



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:43 AM GMT

PDB ID : 2CBI
Title : STRUCTURE OF THE CLOSTRIDIUM PERFRINGENS NAGJ FAMILY 84 GLYCOSIDE HYDROLASE, A HOMOLOGUE OF HUMAN O-GLCNACASE
Authors : Rao, F.V.; Dorfmueller, H.C.; Villa, F.; Allwood, M.; Eggleston, I.M.; Van Aalten, D.M.F.
Deposited on : 2006-01-04
Resolution : 2.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

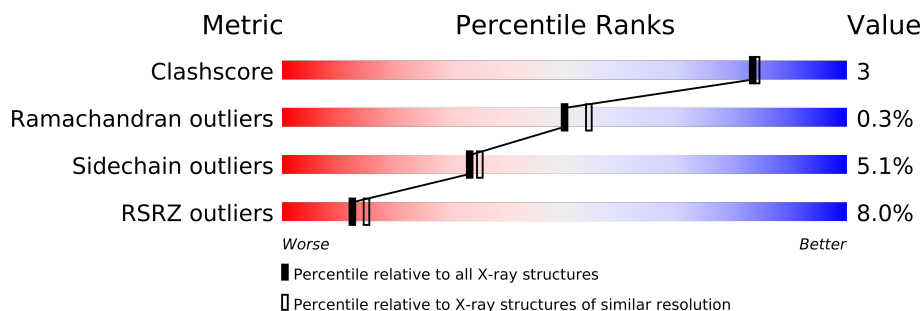
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.25 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	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	594	
1	B	594	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	1625	-	X
3	CL	A	1626	-	X
6	ZN	B	1625	-	X
6	ZN	B	1626	-	X
6	ZN	B	1628	-	X
6	ZN	B	1633	-	X
6	ZN	B	1635	-	X
6	ZN	B	1636	-	X
6	ZN	B	1637	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9931 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HYALURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4620	2908	756	939	17			
1	B	584	Total	C	N	O	S	0	0	0
			4620	2908	756	939	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	GLN	LYS	CONFLICT SEE REMARK 9	UNP Q8XL08
A	234	SER	ASN	CONFLICT SEE REMARK 9	UNP Q8XL08
A	244	ASN	ASP	CONFLICT SEE REMARK 9	UNP Q8XL08
A	268	ASP	GLU	CONFLICT SEE REMARK 9	UNP Q8XL08
A	279	THR	ALA	CONFLICT SEE REMARK 9	UNP Q8XL08
A	348	ALA	THR	CONFLICT SEE REMARK 9	UNP Q8XL08
B	196	GLN	LYS	CONFLICT SEE REMARK 9	UNP Q8XL08
B	234	SER	ASN	CONFLICT SEE REMARK 9	UNP Q8XL08
B	244	ASN	ASP	CONFLICT SEE REMARK 9	UNP Q8XL08
B	268	ASP	GLU	CONFLICT SEE REMARK 9	UNP Q8XL08
B	279	THR	ALA	CONFLICT SEE REMARK 9	UNP Q8XL08
B	348	ALA	THR	CONFLICT SEE REMARK 9	UNP Q8XL08

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

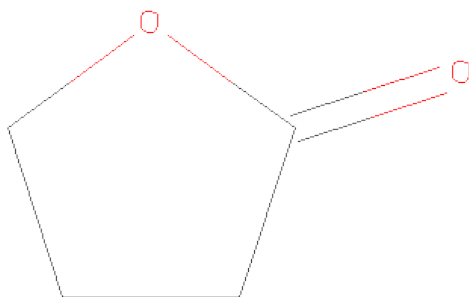


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GAMMA-BUTYROLACTONE (three-letter code: GBL) (formula: C₄H₆O₂).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	11	Total	Zn	0	0
			11	11		

- Molecule 7 is water.

