



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2020 – 07:35 AM EDT

PDB ID : 6W3H  
Title : Brain delivery of therapeutic proteins using an Fc fragment blood-brain barrier transport vehicle in mice and monkeys  
Authors : Srivastava, A.; Kariolis, M.; Wells, R.  
Deposited on : 2020-03-09  
Resolution : 3.38 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.10.1
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.10.1

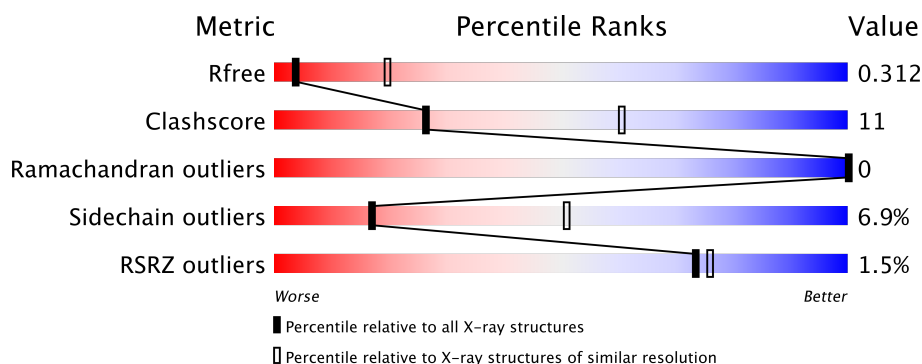
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.38 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))
$R_{free}$	111664	1421 (3.46-3.30)
Clashscore	122126	1489 (3.46-3.30)
Ramachandran outliers	120053	1466 (3.46-3.30)
Sidechain outliers	120020	1465 (3.46-3.30)
RSRZ outliers	108989	1374 (3.46-3.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	
1	B	227	
2	C	166	
2	D	166	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5251 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 ATV Fc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1623	1040	263	315	5			
1	B	190	Total	C	N	O	S	0	0	0
			1464	941	237	281	5			

- Molecule 2 is a protein called Transferrin receptor protein 1,Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	144	Total	C	N	O	S	0	0	0
			1006	627	173	202	4			
2	D	147	Total	C	N	O	S	0	0	0
			1069	678	184	202	5			

There are 18 discrepancies between the modelled and reference sequences:

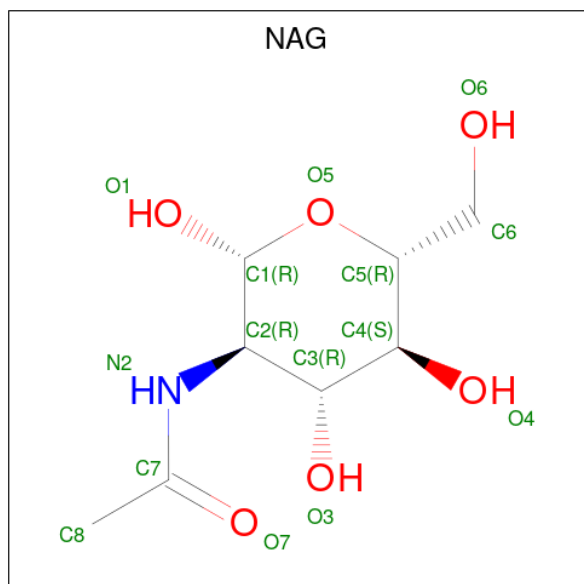
Chain	Residue	Modelled	Actual	Comment	Reference
C	21	THR	-	expression tag	UNP P02786
C	179	ALA	-	linker	UNP P02786
C	180	SER	-	linker	UNP P02786
C	181	HIS	-	expression tag	UNP P02786
C	182	HIS	-	expression tag	UNP P02786
C	183	HIS	-	expression tag	UNP P02786
C	184	HIS	-	expression tag	UNP P02786
C	185	HIS	-	expression tag	UNP P02786
C	186	HIS	-	expression tag	UNP P02786
D	21	THR	-	expression tag	UNP P02786
D	179	ALA	-	linker	UNP P02786
D	180	SER	-	linker	UNP P02786
D	181	HIS	-	expression tag	UNP P02786
D	182	HIS	-	expression tag	UNP P02786
D	183	HIS	-	expression tag	UNP P02786
D	184	HIS	-	expression tag	UNP P02786

