



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:38 AM UTC

PDB ID : 2ZUQ / pdb_00002zuq
Title : Crystal structure of DsbB-Fab complex
Authors : Inaba, K.; Suzuki, M.; Murakami, S.
Deposited on : 2008-10-28
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

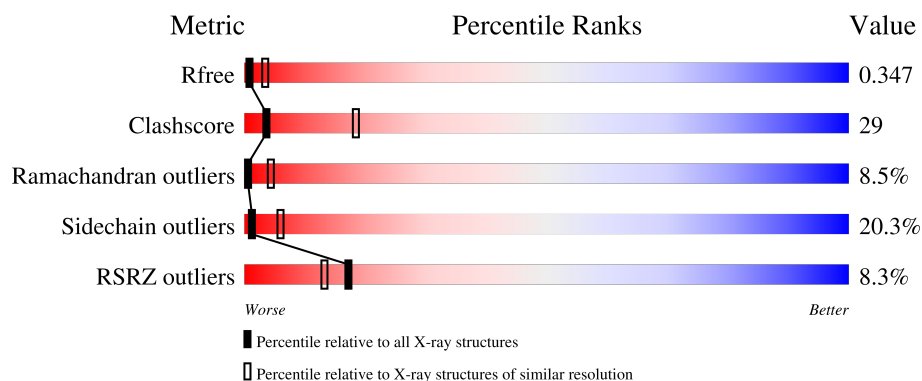
1 Overall quality at a glance

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 of 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	176	
1	D	176	
2	B	239	
2	E	239	
3	C	221	

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Mol	Chain	Length	Quality of chain
3	F	221	9% 41% 42% 13% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8991 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 Disulfide bond formation protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1175	794	183	189	9			
1	D	148	Total	C	N	O	S	0	0	0
			1175	794	183	189	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	CYS	engineered mutation	UNP P0A6M2
A	41	SER	CYS	engineered mutation	UNP P0A6M2
A	49	VAL	CYS	engineered mutation	UNP P0A6M2
D	8	ALA	CYS	engineered mutation	UNP P0A6M2
D	41	SER	CYS	engineered mutation	UNP P0A6M2
D	49	VAL	CYS	engineered mutation	UNP P0A6M2

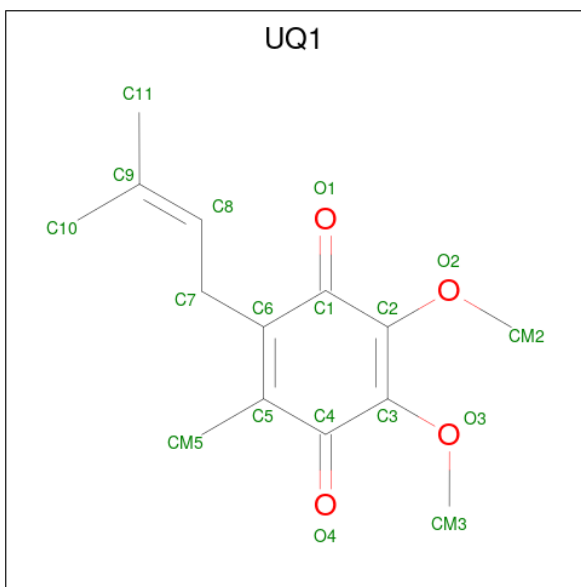
- Molecule 2 is a protein called Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1690	1052	283	347	8			
2	E	218	Total	C	N	O	S	0	0	0
			1690	1052	283	347	8			

- Molecule 3 is a protein called Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	216	Total	C	N	O	S	0	0	0
			1615	1017	264	325	9			
3	F	214	Total	C	N	O	S	0	0	0
			1610	1015	262	324	9			

- Molecule 4 is UBIQUINONE-1 (CCD ID: UQ1) (formula: C₁₄H₁₈O₄).

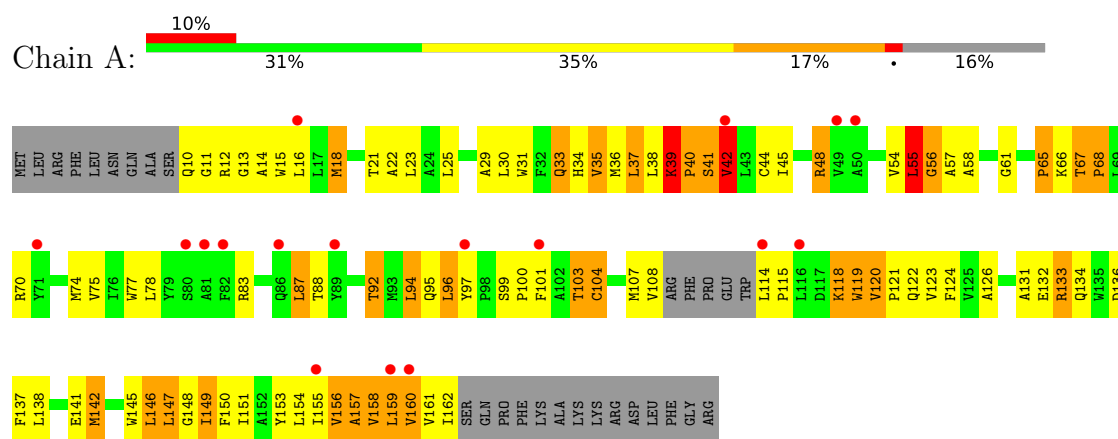


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			18	14	4		
4	D	1	Total	C	O	0	0
			18	14	4		

