



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:10 AM GMT

PDB ID : 2E3X  
Title : Crystal structure of Russell's viper venom metalloproteinase  
Authors : Igarashi, T.; Takeda, S.  
Deposited on : 2006-11-30  
Resolution : 2.91 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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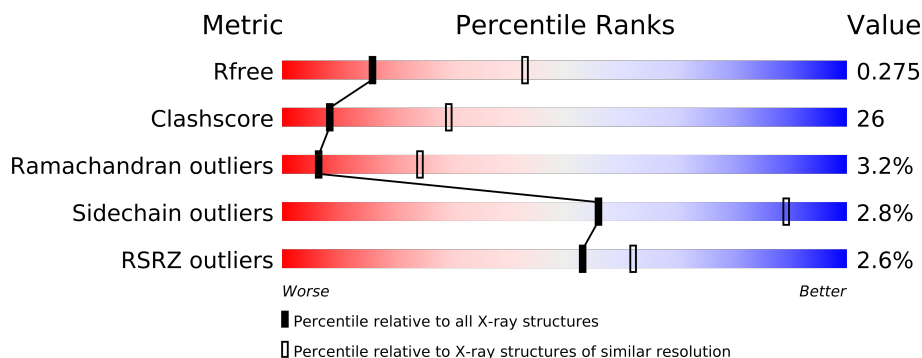
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.91 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))
$R_{free}$	66092	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (2.94-2.90)

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. 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	427	
2	B	134	
3	C	122	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	A	900	-	X
4	NAG	B	903	-	X
8	CA	A	801	-	X
8	CA	B	805	-	X
9	GM6	A	700	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5438 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 Coagulation factor X-activating enzyme heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3235	1983	584	620	48			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	GLU	SEE REMARK 999	UNP Q7LZ61
A	?	-	THR	SEE REMARK 999	UNP Q7LZ61
A	?	-	ARG	SEE REMARK 999	UNP Q7LZ61

- Molecule 2 is a protein called Coagulation factor X-activating enzyme light chain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	129	Total	C	N	O	S	0	0	0
			1078	684	179	203	12			

- Molecule 3 is a protein called Coagulation factor X-activating enzyme light chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	S	0	0	0
			985	628	164	182	11			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	4	Total	C	N	O	0	0
			50	28	2	20		

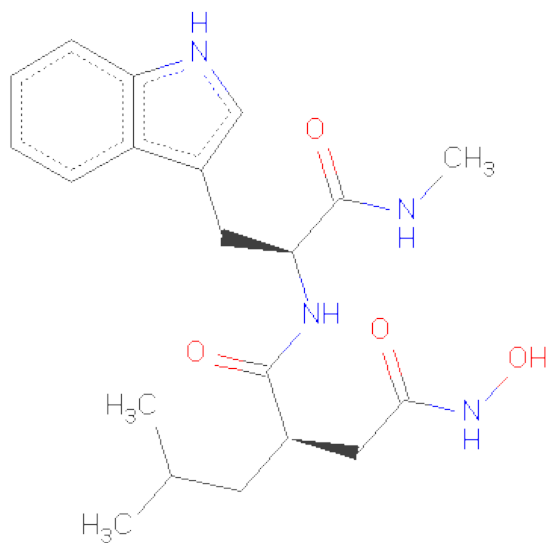
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	A	4	Total	Ca	0	0
			4	4		

- Molecule 9 is 3-(N-HYDROXYCARBOXAMIDO)-2-ISOBUTYLPROPANOYL-TRP-MET HYLAMIDE (three-letter code: GM6) (formula:  $C_{20}H_{28}N_4O_4$ ).



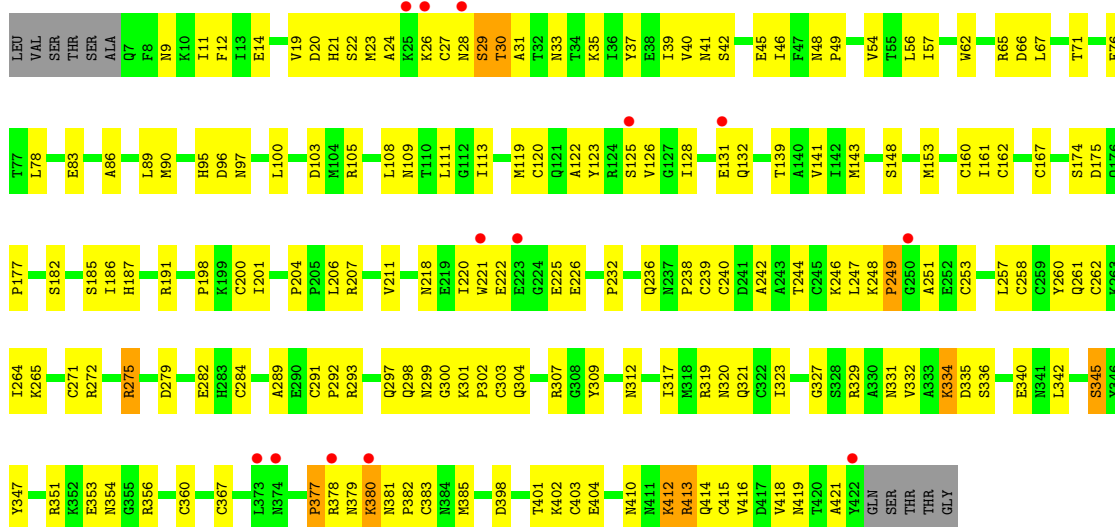
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			28	20	4	4		