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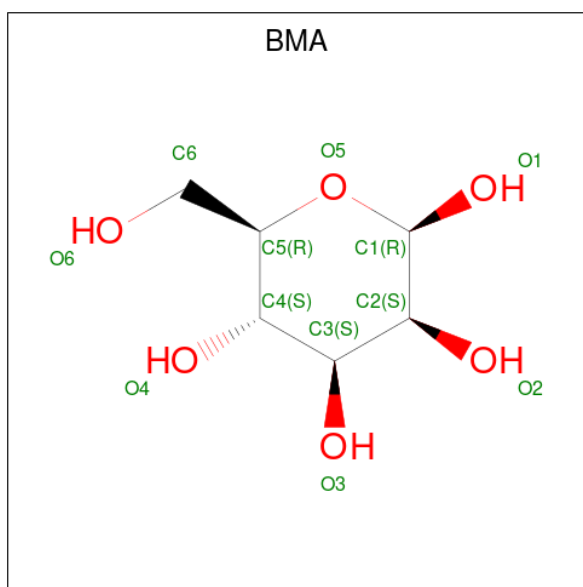
Chain	Residue	Modelled	Actual	Comment	Reference
D	185	HIS	-	expression tag	UNP P02786
D	186	HIS	-	expression tag	UNP P02786

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



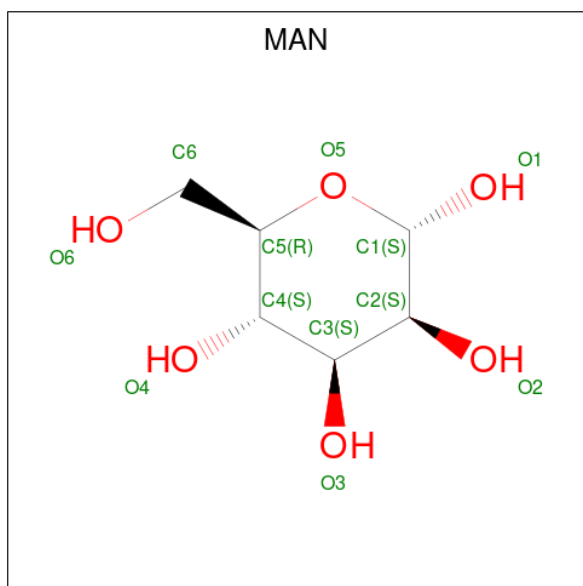
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

