



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:07 am GMT

PDB ID : 4UT6
Title : Crystal structure of dengue 2 virus envelope glycoprotein in complex with the Fab fragment of the broadly neutralizing human antibody EDE2 B7
Authors : Rouvinski, A.; Guardado-Calvo, P.; Barba-Spaeth, G.; Duquerroy, S.; Vaney, M.C.; Rey, F.A.
Deposited on : 2014-07-18
Resolution : 3.20 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : trunk28620
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) : recalc28949

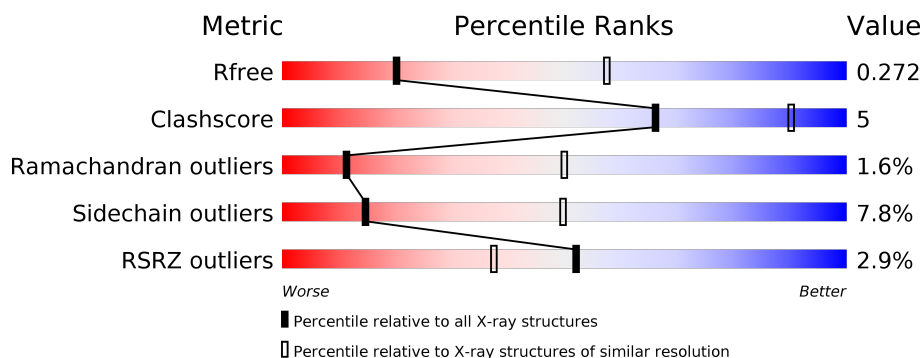
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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 ≥ 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	422	<div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 7%</div> </div> </div>
1	B	422	<div> <div> <div>3%</div> <div>76%</div> <div>16%</div> <div>• 7%</div> </div> </div>
2	H	283	<div> <div> <div></div> <div>38%</div> <div>8%</div> <div>54%</div> </div> </div>
2	I	283	<div> <div> <div>2%</div> <div>39%</div> <div>7%</div> <div>• 54%</div> </div> </div>
3	L	218	<div> <div> <div>2%</div> <div>39%</div> <div>8%</div> <div>• 51%</div> </div> </div>
3	M	218	<div> <div> <div>4%</div> <div>39%</div> <div>10%</div> <div>51%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	567	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9869 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 ENVELOPE GLYCOPROTEIN E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3059	1926	527	582	24			
1	B	391	Total	C	N	O	S	0	0	0
			3036	1911	523	578	24			

- Molecule 2 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 B7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	130	Total	C	N	O	S	0	0	0
			1012	639	175	193	5			
2	I	130	Total	C	N	O	S	0	0	0
			1012	639	175	193	5			

- Molecule 3 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	106	Total	C	N	O	S	0	0	0
			773	480	130	160	3			
3	M	107	Total	C	N	O	S	0	0	0
			781	486	131	161	3			

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	6	Total	C	N	O	0	0
			71	40	2	29		
4	B	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

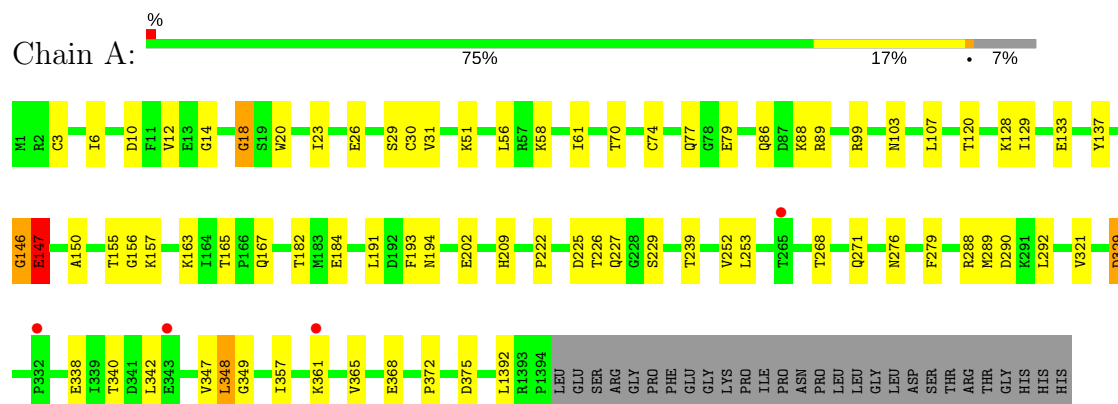
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	8	Total	O	0	0
			8	8		
6	H	1	Total	O	0	0
			1	1		
6	I	2	Total	O	0	0
			2	2		
6	L	2	Total	O	0	0
			2	2		

