



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3N85  
Title : Crystallographic trimer of HER2 extracellular regions in complex with tryptophan-rich antibody fragment  
Authors : Eigenbrot, C.  
Deposited on : 2010-05-27  
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](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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

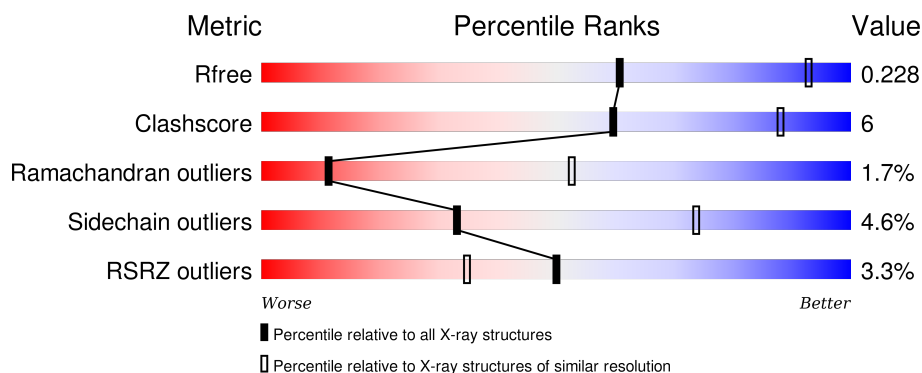
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	624	<div> <div>3%</div> <div>82%</div> <div>13%</div> <div>..</div> </div>
2	L	217	<div> <div>%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
3	H	224	<div> <div>4%</div> <div>86%</div> <div>8%</div> <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	SO4	A	633	-	-	-	X
5	SO4	A	636	-	-	-	X
6	NAG	A	1165	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8114 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 Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	0	0
			4657	2891	833	877	56			

- Molecule 2 is a protein called Fab37 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	1	0
			1669	1051	279	333	6			

- Molecule 3 is a protein called Fab37 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	214	Total	C	N	O	S	0	1	0
			1619	1032	270	311	6			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	4	Total	C	N	O	0	0
			49	28	2	19		

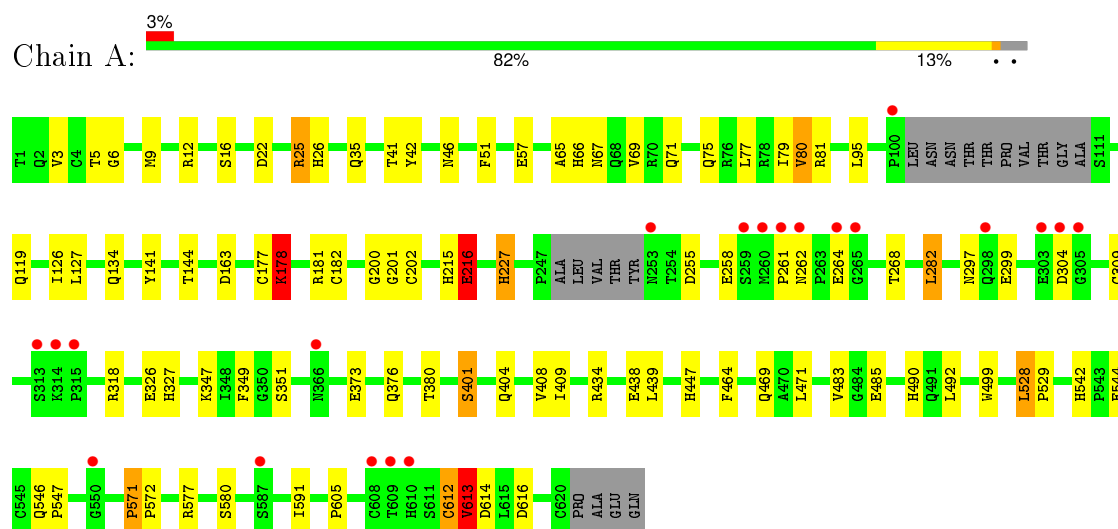
- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	3	Total	C	N	O	0	0
			39	22	2	15		

