



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 03:20 AM EDT

PDB ID : 4EN9  
Title : Crystal structure of HA70 (HA3) subcomponent of Clostridium botulinum type C progenitor toxin in complex with alpha 2-6-sialyllactosamine  
Authors : Yamashita, S.; Yoshida, H.; Tono-zuka, T.; Nishikawa, A.; Kamitori, S.  
Deposited on : 2012-04-12  
Resolution : 2.64 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](mailto: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.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

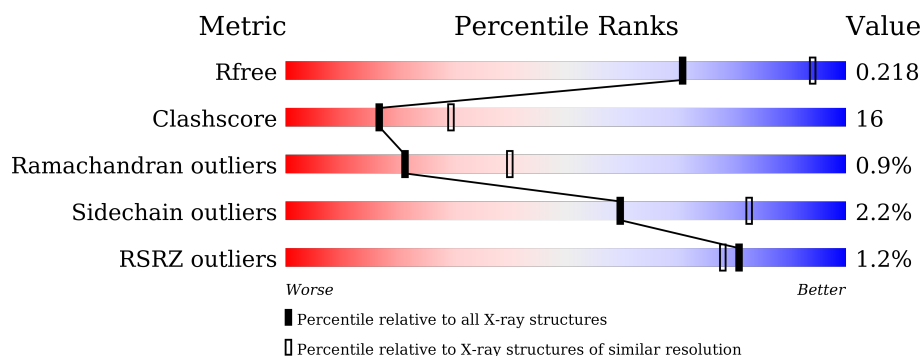
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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. 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	224	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>19%</div> <div>•</div> <div>24%</div> </div> </div>
2	B	420	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>26%</div> <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	MRD	A	301	-	-	-	X
3	MRD	A	302	-	-	-	X
3	MRD	A	303	-	-	-	X
3	MRD	B	705	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5092 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 Hemagglutinin components HA-22/23/53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1382	882	226	271	3			

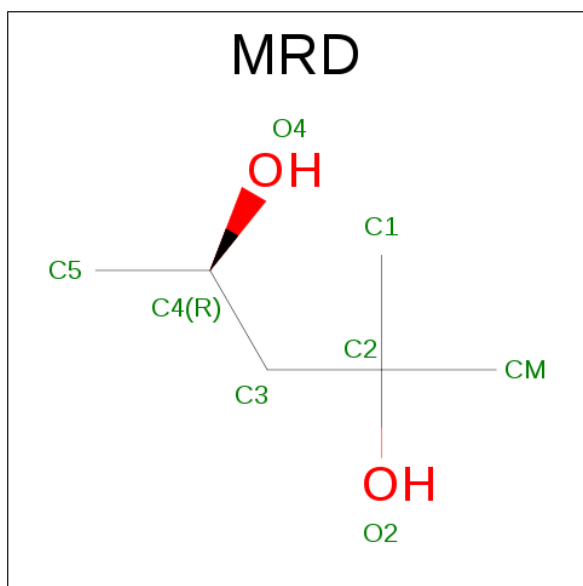
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	ILE	-	EXPRESSION TAG	UNP P46085
A	-19	SER	-	EXPRESSION TAG	UNP P46085
A	-18	GLU	-	EXPRESSION TAG	UNP P46085
A	-17	PHE	-	EXPRESSION TAG	UNP P46085
A	-16	ASP	-	EXPRESSION TAG	UNP P46085
A	-15	TYR	-	EXPRESSION TAG	UNP P46085
A	-14	LYS	-	EXPRESSION TAG	UNP P46085
A	-13	ASP	-	EXPRESSION TAG	UNP P46085
A	-12	HIS	-	EXPRESSION TAG	UNP P46085
A	-11	ASP	-	EXPRESSION TAG	UNP P46085
A	-10	ILE	-	EXPRESSION TAG	UNP P46085
A	-9	ASP	-	EXPRESSION TAG	UNP P46085
A	-8	TYR	-	EXPRESSION TAG	UNP P46085
A	-7	LYS	-	EXPRESSION TAG	UNP P46085
A	-6	ASP	-	EXPRESSION TAG	UNP P46085
A	-5	ASP	-	EXPRESSION TAG	UNP P46085
A	-4	ASP	-	EXPRESSION TAG	UNP P46085
A	-3	ASP	-	EXPRESSION TAG	UNP P46085
A	-2	LYS	-	EXPRESSION TAG	UNP P46085
A	-1	TRP	-	EXPRESSION TAG	UNP P46085
A	0	ILE	-	EXPRESSION TAG	UNP P46085

