



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:44 AM GMT

PDB ID : 3FRU  
Title : NEONATAL FC RECEPTOR, PH 6.5  
Authors : Vaughn, D.E.; Burmeister, W.P.; Bjorkman, P.J.  
Deposited on : 1997-12-22  
Resolution : 2.20 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

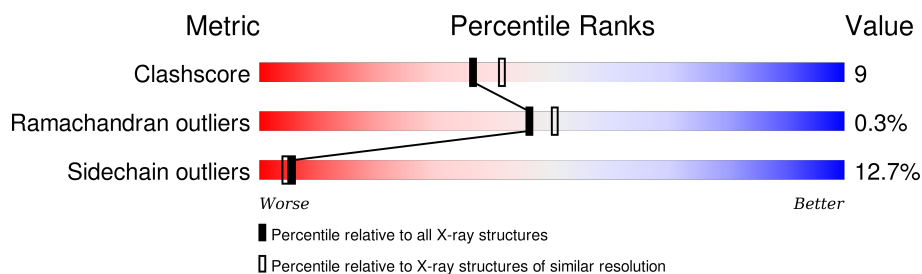
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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	269	
1	C	269	
1	E	269	
2	B	99	
2	D	99	
2	F	99	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9717 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 NEONATAL FC RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2138	1354	370	404	10			
1	C	269	Total	C	N	O	S	0	0	0
			2138	1354	370	404	10			
1	E	269	Total	C	N	O	S	0	0	0
			2138	1354	370	404	10			

- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	528	137	152	4			
2	D	99	Total	C	N	O	S	0	0	0
			821	528	137	152	4			
2	F	99	Total	C	N	O	S	0	0	0
			821	528	137	152	4			

- Molecule 3 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
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	7	Total	C	N	O	0	0
			85	48	3	34		

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	7	Total	C	N	O	0	0
			85	48	3	34		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	S	0	0
			4	2	1	1		
7	C	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 8 is water.

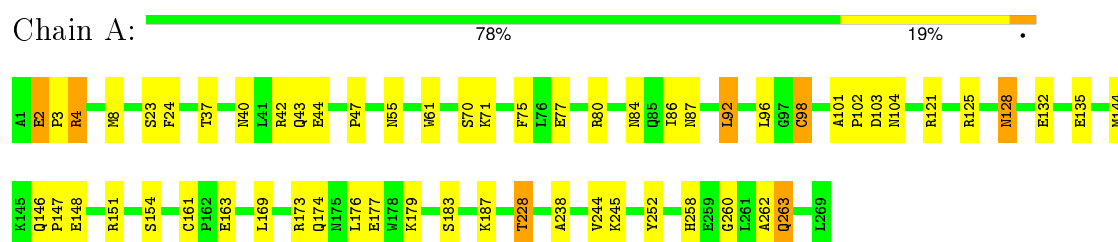
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	147	Total	O	0	0
			147	147		
8	B	83	Total	O	0	0
			83	83		
8	C	164	Total	O	0	0
			164	164		
8	D	81	Total	O	0	0
			81	81		
8	E	91	Total	O	0	0
			91	91		
8	F	54	Total	O	0	0
			54	54		

### 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.

Note EDS was not executed.

#### • Molecule 1: NEONATAL FC RECEPTOR

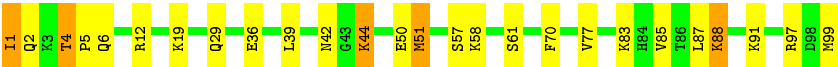




• Molecule 2: BETA-2-MICROGLOBULIN



• Molecule 2: BETA-2-MICROGLOBULIN





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.50 Å   191.70 Å   149.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	25.00 – 2.20	Depositor
% Data completeness (in resolution range)	86.0 (25.00-2.20)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS DEVELOPMENTAL	Depositor
R, $R_{free}$	0.232 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	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: BMA, NAG, BME, NDG, FUC, GAL, SO4, FUL, 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	0.71	0/2200	0.79	0/2991
1	C	0.74	0/2200	0.82	1/2991 (0.0%)
1	E	0.49	0/2200	0.67	0/2991
2	B	0.77	0/846	0.81	0/1149
2	D	0.81	0/846	0.81	0/1149
2	F	0.64	0/846	0.76	0/1149
All	All	0.68	0/9138	0.77	1/12420 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	LEU	CA-CB-CG	5.38	127.69	115.30

