)
All	All	0.69	0/4493	1.30	23/6083 (0.4%)

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	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ASP	CA-CB-CG	7.09	119.69	112.60
1	A	239	ARG	CA-C-N	6.95	129.59	120.28
1	A	239	ARG	C-N-CA	6.95	129.59	120.28
1	B	184	ARG	CG-CD-NE	6.18	125.59	112.00
1	B	18	ARG	CB-CA-C	6.12	121.89	110.70
1	A	168	ASN	CA-C-N	-5.96	114.33	122.92
1	A	168	ASN	C-N-CA	-5.96	114.33	122.92
1	A	55	ASP	N-CA-CB	5.87	118.85	110.16
1	A	18	ARG	CB-CA-C	5.77	121.26	110.70
1	A	101	ARG	CG-CD-NE	5.73	124.61	112.00
1	A	165	GLU	CB-CG-CD	5.62	122.15	112.60
1	A	144	ASP	CB-CA-C	-5.57	102.14	110.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	GLU	CB-CG-CD	5.52	121.98	112.60
1	A	85	VAL	N-CA-C	-5.39	107.22	112.29
1	B	216	ASP	CB-CA-C	5.26	118.90	110.16
1	B	177	GLU	CB-CG-CD	5.21	121.45	112.60
1	A	281	VAL	CA-C-N	5.17	128.98	122.16
1	A	281	VAL	C-N-CA	5.17	128.98	122.16
1	A	115	PRO	CB-CA-C	-5.14	104.37	111.21
1	B	108	VAL	CA-CB-CG1	5.12	119.11	110.40
1	B	10	TYR	CB-CA-C	5.05	120.48	110.42
1	A	131	THR	N-CA-CB	-5.05	102.42	109.94
1	A	103	ASP	CA-C-O	-5.04	115.50	120.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	162	GLY	Peptide
1	B	18	ARG	Sidechain
1	B	239	ARG	Sidechain

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	2252	0	2224	65	1
1	B	2140	0	2110	59	1
2	A	144	0	0	17	0
2	B	48	0	0	4	0
3	A	3	0	0	2	0
3	B	3	0	0	1	0
4	A	4	0	6	6	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	4	0	3	0	0
7	A	12	0	0	0	0
7	B	9	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4629	0	4343	118	1

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 13.

