



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:01 PM GMT

PDB ID : 2R1D  
Title : Crystal structure of rat neurexin 1beta in the Ca<sup>2+</sup> containing form  
Authors : Rudenko, G.  
Deposited on : 2007-08-22  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

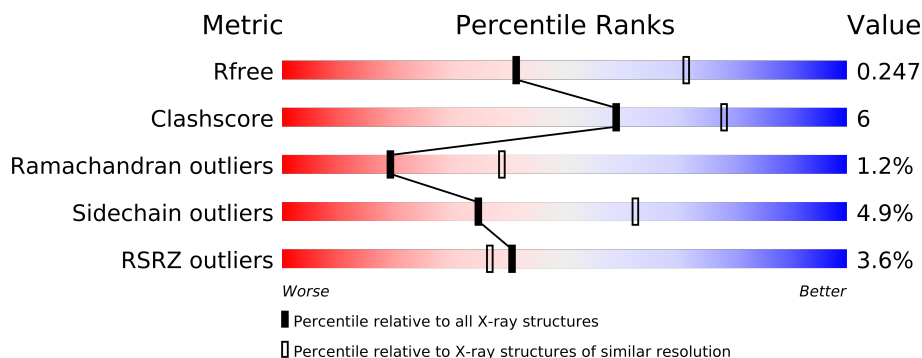
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	226	
1	B	226	
1	C	226	
1	D	226	
1	E	226	
1	F	226	
1	G	226	
1	H	226	
1	I	226	
1	W	226	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12217 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Neurexin-1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1373	866	241	265	1			
1	B	180	Total	C	N	O	S	0	0	0
			1359	857	240	261	1			
1	C	183	Total	C	N	O	S	0	0	0
			1378	869	242	266	1			
1	D	179	Total	C	N	O	S	0	0	0
			1357	855	241	260	1			
1	E	182	Total	C	N	O	S	0	0	0
			1364	860	240	263	1			
1	F	178	Total	C	N	O	S	0	0	0
			1343	847	236	259	1			
1	G	182	Total	C	N	O	S	0	0	0
			1382	871	247	263	1			
1	H	176	Total	C	N	O	S	0	0	0
			1340	843	239	257	1			
1	I	151	Total	C	N	O	S	0	0	0
			1150	734	199	216	1			
1	W	7	Total	C	N	O		0	0	0
			55	35	13	7				

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	I	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

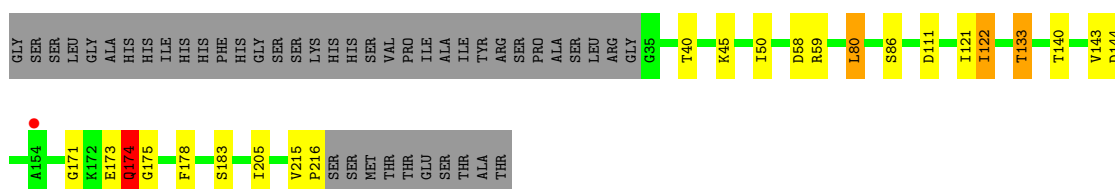
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	O 6	0	0
3	B	22	Total 22	O 22	0	0
3	C	7	Total 7	O 7	0	0
3	D	20	Total 20	O 20	0	0
3	E	11	Total 11	O 11	0	0
3	F	16	Total 16	O 16	0	0
3	G	18	Total 18	O 18	0	0
3	H	10	Total 10	O 10	0	0
3	I	3	Total 3	O 3	0	0

### 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.

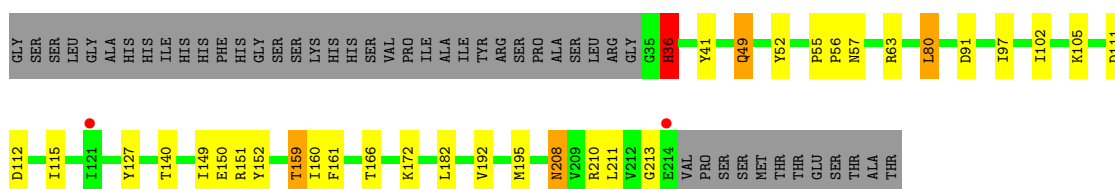
#### • Molecule 1: Neurexin-1-beta

Chain A:



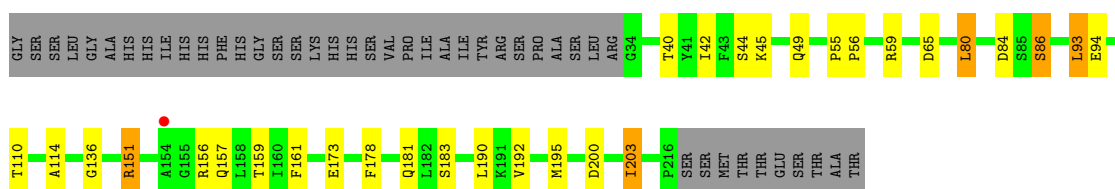
#### • Molecule 1: Neurexin-1-beta

Chain B:



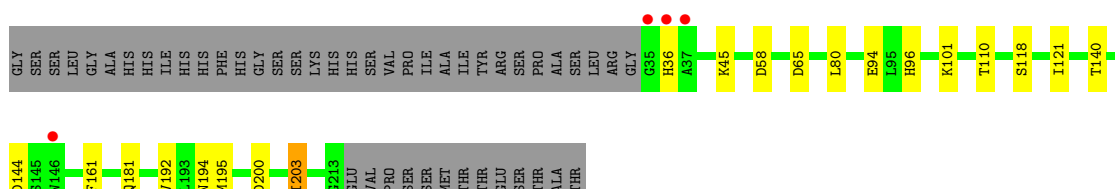
#### • Molecule 1: Neurexin-1-beta

Chain C:



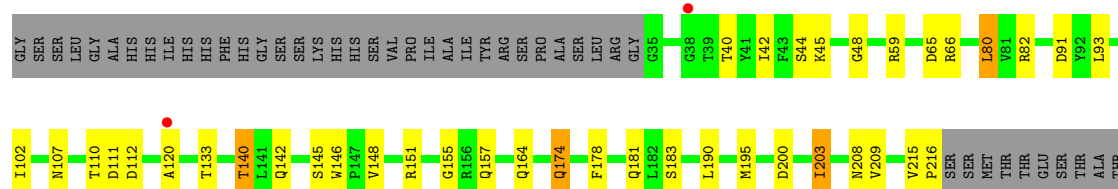
#### • Molecule 1: Neurexin-1-beta

Chain D:



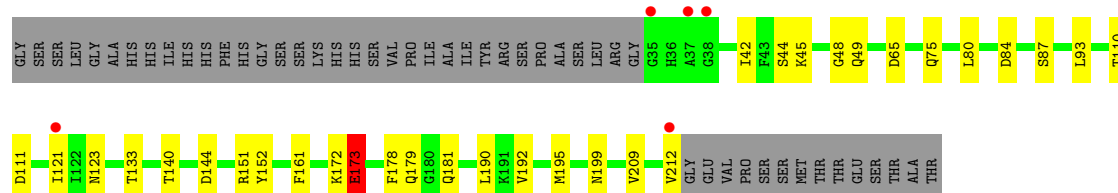
- Molecule 1: Neurexin-1-beta

Chain E:



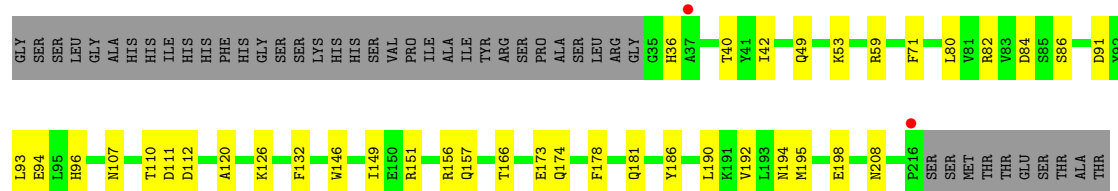
- Molecule 1: Neurexin-1-beta

Chain F:



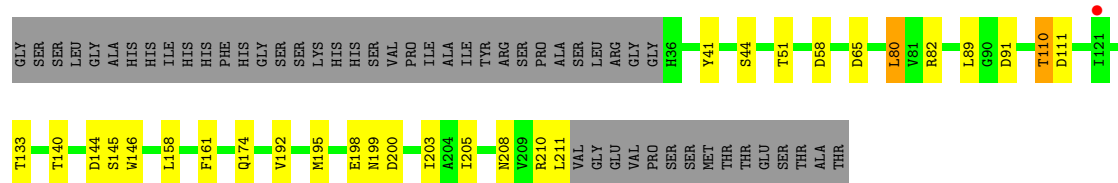
- Molecule 1: Neurexin-1-beta

Chain G:



