Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:10 am BST

PDB ID	:	1QBA
Title	:	BACTERIAL CHITOBIASE, GLYCOSYL HYDROLASE FAMILY 20
Authors	:	Tews, I.; Perrakis, A.; Oppenheim, A.; Dauter, Z.; Wilson, K.S.; Vorgias, C.E.
Deposited on	:	1996-06-06
Resolution	:	1.85 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 following versions of software and data (see references ⓘ) were used in the production of this report:

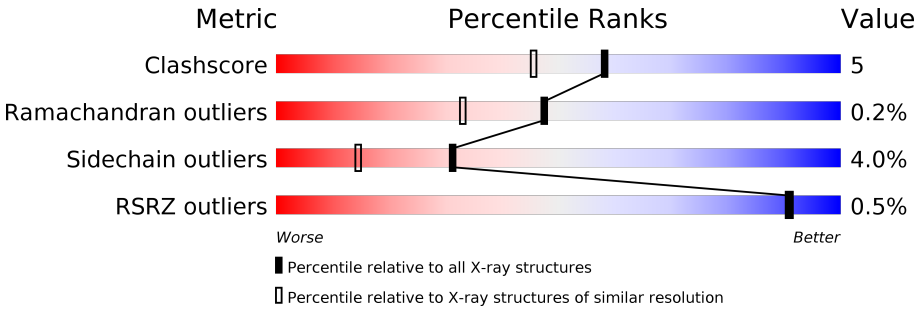
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 >=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	A	858	84% 13% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14096 atoms, of which 6500 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.

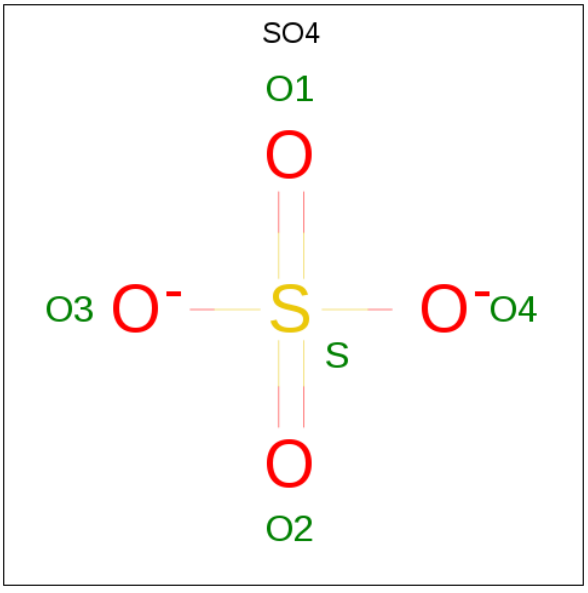
- Molecule 1 is a protein called CHITOBIASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	858	13305	4306	6500	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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 3 is water.

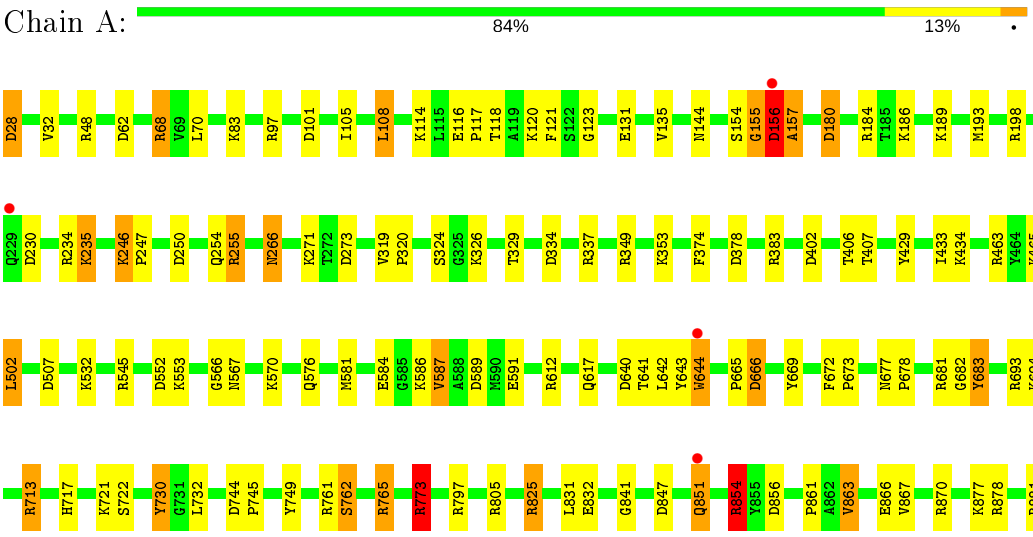
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	771	Total O 771 771	0	0