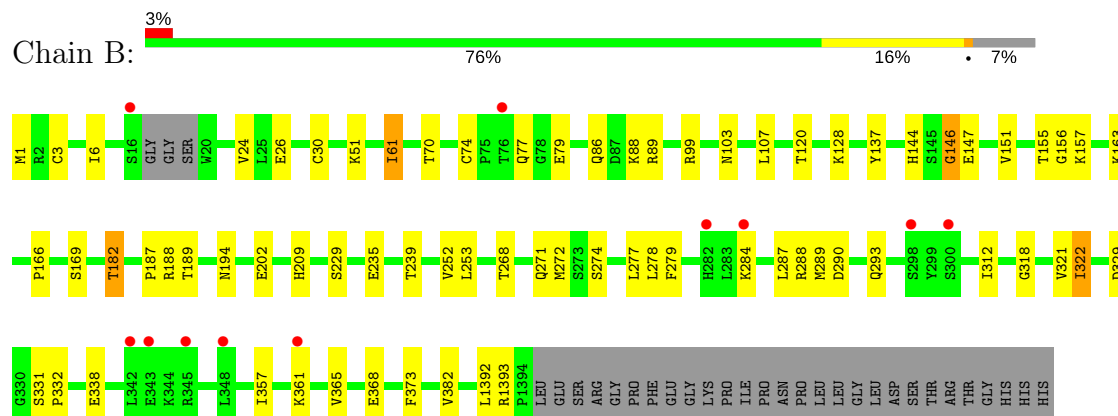
3 Residue-property plots [i](#)

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.

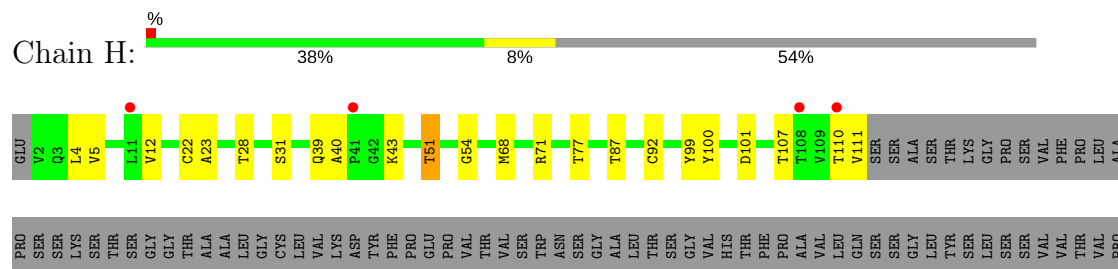
• Molecule 1: ENVELOPE GLYCOPROTEIN E



• Molecule 1: ENVELOPE GLYCOPROTEIN E



• Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 B7



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.28Å 58.98Å 191.57Å 90.00° 96.20° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 29.73 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-3.20) 98.6 (29.73-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.212 , 0.250 0.229 , 0.272	Depositor DCC
R_{free} test set	1990 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	76.2	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9869	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 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	0.42	0/3121	0.68	0/4220
1	B	0.42	0/3095	0.68	0/4183
2	H	0.37	0/1040	0.64	0/1411
2	I	0.40	0/1040	0.65	0/1411
3	L	0.40	0/788	0.67	1/1068 (0.1%)
3	M	0.40	0/796	0.65	0/1079
All	All	0.41	0/9880	0.67	1/13372 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	25	GLY	C-N-CA	5.05	134.34	121.70