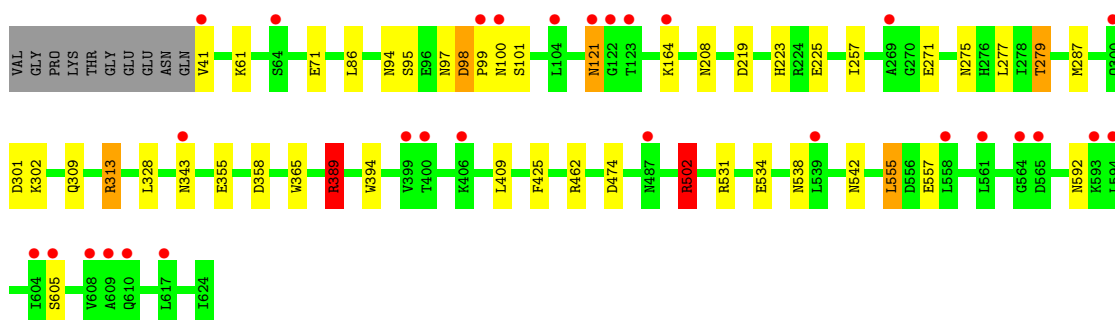
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	313	Total	O	0	0
			313	313		
7	B	337	Total	O	0	0
			337	337		

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 errors 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.

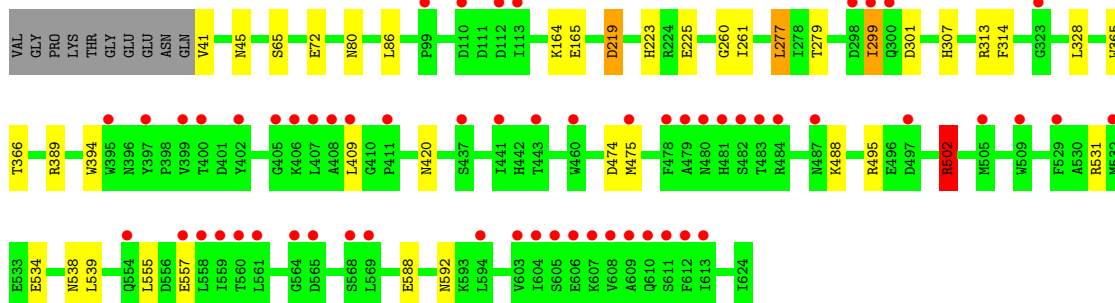
• Molecule 1: HYALURONIDASE

Chain A: 



• Molecule 1: HYALURONIDASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.94Å 147.38Å 157.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.03 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.25) 99.9 (20.03-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.40 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.169 , 0.220 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 17.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 65955 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9931	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, ZN, GBL, CL

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	0.79	1/4716 (0.0%)	0.74	5/6403 (0.1%)
1	B	0.82	1/4716 (0.0%)	0.75	5/6403 (0.1%)
All	All	0.80	2/9432 (0.0%)	0.74	10/12806 (0.1%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	534	GLU	CG-CD	5.84	1.60	1.51
1	A	534	GLU	CG-CD	5.17	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	A	502	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	B	502	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	B	502	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	B	495	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	389	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	389	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	495	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	219	ASP	CB-CG-OD1	5.69	123.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	555	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	ASN	Peptide
1	A	98	ASP	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4620	0	0	13	0
1	B	4620	0	0	14	0
2	A	5	0	0	0	0
3	A	1	0	0	2	0
4	A	6	0	6	0	0
4	B	6	0	6	2	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	B	11	0	0	0	0
7	A	313	0	0	3	0
7	B	337	0	0	4	0
All	All	9931	0	28	28	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (28) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:299:ILE:CD1	1:B:307:HIS:CE1	2.68	0.77
1:B:366:THR:CG2	4:B:1629:GBL:HAC1	2.31	0.61
1:A:462:ARG:NE	7:A:2193:HOH:O	2.34	0.60
1:A:474:ASP:OD1	1:A:531:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:302:LYS:O	1:A:302:LYS:CG	2.52	0.57
1:A:592:ASN:ND2	7:A:2284:HOH:O	2.38	0.56
1:A:271:GLU:OE1	1:A:313:ARG:NH2	2.38	0.56
1:A:98:ASP:C	1:A:100:ASN:N	2.60	0.54
1:B:488:LYS:NZ	7:B:2221:HOH:O	2.43	0.51
1:B:474:ASP:OD2	1:B:538:ASN:ND2	2.45	0.50
1:B:277:LEU:CD1	1:B:314:PHE:CD1	2.95	0.49
1:A:98:ASP:O	1:A:98:ASP:CG	2.51	0.48
1:B:45:ASN:ND2	7:B:2006:HOH:O	2.45	0.48
1:A:275:ASN:O	1:A:279:THR:CG2	2.61	0.48
3:A:1626:CL:CL	7:A:2063:HOH:O	2.58	0.47
1:B:260:GLY:CA	1:B:299:ILE:CG2	2.92	0.47
1:A:94:ASN:ND2	1:A:101:SER:OG	2.48	0.46
1:B:502:ARG:CD	1:B:502:ARG:O	2.63	0.46
1:A:358:ASP:O	1:A:389:ARG:NH2	2.49	0.46
1:A:502:ARG:O	1:A:502:ARG:CD	2.64	0.46
1:B:80:ASN:ND2	7:B:2024:HOH:O	2.48	0.45
1:A:538:ASN:OD1	1:A:542:ASN:ND2	2.49	0.44
1:B:474:ASP:OD1	1:B:531:ARG:NH2	2.52	0.43
1:B:475:MET:CE	1:B:539:LEU:CD2	2.97	0.43
1:B:394:TRP:CD2	4:B:1629:GBL:HAC2	2.54	0.42
1:B:502:ARG:CD	1:B:502:ARG:C	2.87	0.42
1:B:592:ASN:ND2	7:B:2308:HOH:O	2.52	0.42
1:A:208:ASN:OD1	3:A:1626:CL:CL	2.75	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	582/594 (98%)	560 (96%)	19 (3%)	3 (0%)	38	38
1	B	582/594 (98%)	565 (97%)	16 (3%)	1 (0%)	56	63
All	All	1164/1188 (98%)	1125 (97%)	35 (3%)	4 (0%)	50	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	301	ASP
1	B	261	ILE
1	A	99	PRO

