



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:57 PM GMT

PDB ID : 3VKF  
Title : Crystal Structure of Neurexin 1beta/Neurologin 1 complex  
Authors : Tanaka, H.; Miyazaki, N.; Nogi, T.; Iwasaki, K.; Takagi, J.  
Deposited on : 2011-11-15  
Resolution : 3.30 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

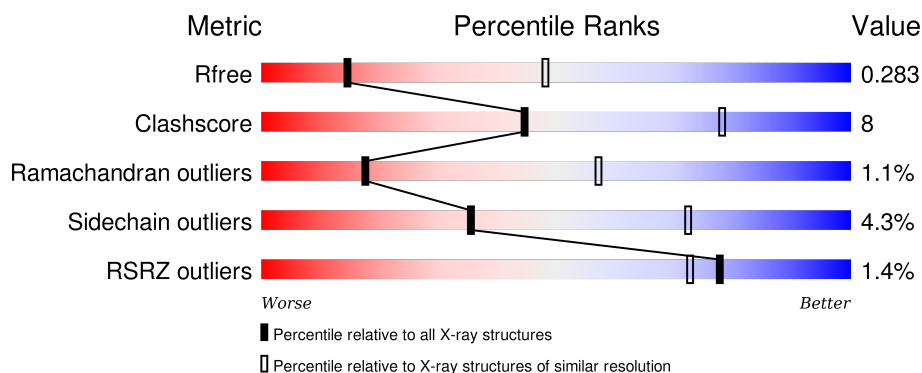
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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.

Mol	Chain	Length	Quality of chain
1	A	585	<div> <div>2%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	B	585	<div> <div>2%</div> <div>75%</div> <div>14%</div> <div>• 10%</div> </div>
2	C	181	<div> <div>72%</div> <div>24%</div> <div>• •</div> </div>
2	D	181	<div> <div>2%</div> <div>72%</div> <div>25%</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
4	NAG	B	2001	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11320 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 Neuroligin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			4399	2820	739	822	18			
1	B	527	Total	C	N	O	S	0	0	0
			4144	2666	688	774	16			

- Molecule 2 is a protein called Neurexin-1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	177	Total	C	N	O	S	0	0	0
			1354	853	241	259	1			
2	D	177	Total	C	N	O	S	0	0	0
			1354	853	241	259	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	81	GLY	-	EXPRESSION TAG	UNP Q28142
C	82	SER	-	EXPRESSION TAG	UNP Q28142
C	291	SER	-	EXPRESSION TAG	UNP Q28142
D	81	GLY	-	EXPRESSION TAG	UNP Q28142
D	82	SER	-	EXPRESSION TAG	UNP Q28142
D	291	SER	-	EXPRESSION TAG	UNP Q28142

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 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
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		

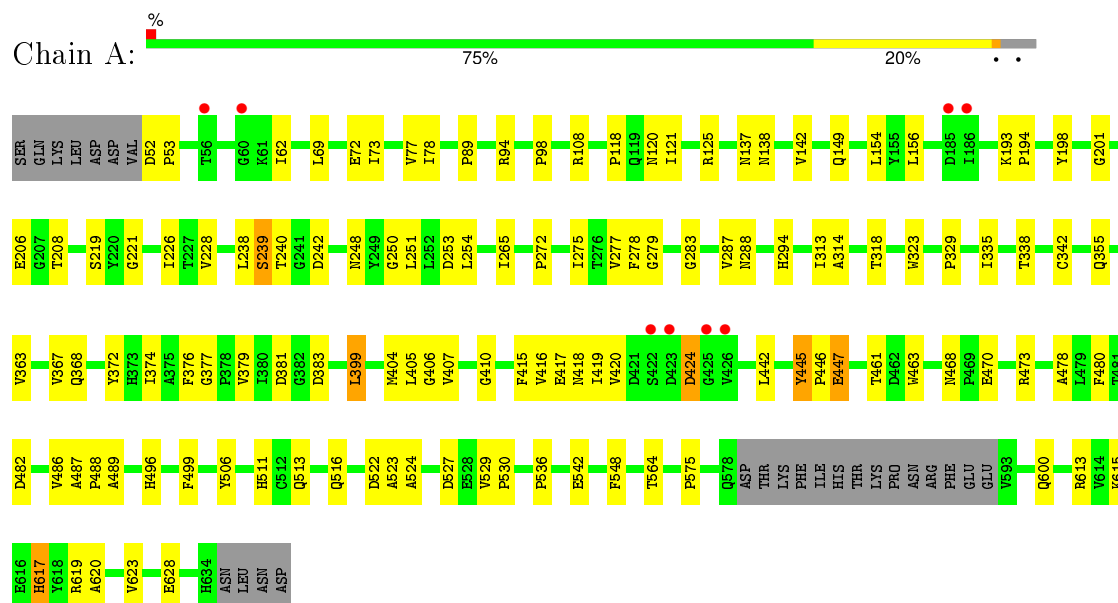
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

