



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:04 am BST

PDB ID : 2R1D
Title : Crystal structure of rat neurexin 1beta in the Ca²⁺ containing form
Authors : Rudenko, G.
Deposited on : 2007-08-22
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

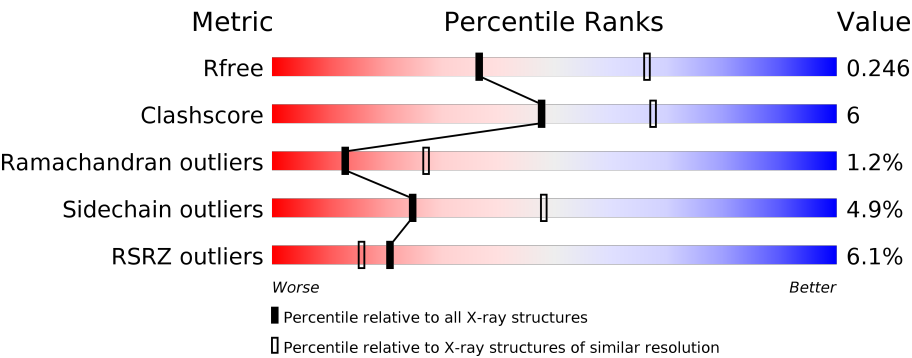
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	226	<div><div>%</div><div><div></div><div>70%</div><div>8%</div><div>•</div><div>19%</div></div></div>
1	B	226	<div><div>2%</div><div><div></div><div>65%</div><div>13%</div><div>•</div><div>20%</div></div></div>
1	C	226	<div><div>%</div><div><div></div><div>67%</div><div>12%</div><div>•</div><div>19%</div></div></div>
1	D	226	<div><div>2%</div><div><div></div><div>70%</div><div>8%</div><div>21%</div></div></div>
1	E	226	<div><div>3%</div><div><div></div><div>63%</div><div>16%</div><div>•</div><div>19%</div></div></div>
1	F	226	<div><div>4%</div><div><div></div><div>65%</div><div>14%</div><div>21%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	226	<div><div>%</div><div><div></div><div>63%</div><div>17%</div><div>19%</div></div></div>
1	H	226	<div><div>2%</div><div><div></div><div>65%</div><div>12%</div><div>22%</div></div></div>
1	I	226	<div><div>25%</div><div><div></div><div>55%</div><div>9%</div><div>33%</div></div></div>
1	W	226	<div><div>3%</div><div><div></div><div>97%</div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12217 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 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		

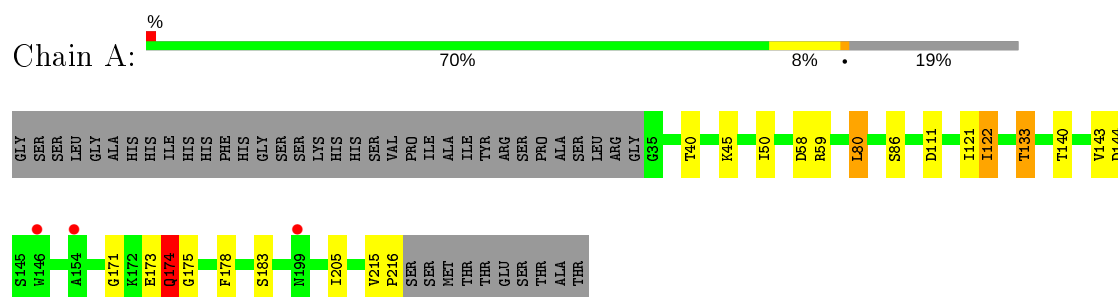
- Molecule 3 is water.

