



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:56 PM GMT

PDB ID : 4QD2
Title : Molecular basis for disruption of E-cadherin adhesion by botulinum neurotoxin A complex
Authors : Lee, K.; Zhong, X.; Gu, S.; Kruel, A.; Dorner, M.B.; Perry, K.; Rummel, A.; Dong, M.; Jin, R.
Deposited on : 2014-05-13
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

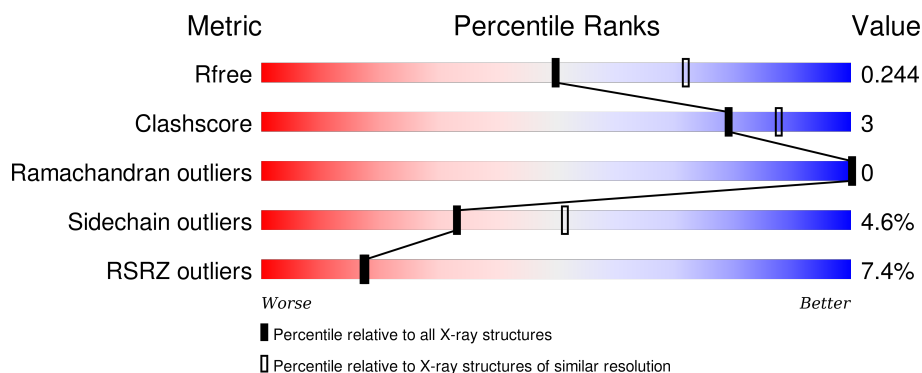
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



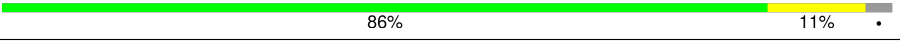




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	296	<div> <div>8%</div> <div>85%</div> <div>11%</div> <div>••</div> </div>
1	D	296	<div> <div>21%</div> <div>80%</div> <div>16%</div> <div>••</div> </div>
1	H	296	<div> <div>7%</div> <div>84%</div> <div>12%</div> <div>••</div> </div>
1	I	296	<div> <div>3%</div> <div>86%</div> <div>9%</div> <div>••</div> </div>
2	B	147	<div> <div>%</div> <div>88%</div> <div>10%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	147	
3	A	254	
3	F	254	
4	E	213	
4	J	213	

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	CA	E	301	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19012 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 Hemagglutinin component HA33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	286	Total	C	N	O	S	0	0	0
			2333	1476	399	455	3			
1	C	286	Total	C	N	O	S	0	0	0
			2333	1476	399	455	3			
1	I	286	Total	C	N	O	S	0	0	0
			2333	1476	399	455	3			
1	H	286	Total	C	N	O	S	0	0	0
			2333	1476	399	455	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	294	PRO	-	EXPRESSION TAG	UNP A5HZZ6
D	295	GLY	-	EXPRESSION TAG	UNP A5HZZ6
D	296	SER	-	EXPRESSION TAG	UNP A5HZZ6
D	297	ALA	-	EXPRESSION TAG	UNP A5HZZ6
C	294	PRO	-	EXPRESSION TAG	UNP A5HZZ6
C	295	GLY	-	EXPRESSION TAG	UNP A5HZZ6
C	296	SER	-	EXPRESSION TAG	UNP A5HZZ6
C	297	ALA	-	EXPRESSION TAG	UNP A5HZZ6
I	294	PRO	-	EXPRESSION TAG	UNP A5HZZ6
I	295	GLY	-	EXPRESSION TAG	UNP A5HZZ6
I	296	SER	-	EXPRESSION TAG	UNP A5HZZ6
I	297	ALA	-	EXPRESSION TAG	UNP A5HZZ6
H	294	PRO	-	EXPRESSION TAG	UNP A5HZZ6
H	295	GLY	-	EXPRESSION TAG	UNP A5HZZ6
H	296	SER	-	EXPRESSION TAG	UNP A5HZZ6
H	297	ALA	-	EXPRESSION TAG	UNP A5HZZ6

- Molecule 2 is a protein called Hemagglutinin component HA17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	143	Total	C	N	O	S	0	0	0
			1180	762	188	225	5			
2	G	143	Total	C	N	O	S	0	0	0
			1180	762	188	225	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	EXPRESSION TAG	UNP A5HZZ5
B	1	PRO	-	EXPRESSION TAG	UNP A5HZZ5
G	0	GLY	-	EXPRESSION TAG	UNP A5HZZ5
G	1	PRO	-	EXPRESSION TAG	UNP A5HZZ5