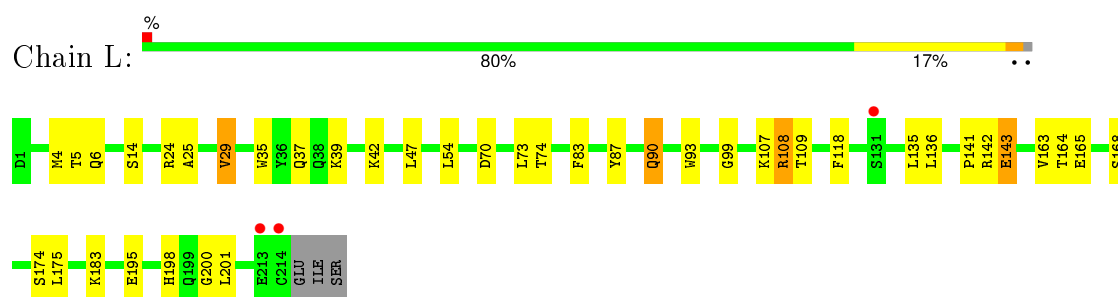
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

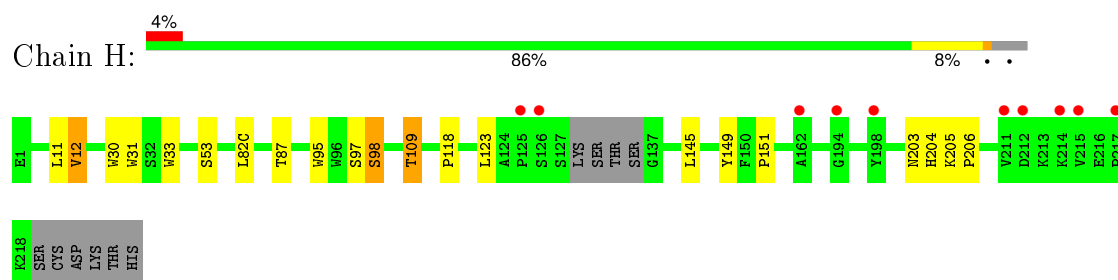
- Molecule 1: Receptor tyrosine-protein kinase erbB-2



- Molecule 2: Fab37 Light Chain



- Molecule 3: Fab37 Heavy Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.22Å 182.22Å 330.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 48.38 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-3.20) 96.3 (48.38-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.206 , 0.230 0.205 , 0.228	Depositor DCC
$R_{free}$ test set	1636 reflections (3.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 52198 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CL, BMA, NAG, FUC, SO4

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	0.37	1/4768 (0.0%)	0.55	0/6486
2	L	0.36	0/1711	0.53	0/2327
3	H	0.33	0/1667	0.50	0/2280
All	All	0.36	1/8146 (0.0%)	0.54	0/11093

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	485	GLU	CD-OE2	7.43	1.33	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4657	0	4440	58	0
2	L	1669	0	1610	22	0
3	H	1619	0	1565	13	0
4	A	1	0	0	0	0
5	A	65	0	0	0	0
5	H	5	0	0	0	0
5	L	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	49	0	43	2	0
7	A	39	0	34	0	0
All	All	8114	0	7692	90	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 6.

