



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 04:41 pm GMT

PDB ID : 1FC1  
Title : CRYSTALLOGRAPHIC REFINEMENT AND ATOMIC MODELS OF A HUMAN FC FRAGMENT AND ITS COMPLEX WITH FRAGMENT B OF PROTEIN A FROM STAPHYLOCOCCUS AUREUS AT 2.9-AND 2.8-ANGSTROMS RESOLUTION  
Authors : Deisenhofer, J.  
Deposited on : 1981-05-21  
Resolution : 2.90 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

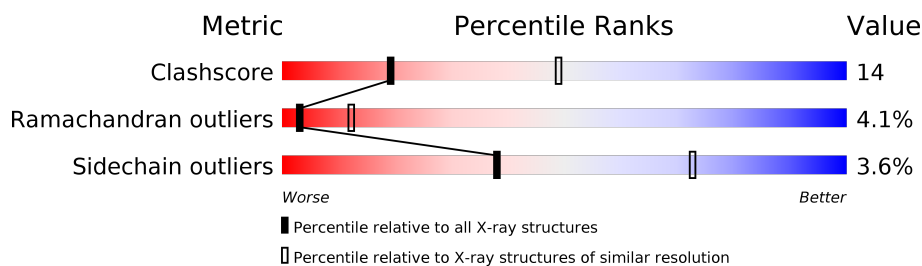
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122078	1924 (2.90-2.90)
Ramachandran outliers	120005	1884 (2.90-2.90)
Sidechain outliers	119972	1886 (2.90-2.90)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	224	
1	B	224	

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	FUC	A	2	X	-	-	-
3	FUC	B	2	X	-	-	-
4	MAN	A	4	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	B	4	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3532 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 FC FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	60	0	1
			1656	1054	282	313	7			
1	B	207	Total	C	N	O	S	217	0	1
			1656	1054	282	313	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	GLN	GLU	CONFLICT	UNP P01857
A	283	GLN	GLU	CONFLICT	UNP P01857
A	294	GLN	GLU	CONFLICT	UNP P01857
A	312	ASN	ASP	CONFLICT	UNP P01857
A	315	ASP	ASN	CONFLICT	UNP P01857
A	356	GLU	ASP	CONFLICT	UNP P01857
A	358	MET	LEU	CONFLICT	UNP P01857
B	272	GLN	GLU	CONFLICT	UNP P01857
B	283	GLN	GLU	CONFLICT	UNP P01857
B	294	GLN	GLU	CONFLICT	UNP P01857
B	312	ASN	ASP	CONFLICT	UNP P01857
B	315	ASP	ASN	CONFLICT	UNP P01857
B	356	GLU	ASP	CONFLICT	UNP P01857
B	358	MET	LEU	CONFLICT	UNP P01857

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



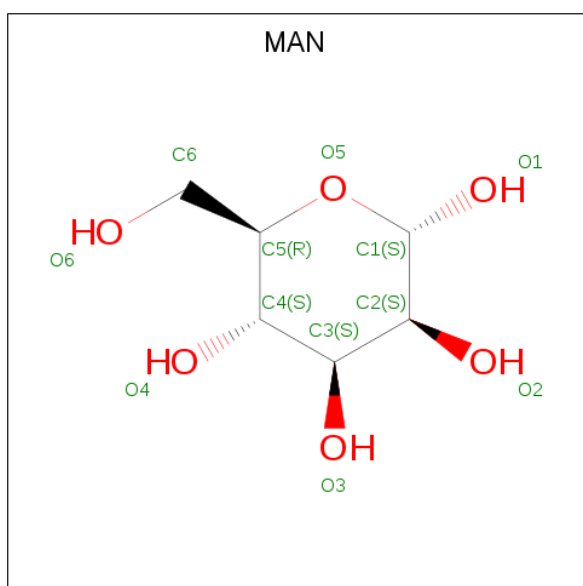
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	3	0
			14	8	1	5		
2	A	1	Total	C	N	O	8	0
			14	8	1	5		
2	B	1	Total	C	N	O	14	0
			14	8	1	5		
2	B	1	Total	C	N	O	1	0
			14	8	1	5		
2	B	1	Total	C	N	O	4	0
			14	8	1	5		
2	B	1	Total	C	N	O	14	0
			14	8	1	5		

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	4	0
			10	6	4		
3	B	1	Total	C	O	10	0
			10	6	4		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



