



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:51 am GMT

PDB ID : 1QBB  
Title : BACTERIAL CHITOBIASE COMPLEXED WITH CHITOBIOSE (DINAG)  
Authors : Tews, I.; Perrakis, A.; Oppenheim, A.; Dauter, Z.; Wilson, K.S.; Vorgias, C.E.  
Deposited on : 1996-06-07  
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

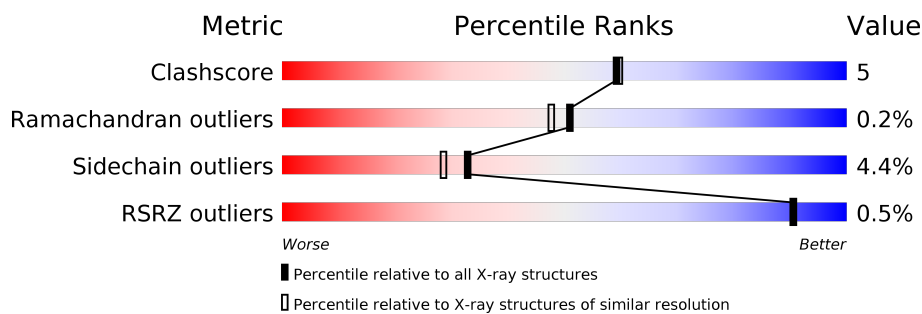
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.00 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))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	858	

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	SO4	A	3	-	-	-	X
3	SO4	A	4	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14056 atoms, of which 6501 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.

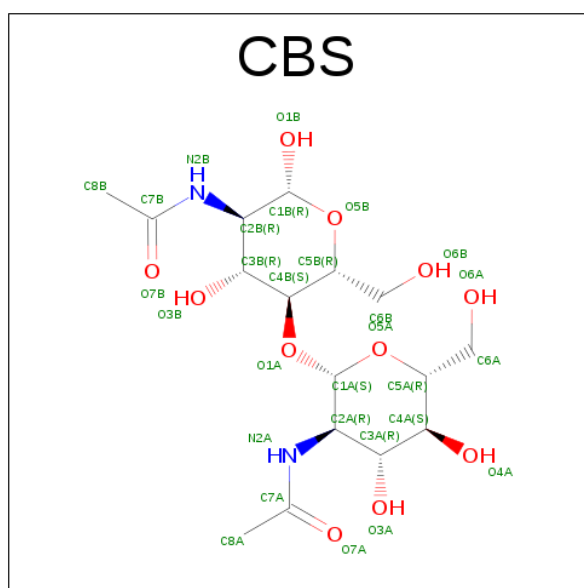
- Molecule 1 is a protein called CHITOBIASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	858	13306	4306	6501	1189	1286	24	0	13	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	566	GLY	SER	CONFLICT	UNP Q54468
A	828	GLY	ALA	CONFLICT	UNP Q54468

- Molecule 2 is SUGAR (DI(N-ACETYL-D-GLUCOSAMINE)) (three-letter code: CBS) (formula:  $C_{16}H_{28}N_2O_{11}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	16	2	12	0	1