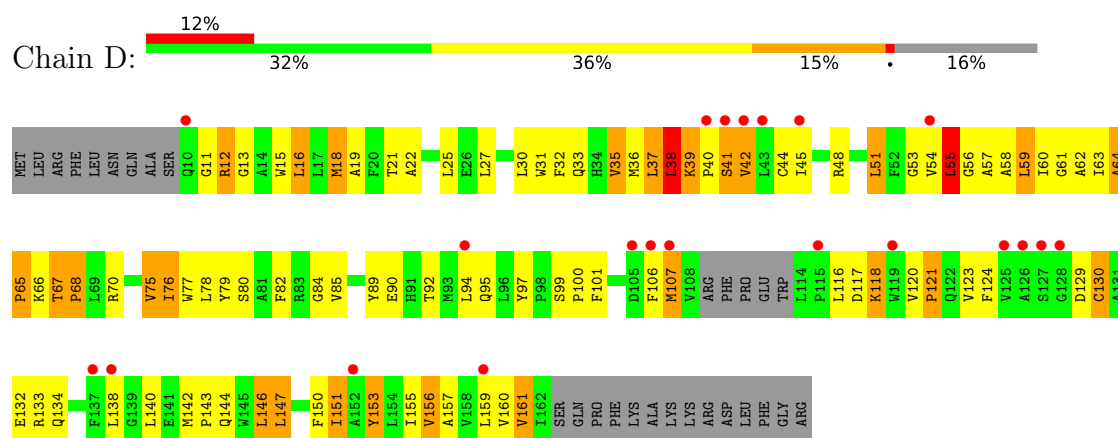
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

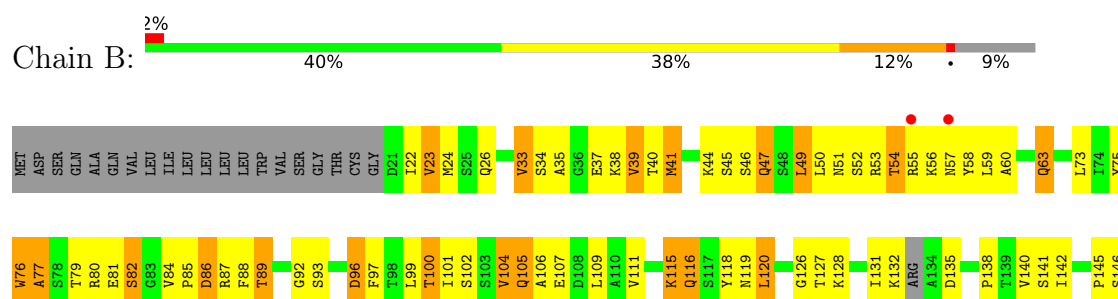
• Molecule 1: Disulfide bond formation protein B

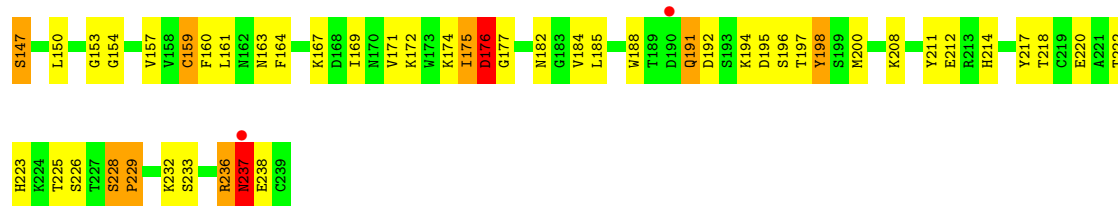


• Molecule 1: Disulfide bond formation protein B

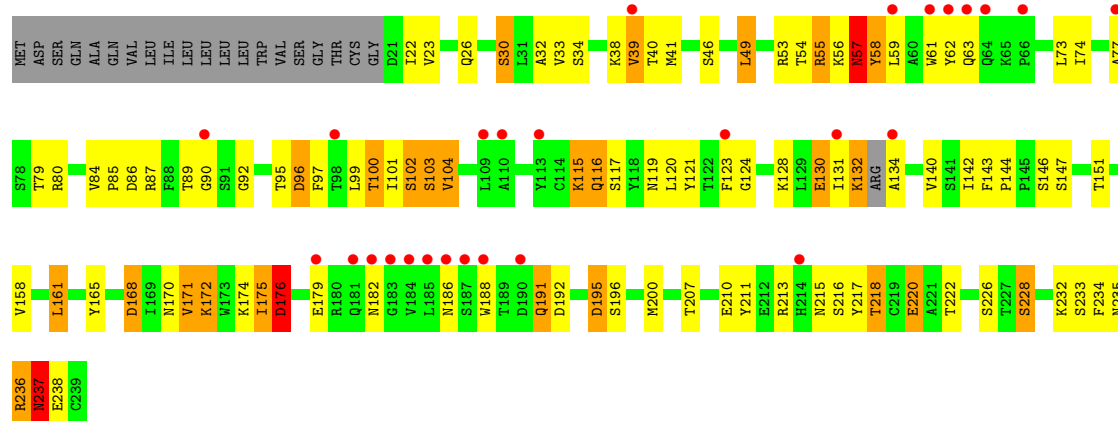


• Molecule 2: Fab fragment light chain

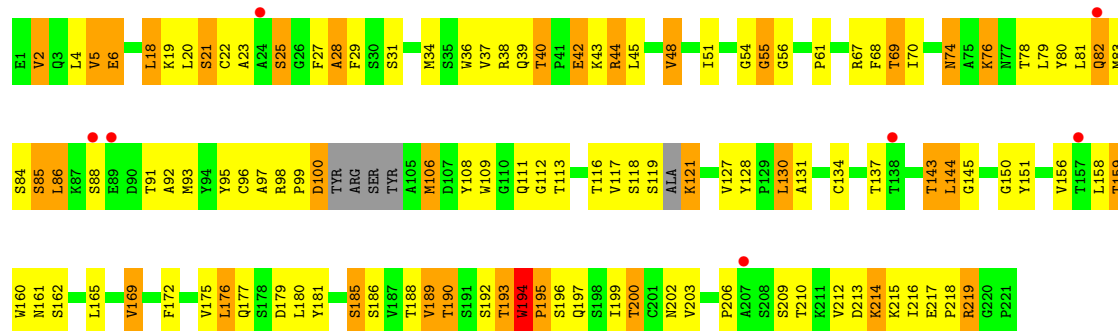
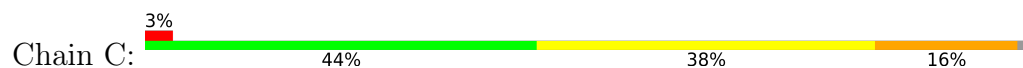




