



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:48 PM UTC

PDB ID : 1QBA / pdb_00001qba
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 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

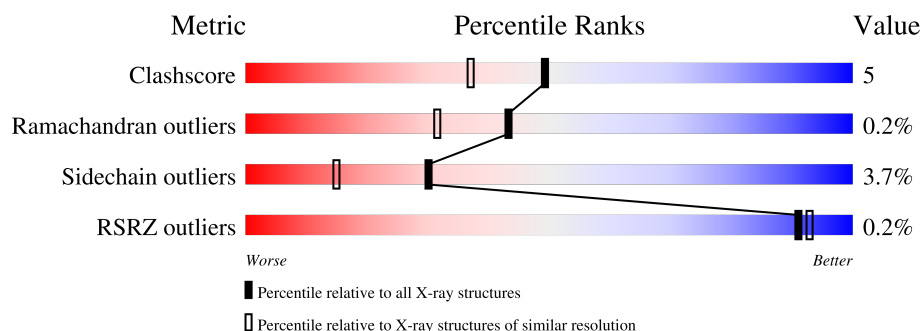
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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 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	858	

2 Entry composition [i](#)

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
1	A	858	Total	C	H	N	O	S	0	13	0
			13305	4306	6500	1189	1286	24			

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 (CCD ID: SO4) (formula: O₄S).



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

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

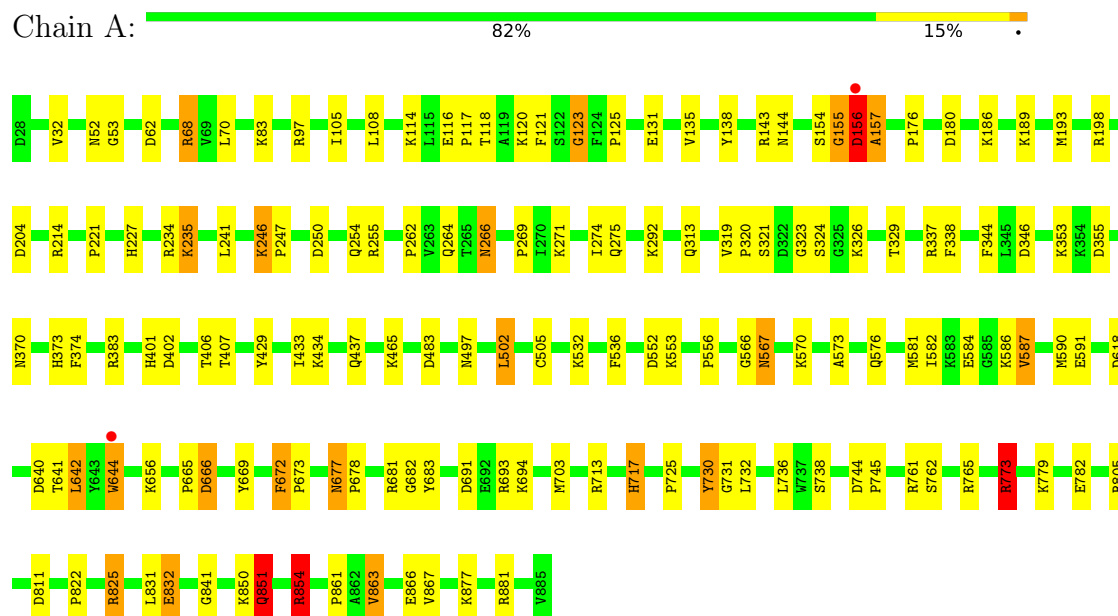
- Molecule 3 is water.

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

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: CHITOBIASE



4 Data and refinement statistics

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) 99.1 (10.00-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.85Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.139 , 0.196 0.131 , (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)	0.40 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	1.25	11/7040 (0.2%)	1.63	86/9534 (0.9%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	566	GLY	C-N	-12.04	1.17	1.33
1	A	157	ALA	N-CA	-8.34	1.35	1.46
1	A	68	ARG	CD-NE	-7.13	1.36	1.46
1	A	693	ARG	CD-NE	-6.36	1.37	1.46
1	A	156	ASP	CA-CB	5.79	1.63	1.53
1	A	337	ARG	NE-CZ	5.51	1.39	1.33
1	A	825	ARG	NE-CZ	-5.51	1.26	1.33
1	A	825	ARG	CZ-NH1	5.21	1.40	1.32
1	A	68	ARG	NE-CZ	-5.19	1.27	1.33
1	A	832	GLU	CA-C	5.12	1.58	1.52
1	A	567	ASN	CA-CB	-5.09	1.45	1.53