- Molecule 3 is a protein called Hemagglutinin component HA70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	224	Total	C	N	O	S	0	0	0
			1825	1154	310	360	1			
3	F	225	Total	C	N	O	S	0	0	0
			1833	1158	312	362	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	GLY	-	EXPRESSION TAG	UNP A5HZZ4
A	374	PRO	-	EXPRESSION TAG	UNP A5HZZ4
A	375	LEU	-	EXPRESSION TAG	UNP A5HZZ4
A	376	GLY	-	EXPRESSION TAG	UNP A5HZZ4
A	377	SER	-	EXPRESSION TAG	UNP A5HZZ4
F	373	GLY	-	EXPRESSION TAG	UNP A5HZZ4
F	374	PRO	-	EXPRESSION TAG	UNP A5HZZ4
F	375	LEU	-	EXPRESSION TAG	UNP A5HZZ4
F	376	GLY	-	EXPRESSION TAG	UNP A5HZZ4
F	377	SER	-	EXPRESSION TAG	UNP A5HZZ4

- Molecule 4 is a protein called Cadherin-1.

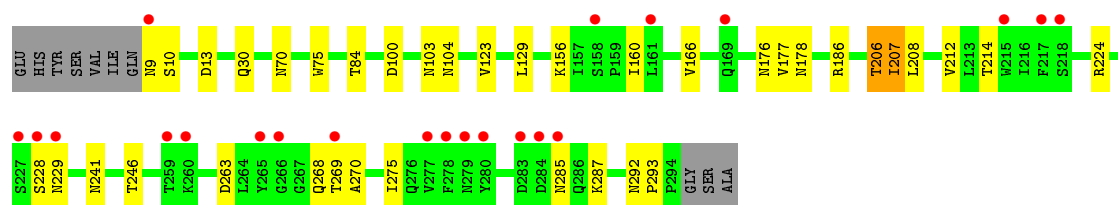
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	212	Total	C	N	O	S	0	0	0
			1627	1023	266	334	4			
4	J	212	Total	C	N	O	S	0	0	0
			1627	1023	266	334	4			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

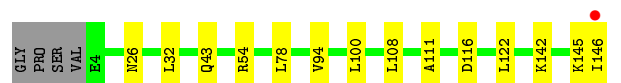
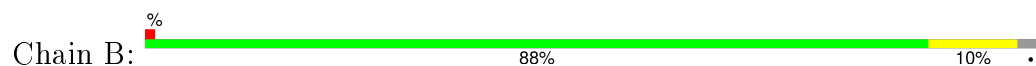
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	3	Total	Ca	0	0
			3	3		
5	E	3	Total	Ca	0	0
			3	3		

- Molecule 6 is water.

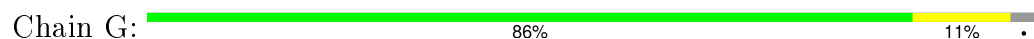
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	37	Total	O	0	0
			37	37		
6	B	44	Total	O	0	0
			44	44		
6	C	47	Total	O	0	0
			47	47		
6	A	31	Total	O	0	0
			31	31		
6	E	46	Total	O	0	0
			46	46		
6	I	50	Total	O	0	0
			50	50		
6	G	50	Total	O	0	0
			50	50		
6	H	43	Total	O	0	0
			43	43		
6	F	28	Total	O	0	0
			28	28		
6	J	26	Total	O	0	0
			26	26		



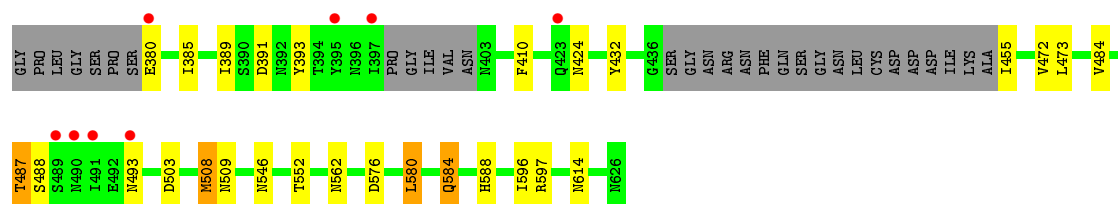
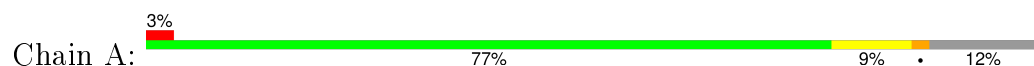
- Molecule 2: Hemagglutinin component HA17



