



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2017 – 01:45 PM EDT

PDB ID : 4QWW  
Title : Crystal structure of the Fab410-BfAChE complex  
Authors : Bourne, Y.; Renault, L.; Marchot, P.  
Deposited on : 2014-07-17  
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029077

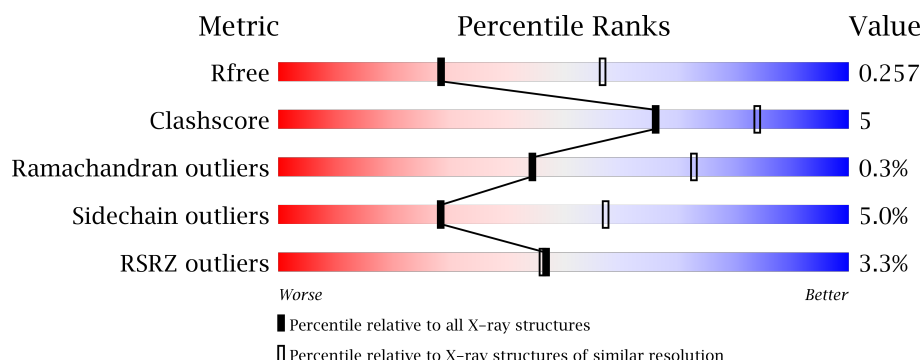
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	542	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	542	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
2	C	213	<div> <div></div> <div> <div></div> <div>86%</div> <div>13%</div> </div> </div>
2	E	213	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
3	D	234	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	234	 .% 79% 12% 6%

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
8	EDO	B	613	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15524 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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	1	0
			4173	2678	711	767	17			
1	B	529	Total	C	N	O	S	0	1	0
			4173	2678	711	767	17			

- Molecule 2 is a protein called Fab410 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	212	Total	C	N	O	S	0	0	0
			1626	1011	272	334	9			
2	E	212	Total	C	N	O	S	0	1	0
			1632	1015	272	336	9			

- Molecule 3 is a protein called Fab410 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	225	Total	C	N	O	S	0	1	0
			1723	1089	285	339	10			
3	F	219	Total	C	N	O	S	0	1	0
			1683	1067	277	329	10			

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



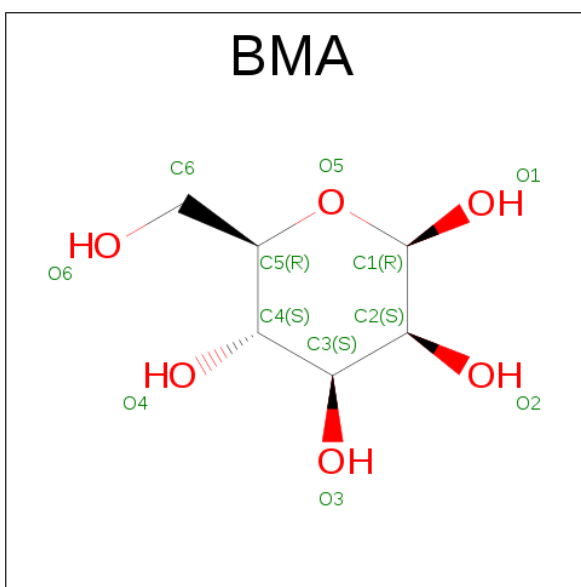
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1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

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



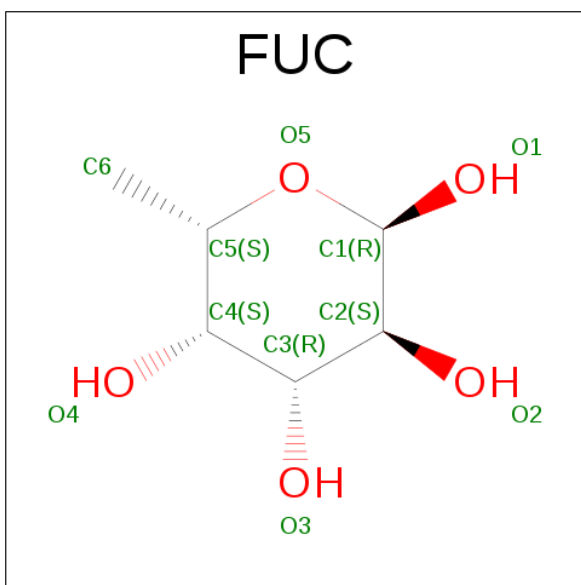
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

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



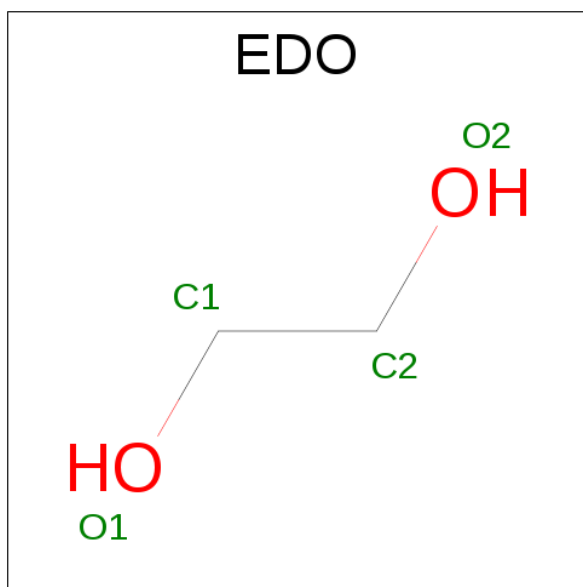
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 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
7	A	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 9 is water.