All (118) 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:221:GLU:OE1	2:A:305:TBR:BR8	2.23	1.11
1:A:270:TRP:NE1	1:B:220:PRO:HD2	1.71	1.05
1:A:270:TRP:HE1	1:B:220:PRO:HD2	0.86	1.00
1:A:7:PRO:HG3	2:A:301[A]:TBR:BR4	2.17	0.99
1:A:131:THR:CG2	1:A:137:GLU:OE1	2.19	0.90
1:B:131:THR:CG2	1:B:137:GLU:OE1	2.23	0.86
1:A:278:ARG:CD	2:A:302:TBR:BR4	2.79	0.86
1:A:278:ARG:HD2	2:A:302:TBR:BR4	2.33	0.82
1:A:270:TRP:HE1	1:B:220:PRO:CD	1.82	0.82
1:B:215:LEU:CD2	1:B:220:PRO:HD3	2.10	0.81
1:A:223:THR:HG22	1:A:225:ILE:H	1.44	0.80
1:B:215:LEU:HD23	1:B:220:PRO:HD3	1.68	0.76
1:B:131:THR:HG21	1:B:137:GLU:OE1	1.87	0.75
1:B:263:ASN:ND2	7:B:401:HOH:O	2.17	0.73
1:B:261:VAL:HG12	1:B:262:MET:HE2	1.69	0.73
1:A:278:ARG:HG2	2:A:302:TBR:BRB	2.45	0.72
1:A:221:GLU:CD	2:A:305:TBR:BR8	2.88	0.71
1:B:99:PHE:CE1	1:B:262:MET:HE3	2.26	0.71
1:A:131:THR:HG21	1:A:137:GLU:OE1	1.90	0.68
1:B:101:ARG:NH2	7:B:402:HOH:O	2.25	0.68
1:A:160:HIS:CD2	2:A:306:TBR:BR4	3.02	0.68
1:B:120:LEU:HD11	1:B:143:LYS:HB2	1.76	0.68
1:B:99:PHE:HE1	1:B:262:MET:HE3	1.58	0.68
1:A:276:LEU:O	1:B:233:HIS:HB3	1.95	0.67
1:A:267:LYS:HE3	2:A:304:TBR:BR8	2.49	0.67
1:B:233:HIS:HE1	1:B:250:ASP:OD2	1.78	0.67
1:A:120:LEU:HD11	1:A:143:LYS:HB2	1.75	0.67
1:A:131:THR:HG23	1:A:137:GLU:OE1	1.94	0.66
1:A:278:ARG:HD3	2:A:302:TBR:BR4	2.52	0.64
1:A:121:SER:HB2	4:A:311:EDO:H21	1.77	0.64
1:B:223:THR:HG22	1:B:224:GLU:N	2.12	0.63
1:A:114:HIS:HB2	1:A:115:PRO:HD2	1.80	0.62
1:B:223:THR:HG22	1:B:224:GLU:H	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:THR:HG21	1:A:225:ILE:HD12	1.81	0.61
1:B:127:HIS:HD2	1:B:128:ASN:ND2	1.99	0.61
1:B:191:ALA:HB1	1:B:223:THR:HB	1.82	0.60
1:A:36:MET:HE3	1:A:36:MET:HA	1.83	0.60
1:A:234:GLN:HE22	1:A:246:PRO:HA	1.66	0.60
1:B:106:VAL:HG13	1:B:108:VAL:HG13	1.83	0.60
1:B:79:LEU:HB2	1:B:83:GLN:HB3	1.85	0.59
1:A:80:ASN:O	1:A:83:GLN:HB3	2.02	0.59
1:B:184:ARG:HH11	1:B:184:ARG:HG2	1.68	0.58
1:B:20:SER:HA	1:B:27:SER:HB2	1.85	0.58
1:A:7:PRO:CG	2:A:301[A]:TBR:BRA	3.03	0.57
1:B:223:THR:HG22	1:B:224:GLU:CG	2.34	0.57
1:A:270:TRP:CZ2	1:B:219:ALA:HA	2.39	0.57
1:A:8:LEU:HD23	3:A:309:BR:BR	2.60	0.57
1:A:11:THR:O	1:A:15:LYS:HG2	2.05	0.56
1:B:131:THR:HG23	1:B:137:GLU:OE1	2.04	0.56
1:B:267:LYS:HD3	2:B:303:TBR:BRC	2.60	0.55
1:B:83:GLN:C	1:B:85:VAL:H	2.15	0.55
1:A:270:TRP:HZ2	1:B:219:ALA:HA	1.72	0.54
1:A:158:GLN:NE2	1:A:162:GLY:O	2.42	0.53
1:B:215:LEU:CD2	1:B:220:PRO:CD	2.84	0.53
1:A:223:THR:HG22	1:A:224:GLU:N	2.24	0.53
1:B:114:HIS:HB2	1:B:115:PRO:HD2	1.90	0.53
1:B:127:HIS:H	1:B:131:THR:HG21	1.73	0.52
1:B:116:ALA:HB3	1:B:148:ILE:HD12	1.90	0.52