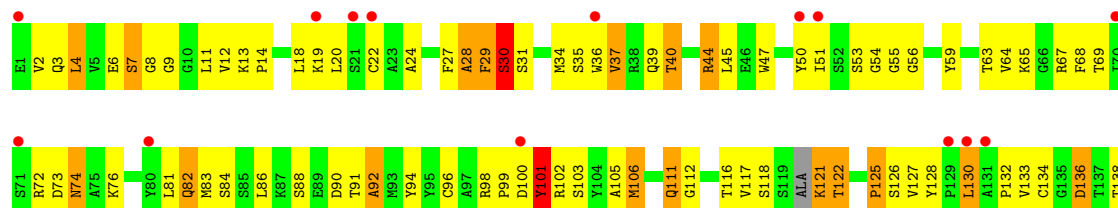
• Molecule 2: Fab fragment light chain

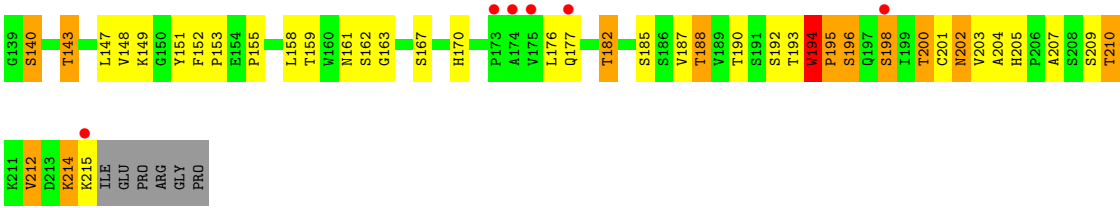


• Molecule 3: Fab fragment heavy chain



• Molecule 3: Fab fragment heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	269.31Å 51.48Å 125.84Å 90.00° 106.89° 90.00°	Depositor
Resolution (Å)	45.64 – 3.30 45.64 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.64-3.30) 99.3 (45.64-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.275 , 0.351 0.272 , 0.347	Depositor DCC
R_{free} test set	1316 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	107.8	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8991	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, 0.333 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: UQ1

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	0.70	0/1210	0.99	3/1654 (0.2%)
1	D	0.67	0/1210	1.06	4/1654 (0.2%)
2	B	0.70	0/1725	1.02	1/2336 (0.0%)
2	E	0.63	0/1725	1.00	5/2336 (0.2%)
3	C	0.69	0/1654	1.00	5/2254 (0.2%)
3	F	0.63	0/1650	0.98	4/2249 (0.2%)
All	All	0.67	0/9174	1.01	22/12483 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
3	C	0	1
3	F	0	1
All	All	0	3

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	153	TYR	N-CA-C	-8.10	105.38	114.62
3	F	151	TYR	N-CA-C	6.89	118.58	108.86
1	D	134	GLN	N-CA-C	6.78	120.21	109.50
3	F	3	GLN	N-CA-C	6.76	120.55	109.06
1	D	64	ALA	CA-C-N	6.32	127.74	119.84
1	D	64	ALA	C-N-CA	6.32	127.74	119.84
2	B	163	ASN	N-CA-C	6.27	120.06	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	143	PHE	CA-C-N	5.97	126.53	120.38
2	E	143	PHE	C-N-CA	5.97	126.53	120.38
1	A	137	PHE	N-CA-C	5.81	117.80	110.24
3	F	133	VAL	N-CA-C	5.81	116.77	108.93
2	E	84	VAL	CA-C-N	5.65	126.91	119.84
2	E	84	VAL	C-N-CA	5.65	126.91	119.84
3	C	25	SER	N-CA-C	5.58	117.20	107.49
3	C	185	SER	N-CA-C	5.46	117.10	107.61
3	C	69	THR	N-CA-C	5.32	116.11	107.23
3	C	172	PHE	CA-C-N	5.09	126.20	119.84
3	C	172	PHE	C-N-CA	5.09	126.20	119.84
3	F	7	SER	N-CA-C	5.04	114.98	107.88
2	E	39	VAL	CB-CA-C	-5.03	106.06	111.59
1	A	39	LYS	CA-C-N	5.02	126.11	119.84
1	A	39	LYS	C-N-CA	5.02	126.11	119.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	194	TRP	Peptide
2	E	57	ASN	Peptide
3	F	194	TRP	Peptide

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	1175	0	1208	111	0
1	D	1175	0	1208	70	0
2	B	1690	0	1625	103	0
2	E	1690	0	1625	71	0
3	C	1615	0	1570	90	0
3	F	1610	0	1560	90	0
4	A	18	0	18	2	0
4	D	18	0	18	2	0
All	All	8991	0	8832	522	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 29.