All (90) 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:25:ARG:HH11	1:A:25:ARG:HG2	1.09	1.10
1:A:326:GLU:HG3	1:A:327:HIS:H	1.33	0.91
1:A:408:VAL:HG12	1:A:438:GLU:HB3	1.57	0.84
1:A:25:ARG:NH1	1:A:25:ARG:HG2	1.87	0.82
1:A:528:LEU:HB2	1:A:529:PRO:CD	2.11	0.80
2:L:90:GLN:HE22	2:L:93:TRP:H	1.30	0.79
1:A:528:LEU:CB	1:A:529:PRO:HD3	2.13	0.78
1:A:326:GLU:HG3	1:A:327:HIS:N	1.98	0.78
1:A:528:LEU:CB	1:A:529:PRO:CD	2.65	0.75
2:L:24:ARG:NH1	2:L:70:ASP:HB2	2.04	0.71
2:L:24:ARG:HH11	2:L:70:ASP:HB2	1.55	0.71
1:A:144:THR:CG2	1:A:181:ARG:HA	2.21	0.70
1:A:144:THR:HG23	1:A:181:ARG:HA	1.72	0.69
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.75	0.67
1:A:25:ARG:HH11	1:A:25:ARG:CG	1.97	0.67
3:H:87:THR:HG23	3:H:109:THR:HA	1.76	0.66
1:A:25:ARG:HG3	1:A:51:PHE:CD2	2.33	0.64
2:L:6:GLN:HE21	2:L:99:GLY:HA3	1.61	0.63
1:A:144:THR:HG21	1:A:182:CYS:H	1.63	0.63
1:A:215:HIS:CD2	1:A:227:HIS:HB3	2.35	0.62
1:A:401:SER:O	1:A:404:GLN:HB2	1.99	0.61
1:A:141:TYR:O	1:A:144:THR:HB	2.01	0.61
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.81	0.61
1:A:297:ASN:HD22	1:A:309:CYS:HB3	1.67	0.60
1:A:528:LEU:HB2	1:A:529:PRO:HD3	1.77	0.59
1:A:178:LYS:HD2	1:A:178:LYS:H	1.68	0.58
6:A:1165:NAG:H61	6:A:1170:FUC:H5	1.86	0.57
2:L:118:PHE:CD1	3:H:123:LEU:HB3	2.39	0.57
1:A:546:GLN:HE21	1:A:547:PRO:HD2	1.69	0.57
1:A:542:HIS:HD2	1:A:544:GLU:H	1.53	0.57
2:L:164:THR:HG22	2:L:165:GLU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:LYS:HG3	2:L:42:LYS:HE3	1.87	0.55
2:L:198:HIS:CD2	2:L:200:GLY:H	2.25	0.55
2:L:6:GLN:HE22	2:L:87:TYR:HA	1.72	0.55
2:L:142:ARG:HD2	2:L:163:VAL:HG11	1.88	0.54
1:A:9:MET:HA	1:A:12:ARG:HH12	1.73	0.53
2:L:29:VAL:HG21	2:L:90:GLN:HB2	1.90	0.53
1:A:144:THR:CG2	1:A:182:CYS:H	2.22	0.53
6:A:1165:NAG:H61	6:A:1170:FUC:H3	1.91	0.53
1:A:282:LEU:HD21	1:A:299:GLU:HG3	1.89	0.53
1:A:490:HIS:HD2	1:A:492:LEU:HB2	1.75	0.52
3:H:123:LEU:HD11	3:H:145:LEU:HB2	1.93	0.51
2:L:35:TRP:CD2	2:L:73:LEU:HB2	2.46	0.51
1:A:376:GLN:HG2	3:H:31:TRP:NE1	2.24	0.51
3:H:33:TRP:HB3	3:H:95:TRP:HB3	1.93	0.51
3:H:11:LEU:HB2	3:H:151:PRO:HG3	1.93	0.51
1:A:528:LEU:HB2	1:A:529:PRO:HD2	1.91	0.50
1:A:57:GLU:HG3	1:A:79:ILE:HG23	1.92	0.50
2:L:136:LEU:HB2	2:L:175:LEU:HB3	1.94	0.50
1:A:376:GLN:HG2	3:H:31:TRP:HE1	1.76	0.50
3:H:205:LYS:HB2	3:H:206:PRO:HD3	1.93	0.49
1:A:25:ARG:NH1	1:A:25:ARG:CG	2.62	0.49
1:A:542:HIS:CD2	1:A:544:GLU:H	2.31	0.48
1:A:434:ARG:HA	1:A:499:TRP:CD1	2.49	0.48
3:H:12:VAL:HG21	3:H:82(C):LEU:HD13	1.96	0.47
1:A:612:CYS:O	1:A:613:VAL:HG13	2.15	0.47
3:H:118:PRO:HD3	3:H:204:HIS:CD2	2.50	0.47
2:L:29:VAL:CG2	2:L:90:GLN:HB2	2.44	0.47
1:A:215:HIS:CG	1:A:227:HIS:HB3	2.50	0.47
2:L:141:PRO:O	2:L:198:HIS:HE1	1.98	0.46
1:A:41:THR:HA	1:A:65:ALA:O	2.16	0.46
1:A:42:TYR:HA	1:A:66:HIS:O	2.15	0.46
1:A:376:GLN:CG	3:H:31:TRP:HE1	2.29	0.45
1:A:5:THR:HG22	1:A:6:GLY:N	2.32	0.45
1:A:490:HIS:CD2	1:A:492:LEU:H	2.35	0.45
1:A:81:ARG:HG2	1:A:127:LEU:HD12	1.98	0.45
2:L:164:THR:HB	2:L:174:SER:H	1.82	0.45
1:A:571:PRO:HA	1:A:572:PRO:HA	1.72	0.44
1:A:326:GLU:CG	1:A:327:HIS:N	2.71	0.44
1:A:16:SER:HB3	1:A:447:HIS:CE1	2.53	0.43
1:A:347:LYS:HE2	1:A:349:PHE:CZ	2.53	0.43
1:A:409:ILE:HB	1:A:439:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASN:HB3	1:A:69:VAL:HG12	2.00	0.43
2:L:143:GLU:H	2:L:143:GLU:CD	2.22	0.43
1:A:216:GLU:HG3	1:A:216:GLU:H	1.45	0.43
1:A:178:LYS:CD	1:A:178:LYS:H	2.32	0.43
1:A:80:VAL:HG22	1:A:126:ILE:HG12	2.01	0.42
2:L:108:ARG:HD3	2:L:109:THR:O	2.20	0.42
1:A:404:GLN:NE2	3:H:53:SER:O	2.52	0.42
3:H:118:PRO:HB3	3:H:149:TYR:HB3	2.01	0.42
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.56	0.41
1:A:577:ARG:HH12	1:A:580:SER:HB2	1.86	0.41
1:A:134:GLN:HA	1:A:163:ASP:HB3	2.02	0.41
1:A:75:GLN:NE2	1:A:119:GLN:HB3	2.36	0.41
1:A:65:ALA:HA	1:A:95:LEU:O	2.21	0.40
1:A:3:VAL:HG13	1:A:35:GLN:HG2	2.04	0.40
1:A:22:ASP:O	1:A:26:HIS:HD2	2.03	0.40
1:A:464:PHE:HB3	1:A:469:GLN:HG3	2.04	0.40
2:L:83[B]:PHE:HE2	2:L:168:SER:HB3	1.85	0.40
2:L:4:MET:HE2	2:L:25:ALA:HA	2.04	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	599/624 (96%)	542 (90%)	42 (7%)	15 (2%)	7	41
2	L	213/217 (98%)	204 (96%)	9 (4%)	0	100	100
3	H	211/224 (94%)	201 (95%)	8 (4%)	2 (1%)	21	67
All	All	1023/1065 (96%)	947 (93%)	59 (6%)	17 (2%)	11	52