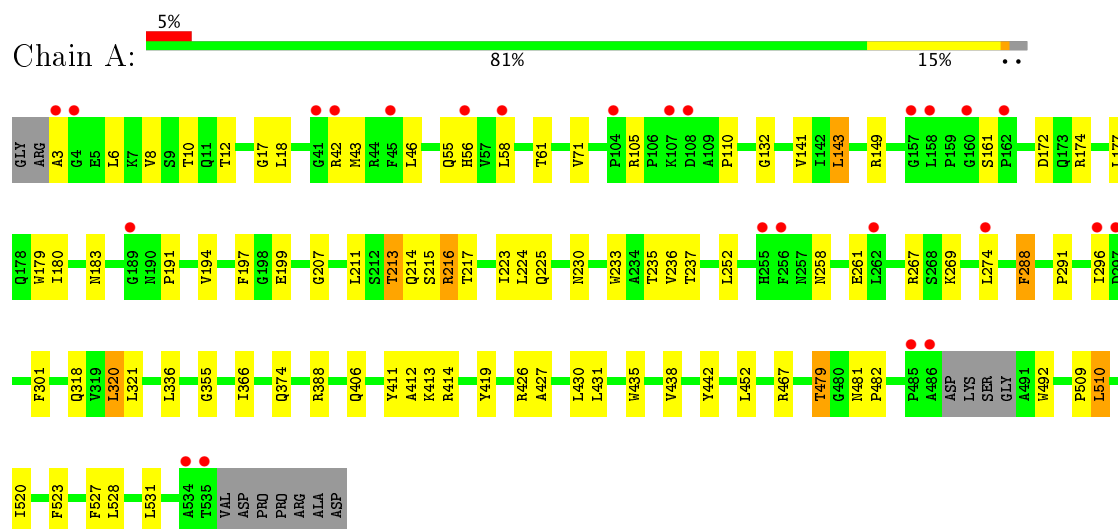
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	48	Total	O	0	0
			48	48		
9	B	40	Total	O	0	0
			40	40		
9	C	44	Total	O	0	0
			44	44		
9	D	26	Total	O	0	0
			26	26		
9	E	54	Total	O	0	0
			54	54		
9	F	16	Total	O	0	0
			16	16		



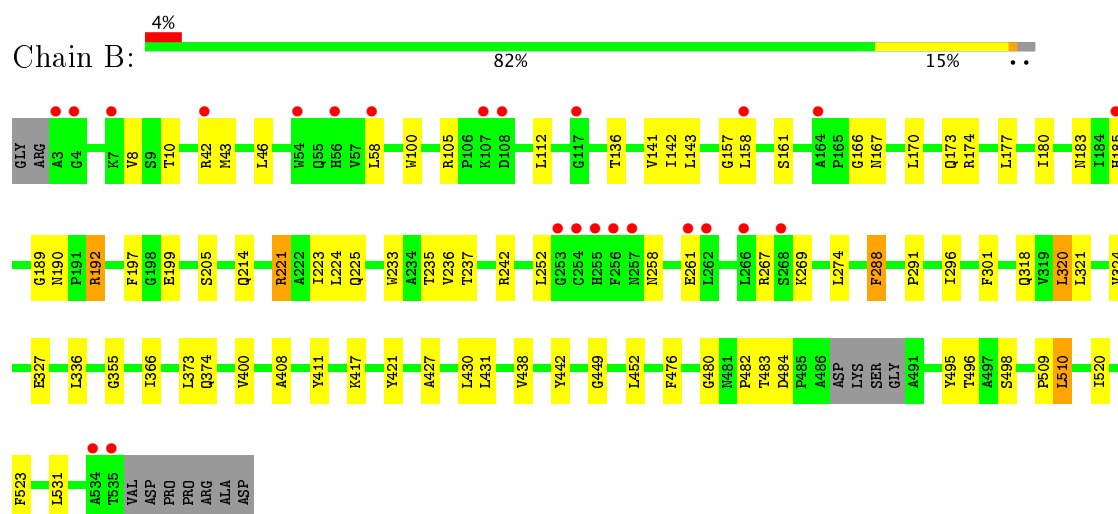
### 3 Residue-property plots

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.