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

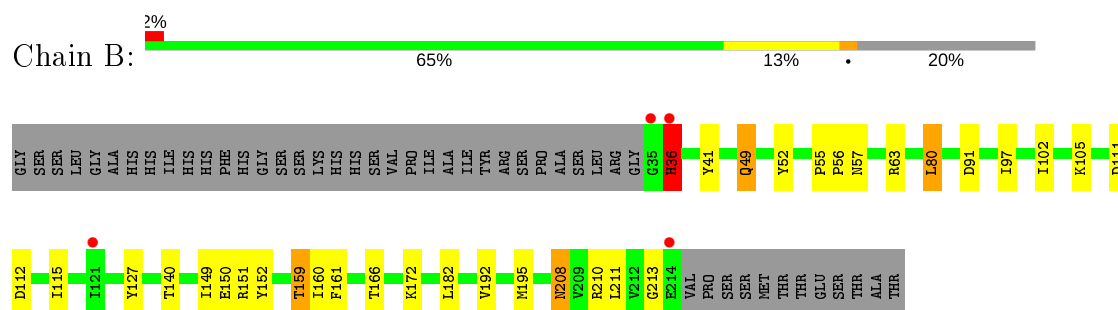
3 Residue-property plots [i](#)

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.

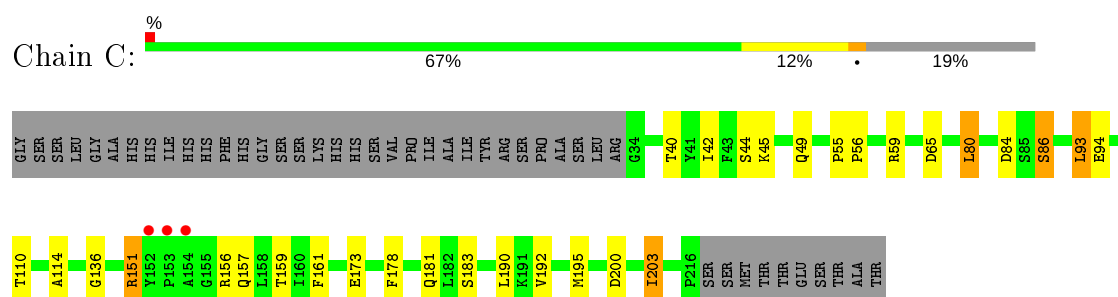
• Molecule 1: Neurexin-1-beta



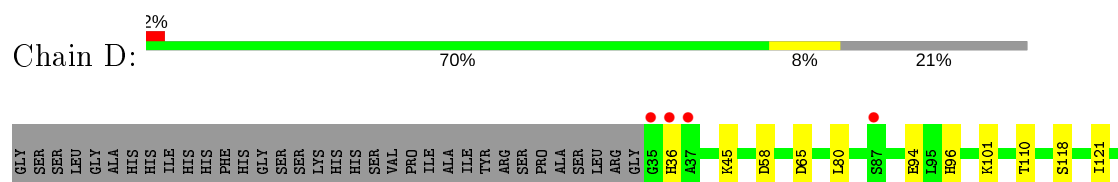
• Molecule 1: Neurexin-1-beta

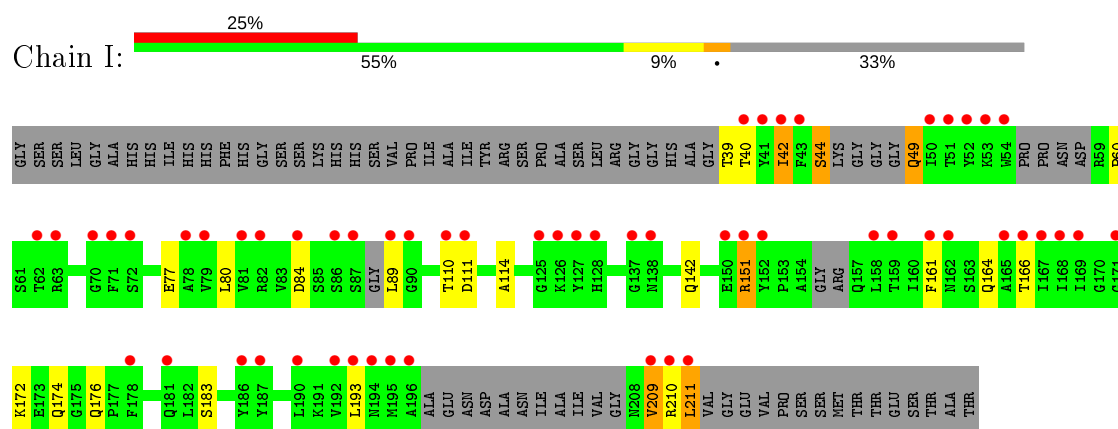


• Molecule 1: Neurexin-1-beta

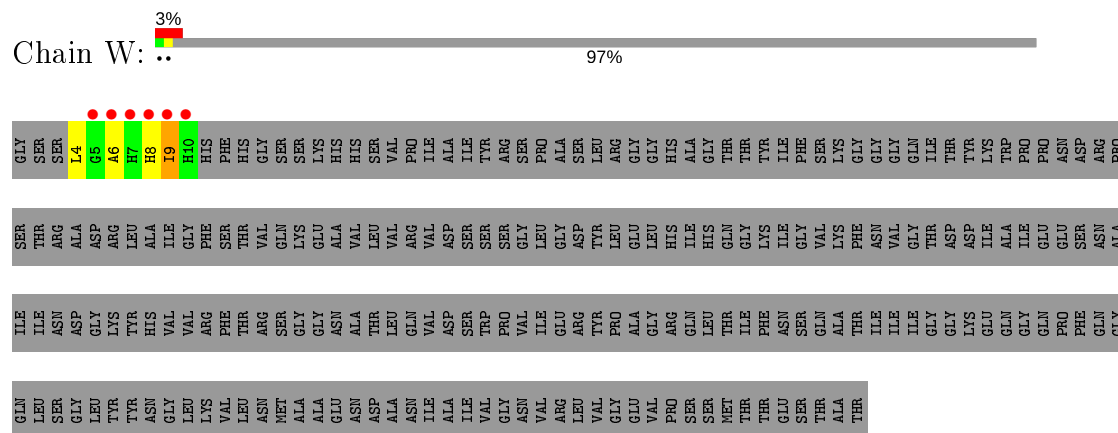


• Molecule 1: Neurexin-1-beta





- Molecule 1: Neurexin-1-beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.203 , 0.244 0.206 , 0.246	Depositor DCC
R_{free} test set	3755 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12217	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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 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	1373	0	1338	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 (146) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:80:LEU:HD22	1:F:178:PHE:CD1	2.40	0.56
1:G:93:LEU:HD11	1:G:132:PHE:CE2	2.40	0.56
1:F:133:THR:HG22	3:F:238:HOH:O	2.04	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:E:80:LEU:HD22	1:E:178:PHE:CD1	2.41	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:C:42:ILE:HD13	1:C:181:GLN:CG	2.28	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:57:ASN:HB2	3:B:1008:HOH:O	2.11	0.51
1:C:190:LEU:HB3	1:C:195:MET:CE	2.41	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:D:200:ASP:HB3	1:D:203:ILE:HG13	1.96	0.48