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	3059	0	3056	28	0
1	B	3036	0	3036	21	0
2	H	1012	0	945	9	0
2	I	1012	0	945	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	773	0	747	9	0
3	M	781	0	758	12	0
4	A	71	0	61	2	0
4	B	71	0	61	2	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	13	0	0	0	0
6	B	8	0	0	0	0
6	H	1	0	0	0	0
6	I	2	0	0	0	0
6	L	2	0	0	0	0
All	All	9869	0	9635	89	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 (89) 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:26:GLU:HG2	1:A:29:SER:HB2	1.62	0.81
1:A:155:THR:HG21	2:I:31:SER:HB2	1.66	0.78
3:M:19:ILE:HG13	3:M:20:THR:H	1.56	0.70
1:A:56:LEU:HD22	1:A:129:ILE:HD11	1.78	0.65
1:A:342:LEU:HD11	1:A:375:ASP:HB2	1.81	0.61
1:B:24:VAL:HG22	1:B:284:LYS:HG3	1.82	0.61
1:A:14:GLY:HA3	1:A:18:GLY:HA2	1.83	0.61
1:B:166:PRO:HB3	1:B:187:PRO:HB3	1.83	0.60
3:L:65:SER:HB3	3:L:72:SER:HB2	1.84	0.59
3:M:65:SER:HB3	3:M:72:SER:HB2	1.84	0.59
1:A:348:LEU:HB2	1:A:372:PRO:HG3	1.83	0.59
2:I:19:LYS:HG3	2:I:81:HIS:HD1	1.68	0.59
1:A:56:LEU:HB2	1:A:129:ILE:HD13	1.86	0.58
1:B:155:THR:HG21	2:H:31:SER:HB2	1.87	0.57
1:A:56:LEU:HB2	1:A:129:ILE:CD1	2.35	0.56
1:A:222:PRO:HD2	1:A:225:ASP:HB3	1.89	0.55
4:A:501:NAG:H5	2:I:99:TYR:CE2	2.41	0.55
1:A:146:GLY:HA3	1:A:365:VAL:HG13	1.88	0.55
3:L:4:LEU:HA	3:L:25:GLY:HA3	1.89	0.55
1:B:146:GLY:HA3	1:B:365:VAL:HG13	1.88	0.55
1:A:58:LYS:NZ	1:A:226:THR:HG23	2.22	0.54
2:I:87:THR:HG23	2:I:110:THR:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:HG11	1:A:23:ILE:HG22	1.89	0.54
1:A:20:TRP:CD1	1:A:288:ARG:HG2	2.43	0.53
2:H:51:THR:HG22	2:H:54:GLY:HA2	1.90	0.53
2:I:51:THR:HG22	2:I:54:GLY:HA2	1.91	0.53
3:M:63:SER:HB2	3:M:74:ALA:HB3	1.90	0.53
2:H:87:THR:HG23	2:H:110:THR:HA	1.89	0.53
1:A:10:ASP:HB2	1:A:31:VAL:HG22	1.91	0.53
3:M:33:VAL:HG11	3:M:71:ALA:HB1	1.91	0.53
3:M:4:LEU:HA	3:M:25:GLY:HA3	1.91	0.53
3:L:63:SER:HB2	3:L:74:ALA:HB3	1.91	0.52
3:L:33:VAL:HG11	3:L:71:ALA:HB1	1.91	0.52
1:B:89:ARG:HG2	1:B:229:SER:HB2	1.92	0.52
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.92	0.52
2:H:23:ALA:HA	2:H:77:THR:HG22	1.91	0.52
1:A:155:THR:HG21	2:I:31:SER:CB	2.39	0.51
2:I:23:ALA:HA	2:I:77:THR:HG22	1.91	0.51