- Molecule 2 is a protein called Hemagglutinin components HA-22/23/53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3339	2109	553	672	5			

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	3	Total	C	N	O	0	0
			46	25	2	19		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total 83	O 83	0	0
5	B	202	Total 202	O 202	0	0

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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:
- 
- | Category | Residue Count |
|----------|---------------|
| ASP      | 1             |
| ILE      | 1             |
| SER      | 1             |
| GLU      | 1             |
| PHE      | 1             |
| ASP      | 1             |
| THR      | 1             |
| LYS      | 1             |
| ASP      | 1             |
| HIS      | 1             |
| ASP      | 1             |
| ILE      | 1             |
| ASP      | 1             |
| TYR      | 1             |
| LYS      | 1             |
| ASP      | 1             |
| ASP      | 1             |
| ASP      | 1             |
| ASP      | 1             |
| LYS      | 1             |
| TRP      | 1             |
| ILE      | 1             |
| MET      | 1             |
| SER      | 1             |
| LEU      | 1             |
| SER      | 1             |
| ILE      | 1             |
| LYS      | 1             |
| GLU      | 1             |
| LEU      | 1             |
| TYR      | 1             |
| THR      | 1             |
| LYS      | 1             |
| ASP      | 1             |
| LYS      | 1             |
| S15      | 1             |
| I16      | 1             |
| M17      | 1             |
| M18      | 1             |
| L21      | 1             |
| R30      | 1             |
| S37      | 1             |
| R38      | 1             |
| G39      | 1             |
| M40      | 1             |
| M46      | 1             |
| I47      | 1             |
| A54      | 1             |
| D58      | 1             |
| L59      | 1             |
| R60      | 1             |
| I61      | 1             |
| R62      | 1             |
| A65      | 1             |
| T66      | 1             |
| P67      | 1             |
| Y68      | 1             |
| Y69      | 1             |
| Q85      | 1             |
| F88      | 1             |
| T92      | 1             |
| E93      | 1             |
| A94      | 1             |
| S95      | 1             |
| E96      | 1             |
| I97      | 1             |
| P98      | 1             |
| F101     | 1             |
| S104     | 1             |
| M115     | 1             |
| L130     | 1             |
| R137     | 1             |
| L140     | 1             |
| G146     | 1             |
| K149     | 1             |
| M154     | 1             |
| S155     | 1             |
| E156     | 1             |
| E157     | 1             |
| K161     | 1             |
| Y164     | 1             |
| F165     | 1             |
| K175     | 1             |
| K176     | 1             |
| D184     | 1             |
| THR      | 1             |
| ILE      | 1             |
| THR      | 1             |
| VAL      | 1             |
| LYS      | 1             |
| GLU      | 1             |
| SER      | 1             |
| LYS      | 1             |
| ASN      | 1             |
| SER      | 1             |
| ASN      | 1             |
| ASN      | 1             |
| ASN      | 1             |
| PHE      | 1             |
| THR      | 1             |
| SER      | 1             |

- Chain B:

L587	F472	E366	Q204
L588	K473	N367	T205
N589	D474	N368	I206
V590	K475	I373	T216
E591	I484	N378	N317
S594	S490	I394	K218
L596	E496	P395	G221
T600	E497	T396	N226
Y601	N500	Q399	E237
E609	I501	K408	T240
N612	D503	T412	G242
Y613	L504	G413	S243
N614	A505	V414	I244
I615	D506	Y415	Q246
I616	S507	K416	P247
R621	L512	K420	R248
N622	L515	M421	L249
S623	N516	M422	R250
	T517	L423	N251
	P528	P425	R254
	N532	L426	P255
	Y533	I427	L256
	I534	I428	F257
	S535	Y429	N258
	Y536	E430	T259
	Q537	S435	S260
	L538	M436	N261
	N545	R437	I264
	I547	N438	R273
	A548	M439	L274
	S549	L444	N275
	I551	S445	D276
	F552	N446	N279
	S553	D447	T285
	F554	N448	Y330
	R555	I449	K336
	T556	I452	C337
	R557	I455	E338
	Q560	T456	V354
	R567	G457	D355
	I572	R460	Q356
	N573	K464	D357
	I577	L467	T362
		T468	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.98 Å   175.98 Å   80.64 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	33.26 – 2.64 33.26 – 2.64	Depositor EDS
% Data completeness (in resolution range)	95.8 (33.26-2.64) 95.8 (33.26-2.64)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.25 (at 2.65 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.193 , 0.220 0.191 , 0.218	Depositor DCC
$R_{free}$ test set	4066 reflections (11.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.6	EDS
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 41955 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MRD, SIA, GAL, NAG

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	0.37	0/1411	0.66	0/1914
2	B	0.35	0/3405	0.68	0/4642
All	All	0.35	0/4816	0.67	0/6556

There are no bond length outliers.

There are no bond angle outliers.

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	1382	0	1336	40	0
2	B	3339	0	3275	112	0
3	A	24	0	42	8	0
3	B	16	0	28	1	0
4	B	46	0	40	5	0
5	A	83	0	0	11	0
5	B	202	0	0	16	0
All	All	5092	0	4721	157	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 16.