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	CYS
1	A	528	LEU
1	A	178	LYS
1	A	216	GLU
1	A	264	GLU
1	A	605	PRO
1	A	614	ASP
1	A	616	ASP
3	H	97	SER
1	A	200	GLY
1	A	612	CYS
3	H	98	SER
1	A	261	PRO
1	A	262	ASN
1	A	571	PRO
1	A	201	GLY
1	A	613	VAL

### 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	523/538 (97%)	500 (96%)	23 (4%)	35	74
2	L	190/192 (99%)	177 (93%)	13 (7%)	20	59
3	H	178/187 (95%)	172 (97%)	6 (3%)	44	80
All	All	891/917 (97%)	849 (95%)	42 (5%)	33	73

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	46	ASN
1	A	71	GLN
1	A	77	LEU
1	A	80	VAL
1	A	177	CYS

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Mol	Chain	Res	Type
1	A	178	LYS
1	A	216	GLU
1	A	227	HIS
1	A	255	ASP
1	A	258	GLU
1	A	268	THR
1	A	282	LEU
1	A	304	ASP
1	A	318	ARG
1	A	351	SER
1	A	373	GLU
1	A	380	THR
1	A	401	SER
1	A	471	LEU
1	A	483	VAL
1	A	591	ILE
1	A	613	VAL
2	L	5	THR
2	L	14	SER
2	L	29	VAL
2	L	54	LEU
2	L	74	THR
2	L	90	GLN
2	L	107	LYS
2	L	108	ARG
2	L	135	LEU
2	L	143	GLU
2	L	183	LYS
2	L	195	GLU
2	L	201	LEU
3	H	12	VAL
3	H	30[A]	TRP
3	H	30[B]	TRP
3	H	98	SER
3	H	109	THR
3	H	203	ASN