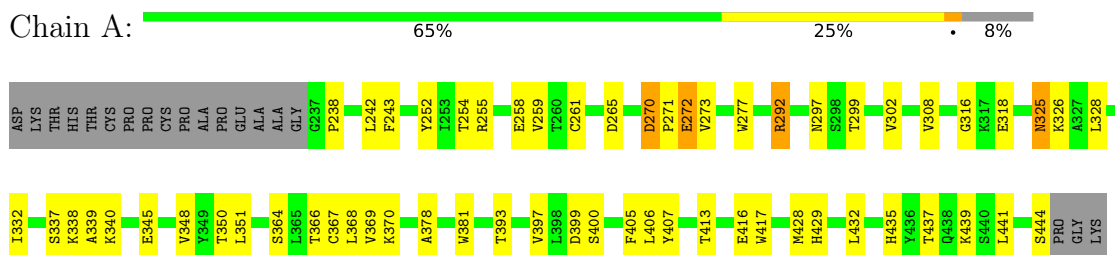


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

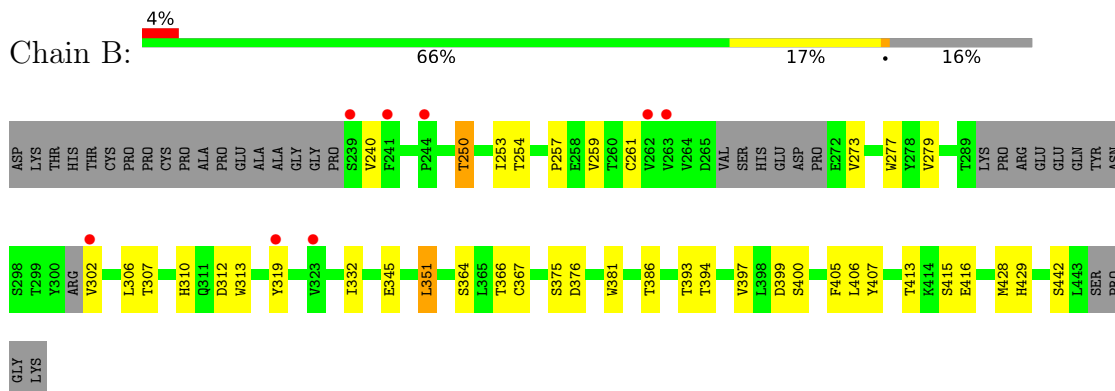
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

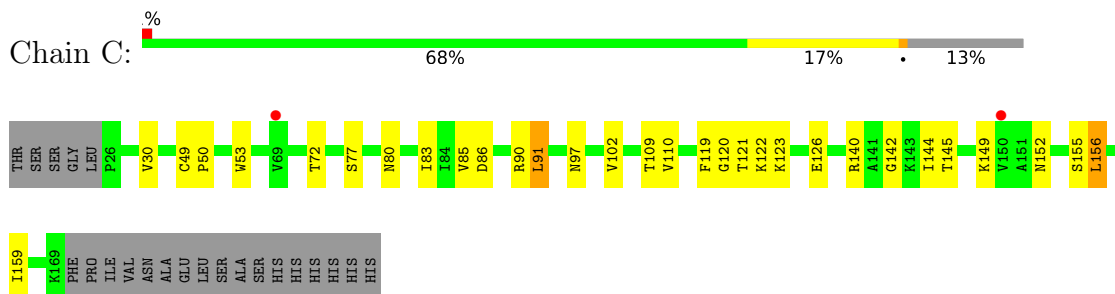
- Molecule 1: ATV Fc



- Molecule 1: ATV Fc

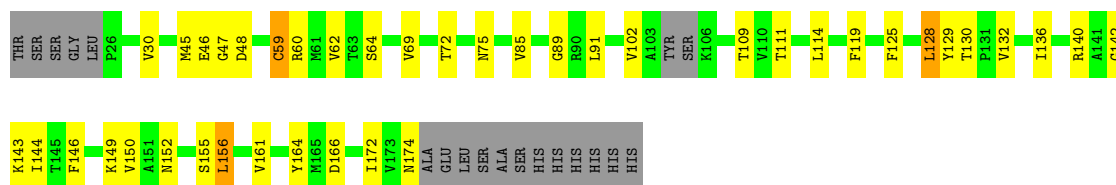


- Molecule 2: Transferrin receptor protein 1,Transferrin receptor protein 1



- Molecule 2: Transferrin receptor protein 1,Transferrin receptor protein 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.37Å 126.37Å 113.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.30 – 3.38 55.24 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.8 (55.30-3.38) 99.8 (55.24-3.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.238 , 0.318 0.236 , 0.312	Depositor DCC
$R_{free}$ test set	657 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.2	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	0.66	0/1670	0.81	0/2284
1	B	0.66	0/1504	0.79	0/2057
2	C	0.67	0/1020	0.87	0/1396
2	D	0.67	0/1085	0.94	0/1477
All	All	0.67	0/5279	0.84	0/7214

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 [i](#)

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	1623	0	1534	41	0
1	B	1464	0	1363	24	0
2	C	1006	0	923	28	0
2	D	1069	0	1057	25	0
3	A	56	0	50	3	0
4	A	11	0	8	0	0
5	A	22	0	18	1	0
All	All	5251	0	4953	113	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 11.