All (522) 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:115:LYS:HB2	2:B:115:LYS:NZ	1.48	1.17
2:B:26:GLN:NE2	2:B:126:GLY:H	1.46	1.13
2:B:40:THR:HG22	2:B:100:THR:HB	1.23	1.10
2:B:44:LYS:NZ	2:B:96:ASP:OD1	1.85	1.06
2:B:115:LYS:HB2	2:B:115:LYS:HZ3	0.97	1.06
1:A:151:ILE:O	1:A:155:ILE:HG12	1.56	1.05
1:A:65:PRO:HB2	1:A:66:LYS:HA	1.05	1.02
1:A:78:LEU:HD21	1:A:158:VAL:HG23	1.41	1.02
2:B:145:PRO:HD3	2:B:157:VAL:HG22	1.40	1.01
2:B:115:LYS:NZ	2:B:115:LYS:CB	2.23	0.98
2:B:115:LYS:HZ3	2:B:115:LYS:CB	1.78	0.97
3:C:162:SER:H	3:C:202:ASN:HD21	1.07	0.96
1:A:65:PRO:HB3	1:A:70:ARG:NH2	1.82	0.94
1:D:58:ALA:HB2	1:D:77:TRP:HZ3	1.29	0.94
1:A:65:PRO:HB2	1:A:66:LYS:CA	1.97	0.93
1:A:65:PRO:CB	1:A:66:LYS:HA	1.95	0.93
2:E:237:ASN:HD22	2:E:238:GLU:H	1.17	0.93
1:A:67:THR:H	1:A:68:PRO:HD2	1.29	0.91
3:C:159:THR:HG23	3:C:202:ASN:HB2	1.50	0.91
3:F:149:LYS:HG3	3:F:182:THR:HG23	1.51	0.90
1:D:58:ALA:HB2	1:D:77:TRP:CZ3	2.05	0.90
1:A:48:ARG:CG	1:A:48:ARG:HH11	1.85	0.90
2:B:237:ASN:HD22	2:B:238:GLU:H	1.15	0.90
2:B:26:GLN:NE2	2:B:126:GLY:N	2.21	0.88
2:B:26:GLN:HE22	2:B:126:GLY:N	1.70	0.88
3:C:44:ARG:NH1	3:C:45:LEU:H	1.73	0.86
1:A:77:TRP:CD1	1:A:157:ALA:HB2	2.11	0.86
1:A:74:MET:HE1	1:A:161:VAL:HG11	1.58	0.85
1:A:58:ALA:HB2	1:A:77:TRP:HZ3	1.40	0.85
1:A:67:THR:H	1:A:68:PRO:CD	1.87	0.85
1:A:96:LEU:O	1:A:97:TYR:CD1	2.30	0.84
1:A:12:ARG:O	1:A:16:LEU:HB2	1.79	0.82
1:A:74:MET:HE2	1:A:162:ILE:HG23	1.60	0.82
1:A:39:LYS:N	1:A:40:PRO:HD2	1.94	0.82
3:C:175:VAL:HG12	3:C:176:LEU:H	1.44	0.82
2:E:171:VAL:HG21	2:E:200:MET:HE1	1.60	0.81
2:B:26:GLN:HE22	2:B:126:GLY:H	1.22	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:MET:HG2	1:A:77:TRP:HH2	1.44	0.81
1:A:136:ASP:HB2	1:A:141:GLU:HA	1.61	0.81
1:A:15:TRP:HE3	1:A:58:ALA:HA	1.44	0.80
2:B:40:THR:HG22	2:B:100:THR:CB	2.08	0.80
2:B:115:LYS:HB2	2:B:115:LYS:HZ2	1.46	0.80
3:C:210:THR:HG22	3:C:212:VAL:HG23	1.64	0.79
2:E:237:ASN:ND2	2:E:238:GLU:H	1.80	0.78
1:A:57:ALA:HB1	1:A:77:TRP:HB2	1.65	0.78
2:E:176:ASP:HB3	2:E:216:SER:HB3	1.66	0.78
3:C:19:LYS:HB2	3:C:82:GLN:HE21	1.49	0.77
3:C:219:ARG:N	3:C:219:ARG:HE	1.82	0.77
1:D:31:TRP:NE1	1:D:35:VAL:HG21	1.99	0.77
1:A:156:VAL:HG12	1:A:157:ALA:N	2.00	0.76
1:D:65:PRO:HB3	1:D:70:ARG:HH12	1.51	0.75
2:B:26:GLN:HE21	2:B:126:GLY:H	1.32	0.75
2:E:237:ASN:HD22	2:E:238:GLU:N	1.84	0.75
2:B:80:ARG:HH21	2:B:89:THR:HG23	1.52	0.75
1:A:142:MET:HG2	4:A:177:UQ1:H8	1.68	0.74
3:C:161:ASN:ND2	3:C:200:THR:H	1.85	0.74
1:A:48:ARG:HH11	1:A:48:ARG:HG3	1.49	0.74
1:A:65:PRO:HB3	1:A:70:ARG:HH21	1.51	0.74
1:D:57:ALA:HB1	1:D:77:TRP:HB2	1.69	0.74
3:F:6:GLU:OE2	3:F:96:CYS:HB3	1.88	0.74
1:A:120:VAL:HG11	1:A:123:VAL:HG12	1.70	0.73
3:C:188:THR:O	3:C:189:VAL:HB	1.87	0.73
3:F:19:LYS:HG3	3:F:82:GLN:HG2	1.71	0.73
3:F:83:MET:HB3	3:F:86:LEU:HD21	1.71	0.73
3:C:19:LYS:HD2	3:C:82:GLN:HG2	1.70	0.72
1:D:18:MET:HA	1:D:21:THR:HG22	1.71	0.71
2:B:41:MET:HE2	2:B:41:MET:H	1.56	0.71
2:B:237:ASN:HD22	2:B:238:GLU:N	1.88	0.70
1:D:151:ILE:O	1:D:155:ILE:HG12	1.89	0.70