1:B:196:ARG:N	2:B:302:TBR:BRB	2.97	0.52
1:B:233:HIS:CE1	1:B:250:ASP:OD2	2.62	0.52
1:B:51:GLN:HE21	1:B:51:GLN:HA	1.74	0.51
1:A:213:LEU:HD11	1:A:215:LEU:HD23	1.92	0.51
1:A:268:ILE:CG2	1:A:271:ASP:HB2	2.41	0.51
1:A:207:PHE:CD1	1:A:227:GLU:HB2	2.45	0.50
1:B:215:LEU:HG	1:B:218:GLY:O	2.11	0.50
1:B:127:HIS:CD2	1:B:128:ASN:ND2	2.79	0.50
1:A:223:THR:HG21	1:A:225:ILE:CD1	2.40	0.49
1:A:234:GLN:NE2	1:A:247:ASN:H	2.10	0.49
1:A:122:LEU:H	4:A:311:EDO:H21	1.77	0.49
1:B:51:GLN:HA	1:B:51:GLN:NE2	2.28	0.49
1:B:232:ARG:O	1:B:234:GLN:HG3	2.13	0.49
1:B:172:PRO:HD2	1:B:201:THR:HG21	1.94	0.49
1:A:199:ARG:NH2	2:A:307:TBR:BR6	3.02	0.48
1:A:235:ARG:HG2	1:A:237:SER:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:HIS:HB2	1:A:115:PRO:CD	2.44	0.48
1:A:279:GLY:HA3	1:B:253:LEU:HD21	1.94	0.48
1:B:223:THR:HG22	1:B:224:GLU:HG2	1.95	0.48
1:A:127:HIS:H	1:A:131:THR:HG21	1.78	0.47
1:A:195:GLU:OE1	2:A:305:TBR:BRA	2.88	0.47
1:A:223:THR:CG2	1:A:224:GLU:N	2.77	0.47
1:A:160:HIS:NE2	2:A:306:TBR:BR4	3.03	0.47
1:A:199:ARG:HH22	4:A:311:EDO:H12	1.80	0.46
1:A:83:GLN:O	1:A:83:GLN:HG2	2.13	0.46
1:A:199:ARG:NH1	3:A:310:BR:BR	3.03	0.46
1:A:122:LEU:O	4:A:311:EDO:H22	2.15	0.46
1:A:172:PRO:HD2	1:A:201:THR:HG21	1.97	0.46
2:B:301:TBR:BR9	3:B:306:BR:BR	3.44	0.46
1:B:114:HIS:HB2	1:B:115:PRO:CD	2.45	0.46
1:B:179:LYS:O	1:B:210:ALA:HA	2.16	0.46
1:A:122:LEU:H	4:A:311:EDO:C2	2.29	0.46
1:B:196:ARG:HD2	2:B:302:TBR:BR8	2.71	0.46
1:A:19:LYS:NZ	1:A:82:ALA:HB1	2.32	0.45
1:B:241:LYS:HB3	1:B:242:PRO:HD2	1.98	0.45
1:A:125:ASN:ND2	1:A:139:THR:OG1	2.49	0.45
1:A:160:HIS:HD2	2:A:306:TBR:BR4	2.51	0.44
1:A:103:ASP:HB2	2:A:301[B]:TBR:BR2	2.73	0.44
1:B:207:PHE:CD1	1:B:227:GLU:HB2	2.53	0.44
1:B:184:ARG:HH11	1:B:184:ARG:CG	2.30	0.44
1:B:223:THR:CG2	1:B:224:GLU:HG2	2.48	0.44
1:A:199:ARG:NH2	4:A:311:EDO:H12	2.32	0.43
1:B:215:LEU:HD21	1:B:220:PRO:HD3	1.98	0.43
1:A:59:LYS:HE3	1:A:59:LYS:HB2	1.82	0.43
1:B:207:PHE:CE1	1:B:227:GLU:HB2	2.54	0.42
1:A:121:SER:OG	1:A:141:ARG:NE	2.52	0.42
1:A:221:GLU:HB3	2:A:305:TBR:BR8	2.75	0.42
1:B:131:THR:CG2	1:B:137:GLU:CD	2.92	0.42
1:A:67:TYR:CZ	1:A:71:VAL:HG11	2.55	0.42
1:A:195:GLU:CD	2:A:305:TBR:BRA	3.18	0.41
1:B:257:LEU:HD23	1:B:257:LEU:C	2.45	0.41
1:B:19:LYS:NZ	1:B:82:ALA:HB1	2.35	0.41
1:B:80:ASN:HB3	1:B:81:SER:H	1.80	0.41
1:A:184:ARG:HA	1:A:184:ARG:HD3	1.85	0.41
1:B:125:ASN:ND2	1:B:139:THR:OG1	2.53	0.41
1:A:184:ARG:CZ	1:A:217:ASP:OD1	2.69	0.41
1:A:207:PHE:CE1	1:A:227:GLU:HB2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:THR:HG21	1:B:137:GLU:CD	2.46	0.41
1:B:223:THR:CG2	1:B:224:GLU:N	2.80	0.41
1:A:194:ALA:O	1:A:198:LYS:HG2	2.21	0.40