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ASN	CA-CB-CG	26.16	138.76	112.60
1	A	68	ARG	CD-NE-CZ	18.59	150.43	124.40
1	A	825	ARG	CD-NE-CZ	14.14	144.20	124.40
1	A	266	ASN	OD1-CG-ND2	-11.99	110.61	122.60
1	A	773	ARG	CD-NE-CZ	10.77	139.48	124.40
1	A	567	ASN	CA-CB-CG	10.46	123.06	112.60
1	A	811	ASP	CA-CB-CG	8.95	121.55	112.60
1	A	693	ARG	CD-NE-CZ	8.06	135.68	124.40
1	A	681	ARG	NE-CZ-NH2	-7.99	112.00	119.20
1	A	156	ASP	CA-C-N	7.96	136.74	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ASP	C-N-CA	7.96	136.74	121.54
1	A	97	ARG	NE-CZ-NH2	7.72	126.15	119.20
1	A	552	ASP	CA-C-N	7.62	131.51	120.38
1	A	552	ASP	C-N-CA	7.62	131.51	120.38
1	A	681	ARG	CD-NE-CZ	7.26	134.56	124.40
1	A	681	ARG	NE-CZ-NH1	7.14	128.64	121.50
1	A	313	GLN	OE1-CD-NE2	-7.11	115.49	122.60
1	A	269	PRO	N-CA-CB	6.99	109.16	103.36
1	A	204	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	854	ARG	CD-NE-CZ	6.86	134.00	124.40
1	A	761	ARG	CD-NE-CZ	6.82	133.94	124.40
1	A	125	PRO	N-CA-CB	6.80	109.27	103.35
1	A	851	GLN	CB-CG-CD	6.71	124.01	112.60
1	A	738[A]	SER	N-CA-C	6.68	120.75	112.59
1	A	738[B]	SER	N-CA-C	6.68	120.75	112.59
1	A	825	ARG	NE-CZ-NH2	6.64	125.18	119.20
1	A	730	TYR	CA-C-O	6.60	127.32	119.60
1	A	355	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	437	GLN	OE1-CD-NE2	-6.52	116.08	122.60
1	A	52	ASN	CA-CB-CG	-6.45	106.15	112.60
1	A	338	PHE	CA-CB-CG	6.45	120.25	113.80
1	A	717	HIS	CA-CB-CG	-6.33	107.47	113.80
1	A	666	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	573	ALA	CA-C-O	-6.28	113.90	120.55
1	A	274	ILE	CA-C-N	6.25	129.36	122.74
1	A	274	ILE	C-N-CA	6.25	129.36	122.74
1	A	618	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	805	ARG	CD-NE-CZ	6.12	132.97	124.40
1	A	337	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	A	53	GLY	N-CA-C	6.08	122.82	114.92
1	A	881	ARG	CA-CB-CG	6.04	126.17	114.10
1	A	241	LEU	CA-C-N	6.03	128.96	120.28
1	A	241	LEU	C-N-CA	6.03	128.96	120.28
1	A	765	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	A	691	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	262	PRO	N-CA-CB	5.89	108.47	103.35
1	A	275	GLN	CA-C-N	5.79	125.92	119.32
1	A	275	GLN	C-N-CA	5.79	125.92	119.32
1	A	176	PRO	N-CA-CB	5.75	108.35	103.35
1	A	730	TYR	O-C-N	-5.70	114.27	122.36
1	A	323	GLY	CA-C-N	5.70	130.23	120.72
1	A	323	GLY	C-N-CA	5.70	130.23	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	GLY	N-CA-C	5.69	118.66	112.29
1	A	805	ARG	CG-CD-NE	5.67	124.46	112.00
1	A	556	PRO	N-CA-CB	5.63	108.18	103.17
1	A	672	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	373	HIS	CA-CB-CG	5.60	119.40	113.80
1	A	346	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	62	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	221	PRO	N-CA-CB	5.50	108.44	103.33
1	A	214	ARG	CD-NE-CZ	-5.49	116.72	124.40
1	A	765	ARG	NE-CZ-NH1	-5.43	116.06	121.50
1	A	370	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	A	143	ARG	CA-C-N	5.41	129.25	120.60
1	A	143	ARG	C-N-CA	5.41	129.25	120.60
1	A	374	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	383	ARG	N-CA-C	5.37	119.81	112.88
1	A	642	LEU	CB-CA-C	-5.35	102.44	110.90
1	A	822	PRO	N-CA-CB	5.30	107.96	103.35
1	A	264	GLN	CB-CA-C	5.29	120.16	109.68
1	A	536	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	725	PRO	N-CA-CB	5.22	107.95	103.31
1	A	483	ASP	CA-C-N	5.17	124.84	119.56
1	A	483	ASP	C-N-CA	5.17	124.84	119.56
1	A	567	ASN	N-CA-C	-5.17	105.64	112.94
1	A	640	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	731	GLY	N-CA-C	5.16	119.01	110.55
1	A	157	ALA	CA-C-O	5.15	127.87	120.51
1	A	138	TYR	CA-C-N	5.13	130.62	121.75
1	A	138	TYR	C-N-CA	5.13	130.62	121.75
1	A	677	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	A	337	ARG	NH1-CZ-NH2	5.10	125.93	119.30
1	A	851	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	502	LEU	CA-CB-CG	5.04	133.92	116.30
1	A	401	HIS	CA-CB-CG	-5.03	108.77	113.80
1	A	321	SER	CA-CB-OG	-5.03	101.04	111.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6805	6500	6596	73	0
2	A	20	0	0	2	0
3	A	771	0	0	13	0
All	All	7596	6500	6596	73	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 (73) 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: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:NZ	1:A:591:GLU:CD	2.45	0.75
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:193[A]:MET:HE1	1:A:198:ARG:HA	1.72	0.71
1:A:532:LYS:HD2	3:A:1063:HOH:O	1.90	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:570:LYS:HZ2	1:A:591:GLU:HG2	1.60	0.66
1:A:773:ARG:HH11	1:A:773:ARG:HB3	1.59	0.65
1:A:730:TYR:OH	2:A:3:SO4:O2	2.16	0.64
1:A:642:LEU:HD21	1:A:703[B]:MET:HE3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:581:MET:HE3	3:A:1432:HOH:O	2.08	0.53
1:A:570:LYS:HZ2	1:A:591:GLU:CD	2.13	0.53
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
1:A:154:SER:O	1:A:155:GLY:C	2.54	0.50
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:505:CYS:HA	1:A:581:MET:HE1	1.96	0.47
1:A:250:ASP:O	1:A:254[A]:GLN:HG2	2.15	0.46
1:A:570:LYS:HZ1	1:A:591:GLU:CD	2.22	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: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:642:LEU:HD21	1:A:703[B]:MET:CE	2.46	0.44
1:A:235:LYS:HE3	1:A:235:LYS:HB2	1.57	0.44
1:A:193[A]:MET:HE2	3:A:1027:HOH:O	2.18	0.43
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:HH11	1:A:255[A]:ARG:HD3	1.15	0.42
1:A:344:PHE:CD1	1:A:344:PHE:C	2.96	0.42
1:A:193[A]:MET:CE	1:A:198:ARG:HA	2.43	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:582:ILE:HD12	1:A:590:MET:HE2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:779:LYS:HE3	1:A:782:GLU:CD	2.46	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%)	43 31