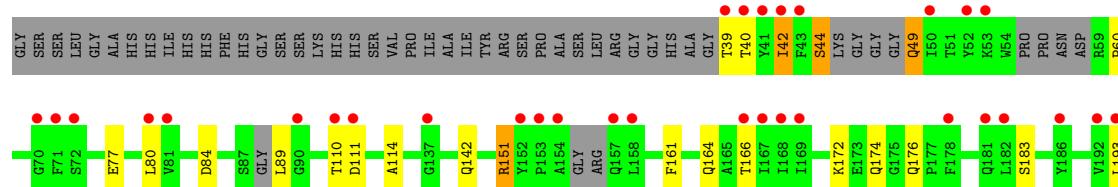
- Molecule 1: Neurexin-1-beta

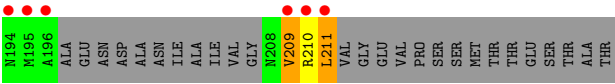
Chain H:



- Molecule 1: Neurexin-1-beta

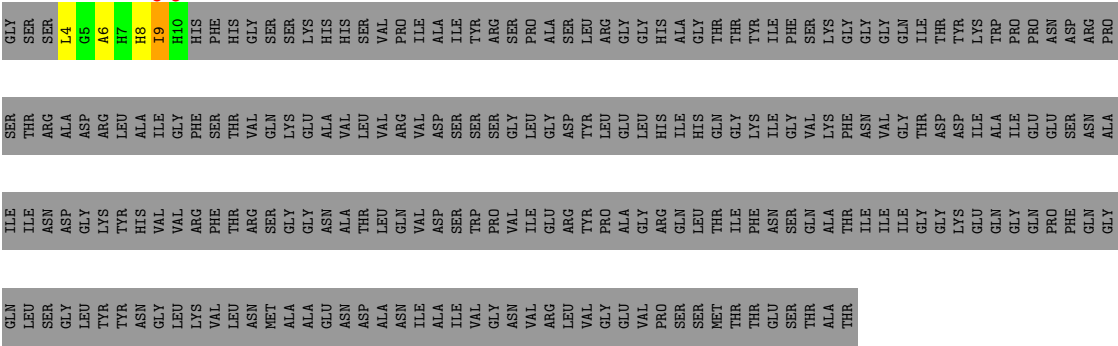
Chain I:





● Molecule 1: Neurexin-1-beta

Chain W: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.68Å 195.72Å 103.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 40.63 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 99.6 (40.63-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.203 , 0.244 0.207 , 0.247	Depositor DCC
$R_{free}$ test set	3755 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 73861 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12217	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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 30.00 % 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 1.4078e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.66	0/1400	0.84	1/1901 (0.1%)
1	B	0.85	0/1385	0.96	5/1878 (0.3%)
1	C	0.67	0/1405	0.83	2/1908 (0.1%)
1	D	0.77	0/1383	0.88	3/1876 (0.2%)
1	E	0.67	0/1390	0.88	4/1889 (0.2%)
1	F	0.76	1/1369 (0.1%)	0.99	5/1860 (0.3%)
1	G	0.75	0/1409	0.91	3/1912 (0.2%)
1	H	0.72	0/1366	0.90	7/1855 (0.4%)
1	I	1.35	5/1168 (0.4%)	0.78	3/1578 (0.2%)
1	W	0.77	0/57	0.94	0/76
All	All	0.81	6/12332 (0.0%)	0.89	33/16733 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	44	SER	C-O	27.59	1.75	1.23
1	I	211	LEU	C-O	27.58	1.75	1.23
1	I	49	GLN	CA-CB	10.19	1.76	1.53
1	I	39	THR	C-O	5.42	1.33	1.23
1	F	212	VAL	C-O	5.22	1.33	1.23
1	I	49	GLN	N-CA	5.07	1.56	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	212	VAL	CA-C-O	13.62	148.70	120.10
1	E	112	ASP	CB-CG-OD2	9.08	126.47	118.30
1	B	151	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	58	ASP	CB-CG-OD2	7.19	124.77	118.30
1	E	65	ASP	CB-CG-OD2	6.66	124.29	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ASP	CB-CG-OD2	6.57	124.21	118.30
1	F	144	ASP	CB-CG-OD2	6.50	124.15	118.30
1	F	111	ASP	CB-CG-OD2	6.46	124.12	118.30
1	I	111	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	112	ASP	CB-CG-OD2	6.13	123.82	118.30
1	H	144	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	65	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	151	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	H	111	ASP	CB-CG-OD2	6.03	123.73	118.30
1	E	111	ASP	CB-CG-OD2	5.94	123.65	118.30
1	H	211	LEU	CA-CB-CG	5.93	128.94	115.30
1	I	84	ASP	CB-CG-OD2	5.91	123.62	118.30
1	G	111	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	65	ASP	CB-CG-OD2	5.77	123.50	118.30
1	H	65	ASP	CB-CG-OD2	5.67	123.40	118.30
1	G	84	ASP	CB-CG-OD2	5.63	123.37	118.30
1	C	84	ASP	CB-CG-OD2	5.62	123.36	118.30
1	G	112	ASP	CB-CG-OD2	5.61	123.35	118.30
1	H	91	ASP	CB-CG-OD2	5.46	123.21	118.30
1	D	58	ASP	CB-CG-OD2	5.31	123.08	118.30
1	F	84	ASP	CB-CG-OD2	5.31	123.08	118.30
1	F	65	ASP	CB-CG-OD2	5.30	123.07	118.30
1	H	58	ASP	CB-CG-OD2	5.24	123.02	118.30
1	I	211	LEU	CA-C-O	-5.20	109.19	120.10
1	E	80	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	111	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	144	ASP	CB-CG-OD2	5.10	122.89	118.30
1	H	80	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1373	0	1338	16	0
1	B	1359	0	1332	18	0
1	C	1378	0	1345	22	0
1	D	1357	0	1331	9	0
1	E	1364	0	1321	19	0
1	F	1343	0	1306	18	0
1	G	1382	0	1360	23	0
1	H	1340	0	1305	9	0
1	I	1150	0	1116	14	0
1	W	55	0	50	2	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	I	1	0	0	0	0
3	A	6	0	0	0	0
3	B	22	0	0	1	0
3	C	7	0	0	0	0
3	D	20	0	0	0	0
3	E	11	0	0	0	0
3	F	16	0	0	1	0
3	G	18	0	0	0	0
3	H	10	0	0	1	0
3	I	3	0	0	0	0