3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	110.70Å 99.90Å 87.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.85 10.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.00-1.85) 99.9 (10.00-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 1.85Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.139 , 0.196 0.145 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 76.3	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	0.97	EDS
Total number of atoms	14096	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 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	1.00	10/7040 (0.1%)	1.45	79/9534 (0.8%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255[A]	ARG	CD-NE	10.35	1.64	1.46
1	A	255[B]	ARG	CD-NE	10.35	1.64	1.46
1	A	566	GLY	C-N	-7.13	1.17	1.34
1	A	68	ARG	CD-NE	-5.99	1.36	1.46
1	A	762	SER	CB-OG	-5.71	1.34	1.42
1	A	255[A]	ARG	CZ-NH1	5.57	1.40	1.33
1	A	255[B]	ARG	CZ-NH1	5.57	1.40	1.33
1	A	157	ALA	N-CA	-5.46	1.35	1.46
1	A	825	ARG	CZ-NH1	5.38	1.40	1.33
1	A	693	ARG	CD-NE	-5.35	1.37	1.46

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	ARG	CD-NE-CZ	19.16	150.43	123.60
1	A	255[A]	ARG	NE-CZ-NH1	-18.29	111.16	120.30
1	A	255[B]	ARG	NE-CZ-NH1	-18.29	111.16	120.30
1	A	681	ARG	NE-CZ-NH1	16.68	128.64	120.30
1	A	681	ARG	NE-CZ-NH2	-16.59	112.00	120.30
1	A	825	ARG	CD-NE-CZ	14.72	144.20	123.60
1	A	255[A]	ARG	NE-CZ-NH2	14.20	127.40	120.30
1	A	255[B]	ARG	NE-CZ-NH2	14.20	127.40	120.30
1	A	97	ARG	NE-CZ-NH2	11.70	126.15	120.30
1	A	266	ASN	CA-CB-CG	11.53	138.76	113.40
1	A	773	ARG	CD-NE-CZ	11.34	139.48	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	255[A]	ARG	CD-NE-CZ	-10.59	108.78	123.60
1	A	255[B]	ARG	CD-NE-CZ	-10.59	108.78	123.60
1	A	878	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	A	337	ARG	NE-CZ-NH1	-9.78	115.41	120.30
1	A	825	ARG	NE-CZ-NH2	9.76	125.18	120.30
1	A	693	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	A	773	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	230	ASP	CB-CG-OD1	8.89	126.30	118.30
1	A	545	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	730	TYR	CB-CG-CD2	-8.71	115.77	121.00
1	A	693	ARG	CD-NE-CZ	8.63	135.68	123.60
1	A	765	ARG	NE-CZ-NH1	-8.47	116.06	120.30
1	A	765	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	A	502	LEU	CA-CB-CG	8.10	133.92	115.30
1	A	48	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	681	ARG	CD-NE-CZ	7.83	134.56	123.60
1	A	552	ASP	CB-CG-OD1	7.82	125.34	118.30
1	A	68	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	854	ARG	CD-NE-CZ	7.43	134.00	123.60
1	A	797	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	761	ARG	CD-NE-CZ	7.39	133.94	123.60
1	A	847	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	97	ARG	NE-CZ-NH1	-7.09	116.76	120.30
1	A	878	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	870	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	A	805	ARG	CD-NE-CZ	6.70	132.97	123.60
1	A	180[A]	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	180[B]	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	28	ASP	CB-CG-OD1	6.64	124.27	118.30
1	A	825	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	A	854	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	230	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	214	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	A	378	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	589	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	A	713	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	101	ASP	CB-CG-OD1	6.22	123.89	118.30
1	A	62	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	273	ASP	CB-CG-OD1	6.15	123.84	118.30
1	A	108	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	856	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	68	ARG	NE-CZ-NH2	-6.09	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	498	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	643	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	A	683	TYR	CB-CG-CD1	6.05	124.63	121.00
1	A	805	ARG	CG-CD-NE	6.03	124.46	111.80
1	A	156	ASP	C-N-CA	6.02	136.74	121.70
1	A	334	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	463	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	A	337	ARG	NH1-CZ-NH2	5.94	125.93	119.40
1	A	612	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	870	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	881	ARG	CA-CB-CG	5.80	126.17	113.40
1	A	683	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	A	761	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	713	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	805	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	184	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	383	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	507	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	722	SER	N-CA-CB	5.52	118.78	110.50
1	A	643	TYR	CB-CG-CD2	5.49	124.30	121.00
1	A	640	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	749	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	730	TYR	O-C-N	-5.25	114.27	123.20
1	A	589	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	101	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	666	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	6805	6500	6596	65	0
2	A	20	0	0	2	0
3	A	771	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7596	6500	6596	65	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 5.