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%)	692 (96%)	26 (4%)	31 16

All (26) 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	292	LYS
1	A	502	LEU
1	A	553	LYS
1	A	567	ASN
1	A	576	GLN
1	A	587	VAL
1	A	644	TRP
1	A	656	LYS
1	A	666	ASP
1	A	736	LEU
1	A	773	ARG
1	A	850	LYS
1	A	851	GLN
1	A	854	ARG
1	A	863	VAL
1	A	877	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	140	GLN
1	A	144	ASN
1	A	172	GLN
1	A	440	GLN
1	A	567	ASN
1	A	599	GLN
1	A	717	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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	1	-	4,4,4	0.76	0	6,6,6	0.53	0
2	SO4	A	3	-	4,4,4	0.62	0	6,6,6	0.52	0
2	SO4	A	2	-	4,4,4	0.80	0	6,6,6	0.55	0
2	SO4	A	4	-	4,4,4	0.68	0	6,6,6	0.60	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	1	SO4	1	0
2	A	3	SO4	1	0

5.7 Other polymers [i](#)

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 [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, 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	858/858 (100%)	-1.05	2 (0%) 91 93	5, 14, 40, 78	13 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644	TRP	5.5
1	A	156	ASP	2.1

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
2	SO4	A	4	5/5	0.86	0.18	22,30,33,33	5
2	SO4	A	2	5/5	0.96	0.10	55,55,57,60	0
2	SO4	A	3	5/5	0.97	0.06	28,33,35,35	0
2	SO4	A	1	5/5	0.99	0.04	13,18,20,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.