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	2138	0	2034	29	0
1	C	2138	0	2033	37	0
1	E	2138	0	2036	46	0
2	B	821	0	807	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	821	0	807	13	0
2	F	821	0	807	13	0
3	A	14	0	13	1	0
3	C	14	0	13	2	0
4	A	85	0	73	5	0
5	C	85	0	73	8	0
6	A	10	0	0	0	0
7	B	4	0	6	3	0
7	C	4	0	6	3	0
7	E	4	0	6	1	0
8	A	147	0	0	6	0
8	B	83	0	0	7	0
8	C	164	0	0	10	0
8	D	81	0	0	3	0
8	E	91	0	0	9	0
8	F	54	0	0	4	0
All	All	9717	0	8714	169	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 9.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:HG2	8:A:652:HOH:O	1.64	0.96
1:C:2:GLU:HG3	1:C:3:PRO:HD2	1.53	0.88
1:E:146:GLN:HB2	8:E:432:HOH:O	1.74	0.87
4:A:502:FUL:H63	4:A:503:NDG:H5	1.62	0.82
1:A:148:GLU:HB2	8:A:655:HOH:O	1.77	0.82
1:A:252:TYR:OH	5:C:509:NDG:H8C1	1.79	0.82
1:C:52:ILE:HG23	8:C:646:HOH:O	1.78	0.81
1:A:80:ARG:HB3	8:A:639:HOH:O	1.81	0.79
1:E:2:GLU:HG2	1:E:3:PRO:HD2	1.63	0.79
1:C:4:ARG:HD3	1:C:99:GLU:OE1	1.90	0.71
1:C:125:ARG:HD3	8:C:544:HOH:O	1.91	0.71
2:F:58:LYS:HE3	8:F:144:HOH:O	1.91	0.70
1:E:39:ASN:HD22	1:E:41:LEU:H	1.38	0.70
2:B:69:GLU:HG2	8:B:425:HOH:O	1.90	0.70
7:C:420:BME:H21	8:C:584:HOH:O	1.91	0.69
1:E:39:ASN:ND2	1:E:41:LEU:H	1.92	0.68
2:B:43:GLY:C	2:B:44:LYS:HD2	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:CYS:SG	7:C:420:BME:S2	2.69	0.67
1:E:43:GLN:OE1	1:E:69:LYS:HE2	1.94	0.67
4:A:503:NDG:H6C1	4:A:504:BMA:C1	2.24	0.67
3:A:401:NAG:O7	3:A:401:NAG:H3	1.93	0.66
1:C:179:LYS:HE3	1:C:259:GLU:OE1	1.94	0.66
4:A:510:GAL:O6	1:C:221:SER:HA	1.94	0.66
1:A:258:HIS:CD2	1:A:260:GLY:H	2.14	0.66
1:C:111:VAL:HG13	1:C:121:ARG:HG3	1.78	0.65
5:C:509:NDG:H3	5:C:509:NDG:O7	1.96	0.64
1:E:258:HIS:CD2	1:E:260:GLY:H	2.16	0.63
1:E:55:ASN:O	1:E:171:ARG:HD3	1.98	0.63
1:A:174:GLN:HG3	8:A:632:HOH:O	1.97	0.63
1:A:187:LYS:HE3	8:B:447:HOH:O	1.97	0.63
1:C:146:GLN:HG2	8:C:631:HOH:O	1.99	0.62
1:C:262:ALA:C	1:C:263:GLN:HG3	2.19	0.62
1:A:75:PHE:CD2	1:A:92:LEU:HD13	2.35	0.61
1:E:47:PRO:HB3	1:E:61:TRP:CZ2	2.35	0.61
1:C:246:ARG:NH2	8:C:582:HOH:O	2.34	0.59
2:D:85:VAL:HG22	8:D:168:HOH:O	2.01	0.59
1:C:43:GLN:HB3	1:C:69:LYS:HE2	1.83	0.59