All (65) 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:156:ASP:HA	3:A:1472:HOH:O	1.64	0.95
1:A:570:LYS:NZ	1:A:591:GLU:OE2	1.99	0.95
1:A:773:ARG:NH2	3:A:1557:HOH:O	2.02	0.89
1:A:570:LYS:NZ	1:A:591:GLU:CG	2.36	0.88
1:A:193[A]:MET:HE1	1:A:198:ARG:HA	1.55	0.88
1:A:854:ARG:HH11	1:A:854:ARG:HG2	1.44	0.82
1:A:570:LYS:HZ2	1:A:591:GLU:CG	1.95	0.80
1:A:180[B]:ASP:OD1	3:A:1312:HOH:O	2.00	0.79
1:A:465:LYS:HD2	3:A:1270:HOH:O	1.84	0.78
1:A:866:GLU:HG3	3:A:1613:HOH:O	1.85	0.76
1:A:570:LYS:HZ1	1:A:591:GLU:HG3	1.51	0.74
1:A:570:LYS:HZ1	1:A:591:GLU:CG	2.03	0.72
1:A:532:LYS:HD2	3:A:1063:HOH:O	1.90	0.70
1:A:570:LYS:NZ	1:A:591:GLU:CD	2.45	0.70
1:A:434:LYS:HE3	3:A:1488:HOH:O	1.92	0.68
1:A:825:ARG:NH1	1:A:832:GLU:OE1	2.27	0.67
1:A:28:ASP:N	1:A:154:SER:HG	1.93	0.67
1:A:570:LYS:HZ2	1:A:591:GLU:HG2	1.60	0.66
1:A:773:ARG:HB3	1:A:773:ARG:HH11	1.59	0.65
1:A:730:TYR:OH	2:A:3:SO4:O2	2.16	0.64
1:A:324:SER:O	1:A:326:LYS:HG2	1.98	0.63
1:A:406:THR:HG23	1:A:407[A]:THR:HG23	1.80	0.63
1:A:851:GLN:NE2	3:A:1646:HOH:O	2.29	0.63
1:A:570:LYS:NZ	1:A:591:GLU:HG3	2.10	0.63
1:A:713:ARG:NH1	3:A:1188:HOH:O	2.10	0.63
1:A:429:TYR:CE2	1:A:433:ILE:HD11	2.36	0.60
1:A:641:THR:OG1	1:A:644:TRP:HB3	2.03	0.59
1:A:83:LYS:HE3	1:A:118:THR:O	2.05	0.57
1:A:353:LYS:HG2	3:A:1590:HOH:O	2.06	0.56
1:A:673:PRO:HD3	1:A:683:TYR:O	2.05	0.56
1:A:250:ASP:O	1:A:254[B]:GLN:HG3	2.06	0.54
1:A:831:LEU:HB3	1:A:861:PRO:HG2	1.90	0.52
1:A:854:ARG:HG2	1:A:854:ARG:NH1	2.16	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:LEU:HD23	1:A:762:SER:HB3	1.95	0.49
1:A:717:HIS:CE1	3:A:1303:HOH:O	2.65	0.49
1:A:581:MET:HG2	1:A:587:VAL:HG23	1.95	0.49
1:A:665:PRO:HA	1:A:669:TYR:CD1	2.48	0.48
1:A:570:LYS:HZ2	1:A:591:GLU:CD	2.13	0.48
1:A:250:ASP:O	1:A:254[A]:GLN:HG2	2.15	0.46
1:A:154:SER:O	1:A:155:GLY:C	2.54	0.46
1:A:227:HIS:HB2	1:A:329:THR:OG1	2.16	0.46
1:A:584:GLU:HG3	1:A:586:LYS:HG3	1.97	0.45
1:A:642:LEU:HD21	1:A:703[B]:MET:CE	2.46	0.45
1:A:144:ASN:ND2	1:A:682:GLY:H	2.15	0.45
1:A:116:GLU:HB3	1:A:117:PRO:HD2	1.99	0.44
1:A:235:LYS:HE3	1:A:235:LYS:HB2	1.57	0.44
1:A:863:VAL:HG11	1:A:867:VAL:HG21	2.01	0.43
1:A:32:VAL:HG23	1:A:154:SER:HB3	2.00	0.43
1:A:841:GLY:HA3	1:A:854:ARG:HH22	1.84	0.43
1:A:841:GLY:CA	1:A:854:ARG:HH22	2.32	0.43
1:A:105:ILE:HA	1:A:114:LYS:O	2.19	0.42
1:A:121:PHE:CZ	1:A:123:GLY:HA2	2.54	0.42
1:A:255[A]:ARG:HD3	1:A:255[A]:ARG:HH11	1.15	0.42
1:A:497:ASN:HB3	2:A:1:SO4:O1	2.20	0.42
1:A:744:ASP:N	1:A:745:PRO:CD	2.82	0.42
1:A:677:ASN:HA	1:A:678:PRO:HD3	1.89	0.41
1:A:326:LYS:HE2	1:A:326:LYS:HB3	1.88	0.41
1:A:402:ASP:OD2	1:A:407[B]:THR:HG22	2.20	0.41
1:A:319:VAL:HA	1:A:320:PRO:HD3	1.88	0.41
1:A:672:PHE:HA	1:A:683:TYR:O	2.20	0.41
1:A:863:VAL:CG1	1:A:867:VAL:HG21	2.51	0.41
1:A:68:ARG:HG2	1:A:135:VAL:HG22	2.03	0.41
1:A:70:LEU:HD11	1:A:131:GLU:HB3	2.02	0.41
1:A:246:LYS:N	1:A:247:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