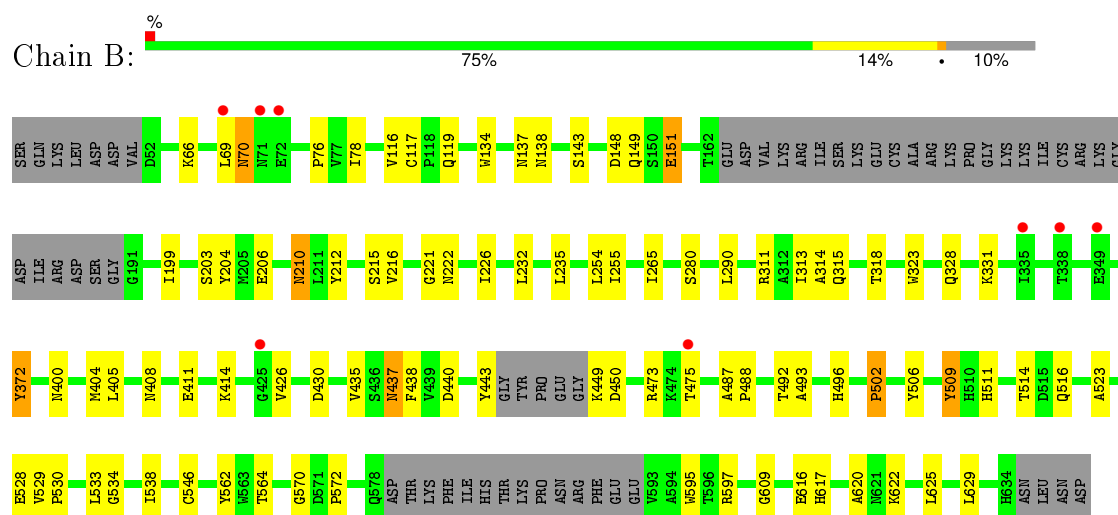
### 3 Residue-property plots

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.

#### • Molecule 1: Neuroligin-1



#### • Molecule 1: Neuroligin-1



#### • Molecule 2: Neurexin-1-beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.26Å 95.19Å 120.40Å 90.00° 108.62° 90.00°	Depositor
Resolution (Å)	48.91 – 3.30 48.31 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.91-3.30) 96.8 (48.31-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.04 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.205 , 0.287 0.203 , 0.283	Depositor DCC
$R_{free}$ test set	2586 reflections (11.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.2	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 30.8	EDS
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 25507 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11320	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% 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: CA, BMA, NAG

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	0.38	0/4521	0.52	0/6165
1	B	0.36	0/4261	0.51	0/5819
2	C	0.38	0/1379	0.56	0/1868
2	D	0.35	0/1379	0.54	0/1868
All	All	0.37	0/11540	0.52	0/15720

There are no bond length outliers.

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	4399	0	4269	68	0
1	B	4144	0	4005	46	0
2	C	1354	0	1343	37	0
2	D	1354	0	1343	29	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	39	0	34	0	0
All	All	11320	0	11020	176	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 8.