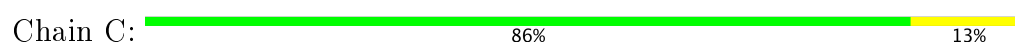
#### • Molecule 1: Acetylcholinesterase

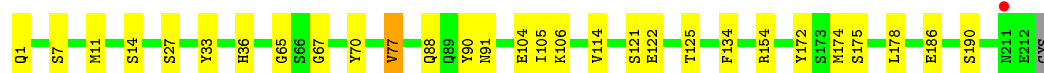


#### • Molecule 1: Acetylcholinesterase

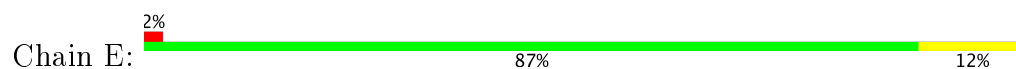


#### • Molecule 2: Fab410 antibody light chain

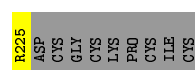
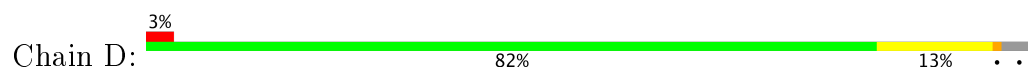




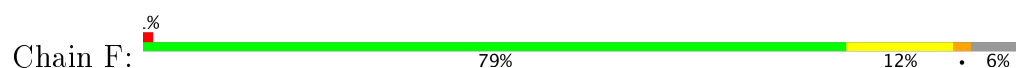
- Molecule 2: Fab410 antibody light chain



- Molecule 3: Fab410 antibody heavy chain



- Molecule 3: Fab410 antibody heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.59 Å   251.34 Å   73.98 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	39.53 – 2.70 39.15 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.53-2.70) 99.9 (39.15-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.69 Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.199   ,   0.239 0.218   ,   0.257	Depositor DCC
$R_{free}$ test set	4060 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.32 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7941e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: FUC, MAN, BMA, NAG, EDO

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	0.54	0/4303	0.74	2/5873 (0.0%)
1	B	0.56	0/4303	0.74	1/5873 (0.0%)
2	C	0.51	0/1667	0.74	0/2266
2	E	0.51	0/1676	0.76	0/2278
3	D	0.50	0/1772	0.80	1/2418 (0.0%)
3	F	0.46	0/1731	0.76	0/2360
All	All	0.53	0/15452	0.75	4/21068 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	THR	N-CA-C	6.41	128.30	111.00
1	A	510	LEU	CB-CA-C	5.89	121.39	110.20
1	B	510	LEU	CB-CA-C	5.42	120.49	110.20
3	D	142	ALA	CB-CA-C	-5.07	102.50	110.10

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	4173	0	4027	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4173	0	4026	46	0
2	C	1626	0	1544	9	0
2	E	1632	0	1550	8	0
3	D	1723	0	1674	14	0
3	F	1683	0	1637	19	0
4	A	56	0	47	0	0
4	B	70	0	60	0	0
5	A	44	0	40	0	0
5	B	44	0	40	0	0
6	A	22	0	16	0	0
6	B	22	0	16	0	0
7	A	10	0	10	0	0
7	B	10	0	10	0	0
8	A	4	0	6	0	0
8	B	4	0	6	0	0
9	A	48	0	0	0	0
9	B	40	0	0	1	0
9	C	44	0	0	0	0
9	D	26	0	0	0	0
9	E	54	0	0	0	0
9	F	16	0	0	0	0
All	All	15524	0	14709	139	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 5.