All	All	12217	0	11804	146	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (146) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:49:GLN:CB	1:I:49:GLN:CA	1.76	1.62
1:I:44:SER:O	1:I:44:SER:C	1.75	1.24
1:I:211:LEU:C	1:I:211:LEU:O	1.75	1.24
1:C:192:VAL:HA	1:C:195:MET:HE3	1.30	1.09
1:G:192:VAL:HA	1:G:195:MET:HE3	1.34	1.05
1:B:192:VAL:HA	1:B:195:MET:HE3	1.36	1.03
1:C:42:ILE:HD13	1:C:181:GLN:HG2	1.42	0.99
1:F:49:GLN:HE22	1:F:173:GLU:HB2	1.31	0.96
1:C:49:GLN:OE1	1:C:173:GLU:HB2	1.67	0.94
1:B:208:ASN:HD21	1:B:210:ARG:HH21	1.18	0.90
1:H:192:VAL:HA	1:H:195:MET:HE2	1.58	0.83
1:D:192:VAL:HA	1:D:195:MET:HE3	1.60	0.82
1:A:122:ILE:HD11	1:A:143:VAL:HG11	1.63	0.80
1:B:192:VAL:HA	1:B:195:MET:CE	2.12	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:121:ILE:HD13	1:I:110:THR:HG23	1.65	0.78
1:A:174:GLN:H	1:A:174:GLN:NE2	1.81	0.78
1:D:192:VAL:HA	1:D:195:MET:CE	2.14	0.78
1:F:49:GLN:NE2	1:F:173:GLU:H	1.83	0.76
1:C:40:THR:HG23	1:C:183:SER:HB3	1.67	0.75
1:E:120:ALA:HB3	1:E:146:TRP:CZ3	2.24	0.72
1:I:40:THR:HG23	1:I:183:SER:HB3	1.72	0.72
1:F:48:GLY:HA3	1:F:209:VAL:HG23	1.72	0.71
1:E:120:ALA:CB	1:E:146:TRP:CZ3	2.74	0.71
1:H:205:ILE:HD12	1:W:9:ILE:HG23	1.72	0.70
1:C:42:ILE:CD1	1:C:181:GLN:HG2	2.18	0.69
1:G:192:VAL:HA	1:G:195:MET:CE	2.19	0.68
1:F:192:VAL:HA	1:F:195:MET:HE3	1.76	0.68
1:C:49:GLN:OE1	1:C:173:GLU:CB	2.42	0.67
1:F:133:THR:HB	1:F:140:THR:OG1	1.96	0.66
1:D:36:HIS:CE1	1:D:181:GLN:HB3	2.34	0.63
1:F:48:GLY:HA3	1:F:209:VAL:CG2	2.29	0.62
1:I:49:GLN:CB	1:I:49:GLN:C	2.63	0.62
1:A:40:THR:HG23	1:A:183:SER:HB3	1.82	0.62
1:A:174:GLN:H	1:A:174:GLN:HE21	1.46	0.61
1:G:192:VAL:CA	1:G:195:MET:HE3	2.20	0.61
1:B:159:THR:HG22	1:B:160:ILE:HG13	1.82	0.60
1:E:42:ILE:HG12	1:E:181:GLN:HG2	1.84	0.60
1:E:200:ASP:HB3	1:E:203:ILE:HG13	1.84	0.59
1:E:133:THR:HB	1:E:140:THR:HB	1.83	0.59
1:B:36:HIS:HB2	1:B:127:TYR:CZ	2.38	0.59
1:C:93:LEU:HD12	1:C:93:LEU:C	2.22	0.59
1:F:49:GLN:NE2	1:F:173:GLU:HB2	2.11	0.58
1:F:75:GLN:O	1:F:123:ASN:ND2	2.36	0.57
1:C:80:LEU:HD22	1:C:178:PHE:CD1	2.40	0.57
1:F:133:THR:HG22	3:F:238:HOH:O	2.04	0.56
1:G:93:LEU:HD11	1:G:132:PHE:CE2	2.40	0.56
1:F:80:LEU:HD22	1:F:178:PHE:CD1	2.40	0.56
1:G:59:ARG:NH1	1:G:86:SER:HB3	2.22	0.55
1:C:114:ALA:O	1:C:151:ARG:HD3	2.07	0.54
1:F:49:GLN:HE22	1:F:173:GLU:H	1.50	0.54
1:F:190:LEU:HB3	1:F:195:MET:HE1	1.89	0.54
1:E:80:LEU:HD22	1:E:178:PHE:CD1	2.41	0.54
1:C:42:ILE:HD13	1:C:181:GLN:CG	2.28	0.54
1:B:115:ILE:HD11	1:B:149:ILE:HG22	1.90	0.54
1:I:114:ALA:O	1:I:151:ARG:HD3	2.08	0.54
1:F:192:VAL:HA	1:F:195:MET:CE	2.38	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:190:LEU:HB3	1:E:195:MET:HE3	1.90	0.53
1:E:142:GLN:HG3	1:E:148:VAL:HG22	1.89	0.53
1:A:80:LEU:HD22	1:A:178:PHE:CD1	2.44	0.53
1:G:94:GLU:OE1	1:G:96:HIS:HD2	1.90	0.53
1:E:190:LEU:HB3	1:E:195:MET:CE	2.39	0.53
1:A:133:THR:HB	1:A:140:THR:OG1	2.10	0.52
1:A:111:ASP:OD1	1:F:151:ARG:HD2	2.09	0.52
1:H:146:TRP:N	1:H:146:TRP:CD1	2.76	0.52
1:G:49:GLN:OE1	1:G:173:GLU:HB3	2.10	0.52
1:C:200:ASP:HB3	1:C:203:ILE:HG13	1.92	0.52
1:G:110:THR:HB	1:G:157:GLN:OE1	2.10	0.52
1:E:120:ALA:HB1	1:E:146:TRP:CH2	2.45	0.51
1:A:215:VAL:HG13	1:A:216:PRO:HD2	1.93	0.51
1:I:42:ILE:HG22	1:I:210:ARG:O	2.10	0.51
1:C:190:LEU:HB3	1:C:195:MET:CE	2.41	0.51
1:B:57:ASN:HB2	3:B:1008:HOH:O	2.11	0.51
1:D:121:ILE:HG13	1:D:121:ILE:O	2.11	0.50
1:G:120:ALA:HB3	1:G:146:TRP:CZ3	2.46	0.50
1:A:50:ILE:HG12	1:A:205:ILE:HG12	1.92	0.50
1:I:49:GLN:CB	1:I:49:GLN:N	2.70	0.50
1:G:53:LYS:HG2	1:G:166:THR:HG22	1.93	0.50
1:C:59:ARG:NH1	1:C:86:SER:HB3	2.27	0.50
1:C:42:ILE:CD1	1:C:181:GLN:CG	2.88	0.49