2:E:144:PRO:HB3	2:E:234:PHE:CE1	2.25	0.70
1:A:18:MET:O	1:A:21:THR:HG22	1.92	0.70
3:F:214:LYS:HD2	3:F:214:LYS:N	2.05	0.70
2:B:63:GLN:HB3	2:B:73:LEU:HD22	1.73	0.70
3:C:162:SER:H	3:C:202:ASN:ND2	1.85	0.70
1:D:155:ILE:C	1:D:157:ALA:H	1.98	0.70
2:E:123:PHE:CD1	3:F:45:LEU:HB3	2.27	0.70
1:A:18:MET:HA	1:A:21:THR:HG22	1.74	0.69
1:A:18:MET:HG2	1:A:77:TRP:CH2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:HG11	1:A:153:TYR:CE2	2.26	0.69
2:B:153:GLY:HA2	2:B:208:LYS:HD2	1.74	0.69
3:F:162:SER:H	3:F:202:ASN:ND2	1.90	0.69
1:A:114:LEU:HD12	1:A:115:PRO:HD2	1.75	0.69
3:F:143:THR:HB	3:F:188:THR:HG23	1.75	0.68
1:A:58:ALA:HB2	1:A:77:TRP:CZ3	2.27	0.68
1:A:77:TRP:HD1	1:A:157:ALA:HB2	1.56	0.68
1:A:36:MET:O	1:A:38:LEU:HB2	1.93	0.68
1:A:99:SER:O	1:A:101:PHE:N	2.27	0.68
3:F:50:TYR:HB3	3:F:59:TYR:HB2	1.76	0.68
2:B:237:ASN:ND2	2:B:238:GLU:H	1.91	0.68
1:D:65:PRO:HB2	1:D:66:LYS:HA	1.76	0.68
3:F:44:ARG:HA	3:F:44:ARG:HH11	1.59	0.68
1:A:29:ALA:HB2	4:A:177:UQ1:H113	1.74	0.68
1:A:95:GLN:C	1:A:97:TYR:H	2.01	0.68
2:B:192:ASP:O	2:B:196:SER:HA	1.93	0.68
3:F:67:ARG:NH2	3:F:90:ASP:OD2	2.27	0.67
3:C:74:ASN:OD1	3:C:74:ASN:N	2.27	0.67
2:E:170:ASN:HB3	2:E:222:THR:OG1	1.95	0.67
2:B:146:SER:OG	3:C:128:TYR:HB3	1.94	0.67
3:C:194:TRP:HD1	3:C:199:ILE:HD12	1.59	0.67
3:C:194:TRP:CE3	3:C:195:PRO:HD3	2.30	0.67
3:C:67:ARG:C	3:C:68:PHE:HD1	2.03	0.67
2:B:22:ILE:HG12	2:B:47:GLN:HB2	1.77	0.67
2:B:88:PHE:HD2	2:B:101:ILE:HG12	1.60	0.66
3:F:212:VAL:HG12	3:F:214:LYS:HE3	1.76	0.66
1:D:106:PHE:O	1:D:107:MET:HB3	1.97	0.65
1:A:18:MET:CG	1:A:77:TRP:HH2	2.10	0.65
3:C:28:ALA:O	3:C:31:SER:OG	2.14	0.65
1:D:75:VAL:C	1:D:77:TRP:H	2.05	0.65
1:A:156:VAL:HG12	1:A:157:ALA:H	1.61	0.65
1:A:39:LYS:N	1:A:40:PRO:CD	2.60	0.64
3:C:44:ARG:HA	3:C:44:ARG:HH11	1.62	0.64
1:A:48:ARG:CG	1:A:48:ARG:NH1	2.53	0.64
3:C:42:GLU:O	3:C:43:LYS:HB2	1.97	0.64
3:F:205:HIS:HE1	3:F:207:ALA:HB3	1.62	0.64
1:A:15:TRP:CE3	1:A:58:ALA:HA	2.31	0.64
3:C:83:MET:HE2	3:C:86:LEU:HD21	1.78	0.64
2:B:174:LYS:HB2	2:B:218:THR:HG23	1.79	0.64
1:A:48:ARG:HH11	1:A:48:ARG:HG2	1.61	0.63
3:F:200:THR:HA	3:F:214:LYS:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:TRP:CE2	1:A:35:VAL:HG21	2.33	0.63
2:B:24:MET:SD	2:B:45:SER:HB2	2.38	0.63
1:A:22:ALA:HB3	1:A:55:LEU:HD23	1.79	0.63
2:B:116:GLN:HE22	2:B:119:ASN:H	1.45	0.63
3:C:175:VAL:HG12	3:C:176:LEU:N	2.14	0.63
3:F:54:GLY:O	3:F:56:GLY:N	2.32	0.63
1:D:51:LEU:C	1:D:53:GLY:H	2.07	0.63
2:E:218:THR:HB	2:E:233:SER:HB2	1.81	0.62
2:E:174:LYS:HB2	2:E:218:THR:HG23	1.80	0.62
3:C:119:SER:O	3:C:121:LYS:N	2.32	0.62
2:E:218:THR:HB	2:E:233:SER:CB	2.30	0.62
3:C:193:THR:O	3:C:197:GLN:HB3	1.99	0.61
1:A:67:THR:N	1:A:68:PRO:CD	2.59	0.61
3:C:194:TRP:CD1	3:C:199:ILE:HD12	2.35	0.61
3:F:24:ALA:HB1	3:F:27:PHE:CE2	2.36	0.61
1:A:70:ARG:O	1:A:74:MET:HG2	2.01	0.61
2:E:116:GLN:HE22	2:E:119:ASN:H	1.47	0.60
2:B:41:MET:HE3	2:B:99:LEU:HB3	1.83	0.60
2:E:211:TYR:CE1	2:E:217:TYR:CE2	2.89	0.60
3:F:161:ASN:C	3:F:163:GLY:H	2.09	0.60
1:A:136:ASP:CB	1:A:141:GLU:HA	2.31	0.60