All (176) 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:445:TYR:HB2	1:A:446:PRO:HD3	1.32	1.07
1:A:445:TYR:CB	1:A:446:PRO:HD3	2.01	0.89
1:A:445:TYR:HB2	1:A:446:PRO:CD	2.02	0.89
2:D:147:ILE:H	2:D:167:ILE:HD13	1.40	0.86
1:A:314:ALA:HB3	1:A:405:LEU:HD23	1.63	0.81
1:B:514:THR:HB	1:B:546:CYS:HB3	1.66	0.76
2:C:114:ILE:HG22	2:C:175:VAL:HG12	1.69	0.74
2:D:138:LEU:HD11	2:D:177:PHE:CE2	2.24	0.73
1:A:329:PRO:HB3	1:A:379:VAL:HG11	1.68	0.73
1:A:201:GLY:HA3	1:A:283:GLY:N	2.04	0.73
2:C:269:ASN:O	2:C:273:GLU:HG2	1.89	0.71
1:A:201:GLY:HA3	1:A:283:GLY:H	1.56	0.69
1:A:288:ASN:HD22	1:A:318:THR:HA	1.57	0.69
2:C:95:ILE:HG22	2:C:280:ILE:HG23	1.76	0.67
1:B:134:TRP:O	1:B:138:ASN:HB2	1.96	0.66
1:A:446:PRO:O	1:A:447:GLU:HB2	1.96	0.66
1:A:478:ALA:HB1	1:A:619:ARG:HH22	1.60	0.65
1:B:408:ASN:O	1:B:411:GLU:HG2	1.96	0.64
2:D:109:ALA:HA	2:D:179:ARG:O	1.98	0.64
2:C:138:LEU:HD12	2:C:151:PHE:HB3	1.81	0.63
2:D:183:ASN:HD22	2:D:198:PRO:HD2	1.64	0.63
1:B:69:LEU:HD21	1:B:215:SER:HB3	1.81	0.62
1:A:381:ASP:OD2	1:A:383:ASP:HB3	2.00	0.62
1:A:511:HIS:HB3	1:A:523:ALA:HA	1.80	0.61
1:A:288:ASN:ND2	1:A:318:THR:HA	2.16	0.60
1:B:313:ILE:HG12	1:B:404:MET:HB3	1.83	0.60
1:A:511:HIS:HE1	1:A:513:GLN:HE21	1.49	0.60
1:A:277:VAL:HG12	1:A:287:VAL:HG22	1.81	0.60
2:C:116:PHE:HZ	2:C:167:ILE:HG21	1.67	0.58
1:B:616:GLU:HG2	1:B:617:HIS:CD2	2.38	0.58
2:D:110:ASP:CG	2:D:179:ARG:HH21	2.06	0.58
2:C:187:GLN:HB2	2:C:193:VAL:HG13	1.86	0.58
2:C:246:GLY:HA2	2:C:249:GLN:OE1	2.03	0.57
2:C:270:MET:O	2:C:275:ASP:HB2	2.04	0.57
1:A:118:PRO:HB2	1:A:363:VAL:HG21	1.87	0.56
2:C:101:PRO:HB2	2:C:102:ASN:HD22	1.70	0.56
2:D:122:GLU:HG2	2:D:143:HIS:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:HIS:HB3	1:A:620:ALA:HB2	1.86	0.56
2:D:110:ASP:HB2	2:D:179:ARG:HB3	1.88	0.56
2:D:275:ASP:HB3	2:D:278:ILE:HD12	1.87	0.56
1:A:407:VAL:HG21	1:A:486:VAL:HG22	1.87	0.55
2:C:96:THR:HG23	2:C:243:ILE:HD13	1.87	0.55
2:D:107:THR:HG22	2:D:239:GLN:HE22	1.72	0.54
2:D:97:TYR:HD1	2:D:278:ILE:HG13	1.73	0.54
1:B:226:ILE:HD11	1:B:265:ILE:HD13	1.89	0.54
2:C:95:ILE:HD11	2:C:268:LEU:HD23	1.89	0.54
1:B:221:GLY:HA3	1:B:564:THR:HG21	1.90	0.53
1:B:328:GLN:NE2	1:B:331:LYS:HD2	2.24	0.53
1:A:226:ILE:HD11	1:A:265:ILE:HD13	1.90	0.53
1:A:399:LEU:HD11	2:C:108:ARG:HH22	1.74	0.52
2:C:138:LEU:HB2	2:C:236:PHE:HE2	1.75	0.52
1:A:251:LEU:HA	1:A:254:LEU:HD12	1.91	0.52
1:B:70:ASN:HD22	1:B:538:ILE:HG21	1.74	0.52
2:C:106:SER:HA	2:C:236:PHE:O	2.09	0.52
1:A:248:ASN:OD1	1:A:251:LEU:HD12	2.10	0.51
1:A:77:VAL:HG22	1:A:219:SER:HB3	1.92	0.51
2:D:84:THR:HG21	2:D:272:ALA:HB2	1.93	0.51
1:A:487:ALA:HB3	1:A:488:PRO:HD3	1.91	0.51
1:A:487:ALA:HA	1:A:623:VAL:HG13	1.93	0.51
1:A:318:THR:HG21	1:A:489:ALA:HA	1.92	0.50