1:G:59:ARG:HH11	1:G:86:SER:HB3	1.77	0.49
1:H:145:SER:HB2	3:H:232:HOH:O	2.12	0.49
1:E:48:GLY:HA3	1:E:209:VAL:HG23	1.95	0.49
1:G:194:ASN:O	1:G:198:GLU:HG3	2.13	0.48
1:W:6:ALA:HB1	1:W:9:ILE:HD12	1.94	0.48
1:D:200:ASP:HB3	1:D:203:ILE:HG13	1.96	0.48
1:D:101:LYS:HE3	1:D:118:SER:O	2.14	0.48
1:G:190:LEU:HB3	1:G:195:MET:CE	2.43	0.47
1:E:82:ARG:HD3	1:E:174:GLN:NE2	2.29	0.47
1:A:173:GLU:C	1:A:175:GLY:H	2.18	0.47
1:G:42:ILE:HG12	1:G:181:GLN:HG2	1.96	0.47
1:C:93:LEU:HD12	1:C:94:GLU:N	2.30	0.46
1:E:110:THR:HB	1:E:157:GLN:OE1	2.15	0.46
1:C:110:THR:HB	1:C:157:GLN:OE1	2.16	0.46
1:F:42:ILE:HG12	1:F:181:GLN:HG2	1.97	0.46
1:D:94:GLU:OE1	1:D:96:HIS:HD2	1.99	0.46
1:F:45:LYS:HA	1:F:179:GLN:NE2	2.30	0.46
1:I:77:GLU:HB3	1:I:176:GLN:HE21	1.80	0.46
1:I:60:PRO:HD2	1:I:164:GLN:HB2	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:GLY:HA2	1:A:174:GLN:NE2	2.31	0.45
1:E:215:VAL:HG12	1:E:216:PRO:O	2.16	0.45
1:F:190:LEU:HB3	1:F:195:MET:CE	2.47	0.45
1:B:49:GLN:HE21	1:B:172:LYS:HB3	1.81	0.45
1:A:143:VAL:O	1:A:144:ASP:C	2.55	0.45
1:B:97:ILE:HG13	1:B:102:ILE:HD12	1.98	0.45
1:G:40:THR:HG21	1:G:181:GLN:OE1	2.17	0.44
1:D:192:VAL:HA	1:D:195:MET:HE2	1.99	0.44
1:C:190:LEU:HB3	1:C:195:MET:HE1	2.00	0.43
1:I:209:VAL:HG22	1:I:209:VAL:O	2.18	0.43
1:G:190:LEU:HB3	1:G:195:MET:HE1	2.00	0.43
1:E:120:ALA:HB1	1:E:146:TRP:CZ3	2.51	0.43
1:B:150:GLU:HB3	1:B:152:TYR:CE1	2.54	0.43
1:E:91:ASP:HA	1:E:107:ASN:O	2.18	0.43
1:B:52:TYR:O	1:B:166:THR:HA	2.19	0.43
1:H:82:ARG:HD3	1:H:174:GLN:NE2	2.33	0.43
1:C:136:GLY:HA2	1:C:159:THR:HB	2.01	0.43
1:I:151:ARG:HE	1:I:151:ARG:HB3	1.67	0.42
1:G:91:ASP:HA	1:G:107:ASN:O	2.19	0.42
1:C:192:VAL:HA	1:C:195:MET:CE	2.22	0.42
1:G:80:LEU:HD22	1:G:178:PHE:CD1	2.54	0.42
1:H:198:GLU:O	1:H:199:ASN:HB3	2.20	0.42
1:B:55:PRO:HA	1:B:56:PRO:HD3	1.95	0.42
1:H:51:THR:O	1:H:203:ILE:HA	2.19	0.42
1:B:105:LYS:HB2	1:B:105:LYS:HE3	1.92	0.42
1:G:82:ARG:HD3	1:G:174:GLN:NE2	2.35	0.42
1:C:55:PRO:HA	1:C:56:PRO:HD3	1.93	0.42
1:E:40:THR:HG23	1:E:183:SER:HB3	2.01	0.42
1:B:140:THR:HA	1:B:149:ILE:O	2.20	0.42
1:G:71:PHE:HA	1:G:181:GLN:O	2.20	0.42
1:G:82:ARG:HD2	1:G:82:ARG:HH11	1.72	0.42
1:A:59:ARG:NH1	1:A:86:SER:HB3	2.35	0.41
1:B:208:ASN:ND2	1:B:210:ARG:HH21	2.00	0.41
1:G:82:ARG:HD3	1:G:174:GLN:HE21	1.84	0.41
1:H:44:SER:HB2	1:H:208:ASN:CG	2.41	0.41
1:G:186:TYR:CD2	1:G:186:TYR:C	2.94	0.41
1:E:215:VAL:CG1	1:E:216:PRO:N	2.83	0.41
1:I:193:LEU:HA	1:I:193:LEU:HD23	1.92	0.41
1:C:190:LEU:HB3	1:C:195:MET:HE2	2.03	0.41
1:B:41:TYR:CZ	1:B:211:LEU:HD13	2.56	0.41
1:B:63:ARG:HD2	1:F:152:TYR:CD1	2.56	0.41
1:A:122:ILE:HD11	1:A:143:VAL:CG1	2.41	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:GLN:N	1:A:174:GLN:HE21	2.16	0.40
1:E:59:ARG:HG2	1:E:164:GLN:O	2.22	0.40
1:H:41:TYR:HA	1:H:210:ARG:O	2.20	0.40
1:A:173:GLU:O	1:A:175:GLY:N	2.55	0.40
1:C:192:VAL:CA	1:C:195:MET:HE3	2.22	0.40
1:B:80:LEU:HD13	1:B:182:LEU:HD21	2.04	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	180/226 (80%)	170 (94%)	8 (4%)	2 (1%)	21	42
1	B	178/226 (79%)	167 (94%)	9 (5%)	2 (1%)	21	42
1	C	181/226 (80%)	174 (96%)	5 (3%)	2 (1%)	21	42
1	D	177/226 (78%)	170 (96%)	6 (3%)	1 (1%)	33	63
1	E	180/226 (80%)	170 (94%)	7 (4%)	3 (2%)	14	26
1	F	176/226 (78%)	164 (93%)	9 (5%)	3 (2%)	14	26
1	G	180/226 (80%)	173 (96%)	6 (3%)	1 (1%)	33	63
1	H	174/226 (77%)	161 (92%)	11 (6%)	2 (1%)	21	42
1	I	139/226 (62%)	128 (92%)	9 (6%)	2 (1%)	16	32
1	W	5/226 (2%)	2 (40%)	2 (40%)	1 (20%)	0	0
All	All	1570/2260 (70%)	1479 (94%)	72 (5%)	19 (1%)	19	39