1:B:271:GLN:HB2	1:B:278:LEU:HB2	1.92	0.51
1:A:137:TYR:O	1:A:163:LYS:HA	2.11	0.50
1:B:321:VAL:HG22	1:B:368:GLU:HG3	1.94	0.50
1:B:277:LEU:HB2	1:B:279:PHE:CE2	2.46	0.50
1:B:137:TYR:O	1:B:163:LYS:HA	2.11	0.50
1:A:89:ARG:HG2	1:A:229:SER:HB3	1.93	0.50
3:M:24:THR:HB	3:M:70:THR:HG23	1.94	0.49
1:A:342:LEU:HD11	1:A:375:ASP:CB	2.41	0.49
2:H:12:VAL:HG13	2:H:111:VAL:HB	1.95	0.49
2:I:5:VAL:HG23	2:I:23:ALA:HB3	1.93	0.49
1:A:321:VAL:HG22	1:A:368:GLU:HG3	1.95	0.49
3:M:19:ILE:CG1	3:M:20:THR:H	2.24	0.49
1:A:340:THR:HG22	1:A:347:VAL:HA	1.95	0.48
2:I:19:LYS:HG3	2:I:81:HIS:ND1	2.29	0.48
3:M:19:ILE:HG13	3:M:20:THR:N	2.27	0.48
2:H:4:LEU:HG	2:H:92:CYS:SG	2.54	0.47
3:L:21:ILE:HD11	3:L:104:LEU:HD13	1.95	0.47
1:B:373:PHE:HA	1:B:1393:ARG:HB3	1.95	0.47
4:A:503:NAG:H4	2:I:100:TYR:CE1	2.50	0.47
3:L:23:CYS:HB3	3:L:71:ALA:HB3	1.96	0.47
3:M:92:ALA:HB3	3:M:95(A):SER:HB2	1.97	0.47
3:M:23:CYS:HB3	3:M:71:ALA:HB3	1.98	0.46
3:L:24:THR:HB	3:L:70:THR:HG23	1.97	0.46
1:A:20:TRP:HD1	1:A:288:ARG:HG2	1.80	0.46
1:B:188:ARG:HG3	1:B:284:LYS:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:92:ALA:HB3	3:L:95(A):SER:HB2	1.97	0.46
1:B:312:ILE:HG12	1:B:322:ILE:HG23	1.97	0.46
2:I:40:ALA:HB3	2:I:43:LYS:HB2	1.98	0.45
4:B:503:NAG:H4	2:H:100:TYR:CE1	2.50	0.45
1:B:1:MET:HG2	1:B:144:HIS:HA	1.99	0.45
1:B:318:GLY:HA3	1:B:1393:ARG:HH21	1.81	0.45
1:A:147:GLU:HB3	1:A:150:ALA:HB2	1.99	0.44
3:L:47:ILE:HA	3:L:58:VAL:HG21	2.00	0.44
3:M:47:ILE:HA	3:M:58:VAL:HG21	1.99	0.44
1:B:329:ASP:HA	1:B:361:LYS:HE2	2.00	0.44
1:B:331:SER:HA	1:B:332:PRO:C	2.38	0.44
1:B:74:CYS:O	1:B:77:GLN:HB2	2.18	0.44
2:I:70:SER:HB2	2:I:79:TYR:HB2	1.99	0.43
1:A:133:GLU:HB3	1:A:167:GLN:HB2	2.01	0.43
1:B:3:CYS:HA	1:B:6:ILE:HD12	2.01	0.43
1:A:3:CYS:HA	1:A:6:ILE:HD12	2.00	0.43
1:A:193:PHE:HZ	1:A:279:PHE:CE2	2.36	0.43
1:A:74:CYS:O	1:A:77:GLN:HB2	2.19	0.42
1:B:61:ILE:H	1:B:61:ILE:HG13	1.80	0.42
2:I:51:THR:HG23	2:I:57:THR:HG22	2.02	0.42
1:B:99:ARG:HA	1:B:103:ASN:HD21	1.85	0.41
1:A:99:ARG:HA	1:A:103:ASN:HD21	1.86	0.41
3:M:11:VAL:HG21	3:M:21:ILE:HG12	2.02	0.41
1:B:182:THR:HG23	1:B:288:ARG:HB2	2.02	0.41
4:B:501:NAG:H5	2:H:99:TYR:CE2	2.56	0.41
1:A:329:ASP:HA	1:A:361:LYS:HE2	2.02	0.41