All (157) 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)
2:B:505:ALA:HA	5:B:901:HOH:O	1.51	1.09
2:B:545:ASN:HD21	2:B:548:ALA:HB3	1.29	0.96
2:B:512:LEU:HD22	2:B:538:LEU:HD21	1.47	0.95
2:B:273:ARG:NH1	2:B:276:ASP:OD2	2.12	0.82
2:B:226:ASN:HD21	2:B:355:ASP:H	1.30	0.79
3:A:303:MRD:HMC1	3:A:303:MRD:H5C3	1.62	0.79
2:B:378:ASN:HD22	2:B:378:ASN:H	1.30	0.78
2:B:545:ASN:HD21	2:B:548:ALA:CB	1.97	0.77
2:B:460:ARG:NH1	4:B:703:NAG:H3	2.01	0.76
5:A:411:HOH:O	3:B:705:MRD:H1C1	1.85	0.75
2:B:612:ASN:HD22	2:B:614:ASN:H	1.35	0.74
2:B:420:LYS:HD3	5:B:859:HOH:O	1.87	0.74
1:A:176:LYS:HE3	5:A:412:HOH:O	1.88	0.72
1:A:37:SER:O	1:A:38:ARG:HG2	1.89	0.71
2:B:612:ASN:ND2	2:B:614:ASN:H	1.89	0.69
1:A:62:ARG:HB2	1:A:95:SER:O	1.94	0.67
2:B:460:ARG:HG3	4:B:703:NAG:HN2	1.60	0.66
2:B:545:ASN:ND2	2:B:548:ALA:HB3	2.08	0.66
2:B:528:PRO:HG2	2:B:534:ILE:HB	1.77	0.66
4:B:702:GAL:H3	5:B:803:HOH:O	1.94	0.65
1:A:85:GLN:NE2	1:A:92:THR:H	1.95	0.65
2:B:512:LEU:CD2	2:B:538:LEU:HD21	2.23	0.65
2:B:447:ASP:HB2	2:B:449:ILE:HG13	1.78	0.65
2:B:507:SER:HA	5:B:952:HOH:O	1.96	0.65
2:B:245:ILE:HD11	5:B:904:HOH:O	1.97	0.64
1:A:161:LYS:HD3	3:A:303:MRD:HMC2	1.79	0.64
2:B:221:GLY:O	2:B:362:THR:HB	1.97	0.63
2:B:515:LEU:HD11	2:B:538:LEU:HD22	1.80	0.63
2:B:424:PRO:HG3	2:B:484:ILE:HD11	1.80	0.62
2:B:428:ILE:HG23	2:B:455:ILE:HB	1.82	0.62
3:A:301:MRD:O4	3:A:301:MRD:H1C2	2.01	0.61
2:B:612:ASN:HB2	5:B:948:HOH:O	2.00	0.61
2:B:243:SER:HB3	5:B:904:HOH:O	2.00	0.61
2:B:336:LYS:HD2	2:B:362:THR:HG21	1.81	0.60
2:B:435:SER:HB3	2:B:475:LYS:HG2	1.83	0.60
2:B:261:ASN:OD1	2:B:264:ILE:HG22	2.02	0.60
2:B:545:ASN:HD22	2:B:545:ASN:N	1.97	0.60
3:A:303:MRD:H1C1	5:A:451:HOH:O	2.02	0.59
1:A:88:PHE:HB3	5:A:406:HOH:O	2.03	0.59
1:A:40:ASN:HD22	1:A:40:ASN:H	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:LYS:NZ	2:B:338:GLU:HG3	2.19	0.58
2:B:422:ASN:HD22	2:B:464:LYS:HE2	1.68	0.58
1:A:16:ILE:O	1:A:16:ILE:HD13	2.04	0.58
2:B:430:GLU:HG2	5:B:842:HOH:O	2.04	0.57
2:B:256:LEU:HB2	2:B:330:TYR:HB2	1.87	0.57
2:B:216:ILE:CD1	2:B:369:ILE:HG23	2.35	0.57
1:A:69:TYR:CE1	1:A:140:LEU:HD13	2.40	0.56
1:A:154:ASN:OD1	1:A:157:GLU:HG3	2.05	0.56
2:B:547:ILE:HG13	2:B:548:ALA:N	2.20	0.56
2:B:226:ASN:HD21	2:B:355:ASP:N	2.00	0.56
2:B:423:LEU:HD13	2:B:464:LYS:HA	1.87	0.56
2:B:336:LYS:CD	2:B:362:THR:HG21	2.36	0.56
2:B:420:LYS:HG2	5:B:885:HOH:O	2.05	0.56