All (113) 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:B:273:VAL:HG21	1:B:302:VAL:HG11	1.70	0.73
2:C:119:PHE:HD2	2:C:142:GLY:HA3	1.54	0.72
2:D:30:VAL:HG21	2:D:150:VAL:HG21	1.75	0.69
1:B:240:VAL:HG21	1:B:332:ILE:HD11	1.75	0.67
2:C:72:THR:HG23	2:C:109:THR:HG22	1.74	0.67
3:A:502:NAG:H82	5:A:504:MAN:O4	1.94	0.67
2:C:119:PHE:CD2	2:C:142:GLY:HA3	2.29	0.66
2:D:30:VAL:HG22	2:D:161:VAL:HB	1.77	0.65
2:D:59:CYS:SG	2:D:59:CYS:O	2.55	0.64
2:D:30:VAL:HG21	2:D:150:VAL:CG2	2.27	0.64
1:A:413:THR:HG23	1:A:416:GLU:HG3	1.81	0.63
1:A:351:LEU:N	1:A:351:LEU:HD12	2.14	0.63
1:A:238:PRO:HA	1:A:265:ASP:O	2.01	0.60
2:D:69:VAL:HG13	2:D:136:ILE:HD12	1.84	0.60
1:A:328:LEU:HD21	1:A:332:ILE:HD12	1.84	0.60
1:A:413:THR:CG2	1:A:416:GLU:HG3	2.32	0.60
2:D:45:MET:HE3	2:D:114:LEU:HB3	1.84	0.59
2:C:30:VAL:HG13	2:C:102:VAL:HG11	1.84	0.59
2:C:83:ILE:HD12	2:C:91:LEU:HD13	1.85	0.58
1:A:366:THR:HG23	1:B:407:TYR:CZ	2.39	0.58
2:C:121:THR:HG22	2:C:123:LYS:H	1.68	0.58
1:A:350:THR:C	1:A:351:LEU:HD12	2.25	0.57
1:A:318:GLU:HA	1:A:337:SER:HB3	1.86	0.57
1:A:252:TYR:HB2	1:A:255:ARG:HG3	1.87	0.55
1:A:397:VAL:HB	1:A:405:PHE:CE1	2.41	0.55
2:D:125:PHE:HE1	2:D:132:VAL:HG21	1.71	0.55
1:A:316:GLY:O	1:A:340:LYS:HE3	2.08	0.54
1:A:368:LEU:HD23	1:A:368:LEU:C	2.29	0.53
2:C:91:LEU:HD22	1:B:386:THR:HB	1.90	0.53
1:B:257:PRO:HD3	1:B:310:HIS:NE2	2.23	0.52
2:D:152:ASN:O	2:D:156:LEU:HD12	2.09	0.52
1:A:345:GLU:HG3	1:A:432:LEU:HD23	1.91	0.52
2:C:122:LYS:H	2:C:122:LYS:HD2	1.73	0.52
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.45	0.52
1:A:297:ASN:OD1	1:A:299:THR:OG1	2.17	0.52
2:C:120:GLY:O	2:C:152:ASN:ND2	2.36	0.51
2:C:53:TRP:N	2:C:53:TRP:CD1	2.77	0.51
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ILE:HA	1:B:310:HIS:CE1	2.46	0.51
2:D:140:ARG:HD3	2:D:166:ASP:OD2	2.11	0.51
1:A:272:GLU:O	1:A:325:ASN:ND2	2.44	0.51
2:D:85:VAL:CG1	2:D:89:GLY:HA2	2.41	0.50
2:C:126:GLU:HA	2:C:126:GLU:OE1	2.10	0.50
1:B:397:VAL:HB	1:B:405:PHE:CE1	2.45	0.50
1:A:242:LEU:HD11	1:A:259:VAL:CG1	2.42	0.50
1:A:243:PHE:HD2	3:A:506:NAG:H62	1.76	0.50
1:B:413:THR:OG1	1:B:416:GLU:HG3	2.11	0.50
2:D:47:GLY:O	2:D:60:ARG:CD	2.60	0.50
1:B:351:LEU:HD12	1:B:366:THR:HB	1.93	0.49
2:C:144:ILE:HG22	2:C:145:THR:O	2.11	0.49
1:A:243:PHE:CD2	3:A:506:NAG:H62	2.46	0.49
2:D:174:ASN:N	2:D:174:ASN:OD1	2.45	0.49
2:C:85:VAL:HA	2:C:90:ARG:O	2.13	0.49
1:A:270:ASP:OD2	1:A:326:LYS:CB	2.61	0.48
1:B:279:VAL:HG22	1:B:319:TYR:CD1	2.48	0.48
2:D:140:ARG:HG2	2:D:164:TYR:CZ	2.48	0.48
2:D:125:PHE:CE1	2:D:132:VAL:HG21	2.49	0.48
2:D:62:VAL:HG11	2:D:130:THR:HG21	1.95	0.48
2:C:30:VAL:HG22	2:C:102:VAL:HG21	1.95	0.48
2:C:122:LYS:H	2:C:122:LYS:CD	2.26	0.47
2:C:152:ASN:O	2:C:156:LEU:HD12	2.14	0.47
2:C:80:ASN:O	2:C:97:ASN:ND2	2.47	0.47
2:C:121:THR:HA	2:C:144:ILE:HD11	1.97	0.47