2:C:95:ILE:HB	2:C:280:ILE:HG12	1.92	0.50
1:B:216:VAL:HG11	1:B:534:GLY:O	2.11	0.50
1:A:374:ILE:HD12	1:A:377:GLY:HA3	1.93	0.50
1:B:625:LEU:HD12	1:B:629:LEU:HD23	1.92	0.50
1:A:415:PHE:CD2	1:A:480:PHE:HB2	2.47	0.50
2:D:116:PHE:HZ	2:D:167:ILE:CG2	2.25	0.50
2:C:102:ASN:N	2:C:102:ASN:HD22	2.09	0.50
2:D:107:THR:HG21	2:D:110:ASP:OD1	2.12	0.50
2:C:179:ARG:NH2	2:C:236:PHE:HB2	2.27	0.50
1:B:280:SER:HA	1:B:315:GLN:O	2.12	0.49
2:C:147:ILE:H	2:C:167:ILE:HD13	1.78	0.49
1:B:509:TYR:CE1	1:B:609:GLY:HA3	2.48	0.49
1:B:617:HIS:HB3	1:B:620:ALA:HB2	1.94	0.49
1:A:52:ASP:N	1:A:53:PRO:HD3	2.26	0.49
1:B:443:TYR:C	1:B:449:LYS:HE3	2.33	0.48
2:C:112:LEU:HA	2:C:261:TYR:O	2.13	0.48
1:A:120:ASN:HD21	1:A:125:ARG:HH22	1.60	0.48
1:A:613:ARG:HD2	1:A:615:LYS:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ALA:HB3	1:B:405:LEU:HD23	1.96	0.48
1:A:470:GLU:O	1:A:473:ARG:HB3	2.14	0.48
1:B:137:ASN:HD22	1:B:516:GLN:HG2	1.78	0.47
1:A:294:HIS:HD2	2:C:108:ARG:CD	2.27	0.47
1:B:435:VAL:O	1:B:438:PHE:HB3	2.14	0.47
2:D:155:THR:HG23	2:D:233:LEU:HG	1.95	0.47
2:C:94:GLN:HE22	2:C:248:GLU:HB2	1.80	0.47
1:A:221:GLY:HA3	1:A:564:THR:HG21	1.97	0.47
1:A:238:LEU:HD12	1:A:376:PHE:HE1	1.79	0.47
2:D:128:VAL:HG22	2:D:242:ILE:HG12	1.96	0.47
2:D:198:PRO:HB2	2:D:232:GLN:HE22	1.78	0.47
1:A:53:PRO:HB3	1:A:78:ILE:HD13	1.97	0.47
1:B:116:VAL:HG23	1:B:149:GLN:HG2	1.96	0.47
2:C:114:ILE:HG22	2:C:175:VAL:CG1	2.43	0.46
1:B:212:TYR:HD1	1:B:533:LEU:HD11	1.79	0.46
2:D:173:HIS:ND1	2:D:189:ASP:OD1	2.37	0.46
1:A:137:ASN:HB3	1:A:516:GLN:NE2	2.30	0.46
1:A:250:GLY:O	1:A:253:ASP:HB2	2.16	0.46
1:A:198:TYR:CE1	1:A:279:GLY:HA2	2.50	0.46
1:A:313:ILE:HG12	1:A:404:MET:HB3	1.98	0.46
1:B:66:LYS:HE2	1:B:76:PRO:HB3	1.97	0.46
1:A:120:ASN:ND2	1:A:125:ARG:HH22	2.14	0.46
1:A:239:SER:HB3	1:A:329:PRO:HB2	1.98	0.46
1:A:98:PRO:HG3	1:A:253:ASP:HA	1.98	0.46
1:B:506:TYR:HB3	1:B:595:TRP:CZ2	2.52	0.45
2:C:154:GLY:HA3	2:C:233:LEU:HD12	1.99	0.45
1:B:616:GLU:HG2	1:B:617:HIS:HD2	1.80	0.45
1:B:437:ASN:HA	1:B:440:ASP:HB2	1.98	0.45
1:A:482:ASP:OD1	1:A:619:ARG:NH2	2.49	0.45
2:C:147:ILE:N	2:C:167:ILE:HD13	2.31	0.45
1:B:426:VAL:HG23	1:B:473:ARG:HG3	1.99	0.45
2:C:164:ASN:O	2:C:165:ALA:HB2	2.16	0.45
1:A:198:TYR:HB2	1:A:278:PHE:CZ	2.52	0.45
1:A:156:LEU:HD22	1:A:228:VAL:HG22	1.97	0.45
1:A:314:ALA:HB3	1:A:405:LEU:CD2	2.40	0.44
1:B:487:ALA:HB3	1:B:488:PRO:HD3	1.98	0.44
1:B:405:LEU:HD12	1:B:493:ALA:HB2	1.99	0.44
1:A:529:VAL:N	1:A:530:PRO:HD2	2.31	0.44
2:C:145:GLY:HA3	2:C:166:ILE:HG12	2.00	0.44
1:B:199:ILE:HG12	1:B:254:LEU:HD22	1.97	0.44
1:A:198:TYR:HA	1:A:278:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:PRO:HG3	1:A:548:PHE:CD2	2.52	0.44
2:C:116:PHE:CZ	2:C:167:ILE:HG21	2.52	0.44