All (139) 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:374:GLN:HE22	1:B:374:GLN:HE22	1.25	0.84
3:F:99:VAL:HG11	3:F:112:MET:HB3	1.65	0.76
3:F:35:HIS:HD2	3:F:47:TRP:HE1	1.33	0.75
3:F:168:SER:H	3:F:208:ASN:HD21	1.33	0.74
1:A:427:ALA:HB3	1:A:430:LEU:HB2	1.70	0.73
1:B:366:ILE:HG23	1:B:531:LEU:HD21	1.71	0.73
1:A:366:ILE:HG23	1:A:531:LEU:HD21	1.72	0.72
1:B:112:LEU:HD12	1:B:141:VAL:HG11	1.73	0.71
3:F:165:THR:HG23	3:F:208:ASN:HB2	1.73	0.70
1:A:224:LEU:HB2	1:A:321:LEU:HD23	1.74	0.69
1:A:12:THR:HG21	1:A:179:TRP:HE1	1.59	0.68
1:B:427:ALA:HB2	1:B:442[B]:TYR:OH	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:TRP:HB3	1:B:136:THR:HG21	1.78	0.66
1:A:149:ARG:HD3	1:A:172:ASP:OD2	1.95	0.65
1:B:224:LEU:HB2	1:B:321:LEU:HD23	1.79	0.65
3:F:66:VAL:HG13	3:F:70:PHE:HB2	1.80	0.64
1:A:419:TYR:HD1	1:A:492:TRP:CD1	2.15	0.63
1:A:427:ALA:HB2	1:A:442[B]:TYR:OH	1.98	0.63
3:F:99:VAL:CG1	3:F:112:MET:HB3	2.29	0.62
1:B:417:LYS:HD3	9:B:704:HOH:O	1.98	0.62
1:A:258:ASN:HB2	1:A:261:GLU:HB2	1.82	0.61
3:F:11:LEU:HB2	3:F:159:PRO:HG3	1.82	0.61
3:D:99:VAL:HG11	3:D:112:MET:HB3	1.83	0.61
1:B:258:ASN:HB2	1:B:261:GLU:HB2	1.83	0.60
3:D:66:VAL:HG13	3:D:70:PHE:HB2	1.84	0.60
3:D:11:LEU:HB2	3:D:159:PRO:HG3	1.84	0.59
1:B:8:VAL:HG22	1:B:105:ARG:HH21	1.67	0.59
1:B:43:MET:HA	1:B:46:LEU:HD12	1.85	0.59
1:A:43:MET:HA	1:A:46:LEU:HD12	1.85	0.59
1:A:174:ARG:HA	1:A:177:LEU:HD12	1.86	0.57
2:C:154:ARG:HG2	2:C:178:LEU:HD11	1.86	0.56
3:F:35:HIS:HD2	3:F:47:TRP:NE1	2.03	0.56
1:A:8:VAL:HG22	1:A:105:ARG:HH21	1.70	0.56
1:B:174:ARG:HA	1:B:177:LEU:HD12	1.86	0.56
1:A:427:ALA:HB2	1:A:442[B]:TYR:CZ	2.42	0.55
1:A:426:ARG:HB2	1:A:438:VAL:HG22	1.89	0.54
1:B:167:ASN:HB3	1:B:170:LEU:HD12	1.89	0.54
1:B:427:ALA:HB3	1:B:430:LEU:HB2	1.90	0.54
3:F:168:SER:H	3:F:208:ASN:ND2	2.04	0.54
1:B:496:THR:HG22	1:B:498:SER:H	1.73	0.53
1:B:173:GLN:OE1	1:B:205:SER:HB3	2.08	0.53
1:A:252:LEU:HD22	1:A:269:LYS:HG2	1.90	0.53
3:D:99:VAL:CG1	3:D:112:MET:HB3	2.38	0.52
1:A:132:GLY:HA3	1:A:143:LEU:HD22	1.91	0.52
1:A:199:GLU:HA	1:A:225:GLN:O	2.09	0.52
3:F:35:HIS:CD2	3:F:47:TRP:HE1	2.21	0.52
1:B:252:LEU:HD22	1:B:269:LYS:HG2	1.90	0.52
1:B:296:ILE:HA	1:B:301:PHE:HB2	1.90	0.52
1:A:296:ILE:HA	1:A:301:PHE:HB2	1.90	0.52
1:A:17:GLY:O	1:A:61:THR:HG22	2.10	0.52
1:B:199:GLU:HA	1:B:225:GLN:O	2.10	0.51
2:C:104:GLU:HG3	2:C:172:TYR:OH	2.11	0.51
1:A:412:ALA:C	1:A:414:ARG:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:14:SER:HA	2:E:106:LYS:HB2	1.93	0.50
2:E:104:GLU:HG3	2:E:172:TYR:OH	2.12	0.50
2:C:14:SER:HA	2:C:106:LYS:HB2	1.93	0.49
1:B:324:VAL:HG22	1:B:327:GLU:OE2	2.13	0.49
1:A:12:THR:HG21	1:A:179:TRP:NE1	2.26	0.49
1:A:233:TRP:HB3	1:A:288:PHE:O	2.12	0.49
1:B:221:ARG:HD3	1:B:480:GLY:HA2	1.94	0.49
3:D:29:PHE:HB2	3:D:79:THR:HG23	1.95	0.49
1:B:233:TRP:HB3	1:B:288:PHE:O	2.13	0.48
3:D:85:MET:HE2	3:D:88:LEU:HD21	1.95	0.48
1:A:207:GLY:O	1:A:211:LEU:HG	2.13	0.48
2:E:77:VAL:HG13	2:E:105:ILE:HD12	1.94	0.48
1:B:427:ALA:HB2	1:B:442[B]:TYR:CZ	2.49	0.47
2:C:122:GLU:HA	2:C:125:THR:HG22	1.97	0.47