3:C:67:ARG:HD2	3:C:85:SER:HB2	1.84	0.60
2:B:51:ASN:OD1	2:B:58:TYR:HE1	1.84	0.60
2:B:107:GLU:OE2	2:B:194:LYS:HA	2.02	0.60
1:A:157:ALA:O	1:A:161:VAL:HB	2.00	0.60
3:C:36:TRP:HD1	3:C:70:ILE:HD12	1.67	0.60
1:A:77:TRP:HD1	1:A:157:ALA:CB	2.14	0.60
2:B:88:PHE:CD2	2:B:101:ILE:HG12	2.37	0.60
3:F:103:SER:C	3:F:105:ALA:H	2.08	0.59
1:A:74:MET:HE1	1:A:161:VAL:CG1	2.31	0.59
1:A:41:SER:O	1:A:44:CYS:HB3	2.02	0.59
3:C:6:GLU:HA	3:C:22:CYS:HA	1.84	0.59
2:E:30:SER:HB3	2:E:128:LYS:HB3	1.83	0.59
1:A:78:LEU:CD2	1:A:158:VAL:HG23	2.27	0.59
3:C:36:TRP:O	3:C:48:VAL:HB	2.03	0.59
2:E:123:PHE:HE1	3:F:37:VAL:HG11	1.68	0.59
2:E:40:THR:HG22	2:E:100:THR:HB	1.85	0.58
2:E:131:ILE:H	2:E:191:GLN:HE22	1.50	0.58
3:F:24:ALA:HB1	3:F:27:PHE:HE2	1.66	0.58
3:F:162:SER:H	3:F:202:ASN:CG	2.10	0.58
2:B:120:LEU:HD23	2:B:120:LEU:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:ARG:NH1	3:C:45:LEU:N	2.50	0.58
2:B:34:SER:O	2:B:37:GLU:HG3	2.04	0.58
1:D:51:LEU:C	1:D:53:GLY:N	2.59	0.58
2:E:132:LYS:O	2:E:134:ALA:N	2.36	0.58
2:E:192:ASP:O	2:E:196:SER:HA	2.04	0.58
3:F:34:MET:HB2	3:F:51:ILE:CG2	2.34	0.57
3:F:205:HIS:CE1	3:F:207:ALA:HB3	2.39	0.57
1:A:77:TRP:CD1	1:A:157:ALA:CB	2.86	0.57
1:A:132:GLU:O	2:B:52:SER:OG	2.22	0.57
1:A:55:LEU:O	1:A:56:GLY:C	2.46	0.57
1:A:48:ARG:NH1	1:A:48:ARG:HG2	2.18	0.57
2:E:175:ILE:HG23	2:E:217:TYR:CE1	2.39	0.57
1:A:10:GLN:HG2	1:A:70:ARG:HH11	1.70	0.56
1:D:155:ILE:C	1:D:157:ALA:N	2.63	0.56
3:F:201:CYS:N	3:F:214:LYS:O	2.29	0.56
3:C:22:CYS:HB3	3:C:79:LEU:HB3	1.86	0.56
3:C:37:VAL:O	3:C:95:TYR:N	2.39	0.56
3:F:6:GLU:HG2	3:F:111:GLN:HE22	1.70	0.56
3:F:170:HIS:O	3:F:185:SER:HA	2.04	0.56
3:F:194:TRP:O	3:F:196:SER:N	2.38	0.56
1:A:10:GLN:HG2	1:A:70:ARG:NH1	2.20	0.56
2:B:175:ILE:C	2:B:177:GLY:H	2.13	0.56
3:C:6:GLU:OE1	3:C:111:GLN:HG2	2.06	0.56
1:A:35:VAL:HG23	1:A:36:MET:N	2.20	0.56
2:E:238:GLU:HB3	3:F:134:CYS:SG	2.46	0.56
3:C:219:ARG:HE	3:C:219:ARG:H	1.54	0.56
3:F:6:GLU:HA	3:F:22:CYS:HA	1.85	0.56
1:A:35:VAL:CG2	1:A:36:MET:N	2.69	0.56
3:C:200:THR:HG22	3:C:215:LYS:HG3	1.87	0.56
2:E:57:ASN:HA	2:E:58:TYR:HB2	1.88	0.56
2:B:218:THR:HB	2:B:233:SER:OG	2.06	0.56
2:E:103:SER:O	2:E:104:VAL:C	2.49	0.56
1:A:148:GLY:HA2	1:A:151:ILE:HD12	1.88	0.55
2:B:184:VAL:HG12	2:B:184:VAL:O	2.06	0.55
3:C:67:ARG:O	3:C:68:PHE:HD1	1.88	0.55
1:A:18:MET:CB	1:A:77:TRP:HH2	2.20	0.55
1:A:74:MET:HE2	1:A:162:ILE:CG2	2.36	0.55
3:F:40:THR:OG1	3:F:44:ARG:HB3	2.07	0.55
1:A:155:ILE:O	1:A:160:VAL:HG23	2.06	0.55
2:B:211:TYR:O	2:B:217:TYR:OH	2.21	0.55
3:C:51:ILE:HD12	3:C:70:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:194:TRP:CG	3:C:195:PRO:N	2.74	0.55
1:D:22:ALA:HA	1:D:25:LEU:HD12	1.87	0.55
1:A:18:MET:HA	1:A:21:THR:CG2	2.36	0.55
1:D:97:TYR:CD2	3:F:102:ARG:HB3	2.42	0.55
2:E:23:VAL:HG23	2:E:46:SER:HB3	1.89	0.55
1:A:13:GLY:C	1:A:15:TRP:H	2.15	0.55
1:A:41:SER:O	1:A:44:CYS:CB	2.55	0.55
1:A:41:SER:HB2	1:A:45:ILE:HG23	1.89	0.55
1:D:39:LYS:N	1:D:40:PRO:CD	2.70	0.55
3:F:68:PHE:CZ	3:F:83:MET:HG2	2.42	0.55