### 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.

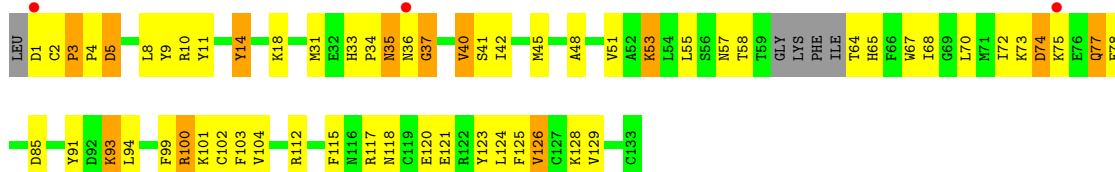
- Molecule 1: Coagulation factor X-activating enzyme heavy chain

Chain A: 



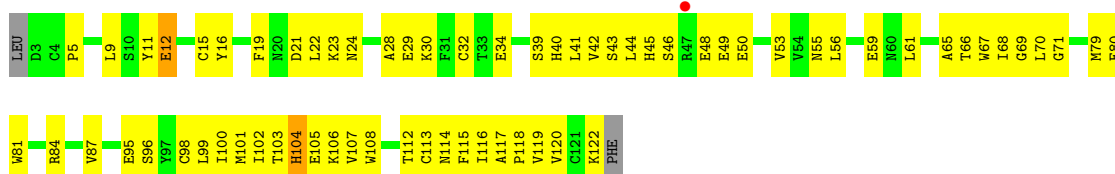
- Molecule 2: Coagulation factor X-activating enzyme light chain 2

Chain B: 



- Molecule 3: Coagulation factor X-activating enzyme light chain 1

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.35Å 91.73Å 152.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.60 – 2.91 44.56 – 2.91	Depositor EDS
% Data completeness (in resolution range)	95.9 (44.60-2.91) 95.9 (44.56-2.91)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.35 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.273 0.219 , 0.275	Depositor DCC
$R_{free}$ test set	1084 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21482 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: ZN, GM6, NAG, CA, MAN

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	0.28	0/3298	0.56	0/4453
2	B	0.32	0/1108	0.58	0/1488
3	C	0.29	0/1012	0.53	0/1366
All	All	0.29	0/5418	0.56	0/7307

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
6	E	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	906	MAN	C1
6	E	907	MAN	C1

There are no planarity outliers.

### 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	3235	0	3075	150	0
2	B	1078	0	1002	72	0
3	C	985	0	937	62	0
4	A	14	0	13	0	0
4	B	14	0	13	1	0
5	D	28	0	25	3	0
6	E	50	0	43	2	0
7	A	1	0	0	0	0
8	A	4	0	0	0	0
8	B	1	0	0	0	0
9	A	28	0	27	4	0
All	All	5438	0	5135	276	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 26.