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

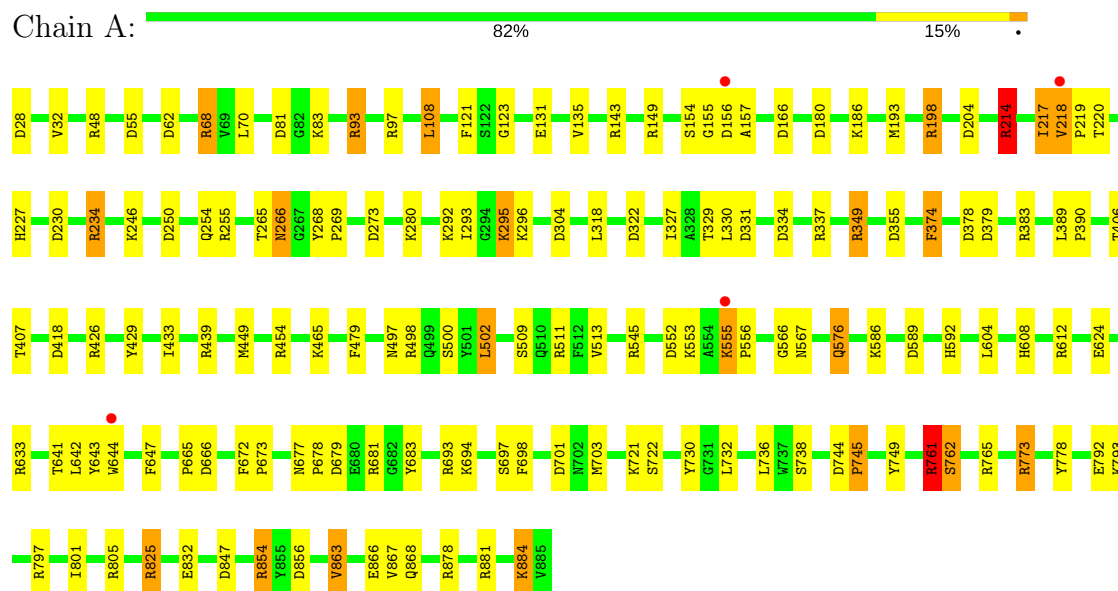
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	700	Total	O	0	0
			700	700		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: CHITOBIASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.70Å 99.90Å 87.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.00) 99.5 (10.00-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.01Å)	Xtriage
Refinement program	ARP/WARP, PROLSQ	Depositor
R, $R_{free}$	0.151 , 0.212 0.143 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 66.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14056	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CBS, 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	1.73	18/7040 (0.3%)	1.63	107/9534 (1.1%)

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	A	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218[A]	VAL	CB-CG1	64.17	2.87	1.52
1	A	218[B]	VAL	CB-CG1	64.17	2.87	1.52
1	A	218[A]	VAL	CB-CG2	37.33	2.31	1.52
1	A	218[B]	VAL	CB-CG2	37.33	2.31	1.52
1	A	218[A]	VAL	CA-C	21.98	2.10	1.52
1	A	218[B]	VAL	CA-C	21.98	2.10	1.52
1	A	217	ILE	C-N	13.03	1.64	1.34
1	A	255[A]	ARG	CD-NE	8.56	1.61	1.46
1	A	255[B]	ARG	CD-NE	8.56	1.61	1.46
1	A	762	SER	CB-OG	-5.99	1.34	1.42
1	A	881	ARG	CB-CG	-5.82	1.36	1.52
1	A	722	SER	CB-OG	5.67	1.49	1.42
1	A	218[A]	VAL	CA-CB	-5.33	1.43	1.54
1	A	218[B]	VAL	CA-CB	-5.33	1.43	1.54
1	A	500[A]	SER	CB-OG	-5.30	1.35	1.42
1	A	500[B]	SER	CB-OG	-5.30	1.35	1.42
1	A	693	ARG	CG-CD	5.21	1.65	1.51
1	A	693	ARG	CD-NE	-5.14	1.37	1.46