1:A:145:TRP:O	1:A:148:GLY:N	2.40	0.54
1:A:48:ARG:HD3	1:A:123:VAL:HG22	1.90	0.54
1:A:54:VAL:HG11	1:A:153:TYR:CD2	2.42	0.54
1:A:103:THR:O	1:A:104:CYS:HB3	2.06	0.54
3:C:213:ASP:O	3:C:214:LYS:HD2	2.06	0.54
2:E:32:ALA:HA	2:E:130:GLU:O	2.08	0.54
2:E:174:LYS:HG2	2:E:179:GLU:HG2	1.89	0.54
3:C:106:MET:HB2	3:C:109:TRP:NE1	2.23	0.54
1:D:18:MET:CG	1:D:77:TRP:HH2	2.21	0.54
2:B:38:LYS:HE3	2:B:102:SER:HB3	1.88	0.54
3:F:68:PHE:CE2	3:F:83:MET:HG2	2.42	0.54
3:F:88:SER:HA	3:F:117:VAL:HB	1.90	0.54
3:C:158:LEU:HD13	3:C:185:SER:HB2	1.90	0.53
2:E:171:VAL:CG2	2:E:200:MET:HE1	2.34	0.53
2:B:115:LYS:CB	2:B:115:LYS:HZ2	2.11	0.53
3:F:149:LYS:HG3	3:F:182:THR:CG2	2.32	0.53
2:E:74:ILE:HG21	2:E:77:ALA:O	2.09	0.53
2:B:172:LYS:HG3	2:B:220:GLU:HB2	1.91	0.53
3:F:190:THR:HG22	3:F:192:SER:H	1.73	0.53
1:A:88:THR:OG1	1:A:147:LEU:HA	2.08	0.53
1:D:147:LEU:HD22	1:D:147:LEU:O	2.08	0.53
1:A:39:LYS:H	1:A:40:PRO:HD2	1.70	0.52
1:A:156:VAL:O	1:A:157:ALA:C	2.52	0.52
3:C:78:THR:OG1	3:C:80:TYR:CZ	2.57	0.52
2:E:123:PHE:CE1	3:F:37:VAL:HG11	2.44	0.52
1:D:37:LEU:HA	1:D:38:LEU:O	2.09	0.52
2:B:76:TRP:O	2:B:77:ALA:HB2	2.09	0.52
3:C:34:MET:HB3	3:C:79:LEU:HD22	1.92	0.52
1:D:33:GLN:HE22	1:D:123:VAL:HG23	1.74	0.52
1:D:146:LEU:HD21	4:D:177:UQ1:H103	1.90	0.52
2:E:192:ASP:HB3	2:E:196:SER:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLN:HB3	1:A:34:HIS:ND1	2.24	0.52
2:E:192:ASP:HB3	2:E:196:SER:N	2.23	0.52
1:D:156:VAL:HG12	1:D:156:VAL:O	2.10	0.52
2:B:140:VAL:HG22	2:B:141:SER:N	2.25	0.52
2:B:171:VAL:HA	2:B:220:GLU:O	2.10	0.52
2:B:40:THR:HA	2:B:99:LEU:O	2.10	0.51
3:C:98:ARG:O	3:C:106:MET:HA	2.10	0.51
1:D:92:THR:HG21	1:D:144:GLN:HG3	1.92	0.51
2:B:75:TYR:O	2:B:77:ALA:N	2.43	0.51
2:B:131:ILE:HB	2:B:191:GLN:HE22	1.75	0.51
1:A:54:VAL:HG11	1:A:153:TYR:HE2	1.71	0.51
3:C:51:ILE:HD11	3:C:55:GLY:HA2	1.92	0.51
1:D:36:MET:HA	1:D:36:MET:HE2	1.92	0.51
3:F:34:MET:HB2	3:F:51:ILE:HG22	1.91	0.51
2:B:33:VAL:C	2:B:132:LYS:HG3	2.35	0.51
2:B:26:GLN:HE22	2:B:126:GLY:CA	2.23	0.51
3:F:128:TYR:HD2	3:F:147:LEU:HD23	1.76	0.51
1:D:85:VAL:HG23	1:D:150:PHE:HB3	1.93	0.51
2:B:24:MET:HE1	2:B:45:SER:HB3	1.92	0.51
2:E:62:TYR:OH	2:E:115:LYS:HE2	2.11	0.51
2:B:92:GLY:HA3	2:B:97:PHE:HA	1.93	0.51
3:C:2:VAL:HG11	3:C:108:TYR:CE2	2.46	0.51
3:C:42:GLU:N	3:C:42:GLU:CD	2.69	0.51
1:D:64:ALA:C	1:D:66:LYS:HG3	2.36	0.51
2:B:145:PRO:CD	2:B:157:VAL:HG22	2.28	0.51
2:B:73:LEU:O	2:B:84:VAL:HG21	2.12	0.50
2:B:220:GLU:OE1	2:B:229:PRO:HB2	2.10	0.50
2:E:161:LEU:HG	2:E:200:MET:HE2	1.93	0.50
1:A:66:LYS:C	1:A:70:ARG:HE	2.19	0.50
2:E:38:LYS:HA	2:E:101:ILE:O	2.11	0.50
2:B:142:ILE:H	2:B:232:LYS:HD2	1.76	0.50
3:C:5:VAL:HG23	3:C:23:ALA:HB3	1.93	0.50
1:A:158:VAL:HG12	1:A:159:LEU:N	2.27	0.50
2:B:54:THR:CG2	2:B:56:LYS:HG2	2.42	0.50
3:F:125:PRO:HB2	3:F:148:VAL:HG13	1.94	0.50
1:A:45:ILE:HG12	1:A:126:ALA:HB2	1.94	0.50
3:C:88:SER:HA	3:C:117:VAL:HB	1.94	0.50
3:F:91:THR:O	3:F:92:ALA:HB2	2.11	0.50
2:B:37:GLU:O	2:B:104:VAL:HG23	2.10	0.50
2:E:74:ILE:HD13	2:E:90:GLY:H	1.77	0.50
