



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:08 PM GMT

PDB ID : 1E6N
Title : CHITINASE B FROM SERRATIA MARCESCENS INACTIVE MUTANT
E144Q IN COMPLEX WITH N-ACETYLGLUCOSAMINE-PENTAMER
Authors : Komander, D.; Synstad, B.; Eijsink, V.G.H.; Van Aalten, D.M.F.
Deposited on : 2000-08-21
Resolution : 2.25 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

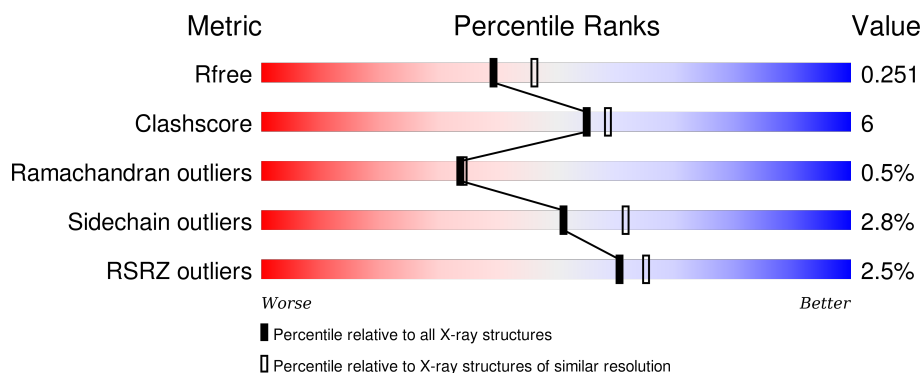
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
R_{free}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (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. 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	499	<div> <div>3%</div> <div>85%</div> <div>14%</div> <div>..</div> </div>
1	B	499	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>

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	1504	-	-	-	X
3	SO4	A	1507	-	-	-	X
3	SO4	A	1510	-	-	-	X
3	SO4	A	1511	-	-	-	X
3	SO4	B	1508	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8440 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 CHITINASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	1	0
			3899	2492	662	731	14			
1	B	497	Total	C	N	O	S	1	0	0
			3892	2490	657	731	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	GLN	GLU	CONFLICT	UNP Q54276
B	144	GLN	GLU	CONFLICT	UNP Q54276

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			71	40	5	26		
2	B	5	Total	C	N	O	0	0
			71	40	5	26		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

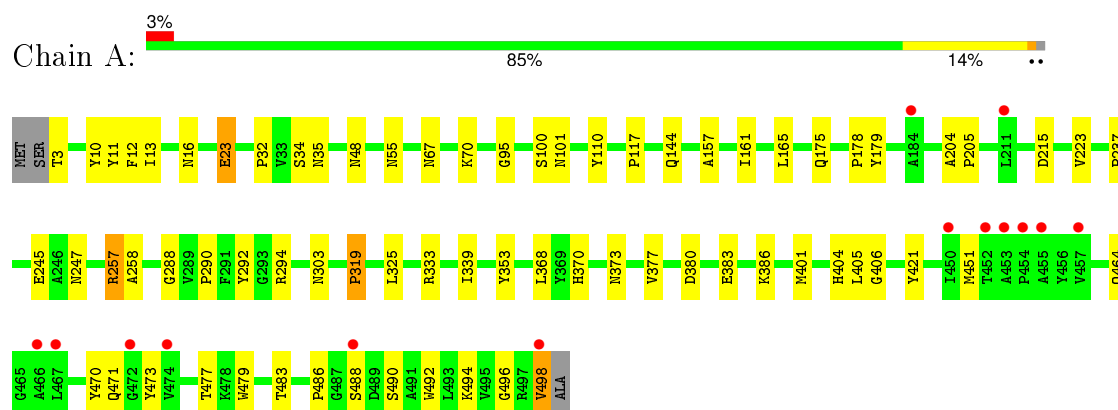
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	236	Total	O	0	0
			236	236		
5	B	205	Total	O	0	0
			205	205		