1:W:6:ALA:HB1	1:W:9:ILE:HD12	1.94	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:110:THR:HB	1:C:157:GLN:OE1	2.16	0.46
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:F:42:ILE:HG12	1:F:181:GLN:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:49:GLN:HE21	1:B:172:LYS:HB3	1.81	0.45
1:F:190:LEU:HB3	1:F:195:MET:CE	2.47	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:E:120:ALA:HB1	1:E:146:TRP:CZ3	2.51	0.43
1:G:190:LEU:HB3	1:G:195:MET:HE1	2.00	0.43
1:B:150:GLU:HB3	1:B:152:TYR:CE1	2.54	0.43
1:B:52:TYR:O	1:B:166:THR:HA	2.19	0.43
1:E:91:ASP:HA	1:E:107:ASN:O	2.18	0.43
1:C:136:GLY:HA2	1:C:159:THR:HB	2.01	0.43
1:H:82:ARG:HD3	1:H:174:GLN:NE2	2.33	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:B:55:PRO:HA	1:B:56:PRO:HD3	1.95	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:105:LYS:HB2	1:B:105:LYS:HE3	1.92	0.42
1:H:51:THR:O	1:H:203:ILE:HA	2.19	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:G:82:ARG:HD3	1:G:174:GLN:NE2	2.35	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:G:186:TYR:CD2	1:G:186:TYR:C	2.94	0.41
1:H:44:SER:HB2	1:H:208:ASN:CG	2.41	0.41
1:E:215:VAL:CG1	1:E:216:PRO:N	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:193:LEU:HA	1:I:193:LEU:HD23	1.92	0.41
1:B:41:TYR:CZ	1:B:211:LEU:HD13	2.56	0.41
1:C:190:LEU:HB3	1:C:195:MET:HE2	2.03	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