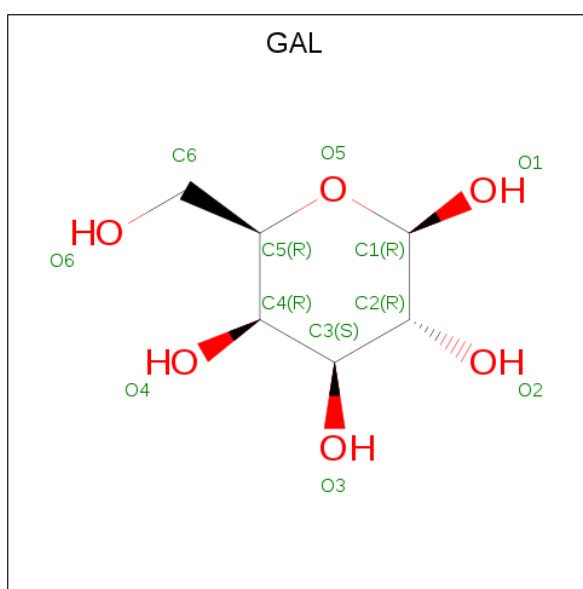
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	3	0
			11	6	5		
4	B	1	Total	C	O	1	0
			11	6	5		
4	B	1	Total	C	O	3	0
			11	6	5		
4	B	1	Total	C	O	3	0
			11	6	5		

- Molecule 5 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



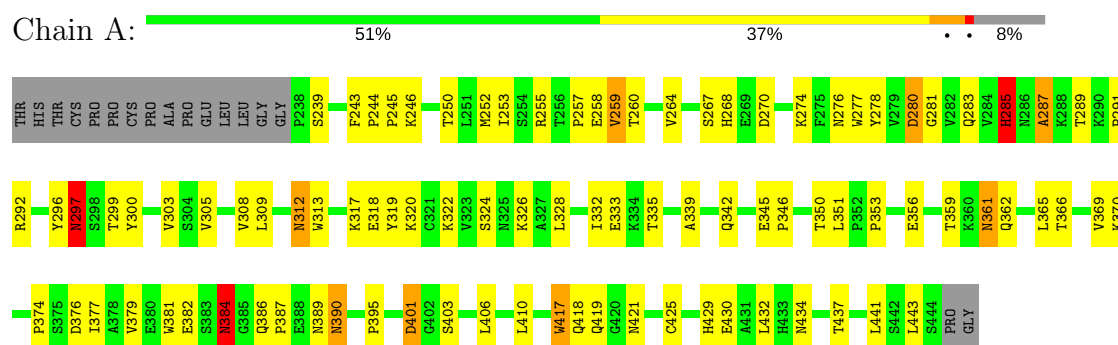
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	5	0
			11	6	5		

### 3 Residue-property plots [i](#)

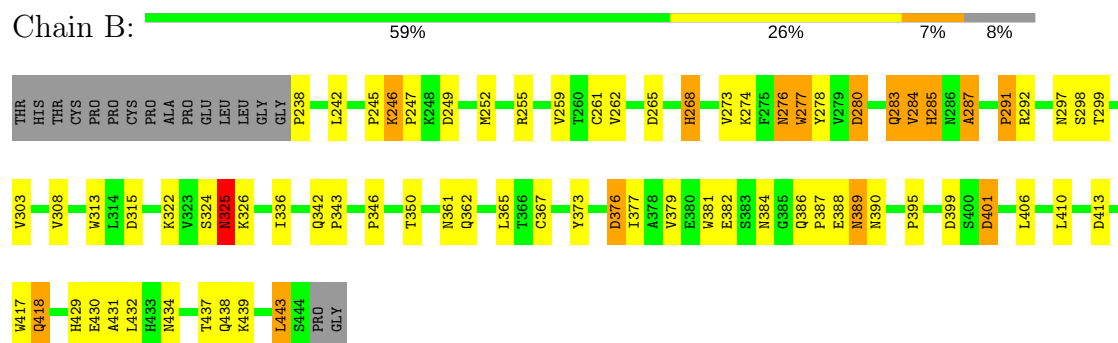
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: FC FRAGMENT



#### • Molecule 1: FC FRAGMENT





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.40Å 146.40Å 50.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, GAL, 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	1.01	4/1702 (0.2%)	1.22	2/2318 (0.1%)
1	B	1.01	4/1702 (0.2%)	1.21	1/2318 (0.0%)
All	All	1.01	8/3404 (0.2%)	1.22	3/4636 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17
1	B	0	22
All	All	0	39