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218[A]	VAL	CG1-CB-CG2	-26.02	69.26	110.90
1	A	218[B]	VAL	CG1-CB-CG2	-26.02	69.26	110.90
1	A	773	ARG	CD-NE-CZ	22.54	155.16	123.60
1	A	255[A]	ARG	NE-CZ-NH1	-16.74	111.93	120.30
1	A	255[B]	ARG	NE-CZ-NH1	-16.74	111.93	120.30
1	A	612	ARG	NE-CZ-NH2	-15.60	112.50	120.30
1	A	693	ARG	CD-NE-CZ	15.07	144.69	123.60
1	A	217	ILE	O-C-N	-14.27	99.86	122.70
1	A	266	ASN	CA-CB-CG	14.06	144.33	113.40
1	A	255[A]	ARG	NE-CZ-NH2	13.01	126.81	120.30
1	A	255[B]	ARG	NE-CZ-NH2	13.01	126.81	120.30
1	A	218[A]	VAL	N-CA-C	-12.55	77.11	111.00
1	A	218[B]	VAL	N-CA-C	-12.55	77.11	111.00
1	A	681	ARG	NE-CZ-NH2	-12.39	114.11	120.30
1	A	218[A]	VAL	CA-CB-CG2	-12.25	92.52	110.90
1	A	218[B]	VAL	CA-CB-CG2	-12.25	92.52	110.90
1	A	854	ARG	CD-NE-CZ	11.47	139.66	123.60
1	A	730	TYR	CB-CG-CD2	-10.98	114.41	121.00
1	A	797	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	A	218[A]	VAL	O-C-N	10.66	141.36	121.10
1	A	218[B]	VAL	O-C-N	10.66	141.36	121.10
1	A	545	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	A	681	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	A	805	ARG	CD-NE-CZ	10.23	137.93	123.60
1	A	825	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	A	214	ARG	CA-CB-CG	9.66	134.66	113.40
1	A	93[A]	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	A	93[B]	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	A	255[A]	ARG	CD-NE-CZ	-9.16	110.77	123.60
1	A	255[B]	ARG	CD-NE-CZ	-9.16	110.77	123.60
1	A	337	ARG	NE-CZ-NH1	-8.94	115.83	120.30
1	A	502	LEU	CA-CB-CG	8.93	135.83	115.30
1	A	681	ARG	CD-NE-CZ	8.74	135.83	123.60
1	A	761	ARG	CD-NE-CZ	8.61	135.66	123.60
1	A	383	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	A	805	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	A	426	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	A	218[A]	VAL	CA-C-N	-7.92	94.92	117.10
1	A	218[B]	VAL	CA-C-N	-7.92	94.92	117.10
1	A	454	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	A	374	PHE	CB-CG-CD1	7.55	126.08	120.80
1	A	878	ARG	NE-CZ-NH2	-7.54	116.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	881	ARG	CA-CB-CG	7.49	129.88	113.40
1	A	198	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	805	ARG	CG-CD-NE	7.43	127.39	111.80
1	A	761	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	730	TYR	CB-CG-CD1	7.30	125.38	121.00
1	A	180[A]	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	180[B]	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	383	ARG	CD-NE-CZ	7.18	133.66	123.60
1	A	334	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	108	LEU	CA-CB-CG	6.90	131.18	115.30
1	A	730	TYR	O-C-N	-6.88	111.50	123.20
1	A	643	TYR	CB-CG-CD2	-6.81	116.91	121.00
1	A	778	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	A	439	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	A	156	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	68	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	511	ARG	CB-CG-CD	6.64	128.86	111.60
1	A	778	TYR	CB-CG-CD1	6.61	124.97	121.00
1	A	749	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	A	378	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	217	ILE	CA-C-N	6.50	131.50	117.20
1	A	797	ARG	CD-NE-CZ	6.38	132.53	123.60
1	A	349	ARG	CD-NE-CZ	6.32	132.45	123.60
1	A	881	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	A	304	ASP	CB-CG-OD1	6.25	123.93	118.30
1	A	773	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	97	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	A	612	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	693	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	878	ARG	CD-NE-CZ	6.08	132.11	123.60
1	A	633	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	866	GLU	CA-CB-CG	5.99	126.58	113.40
1	A	355	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	337	ARG	NH1-CZ-NH2	5.92	125.91	119.40
1	A	749	TYR	CB-CG-CD1	5.91	124.55	121.00
1	A	374	PHE	CB-CG-CD2	-5.80	116.74	120.80
1	A	511	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	A	552	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	62	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	390	PRO	N-CA-CB	5.58	110.00	103.30
1	A	765	ARG	NE-CZ-NH1	-5.56	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	745	PRO	N-CA-CB	5.49	109.89	103.30
1	A	234	ARG	CD-NE-CZ	5.48	131.27	123.60
1	A	322	ASP	CB-CG-OD1	5.47	123.23	118.30
1	A	449	MET	CA-CB-CG	5.45	122.56	113.30
1	A	204	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	552	ASP	C-N-CA	5.33	135.04	121.70
1	A	273	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	218[A]	VAL	N-CA-CB	5.30	123.16	111.50
1	A	218[B]	VAL	N-CA-CB	5.30	123.16	111.50
1	A	379	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	511	ARG	CD-NE-CZ	5.26	130.97	123.60
1	A	679	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	856	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	847	ASP	CB-CG-OD1	5.22	122.99	118.30
1	A	624	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	A	81	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	143	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	418	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	55	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	773	ARG	CG-CD-NE	5.05	122.40	111.80
1	A	498	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	A	156	ASP	C-N-CA	5.01	134.24	121.70
1	A	355	ASP	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	ILE	Mainchain