1:E:4:ARG:HD3	1:E:99:GLU:OE1	2.04	0.58
1:A:37:THR:HG21	7:B:420:BME:H12	1.85	0.58
2:F:88:LYS:HG2	8:F:150:HOH:O	2.04	0.58
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.86	0.57
1:C:2:GLU:CG	1:C:3:PRO:HD2	2.29	0.57
1:E:39:ASN:HD22	1:E:39:ASN:C	2.07	0.57
1:A:258:HIS:HD2	1:A:260:GLY:H	1.53	0.56
2:D:44:LYS:N	2:D:44:LYS:HD2	2.18	0.56
1:A:98:CYS:SG	1:A:161:CYS:HB3	2.46	0.56
2:D:44:LYS:HB2	8:D:141:HOH:O	2.05	0.56
2:B:44:LYS:HD2	2:B:44:LYS:N	2.18	0.55
1:E:179:LYS:HE3	1:E:259:GLU:OE1	2.06	0.55
1:A:2:GLU:OE2	1:A:3:PRO:HD2	2.06	0.55
1:C:98:CYS:SG	1:C:161:CYS:HB3	2.46	0.55
2:D:42:ASN:OD1	2:D:77:VAL:HG12	2.07	0.55
1:A:147:PRO:HB2	1:A:151:ARG:NH2	2.21	0.55
1:E:146:GLN:HG3	8:E:435:HOH:O	2.05	0.54
1:E:71:LYS:NZ	1:E:156:PHE:CD2	2.73	0.54
1:C:66:THR:HG22	8:C:554:HOH:O	2.05	0.54
1:E:98:CYS:SG	1:E:161:CYS:HB3	2.47	0.54
4:A:503:NDG:C6	4:A:504:BMA:C1	2.84	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:597:HOH:O	5:C:503:NAG:H62	2.07	0.54
2:F:42:ASN:OD1	2:F:77:VAL:HG12	2.08	0.54
5:C:509:NDG:C3	5:C:509:NDG:O7	2.56	0.54
2:F:36:GLU:OE1	2:F:83:LYS:HE2	2.08	0.54
2:F:4:THR:HG22	2:F:5:PRO:HD2	1.89	0.53
1:A:4:ARG:CZ	8:A:653:HOH:O	2.56	0.53
2:B:44:LYS:HD3	8:B:473:HOH:O	2.06	0.53
1:E:39:ASN:HD22	1:E:41:LEU:N	2.04	0.53
1:C:49:GLY:O	1:C:52:ILE:HD12	2.09	0.52
2:B:4:THR:HG22	2:B:5:PRO:HD2	1.92	0.52
1:A:244:VAL:HA	5:C:508:MAN:H62	1.91	0.52
2:F:1:ILE:HG13	2:F:2:GLN:N	2.24	0.52
1:E:75:PHE:CD2	1:E:92:LEU:HD13	2.45	0.51
1:C:228:THR:HB	1:C:238:ALA:HB2	1.92	0.51
1:A:47:PRO:HB3	1:A:61:TRP:CZ2	2.46	0.51
1:E:49:GLY:O	1:E:52:ILE:HD12	2.10	0.51
2:F:29:GLN:HA	2:F:61:SER:HB2	1.92	0.51
1:E:36:LEU:C	1:E:36:LEU:HD23	2.31	0.51
2:D:38:GLU:OE2	2:D:81:ARG:NH1	2.45	0.50
1:A:24:PHE:N	1:A:40:ASN:OD1	2.35	0.50
1:C:57:VAL:HG21	1:C:59:TRP:CE2	2.47	0.50
1:E:39:ASN:C	1:E:39:ASN:ND2	2.65	0.50
2:B:36:GLU:OE1	2:B:83:LYS:HE2	2.12	0.50
4:A:504:BMA:O4	4:A:508:MAN:H5	2.12	0.49
2:F:99:MET:HG2	8:F:108:HOH:O	2.12	0.49
1:E:38:TYR:CD1	1:E:38:TYR:C	2.86	0.49
1:A:43:GLN:O	1:A:43:GLN:HG3	2.12	0.49
1:E:258:HIS:HD2	1:E:260:GLY:H	1.58	0.49
2:B:51:MET:HE2	2:B:64:ILE:HD11	1.95	0.49