1:B:562:TYR:HD1	1:B:572:PRO:HB2	1.82	0.44
1:B:372:TYR:CD1	1:B:372:TYR:N	2.84	0.44
2:C:179:ARG:HH22	2:C:236:PHE:HB2	1.82	0.43
1:A:406:GLY:HA3	1:A:506:TYR:CE2	2.52	0.43
1:B:414:LYS:HA	1:B:414:LYS:HE2	2.00	0.43
1:A:542:GLU:CD	1:A:542:GLU:H	2.22	0.43
1:A:138:ASN:O	1:A:142:VAL:HG23	2.19	0.43
1:A:420:VAL:HG12	1:A:424:ASP:HA	2.00	0.43
2:C:94:GLN:HE21	2:C:248:GLU:H	1.67	0.43
1:B:511:HIS:HB3	1:B:523:ALA:HA	2.00	0.43
2:D:237:ASN:O	2:D:238:SER:C	2.57	0.43
1:A:446:PRO:O	1:A:447:GLU:CB	2.65	0.43
1:B:117:CYS:O	1:B:119:GLN:HG2	2.19	0.43
2:D:95:ILE:HG12	2:D:280:ILE:HG12	2.00	0.43
1:B:203:SER:O	1:B:204:TYR:HB2	2.19	0.43
2:D:116:PHE:CZ	2:D:167:ILE:HG22	2.53	0.42
1:B:492:THR:HG22	1:B:496:HIS:HD2	1.83	0.42
1:A:89:PRO:HG3	1:A:154:LEU:HD11	2.01	0.42
1:B:622:LYS:O	1:B:625:LEU:HB3	2.18	0.42
1:B:66:LYS:HG3	1:B:78:ILE:HD13	2.01	0.42
2:C:109:ALA:HA	2:C:179:ARG:O	2.19	0.42
2:D:134:LEU:HD12	2:D:134:LEU:N	2.34	0.42
2:D:130:SER:HA	2:D:239:GLN:HA	2.00	0.42
2:D:86:TYR:HD2	2:D:268:LEU:HD22	1.84	0.42
1:A:410:GLY:O	1:A:524:ALA:HA	2.20	0.42
2:D:114:ILE:HD12	2:D:260:LEU:HD13	2.02	0.42
2:C:128:VAL:HG22	2:C:242:ILE:HG12	2.02	0.42
2:D:104:ARG:HA	2:D:105:PRO:HD3	1.82	0.42
1:A:445:TYR:CB	1:A:446:PRO:CD	2.71	0.42
1:A:399:LEU:HD11	2:C:108:ARG:NH2	2.34	0.42
1:A:193:LYS:HA	1:A:194:PRO:HD3	1.97	0.42
1:A:94:ARG:HD2	1:A:355:GLN:HA	2.02	0.41
1:B:311:ARG:HD3	1:B:570:GLY:HA2	2.02	0.41
1:B:255:ILE:HD11	1:B:290:LEU:HD22	2.01	0.41
2:C:110:ASP:OD2	2:C:179:ARG:NE	2.48	0.41
1:A:272:PRO:HA	1:A:275:ILE:HD11	2.02	0.41
1:A:62:ILE:HG22	1:A:108:ARG:HG2	2.02	0.41
2:C:128:VAL:HB	2:C:138:LEU:HB3	2.03	0.41
2:D:116:PHE:HZ	2:D:167:ILE:HG21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ASP:HA	1:A:486:VAL:HB	2.03	0.41
2:C:116:PHE:HZ	2:C:167:ILE:CG2	2.34	0.41
1:B:70:ASN:ND2	1:B:70:ASN:H	2.18	0.41
1:A:416:VAL:O	1:A:418:ASN:N	2.39	0.41
2:D:100:PRO:HA	2:D:101:PRO:HD3	1.94	0.41
1:A:468:ASN:HD21	1:A:470:GLU:HB2	1.86	0.41
1:B:210:ASN:N	1:B:210:ASN:OD1	2.54	0.41
1:B:502:PRO:HA	1:B:597:ARG:HD2	2.02	0.41
2:D:147:ILE:HG13	2:D:148:GLY:N	2.36	0.41
1:A:499:PHE:CD2	2:C:134:LEU:HD21	2.57	0.40
1:A:461:THR:O	1:A:463:TRP:CD1	2.74	0.40
2:C:110:ASP:OD2	2:C:179:ARG:NH2	2.53	0.40
1:B:151:GLU:HG2	1:B:235:LEU:HD21	2.02	0.40
1:B:529:VAL:N	1:B:530:PRO:HD2	2.37	0.40
2:D:271:ALA:HB2	2:D:278:ILE:HG21	2.04	0.40
1:B:70:ASN:HD22	1:B:538:ILE:CG2	2.34	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	556/585 (95%)	500 (90%)	47 (8%)	9 (2%)	12	48
1	B	519/585 (89%)	480 (92%)	38 (7%)	1 (0%)	52	85
2	C	175/181 (97%)	156 (89%)	16 (9%)	3 (2%)	11	47
2	D	175/181 (97%)	158 (90%)	15 (9%)	2 (1%)	17	57
All	All	1425/1532 (93%)	1294 (91%)	116 (8%)	15 (1%)	17	57