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:B:80:LEU:HD13	1:B:182:LEU:HD21	2.04	0.40
1:C:192:VAL:CA	1:C:195:MET:HE3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/226 (80%)	170 (94%)	8 (4%)	2 (1%)	14	30
1	B	178/226 (79%)	167 (94%)	9 (5%)	2 (1%)	14	30
1	C	181/226 (80%)	174 (96%)	5 (3%)	2 (1%)	14	30
1	D	177/226 (78%)	170 (96%)	6 (3%)	1 (1%)	25	47
1	E	180/226 (80%)	170 (94%)	7 (4%)	3 (2%)	9	18
1	F	176/226 (78%)	164 (93%)	9 (5%)	3 (2%)	9	18
1	G	180/226 (80%)	173 (96%)	6 (3%)	1 (1%)	25	47
1	H	174/226 (77%)	161 (92%)	11 (6%)	2 (1%)	14	30
1	I	139/226 (62%)	128 (92%)	9 (6%)	2 (1%)	11	22
1	W	5/226 (2%)	2 (40%)	2 (40%)	1 (20%)	0	0
All	All	1570/2260 (70%)	1479 (94%)	72 (5%)	19 (1%)	13	27

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
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%)	36	62
1	B	141/182 (78%)	135 (96%)	6 (4%)	29	54
1	C	143/182 (79%)	136 (95%)	7 (5%)	25	48
1	D	141/182 (78%)	135 (96%)	6 (4%)	29	54
1	E	140/182 (77%)	131 (94%)	9 (6%)	17	35
1	F	139/182 (76%)	132 (95%)	7 (5%)	24	47
1	G	144/182 (79%)	139 (96%)	5 (4%)	36	62
1	H	139/182 (76%)	132 (95%)	7 (5%)	24	47
1	I	119/182 (65%)	111 (93%)	8 (7%)	16	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	5/182 (3%)	3 (60%)	2 (40%)	0	0
All	All	1254/1820 (69%)	1192 (95%)	62 (5%)	25	48

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 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 ⓘ

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.