1:C:178:TRP:C	1:C:179:LYS:HG2	2.32	0.49
1:A:262:ALA:C	1:A:263:GLN:HG2	2.33	0.49
1:E:225:ASN:ND2	8:E:463:HOH:O	2.46	0.49
1:E:43:GLN:HB3	1:E:69:LYS:HE2	1.94	0.48
1:E:2:GLU:CG	1:E:3:PRO:HD2	2.41	0.48
2:D:81:ARG:HG2	2:D:81:ARG:HH11	1.78	0.48
2:B:91:LYS:NZ	8:B:481:HOH:O	2.46	0.48
1:E:8:MET:HE2	1:E:95:LEU:HG	1.95	0.48
2:B:43:GLY:O	2:B:44:LYS:HD2	2.14	0.48
1:A:228:THR:HB	1:A:238:ALA:HB2	1.96	0.48
7:B:420:BME:H21	8:B:484:HOH:O	2.14	0.47
2:D:4:THR:HG22	2:D:5:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:ARG:NH2	8:E:504:HOH:O	2.46	0.47
1:E:146:GLN:CG	8:E:435:HOH:O	2.63	0.47
2:B:51:MET:HE2	2:B:64:ILE:CD1	2.44	0.47
1:A:2:GLU:CD	1:A:3:PRO:HD2	2.35	0.47
1:C:104:ASN:ND2	3:C:401:NAG:H4	2.29	0.47
1:E:39:ASN:ND2	1:E:41:LEU:N	2.60	0.47
1:E:36:LEU:CD1	1:E:64:GLU:HG2	2.45	0.47
1:E:103:ASP:O	1:E:104:ASN:HB2	2.15	0.47
1:E:147:PRO:HB2	1:E:151:ARG:NH2	2.31	0.47
1:C:146:GLN:CG	8:C:631:HOH:O	2.60	0.46
1:C:86:ILE:HG22	1:C:87:ASN:N	2.30	0.46
1:E:160:SER:O	1:E:164:ARG:HG3	2.16	0.46
1:A:86:ILE:HG22	1:A:87:ASN:N	2.31	0.46
1:E:57:VAL:HG21	1:E:59:TRP:CE2	2.50	0.46
1:A:2:GLU:CG	1:A:3:PRO:HD2	2.46	0.46
1:E:249:GLU:CD	1:E:249:GLU:H	2.20	0.46
1:E:211:LYS:HE2	8:E:486:HOH:O	2.16	0.46
1:A:42:ARG:O	1:A:43:GLN:CG	2.64	0.45
2:D:51:MET:HE2	2:D:64:ILE:CD1	2.46	0.45
1:C:203:PHE:CE2	1:C:237:HIS:HE1	2.35	0.45
1:A:103:ASP:O	1:A:104:ASN:HB2	2.17	0.45
1:E:219:LEU:HA	8:E:471:HOH:O	2.16	0.45
2:F:44:LYS:HD2	2:F:44:LYS:N	2.32	0.45
1:C:259:GLU:HB2	8:C:603:HOH:O	2.17	0.45
1:A:101:ALA:HB1	1:A:102:PRO:HD2	1.99	0.45
1:C:47:PRO:HB3	1:C:61:TRP:CZ2	2.52	0.44
2:D:59:ASP:O	2:D:60:TRP:HB2	2.18	0.44
1:C:106:SER:HB2	1:C:162:PRO:HG3	1.99	0.44
1:C:103:ASP:OD1	1:C:105:SER:HB3	2.19	0.43
1:C:75:PHE:CD2	1:C:92:LEU:HD13	2.53	0.43
2:F:6:GLN:HG2	8:F:102:HOH:O	2.19	0.43
1:E:62:GLU:HA	1:E:62:GLU:OE1	2.17	0.43
2:D:43:GLY:C	2:D:44:LYS:HD2	2.39	0.43
2:D:7:ILE:HD13	2:D:82:VAL:HG13	2.01	0.43
1:A:8:MET:HB3	1:A:8:MET:HE2	1.89	0.43
1:C:44:GLU:OE2	1:C:46:ASP:OD1	2.37	0.43
1:C:103:ASP:O	1:C:104:ASN:HB2	2.19	0.42
1:E:246:ARG:NH2	8:E:473:HOH:O	2.52	0.42
2:B:48:ASN:N	8:B:486:HOH:O	2.51	0.42
2:B:53:ASP:OD2	7:B:420:BME:H11	2.19	0.42