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	392/422 (93%)	364 (93%)	20 (5%)	8 (2%)	9	44
1	B	387/422 (92%)	357 (92%)	21 (5%)	9 (2%)	7	40
2	H	128/283 (45%)	115 (90%)	12 (9%)	1 (1%)	22	65
2	I	128/283 (45%)	120 (94%)	8 (6%)	0	100	100
3	L	104/218 (48%)	90 (86%)	13 (12%)	1 (1%)	18	61
3	M	105/218 (48%)	90 (86%)	14 (13%)	1 (1%)	18	61
All	All	1244/1846 (67%)	1136 (91%)	88 (7%)	20 (2%)	11	50

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	LYS
1	B	157	LYS
3	L	26	ILE
1	A	146	GLY
1	A	147	GLU
1	A	194	ASN
1	A	202	GLU
1	B	194	ASN
3	M	26	ILE
1	B	147	GLU
1	B	202	GLU
1	A	349	GLY
1	B	274	SER
1	A	18	GLY
1	B	189	THR
2	H	101	ASP
1	A	156	GLY
1	B	146	GLY
1	B	151	VAL
1	B	156	GLY

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	342/366 (93%)	311 (91%)	31 (9%)	11	39
1	B	340/366 (93%)	311 (92%)	29 (8%)	12	44
2	H	107/235 (46%)	99 (92%)	8 (8%)	16	52
2	I	107/235 (46%)	101 (94%)	6 (6%)	25	64
3	L	85/181 (47%)	80 (94%)	5 (6%)	23	62
3	M	86/181 (48%)	82 (95%)	4 (5%)	30	69
All	All	1067/1564 (68%)	984 (92%)	83 (8%)	15	50

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	CYS
1	A	51	LYS
1	A	61	ILE
1	A	70	THR
1	A	79	GLU
1	A	86	GLN
1	A	88	LYS
1	A	107	LEU
1	A	120	THR
1	A	128	LYS
1	A	147	GLU
1	A	165	THR
1	A	182	THR
1	A	184	GLU
1	A	191	LEU
1	A	209	HIS
1	A	227	GLN
1	A	239	THR
1	A	252	VAL
1	A	253	LEU
1	A	268	THR
1	A	271	GLN
1	A	276	ASN
1	A	289	MET
1	A	290	ASP
1	A	292	LEU
1	A	329	ASP
1	A	338	GLU
1	A	348	LEU
1	A	357	ILE

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Mol	Chain	Res	Type
1	A	1392	LEU
1	B	26	GLU
1	B	30	CYS
1	B	51	LYS
1	B	61	ILE
1	B	70	THR
1	B	79	GLU
1	B	86	GLN
1	B	88	LYS
1	B	107	LEU
1	B	120	THR
1	B	128	LYS
1	B	169	SER
1	B	182	THR
1	B	209	HIS
1	B	235	GLU
1	B	239	THR
1	B	252	VAL
1	B	253	LEU
1	B	268	THR
1	B	272	MET
1	B	287	LEU
1	B	289	MET
1	B	290	ASP
1	B	293	GLN
1	B	322	ILE
1	B	338	GLU
1	B	357	ILE
1	B	382	VAL
1	B	1392	LEU
2	H	5	VAL
2	H	22	CYS
2	H	28	THR
2	H	39	GLN
2	H	51	THR
2	H	68	MET
2	H	71	ARG
2	H	107	THR
2	I	5	VAL
2	I	22	CYS
2	I	28	THR
2	I	39	GLN