All (1) 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:127:HIS:O	1:B:268:ILE:O[3_555]	1.98	0.22

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	278/285 (98%)	261 (94%)	15 (5%)	2 (1%)	18	20
1	B	264/285 (93%)	246 (93%)	14 (5%)	4 (2%)	8	7
All	All	542/570 (95%)	507 (94%)	29 (5%)	6 (1%)	11	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	THR
1	B	242	PRO
1	A	80	ASN
1	B	269	TRP
1	A	162	GLY
1	B	80	ASN

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	244/250 (98%)	220 (90%)	24 (10%)	7	7
1	B	233/250 (93%)	213 (91%)	20 (9%)	10	10
All	All	477/500 (95%)	433 (91%)	44 (9%)	8	9

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	8	LEU
1	A	21	LYS
1	A	22	LYS
1	A	25	THR
1	A	51	GLN
1	A	59	LYS
1	A	71	VAL
1	A	83	GLN
1	A	85	VAL
1	A	106	VAL
1	A	110	ILE
1	A	131	THR
1	A	133	ILE
1	A	141	ARG
1	A	184	ARG
1	A	185	ASN
1	A	189	GLU
1	A	199	ARG
1	A	215	LEU
1	A	235	ARG
1	A	260	GLU
1	A	276	LEU
1	A	282	PHE
1	B	9	VAL
1	B	21	LYS
1	B	22	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	59	LYS
1	B	71	VAL
1	B	80	ASN
1	B	85	VAL
1	B	86	LEU
1	B	101	ARG
1	B	104	SER
1	B	106	VAL
1	B	108	VAL
1	B	131	THR
1	B	133	ILE
1	B	184	ARG
1	B	189	GLU
1	B	195	GLU
1	B	199	ARG
1	B	205	LEU
1	B	235	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	125	ASN
1	A	127	HIS
1	A	234	GLN
1	B	51	GLN
1	B	83	GLN
1	B	87	GLN
1	B	125	ASN
1	B	127	HIS
1	B	233	HIS
1	B	259	GLN

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 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 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	$\# Z > 2$
2	TBR	A	305	-	0,36,36	-	-	-		
4	EDO	A	311	-	3,3,3	0.54	0	2,2,2	0.64	0
2	TBR	A	304	-	0,36,36	-	-	-		
2	TBR	A	302	-	0,36,36	-	-	-		
2	TBR	A	307	-	0,36,36	-	-	-		
6	ACT	A	313	-	3,3,3	0.77	0	3,3,3	0.97	0
2	TBR	A	303	-	0,36,36	-	-	-		
2	TBR	B	302	-	0,36,36	-	-	-		
2	TBR	A	301[A]	-	0,36,36	-	-	-		
2	TBR	B	303	-	0,24,36	-	-	-		
5	SO4	A	312	-	4,4,4	0.54	0	6,6,6	0.48	0
5	SO4	B	307	-	4,4,4	0.45	0	6,6,6	0.28	0
2	TBR	B	301	-	0,36,36	-	-	-		
2	TBR	A	306	-	0,36,36	-	-	-		
2	TBR	A	301[B]	-	0,36,36	-	-	-		

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
4	EDO	A	311	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	311	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	305	TBR	5	0
4	A	311	EDO	6	0
2	A	304	TBR	1	0
2	A	302	TBR	4	0
2	A	307	TBR	1	0
2	B	302	TBR	2	0
2	A	301[A]	TBR	2	0
2	B	303	TBR	1	0
2	B	301	TBR	1	0
2	A	306	TBR	3	0
2	A	301[B]	TBR	1	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 ⓘ