5:C:501:NAG:H62	5:C:502:FUC:H2	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:O	1:A:43:GLN:HG2	2.19	0.42
2:B:55:SER:OG	2:B:56:PHE:N	2.50	0.42
1:C:177:GLU:O	1:C:179:LYS:HG2	2.20	0.42
5:C:503:NAG:H3	8:C:670:HOH:O	2.18	0.42
1:E:219:LEU:HD23	8:E:471:HOH:O	2.19	0.42
1:C:104:ASN:ND2	3:C:401:NAG:C4	2.80	0.42
1:E:48:CYS:SG	7:E:420:BME:S2	3.03	0.42
1:E:221:SER:OG	1:E:221:SER:O	2.32	0.42
2:B:88:LYS:HE2	2:B:88:LYS:HB3	1.94	0.41
1:C:225:ASN:OD1	5:C:501:NAG:C7	2.68	0.41
2:F:42:ASN:HA	2:F:77:VAL:HG13	2.01	0.41
1:E:101:ALA:HB2	1:E:107:LEU:CD2	2.50	0.41
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.99	0.41
1:E:100:LEU:HG	1:E:165:LEU:HD23	2.02	0.41
2:B:92:THR:O	1:C:247:GLY:HA2	2.21	0.41
2:F:50:GLU:O	2:F:51:MET:HG2	2.21	0.41
1:C:187:LYS:HG3	8:D:124:HOH:O	2.21	0.41
2:B:85:VAL:HG22	8:B:476:HOH:O	2.20	0.41
1:C:49:GLY:H	7:C:420:BME:C1	2.33	0.41
2:D:4:THR:HG23	2:D:86:THR:OG1	2.21	0.41
1:E:195:SER:O	1:E:246:ARG:NH1	2.54	0.41
2:F:51:MET:HB3	2:F:51:MET:HE2	1.92	0.41
1:A:128:ASN:ND2	1:A:144:MET:CE	2.84	0.41
1:E:36:LEU:HD12	1:E:64:GLU:HG2	2.02	0.40
2:D:81:ARG:HG2	2:D:81:ARG:NH1	2.37	0.40
2:B:7:ILE:HD13	2:B:82:VAL:HG13	2.03	0.40
1:E:86:ILE:HG22	1:E:87:ASN:N	2.37	0.40
2:B:51:MET:HE2	2:B:51:MET:HB3	1.86	0.40
1:C:132:GLU:CD	8:C:643:HOH:O	2.60	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	267/269 (99%)	258 (97%)	9 (3%)	0	100	100
1	C	267/269 (99%)	255 (96%)	12 (4%)	0	100	100
1	E	267/269 (99%)	255 (96%)	11 (4%)	1 (0%)	39	42
2	B	97/99 (98%)	89 (92%)	7 (7%)	1 (1%)	19	16
2	D	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
2	F	97/99 (98%)	90 (93%)	6 (6%)	1 (1%)	19	16
All	All	1092/1104 (99%)	1038 (95%)	51 (5%)	3 (0%)	46	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97	ARG
2	F	97	ARG
1	E	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	227/227 (100%)	199 (88%)	28 (12%)	6	5
1	C	227/227 (100%)	195 (86%)	32 (14%)	4	3
1	E	227/227 (100%)	200 (88%)	27 (12%)	6	5
2	B	95/95 (100%)	83 (87%)	12 (13%)	5	4
2	D	95/95 (100%)	84 (88%)	11 (12%)	7	6
2	F	95/95 (100%)	82 (86%)	13 (14%)	4	3
All	All	966/966 (100%)	843 (87%)	123 (13%)	5	4