All (276) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:248:LYS:HB3	1:A:249:PRO:HD2	1.29	1.10
1:A:226:GLU:HG2	1:A:247:LEU:HG	1.53	0.90
1:A:351:ARG:HH21	1:A:412:LYS:HG2	1.35	0.89
2:B:93:LYS:NZ	2:B:93:LYS:HB2	1.89	0.86
2:B:64:THR:HG22	2:B:65:HIS:H	1.39	0.85
1:A:382:PRO:HD2	2:B:10:ARG:NH2	1.92	0.85
1:A:30:THR:HG23	1:A:31:ALA:H	1.42	0.82
1:A:78:LEU:HD22	1:A:113:ILE:HG23	1.62	0.80
2:B:93:LYS:HE3	3:C:107:VAL:HA	1.64	0.80
3:C:22:LEU:HB3	3:C:116:ILE:HG22	1.64	0.79
5:D:901:NAG:H61	5:D:902:NAG:HN2	1.50	0.77
1:A:410:ASN:HD21	1:A:414:GLN:HE21	1.33	0.77
2:B:68:ILE:HG23	2:B:70:LEU:H	1.51	0.76
1:A:111:LEU:HD13	9:A:700:GM6:HBB	1.51	0.75
2:B:34:PRO:HB2	2:B:129:VAL:HG11	1.69	0.74
3:C:112:THR:HG22	3:C:114:ASN:H	1.51	0.74
1:A:232:PRO:HA	1:A:242:ALA:HB1	1.70	0.74
1:A:275:ARG:HH11	1:A:275:ARG:HB3	1.53	0.74
1:A:236:GLN:O	1:A:238:PRO:HD3	1.89	0.72
1:A:351:ARG:NH2	1:A:412:LYS:HG2	2.04	0.72
1:A:48:ASN:HB3	1:A:49:PRO:HD3	1.71	0.72
2:B:93:LYS:CE	3:C:107:VAL:HA	2.20	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:118:ASN:HD21	2:B:120:GLU:HB3	1.54	0.71
1:A:379:ASN:O	1:A:380:LYS:HG3	1.92	0.69
1:A:218:ASN:O	1:A:220:ILE:HG13	1.93	0.69
3:C:55:ASN:O	3:C:59:GLU:HG2	1.93	0.69
1:A:206:LEU:HD11	1:A:293:ARG:HA	1.75	0.68
6:E:905:NAG:H83	6:E:907:MAN:H3	1.76	0.68
1:A:307:ARG:HE	1:A:307:ARG:HA	1.58	0.68
2:B:118:ASN:HB3	2:B:121:GLU:HG3	1.75	0.68
1:A:299:ASN:HD21	1:A:312:ASN:H	1.43	0.68
1:A:162:CYS:SG	1:A:182:SER:HA	2.34	0.67
1:A:248:LYS:HB3	1:A:249:PRO:CD	2.16	0.67
2:B:2:CYS:C	2:B:4:PRO:HD2	2.16	0.66
5:D:901:NAG:H61	5:D:902:NAG:N2	2.10	0.66
1:A:271:CYS:HB3	1:A:284:CYS:SG	2.35	0.66
1:A:309:TYR:HE1	1:A:402:LYS:HG3	1.58	0.66
1:A:30:THR:HG23	1:A:31:ALA:N	2.09	0.66
2:B:4:PRO:O	2:B:5:ASP:HB2	1.96	0.66
1:A:207:ARG:HG2	1:A:221:TRP:O	1.96	0.66
2:B:40:VAL:CG2	2:B:126:VAL:HG13	2.26	0.65
1:A:410:ASN:HD21	1:A:414:GLN:NE2	1.95	0.65
2:B:40:VAL:HG21	2:B:126:VAL:HG13	1.79	0.64
2:B:53:LYS:HA	2:B:53:LYS:HE2	1.79	0.64
1:A:153:MET:CE	1:A:185:SER:HB3	2.28	0.63
3:C:67:TRP:CE3	3:C:100:ILE:HG12	2.34	0.63
2:B:93:LYS:HZ2	2:B:93:LYS:HB2	1.62	0.62
1:A:11:ILE:HG23	1:A:201:ILE:HB	1.81	0.62
1:A:261:GLN:O	1:A:262:CYS:HB2	1.98	0.62
6:E:905:NAG:C8	6:E:907:MAN:H3	2.29	0.62
1:A:307:ARG:HA	1:A:307:ARG:NE	2.15	0.61
1:A:321:GLN:HE22	1:A:398:ASP:H	1.48	0.61
2:B:2:CYS:O	2:B:4:PRO:HD2	2.01	0.61
1:A:222:GLU:HB2	1:A:225:GLU:OE2	2.01	0.61
2:B:93:LYS:HZ3	2:B:93:LYS:HB2	1.66	0.61
2:B:35:ASN:C	2:B:37:GLY:H	2.03	0.61
2:B:18:LYS:O	2:B:18:LYS:HG2	2.01	0.61
1:A:261:GLN:HE21	1:A:261:GLN:HA	1.66	0.60
3:C:65:ALA:O	3:C:118:PRO:HG2	2.00	0.60
1:A:83:GLU:HG3	1:A:123:TYR:HE2	1.65	0.60
3:C:22:LEU:HB3	3:C:116:ILE:CG2	2.31	0.60
2:B:14:TYR:N	2:B:14:TYR:CD2	2.70	0.60
3:C:70:LEU:HD12	3:C:99:LEU:HD22	1.84	0.59
2:B:118:ASN:ND2	2:B:120:GLU:HB3	2.16	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:382:PRO:HD2	2:B:10:ARG:HH22	1.64	0.59
2:B:117:ARG:HD2	2:B:123:TYR:OH	2.03	0.59
2:B:2:CYS:C	2:B:4:PRO:CD	2.71	0.59