2:C:77:VAL:HG13	2:C:105:ILE:HD12	1.95	0.47
3:F:131:PRO:HB3	3:F:157:TYR:HB3	1.96	0.46
1:A:191:PRO:HA	1:A:194:VAL:HG23	1.97	0.46
2:E:185:TYR:HA	2:E:191:TYR:OH	2.15	0.46
3:F:12:VAL:HG21	3:F:18:LEU:HB2	1.96	0.46
3:D:131:PRO:HB3	3:D:157:TYR:HB3	1.96	0.46
3:F:85:MET:HE2	3:F:88:LEU:HD21	1.96	0.46
3:D:12:VAL:HG21	3:D:18:LEU:HB2	1.97	0.46
3:D:29:PHE:CB	3:D:79:THR:HG23	2.46	0.46
1:A:18:LEU:HD13	1:A:61:THR:HB	1.96	0.45
3:F:29:PHE:HB2	3:F:79:THR:HG23	1.98	0.45
1:A:479:THR:HB	1:A:481:ASN:H	1.82	0.45
2:E:149:ILE:HD11	2:E:178:LEU:HD21	1.99	0.45
1:A:10:THR:HB	1:A:183:ASN:OD1	2.17	0.45
1:A:132:GLY:CA	1:A:143:LEU:HD22	2.47	0.45
1:B:141:VAL:HG12	1:B:142:ILE:N	2.32	0.45
1:B:190:ASN:HD22	1:B:192:ARG:HG3	1.82	0.44
1:A:42:ARG:HA	1:A:267:ARG:HD3	1.99	0.44
1:A:509:PRO:O	1:A:510:LEU:C	2.55	0.44
1:B:10:THR:HB	1:B:183:ASN:OD1	2.17	0.44
1:B:42:ARG:HA	1:B:267:ARG:HD3	2.00	0.44
2:C:114:VAL:HA	2:C:134:PHE:O	2.17	0.44
2:C:33:TYR:HB2	2:C:88:GLN:OE1	2.18	0.44
3:D:101:GLU:HA	3:D:111:ALA:O	2.17	0.44
1:A:230:ASN:HD22	1:A:406:GLN:HE21	1.64	0.43
1:A:110:PRO:HG2	1:A:141:VAL:HG22	1.99	0.43
1:A:336:LEU:HD22	1:A:355:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:29:PHE:CB	3:F:79:THR:HG23	2.49	0.43
2:E:114:VAL:HA	2:E:134:PHE:O	2.18	0.43
1:A:452:LEU:HD11	1:A:467:ARG:HG3	2.00	0.43
1:B:438:VAL:HG13	1:B:442[B]:TYR:HD2	1.84	0.43
3:D:198:SER:HB2	3:D:199:PRO:HD3	2.00	0.43
1:A:223:ILE:HG12	1:A:320:LEU:HB3	2.01	0.42
1:A:177:LEU:HA	1:A:180:ILE:HD12	2.01	0.42
1:B:157:GLY:HA2	1:B:166:GLY:HA2	2.01	0.42
1:B:476:PHE:HD1	1:B:482:PRO:HD3	1.84	0.42
1:A:213:THR:HA	1:A:216:ARG:HE	1.85	0.42
1:B:336:LEU:HD22	1:B:355:GLY:HA2	2.01	0.42
2:C:174:MET:HG2	2:C:175:SER:N	2.34	0.42
3:F:198:SER:HB2	3:F:199:PRO:HD3	2.01	0.42
1:B:177:LEU:HA	1:B:180:ILE:HD12	2.01	0.42
3:D:139:GLY:HA2	3:D:225:ARG:HG3	2.01	0.42
1:A:71:VAL:HG11	3:F:104[A]:TYR:CG	2.55	0.42
1:B:520:ILE:O	1:B:523:PHE:HB3	2.20	0.42
3:F:196:PRO:O	3:F:199:PRO:HD2	2.20	0.42
1:B:158:LEU:HD23	1:B:242:ARG:HG2	2.02	0.41
1:A:388:ARG:HD3	1:A:435:TRP:CE3	2.56	0.41
1:B:438:VAL:HG13	1:B:442[B]:TYR:CD2	2.56	0.41
1:B:8:VAL:CG2	1:B:105:ARG:HH21	2.33	0.41
3:D:196:PRO:O	3:D:199:PRO:HD2	2.20	0.41
1:A:520:ILE:O	1:A:523:PHE:HB3	2.21	0.41
1:A:527:PHE:HB2	1:B:373:LEU:HD13	2.03	0.41
2:E:174:MET:HG2	2:E:175:SER:N	2.35	0.41
1:A:528:LEU:HD12	1:A:528:LEU:HA	1.94	0.41
1:B:223:ILE:HG12	1:B:320:LEU:HB3	2.03	0.41
1:B:327:GLU:OE1	1:B:400:VAL:HG11	2.20	0.41
1:B:449:GLY:O	1:B:452:LEU:HB2	2.20	0.41
2:C:65:GLY:HA3	2:C:70:TYR:HA	2.03	0.41
1:B:225:GLN:HG2	1:B:421:TYR:OH	2.20	0.41
1:B:221:ARG:CG	1:B:318:GLN:HE21	2.34	0.41
1:B:509:PRO:O	1:B:510:LEU:C	2.59	0.41
3:D:196:PRO:HD2	3:D:199:PRO:HG2	2.03	0.41
3:F:196:PRO:HD2	3:F:199:PRO:HG2	2.02	0.41
1:A:8:VAL:CG2	1:A:105:ARG:HH21	2.34	0.40
1:A:3:ALA:HB2	1:A:6:LEU:HD12	2.03	0.40
1:B:408:ALA:HB1	1:B:495:TYR:CD1	2.57	0.40
2:E:65:GLY:HA3	2:E:70:TYR:HA	2.04	0.40
1:A:55:GLN:HA	1:A:56:HIS:HA	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:HIS:HA	1:B:189:GLY:O	2.22	0.40