## 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	6805	6501	6597	70	0
2	A	30	0	3	0	0
3	A	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	700	0	0	10	2
All	All	7555	6501	6600	70	2

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 5.

All (70) 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:218[A]:VAL:CG2	1:A:218[A]:VAL:CB	2.31	1.08
1:A:193[A]:MET:HE1	1:A:198:ARG:HA	1.51	0.92
1:A:218[A]:VAL:CG1	1:A:801:ILE:HD13	1.98	0.92
1:A:566:GLY:HA3	4:A:1256:HOH:O	1.70	0.90
1:A:218[A]:VAL:HG11	1:A:801:ILE:HG21	1.59	0.85
1:A:292:LYS:HG3	1:A:331:ASP:OD1	1.85	0.77
1:A:218[A]:VAL:HG11	1:A:801:ILE:HD13	1.70	0.72
1:A:218[A]:VAL:HG12	1:A:801:ILE:HD13	1.72	0.71
1:A:832:GLU:OE1	4:A:1366:HOH:O	2.11	0.68
1:A:465:LYS:HD2	4:A:1228:HOH:O	1.93	0.67
1:A:218[A]:VAL:CG1	1:A:801:ILE:HG21	2.25	0.67
1:A:825:ARG:NH2	4:A:1366:HOH:O	2.30	0.65
1:A:28:ASP:N	1:A:154:SER:HG	1.95	0.64
1:A:697[B]:SER:OG	4:A:1270:HOH:O	2.14	0.64
1:A:250:ASP:O	1:A:254[B]:GLN:HG3	1.98	0.64
1:A:732:LEU:HD23	1:A:762:SER:HB3	1.85	0.58
1:A:497:ASN:HB3	3:A:1:SO4:O1	2.05	0.55
1:A:641:THR:HG22	1:A:665:PRO:HG2	1.88	0.55
1:A:218[A]:VAL:CB	1:A:218[A]:VAL:CG1	2.87	0.53
1:A:295:LYS:HD2	1:A:295:LYS:O	2.11	0.50
1:A:673:PRO:HD3	1:A:683:TYR:O	2.12	0.50
1:A:642:LEU:HD21	1:A:703[B]:MET:HB3	1.94	0.49
1:A:642:LEU:HD22	1:A:647:PHE:HB3	1.96	0.48
1:A:576:GLN:HG3	4:A:1315:HOH:O	2.13	0.47
1:A:68:ARG:HG2	1:A:135:VAL:HG22	1.96	0.47
1:A:296:LYS:HD2	1:A:296:LYS:HA	1.69	0.47
1:A:318:LEU:HD11	1:A:330:LEU:HD21	1.96	0.47
1:A:744:ASP:N	1:A:745:PRO:CD	2.77	0.47
1:A:698:PHE:O	1:A:761:ARG:HD2	2.15	0.46
1:A:429:TYR:CE2	1:A:433:ILE:HD11	2.50	0.46
1:A:604:LEU:O	1:A:608:HIS:HD2	1.99	0.45
1:A:589:ASP:OD1	1:A:592:HIS:ND1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LYS:HD2	4:A:1267:HOH:O	2.16	0.45
1:A:70:LEU:HD11	1:A:131:GLU:HB3	1.99	0.44
1:A:214:ARG:NH2	1:A:230:ASP:OD1	2.44	0.43
1:A:863:VAL:HG11	1:A:867:VAL:HG21	1.99	0.43
1:A:389:LEU:HD21	1:A:479:PHE:CD2	2.53	0.43
1:A:227:HIS:HB2	1:A:329:THR:OG1	2.19	0.43
1:A:268:TYR:HA	1:A:269:PRO:HD3	1.75	0.42
1:A:509:SER:O	1:A:513:VAL:HG23	2.20	0.42
1:A:149:ARG:HG2	1:A:166:ASP:HA	2.02	0.42
1:A:218[A]:VAL:CG2	1:A:218[A]:VAL:CG1	2.98	0.42
1:A:121:PHE:CZ	1:A:123:GLY:HA2	2.54	0.41
1:A:293:ILE:HD13	1:A:327:ILE:HD12	2.01	0.41
1:A:32:VAL:HG23	1:A:154:SER:HB3	2.02	0.41
1:A:269:PRO:HD2	1:A:296:LYS:O	2.21	0.41
1:A:672:PHE:HA	1:A:683:TYR:O	2.21	0.41
1:A:566:GLY:CA	4:A:1256:HOH:O	2.48	0.41
1:A:406:THR:HG23	1:A:407[A]:THR:HG23	2.02	0.41
1:A:576:GLN:CG	4:A:1315:HOH:O	2.68	0.41
1:A:677:ASN:HA	1:A:678:PRO:HD3	1.94	0.41
1:A:555:LYS:N	1:A:556:PRO:HD3	2.36	0.40
1:A:68:ARG:HD3	4:A:1151:HOH:O	2.22	0.40
1:A:868:GLN:HG2	1:A:884:LYS:HG3	2.04	0.40