3:C:102:ILE:HD12	3:C:104:HIS:CE1	2.37	0.58
2:B:40:VAL:HG22	2:B:126:VAL:O	2.04	0.58
1:A:377:PRO:O	1:A:378:ARG:HB2	2.03	0.58
1:A:297:GLN:NE2	1:A:298:GLN:H	2.01	0.58
1:A:111:LEU:HD13	9:A:700:GM6:NBB	2.18	0.58
1:A:272:ARG:HD2	1:A:282:GLU:OE1	2.04	0.58
1:A:297:GLN:HE21	1:A:298:GLN:H	1.50	0.58
1:A:39:ILE:HD13	1:A:139:THR:HG21	1.85	0.58
1:A:119:MET:HE3	1:A:125:SER:OG	2.04	0.57
2:B:93:LYS:HD3	3:C:50:GLU:OE2	2.04	0.57
1:A:153:MET:HE2	1:A:185:SER:HB3	1.85	0.57
1:A:248:LYS:CB	1:A:249:PRO:HD2	2.17	0.57
2:B:10:ARG:O	2:B:11:TYR:HB2	2.04	0.57
1:A:271:CYS:SG	1:A:292:PRO:HD2	2.45	0.57
1:A:39:ILE:HD11	1:A:131:GLU:OE2	2.05	0.57
3:C:66:THR:HG21	3:C:120:VAL:HG23	1.87	0.57
2:B:18:LYS:HA	2:B:124:LEU:HD22	1.85	0.57
2:B:9:TYR:CZ	2:B:10:ARG:HD3	2.40	0.56
1:A:29:SER:O	1:A:31:ALA:N	2.39	0.56
3:C:46:SER:OG	3:C:48:GLU:HG2	2.05	0.56
2:B:65:HIS:HB2	2:B:123:TYR:CD2	2.41	0.56
1:A:239:CYS:HA	1:A:248:LYS:HG3	1.87	0.56
1:A:253:CYS:SG	1:A:264:ILE:HD13	2.46	0.56
1:A:301:LYS:HD2	1:A:302:PRO:HD2	1.89	0.55
2:B:64:THR:HG22	2:B:65:HIS:N	2.16	0.55
1:A:35:LYS:O	1:A:39:ILE:HG13	2.07	0.55
1:A:71:THR:HG21	1:A:76:GLU:OE2	2.06	0.55
1:A:334:LYS:HD2	1:A:335:ASP:N	2.22	0.55
1:A:207:ARG:HD3	1:A:221:TRP:CD2	2.41	0.55
1:A:342:LEU:HD23	1:A:360:CYS:O	2.05	0.55
2:B:45:MET:HG3	2:B:112:ARG:HH22	1.72	0.55
1:A:41:ASN:O	1:A:45:GLU:HG3	2.06	0.55
1:A:111:LEU:HD22	9:A:700:GM6:OAZ	2.07	0.55
3:C:117:ALA:HB1	3:C:118:PRO:HD2	1.88	0.54
2:B:40:VAL:HG13	2:B:126:VAL:HG22	1.89	0.54
1:A:26:LYS:O	1:A:28:ASN:N	2.40	0.54
1:A:14:GLU:HG3	1:A:96:ASP:OD2	2.08	0.54
3:C:19:PHE:HB2	3:C:119:VAL:HG13	1.90	0.54
3:C:43:SER:O	3:C:44:LEU:HD23	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:66:THR:HG21	3:C:120:VAL:CG2	2.38	0.54
2:B:1:ASP:HA	2:B:8:LEU:HD22	1.89	0.54
1:A:319:ARG:NH1	1:A:331:ASN:ND2	2.55	0.54
3:C:15:CYS:O	3:C:122:LYS:HA	2.08	0.54
3:C:11:TYR:CE2	3:C:49:GLU:HA	2.43	0.53
3:C:102:ILE:HD12	3:C:104:HIS:HE1	1.72	0.53
1:A:334:LYS:NZ	1:A:336:SER:H	2.06	0.53
2:B:35:ASN:O	2:B:37:GLY:N	2.41	0.53
1:A:97:ASN:HB2	1:A:119:MET:HE1	1.91	0.53
1:A:62:TRP:NE1	1:A:67:LEU:HD12	2.23	0.53
2:B:42:ILE:HD12	2:B:68:ILE:HD11	1.90	0.52
2:B:99:PHE:C	2:B:100:ARG:HD2	2.30	0.52
1:A:11:ILE:CG2	1:A:201:ILE:HD12	2.40	0.52
1:A:416:VAL:HG23	1:A:421:ALA:HB2	1.92	0.52
1:A:418:VAL:HG13	1:A:419:ASN:N	2.24	0.52
3:C:41:LEU:HB3	3:C:68:ILE:O	2.10	0.52
2:B:41:SER:HA	3:C:81:TRP:CE3	2.44	0.52
2:B:67:TRP:CE3	2:B:104:VAL:HG12	2.45	0.52
1:A:403:CYS:O	1:A:404:GLU:HG3	2.11	0.51
1:A:187:HIS:O	1:A:191:ARG:HG3	2.10	0.51
1:A:309:TYR:CE1	1:A:402:LYS:HG3	2.41	0.51
1:A:148:SER:HB3	1:A:153:MET:SD	2.50	0.51
1:A:174:SER:O	1:A:177:PRO:HG3	2.09	0.51
1:A:240:CYS:N	1:A:248:LYS:HG3	2.25	0.51
1:A:416:VAL:CG2	1:A:421:ALA:HB2	2.40	0.51
3:C:81:TRP:NE1	3:C:87:VAL:HG22	2.25	0.51
2:B:33:HIS:N	2:B:34:PRO:HD2	2.25	0.51
1:A:42:SER:O	1:A:46:ILE:HG13	2.11	0.51
2:B:67:TRP:CZ3	2:B:102:CYS:HB3	2.45	0.51
2:B:31:MET:HB3	2:B:37:GLY:O	2.09	0.51
1:A:261:GLN:NE2	1:A:261:GLN:HA	2.26	0.51