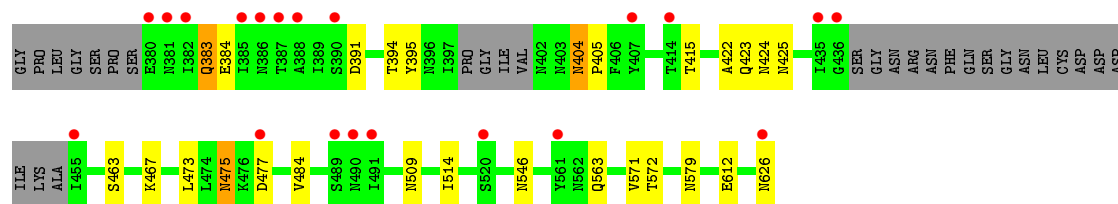
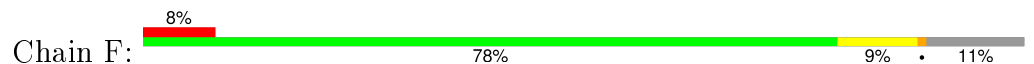
- Molecule 2: Hemagglutinin component HA17



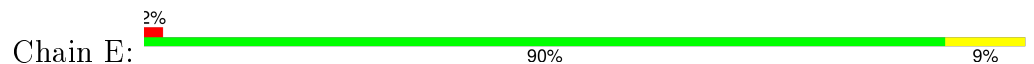
- Molecule 3: Hemagglutinin component HA70



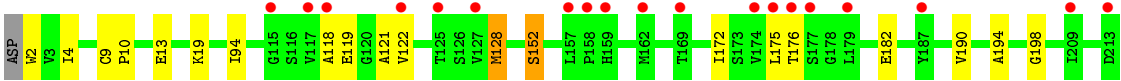
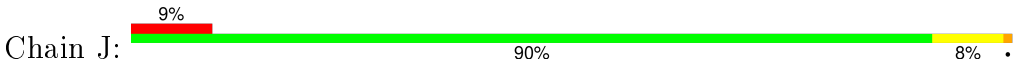
- Molecule 3: Hemagglutinin component HA70



- Molecule 4: Cadherin-1



- Molecule 4: Cadherin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.99Å 95.73Å 96.14Å 116.89° 96.34° 93.70°	Depositor
Resolution (Å)	47.73 – 2.40 47.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.7 (47.73-2.40) 81.9 (47.73-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.2_869)	Depositor
R, R_{free}	0.208 , 0.247 0.206 , 0.244	Depositor DCC
R_{free} test set	5232 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.2	EDS
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 104475 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19012	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	C	0.23	0/2384	0.41	0/3255
1	D	0.23	0/2384	0.42	0/3255
1	H	0.23	0/2384	0.42	0/3255
1	I	0.24	0/2384	0.42	0/3255
2	B	0.25	0/1210	0.41	0/1643
2	G	0.25	0/1210	0.42	0/1643
3	A	0.24	0/1857	0.45	1/2527 (0.0%)
3	F	0.23	0/1865	0.44	1/2538 (0.0%)
4	E	0.23	0/1658	0.42	0/2263
4	J	0.22	0/1658	0.42	0/2263
All	All	0.23	0/18994	0.42	2/25897 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	391	ASP	CB-CG-OD2	5.23	123.01	118.30
3	A	391	ASP	CB-CG-OD2	5.12	122.91	118.30

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	C	2333	0	2250	16	0
1	D	2333	0	2250	17	0
1	H	2333	0	2250	15	0
1	I	2333	0	2250	13	0
2	B	1180	0	1141	16	0
2	G	1180	0	1141	14	0
3	A	1825	0	1779	14	0
3	F	1833	0	1785	10	0
4	E	1627	0	1595	10	0
4	J	1627	0	1595	11	0
5	E	3	0	0	0	0
5	J	3	0	0	0	0
6	A	31	0	0	0	0
6	B	44	0	0	0	0
6	C	47	0	0	3	0
6	D	37	0	0	1	0
6	E	46	0	0	1	0
6	F	28	0	0	0	0
6	G	50	0	0	0	0
6	H	43	0	0	2	0
6	I	50	0	0	0	0
6	J	26	0	0	1	0
All	All	19012	0	18036	127	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 3.