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	26	HIS
1	A	46	ASN

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Mol	Chain	Res	Type
1	A	53	GLN
1	A	71	GLN
1	A	297	ASN
1	A	298	GLN
1	A	416	ASN
1	A	490	HIS
1	A	542	HIS
1	A	546	GLN
2	L	6	GLN
2	L	38	GLN
2	L	90	GLN
2	L	198	HIS
3	H	39	GLN
3	H	203	ASN
3	H	204	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 ⓘ

7 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	$\# Z  > 2$
6	NAG	A	1165	1,6	14,14,15	0.52	0	15,19,21	0.94	0
6	NAG	A	1166	6	14,14,15	0.51	0	15,19,21	1.29	3 (20%)
6	BMA	A	1167	6	11,11,12	0.63	0	14,15,17	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	FUC	A	1170	6	10,10,11	0.66	0	14,14,16	1.34	3 (21%)
7	NAG	A	1237	1,7	14,14,15	0.58	0	15,19,21	1.03	1 (6%)
7	NAG	A	1238	7	14,14,15	0.62	0	15,19,21	1.49	3 (20%)
7	BMA	A	1239	7	11,11,12	0.60	0	14,15,17	1.07	1 (7%)

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	NAG	A	1165	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1166	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1167	6	-	0/2/19/22	0/1/1/1
6	FUC	A	1170	6	-	0/0/17/20	0/1/1/1
7	NAG	A	1237	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1238	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1239	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1166	NAG	C4-C3-C2	2.04	114.40	111.23
7	A	1238	NAG	O4-C4-C5	2.07	114.73	109.24
7	A	1238	NAG	C2-N2-C7	2.10	125.73	123.04
6	A	1170	FUC	C1-C2-C3	2.11	112.04	109.54
6	A	1166	NAG	O4-C4-C3	2.25	115.39	110.34
7	A	1237	NAG	C4-C3-C2	2.43	115.01	111.23
7	A	1239	BMA	C1-C2-C3	2.82	112.88	109.54
6	A	1170	FUC	O5-C5-C6	2.86	110.86	106.13
6	A	1166	NAG	C1-O5-C5	2.95	116.00	112.25
6	A	1170	FUC	C1-O5-C5	3.22	117.36	112.38
7	A	1238	NAG	C1-O5-C5	3.53	116.73	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1165	NAG	2	0
6	A	1170	FUC	2	0