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	4	ARG

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Mol	Chain	Res	Type
1	A	23	SER
1	A	44	GLU
1	A	55	ASN
1	A	70	SER
1	A	71	LYS
1	A	77	GLU
1	A	84	ASN
1	A	92	LEU
1	A	96	LEU
1	A	98	CYS
1	A	121	ARG
1	A	125	ARG
1	A	128	ASN
1	A	132	GLU
1	A	135	GLU
1	A	146	GLN
1	A	154	SER
1	A	169	LEU
1	A	173	ARG
1	A	176	LEU
1	A	177	GLU
1	A	179	LYS
1	A	183	SER
1	A	228	THR
1	A	245	LYS
1	A	263	GLN
2	B	4	THR
2	B	6	GLN
2	B	12	ARG
2	B	19	LYS
2	B	39	LEU
2	B	44	LYS
2	B	51	MET
2	B	57	SER
2	B	70	PHE
2	B	82	VAL
2	B	85	VAL
2	B	87	LEU
1	C	2	GLU
1	C	4	ARG
1	C	42	ARG
1	C	55	ASN

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Mol	Chain	Res	Type
1	C	70	SER
1	C	77	GLU
1	C	84	ASN
1	C	89	THR
1	C	92	LEU
1	C	96	LEU
1	C	98	CYS
1	C	107	LEU
1	C	111	VAL
1	C	121	ARG
1	C	128	ASN
1	C	132	GLU
1	C	135	GLU
1	C	145	LYS
1	C	146	GLN
1	C	148	GLU
1	C	161	CYS
1	C	169	LEU
1	C	173	ARG
1	C	174	GLN
1	C	176	LEU
1	C	177	GLU
1	C	179	LYS
1	C	183	SER
1	C	192	ASN
1	C	228	THR
1	C	246	ARG
1	C	263	GLN
2	D	4	THR
2	D	6	GLN
2	D	12	ARG
2	D	39	LEU
2	D	44	LYS
2	D	51	MET
2	D	57	SER
2	D	70	PHE
2	D	85	VAL
2	D	87	LEU
2	D	88	LYS
1	E	4	ARG
1	E	39	ASN
1	E	42	ARG

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Mol	Chain	Res	Type
1	E	77	GLU
1	E	84	ASN
1	E	92	LEU
1	E	96	LEU
1	E	98	CYS
1	E	121	ARG
1	E	128	ASN
1	E	132	GLU
1	E	135	GLU
1	E	144	MET
1	E	145	LYS
1	E	146	GLN
1	E	161	CYS
1	E	169	LEU
1	E	173	ARG
1	E	176	LEU
1	E	177	GLU
1	E	179	LYS
1	E	196	SER
1	E	210	LEU
1	E	228	THR
1	E	240	SER
1	E	245	LYS
1	E	246	ARG
2	F	1	ILE
2	F	4	THR
2	F	12	ARG
2	F	19	LYS
2	F	39	LEU
2	F	44	LYS
2	F	51	MET
2	F	57	SER
2	F	70	PHE
2	F	85	VAL
2	F	87	LEU
2	F	88	LYS
2	F	91	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN

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Mol	Chain	Res	Type
1	A	258	HIS
1	A	263	GLN
1	C	84	ASN
1	C	128	ASN
1	C	141	ASN
1	C	146	GLN
1	C	192	ASN
1	E	39	ASN
1	E	84	ASN
1	E	128	ASN
1	E	146	GLN
1	E	192	ASN
1	E	258	HIS