2:C:30:VAL:CG1	2:C:102:VAL:HG11	2.46	0.46
2:C:119:PHE:CE2	2:C:140:ARG:HG3	2.50	0.46
2:C:122:LYS:HD2	2:C:122:LYS:N	2.30	0.46
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.51	0.46
1:A:366:THR:HG21	1:B:407:TYR:CE1	2.50	0.46
1:A:417:TRP:HH2	1:A:441:LEU:HD11	1.81	0.46
1:A:271:PRO:HB2	1:A:292:ARG:NH1	2.31	0.46
1:A:297:ASN:O	1:A:299:THR:HG23	2.15	0.46
2:C:144:ILE:O	2:C:149:LYS:HE2	2.16	0.46
1:B:393:THR:HG23	1:B:406:LEU:HD13	1.98	0.45
2:D:30:VAL:HG12	2:D:102:VAL:HG21	1.98	0.45
2:D:47:GLY:O	2:D:60:ARG:HD2	2.17	0.45
2:D:47:GLY:O	2:D:60:ARG:HD3	2.17	0.45
1:B:406:LEU:HD12	1:B:406:LEU:C	2.36	0.45
2:D:128:LEU:HD12	2:D:129:TYR:N	2.31	0.44
1:A:429:HIS:O	1:A:435:HIS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TYR:CB	1:A:255:ARG:HG3	2.48	0.44
1:B:259:VAL:HG23	1:B:306:LEU:HB3	1.99	0.44
2:C:110:VAL:HG11	2:C:159:ILE:HG13	2.00	0.44
1:A:393:THR:HG23	1:A:406:LEU:HD13	2.01	0.43
2:C:86:ASP:HB3	2:C:90:ARG:H	1.82	0.43
1:A:273:VAL:HG21	1:A:302:VAL:HG11	1.99	0.43
2:D:119:PHE:CD1	2:D:142:GLY:HA3	2.53	0.43
2:D:140:ARG:CD	2:D:166:ASP:OD2	2.67	0.43
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.53	0.43
1:B:376:ASP:O	1:B:429:HIS:HD2	2.02	0.43
2:C:119:PHE:CE1	2:C:140:ARG:HD3	2.54	0.43
2:C:49:CYS:HA	2:C:50:PRO:HD3	1.87	0.43
1:B:279:VAL:HG22	1:B:319:TYR:CE1	2.54	0.43
1:B:351:LEU:HD12	1:B:366:THR:CG2	2.49	0.42
2:D:72:THR:OG1	2:D:109:THR:HG23	2.18	0.42
1:A:338:LYS:NZ	1:A:339:ALA:O	2.47	0.42
1:B:406:LEU:HD12	1:B:407:TYR:N	2.34	0.42
1:A:368:LEU:HD21	1:A:370:LYS:HB3	2.00	0.42
1:A:259:VAL:HG23	1:A:308:VAL:HG11	2.00	0.42
1:A:406:LEU:HD12	1:A:406:LEU:C	2.39	0.42
1:B:250:THR:HG21	1:B:313:TRP:CD1	2.55	0.42
1:A:397:VAL:HG21	1:B:394:THR:HA	2.02	0.42
1:A:348:VAL:O	1:A:439:LYS:HG3	2.20	0.41
2:D:143:LYS:O	2:D:172:ILE:HA	2.20	0.41
1:A:368:LEU:HD23	1:A:369:VAL:N	2.34	0.41
2:C:86:ASP:HB2	2:C:90:ARG:HB2	2.02	0.41
1:A:366:THR:HG23	1:B:407:TYR:OH	2.20	0.41
2:D:144:ILE:O	2:D:149:LYS:HE2	2.20	0.41
2:D:146:PHE:O	2:D:150:VAL:HG23	2.21	0.40
1:A:366:THR:CG2	1:B:407:TYR:CE1	3.04	0.40
1:A:406:LEU:HD12	1:A:407:TYR:N	2.36	0.40
1:A:351:LEU:N	1:A:351:LEU:CD1	2.81	0.40
1:A:378:ALA:HB3	1:A:428:MET:HB2	2.02	0.40
2:C:90:ARG:HG3	2:C:90:ARG:HH11	1.86	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	206/227 (91%)	205 (100%)	1 (0%)	0	100	100
1	B	182/227 (80%)	180 (99%)	2 (1%)	0	100	100
2	C	142/166 (86%)	136 (96%)	6 (4%)	0	100	100
2	D	143/166 (86%)	139 (97%)	4 (3%)	0	100	100
All	All	673/786 (86%)	660 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	181/207 (87%)	170 (94%)	11 (6%)	20	55
1	B	160/207 (77%)	147 (92%)	13 (8%)	13	42
2	C	98/140 (70%)	94 (96%)	4 (4%)	33	66
2	D	112/140 (80%)	102 (91%)	10 (9%)	11	37
All	All	551/694 (79%)	513 (93%)	38 (7%)	17	51