2:B:512:LEU:HD22	2:B:538:LEU:CD2	2.29	0.55
3:A:301:MRD:H3C1	5:A:427:HOH:O	2.06	0.55
2:B:532:ASN:HA	5:B:996:HOH:O	2.06	0.55
2:B:552:PHE:CD2	2:B:595:LEU:HD12	2.42	0.55
1:A:66:THR:HG23	5:A:467:HOH:O	2.06	0.55
2:B:336:LYS:HE2	2:B:362:THR:HG23	1.88	0.55
4:B:701:SIA:H6	4:B:701:SIA:O1B	2.04	0.55
2:B:515:LEU:CD1	2:B:538:LEU:HD22	2.37	0.54
2:B:547:ILE:HG13	2:B:548:ALA:H	1.72	0.54
2:B:444:LEU:C	2:B:444:LEU:HD23	2.27	0.54
2:B:528:PRO:CG	2:B:534:ILE:HB	2.37	0.54
2:B:557:ARG:HG2	2:B:557:ARG:HH11	1.71	0.54
2:B:556:THR:HA	2:B:616:ILE:O	2.08	0.53
2:B:512:LEU:HB2	2:B:538:LEU:HD23	1.91	0.53
2:B:424:PRO:HB2	2:B:425:PRO:HD2	1.91	0.53
2:B:512:LEU:HD11	2:B:536:TYR:HB3	1.91	0.53
2:B:436:ASN:HB3	5:B:960:HOH:O	2.08	0.53
1:A:60:ARG:NH2	5:A:452:HOH:O	2.38	0.53
2:B:555:ARG:NH1	2:B:589:ASN:O	2.38	0.52
3:A:302:MRD:HMC2	3:A:302:MRD:O4	2.09	0.52
2:B:497:GLU:HB3	2:B:501:ILE:HG21	1.90	0.52
2:B:216:ILE:HD12	2:B:369:ILE:HG12	1.92	0.52
2:B:545:ASN:O	2:B:547:ILE:N	2.43	0.51
2:B:591:GLU:HG2	5:B:916:HOH:O	2.09	0.51
1:A:93:GLU:O	1:A:96:GLU:HG2	2.11	0.51
1:A:40:ASN:ND2	1:A:40:ASN:H	2.08	0.51
1:A:30:ARG:NH1	1:A:175:GLU:OE2	2.44	0.50
2:B:545:ASN:O	2:B:545:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:C	1:A:38:ARG:HG2	2.32	0.50
2:B:545:ASN:O	2:B:546:ASN:C	2.49	0.50
1:A:15:SER:N	1:A:18:ASN:ND2	2.59	0.50
2:B:378:ASN:ND2	2:B:378:ASN:H	2.05	0.50
1:A:164:TYR:CZ	2:B:366:GLU:HB2	2.48	0.49
1:A:62:ARG:NH1	5:A:441:HOH:O	2.45	0.49
2:B:226:ASN:ND2	2:B:354:VAL:HG22	2.28	0.49
2:B:273:ARG:NH2	5:B:818:HOH:O	2.31	0.48
1:A:60:ARG:O	1:A:60:ARG:HG3	2.12	0.48
1:A:85:GLN:HE22	1:A:92:THR:H	1.60	0.48
2:B:468:ILE:HG21	2:B:504:LEU:HB2	1.96	0.48
2:B:595:LEU:HB3	2:B:601:TYR:CE2	2.48	0.47
2:B:546:ASN:O	2:B:596:LEU:HG	2.13	0.47
2:B:560:GLN:HB3	2:B:609:GLU:HB3	1.97	0.47
2:B:550:SER:HB3	2:B:623:SER:O	2.15	0.47
2:B:373:ILE:HD12	2:B:452:ILE:HD13	1.96	0.47
1:A:115:MET:HA	1:A:149:LYS:O	2.15	0.47
1:A:161:LYS:HD3	3:A:303:MRD:CM	2.43	0.47
1:A:98:PRO:HA	5:A:407:HOH:O	2.15	0.46
1:A:58:ASP:OD2	1:A:59:LEU:N	2.45	0.46
2:B:226:ASN:CG	2:B:354:VAL:HG22	2.36	0.46
1:A:137:ARG:O	2:B:438:ASN:HA	2.16	0.46
2:B:551:ILE:HD13	2:B:594:SER:HB3	1.98	0.46
2:B:261:ASN:CG	2:B:264:ILE:HG22	2.36	0.46
2:B:438:ASN:ND2	2:B:445:SER:HB3	2.31	0.46
2:B:560:GLN:HB2	2:B:587:LEU:HD22	1.98	0.46
2:B:336:LYS:HE2	2:B:362:THR:CG2	2.45	0.46
2:B:254:ARG:HG2	2:B:254:ARG:HH11	1.80	0.45