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	869/858 (101%)	850 (98%)	17 (2%)	2 (0%)	47 33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	GLY
1	A	157	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	718/705 (102%)	690 (96%)	28 (4%)	32 15

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	120	LYS
1	A	156	ASP
1	A	186	LYS
1	A	189	LYS
1	A	234	ARG
1	A	235	LYS
1	A	246	LYS
1	A	266	ASN
1	A	271	LYS
1	A	349	ARG
1	A	374	PHE
1	A	502	LEU
1	A	553	LYS
1	A	567	ASN
1	A	576	GLN
1	A	587	VAL

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Mol	Chain	Res	Type
1	A	617	GLN
1	A	644	TRP
1	A	666	ASP
1	A	701	ASP
1	A	721	LYS
1	A	765	ARG
1	A	773	ARG
1	A	851	GLN
1	A	854	ARG
1	A	863	VAL
1	A	877	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	599	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)

4 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	$\#\|Z\| > 2$
2	SO4	A	3	-	4,4,4	0.60	0	6,6,6	0.57	0
2	SO4	A	2	-	4,4,4	0.74	0	6,6,6	0.55	0
2	SO4	A	4	-	4,4,4	0.63	0	6,6,6	0.56	0
2	SO4	A	1	-	4,4,4	0.70	0	6,6,6	0.56	0

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.

2 monomers are involved in 2 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	566:GLY	C	567:ASN	N	1.17

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	858/858 (100%)	-0.93	4 (0%)	91	91	5, 13, 38, 77	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644	TRP	8.2
1	A	156	ASP	2.6
1	A	851	GLN	2.4
1	A	229	GLN	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	4	5/5	0.92	0.14	22,30,33,33	5
2	SO4	A	2	5/5	0.97	0.10	55,55,57,60	0
2	SO4	A	3	5/5	0.98	0.08	28,33,35,35	0
2	SO4	A	1	5/5	0.99	0.05	13,18,20,25	0

6.5 Other polymers (i)

There are no such residues in this entry.