There are no symmetry-related clashes.

## 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	526/542 (97%)	488 (93%)	36 (7%)	2 (0%)	38	66
1	B	526/542 (97%)	496 (94%)	28 (5%)	2 (0%)	38	66
2	C	210/213 (99%)	205 (98%)	4 (2%)	1 (0%)	32	60
2	E	211/213 (99%)	205 (97%)	5 (2%)	1 (0%)	32	60
3	D	224/234 (96%)	211 (94%)	13 (6%)	0	100	100
3	F	216/234 (92%)	205 (95%)	11 (5%)	0	100	100
All	All	1913/1978 (97%)	1810 (95%)	97 (5%)	6 (0%)	44	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	484	ASP
1	A	482	PRO
2	C	67	GLY
2	E	67	GLY
1	A	291	PRO
1	B	291	PRO

### 5.3.2 Protein sidechains [i](#)

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	448/457 (98%)	429 (96%)	19 (4%)	34	65
1	B	448/457 (98%)	432 (96%)	16 (4%)	40	70
2	C	186/187 (100%)	175 (94%)	11 (6%)	23	49
2	E	187/187 (100%)	177 (95%)	10 (5%)	26	54
3	D	194/201 (96%)	182 (94%)	12 (6%)	21	46
3	F	190/201 (94%)	176 (93%)	14 (7%)	16	37
All	All	1653/1690 (98%)	1571 (95%)	82 (5%)	28	57

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	143	LEU
1	A	161	SER
1	A	197	PHE
1	A	214	GLN
1	A	215	SER
1	A	216	ARG
1	A	217	THR
1	A	235	THR
1	A	236	VAL
1	A	237	THR
1	A	274	LEU
1	A	288	PHE
1	A	318	GLN
1	A	320	LEU
1	A	411	TYR
1	A	413	LYS
1	A	431	LEU
1	A	479	THR
1	B	58	LEU
1	B	143	LEU
1	B	161	SER
1	B	192	ARG
1	B	197	PHE
1	B	214	GLN
1	B	221	ARG

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Mol	Chain	Res	Type
1	B	235	THR
1	B	236	VAL
1	B	237	THR
1	B	274	LEU
1	B	288	PHE
1	B	320	LEU
1	B	411	TYR
1	B	431	LEU
1	B	483	THR
2	C	1	GLN
2	C	7	SER
2	C	11	MET
2	C	27	SER
2	C	36	HIS
2	C	77	VAL
2	C	90	TYR
2	C	91	ASN
2	C	121	SER
2	C	186	GLU
2	C	190	SER
3	D	13	GLN
3	D	21	SER
3	D	25	SER
3	D	66	VAL
3	D	91	GLU
3	D	98	CYS
3	D	140	SER
3	D	155	LYS
3	D	162	VAL
3	D	163	THR
3	D	171	LEU
3	D	198	SER
2	E	1	GLN
2	E	7	SER
2	E	11	MET
2	E	27	SER
2	E	36	HIS
2	E	77	VAL
2	E	90	TYR
2	E	91	ASN
2	E	180	LEU
2	E	190	SER

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Mol	Chain	Res	Type
3	F	13	GLN
3	F	21	SER
3	F	25	SER
3	F	66	VAL
3	F	91	GLU
3	F	98	CYS
3	F	100	ARG
3	F	162	VAL
3	F	163	THR
3	F	165	THR
3	F	171	LEU
3	F	172	SER
3	F	198	SER
3	F	208	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	374	GLN
1	A	406	GLN
1	B	11	GLN
1	B	190	ASN
1	B	209	HIS
1	B	220	GLN
1	B	318	GLN
1	B	504	GLN
2	C	36	HIS
2	C	93	HIS
3	F	35	HIS
3	F	208	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