2:B:421:ASN:N	5:B:991:HOH:O	2.34	0.45
1:A:101:PHE:CE1	1:A:146:GLY:HA3	2.52	0.45
2:B:512:LEU:CD1	2:B:536:TYR:HB3	2.46	0.45
4:B:703:NAG:H82	4:B:703:NAG:O1	2.17	0.45
2:B:500:ASN:HD21	2:B:577:LEU:HB2	1.82	0.45
2:B:247:PRO:HG2	2:B:249:LEU:HD22	1.99	0.45
1:A:161:LYS:HE2	1:A:161:LYS:HB3	1.69	0.45
2:B:336:LYS:HE3	2:B:338:GLU:OE2	2.17	0.45
1:A:46:ASN:HD21	1:A:54:ALA:HB1	1.82	0.44
1:A:96:GLU:HG3	1:A:97:ILE:CD1	2.48	0.44
2:B:378:ASN:N	2:B:378:ASN:HD22	2.05	0.44
2:B:424:PRO:HG3	2:B:484:ILE:CD1	2.46	0.44
1:A:46:ASN:ND2	1:A:54:ALA:HB1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASN:CG	1:A:157:GLU:HG3	2.38	0.44
2:B:237:GLU:O	2:B:240:THR:HB	2.18	0.44
2:B:247:PRO:CG	2:B:249:LEU:HD22	2.48	0.44
2:B:567:ARG:HD3	2:B:601:TYR:CE1	2.54	0.43
1:A:47:ILE:HD13	2:B:362:THR:HG22	2.00	0.43
1:A:66:THR:HA	1:A:67:PRO:HD3	1.83	0.43
2:B:396:THR:O	2:B:399:GLN:HG3	2.19	0.43
2:B:439:MET:SD	2:B:439:MET:C	2.97	0.43
2:B:427:ILE:HA	2:B:457:GLY:HA3	2.00	0.43
2:B:394:ILE:HD12	2:B:490:SER:HB2	2.01	0.43
2:B:218:LYS:HE2	5:B:990:HOH:O	2.19	0.42
2:B:512:LEU:N	2:B:512:LEU:HD12	2.34	0.42
5:A:469:HOH:O	2:B:436:ASN:HB2	2.18	0.42
2:B:500:ASN:ND2	2:B:577:LEU:HB2	2.34	0.42
2:B:240:THR:HG22	2:B:241:SER:N	2.33	0.42
2:B:414:VAL:HG21	2:B:502:SER:CB	2.49	0.42
2:B:567:ARG:HG3	2:B:567:ARG:HH11	1.85	0.42
1:A:156:GLU:OE1	1:A:156:GLU:N	2.52	0.42
2:B:435:SER:HA	2:B:474:ASP:O	2.19	0.42
1:A:104:SER:HB3	3:A:301:MRD:HMC1	2.01	0.42
2:B:512:LEU:HB2	2:B:538:LEU:CD2	2.50	0.41
2:B:206:ILE:N	2:B:206:ILE:HD12	2.35	0.41
1:A:69:TYR:CD1	1:A:140:LEU:HD13	2.54	0.41
2:B:412:THR:HG23	2:B:472:PHE:HA	2.02	0.41
1:A:165:PHE:HB2	2:B:368:ILE:HD13	2.02	0.41
2:B:517:THR:O	2:B:621:ARG:HD3	2.20	0.41
2:B:273:ARG:NE	5:B:818:HOH:O	2.40	0.41
2:B:415:TYR:CE1	2:B:496:ARG:HB2	2.55	0.41
1:A:30:ARG:HA	1:A:176:LYS:O	2.21	0.41
2:B:275:ASN:O	2:B:279:ASN:HA	2.21	0.41
1:A:60:ARG:C	5:A:407:HOH:O	2.59	0.41
2:B:538:LEU:O	2:B:600:THR:HA	2.20	0.41
2:B:257:PHE:CZ	2:B:259:THR:HB	2.56	0.40
2:B:251:ASN:O	2:B:285:THR:HA	2.22	0.40
2:B:416:LYS:HA	2:B:467:LEU:O	2.22	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	168/224 (75%)	156 (93%)	9 (5%)	3 (2%)	11	19
2	B	418/420 (100%)	397 (95%)	19 (4%)	2 (0%)	34	57
All	All	586/644 (91%)	553 (94%)	28 (5%)	5 (1%)	21	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	546	ASN
1	A	65	ALA
2	B	505	ALA
1	A	155	SER
1	A	60	ARG