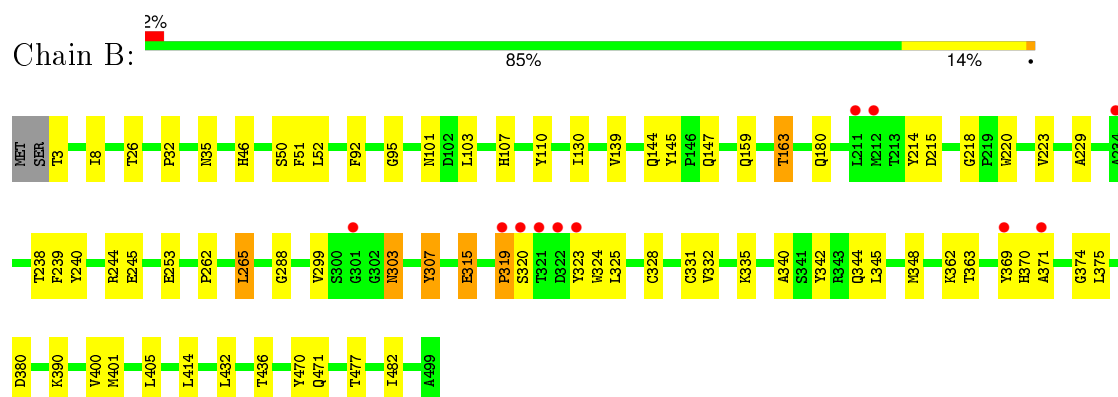
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CHITINASE B



• Molecule 1: CHITINASE B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.73Å 104.48Å 186.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.58 – 2.25 38.58 – 2.24	Depositor EDS
% Data completeness (in resolution range)	90.6 (38.58-2.25) 89.9 (38.58-2.24)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.81 (at 2.24Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.189 , 0.239 0.205 , 0.251	Depositor DCC
R_{free} test set	985 reflections (2.06%)	DCC
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 47841 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8440	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, NAG, 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	0.50	0/4013	0.69	1/5468 (0.0%)
1	B	0.49	0/4003	0.67	0/5457
All	All	0.49	0/8016	0.68	1/10925 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	100	SER	N-CA-C	5.62	126.18	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	TYR	Sidechain

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	3899	0	3736	50	0
1	B	3892	0	3717	52	0
2	A	71	0	63	0	0
2	B	71	0	63	1	0
3	A	40	0	0	3	0
3	B	20	0	0	0	0
4	B	6	0	8	0	0
5	A	236	0	0	4	0
5	B	205	0	0	1	0
All	All	8440	0	7587	98	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 6.