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	TRP	NE1-CE2	-7.99	1.27	1.37
1	A	277	TRP	NE1-CE2	-7.94	1.27	1.37
1	B	277	TRP	NE1-CE2	-7.76	1.27	1.37
1	B	313	TRP	NE1-CE2	-7.71	1.27	1.37
1	A	417	TRP	NE1-CE2	-7.63	1.27	1.37
1	A	313	TRP	NE1-CE2	-7.57	1.27	1.37
1	B	417	TRP	NE1-CE2	-7.53	1.27	1.37
1	A	381	TRP	NE1-CE2	-7.30	1.28	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	ASP	CB-CA-C	-5.71	98.98	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASN	N-CA-CB	-5.52	100.66	110.60
1	A	285	HIS	CA-CB-CG	-5.42	104.39	113.60

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	VAL	Mainchain
1	A	276	ASN	Sidechain
1	A	280	ASP	Mainchain
1	A	287	ALA	Mainchain
1	A	309	LEU	Mainchain
1	A	312	ASN	Sidechain
1	A	318	GLU	Sidechain
1	A	342	GLN	Sidechain
1	A	361	ASN	Sidechain
1	A	362	GLN	Sidechain
1	A	376	ASP	Sidechain
1	A	382	GLU	Sidechain
1	A	384	ASN	Mainchain
1	A	401	ASP	Mainchain
1	A	417	TRP	Mainchain
1	A	419	GLN	Sidechain
1	A	430	GLU	Sidechain
1	B	246	LYS	Mainchain
1	B	249	ASP	Sidechain
1	B	268	HIS	Mainchain
1	B	276	ASN	Sidechain
1	B	280	ASP	Sidechain
1	B	283	GLN	Sidechain
1	B	287	ALA	Mainchain
1	B	298	SER	Mainchain
1	B	315	ASP	Sidechain,Mainchain
1	B	325	ASN	Sidechain
1	B	342	GLN	Sidechain
1	B	376	ASP	Sidechain
1	B	382	GLU	Sidechain
1	B	388	GLU	Sidechain
1	B	389	ASN	Mainchain
1	B	399	ASP	Sidechain
1	B	401	ASP	Mainchain
1	B	413	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	B	418	GLN	Sidechain
1	B	438	GLN	Sidechain
1	B	443	LEU	Mainchain

## 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	1656	0	1629	51	4
1	B	1656	0	1629	36	1
2	A	56	0	48	2	0
2	B	56	0	48	0	0
3	A	10	0	10	0	0
3	B	10	0	10	0	0
4	A	33	0	26	0	0
4	B	33	0	26	0	0
5	A	11	0	10	3	0
5	B	11	0	10	1	0
All	All	3532	0	3446	86	4

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 14.