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	499/507 (98%)	471 (94%)	28 (6%)	30	30
1	B	499/507 (98%)	476 (95%)	23 (5%)	37	41
All	All	998/1014 (98%)	947 (95%)	51 (5%)	33	35

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	61	LYS
1	A	71	GLU
1	A	86	LEU
1	A	95	SER
1	A	121	ASN
1	A	164	LYS
1	A	219	ASP
1	A	223	HIS
1	A	225	GLU
1	A	257	ILE
1	A	277	LEU
1	A	279	THR
1	A	287	MET
1	A	309	GLN
1	A	313	ARG
1	A	328	LEU
1	A	343	ASN
1	A	355	GLU
1	A	365	TRP

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Mol	Chain	Res	Type
1	A	389	ARG
1	A	394	TRP
1	A	409	LEU
1	A	425	PHE
1	A	502	ARG
1	A	555	LEU
1	A	557	GLU
1	A	605	SER
1	B	41	VAL
1	B	65	SER
1	B	72	GLU
1	B	86	LEU
1	B	164	LYS
1	B	165	GLU
1	B	219	ASP
1	B	223	HIS
1	B	225	GLU
1	B	277	LEU
1	B	279	THR
1	B	299	ILE
1	B	301	ASP
1	B	313	ARG
1	B	328	LEU
1	B	365	TRP
1	B	389	ARG
1	B	409	LEU
1	B	420	ASN
1	B	502	ARG
1	B	555	LEU
1	B	557	GLU
1	B	588	GLU

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

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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	SO4	A	1625	6	4,4,4	0.26	0	6,6,6	0.85	0
4	GBL	A	1627	-	6,6,6	0.57	0	7,7,7	1.16	0
5	GOL	A	1628	-	5,5,5	0.26	0	5,5,5	0.68	0
4	GBL	B	1629	-	6,6,6	1.00	0	7,7,7	1.36	0
5	GOL	B	1630	-	5,5,5	0.42	0	5,5,5	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1625	6	-	0/0/0/0	0/0/0/0
4	GBL	A	1627	-	-	0/0/7/7	0/1/1/1
5	GOL	A	1628	-	-	0/4/4/4	0/0/0/0
4	GBL	B	1629	-	-	0/0/7/7	0/1/1/1
5	GOL	B	1630	-	-	0/4/4/4	0/0/0/0

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.