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	A	280/285 (98%)	0.91	48 (17%) 4 4	35, 53, 119, 190	1 (0%)
1	B	266/285 (93%)	0.94	40 (15%) 5 6	33, 52, 112, 159	1 (0%)
All	All	546/570 (95%)	0.92	88 (16%) 4 5	33, 53, 117, 190	2 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	PHE	8.4
1	B	213	LEU	7.6
1	A	281	VAL	6.6
1	A	85	VAL	6.4
1	B	82	ALA	6.1
1	A	82	ALA	5.9
1	A	220	PRO	5.7
1	A	219	ALA	5.6
1	B	215	LEU	5.4
1	A	283	ASN	5.3
1	B	222	LEU	5.3
1	B	220	PRO	5.1
1	A	270	TRP	5.0
1	B	219	ALA	4.6
1	B	85	VAL	4.4
1	B	223	THR	4.4
1	A	234	GLN	4.4
1	A	84	GLU	4.3
1	A	276	LEU	4.3
1	B	274	SER	4.1
1	A	222	LEU	4.1
1	A	279	GLY	3.8
1	B	218	GLY	3.8
1	A	275	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	236	ASN	3.7
1	A	274	SER	3.7
1	A	263	ASN	3.6
1	A	217	ASP	3.5
1	B	9	VAL	3.4
1	B	199	ARG	3.4
1	A	244	PHE	3.3
1	B	230	ILE	3.3
1	A	242	PRO	3.3
1	B	103	ASP	3.3
1	B	241	LYS	3.3
1	A	213	LEU	3.2
1	B	184	ARG	3.1
1	A	233	HIS	3.0
1	A	18	ARG	3.0
1	B	217	ASP	3.0
1	B	83	GLN	3.0
1	A	182	LEU	3.0
1	B	81	SER	2.9
1	A	280	LYS	2.8
1	B	221	GLU	2.8
1	B	235	ARG	2.8
1	A	272	PRO	2.7
1	A	221	GLU	2.7
1	A	215	LEU	2.7
1	B	80	ASN	2.6
1	B	25	THR	2.6
1	A	161	GLY	2.6
1	A	162	GLY	2.6
1	B	33	PHE	2.6
1	B	47	LEU	2.6
1	A	4	GLN	2.5
1	B	273	ASN	2.5
1	A	218	GLY	2.4
1	A	205	LEU	2.4
1	B	268	ILE	2.4
1	A	223	THR	2.3
1	B	18	ARG	2.3
1	B	24	LYS	2.3
1	A	25	THR	2.3
1	A	186	MET	2.3
1	A	203	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	243	GLY	2.3
1	A	165	GLU	2.3
1	B	227	GLU	2.3
1	A	79	LEU	2.2
1	A	277	GLN	2.2
1	A	181	TYR	2.2
1	A	29	VAL	2.2
1	A	256	ASP	2.2
1	B	271	ASP	2.2
1	A	163	GLU	2.2
1	B	212	TYR	2.1
1	A	22	LYS	2.1
1	A	238	GLU	2.1
1	B	229	TYR	2.1
1	B	185	ASN	2.1
1	B	216	ASP	2.1
1	B	242	PRO	2.1
1	B	10	TYR	2.1
1	B	84	GLU	2.1
1	A	278	ARG	2.1
1	A	83	GLN	2.0
1	A	273	ASN	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 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, 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
6	ACT	A	313	4/4	0.41	0.31	68,82,90,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	A	312	5/5	0.65	0.14	82,82,82,97	0
5	SO4	B	307	5/5	0.68	0.16	98,110,119,121	0
2	TBR	B	303	12/18	0.82	0.17	103,117,120,121	12
2	TBR	A	306	18/18	0.84	0.17	101,114,117,117	18
2	TBR	A	304	18/18	0.86	0.15	73,77,83,85	18
2	TBR	A	305	18/18	0.87	0.12	112,121,128,129	18
3	BR	B	304	1/1	0.89	0.17	189,189,189,189	0
4	EDO	A	311	4/4	0.89	0.12	45,46,52,53	0
2	TBR	A	307	18/18	0.89	0.12	75,81,89,91	18
3	BR	A	308	1/1	0.89	0.09	112,112,112,112	1
3	BR	A	309	1/1	0.89	0.17	105,105,105,105	0
2	TBR	B	302	18/18	0.90	0.12	76,94,100,103	18
3	BR	A	310	1/1	0.94	0.12	107,107,107,107	0
3	BR	B	306	1/1	0.96	0.14	130,130,130,130	0
3	BR	B	305	1/1	0.97	0.14	106,106,106,106	0
2	TBR	A	302	18/18	0.97	0.07	79,88,95,96	18
2	TBR	A	303	18/18	0.97	0.06	55,64,69,71	18
2	TBR	A	301[A]	18/18	0.98	0.07	64,84,103,104	18
2	TBR	A	301[B]	18/18	0.98	0.07	25,28,34,35	18
2	TBR	B	301	18/18	0.99	0.04	48,53,57,62	0

6.5 Other polymers

There are no such residues in this entry.