All (2) 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)
4:A:1388:HOH:O	4:A:1388:HOH:O[2_565]	1.63	0.57
4:A:1338:HOH:O	4:A:1441:HOH:O[3_556]	2.15	0.05

## 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	869/858 (101%)	847 (98%)	20 (2%)	2 (0%)	51	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
1	A	155	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	718/705 (102%)	686 (96%)	32 (4%)	32	27

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	108	LEU
1	A	186	LYS
1	A	214	ARG
1	A	234	ARG
1	A	246	LYS
1	A	265	THR
1	A	266	ASN
1	A	280	LYS
1	A	295	LYS
1	A	349	ARG
1	A	374	PHE
1	A	502	LEU
1	A	553	LYS
1	A	555	LYS
1	A	567	ASN
1	A	576	GLN
1	A	586	LYS
1	A	644	TRP

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Mol	Chain	Res	Type
1	A	666	ASP
1	A	701	ASP
1	A	721	LYS
1	A	736	LEU
1	A	738[A]	SER
1	A	738[B]	SER
1	A	761	ARG
1	A	773	ARG
1	A	792	GLU
1	A	793	LYS
1	A	854	ARG
1	A	863	VAL
1	A	884	LYS

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

Mol	Chain	Res	Type
1	A	144	ASN
1	A	172	GLN
1	A	567	ASN
1	A	576	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