All (98) 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:67:ASN:ND2	1:A:70:LYS:HG3	1.80	0.95
1:B:344:GLN:HG3	1:B:348:MET:HE3	1.59	0.84
1:A:11:TYR:CE2	1:A:13:ILE:HD11	2.17	0.79
1:A:383:GLU:HG2	5:A:2172:HOH:O	1.84	0.77
1:B:159:GLN:O	1:B:163:THR:HG22	1.86	0.76
1:B:328:CYS:HB2	1:B:348:MET:HE1	1.68	0.75
1:B:344:GLN:HG3	1:B:348:MET:CE	2.18	0.74
1:A:32:PRO:HD2	1:A:35:ASN:ND2	2.02	0.74
1:A:67:ASN:HD22	1:A:70:LYS:HG3	1.52	0.73
1:A:370:HIS:HD2	1:A:373:ASN:H	1.35	0.72
1:A:470:TYR:CD2	1:A:471:GLN:HG2	2.25	0.71
1:A:23:GLU:OE1	1:A:34:SER:HB3	1.92	0.70
1:A:498:VAL:HG12	1:A:498:VAL:OXT	1.94	0.66
1:B:315:GLU:HB2	1:B:319:PRO:HD3	1.81	0.63
1:B:223:VAL:HG13	1:B:307:TYR:HA	1.81	0.62
1:B:32:PRO:HD2	1:B:35:ASN:HD21	1.63	0.62
1:B:144:GLN:HA	1:B:145:TYR:CG	2.41	0.56
1:B:325:LEU:HD23	1:B:331:CYS:SG	2.45	0.56
1:B:218:GLY:HA3	1:B:220:TRP:CZ2	2.40	0.56
1:B:331:CYS:O	1:B:335:LYS:N	2.37	0.56
1:A:288:GLY:HA2	1:A:401:MET:O	2.05	0.55
1:B:92:PHE:CE1	1:B:139:VAL:HG22	2.41	0.55
1:B:223:VAL:CG1	1:B:307:TYR:HA	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:TYR:CG	1:B:414:LEU:HD11	2.42	0.54
1:A:370:HIS:CD2	1:A:373:ASN:H	2.24	0.53
1:B:362:LYS:NZ	1:B:436:THR:OG1	2.40	0.51
1:A:117:PRO:HD2	5:A:2048:HOH:O	2.10	0.51
1:A:11:TYR:HE2	1:A:13:ILE:HD11	1.71	0.51
1:A:483:THR:HG21	1:B:103:LEU:HD21	1.93	0.50
1:B:238:THR:HB	1:B:262:PRO:HB2	1.93	0.50
1:B:299:VAL:HG22	1:B:374:GLY:C	2.32	0.49
1:B:214:TYR:O	1:B:215:ASP:HB2	2.11	0.49
1:A:490:SER:HB2	1:B:245:GLU:O	2.13	0.49
1:B:328:CYS:CB	1:B:348:MET:HE1	2.39	0.48
1:A:55:ASN:HB2	3:A:1504:SO4:O2	2.12	0.48
1:A:353:TYR:O	1:A:370:HIS:HE1	1.95	0.48
1:A:165:LEU:HD22	1:A:179:TYR:HB3	1.95	0.48
1:B:374:GLY:C	1:B:375:LEU:HD12	2.34	0.48
1:A:101:ASN:HA	1:A:144:GLN:O	2.14	0.48
1:B:323:TYR:HD2	1:B:332:VAL:HG22	1.79	0.48
1:B:50:SER:HA	1:B:51:PHE:HA	1.71	0.48
1:B:32:PRO:HD2	1:B:35:ASN:ND2	2.27	0.48
1:A:464:GLN:HG3	1:A:479:TRP:HA	1.97	0.47
1:A:204:ALA:HB3	1:A:205:PRO:HD3	1.97	0.47
1:A:223:VAL:HG21	1:A:237:PRO:HB3	1.95	0.47
1:B:107:HIS:HE1	5:B:2074:HOH:O	1.97	0.46
1:A:451:MET:CG	1:A:496:GLY:HA3	2.44	0.46
1:A:483:THR:CG2	1:B:103:LEU:HD21	2.44	0.46
1:A:483:THR:HG21	1:B:103:LEU:CD2	2.45	0.46
1:B:240:TYR:CE2	1:B:244:ARG:NH2	2.83	0.46
1:B:477:THR:HG22	1:B:482:ILE:HD11	1.96	0.46
1:B:303:ASN:HD22	1:B:303:ASN:HA	1.52	0.46