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Mol	Chain	Res	Type
2	I	51	THR
2	I	78	VAL
3	L	26	ILE
3	L	69	ASN
3	L	70	THR
3	L	97	VAL
3	L	103	ARG
3	M	27(B)	ASP
3	M	70	THR
3	M	97	VAL
3	M	103	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	194	ASN
2	H	81	HIS
2	H	100(J)	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 ⓘ

12 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	0.29	0	15,19,21	0.56	0
4	FUC	A	502	4	9,10,11	0.43	0	13,14,16	1.40	2 (15%)
4	NAG	A	503	4	14,14,15	0.36	0	15,19,21	1.89	3 (20%)
4	BMA	A	504	4	11,11,12	0.45	0	13,15,17	1.34	2 (15%)
4	MAN	A	505	4	11,11,12	0.37	0	13,15,17	0.93	1 (7%)
4	MAN	A	506	4	11,11,12	0.46	0	13,15,17	1.04	2 (15%)
4	NAG	B	501	1,4	14,14,15	0.31	0	15,19,21	0.48	0
4	FUC	B	502	4	9,10,11	0.45	0	13,14,16	1.43	2 (15%)
4	NAG	B	503	4	14,14,15	0.32	0	15,19,21	1.87	3 (20%)
4	BMA	B	504	4	11,11,12	0.42	0	13,15,17	1.34	1 (7%)
4	MAN	B	505	4	11,11,12	0.32	0	13,15,17	0.85	1 (7%)
4	MAN	B	506	4	11,11,12	0.47	0	13,15,17	1.07	2 (15%)

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	FUC	A	502	4	-	0/0/17/20	0/1/1/1
4	NAG	A	503	4	-	0/6/23/26	0/1/1/1
4	BMA	A	504	4	-	0/2/19/22	1/1/1/1
4	MAN	A	505	4	-	0/2/19/22	0/1/1/1
4	MAN	A	506	4	-	0/2/19/22	0/1/1/1
4	NAG	B	501	1,4	-	0/6/23/26	0/1/1/1
4	FUC	B	502	4	-	0/0/17/20	0/1/1/1
4	NAG	B	503	4	-	0/6/23/26	0/1/1/1
4	BMA	B	504	4	-	0/2/19/22	1/1/1/1
4	MAN	B	505	4	-	0/2/19/22	0/1/1/1
4	MAN	B	506	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	BMA	C1-C2-C3	2.06	112.26	109.65
4	A	506	MAN	C1-C2-C3	2.08	112.29	109.65
4	B	506	MAN	C1-C2-C3	2.21	112.45	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	505	MAN	C1-O5-C5	2.22	115.22	112.17
4	B	502	FUC	C1-C2-C3	2.30	112.57	109.65
4	B	503	NAG	O4-C4-C5	2.30	115.09	109.28
4	A	502	FUC	C1-C2-C3	2.32	112.60	109.65
4	A	503	NAG	O4-C4-C5	2.49	115.56	109.28
4	A	505	MAN	C1-O5-C5	2.55	115.67	112.17
4	A	506	MAN	C1-O5-C5	2.78	116.00	112.17
4	B	506	MAN	C1-O5-C5	2.86	116.10	112.17
4	A	504	BMA	C1-O5-C5	3.22	116.61	112.17
4	A	502	FUC	C1-O5-C5	3.27	119.62	112.39
4	B	502	FUC	C1-O5-C5	3.48	120.09	112.39
4	B	504	BMA	C1-O5-C5	3.49	116.98	112.17
4	A	503	NAG	O5-C1-C2	4.41	117.60	111.47
4	B	503	NAG	O5-C1-C2	4.53	117.78	111.47
4	B	503	NAG	C1-O5-C5	4.79	118.76	112.17
4	A	503	NAG	C1-O5-C5	4.79	118.76	112.17

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	BMA	C1-C2-C3-C4-C5-O5
4	B	504	BMA	C1-C2-C3-C4-C5-O5

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	NAG	1	0
4	A	503	NAG	1	0
4	B	501	NAG	1	0
4	B	503	NAG	1	0