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	THR
1	A	258	GLU

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Mol	Chain	Res	Type
1	A	270	ASP
1	A	272	GLU
1	A	292	ARG
1	A	325	ASN
1	A	364	SER
1	A	399	ASP
1	A	400	SER
1	A	437	THR
1	A	444	SER
2	C	77	SER
2	C	91	LEU
2	C	155	SER
2	C	156	LEU
2	D	46	GLU
2	D	48	ASP
2	D	59	CYS
2	D	64	SER
2	D	75	ASN
2	D	91	LEU
2	D	111	THR
2	D	128	LEU
2	D	155	SER
2	D	156	LEU
1	B	250	THR
1	B	254	THR
1	B	307	THR
1	B	312	ASP
1	B	345	GLU
1	B	351	LEU
1	B	364	SER
1	B	375	SER
1	B	399	ASP
1	B	400	SER
1	B	415	SER
1	B	428	MET
1	B	442	SER

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 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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	NAG	A	507	5	14,14,15	0.74	0	17,19,21	1.84	6 (35%)
3	NAG	A	502	3,4	14,14,15	0.73	0	17,19,21	1.25	3 (17%)
5	MAN	A	505	3,4	11,11,12	0.57	0	15,15,17	1.96	5 (33%)
3	NAG	A	506	5	14,14,15	0.45	0	17,19,21	1.93	6 (35%)
3	NAG	A	501	1,3	14,14,15	0.88	1 (7%)	17,19,21	1.85	5 (29%)
5	MAN	A	504	3,4	11,11,12	0.65	0	15,15,17	1.81	4 (26%)
4	BMA	A	503	3,5	11,11,12	0.84	1 (9%)	15,15,17	1.96	6 (40%)