1:A:498:VAL:OXT	1:A:498:VAL:CG1	2.63	0.46
1:A:486:PRO:HA	1:A:492:TRP:CD1	2.50	0.46
1:A:477:THR:HG23	1:A:492:TRP:CZ3	2.51	0.46
1:B:299:VAL:HG22	1:B:374:GLY:O	2.15	0.45
1:B:229:ALA:HB1	1:B:363:THR:HB	1.97	0.45
1:B:323:TYR:CD2	1:B:332:VAL:HG22	2.51	0.45
1:A:294:ARG:NH1	1:A:339:ILE:HD11	2.32	0.45
1:B:470:TYR:CD2	1:B:471:GLN:HG3	2.52	0.45
1:A:157:ALA:O	1:A:161:ILE:HG13	2.17	0.45
1:A:370:HIS:HD2	1:A:373:ASN:N	2.10	0.44
1:A:223:VAL:HG22	5:A:2104:HOH:O	2.17	0.44
1:A:486:PRO:C	1:A:488:SER:H	2.20	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:PHE:H	1:A:404:HIS:CD2	2.35	0.44
1:A:333:ARG:NH2	3:A:1508:SO4:O1	2.51	0.44
1:B:369:TYR:CZ	1:B:371:ALA:HA	2.52	0.44
1:B:52:LEU:CD2	1:B:130:ILE:HG21	2.48	0.43
1:B:229:ALA:CB	1:B:363:THR:HB	2.48	0.43
1:A:451:MET:O	1:A:498:VAL:OXT	2.36	0.43
1:A:245:GLU:OE2	1:B:253:GLU:HG2	2.18	0.43
1:A:95:GLY:HA2	1:A:110:TYR:OH	2.18	0.43
1:A:215:ASP:CG	1:A:294:ARG:HH21	2.21	0.43
1:B:8:ILE:O	1:B:401:MET:HA	2.18	0.43
1:A:257:ARG:HG3	1:A:258:ALA:N	2.32	0.43
1:B:400:VAL:HG22	1:B:401:MET:N	2.35	0.42
1:A:368:LEU:HB2	1:A:377:VAL:HB	2.02	0.42
1:B:144:GLN:HA	1:B:145:TYR:CD2	2.54	0.42
1:A:401:MET:C	1:A:401:MET:SD	2.98	0.42
1:B:95:GLY:HA2	1:B:110:TYR:OH	2.20	0.42
1:A:10:TYR:HA	1:A:48:ASN:HB2	2.01	0.42
1:B:370:HIS:HB3	1:B:375:LEU:HB2	2.02	0.41
1:A:223:VAL:HG23	1:A:223:VAL:O	2.19	0.41
1:B:288:GLY:HA2	1:B:401:MET:O	2.20	0.41
1:B:239:PHE:CD1	1:B:265:LEU:HD22	2.55	0.41
1:A:486:PRO:HA	1:A:492:TRP:CG	2.55	0.41
1:B:46:HIS:NE2	1:B:180:GLN:NE2	2.69	0.41
1:A:178:PRO:HD2	3:A:1505:SO4:O4	2.21	0.41
1:B:340:ALA:HB3	1:B:345:LEU:HD21	2.02	0.41
1:B:218:GLY:HA3	1:B:220:TRP:CE2	2.55	0.41
1:A:386:LYS:HG2	1:A:421:TYR:CZ	2.56	0.41
1:A:473:TYR:CD1	1:A:494:LYS:HD3	2.56	0.41
1:B:315:GLU:N	1:B:315:GLU:OE1	2.54	0.40
1:B:101:ASN:HA	1:B:144:GLN:O	2.21	0.40
1:B:390:LYS:NZ	1:B:432:LEU:O	2.50	0.40
1:A:404:HIS:CD2	1:A:406:GLY:H	2.40	0.40
1:A:205:PRO:HB3	5:A:2024:HOH:O	2.22	0.40
2:B:1504:NAG:H2	2:B:1504:NAG:H83	1.84	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	495/499 (99%)	479 (97%)	15 (3%)	1 (0%)	52	61
1	B	495/499 (99%)	470 (95%)	21 (4%)	4 (1%)	24	21
All	All	990/998 (99%)	949 (96%)	36 (4%)	5 (0%)	34	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	PRO
1	B	320	SER
1	B	315	GLU
1	B	319	PRO
1	B	324	TRP