1:A:83:GLU:HG3	1:A:123:TYR:CE2	2.45	0.51
1:A:412:LYS:HB2	1:A:412:LYS:NZ	2.25	0.51
2:B:34:PRO:O	2:B:35:ASN:O	2.29	0.51
1:A:356:ARG:HB2	1:A:356:ARG:CZ	2.41	0.51
3:C:80:GLU:HA	3:C:87:VAL:HG23	1.93	0.50
1:A:413:ARG:N	1:A:413:ARG:HD2	2.25	0.50
1:A:161:ILE:HG22	1:A:162:CYS:N	2.27	0.50
3:C:24:ASN:HB2	3:C:113:CYS:O	2.11	0.50
3:C:70:LEU:HD12	3:C:99:LEU:CD2	2.41	0.50
2:B:67:TRP:HB2	2:B:125:PHE:HB3	1.92	0.50
1:A:12:PHE:CD2	1:A:204:PRO:HB3	2.47	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:11:ILE:HG21	1:A:201:ILE:HD12	1.94	0.49
1:A:21:HIS:HA	1:A:24:ALA:HB3	1.93	0.49
1:A:86:ALA:HA	1:A:90:MET:HE2	1.93	0.49
3:C:65:ALA:O	3:C:118:PRO:CG	2.60	0.49
1:A:351:ARG:HE	1:A:412:LYS:HB3	1.77	0.49
1:A:97:ASN:HB2	1:A:119:MET:CE	2.42	0.49
3:C:120:VAL:HG12	3:C:120:VAL:O	2.11	0.49
1:A:238:PRO:O	1:A:248:LYS:HE2	2.13	0.48
3:C:102:ILE:HD11	3:C:107:VAL:HG22	1.94	0.48
1:A:30:THR:CG2	1:A:31:ALA:H	2.21	0.48
1:A:300:GLY:O	1:A:309:TYR:HD2	1.96	0.48
1:A:257:LEU:HB2	1:A:291:CYS:HB2	1.94	0.48
1:A:141:VAL:HG21	1:A:177:PRO:HB2	1.94	0.48
1:A:56:LEU:O	1:A:211:VAL:HG22	2.14	0.48
1:A:19:VAL:HG13	1:A:23:MET:HB2	1.95	0.48
1:A:331:ASN:OD1	1:A:332:VAL:N	2.47	0.48
3:C:16:TYR:CD1	3:C:16:TYR:N	2.82	0.48
3:C:102:ILE:O	3:C:106:LYS:HA	2.14	0.48
1:A:113:ILE:HG22	1:A:128:ILE:HB	1.96	0.48
1:A:33:ASN:HB3	1:A:37:TYR:CZ	2.49	0.48
1:A:182:SER:O	1:A:186:ILE:HG12	2.14	0.47
2:B:94:LEU:HD23	2:B:99:PHE:CE2	2.49	0.47
3:C:9:LEU:HD12	3:C:9:LEU:N	2.29	0.47
3:C:104:HIS:ND1	3:C:105:GLU:HG2	2.29	0.47
1:A:260:TYR:CD1	1:A:261:GLN:HG2	2.49	0.47
3:C:39:SER:HA	3:C:122:LYS:O	2.15	0.47
3:C:29:GLU:OE2	3:C:41:LEU:HG	2.13	0.47
1:A:232:PRO:HA	1:A:242:ALA:CB	2.42	0.47
1:A:239:CYS:HB2	1:A:251:ALA:CB	2.44	0.47
3:C:84:ARG:HG3	3:C:84:ARG:HH11	1.80	0.47
2:B:48:ALA:O	2:B:51:VAL:HG22	2.15	0.47
1:A:239:CYS:CA	1:A:248:LYS:HG3	2.45	0.47
1:A:160:CYS:O	1:A:161:ILE:HD13	2.15	0.47
1:A:62:TRP:CE2	1:A:67:LEU:HD12	2.49	0.47
3:C:56:LEU:HD23	3:C:56:LEU:O	2.15	0.47
1:A:329:ARG:O	1:A:329:ARG:HG3	2.14	0.47
1:A:22:SER:HB3	1:A:103:ASP:HB2	1.96	0.46
1:A:282:GLU:HB3	1:A:292:PRO:HG2	1.97	0.46
1:A:264:ILE:CD1	1:A:289:ALA:HB2	2.46	0.46
3:C:32:CYS:O	3:C:39:SER:HB3	2.15	0.46
3:C:42:VAL:O	3:C:68:ILE:O	2.33	0.46
2:B:93:LYS:HG3	2:B:93:LYS:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:239:CYS:C	1:A:248:LYS:HG3	2.36	0.46
2:B:120:GLU:HA	2:B:120:GLU:OE1	2.15	0.46
1:A:334:LYS:HZ2	1:A:336:SER:H	1.61	0.46
2:B:100:ARG:HD2	2:B:100:ARG:N	2.30	0.46
1:A:317:ILE:HB	1:A:320:ASN:ND2	2.30	0.46
2:B:93:LYS:HE2	3:C:107:VAL:HA	1.98	0.45
2:B:35:ASN:C	2:B:37:GLY:N	2.69	0.45
1:A:175:ASP:C	1:A:177:PRO:HD3	2.36	0.45
2:B:93:LYS:HG2	3:C:108:TRP:CE2	2.52	0.45
1:A:304:GLN:HG3	1:A:317:ILE:HD11	1.98	0.45
2:B:14:TYR:OH	2:B:128:LYS:HE3	2.16	0.45
1:A:334:LYS:CE	1:A:336:SER:H	2.29	0.45
2:B:14:TYR:N	2:B:14:TYR:HD2	2.14	0.45
3:C:11:TYR:CE2	3:C:12:GLU:HG2	2.52	0.45
3:C:30:LYS:O	3:C:34:GLU:HG3	2.17	0.45
1:A:377:PRO:O	1:A:378:ARG:CB	2.63	0.45
2:B:94:LEU:HD23	2:B:99:PHE:HE2	1.82	0.44