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	NAG	A	507	5	-	1/6/23/26	0/1/1/1
3	NAG	A	502	3,4	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	A	505	3,4	-	2/2/19/22	0/1/1/1
3	NAG	A	506	5	-	3/6/23/26	0/1/1/1
3	NAG	A	501	1,3	-	2/6/23/26	0/1/1/1
5	MAN	A	504	3,4	-	0/2/19/22	0/1/1/1
4	BMA	A	503	3,5	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	BMA	C2-C3	2.19	1.55	1.52
3	A	501	NAG	C4-C5	2.16	1.57	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	NAG	C1-C2-N2	-4.78	102.33	110.49
5	A	505	MAN	O2-C2-C3	-4.43	101.26	110.14
3	A	501	NAG	C4-C3-C2	-3.78	105.47	111.02
4	A	503	BMA	C6-C5-C4	-3.52	104.77	113.00
5	A	504	MAN	C2-C3-C4	-3.47	104.88	110.89
3	A	507	NAG	C1-C2-N2	3.47	116.42	110.49
4	A	503	BMA	O3-C3-C2	3.43	116.57	109.99
5	A	504	MAN	O3-C3-C2	-3.15	103.97	109.99
5	A	504	MAN	O3-C3-C4	3.11	117.54	110.35
5	A	505	MAN	O3-C3-C2	-3.01	104.23	109.99
3	A	507	NAG	C4-C3-C2	2.97	115.38	111.02
5	A	505	MAN	C1-C2-C3	2.94	113.28	109.67
4	A	503	BMA	C2-C3-C4	-2.85	105.97	110.89
3	A	506	NAG	O5-C1-C2	-2.84	106.80	111.29
3	A	507	NAG	C3-C4-C5	2.83	115.29	110.24
3	A	507	NAG	O5-C5-C6	2.82	111.63	107.20
3	A	501	NAG	O6-C6-C5	2.81	120.94	111.29
3	A	501	NAG	C1-O5-C5	2.67	115.81	112.19
3	A	506	NAG	C6-C5-C4	-2.66	106.77	113.00
4	A	503	BMA	O5-C5-C6	2.62	111.31	107.20
3	A	507	NAG	O3-C3-C2	-2.57	104.15	109.47
3	A	506	NAG	O7-C7-N2	2.57	126.67	121.95
5	A	505	MAN	O5-C1-C2	-2.53	106.87	110.77
3	A	501	NAG	O4-C4-C5	2.49	115.49	109.30
3	A	502	NAG	C3-C4-C5	-2.49	105.80	110.24
3	A	501	NAG	O5-C1-C2	-2.47	107.38	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	MAN	O5-C1-C2	-2.46	106.97	110.77
3	A	507	NAG	C1-O5-C5	-2.45	108.87	112.19
3	A	506	NAG	C4-C3-C2	-2.44	107.44	111.02
3	A	502	NAG	O3-C3-C4	2.43	115.96	110.35
4	A	503	BMA	O3-C3-C4	-2.41	104.78	110.35
5	A	505	MAN	C3-C4-C5	2.33	114.39	110.24
3	A	502	NAG	O5-C1-C2	-2.32	107.62	111.29
4	A	503	BMA	O5-C1-C2	-2.12	107.49	110.77
3	A	506	NAG	O7-C7-C8	-2.01	118.32	122.06

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	NAG	O5-C5-C6-O6
3	A	506	NAG	C4-C5-C6-O6
5	A	505	MAN	C4-C5-C6-O6
4	A	503	BMA	O5-C5-C6-O6
3	A	507	NAG	O5-C5-C6-O6
3	A	506	NAG	C8-C7-N2-C2
3	A	501	NAG	C4-C5-C6-O6
5	A	505	MAN	O5-C5-C6-O6
3	A	501	NAG	C8-C7-N2-C2
3	A	502	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	1	0
3	A	506	NAG	2	0
5	A	504	MAN	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	208/227 (91%)	0.09	0 <span>100</span> <span>100</span>	57, 71, 112, 132	1 (0%)
1	B	190/227 (83%)	0.29	8 (4%) <span>36</span> <span>39</span>	51, 74, 129, 139	0
2	C	144/166 (86%)	0.30	2 (1%) <span>75</span> <span>78</span>	62, 89, 125, 143	0
2	D	147/166 (88%)	0.08	0 <span>100</span> <span>100</span>	55, 73, 111, 133	0
All	All	689/786 (87%)	0.19	10 (1%) <span>73</span> <span>76</span>	51, 76, 124, 143	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	VAL	3.5
1	B	239	SER	3.5
1	B	262	VAL	3.4
1	B	302	VAL	2.9
1	B	323	VAL	2.5
1	B	319	TYR	2.3
2	C	150	VAL	2.3
1	B	241	PHE	2.2
1	B	244	PRO	2.1
2	C	69	VAL	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	501	14/15	0.71	0.23	82,92,97,99	0
3	NAG	A	507	14/15	0.83	0.22	91,98,100,102	0
3	NAG	A	502	14/15	0.89	0.23	79,86,91,95	0
3	NAG	A	506	14/15	0.90	0.20	71,78,93,95	0
5	MAN	A	505	11/12	0.90	0.14	84,86,90,95	0
5	MAN	A	504	11/12	0.92	0.17	80,84,88,89	0
4	BMA	A	503	11/12	0.93	0.15	77,78,81,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.