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	402/405 (99%)	389 (97%)	13 (3%)	46	57
1	B	399/405 (98%)	390 (98%)	9 (2%)	58	69
All	All	801/810 (99%)	779 (97%)	22 (3%)	51	63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	16	ASN
1	A	23	GLU
1	A	175	GLN
1	A	247	ASN
1	A	257	ARG
1	A	290	PRO
1	A	303	ASN
1	A	319	PRO
1	A	325	LEU
1	A	380	ASP
1	A	405	LEU
1	A	498	VAL
1	B	3	THR
1	B	26	THR
1	B	147	GLN
1	B	163	THR
1	B	265	LEU
1	B	303	ASN
1	B	307	TYR
1	B	380	ASP
1	B	405	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	210	ASN
1	A	247	ASN
1	A	273	GLN
1	A	303	ASN
1	A	350	GLN
1	A	370	HIS
1	A	404	HIS
1	A	471	GLN
1	B	35	ASN
1	B	57	ASN
1	B	76	ASN
1	B	147	GLN
1	B	180	GLN
1	B	273	GLN
1	B	303	ASN
1	B	394	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	431	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 ⓘ

10 carbohydrates 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	NAG	A	1499	2	14,14,15	0.47	0	15,19,21	1.00	1 (6%)
2	NAG	A	1500	2	14,14,15	0.74	1 (7%)	15,19,21	2.13	4 (26%)
2	NAG	A	1501	2	14,14,15	0.66	0	15,19,21	0.74	0
2	NAG	A	1502	2	14,14,15	0.64	0	15,19,21	0.77	1 (6%)
2	NAG	A	1503	2	15,15,15	0.63	0	17,21,21	0.61	0
2	NAG	B	1500	2	14,14,15	0.57	0	15,19,21	0.70	1 (6%)
2	NAG	B	1501	2	14,14,15	1.19	1 (7%)	15,19,21	2.22	4 (26%)
2	NAG	B	1502	2	14,14,15	0.52	0	15,19,21	0.85	1 (6%)
2	NAG	B	1503	2	14,14,15	0.62	0	15,19,21	0.67	0
2	NAG	B	1504	2	15,15,15	0.63	0	17,21,21	1.50	3 (17%)

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	NAG	A	1499	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1500	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1501	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1502	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1503	2	-	0/6/26/26	0/1/1/1
2	NAG	B	1500	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1501	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1502	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1503	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1504	2	-	0/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	NAG	C1-C2	2.05	1.55	1.52
2	B	1501	NAG	C7-N2	3.46	1.47	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1501	NAG	C2-N2-C7	-4.52	117.23	123.04
2	A	1500	NAG	C2-N2-C7	-4.25	117.58	123.04
2	B	1501	NAG	C8-C7-N2	-3.80	108.84	116.11
2	A	1500	NAG	C8-C7-N2	-3.68	109.07	116.11
2	A	1499	NAG	C2-N2-C7	-3.38	118.70	123.04
2	B	1504	NAG	C4-C3-C2	-3.08	106.16	110.43
2	B	1504	NAG	C8-C7-N2	-2.52	111.29	116.11
2	B	1502	NAG	C2-N2-C7	-2.41	119.94	123.04
2	A	1502	NAG	C2-N2-C7	-2.20	120.21	123.04
2	B	1500	NAG	C2-N2-C7	-2.10	120.35	123.04
2	B	1504	NAG	O7-C7-N2	3.23	128.46	121.86
2	A	1500	NAG	C1-O5-C5	3.66	116.90	112.25
2	B	1501	NAG	C1-O5-C5	3.97	117.28	112.25
2	A	1500	NAG	O7-C7-N2	4.21	130.44	121.86
2	B	1501	NAG	O7-C7-N2	4.32	130.67	121.86

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
2	B	1504	NAG	1	0

5.6 Ligand geometry

13 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	1504	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	A	1505	-	4,4,4	0.27	0	6,6,6	0.20	0
3	SO4	A	1506	-	4,4,4	0.24	0	6,6,6	0.16	0
3	SO4	A	1507	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	A	1508	-	4,4,4	0.20	0	6,6,6	0.13	0
3	SO4	A	1509	-	4,4,4	0.37	0	6,6,6	0.11	0
3	SO4	A	1510	-	4,4,4	0.26	0	6,6,6	0.26	0
3	SO4	A	1511	-	4,4,4	0.35	0	6,6,6	0.16	0
3	SO4	B	1505	-	4,4,4	0.30	0	6,6,6	0.07	0
3	SO4	B	1506	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	B	1507	-	4,4,4	0.29	0	6,6,6	0.13	0
3	SO4	B	1508	-	4,4,4	0.27	0	6,6,6	0.13	0
4	GOL	B	1509	-	5,5,5	0.41	0	5,5,5	5.09	4 (80%)