All (127) 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)
2:B:145:LYS:CG	2:B:146:ILE:HG22	1.80	1.10
2:B:145:LYS:HG2	2:B:146:ILE:CG2	1.93	0.98
2:B:145:LYS:HG2	2:B:146:ILE:HG22	0.97	0.95
2:G:145:LYS:HB3	2:G:146:ILE:CG2	2.10	0.82
1:C:64:MET:SD	6:C:333:HOH:O	2.43	0.75
2:G:145:LYS:HB3	2:G:146:ILE:HG22	1.69	0.74
4:J:118:ALA:HB3	4:J:121:ALA:HB2	1.75	0.69
1:D:263:ASP:OD2	1:D:285:ASN:ND2	2.30	0.65
2:G:145:LYS:HB3	2:G:146:ILE:HG23	1.77	0.65
1:C:121:ASP:HB2	1:C:128:LYS:HD3	1.80	0.64
3:F:473:LEU:H	3:F:509:ASN:ND2	1.96	0.64
2:G:145:LYS:HD2	2:G:146:ILE:HG22	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:TYR:HA	1:C:47:ARG:HD2	1.82	0.61
2:B:54:ARG:NH1	3:A:576:ASP:OD1	2.33	0.60
1:D:11:LEU:HD12	1:C:101:ILE:HG21	1.83	0.60
1:C:172:VAL:HA	1:C:207:ILE:HD12	1.83	0.60
1:H:9:ASN:N	6:H:312:HOH:O	2.35	0.59
2:B:145:LYS:HB3	2:B:146:ILE:HG23	1.85	0.58
1:C:155:CYS:HA	1:C:293:PRO:HD3	1.85	0.58
1:D:169:GLN:O	1:D:187:ASN:ND2	2.31	0.58
3:F:563:GLN:HB3	3:F:612:GLU:HB2	1.85	0.58
4:J:4:ILE:HD13	4:J:94:ILE:HD11	1.86	0.57
3:A:552:THR:HG21	3:A:597:ARG:HB3	1.86	0.57
3:F:467:LYS:HB3	3:F:514:ILE:HB	1.87	0.56
1:D:9:ASN:N	1:D:59:TYR:HH	2.03	0.56
3:A:472:VAL:HG23	3:A:509:ASN:HD22	1.70	0.55
1:I:266:GLY:O	1:I:285:ASN:ND2	2.40	0.54
3:F:422:ALA:O	3:F:425:ASN:N	2.37	0.54
4:J:2:TRP:N	6:J:401:HOH:O	2.40	0.54
4:E:112:VAL:HG22	4:E:206:LYS:HB2	1.88	0.54
1:H:268:GLN:HG3	1:H:270:ALA:H	1.73	0.54
3:A:503:ASP:HB3	3:A:580:LEU:HB2	1.91	0.53
3:A:552:THR:HG22	3:A:597:ARG:HH11	1.74	0.52
2:B:145:LYS:CG	2:B:146:ILE:CG2	2.68	0.52
1:I:269:THR:O	1:I:269:THR:OG1	2.25	0.51
2:B:145:LYS:CB	2:B:146:ILE:CG2	2.88	0.51
2:B:145:LYS:CB	2:B:146:ILE:HG22	2.38	0.51
1:I:75:TRP:HH2	2:G:108:LEU:HD11	1.75	0.51
1:H:206:THR:O	1:H:206:THR:OG1	2.22	0.50
4:J:128:MET:HG3	4:J:172:ILE:HB	1.92	0.50
3:A:584:GLN:HG3	3:A:596:ILE:HD12	1.94	0.50
1:C:186:ARG:O	1:C:206:THR:OG1	2.27	0.50
1:D:29:TYR:HD1	1:D:46:GLU:HG3	1.77	0.49
1:H:207:ILE:HG13	1:H:208:LEU:H	1.78	0.49
1:C:39:GLN:NE2	6:C:315:HOH:O	2.45	0.49
1:C:263:ASP:OD2	1:C:285:ASN:ND2	2.45	0.49
2:B:145:LYS:HB3	2:B:146:ILE:CG2	2.43	0.49
1:I:266:GLY:HA3	1:I:268:GLN:H	1.78	0.49
2:G:23:LEU:HB3	2:G:34:PHE:HB3	1.95	0.48
2:G:145:LYS:HA	2:G:146:ILE:HA	1.68	0.48