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	87	SER
1	I	174	GLN
1	A	174	GLN
1	B	213	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	45	LYS
1	A	45	LYS
1	D	45	LYS
1	H	200	ASP
1	W	8	HIS
1	B	36	HIS
1	C	156	ARG
1	F	110	THR
1	F	173	GLU
1	I	172	LYS
1	C	45	LYS
1	E	174	GLN
1	H	110	THR
1	E	155	GLY
1	G	36	HIS

### 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	143/182 (79%)	138 (96%)	5 (4%)	48	77
1	B	141/182 (78%)	135 (96%)	6 (4%)	40	69
1	C	143/182 (79%)	136 (95%)	7 (5%)	35	62
1	D	141/182 (78%)	135 (96%)	6 (4%)	40	69
1	E	140/182 (77%)	131 (94%)	9 (6%)	25	47
1	F	139/182 (76%)	132 (95%)	7 (5%)	34	61
1	G	144/182 (79%)	139 (96%)	5 (4%)	48	77
1	H	139/182 (76%)	132 (95%)	7 (5%)	34	61
1	I	119/182 (65%)	111 (93%)	8 (7%)	23	44
1	W	5/182 (3%)	3 (60%)	2 (40%)	0	0
All	All	1254/1820 (69%)	1192 (95%)	62 (5%)	35	62