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

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	584/594 (98%)	0.15	29 (4%) 28 32	-2, 15, 38, 53	1 (0%)
1	B	584/594 (98%)	0.66	59 (10%) 7 9	-5, 13, 34, 48	1 (0%)
All	All	1168/1188 (98%)	0.40	88 (7%) 12 17	-5, 14, 36, 53	2 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	479	ALA	31.3
1	B	608	VAL	27.7
1	B	482	SER	27.7
1	B	564	GLY	23.1
1	A	604	ILE	22.3
1	A	564	GLY	21.7
1	B	408	ALA	21.0
1	B	558	LEU	18.6
1	B	480	ASN	15.2
1	B	609	ALA	14.2
1	B	560	THR	13.8
1	B	613	ILE	13.0
1	B	483	THR	12.6
1	B	561	LEU	12.6
1	B	481	HIS	12.4
1	B	612	PHE	12.0
1	B	484	ARG	11.0
1	A	609	ALA	10.1
1	B	399	VAL	9.5
1	B	610	GLN	8.8
1	B	611	SER	8.3
1	B	604	ILE	8.2
1	A	122	GLY	7.9
1	B	557	GLU	7.8

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Mol	Chain	Res	Type	RSRZ
1	B	529	PHE	7.2
1	B	395	TRP	7.1
1	B	397	TYR	7.0
1	A	558	LEU	6.9
1	B	554	GLN	6.2
1	A	99	PRO	6.0
1	B	443	THR	5.9
1	B	478	PHE	5.9
1	B	437	SER	5.6
1	B	400	THR	5.3
1	A	561	LEU	5.3
1	B	299	ILE	5.0
1	A	594	LEU	5.0
1	A	593	LYS	5.0
1	A	100	ASN	4.9
1	B	487	ASN	4.7
1	B	402	TYR	4.5
1	A	399	VAL	4.5
1	B	605	SER	4.3
1	B	112	ASP	4.3
1	B	559	ILE	4.3
1	B	569	LEU	4.2
1	B	607	LYS	3.9
1	B	509	TRP	3.8
1	B	460	TRP	3.7
1	B	565	ASP	3.5
1	A	104	LEU	3.5
1	A	400	THR	3.4
1	A	605	SER	3.4
1	A	406	LYS	3.3
1	B	594	LEU	3.3
1	B	497	ASP	3.2
1	A	343	ASN	3.2
1	B	300	GLN	2.8
1	B	409	LEU	2.8
1	B	405	GLY	2.7
1	A	565	ASP	2.7
1	B	411	PRO	2.6
1	A	617	LEU	2.6
1	A	164	LYS	2.5
1	A	300	GLN	2.5
1	B	603	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	568	SER	2.4
1	A	487	ASN	2.4
1	A	269	ALA	2.4
1	A	539	LEU	2.4
1	B	99	PRO	2.4
1	B	505	MET	2.4
1	B	406	LYS	2.4
1	A	608	VAL	2.3
1	B	475	MET	2.3
1	B	441	ILE	2.3
1	B	298	ASP	2.2
1	A	41	VAL	2.2
1	B	323	GLY	2.2
1	B	532	MET	2.2
1	B	110	ASP	2.1
1	A	121	ASN	2.1
1	B	407	LEU	2.1
1	A	610	GLN	2.1
1	A	64	SER	2.1
1	B	606	GLU	2.0
1	A	123	THR	2.0
1	B	113	ILE	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. 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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	ZN	B	1625	1/1	2.15	98.06	-4,-4,-4,-4	1
6	ZN	B	1637	1/1	1.70	32.52	183,183,183,183	1
6	ZN	B	1636	1/1	0.84	16.37	48,48,48,48	1
6	ZN	B	1626	1/1	0.44	13.84	25,25,25,25	1
3	CL	A	1626	1/1	0.18	5.23	31,31,31,31	0
6	ZN	B	1633	1/1	0.24	5.00	25,25,25,25	1
6	ZN	B	1628	1/1	0.31	3.44	27,27,27,27	1
6	ZN	B	1635	1/1	0.24	3.00	42,42,42,42	1
2	SO4	A	1625	5/5	0.17	2.94	35,41,46,48	0
4	GBL	B	1629	6/6	0.14	1.13	13,15,20,23	0
4	GBL	A	1627	6/6	0.12	0.63	6,8,13,13	0
6	ZN	B	1627	1/1	0.17	0.40	15,15,15,15	1
5	GOL	A	1628	6/6	0.12	-0.01	9,17,25,30	0
5	GOL	B	1630	6/6	0.11	-0.36	2,13,16,16	0
6	ZN	B	1634	1/1	0.10	-0.74	23,23,23,23	1
6	ZN	B	1631	1/1	0.13	-1.09	41,41,41,41	1
6	ZN	B	1632	1/1	0.14	-1.13	40,40,40,40	1

6.5 Other polymers ⓘ

There are no such residues in this entry.