1:D:164:ASN:N	1:D:164:ASN:OD1	2.46	0.48
4:J:175:LEU:HG	4:J:176:THR:HG23	1.96	0.48
1:D:60:LYS:HG3	1:D:94:TYR:CE1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:VAL:HG11	1:I:188:GLN:HB3	1.96	0.47
3:A:473:LEU:H	3:A:509:ASN:ND2	2.12	0.47
4:E:77:TYR:CZ	4:E:93:GLU:HB2	2.50	0.47
2:B:100:LEU:HD23	2:B:111:ALA:HB2	1.95	0.47
1:D:181:THR:O	1:D:188:GLN:NE2	2.48	0.47
1:D:175:LEU:HB3	1:D:225:VAL:HG22	1.97	0.47
1:H:10:SER:N	6:H:312:HOH:O	2.47	0.46
1:D:75:TRP:HH2	2:B:108:LEU:HD11	1.79	0.46
1:D:224:ARG:NE	6:D:337:HOH:O	2.46	0.46
2:G:142:LYS:NZ	3:F:546:ASN:OD1	2.45	0.46
4:J:182:GLU:H	4:J:182:GLU:HG2	1.61	0.45
3:A:432:TYR:HB3	3:A:455:ILE:HG23	1.98	0.45
1:I:60:LYS:HG3	1:I:94:TYR:CE1	2.52	0.45
1:C:49:ARG:HB2	6:C:333:HOH:O	2.17	0.44
3:F:415:THR:HG23	3:F:475:ASN:HA	1.98	0.44
1:I:293:PRO:HA	1:I:294:PRO:HD3	1.88	0.44
1:H:212:VAL:O	1:H:214:THR:HG23	2.17	0.44
1:I:75:TRP:CH2	2:G:108:LEU:HD11	2.53	0.44
1:I:170:VAL:HB	1:I:174:ASN:HB3	1.99	0.44
1:I:292:ASN:HA	1:I:293:PRO:HD3	1.90	0.44
1:H:292:ASN:HA	1:H:293:PRO:HD3	1.83	0.44
4:E:82:SER:OG	4:E:84:ASN:OD1	2.35	0.44
4:E:161:ASN:HB3	4:E:175:LEU:HD23	1.99	0.43
1:I:71:LEU:HB3	1:I:84:THR:HG23	2.00	0.43
3:A:487:THR:HB	3:A:488:SER:H	1.53	0.43
3:F:404:ASN:HA	3:F:405:PRO:HD3	1.86	0.43
1:C:214:THR:HG21	1:C:226:SER:OG	2.18	0.43
1:D:62:LYS:HE3	1:D:70:ASN:HA	2.00	0.43
1:D:266:GLY:HA2	1:D:267:GLY:HA2	1.53	0.43
2:G:110:TYR:HB3	2:G:128:LEU:HG	1.99	0.43
1:H:263:ASP:OD1	1:H:285:ASN:ND2	2.51	0.43
4:E:9:CYS:HA	4:E:10:PRO:HD3	1.90	0.43
2:G:13:TYR:CE1	2:G:145:LYS:HG2	2.54	0.43
1:H:186:ARG:O	1:H:206:THR:HG23	2.19	0.43
4:E:194:ALA:HB3	4:E:198:GLY:HA2	1.99	0.42
3:F:383:GLN:HG2	3:F:395:TYR:OH	2.19	0.42
1:D:75:TRP:CH2	2:B:108:LEU:HD11	2.54	0.42
1:I:210:ASN:OD1	1:I:228:SER:OG	2.35	0.42
4:E:154:ASP:HA	4:E:155:PRO:HA	1.82	0.42
1:H:75:TRP:CD1	1:H:129:LEU:HD11	2.55	0.42
2:B:145:LYS:HA	2:B:146:ILE:HA	1.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2:TRP:CD1	4:E:92:MET:HB2	2.55	0.42
4:E:7:ILE:HD12	4:E:94:ILE:HG21	2.01	0.42
1:H:160:ILE:HD13	1:H:287:LYS:HD2	2.01	0.42
4:J:152:SER:HB3	4:J:190:VAL:HB	2.00	0.42
2:B:142:LYS:NZ	3:A:546:ASN:OD1	2.52	0.42
1:C:241:ASN:HA	1:C:242:PRO:HD3	1.77	0.42
1:H:100:ASP:O	1:H:104:ASN:N	2.53	0.42