All (62) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	80	LEU
1	A	121	ILE
1	A	122	ILE
1	A	133	THR
1	A	174	GLN
1	B	36	HIS
1	B	49	GLN
1	B	80	LEU
1	B	159	THR
1	B	161	PHE
1	B	208	ASN
1	C	44	SER
1	C	80	LEU
1	C	86	SER
1	C	93	LEU
1	C	151	ARG
1	C	161	PHE
1	C	203	ILE
1	D	80	LEU
1	D	110	THR
1	D	140	THR
1	D	161	PHE
1	D	194	ASN
1	D	203	ILE
1	E	44	SER
1	E	66	ARG
1	E	93	LEU
1	E	102	ILE
1	E	140	THR
1	E	145	SER
1	E	151	ARG
1	E	203	ILE
1	E	208	ASN
1	F	44	SER
1	F	93	LEU
1	F	121	ILE
1	F	161	PHE
1	F	172	LYS
1	F	173	GLU
1	F	199	ASN
1	G	126	LYS
1	G	149	ILE
1	G	151	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	156	ARG
1	G	208	ASN
1	H	80	LEU
1	H	89	LEU
1	H	110	THR
1	H	133	THR
1	H	140	THR
1	H	158	LEU
1	H	161	PHE
1	I	42	ILE
1	I	80	LEU
1	I	89	LEU
1	I	142	GLN
1	I	151	ARG
1	I	161	PHE
1	I	166	THR
1	I	209	VAL
1	W	4	LEU
1	W	9	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	B	49	GLN
1	B	57	ASN
1	B	176	GLN
1	B	208	ASN
1	C	99	GLN
1	C	142	GLN
1	D	36	HIS
1	D	96	HIS
1	D	179	GLN
1	D	181	GLN
1	D	194	ASN
1	E	208	ASN
1	F	49	GLN
1	F	123	ASN
1	F	199	ASN
1	G	96	HIS
1	I	96	HIS
1	I	176	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

### 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	182/226 (80%)	-0.26	1 (0%) 88 90	34, 39, 47, 59	0
1	B	180/226 (79%)	-0.37	2 (1%) 77 79	34, 39, 50, 71	0
1	C	183/226 (80%)	-0.27	1 (0%) 88 90	32, 39, 50, 61	0
1	D	179/226 (79%)	-0.24	4 (2%) 59 56	33, 39, 51, 71	0
1	E	182/226 (80%)	-0.22	2 (1%) 77 79	32, 39, 47, 56	0
1	F	178/226 (78%)	-0.22	5 (2%) 50 48	32, 39, 48, 55	0
1	G	182/226 (80%)	-0.28	2 (1%) 77 79	35, 39, 49, 59	0
1	H	176/226 (77%)	-0.12	1 (0%) 86 89	32, 39, 48, 55	0
1	I	151/226 (66%)	1.18	38 (25%) 1 1	35, 39, 43, 44	0
1	W	7/226 (3%)	1.53	2 (28%) 1 1	59, 63, 74, 77	0
All	All	1600/2260 (70%)	-0.10	58 (3%) 41 37	32, 39, 49, 77	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	41	TYR	8.8
1	I	40	THR	5.4
1	I	211	LEU	4.7
1	I	195	MET	4.6
1	I	42	ILE	4.3
1	I	209	VAL	4.3
1	I	71	PHE	4.2
1	I	196	ALA	4.1
1	I	50	ILE	4.0
1	W	9	ILE	3.8
1	I	39	THR	3.8
1	I	181	GLN	3.8
1	I	43	PHE	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	194	ASN	3.7
1	I	154	ALA	3.6
1	I	81	VAL	3.5
1	F	37	ALA	3.4
1	G	37	ALA	3.4
1	I	137	GLY	3.4
1	D	36	HIS	3.3
1	C	154	ALA	3.2
1	D	35	GLY	3.2
1	I	152	TYR	3.2
1	I	166	THR	3.1
1	I	167	ILE	3.1
1	I	210	ARG	3.0
1	B	214	GLU	3.0
1	I	186	TYR	3.0
1	G	216	PRO	2.9
1	I	193	LEU	2.7
1	I	169	ILE	2.7
1	I	168	ILE	2.6
1	H	121	ILE	2.6
1	W	10	HIS	2.5
1	F	38	GLY	2.5
1	E	38	GLY	2.5
1	D	146	TRP	2.5
1	I	52	TYR	2.4
1	I	53	LYS	2.3
1	I	158	LEU	2.3
1	F	121	ILE	2.3
1	I	192	VAL	2.3
1	A	154	ALA	2.3
1	I	110	THR	2.2
1	I	72	SER	2.2
1	F	35	GLY	2.2
1	I	90	GLY	2.2
1	I	111	ASP	2.2
1	F	212	VAL	2.2
1	I	80	LEU	2.2
1	I	157	GLN	2.1
1	I	70	GLY	2.1
1	D	37	ALA	2.1
1	E	120	ALA	2.1
1	B	121	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	182	LEU	2.1
1	I	153	PRO	2.1
1	I	178	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	B	1000	1/1	0.16	1.12	50,50,50,50	0
2	CA	I	3000	1/1	0.17	-0.77	33,33,33,33	0
2	CA	D	2000	1/1	0.09	-2.00	46,46,46,46	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.