25 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	$\# Z  > 2$
4	NAG	A	601	4,6	14,14,15	0.25	0	15,19,21	0.44	0
5	MAN	A	602	6	11,11,12	0.31	0	13,15,17	0.83	1 (7%)
6	BMA	A	603	5,4	11,11,12	0.37	0	13,15,17	1.04	2 (15%)
5	MAN	A	604	6	11,11,12	0.41	0	13,15,17	1.07	1 (7%)
4	NAG	A	605	1,4,7	14,14,15	0.41	0	15,19,21	2.14	3 (20%)
7	FUC	A	606	4	9,10,11	0.51	0	13,14,16	1.06	1 (7%)
4	NAG	A	607	4,6	14,14,15	0.24	0	15,19,21	0.81	1 (6%)
4	NAG	A	608	1,4	14,14,15	0.19	0	15,19,21	1.20	2 (13%)
5	MAN	A	609	6	11,11,12	0.25	0	13,15,17	1.00	1 (7%)
6	BMA	A	610	5,4	11,11,12	0.30	0	13,15,17	1.15	1 (7%)
5	MAN	A	611	6	11,11,12	0.46	0	13,15,17	1.04	1 (7%)
8	EDO	A	612	-	3,3,3	0.74	0	2,2,2	0.21	0
4	NAG	B	601	4,6	14,14,15	0.28	0	15,19,21	0.42	0
4	NAG	B	602	1,4,7	14,14,15	0.37	0	15,19,21	2.29	3 (20%)
7	FUC	B	603	4	9,10,11	0.52	0	13,14,16	1.11	1 (7%)
5	MAN	B	604	6	11,11,12	0.34	0	13,15,17	0.82	0
6	BMA	B	605	5,4	11,11,12	0.36	0	13,15,17	1.15	2 (15%)
5	MAN	B	606	6	11,11,12	0.41	0	13,15,17	1.09	1 (7%)
4	NAG	B	607	4,6	14,14,15	0.28	0	15,19,21	0.65	1 (6%)
4	NAG	B	608	1,4	14,14,15	0.25	0	15,19,21	1.21	2 (13%)
5	MAN	B	609	6	11,11,12	0.26	0	13,15,17	0.92	1 (7%)
6	BMA	B	610	5,4	11,11,12	0.24	0	13,15,17	1.13	1 (7%)
5	MAN	B	611	6	11,11,12	0.49	0	13,15,17	1.06	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	612	1	14,14,15	0.32	0	15,19,21	0.90	1 (6%)
8	EDO	B	613	-	3,3,3	0.78	0	2,2,2	0.12	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	601	4,6	-	0/6/23/26	0/1/1/1
5	MAN	A	602	6	-	0/2/19/22	0/1/1/1
6	BMA	A	603	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	604	6	-	0/2/19/22	0/1/1/1
4	NAG	A	605	1,4,7	-	0/6/23/26	0/1/1/1
7	FUC	A	606	4	-	0/0/17/20	0/1/1/1
4	NAG	A	607	4,6	-	0/6/23/26	0/1/1/1
4	NAG	A	608	1,4	-	0/6/23/26	0/1/1/1
5	MAN	A	609	6	-	0/2/19/22	0/1/1/1
6	BMA	A	610	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	611	6	-	0/2/19/22	0/1/1/1
8	EDO	A	612	-	-	0/1/1/1	0/0/0/0
4	NAG	B	601	4,6	-	0/6/23/26	0/1/1/1
4	NAG	B	602	1,4,7	-	0/6/23/26	0/1/1/1
7	FUC	B	603	4	-	0/0/17/20	0/1/1/1
5	MAN	B	604	6	-	0/2/19/22	0/1/1/1
6	BMA	B	605	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	606	6	-	0/2/19/22	0/1/1/1
4	NAG	B	607	4,6	-	0/6/23/26	0/1/1/1
4	NAG	B	608	1,4	-	0/6/23/26	0/1/1/1
5	MAN	B	609	6	-	0/2/19/22	0/1/1/1
6	BMA	B	610	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	611	6	-	0/2/19/22	0/1/1/1
4	NAG	B	612	1	-	0/6/23/26	0/1/1/1
8	EDO	B	613	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	NAG	O5-C1-C2	-5.10	104.37	111.47
4	A	605	NAG	O5-C1-C2	-4.76	104.85	111.47
4	A	608	NAG	O5-C1-C2	-2.77	107.62	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	608	NAG	O5-C1-C2	-2.61	107.84	111.47
6	A	603	BMA	C1-O5-C5	2.05	114.99	112.17
5	A	602	MAN	C1-O5-C5	2.11	115.07	112.17
4	B	607	NAG	C1-O5-C5	2.16	115.14	112.17
4	A	607	NAG	C1-O5-C5	2.55	115.68	112.17
6	B	605	BMA	O3-C3-C2	2.75	115.03	110.02
6	A	603	BMA	O3-C3-C2	2.79	115.10	110.02
6	B	605	BMA	C1-O5-C5	2.81	116.05	112.17
4	B	612	NAG	C1-C2-N2	2.84	115.35	110.49
7	A	606	FUC	C1-O5-C5	2.89	118.78	112.39
5	B	609	MAN	C1-O5-C5	2.89	116.16	112.17
5	A	609	MAN	C1-O5-C5	3.09	116.43	112.17
6	A	610	BMA	C1-O5-C5	3.18	116.55	112.17
4	B	608	NAG	C1-O5-C5	3.19	116.57	112.17
6	B	610	BMA	C1-O5-C5	3.21	116.59	112.17
7	B	603	FUC	C1-O5-C5	3.23	119.54	112.39
4	A	605	NAG	C2-N2-C7	3.29	127.74	122.94
4	A	608	NAG	C1-O5-C5	3.44	116.91	112.17
5	A	611	MAN	C1-O5-C5	3.45	116.92	112.17
5	B	611	MAN	C1-O5-C5	3.45	116.92	112.17
5	A	604	MAN	C1-O5-C5	3.52	117.01	112.17
5	B	606	MAN	C1-O5-C5	3.60	117.13	112.17
4	B	602	NAG	C2-N2-C7	4.44	129.42	122.94
4	B	602	NAG	C1-C2-N2	5.32	119.58	110.49
4	A	605	NAG	C1-C2-N2	5.44	119.78	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