6 ligands 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	$\# Z  > 2$
3	SO4	A	1	-	4,4,4	1.05	0	6,6,6	0.83	0
3	SO4	A	2	-	4,4,4	0.92	0	6,6,6	0.52	0
3	SO4	A	3	-	4,4,4	0.99	0	6,6,6	0.92	0
3	SO4	A	4	-	4,4,4	0.88	0	6,6,6	0.61	0
2	CBS	A	891[A]	-	30,30,30	1.32	5 (16%)	42,43,43	2.14	12 (28%)
2	CBS	A	891[B]	-	30,30,30	1.38	6 (20%)	42,43,43	2.22	14 (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
3	SO4	A	1	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3	-	-	0/0/0/0	0/0/0/0
3	SO4	A	4	-	-	0/0/0/0	0/0/0/0
2	CBS	A	891[A]	-	-	0/16/56/56	0/2/2/2
2	CBS	A	891[B]	-	-	0/16/56/56	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	891[A]	CBS	C3A-C2A	-3.12	1.47	1.53
2	A	891[B]	CBS	C3A-C2A	-3.12	1.47	1.53
2	A	891[A]	CBS	O5B-C1B	-2.58	1.38	1.43
2	A	891[B]	CBS	O5B-C1B	-2.58	1.38	1.43
2	A	891[A]	CBS	O5A-C5A	-2.38	1.38	1.44
2	A	891[B]	CBS	O5A-C5A	-2.38	1.38	1.44
2	A	891[B]	CBS	O1B-C1B	-2.28	1.31	1.39
2	A	891[A]	CBS	C3B-C2B	2.03	1.57	1.53
2	A	891[B]	CBS	C3B-C2B	2.03	1.57	1.53
2	A	891[A]	CBS	O1A-C1A	2.04	1.47	1.41
2	A	891[B]	CBS	O1A-C1A	2.04	1.47	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	891[A]	CBS	O3B-C3B-C2B	-3.26	103.01	109.61
2	A	891[B]	CBS	O3B-C3B-C2B	-3.26	103.01	109.61
2	A	891[A]	CBS	O1A-C1A-O5A	-2.07	105.68	110.70
2	A	891[B]	CBS	O1A-C1A-O5A	-2.07	105.68	110.70
2	A	891[A]	CBS	C4A-C3A-C2A	2.10	113.45	110.33
2	A	891[B]	CBS	C4A-C3A-C2A	2.10	113.45	110.33
2	A	891[A]	CBS	O1A-C4B-C5B	2.20	114.77	109.34
2	A	891[B]	CBS	O1A-C4B-C5B	2.20	114.77	109.34
2	A	891[A]	CBS	C1A-O1A-C4B	2.30	123.60	118.00
2	A	891[B]	CBS	C1A-O1A-C4B	2.30	123.60	118.00
2	A	891[B]	CBS	O1B-C1B-O5B	2.33	117.11	110.20
2	A	891[A]	CBS	O4A-C4A-C3A	2.51	115.81	110.36
2	A	891[B]	CBS	O4A-C4A-C3A	2.51	115.81	110.36
2	A	891[A]	CBS	O5A-C5A-C6A	2.54	112.49	106.41
2	A	891[B]	CBS	O5A-C5A-C6A	2.54	112.49	106.41
2	A	891[B]	CBS	O1B-C1B-C2B	3.48	116.44	109.22
2	A	891[A]	CBS	C1B-O5B-C5B	3.56	119.82	113.39
2	A	891[B]	CBS	C1B-O5B-C5B	3.56	119.82	113.39
2	A	891[A]	CBS	O5B-C1B-C2B	4.20	113.74	109.52
2	A	891[B]	CBS	O5B-C1B-C2B	4.20	113.74	109.52
2	A	891[A]	CBS	O5B-C5B-C4B	4.40	118.75	109.75
2	A	891[B]	CBS	O5B-C5B-C4B	4.40	118.75	109.75
2	A	891[A]	CBS	O3A-C3A-C2A	5.34	120.44	109.61
2	A	891[B]	CBS	O3A-C3A-C2A	5.34	120.44	109.61
2	A	891[A]	CBS	C1A-O5A-C5A	6.15	125.29	113.72
2	A	891[B]	CBS	C1A-O5A-C5A	6.15	125.29	113.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	SO4	1	0

## 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	858/858 (100%)	-0.97	4 (0%) 90 90	2, 11, 35, 76	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644	TRP	6.2
1	A	218[A]	VAL	2.6
1	A	156	ASP	2.3
1	A	555	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	4	5/5	0.86	0.15	4.41	15,29,30,32	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	3	5/5	0.95	0.10	3.00	28,28,33,35	0
3	SO4	A	2	5/5	0.85	0.24	1.95	70,71,72,75	0
3	SO4	A	1	5/5	0.95	0.13	1.77	13,14,26,29	0
2	CBS	A	891[A]	29/29	0.98	0.07	1.07	2,6,8,10	1
2	CBS	A	891[B]	29/29	0.98	0.07	1.07	2,6,8,10	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.