All (86) 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:274:LYS:HB3	1:B:324:SER:HB2	1.47	0.96
1:A:297:ASN:HB3	1:A:299:THR:HG22	1.61	0.81
1:A:328:LEU:HD21	1:A:332:ILE:HG13	1.64	0.77
1:A:250:THR:HG22	1:A:257:PRO:HB3	1.68	0.76
1:A:296:TYR:HD2	2:A:1:NAG:H62	1.52	0.75
1:A:432:LEU:HD13	1:A:437:THR:HG22	1.71	0.73
1:B:346:PRO:HD3	1:B:429:HIS:HD2	1.53	0.72
1:A:258:GLU:HG3	5:A:7:GAL:H62	1.71	0.71
1:A:418:GLN:HA	1:A:443:LEU:HD22	1.72	0.70
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LYS:HG3	5:B:7:GAL:H5	1.75	0.69
1:A:296:TYR:CD2	2:A:1:NAG:H62	2.29	0.68
1:B:283:GLN:HG2	1:B:285:HIS:H	1.61	0.65
1:B:238:PRO:HA	1:B:265:ASP:HB2	1.79	0.65
1:B:350:THR:HG22	1:B:367:CYS:HB3	1.77	0.65
1:A:268:HIS:HA	1:A:300:TYR:HE2	1.62	0.65
1:B:278:TYR:HA	1:B:283:GLN:HA	1.79	0.65
1:A:268:HIS:HA	1:A:300:TYR:CE2	2.33	0.63
1:A:351:LEU:HB2	1:A:366:THR:HB	1.82	0.62
1:A:365:LEU:HB2	1:A:410:LEU:HB3	1.83	0.61
1:A:339:ALA:HB3	1:A:374:PRO:HB3	1.83	0.61
1:B:343:PRO:HB2	1:B:431:ALA:HB2	1.83	0.60
1:B:242:LEU:HB3	1:B:336:ILE:HD12	1.85	0.59
1:A:252:MET:HB2	1:A:255:ARG:HD2	1.85	0.58
1:A:369:VAL:HG11	1:A:377:ILE:HD11	1.85	0.58
1:A:259:VAL:HG23	1:A:308:VAL:HG21	1.84	0.58
1:B:259:VAL:HG23	1:B:308:VAL:HG21	1.86	0.58
1:A:283:GLN:HG2	1:A:285:HIS:H	1.70	0.56
1:A:395:PRO:HG2	1:B:395:PRO:HG2	1.89	0.55
1:A:297:ASN:CB	1:A:299:THR:HG22	2.34	0.55
1:A:345:GLU:HG3	1:A:432:LEU:HD23	1.89	0.55
1:B:379:VAL:HG21	1:B:406:LEU:HD11	1.89	0.54
1:A:246:LYS:HE2	5:A:7:GAL:C1	2.38	0.54
1:A:379:VAL:HG21	1:A:406:LEU:HD11	1.89	0.54
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.89	0.53
1:A:283:GLN:C	1:A:285:HIS:H	2.10	0.53
1:B:284:VAL:HB	1:B:287:ALA:HB2	1.90	0.53
1:B:418:GLN:HA	1:B:443:LEU:HD22	1.92	0.52
1:B:259:VAL:HG23	1:B:308:VAL:CG2	2.39	0.52
1:A:260:THR:HG23	1:A:305:VAL:HG22	1.91	0.51
1:A:401:ASP:HB2	1:A:403:SER:H	1.75	0.51
1:A:350:THR:HB	1:A:441:LEU:HG	1.93	0.50
1:B:377:ILE:HG13	1:B:429:HIS:HB2	1.93	0.50
1:A:274:LYS:HB3	1:A:324:SER:HB2	1.92	0.50
1:B:418:GLN:HA	1:B:443:LEU:CD2	2.42	0.50
1:A:278:TYR:HD1	1:A:320:LYS:HD2	1.77	0.49
1:A:278:TYR:CD1	1:A:320:LYS:HD2	2.48	0.48
1:A:245:PRO:HA	5:A:7:GAL:H61	1.95	0.48
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.95	0.48
1:A:346:PRO:HG2	1:A:432:LEU:HD11	1.96	0.48
1:B:365:LEU:CD1	1:B:410:LEU:HD23	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.49	0.48
1:B:361:ASN:ND2	1:B:362:GLN:HG3	2.28	0.48
1:B:245:PRO:HD3	1:B:259:VAL:HG22	1.96	0.48
1:A:280:ASP:HB2	1:A:317:LYS:HD2	1.96	0.48
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.96	0.47
1:B:343:PRO:HG3	1:B:430:GLU:OE2	2.15	0.47
1:A:274:LYS:HE2	1:A:324:SER:HB2	1.97	0.47
1:A:418:GLN:HA	1:A:443:LEU:CD2	2.41	0.47
1:A:289:THR:HA	1:A:305:VAL:O	2.15	0.46
1:B:386:GLN:HA	1:B:387:PRO:HD3	1.83	0.46
1:A:421:ASN:HD22	1:A:421:ASN:N	2.15	0.45
1:A:312:ASN:HB3	1:A:317:LYS:HG3	1.98	0.45
1:B:261:CYS:HB2	1:B:277:TRP:HZ2	1.81	0.44
1:A:239:SER:HB2	1:A:264:VAL:CG2	2.48	0.44
1:A:384:ASN:C	1:A:386:GLN:H	2.21	0.44
1:A:322:LYS:HD2	1:A:333:GLU:OE1	2.17	0.44
1:B:432:LEU:HD13	1:B:437:THR:HG22	2.00	0.43
1:A:291:PRO:HA	1:A:303:VAL:O	2.19	0.43
1:A:374:PRO:O	1:A:429:HIS:HE1	2.02	0.43
1:B:242:LEU:HD13	1:B:336:ILE:HG22	2.01	0.43
1:A:320:LYS:HD3	1:A:333:GLU:HB3	2.01	0.42
1:A:319:TYR:O	1:A:335:THR:HA	2.19	0.42
1:B:262:VAL:HG22	1:B:303:VAL:HG13	2.00	0.42
1:B:246:LYS:HA	1:B:247:PRO:HD3	1.89	0.42
1:B:252:MET:SD	1:B:255:ARG:HD2	2.60	0.42
1:A:356:GLU:O	1:A:359:THR:HB	2.19	0.41
1:A:243:PHE:HA	1:A:244:PRO:HD3	1.88	0.41
1:B:242:LEU:HA	1:B:242:LEU:HD23	1.92	0.41
1:B:346:PRO:HG2	1:B:432:LEU:HD11	2.01	0.41
1:A:253:ILE:H	1:A:253:ILE:HG13	1.58	0.41
1:B:291:PRO:HA	1:B:303:VAL:O	2.21	0.41
1:B:273:VAL:HA	1:B:324:SER:O	2.21	0.40
1:A:390:ASN:HD22	1:A:390:ASN:C	2.24	0.40
1:B:343:PRO:HA	1:B:373:TYR:O	2.21	0.40
1:A:320:LYS:HB2	1:A:335:THR:HG22	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ASN:OD1	1:B:389:ASN:ND2[4_566]	1.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:HIS:CG	1:A:285:HIS:NE2[2_674]	1.81	0.39
1:A:268:HIS:ND1	1:A:285:HIS:NE2[2_674]	2.01	0.19
1:A:268:HIS:CB	1:A:285:HIS:NE2[2_674]	2.16	0.04