## 5.6 Ligand geometry

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

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	SO4	A	626	-	4,4,4	0.31	0	6,6,6	0.26	0
5	SO4	A	627	-	4,4,4	0.19	0	6,6,6	0.13	0
5	SO4	A	628	-	4,4,4	0.18	0	6,6,6	0.14	0
5	SO4	A	629	-	4,4,4	0.17	0	6,6,6	0.11	0
5	SO4	A	630	-	4,4,4	0.20	0	6,6,6	0.17	0
5	SO4	A	631	-	4,4,4	0.21	0	6,6,6	0.13	0
5	SO4	A	632	-	4,4,4	0.21	0	6,6,6	0.17	0
5	SO4	A	633	-	4,4,4	0.19	0	6,6,6	0.09	0
5	SO4	A	634	-	4,4,4	0.22	0	6,6,6	0.10	0
5	SO4	A	635	-	4,4,4	0.22	0	6,6,6	0.10	0
5	SO4	A	636	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	A	637	-	4,4,4	0.18	0	6,6,6	0.11	0
5	SO4	A	638	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	H	225	-	4,4,4	0.18	0	6,6,6	0.09	0
5	SO4	L	218	-	4,4,4	0.22	0	6,6,6	0.17	0
5	SO4	L	219	-	4,4,4	0.20	0	6,6,6	0.08	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
5	SO4	A	626	-	-	0/0/0/0	0/0/0/0
5	SO4	A	627	-	-	0/0/0/0	0/0/0/0
5	SO4	A	628	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	629	-	-	0/0/0/0	0/0/0/0
5	SO4	A	630	-	-	0/0/0/0	0/0/0/0
5	SO4	A	631	-	-	0/0/0/0	0/0/0/0
5	SO4	A	632	-	-	0/0/0/0	0/0/0/0
5	SO4	A	633	-	-	0/0/0/0	0/0/0/0
5	SO4	A	634	-	-	0/0/0/0	0/0/0/0
5	SO4	A	635	-	-	0/0/0/0	0/0/0/0
5	SO4	A	636	-	-	0/0/0/0	0/0/0/0
5	SO4	A	637	-	-	0/0/0/0	0/0/0/0
5	SO4	A	638	-	-	0/0/0/0	0/0/0/0
5	SO4	H	225	-	-	0/0/0/0	0/0/0/0
5	SO4	L	218	-	-	0/0/0/0	0/0/0/0
5	SO4	L	219	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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	605/624 (96%)	-0.11	21 (3%) 48 32	24, 61, 135, 202	3 (0%)
2	L	214/217 (98%)	-0.04	3 (1%) 78 65	46, 80, 133, 175	0
3	H	214/224 (95%)	-0.04	10 (4%) 35 22	39, 71, 146, 180	0
All	All	1033/1065 (96%)	-0.08	34 (3%) 50 35	24, 68, 138, 202	3 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	ASP	5.3
1	A	253	ASN	4.9
1	A	313	SER	4.9
1	A	260	MET	4.2
1	A	303	GLU	4.2
1	A	264	GLU	3.9
2	L	214	CYS	3.8
1	A	610	HIS	3.7
1	A	265	GLY	3.6
1	A	550	GLY	3.3
1	A	314	LYS	3.2
3	H	217	PRO	3.0
1	A	262	ASN	3.0
1	A	100	PRO	2.9
3	H	162	ALA	2.9
1	A	259	SER	2.9
1	A	608	CYS	2.9
1	A	261	PRO	2.8
2	L	131	SER	2.5
1	A	315	PRO	2.5
1	A	298	GLN	2.5
3	H	214	LYS	2.5
1	A	609	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	587	SER	2.4
3	H	211	VAL	2.4
3	H	126	SER	2.3
1	A	366	ASN	2.3
2	L	213	GLU	2.3
3	H	215	VAL	2.2
1	A	305	GLY	2.2
3	H	198	TYR	2.1
3	H	125	PRO	2.1
3	H	212	ASP	2.0
3	H	194	GLY	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, 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
6	NAG	A	1165	14/15	0.89	0.28	2.47	87,93,110,115	0
7	NAG	A	1237	14/15	0.94	0.15	-0.69	60,75,96,98	0
7	BMA	A	1239	11/12	0.71	0.29	-	142,151,168,169	0
6	FUC	A	1170	10/11	0.86	0.41	-	110,118,127,128	0
6	BMA	A	1167	11/12	0.62	0.38	-	138,144,156,158	0
6	NAG	A	1166	14/15	0.90	0.31	-	110,126,134,134	0
7	NAG	A	1238	14/15	0.85	0.24	-	111,120,132,138	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, 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( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	633	5/5	0.89	0.36	4.15	119,122,124,127	0
5	SO4	A	636	5/5	0.92	0.26	3.84	132,133,137,138	0
5	SO4	H	225	5/5	0.93	0.18	0.52	115,117,119,120	0
5	SO4	A	634	5/5	0.84	0.28	0.30	130,132,134,138	0
5	SO4	A	635	5/5	0.91	0.21	0.27	99,103,104,107	0
5	SO4	A	628	5/5	0.92	0.19	0.25	89,89,93,95	0
5	SO4	A	638	5/5	0.87	0.16	-0.41	142,142,145,148	0
5	SO4	A	630	5/5	0.94	0.15	-1.11	105,107,108,109	0
5	SO4	A	627	5/5	0.95	0.14	-1.24	86,90,91,93	0
5	SO4	A	629	5/5	0.96	0.13	-2.27	78,82,85,87	0
5	SO4	A	626	5/5	0.99	0.11	-3.01	55,56,58,59	0
5	SO4	A	637	5/5	0.76	0.33	-	130,131,133,137	0
5	SO4	A	631	5/5	0.94	0.22	-	115,115,116,117	0
5	SO4	L	218	5/5	0.88	0.16	-	109,109,111,113	0
5	SO4	A	632	5/5	0.86	0.25	-	97,100,102,102	0
4	CL	A	625	1/1	0.89	0.14	-	76,76,76,76	0
5	SO4	L	219	5/5	0.95	0.22	-	131,131,132,136	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.