5.6 Ligand geometry

2 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	$\# Z > 2$
5	NAG	A	567	1	14,14,15	0.32	0	15,19,21	0.98	2 (13%)
5	NAG	B	567	1	14,14,15	0.36	0	15,19,21	0.84	1 (6%)

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
5	NAG	A	567	1	-	0/6/23/26	0/1/1/1
5	NAG	B	567	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	567	NAG	C1-C2-N2	-2.51	106.20	110.49
5	B	567	NAG	C1-C2-N2	-2.04	107.00	110.49
5	A	567	NAG	O5-C1-C2	2.08	114.37	111.47

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, 95th 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 ²)	Q<0.9
1	A	394/422 (93%)	-0.09	4 (1%) 82 72	50, 79, 115, 133	0
1	B	391/422 (92%)	0.02	11 (2%) 53 39	50, 88, 130, 151	0
2	H	130/283 (45%)	0.28	4 (3%) 49 33	66, 109, 169, 185	0
2	I	130/283 (45%)	0.18	6 (4%) 33 20	50, 100, 152, 171	0
3	L	106/218 (48%)	0.12	4 (3%) 41 27	78, 110, 131, 146	0
3	M	107/218 (49%)	0.13	8 (7%) 15 8	62, 89, 127, 153	0
All	All	1258/1846 (68%)	0.05	37 (2%) 52 37	50, 90, 137, 185	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	342	LEU	4.3
2	I	110	THR	4.2
3	M	28	GLU	3.8
2	H	11	LEU	3.3
1	B	16	SER	3.3
3	M	27(C)	VAL	3.2
1	B	348	LEU	3.0
2	H	41	PRO	3.0
2	H	110	THR	2.9
3	M	27(B)	ASP	2.8
3	M	40	PRO	2.8
2	I	13	GLN	2.7
2	H	108	THR	2.7
3	M	29	THR	2.7
1	B	343	GLU	2.6
1	B	300	SER	2.6
3	L	105	THR	2.6
1	A	265	THR	2.5
3	M	27	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	M	26	ILE	2.5
2	I	14	PRO	2.4
3	L	104	LEU	2.4
1	B	361	LYS	2.4
3	L	27(B)	ASP	2.3
1	A	343	GLU	2.3
1	A	332	PRO	2.3
1	B	284	LYS	2.2
1	B	282	HIS	2.2
1	A	361	LYS	2.2
1	B	298	SER	2.2
2	I	41	PRO	2.1
2	I	11	LEU	2.1
1	B	76	THR	2.1
1	B	345	ARG	2.1
2	I	42	GLY	2.0
3	M	25	GLY	2.0
3	L	106	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
4	MAN	A	506	11/12	0.81	0.30	0.96	111,113,116,116	0
4	NAG	A	501	14/15	0.91	0.19	-0.51	62,72,76,78	0
4	MAN	B	506	11/12	0.93	0.23	-0.54	119,121,123,125	0
4	NAG	B	501	14/15	0.94	0.16	-0.93	89,93,96,97	0
4	BMA	B	504	11/12	0.86	0.17	-0.93	107,112,118,118	0
4	FUC	B	502	10/11	0.94	0.22	-	80,91,95,96	0
4	FUC	A	502	10/11	0.97	0.19	-	67,68,72,73	0
4	MAN	B	505	11/12	0.87	0.21	-	119,122,126,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	503	14/15	0.96	0.17	-	73,82,87,89	0
4	MAN	A	505	11/12	0.84	0.28	-	108,111,118,119	0
4	NAG	B	503	14/15	0.94	0.20	-	92,102,107,108	0
4	BMA	A	504	11/12	0.91	0.17	-	94,97,105,107	0

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, 95th 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(\AA^2)	Q<0.9
5	NAG	A	567	14/15	0.62	0.41	2.60	140,142,144,145	0
5	NAG	B	567	14/15	0.72	0.43	-	135,140,142,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.