### 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	153/207 (74%)	150 (98%)	3 (2%)	63	85
2	B	385/385 (100%)	376 (98%)	9 (2%)	58	81
All	All	538/592 (91%)	526 (98%)	12 (2%)	60	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE

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Mol	Chain	Res	Type
1	A	21	LEU
1	A	130	LEU
2	B	249	LEU
2	B	279	ASN
2	B	357	ASP
2	B	378	ASN
2	B	408	LYS
2	B	503	ASP
2	B	545	ASN
2	B	553	SER
2	B	596	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	46	ASN
1	A	50	ASN
1	A	85	GLN
2	B	226	ASN
2	B	279	ASN
2	B	378	ASN
2	B	399	GLN
2	B	401	ASN
2	B	422	ASN
2	B	483	GLN
2	B	545	ASN
2	B	558	ASN
2	B	612	ASN
2	B	614	ASN

### 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

3 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	$\# Z  > 2$
4	SIA	B	701	4	17,20,21	0.50	0	18,28,31	0.80	0
4	GAL	B	702	4	11,11,12	0.49	0	15,15,17	0.34	0
4	NAG	B	703	4	15,15,15	0.54	0	17,21,21	0.56	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
4	SIA	B	701	4	-	0/14/34/38	0/1/1/1
4	GAL	B	702	4	-	0/2/19/22	0/1/1/1
4	NAG	B	703	4	-	0/6/26/26	0/1/1/1

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	SIA	1	0
4	B	702	GAL	1	0
4	B	703	NAG	3	0



## 5.6 Ligand geometry

5 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	MRD	A	301	-	6,7,7	0.35	0	6,10,10	0.39	0
3	MRD	A	302	-	6,7,7	0.24	0	6,10,10	0.20	0
3	MRD	A	303	-	6,7,7	0.28	0	6,10,10	0.24	0
3	MRD	B	704	-	6,7,7	0.32	0	6,10,10	0.28	0
3	MRD	B	705	-	6,7,7	0.28	0	6,10,10	0.21	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
3	MRD	A	301	-	-	0/5/5/5	0/0/0/0
3	MRD	A	302	-	-	0/5/5/5	0/0/0/0
3	MRD	A	303	-	-	0/5/5/5	0/0/0/0
3	MRD	B	704	-	-	0/5/5/5	0/0/0/0
3	MRD	B	705	-	-	0/5/5/5	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.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	MRD	3	0
3	A	302	MRD	1	0
3	A	303	MRD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	705	MRD	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 [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, 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	170/224 (75%)	-0.38	3 (1%) 71 66	27, 48, 78, 94	0
2	B	420/420 (100%)	-0.49	4 (0%) 84 81	28, 49, 74, 92	0
All	All	590/644 (91%)	-0.46	7 (1%) 81 78	27, 49, 77, 94	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	572	ILE	3.8
2	B	573	ASN	3.0
2	B	204	GLN	2.5
1	A	16	ILE	2.3
1	A	184	ASP	2.1
2	B	205	THR	2.1
1	A	156	GLU	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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SIA	B	701	20/21	0.94	0.13	-0.37	48,55,59,59	20

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	703	15/15	0.74	0.37	-	83,88,89,90	15
4	GAL	B	702	11/12	0.83	0.30	-	63,78,81,81	11

## 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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MRD	A	301	8/8	0.89	0.35	9.18	63,64,66,66	0
3	MRD	B	705	8/8	0.84	0.44	8.11	73,74,75,77	8
3	MRD	A	302	8/8	0.80	0.41	7.12	72,72,73,76	8
3	MRD	A	303	8/8	0.89	0.29	4.51	73,74,75,76	8
3	MRD	B	704	8/8	0.92	0.17	1.98	64,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.