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	TYR
1	A	447	GLU
2	C	165	ALA
2	D	238	SER
1	A	73	ILE
1	A	242	ASP
2	C	238	SER
1	A	417	GLU
1	A	527	ASP
1	A	72	GLU
1	A	617	HIS
2	C	259	GLY
1	B	502	PRO
2	D	192	PRO
1	A	575	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	478/503 (95%)	456 (95%)	22 (5%)	33	71
1	B	451/503 (90%)	433 (96%)	18 (4%)	38	74
2	C	143/146 (98%)	136 (95%)	7 (5%)	31	69
2	D	143/146 (98%)	138 (96%)	5 (4%)	43	77
All	All	1215/1298 (94%)	1163 (96%)	52 (4%)	35	72

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	121	ILE
1	A	149	GLN
1	A	206	GLU
1	A	208	THR
1	A	239	SER
1	A	240	THR

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Mol	Chain	Res	Type
1	A	323	TRP
1	A	335	ILE
1	A	338	THR
1	A	342	CYS
1	A	367	VAL
1	A	368	GLN
1	A	372	TYR
1	A	399	LEU
1	A	419	ILE
1	A	424	ASP
1	A	442	LEU
1	A	496	HIS
1	A	522	ASP
1	A	600	GLN
1	A	628	GLU
1	B	70	ASN
1	B	143	SER
1	B	148	ASP
1	B	151	GLU
1	B	206	GLU
1	B	210	ASN
1	B	222	ASN
1	B	232	LEU
1	B	318	THR
1	B	323	TRP
1	B	372	TYR
1	B	400	ASN
1	B	430	ASP
1	B	437	ASN
1	B	450	ASP
1	B	475	THR
1	B	509	TYR
1	B	528	GLU
2	C	84	THR
2	C	89	SER
2	C	95	ILE
2	C	166	ILE
2	C	183	ASN
2	C	185	THR
2	C	236	PHE
2	D	120	GLN
2	D	131	SER