3:A:385:ILE:HG13	3:A:410:PHE:HB3	2.02	0.42
2:G:100:LEU:HD23	2:G:111:ALA:HB2	2.02	0.42
3:F:423:GLN:HA	3:F:424:ASN:HA	1.57	0.41
4:J:194:ALA:HB3	4:J:198:GLY:HA2	2.02	0.41
4:J:9:CYS:HA	4:J:10:PRO:HD3	1.88	0.41
1:D:44:TYR:HA	1:D:47:ARG:HD2	2.03	0.41
1:C:60:LYS:HG3	1:C:94:TYR:CE1	2.56	0.41
2:B:26:ASN:ND2	2:B:43:GLN:HE21	2.17	0.41
1:I:80:HIS:HB3	2:G:132:PHE:CG	2.55	0.41
1:C:169:GLN:O	1:C:187:ASN:ND2	2.44	0.41
1:D:154:THR:HA	1:D:191:THR:HA	2.01	0.41
1:C:25:ASN:O	1:C:39:GLN:HA	2.21	0.41
1:H:177:VAL:HG23	1:H:224:ARG:HA	2.02	0.41
1:H:212:VAL:HB	1:H:228:SER:HB3	2.03	0.41
4:E:2:TRP:N	6:E:433:HOH:O	2.54	0.41
4:J:13:GLU:HG3	4:J:19:LYS:HE3	2.03	0.41
3:A:562:ASN:OD1	3:A:614:ASN:N	2.49	0.41
1:D:155:CYS:HA	1:D:293:PRO:HD3	2.03	0.40
3:F:572:THR:OG1	3:F:579:ASN:HB2	2.21	0.40
3:A:389:ILE:HG23	3:A:393:TYR:HB2	2.03	0.40
1:C:263:ASP:N	1:C:276:GLN:O	2.42	0.40
1:H:178:ASN:HA	1:H:275:ILE:HG12	2.03	0.40
2:G:122:LEU:HA	2:G:122:LEU:HD12	1.88	0.40
2:B:78:LEU:HA	2:B:78:LEU:HD23	1.96	0.40
3:A:508:MET:HA	3:A:509:ASN:HA	1.81	0.40
4:J:128:MET:SD	4:J:172:ILE:HD12	2.61	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	C	284/296 (96%)	270 (95%)	14 (5%)	0	100	100
1	D	284/296 (96%)	270 (95%)	14 (5%)	0	100	100
1	H	284/296 (96%)	266 (94%)	18 (6%)	0	100	100
1	I	284/296 (96%)	270 (95%)	14 (5%)	0	100	100
2	B	141/147 (96%)	137 (97%)	4 (3%)	0	100	100
2	G	141/147 (96%)	134 (95%)	7 (5%)	0	100	100
3	A	218/254 (86%)	207 (95%)	11 (5%)	0	100	100
3	F	219/254 (86%)	202 (92%)	17 (8%)	0	100	100
4	E	210/213 (99%)	204 (97%)	6 (3%)	0	100	100
4	J	210/213 (99%)	205 (98%)	5 (2%)	0	100	100
All	All	2275/2412 (94%)	2165 (95%)	110 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	C	262/270 (97%)	250 (95%)	12 (5%)	33	51
1	D	262/270 (97%)	239 (91%)	23 (9%)	12	18
1	H	262/270 (97%)	247 (94%)	15 (6%)	25	40
1	I	262/270 (97%)	247 (94%)	15 (6%)	25	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	135/138 (98%)	131 (97%)	4 (3%)	48	70
2	G	135/138 (98%)	132 (98%)	3 (2%)	60	79
3	A	208/232 (90%)	199 (96%)	9 (4%)	35	55
3	F	209/232 (90%)	199 (95%)	10 (5%)	31	49
4	E	183/184 (100%)	181 (99%)	2 (1%)	80	92
4	J	183/184 (100%)	179 (98%)	4 (2%)	60	79
All	All	2101/2188 (96%)	2004 (95%)	97 (5%)	33	51