### 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 ⓘ

14 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	NAG	A	501	1,4	14,14,15	0.90	0	15,19,21	1.36	4 (26%)
4	FUL	A	502	4	10,10,11	0.43	0	14,14,16	0.57	0
4	NDG	A	503	4	14,14,15	0.87	0	15,19,21	1.25	2 (13%)
4	BMA	A	504	4	11,11,12	0.86	0	14,15,17	0.94	0
4	MAN	A	508	4	11,11,12	0.66	0	14,15,17	1.16	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	509	4	14,14,15	0.66	0	15,19,21	0.81	0
4	GAL	A	510	4	11,11,12	0.67	0	14,15,17	0.48	0
5	NAG	C	501	1,5	14,14,15	1.46	2 (14%)	15,19,21	1.02	1 (6%)
5	FUC	C	502	5	10,10,11	0.65	0	14,14,16	0.88	1 (7%)
5	NAG	C	503	5	14,14,15	0.74	0	15,19,21	0.99	1 (6%)
5	BMA	C	504	5	11,11,12	0.77	0	14,15,17	0.51	0
5	MAN	C	508	5	11,11,12	0.94	0	14,15,17	1.05	1 (7%)
5	NDG	C	509	5	14,14,15	1.10	1 (7%)	15,19,21	0.96	0
5	GAL	C	510	5	11,11,12	0.59	0	14,15,17	0.59	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	NAG	A	501	1,4	-	0/6/23/26	0/1/1/1
4	FUL	A	502	4	-	0/0/17/20	0/1/1/1
4	NDG	A	503	4	-	0/6/23/26	0/1/1/1
4	BMA	A	504	4	-	0/2/19/22	0/1/1/1
4	MAN	A	508	4	-	0/2/19/22	0/1/1/1
4	NAG	A	509	4	-	0/6/23/26	0/1/1/1
4	GAL	A	510	4	-	0/2/19/22	0/1/1/1
5	NAG	C	501	1,5	-	0/6/23/26	0/1/1/1
5	FUC	C	502	5	-	0/0/17/20	0/1/1/1
5	NAG	C	503	5	-	0/6/23/26	0/1/1/1
5	BMA	C	504	5	-	0/2/19/22	0/1/1/1
5	MAN	C	508	5	-	0/2/19/22	1/1/1/1
5	NDG	C	509	5	-	0/6/23/26	0/1/1/1
5	GAL	C	510	5	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	NAG	C3-C2	2.01	1.57	1.52
5	C	509	NDG	C1-C2	3.37	1.57	1.52
5	C	501	NAG	C1-C2	4.17	1.58	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	NDG	C3-C4-C5	-2.51	105.83	110.20
5	C	503	NAG	C2-N2-C7	-2.46	119.88	123.04
4	A	501	NAG	C4-C3-C2	-2.42	107.47	111.23
4	A	501	NAG	C3-C4-C5	-2.35	106.09	110.20
4	A	501	NAG	C2-N2-C7	-2.28	120.11	123.04
4	A	508	MAN	C2-C3-C4	-2.07	107.52	111.04
5	C	502	FUC	C1-O5-C5	2.08	115.60	112.38
5	C	501	NAG	C6-C5-C4	2.10	118.20	113.02
4	A	503	NDG	C1-O-C5	2.38	115.27	112.25
4	A	501	NAG	O4-C4-C3	2.39	115.72	110.34
4	A	508	MAN	C1-O5-C5	3.16	116.25	112.25
5	C	508	MAN	C1-O5-C5	3.45	116.63	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	508	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	FUL	1	0
4	A	503	NDG	3	0
4	A	504	BMA	3	0
4	A	508	MAN	1	0
4	A	510	GAL	1	0
5	C	501	NAG	2	0
5	C	502	FUC	1	0
5	C	503	NAG	2	0
5	C	508	MAN	1	0
5	C	509	NDG	3	0

## 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	$\# Z  > 2$
6	SO4	A	325	-	4,4,4	0.24	0	6,6,6	0.23	0
6	SO4	A	326	-	4,4,4	0.41	0	6,6,6	0.31	0
3	NAG	A	401	1	14,14,15	0.83	1 (7%)	15,19,21	0.77	1 (6%)
7	BME	B	420	-	3,3,3	0.34	0	2,2,2	0.10	0
3	NAG	C	401	1	14,14,15	1.00	1 (7%)	15,19,21	0.74	0
7	BME	C	420	-	3,3,3	0.81	0	2,2,2	0.37	0
7	BME	E	420	-	3,3,3	0.65	0	2,2,2	0.48	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
6	SO4	A	325	-	-	0/0/0/0	0/0/0/0
6	SO4	A	326	-	-	0/0/0/0	0/0/0/0
3	NAG	A	401	1	-	0/6/23/26	0/1/1/1
7	BME	B	420	-	-	0/1/1/1	0/0/0/0
3	NAG	C	401	1	-	0/6/23/26	0/1/1/1
7	BME	C	420	-	-	0/1/1/1	0/0/0/0
7	BME	E	420	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NAG	C1-C2	2.18	1.55	1.52
3	C	401	NAG	C1-C2	2.46	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	C2-N2-C7	-2.13	120.30	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	1	0
7	B	420	BME	3	0
3	C	401	NAG	2	0
7	C	420	BME	3	0
7	E	420	BME	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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.