2:B:72:ILE:HD12	2:B:101:LYS:HB3	1.98	0.44
1:A:304:GLN:O	1:A:307:ARG:HG2	2.18	0.44
1:A:108:LEU:O	1:A:109:ASN:HB2	2.16	0.44
1:A:319:ARG:HH11	1:A:319:ARG:HG3	1.81	0.44
1:A:30:THR:CG2	1:A:31:ALA:N	2.80	0.44
1:A:62:TRP:HB3	1:A:65:ARG:O	2.17	0.44
1:A:340:GLU:HG2	1:A:347:TYR:CE1	2.53	0.44
2:B:34:PRO:HB2	2:B:129:VAL:CG1	2.44	0.44
2:B:70:LEU:HD21	3:C:79:MET:SD	2.57	0.44
1:A:258:CYS:SG	1:A:271:CYS:HB3	2.58	0.44
2:B:40:VAL:HG22	2:B:126:VAL:HG13	1.98	0.44
3:C:49:GLU:O	3:C:53:VAL:HG23	2.17	0.44
3:C:56:LEU:HD23	3:C:56:LEU:C	2.38	0.44
1:A:232:PRO:CA	1:A:242:ALA:HB1	2.45	0.44
5:D:901:NAG:C6	5:D:902:NAG:N2	2.80	0.43
2:B:78:GLU:H	2:B:78:GLU:CD	2.20	0.43
1:A:89:LEU:HG	1:A:95:HIS:CE1	2.53	0.43
3:C:105:GLU:HA	3:C:105:GLU:OE2	2.18	0.43
1:A:78:LEU:HD11	1:A:126:VAL:HG23	2.00	0.43
1:A:111:LEU:CD1	9:A:700:GM6:HBB	2.25	0.43
1:A:275:ARG:CB	1:A:275:ARG:HH11	2.27	0.43
1:A:119:MET:O	1:A:120:CYS:HB2	2.18	0.43
2:B:73:LYS:O	2:B:74:ASP:CG	2.57	0.43
1:A:353:GLU:O	1:A:354:ASN:HB3	2.17	0.43
1:A:403:CYS:C	1:A:404:GLU:HG3	2.38	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:57:ASN:OD1	4:B:903:NAG:H2	2.18	0.43
1:A:244:THR:O	1:A:246:LYS:HG2	2.17	0.43
3:C:24:ASN:HA	3:C:115:PHE:O	2.19	0.43
2:B:85:ASP:HA	3:C:40:HIS:CD2	2.53	0.43
1:A:319:ARG:HH11	1:A:331:ASN:ND2	2.15	0.43
3:C:12:GLU:OE2	3:C:12:GLU:HA	2.19	0.43
1:A:105:ARG:NH1	1:A:109:ASN:OD1	2.52	0.43
1:A:401:THR:HG22	1:A:402:LYS:N	2.34	0.43
2:B:3:PRO:N	2:B:4:PRO:CD	2.82	0.42
2:B:77:GLN:HG3	2:B:99:PHE:CE2	2.55	0.42
1:A:40:VAL:HA	1:A:143:MET:HE1	2.01	0.42
1:A:303:CYS:O	1:A:304:GLN:HB2	2.19	0.42
1:A:14:GLU:HB3	1:A:57:ILE:HD13	2.00	0.42
1:A:23:MET:HG2	1:A:103:ASP:OD2	2.20	0.42
2:B:33:HIS:N	2:B:34:PRO:CD	2.83	0.42
1:A:218:ASN:ND2	1:A:220:ILE:HB	2.34	0.42
1:A:9:ASN:HD22	1:A:9:ASN:HA	1.64	0.42
1:A:323:ILE:HA	1:A:327:GLY:O	2.19	0.42
1:A:19:VAL:CG1	1:A:23:MET:HB2	2.50	0.42
1:A:367:CYS:SG	1:A:415:CYS:HB2	2.59	0.42
3:C:102:ILE:HD11	3:C:107:VAL:CG2	2.49	0.42
3:C:65:ALA:HA	3:C:101:MET:O	2.20	0.42
3:C:65:ALA:O	3:C:66:THR:CG2	2.68	0.42
1:A:198:PRO:HG2	1:A:201:ILE:HD11	2.02	0.41
1:A:410:ASN:HD21	1:A:414:GLN:HB2	1.84	0.41
2:B:93:LYS:HE2	3:C:106:LYS:O	2.20	0.41
2:B:68:ILE:HG21	2:B:103:PHE:HB2	2.02	0.41
1:A:334:LYS:O	1:A:335:ASP:C	2.59	0.41
2:B:55:LEU:O	2:B:58:THR:HB	2.20	0.41
1:A:131:GLU:OE1	1:A:132:GLN:N	2.54	0.41
3:C:95:GLU:HG2	3:C:96:SER:N	2.35	0.41
1:A:153:MET:HE3	1:A:185:SER:HB3	2.00	0.41
2:B:91:TYR:HB2	3:C:45:HIS:C	2.41	0.41
1:A:260:TYR:HB2	1:A:265:LYS:NZ	2.36	0.41
2:B:103:PHE:HA	2:B:115:PHE:O	2.20	0.41
1:A:20:ASP:HB3	1:A:100:LEU:HD11	2.03	0.41
1:A:275:ARG:HG2	1:A:279:ASP:OD1	2.21	0.41
3:C:23:LYS:HD2	3:C:28:ALA:HA	2.02	0.41
2:B:94:LEU:HA	3:C:108:TRP:HB2	2.02	0.40
3:C:19:PHE:N	3:C:61:LEU:HD21	2.36	0.40
3:C:71:GLY:HA2	3:C:98:CYS:SG	2.61	0.40
1:A:381:ASN:ND2	1:A:383:CYS:C	2.75	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:84:ARG:HG3	3:C:84:ARG:NH1	2.36	0.40
3:C:104:HIS:CG	3:C:105:GLU:H	2.36	0.40