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	21	LYS
1	D	54	SER
1	D	80	HIS
1	D	104	ASN
1	D	143	GLU
1	D	164	ASN
1	D	166	VAL
1	D	171	ASP
1	D	196	GLU
1	D	210	ASN
1	D	225	VAL
1	D	229	ASN
1	D	232	ASN
1	D	246	THR
1	D	247	ASP
1	D	248	GLU
1	D	253	THR
1	D	259	THR
1	D	260	LYS
1	D	269	THR
1	D	273	THR
1	D	283	ASP
1	D	291	ARG
2	B	32	LEU
2	B	94	VAL
2	B	116	ASP
2	B	122	LEU
1	C	30	GLN
1	C	70	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	101	ILE
1	C	104	ASN
1	C	128	LYS
1	C	135	SER
1	C	171	ASP
1	C	183	ASP
1	C	208	LEU
1	C	209	SER
1	C	214	THR
1	C	219	ASN
3	A	380	GLU
3	A	424	ASN
3	A	484	VAL
3	A	487	THR
3	A	493	ASN
3	A	508	MET
3	A	580	LEU
3	A	584	GLN
3	A	588	HIS
4	E	76	LEU
4	E	156	GLU
1	I	13	ASP
1	I	80	HIS
1	I	84	THR
1	I	104	ASN
1	I	165	LYS
1	I	179	LEU
1	I	198	LYS
1	I	212	VAL
1	I	225	VAL
1	I	229	ASN
1	I	247	ASP
1	I	269	THR
1	I	283	ASP
1	I	289	ASN
1	I	292	ASN
2	G	4	GLU
2	G	8	LEU
2	G	26	ASN
1	H	13	ASP
1	H	30	GLN
1	H	70	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	84	THR
1	H	103	ASN
1	H	123	VAL
1	H	156	LYS
1	H	166	VAL
1	H	176	ASN
1	H	206	THR
1	H	207	ILE
1	H	229	ASN
1	H	241	ASN
1	H	246	THR
1	H	269	THR
3	F	383	GLN
3	F	384	GLU
3	F	394	THR
3	F	404	ASN
3	F	463	SER
3	F	475	ASN
3	F	477	ASP
3	F	484	VAL
3	F	571	VAL
3	F	626	ASN
4	J	119	GLU
4	J	122	VAL
4	J	128	MET
4	J	152	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	115	ASN
1	D	221	ASN
2	B	26	ASN
2	B	53	ASN
3	A	509	ASN
3	A	579	ASN
3	A	584	GLN
1	I	115	ASN
1	I	229	ASN
1	H	187	ASN
3	F	509	ASN
4	J	159	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	286/296 (96%)	0.41	24 (8%) 14 13	34, 66, 105, 155	0
1	D	286/296 (96%)	1.06	63 (22%) 1 1	34, 72, 150, 180	0
1	H	286/296 (96%)	0.45	22 (7%) 16 16	28, 67, 125, 158	0
1	I	286/296 (96%)	0.14	8 (2%) 56 55	31, 55, 91, 127	0
2	B	143/147 (97%)	0.01	1 (0%) 89 88	31, 44, 67, 95	0
2	G	143/147 (97%)	0.12	0 100 100	29, 44, 67, 92	0
3	A	224/254 (88%)	0.31	8 (3%) 46 47	34, 59, 111, 149	0
3	F	225/254 (88%)	0.44	20 (8%) 12 12	32, 60, 118, 141	0
4	E	212/213 (99%)	0.07	5 (2%) 62 61	34, 57, 98, 116	0
4	J	212/213 (99%)	0.40	19 (8%) 12 11	37, 59, 126, 138	0
All	All	2303/2412 (95%)	0.38	170 (7%) 17 17	28, 57, 120, 180	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	215	TRP	8.6
1	H	228	SER	8.1
1	D	160	ILE	8.0
1	C	231	GLN	7.5
3	F	387	THR	7.4
1	H	229	ASN	7.3
4	J	179	LEU	7.2
3	A	491	ILE	7.0
1	D	270	ALA	6.9
1	D	166	VAL	6.6
1	D	163	LEU	6.5
1	D	287	LYS	6.3
1	D	165	LYS	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	490	ASN	6.2
1	D	279	ASN	6.1
1	D	280	TYR	6.1
1	I	230	ASP	5.7
3	A	490	ASN	5.6
1	D	264	LEU	5.5
1	D	164	ASN	5.2
1	D	179	LEU	5.1
1	D	275	ILE	5.1
3	F	382	ILE	5.1
3	F	386	ASN	4.9
1	C	230	ASP	4.9
4	J	125	THR	4.8
1	D	269	THR	4.8
4	J	213	ASP	4.8
4	J	174	VAL	4.7
1	D	177	VAL	4.7