## 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	205/224 (92%)	179 (87%)	18 (9%)	8 (4%)	3	13
1	B	205/224 (92%)	179 (87%)	17 (8%)	9 (4%)	3	11
All	All	410/448 (92%)	358 (87%)	35 (8%)	17 (4%)	3	12

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	B	268	HIS
1	B	292	ARG
1	B	297	ASN
1	A	285	HIS
1	B	326	LYS
1	A	267	SER
1	A	292	ARG
1	A	326	LYS
1	A	384	ASN
1	B	285	HIS
1	A	281	GLY
1	B	280	ASP
1	B	325	ASN
1	A	287	ALA
1	B	291	PRO
1	B	384	ASN

### 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	193/207 (93%)	186 (96%)	7 (4%)	38	73
1	B	193/207 (93%)	186 (96%)	7 (4%)	38	73
All	All	386/414 (93%)	372 (96%)	14 (4%)	38	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	ASP
1	A	361	ASN
1	A	370	LYS
1	A	387	PRO
1	A	390	ASN
1	A	425	CYS
1	A	434	ASN
1	B	284	VAL
1	B	299	THR
1	B	325	ASN
1	B	376	ASP
1	B	390	ASN
1	B	434	ASN
1	B	439	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	347	GLN
1	A	361	ASN
1	A	390	ASN
1	A	418	GLN
1	A	419	GLN
1	A	421	ASN
1	A	438	GLN

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Mol	Chain	Res	Type
1	B	283	GLN
1	B	342	GLN
1	B	347	GLN
1	B	361	ASN
1	B	390	ASN
1	B	418	GLN
1	B	419	GLN
1	B	429	HIS
1	B	438	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

18 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	$\# Z  > 2$
2	NAG	A	1	1,3,2	14,14,15	0.70	0	17,19,21	1.85	3 (17%)
3	FUC	A	2	2	9,10,11	0.82	0	13,14,16	1.31	1 (7%)
2	NAG	A	3	2,4	14,14,15	0.98	0	17,19,21	1.56	3 (17%)
4	MAN	A	4	2,4	11,11,12	0.52	0	15,15,17	1.46	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	A	5	2,4	11,11,12	0.55	0	15,15,17	1.28	1 (6%)
2	NAG	A	6	5,4	14,14,15	0.93	0	17,19,21	1.65	1 (5%)
5	GAL	A	7	2	11,11,12	0.54	0	15,15,17	1.64	5 (33%)
4	MAN	A	8	2,4	11,11,12	0.76	0	15,15,17	1.52	1 (6%)
2	NAG	A	9	4	14,14,15	0.78	0	17,19,21	1.80	1 (5%)
2	NAG	B	1	1,3,2	14,14,15	0.75	0	17,19,21	1.54	2 (11%)
3	FUC	B	2	2	9,10,11	0.78	0	13,14,16	1.28	1 (7%)
2	NAG	B	3	2,4	14,14,15	0.91	1 (7%)	17,19,21	1.39	1 (5%)
4	MAN	B	4	2,4	11,11,12	0.59	0	15,15,17	1.78	2 (13%)
4	MAN	B	5	2,4	11,11,12	0.62	0	15,15,17	1.52	1 (6%)
2	NAG	B	6	5,4	14,14,15	0.82	0	17,19,21	1.66	1 (5%)
5	GAL	B	7	2	11,11,12	0.59	0	15,15,17	1.29	1 (6%)
4	MAN	B	8	2,4	11,11,12	0.83	1 (9%)	15,15,17	1.59	1 (6%)
2	NAG	B	9	4	14,14,15	0.93	1 (7%)	17,19,21	1.67	2 (11%)