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, 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	182/226 (80%)	0.09	3 (1%) 72 68	34, 39, 47, 59	0
1	B	180/226 (79%)	0.04	4 (2%) 62 56	34, 39, 50, 71	0
1	C	183/226 (80%)	0.11	3 (1%) 72 68	32, 39, 50, 61	0
1	D	179/226 (79%)	0.08	5 (2%) 53 46	33, 39, 51, 71	0
1	E	182/226 (80%)	0.19	6 (3%) 46 39	32, 39, 47, 56	0
1	F	178/226 (78%)	0.15	8 (4%) 33 26	32, 39, 48, 55	0
1	G	182/226 (80%)	0.10	2 (1%) 80 78	35, 39, 49, 59	0
1	H	176/226 (77%)	0.29	4 (2%) 60 54	32, 39, 48, 55	0
1	I	151/226 (66%)	1.70	57 (37%) 0 0	35, 39, 43, 44	0
1	W	7/226 (3%)	3.05	6 (85%) 0 0	59, 63, 74, 77	0
All	All	1600/2260 (70%)	0.29	98 (6%) 21 16	32, 39, 49, 77	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	41	TYR	8.3
1	C	154	ALA	7.2
1	W	9	ILE	5.4
1	I	194	ASN	5.1
1	I	186	TYR	4.6
1	I	71	PHE	4.5
1	D	36	HIS	4.5
1	I	40	THR	4.5
1	I	166	THR	4.5
1	I	50	ILE	4.4
1	I	52	TYR	4.1
1	I	196	ALA	4.1
1	B	121	ILE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	42	ILE	4.1
1	I	195	MET	4.0
1	I	165	ALA	3.9
1	I	86	SER	3.9
1	I	193	LEU	3.9
1	I	111	ASP	3.8
1	I	209	VAL	3.8
1	I	181	GLN	3.7
1	I	79	VAL	3.6
1	I	72	SER	3.5
1	I	152	TYR	3.4
1	W	8	HIS	3.4
1	I	51	THR	3.4
1	G	37	ALA	3.4
1	F	37	ALA	3.4
1	I	167	ILE	3.3
1	I	78	ALA	3.3
1	I	110	THR	3.3
1	F	212	VAL	3.3
1	I	178	PHE	3.2
1	I	89	LEU	3.2
1	H	38	GLY	3.2
1	I	43	PHE	3.2
1	I	62	THR	3.1
1	F	38	GLY	3.1
1	B	214	GLU	3.1
1	I	211	LEU	3.0
1	A	154	ALA	3.0
1	E	38	GLY	3.0
1	W	10	HIS	3.0
1	H	37	ALA	3.0
1	E	121	ILE	3.0
1	I	81	VAL	3.0
1	I	161	PHE	2.9
1	I	187	TYR	2.9
1	W	6	ALA	2.9
1	I	54	TRP	2.8
1	B	35	GLY	2.8
1	I	171	GLY	2.8
1	E	120	ALA	2.8
1	I	192	VAL	2.8
1	I	53	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	152	TYR	2.7
1	I	87	SER	2.7
1	I	63	ARG	2.7
1	I	137	GLY	2.7
1	D	37	ALA	2.7
1	E	37	ALA	2.7
1	I	90	GLY	2.6
1	I	127	TYR	2.6
1	D	35	GLY	2.6
1	I	210	ARG	2.5
1	I	128	HIS	2.5
1	I	126	LYS	2.5
1	I	151	ARG	2.5
1	I	190	LEU	2.5
1	D	146	TRP	2.5
1	I	82	ARG	2.5
1	W	5	GLY	2.4
1	I	158	LEU	2.4
1	W	7	HIS	2.4
1	I	168	ILE	2.4
1	B	36	HIS	2.4
1	F	35	GLY	2.4
1	I	162	ASN	2.4
1	I	125	GLY	2.3
1	A	199	ASN	2.3
1	I	70	GLY	2.2
1	E	148	VAL	2.2
1	I	84	ASP	2.2
1	D	87	SER	2.2
1	H	36	HIS	2.2
1	I	159	THR	2.2
1	F	121	ILE	2.1
1	H	121	ILE	2.1
1	F	39	THR	2.1
1	E	146	TRP	2.1
1	F	199	ASN	2.1
1	I	169	ILE	2.1
1	A	146	TRP	2.1
1	I	150	GLU	2.0
1	F	36	HIS	2.0
1	I	138	ASN	2.0
1	C	153	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	216	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(\AA^2)	Q<0.9
2	CA	B	1000	1/1	0.84	0.16	50,50,50,50	0
2	CA	I	3000	1/1	0.89	0.06	33,33,33,33	0
2	CA	D	2000	1/1	0.96	0.08	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.