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	1504	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1505	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1506	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1507	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1508	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1509	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1510	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1511	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1505	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1506	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1507	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1508	-	-	0/0/0/0	0/0/0/0
4	GOL	B	1509	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1509	GOL	C3-C2-C1	-2.30	102.09	111.12
4	B	1509	GOL	O1-C1-C2	2.84	123.93	110.18
4	B	1509	GOL	O2-C2-C3	4.26	128.19	108.65
4	B	1509	GOL	O3-C3-C2	9.90	158.19	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1504	SO4	1	0
3	A	1505	SO4	1	0
3	A	1508	SO4	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	496/499 (99%)	-0.18	14 (2%) 56 61	11, 24, 45, 57	0
1	B	497/499 (99%)	-0.08	11 (2%) 65 70	15, 26, 52, 66	1 (0%)
All	All	993/998 (99%)	-0.13	25 (2%) 61 65	11, 25, 49, 66	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	GLY	4.2
1	A	498	VAL	3.5
1	A	472	GLY	3.5
1	A	452	THR	3.3
1	A	466	ALA	3.3
1	A	488	SER	3.2
1	B	321	THR	3.1
1	A	454	PRO	2.9
1	B	319	PRO	2.9
1	B	320	SER	2.8
1	A	450	ILE	2.7
1	B	211	LEU	2.7
1	B	369	TYR	2.6
1	A	455	ALA	2.6
1	A	453	ALA	2.4
1	B	371	ALA	2.4
1	B	323	TYR	2.4
1	B	322	ASP	2.3
1	A	474	VAL	2.2
1	B	212	MET	2.2
1	B	234	ALA	2.2
1	A	457	VAL	2.2
1	A	211	LEU	2.2
1	A	184	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	467	LEU	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](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	B	1504	15/15	0.82	0.18	1.64	39,45,52,52	0
2	NAG	A	1500	14/15	0.97	0.21	1.26	8,17,19,20	0
2	NAG	A	1499	14/15	0.98	0.14	0.97	16,19,21,23	0
2	NAG	B	1500	14/15	0.97	0.16	0.39	24,27,29,29	0
2	NAG	B	1503	14/15	0.92	0.15	0.35	30,33,36,39	0
2	NAG	A	1502	14/15	0.96	0.14	0.26	16,19,22,25	0
2	NAG	B	1501	14/15	0.96	0.18	0.23	8,21,24,24	0
2	NAG	A	1501	14/15	0.97	0.15	-0.01	14,18,19,20	0
2	NAG	B	1502	14/15	0.95	0.17	-0.06	22,25,31,34	0
2	NAG	A	1503	15/15	0.96	0.09	-0.67	14,22,24,25	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	A	1511	5/5	0.82	0.19	5.35	63,64,68,69	0
3	SO4	A	1507	5/5	0.94	0.16	4.95	79,80,81,81	0
3	SO4	B	1508	5/5	0.90	0.23	4.20	89,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	A	1510	5/5	0.86	0.17	3.27	76,76,77,78	0
3	SO4	A	1504	5/5	0.92	0.19	3.24	89,89,89,89	0
3	SO4	A	1508	5/5	0.95	0.18	0.48	79,79,79,80	0
3	SO4	A	1506	5/5	0.96	0.12	-	63,63,63,64	0
3	SO4	A	1505	5/5	0.88	0.18	-	84,85,85,86	0
3	SO4	B	1507	5/5	0.90	0.18	-	77,77,79,79	0
3	SO4	A	1509	5/5	0.95	0.09	-	66,66,66,67	0
4	GOL	B	1509	6/6	0.89	0.12	-	31,32,34,36	0
3	SO4	B	1506	5/5	0.95	0.11	-	80,81,81,81	0
3	SO4	B	1505	5/5	0.89	0.14	-	83,83,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.