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	1	1,3,2	-	0/6/23/26	0/1/1/1
3	FUC	A	2	2	2/2/4/5	0/0/17/20	0/1/1/1
2	NAG	A	3	2,4	-	0/6/23/26	0/1/1/1
4	MAN	A	4	2,4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	5	2,4	-	0/2/19/22	0/1/1/1
2	NAG	A	6	5,4	-	0/6/23/26	0/1/1/1
5	GAL	A	7	2	-	0/2/19/22	0/1/1/1
4	MAN	A	8	2,4	-	0/2/19/22	0/1/1/1
2	NAG	A	9	4	-	0/6/23/26	0/1/1/1
2	NAG	B	1	1,3,2	-	0/6/23/26	0/1/1/1
3	FUC	B	2	2	2/2/4/5	0/0/17/20	0/1/1/1
2	NAG	B	3	2,4	-	0/6/23/26	0/1/1/1
4	MAN	B	4	2,4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	5	2,4	-	0/2/19/22	0/1/1/1
2	NAG	B	6	5,4	-	0/6/23/26	0/1/1/1
5	GAL	B	7	2	-	0/2/19/22	0/1/1/1
4	MAN	B	8	2,4	-	0/2/19/22	0/1/1/1
2	NAG	B	9	4	-	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)
2	B	3	NAG	C1-C2	2.02	1.55	1.52
4	B	8	MAN	C2-C3	2.25	1.55	1.52
2	B	9	NAG	C1-C2	2.49	1.55	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	O5-C1-C2	-3.78	106.31	111.52
2	B	1	NAG	O5-C1-C2	-2.73	107.75	111.52
5	A	7	GAL	O5-C1-C2	-2.73	106.53	110.78
2	A	3	NAG	O5-C1-C2	-2.29	108.36	111.52
4	A	4	MAN	O3-C3-C4	-2.29	105.00	110.34
4	B	4	MAN	O3-C3-C4	-2.26	105.08	110.34
2	A	1	NAG	C4-C3-C2	-2.04	108.02	111.02
2	B	9	NAG	O5-C1-C2	-2.03	108.72	111.52
5	A	7	GAL	O2-C2-C3	-2.03	106.23	110.19
5	A	7	GAL	O5-C5-C6	2.23	110.68	107.15
2	A	3	NAG	C2-N2-C7	2.24	126.21	122.94
5	A	7	GAL	O2-C2-C1	2.29	113.80	109.17
3	B	2	FUC	C1-O5-C5	3.63	120.42	112.39
4	A	5	MAN	C1-O5-C5	3.75	117.34	112.19
3	A	2	FUC	C1-O5-C5	3.77	120.72	112.39
5	B	7	GAL	C1-O5-C5	3.86	117.50	112.19
4	A	4	MAN	C1-O5-C5	3.87	117.51	112.19
5	A	7	GAL	C1-O5-C5	3.88	117.53	112.19
2	B	3	NAG	C1-O5-C5	4.05	117.76	112.19
2	A	3	NAG	C1-O5-C5	4.59	118.51	112.19
4	B	5	MAN	C1-O5-C5	4.97	119.03	112.19
4	B	8	MAN	C1-O5-C5	5.07	119.16	112.19
2	A	1	NAG	C1-O5-C5	5.08	119.18	112.19
4	A	8	MAN	C1-O5-C5	5.18	119.31	112.19
2	B	1	NAG	C1-O5-C5	5.27	119.43	112.19
2	A	6	NAG	C1-O5-C5	5.34	119.54	112.19
4	B	4	MAN	C1-O5-C5	5.58	119.86	112.19
2	B	6	NAG	C1-O5-C5	5.61	119.91	112.19
2	B	9	NAG	C1-O5-C5	5.83	120.20	112.19
2	A	9	NAG	C1-O5-C5	7.02	121.84	112.19

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	4	MAN	C1
4	B	4	MAN	C1
3	A	2	FUC	C5
3	A	2	FUC	C1
3	B	2	FUC	C5
3	B	2	FUC	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	2	0
5	A	7	GAL	3	0
5	B	7	GAL	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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.