1	D	223	VAL	4.7
1	C	207	ILE	4.6
1	D	274	ALA	4.6
4	J	176	THR	4.6
1	D	217	PHE	4.6
3	F	436	GLY	4.5
4	J	159	HIS	4.5
3	F	388	ALA	4.5
1	D	265	TYR	4.5
1	D	273	THR	4.5
1	H	279	ASN	4.3
1	D	230	ASP	4.3
1	D	267	GLY	4.2
1	C	265	TYR	4.2
1	D	229	ASN	4.2
1	D	266	GLY	4.2
1	C	229	ASN	4.1
1	I	231	GLN	4.1
1	D	182	TRP	4.0
1	D	180	TYR	4.0
3	F	491	ILE	4.0
1	H	9	ASN	4.0
1	D	218	SER	4.0
1	H	265	TYR	4.0
3	A	380	GLU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	181	THR	3.9
3	F	380	GLU	3.9
4	E	182	GLU	3.9
1	D	252	ILE	3.9
3	F	385	ILE	3.9
1	D	277	VAL	3.8
1	D	231	GLN	3.8
1	D	184	TYR	3.8
4	J	177	SER	3.8
1	I	184	TYR	3.7
1	I	102	GLY	3.7
4	J	175	LEU	3.7
1	D	285	ASN	3.6
3	F	390	SER	3.6
1	D	268	GLN	3.5
1	D	161	LEU	3.5
1	D	178	ASN	3.4
3	F	435	ILE	3.4
1	H	215	TRP	3.4
1	D	216	ILE	3.4
3	A	493	ASN	3.3
1	C	222	THR	3.3
1	C	232	ASN	3.3
1	H	277	VAL	3.3
1	D	221	ASN	3.2
1	C	9	ASN	3.2
1	D	260	LYS	3.1
1	D	289	ASN	3.1
1	D	159	PRO	3.1
1	H	260	LYS	3.1
1	D	278	PHE	3.1
1	C	215	TRP	3.1
1	C	233	ASN	3.1
1	I	229	ASN	3.1
1	H	283	ASP	3.1
3	A	397	ILE	3.0
4	J	209	ILE	3.0
1	H	217	PHE	3.0
4	E	157	LEU	3.0
4	J	127	VAL	2.9
4	J	158	PRO	2.9
2	B	146	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	219	ASN	2.9
1	H	278	PHE	2.9
1	D	257	ASP	2.9
1	D	256	ARG	2.8
3	F	520	SER	2.8
4	J	117	VAL	2.8
3	F	489	SER	2.8
3	F	626	ASN	2.8
1	C	219	ASN	2.8
3	F	407	TYR	2.8
1	D	167	VAL	2.8
3	A	489	SER	2.8
1	H	259	THR	2.7
1	D	294	PRO	2.7
1	H	266	GLY	2.7
1	D	158	SER	2.7
4	J	118	ALA	2.7
1	D	183	ASP	2.7
4	E	213	ASP	2.7
1	D	102	GLY	2.7
3	A	395	TYR	2.7
1	C	173	THR	2.6
1	C	206	THR	2.6
4	J	122	VAL	2.6
4	J	157	LEU	2.6
1	D	262	LEU	2.6
3	F	561	TYR	2.6
1	D	9	ASN	2.5
1	H	161	LEU	2.5
1	C	216	ILE	2.5
4	E	183	SER	2.5
1	D	255	LEU	2.5
1	H	280	TYR	2.5
3	F	455	ILE	2.5
4	J	115	GLY	2.5
3	F	381	ASN	2.5
1	D	234	ASP	2.4
3	F	477	ASP	2.4
4	E	179	LEU	2.4
1	D	170	VAL	2.4
1	C	266	GLY	2.4
1	C	161	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	284	ASP	2.4
1	D	293	PRO	2.4
4	J	187	TYR	2.3
1	C	236	GLN	2.3
4	J	169	THR	2.3
1	D	197	GLU	2.3
1	H	285	ASN	2.3
3	A	423	GLN	2.3
1	H	218	SER	2.3
1	H	269	THR	2.3
1	C	167	VAL	2.3
1	H	169	GLN	2.2
1	D	220	GLY	2.2
1	H	284	ASP	2.2
1	C	169	GLN	2.2
1	C	176	ASN	2.2
3	F	414	THR	2.2
1	H	158	SER	2.2
1	C	247	ASP	2.2
1	D	291	ARG	2.1
1	H	227	SER	2.1
1	I	280	TYR	2.1
4	J	162	MET	2.1
1	D	201	TYR	2.1
1	I	232	ASN	2.1
1	C	264	LEU	2.1
1	I	266	GLY	2.1
1	C	240	ILE	2.0
1	D	272	GLY	2.0
1	D	168	GLN	2.0
1	C	217	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	CA	E	301	1/1	0.95	0.17	4.99	44,44,44,44	0
5	CA	E	302	1/1	0.96	0.14	1.48	36,36,36,36	0
5	CA	E	303	1/1	0.99	0.14	0.28	42,42,42,42	0
5	CA	J	301	1/1	0.97	0.12	-0.65	45,45,45,45	0
5	CA	J	302	1/1	0.99	0.12	-0.73	38,38,38,38	0
5	CA	J	303	1/1	0.91	0.07	-3.51	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.