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	414/427 (97%)	358 (86%)	48 (12%)	8 (2%)	12	41
2	B	125/134 (93%)	106 (85%)	12 (10%)	7 (6%)	3	7
3	C	118/122 (97%)	94 (80%)	18 (15%)	6 (5%)	3	9
All	All	657/683 (96%)	558 (85%)	78 (12%)	21 (3%)	6	24

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	CYS
1	A	29	SER
1	A	30	THR
2	B	5	ASP
2	B	35	ASN
3	C	104	HIS
1	A	249	PRO
1	A	380	LYS
2	B	74	ASP
3	C	21	ASP
1	A	377	PRO
2	B	36	ASN
2	B	37	GLY
3	C	69	GLY
1	A	345	SER
2	B	75	LYS
3	C	5	PRO

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Mol	Chain	Res	Type
3	C	12	GLU
3	C	103	THR
1	A	122	ALA
2	B	3	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	368/377 (98%)	358 (97%)	10 (3%)	57	89
2	B	120/124 (97%)	113 (94%)	7 (6%)	28	64
3	C	109/111 (98%)	109 (100%)	0	100	100
All	All	597/612 (98%)	580 (97%)	17 (3%)	56	89

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	66	ASP
1	A	167	CYS
1	A	200	CYS
1	A	275	ARG
1	A	334	LYS
1	A	345	SER
1	A	385	MET
1	A	412	LYS
1	A	413	ARG
2	B	14	TYR
2	B	40	VAL
2	B	53	LYS
2	B	77	GLN
2	B	93	LYS
2	B	100	ARG
2	B	126	VAL