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	529/542 (97%)	0.26	25 (4%)	32 30	28, 66, 105, 135	0
1	B	529/542 (97%)	0.25	24 (4%)	34 32	33, 65, 100, 135	0
2	C	212/213 (99%)	-0.32	1 (0%)	90 92	30, 43, 66, 103	0
2	E	212/213 (99%)	-0.20	4 (1%)	67 68	25, 47, 76, 100	0
3	D	225/234 (96%)	-0.14	7 (3%)	49 49	33, 51, 79, 122	0
3	F	219/234 (93%)	-0.13	2 (0%)	84 85	31, 59, 91, 124	0
All	All	1926/1978 (97%)	0.05	63 (3%)	47 46	25, 57, 96, 135	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	145	ASN	7.4
1	B	56	HIS	7.0
3	D	143	GLN	6.2
1	B	3	ALA	4.8
1	A	486	ALA	4.7
1	A	108	ASP	4.7
1	A	256	PHE	4.3
1	A	535	THR	4.3
1	B	535	THR	4.2
1	A	3	ALA	4.1
3	D	141	ALA	4.0
3	D	144	THR	4.0
3	D	140	SER	3.8
1	B	42	ARG	3.7
3	D	142	ALA	3.7
1	A	160	GLY	3.4
1	A	255	HIS	3.4
3	D	139	GLY	3.4
1	B	4	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	56	HIS	2.9
3	F	222	ILE	2.9
1	A	157	GLY	2.8
1	B	534	ALA	2.8
1	B	185	HIS	2.8
1	A	42	ARG	2.8
1	A	158	LEU	2.8
1	B	262	LEU	2.8
1	B	58	LEU	2.7
1	B	108	ASP	2.7
1	B	257	ASN	2.7
1	A	162	PRO	2.6
1	B	253	GLY	2.6
2	E	212	GLU	2.5
1	A	485	PRO	2.5
1	B	268	SER	2.5
1	B	255	HIS	2.4
1	B	261	GLU	2.4
1	A	107	LYS	2.4
3	F	171	LEU	2.4
1	B	7	LYS	2.4
1	B	266	LEU	2.4
1	A	274	LEU	2.3
1	A	534	ALA	2.2
1	A	4	GLY	2.2
1	B	107	LYS	2.2
1	B	164	ALA	2.2
1	B	54	TRP	2.2
1	A	104	PRO	2.2
1	A	262	LEU	2.2
1	A	58	LEU	2.2
1	A	296	ILE	2.1
1	A	41	GLY	2.1
2	E	124	LEU	2.1
2	C	211	ASN	2.1
1	A	297	ASP	2.1
1	B	117	GLY	2.1
1	B	256	PHE	2.1
1	A	189	GLY	2.1
1	A	45	PHE	2.1
1	B	254	CYS	2.0
1	B	158	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	125	THR	2.0
2	E	168	LYS	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](#)

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. 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
8	EDO	B	613	4/4	0.89	0.23	2.75	52,56,60,63	0
4	NAG	B	608	14/15	0.92	0.21	0.80	55,57,63,63	0
4	NAG	A	608	14/15	0.95	0.19	0.73	42,49,56,62	0
8	EDO	A	612	4/4	0.94	0.15	0.59	44,44,49,50	0
4	NAG	A	605	14/15	0.95	0.19	0.52	40,42,60,64	0
4	NAG	A	601	14/15	0.95	0.19	0.06	59,63,77,87	0
4	NAG	A	607	14/15	0.96	0.15	0.03	40,49,56,60	0
5	MAN	A	609	11/12	0.93	0.17	-0.08	59,61,67,71	0
7	FUC	A	606	10/11	0.96	0.13	-0.13	31,40,44,46	0
4	NAG	B	601	14/15	0.95	0.15	-0.42	59,70,79,83	0
5	MAN	B	609	11/12	0.96	0.18	-0.47	65,69,71,73	0
7	FUC	B	603	10/11	0.97	0.12	-0.48	25,39,41,42	0
4	NAG	B	607	14/15	0.93	0.14	-	59,61,63,65	0
6	BMA	A	603	11/12	0.83	0.19	-	101,114,125,132	0
5	MAN	B	604	11/12	0.74	0.25	-	107,110,112,113	0
6	BMA	B	605	11/12	0.80	0.17	-	94,102,107,108	0
5	MAN	B	611	11/12	0.45	0.40	-	97,105,110,112	0
6	BMA	A	610	11/12	0.97	0.11	-	50,57,74,84	0
4	NAG	B	602	14/15	0.90	0.19	-	38,46,60,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	BMA	B	610	11/12	0.95	0.10	-	68,73,89,97	0
5	MAN	A	611	11/12	0.62	0.32	-	93,98,103,105	0
5	MAN	A	604	11/12	0.75	0.42	-	138,143,145,145	0
4	NAG	B	612	14/15	0.67	0.39	-	111,117,118,119	0
5	MAN	B	606	11/12	0.78	0.22	-	111,114,118,119	0
5	MAN	A	602	11/12	0.72	0.24	-	115,117,118,119	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.