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Mol	Chain	Res	Type
2	D	134	LEU
2	D	236	PHE
2	D	251	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	120	ASN
1	A	149	GLN
1	A	288	ASN
1	A	294	HIS
1	A	355	GLN
1	A	409	GLN
1	A	468	ASN
1	A	496	HIS
1	A	511	HIS
1	A	600	GLN
1	A	603	GLN
1	B	70	ASN
1	B	137	ASN
1	B	288	ASN
1	B	328	GLN
1	B	418	ASN
1	B	437	ASN
1	B	496	HIS
2	C	94	GLN
2	C	102	ASN
2	C	144	GLN
2	C	164	ASN
2	C	183	ASN
2	D	144	GLN
2	D	152	ASN
2	D	183	ASN
2	D	232	GLN
2	D	239	GLN
2	D	249	GLN
2	D	269	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 ⓘ

3 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	$\# Z  > 2$
5	NAG	A	2002	1,5	14,14,15	0.53	0	15,19,21	0.98	1 (6%)
5	NAG	A	2003	5	14,14,15	0.46	0	15,19,21	0.72	0
5	BMA	A	2004	5	11,11,12	0.58	0	14,15,17	1.29	2 (14%)

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	2002	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2003	5	-	0/6/23/26	0/1/1/1
5	BMA	A	2004	5	-	0/2/19/22	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	2004	BMA	C2-C3-C4	2.08	114.57	111.04
5	A	2002	NAG	C4-C3-C2	2.59	115.25	111.23
5	A	2004	BMA	C1-C2-C3	3.81	114.05	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
4	NAG	A	2001	1	14,14,15	0.47	0	15,19,21	0.73	0
4	NAG	B	2001	1	14,14,15	0.56	0	15,19,21	0.94	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
4	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	NAG	C4-C3-C2	2.61	115.29	111.23

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	560/585 (95%)	-0.11	8 (1%) 78 73	36, 59, 87, 119	0
1	B	527/585 (90%)	-0.01	8 (1%) 76 71	48, 72, 96, 117	0
2	C	177/181 (97%)	-0.10	0 100 100	43, 60, 76, 87	0
2	D	177/181 (97%)	0.18	4 (2%) 64 57	54, 75, 101, 121	0
All	All	1441/1532 (94%)	-0.04	20 (1%) 78 73	36, 66, 94, 121	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	GLU	3.9
1	B	335	ILE	3.9
1	A	185	ASP	3.1
1	B	71	ASN	3.0
1	A	422	SER	2.7
1	B	338	THR	2.5
1	B	349	GLU	2.5
2	D	156	ASP	2.5
2	D	98	LYS	2.5
1	A	56	THR	2.3
1	A	426	VAL	2.3
1	A	186	ILE	2.2
1	A	423	ASP	2.2
1	B	69	LEU	2.1
1	A	60	GLY	2.1
2	D	279	ALA	2.1
1	B	475	THR	2.1
1	A	425	GLY	2.1
2	D	96	THR	2.0
1	B	425	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( $\text{\AA}^2$ )	Q<0.9
5	BMA	A	2004	11/12	0.76	0.15	-	111,114,119,122	0
5	NAG	A	2003	14/15	0.81	0.30	-	98,103,109,109	0
5	NAG	A	2002	14/15	0.87	0.24	-	89,94,97,98	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
4	NAG	B	2001	14/15	0.91	0.45	0.08	98,108,114,119	0
3	CA	C	2001	1/1	0.93	0.13	-1.20	68,68,68,68	0
3	CA	D	2001	1/1	0.96	0.08	-2.67	70,70,70,70	0
4	NAG	A	2001	14/15	0.88	0.24	-	77,83,88,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.