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	9	ASN
1	A	28	ASN
1	A	79	ASN
1	A	163	ASN
1	A	176	GLN
1	A	261	GLN
1	A	297	GLN
1	A	299	ASN
1	A	312	ASN
1	A	320	ASN
1	A	321	GLN
1	A	341	ASN
1	A	374	ASN
1	A	384	ASN
1	A	392	GLN
1	A	414	GLN
2	B	118	ASN
3	C	40	HIS

### 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 ⓘ

6 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	$\# Z  > 2$
5	NAG	D	901	1,5	12,14,15	0.49	0	15,19,21	0.78	0
5	NAG	D	902	5	12,14,15	0.42	0	15,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	E	904	3,6	12,14,15	0.56	0	15,19,21	0.84	1 (6%)
6	NAG	E	905	6	12,14,15	0.51	0	15,19,21	0.70	0
6	MAN	E	906	6	10,11,12	0.46	0	11,15,17	0.36	0
6	MAN	E	907	6	10,11,12	0.45	0	11,15,17	0.36	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
5	NAG	D	901	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	902	5	-	0/6/23/26	0/1/1/1
6	NAG	E	904	3,6	-	0/6/23/26	0/1/1/1
6	NAG	E	905	6	-	0/6/23/26	0/1/1/1
6	MAN	E	906	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	E	907	6	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	904	NAG	C3-C2-N2	-2.33	108.21	111.76

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	907	MAN	C1
6	E	906	MAN	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z  > 2$
9	GM6	A	700	7	29,29,29	1.26	3 (10%)	39,39,39	1.18	4 (10%)
4	NAG	A	900	1	12,14,15	0.45	0	15,19,21	0.65	0
4	NAG	B	903	2	12,14,15	0.47	0	15,19,21	0.65	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
9	GM6	A	700	7	-	0/28/28/28	0/0/2/2
4	NAG	A	900	1	-	0/6/23/26	0/1/1/1
4	NAG	B	903	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	700	GM6	CAX-CAV	2.57	1.42	1.36
9	A	700	GM6	CAT-CAP	-2.23	1.34	1.37
9	A	700	GM6	CAW-CAS	2.12	1.41	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	700	GM6	CAP-CAO-CAN	3.28	119.71	114.55
9	A	700	GM6	CAO-CAN-CAY	-2.71	102.57	110.26
9	A	700	GM6	CBA-NBB-CAY	-2.23	118.17	122.25
9	A	700	GM6	CAP-CAQ-CAR	2.21	109.53	107.01

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, 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	416/427 (97%)	0.20	13 (3%) 47 55	35, 67, 107, 150	0
2	B	129/134 (96%)	0.15	3 (2%) 57 66	41, 68, 116, 130	0
3	C	120/122 (98%)	0.21	1 (0%) 83 89	48, 75, 111, 132	0
All	All	665/683 (97%)	0.19	17 (2%) 53 62	35, 68, 111, 150	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	ARG	6.1
2	B	36	ASN	5.6
1	A	380	LYS	4.5
2	B	1	ASP	4.1
1	A	373	LEU	3.9
1	A	374	ASN	3.5
1	A	223	GLU	3.3
1	A	422	TYR	3.2
2	B	75	LYS	3.0
1	A	250	GLY	3.0
3	C	47	ARG	2.6
1	A	28	ASN	2.5
1	A	221	TRP	2.3
1	A	25	LYS	2.3
1	A	125	SER	2.1
1	A	131	GLU	2.0
1	A	26	LYS	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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	MAN	E	907	11/12	0.40	9.41	149,158,166,174	0
6	NAG	E	905	14/15	0.28	0.95	87,106,121,134	0
5	NAG	D	901	14/15	0.21	-0.14	65,79,97,98	0
6	NAG	E	904	14/15	0.15	-0.47	57,76,85,94	0
5	NAG	D	902	14/15	0.21	-0.59	91,103,111,115	0
6	MAN	E	906	11/12	0.19	-	116,126,134,140	0

### 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	CA	B	805	1/1	0.25	4.86	86,86,86,86	0
8	CA	A	801	1/1	0.30	3.34	55,55,55,55	0
4	NAG	B	903	14/15	0.35	2.85	126,138,145,147	0
9	GM6	A	700	28/28	0.30	2.35	37,70,95,100	0
4	NAG	A	900	14/15	0.27	2.03	99,105,112,122	0
8	CA	A	804	1/1	0.19	1.71	89,89,89,89	0
7	ZN	A	800	1/1	0.21	0.58	56,56,56,56	0
8	CA	A	803	1/1	0.19	0.44	56,56,56,56	0
8	CA	A	802	1/1	0.10	-1.50	76,76,76,76	0

### 6.5 Other polymers

There are no such residues in this entry.