2:B:59:LEU:HD13	2:B:97:PHE:CG	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:TRP:CE2	1:D:35:VAL:HG21	2.46	0.50
1:D:84:GLY:HA3	1:D:150:PHE:CD2	2.47	0.50
3:C:42:GLU:CD	3:C:42:GLU:H	2.19	0.50
1:A:18:MET:CA	1:A:21:THR:HG22	2.42	0.49
1:D:31:TRP:CD1	1:D:35:VAL:HG21	2.46	0.49
1:A:21:THR:HG23	1:A:153:TYR:OH	2.12	0.49
2:E:80:ARG:NH2	2:E:86:ASP:HA	2.27	0.49
1:A:11:GLY:HA2	1:A:70:ARG:HH22	1.77	0.49
3:F:6:GLU:OE1	3:F:112:GLY:N	2.43	0.49
3:C:175:VAL:CG1	3:C:176:LEU:H	2.21	0.49
1:D:48:ARG:HH12	4:D:177:UQ1:H72	1.77	0.49
1:D:106:PHE:O	1:D:107:MET:CB	2.60	0.49
3:C:219:ARG:N	3:C:219:ARG:NE	2.58	0.49
3:C:143:THR:HG22	3:C:188:THR:HG23	1.94	0.49
1:D:18:MET:HG3	1:D:77:TRP:HH2	1.77	0.49
1:A:65:PRO:CB	1:A:70:ARG:HH21	2.22	0.49
2:E:120:LEU:HD22	3:F:47:TRP:CZ3	2.48	0.49
1:A:41:SER:OG	1:A:42:VAL:N	2.43	0.49
1:D:100:PRO:HA	2:E:117:SER:O	2.12	0.49
2:E:49:LEU:C	2:E:57:ASN:ND2	2.71	0.49
1:D:18:MET:HA	1:D:21:THR:CG2	2.42	0.49
1:D:75:VAL:C	1:D:77:TRP:N	2.71	0.49
2:E:216:SER:HA	2:E:235:ASN:HB3	1.94	0.49
3:C:39:GLN:HG3	3:C:44:ARG:O	2.12	0.49
2:B:140:VAL:HG13	2:B:232:LYS:HB2	1.95	0.48
2:B:146:SER:O	2:B:147:SER:C	2.56	0.48
2:E:38:LYS:HD2	2:E:102:SER:HB3	1.95	0.48
3:F:39:GLN:HB2	3:F:45:LEU:HD23	1.95	0.48
3:C:51:ILE:HB	3:C:70:ILE:HG12	1.95	0.48
2:B:142:ILE:HA	2:B:159:CYS:HB3	1.95	0.48
3:F:9:GLY:HA2	3:F:18:LEU:HD11	1.94	0.48
3:C:121:LYS:O	3:C:121:LYS:HG2	2.14	0.48
2:E:182:ASN:OD1	2:E:182:ASN:N	2.43	0.48
3:F:63:THR:HG23	3:F:64:VAL:HG13	1.95	0.48
2:B:39:VAL:O	2:B:100:THR:HA	2.13	0.48
3:C:106:MET:HB2	3:C:109:TRP:HE1	1.79	0.48
1:D:89:TYR:HA	1:D:147:LEU:HG	1.95	0.48
1:D:118:LYS:H	1:D:118:LYS:HD2	1.78	0.48
2:B:140:VAL:HB	2:B:161:LEU:HD13	1.95	0.48
3:C:175:VAL:O	3:C:181:TYR:HA	2.14	0.48
3:C:215:LYS:HD3	3:C:217:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:GLY:O	1:D:60:ILE:N	2.39	0.48
2:E:22:ILE:HD12	2:E:116:GLN:NE2	2.29	0.48
3:F:127:VAL:HG22	3:F:148:VAL:HG22	1.95	0.47
3:C:21:SER:HB3	3:C:80:TYR:CD1	2.48	0.47
3:C:210:THR:CG2	3:C:212:VAL:HG23	2.42	0.47
3:F:73:ASP:OD2	3:F:76:LYS:HB2	2.13	0.47
2:B:153:GLY:C	2:B:208:LYS:HB2	2.39	0.47
3:F:194:TRP:HB3	3:F:195:PRO:CD	2.45	0.47
2:B:97:PHE:CD1	2:B:97:PHE:N	2.82	0.47
1:A:156:VAL:CG1	1:A:157:ALA:N	2.71	0.47
1:A:87:LEU:N	1:A:87:LEU:HD23	2.28	0.47
2:B:54:THR:HG22	2:B:55:ARG:O	2.14	0.47
3:F:161:ASN:N	3:F:202:ASN:HD21	2.13	0.47
1:A:99:SER:C	1:A:101:PHE:H	2.23	0.47
2:E:186:ASN:HB2	2:E:188:TRP:CH2	2.50	0.47
3:F:101:TYR:N	3:F:101:TYR:CD2	2.83	0.47
3:C:131:ALA:HB1	3:C:219:ARG:HD3	1.97	0.47
1:D:12:ARG:O	1:D:16:LEU:HB2	2.14	0.47
3:F:94:TYR:O	3:F:112:GLY:HA2	2.15	0.47
3:F:202:ASN:ND2	3:F:202:ASN:H	2.13	0.47
2:E:174:LYS:HE2	2:E:179:GLU:CD	2.39	0.46
1:D:75:VAL:O	1:D:77:TRP:N	2.48	0.46
1:D:84:GLY:HA3	1:D:150:PHE:CE2	2.50	0.46
3:C:48:VAL:O	3:C:61:PRO:HD2	2.14	0.46
3:C:194:TRP:O	3:C:196:SER:N	2.49	0.46
3:C:4:LEU:HD22	3:C:22:CYS:SG	2.55	0.46
1:D:99:SER:C	1:D:101:PHE:H	2.24	0.46
1:D:142:MET:N	1:D:143:PRO:HD2	2.31	0.46
1:A:92:THR:HG22	1:A:96:LEU:HD11	1.98	0.46
1:D:57:ALA:HB2	1:D:76:ILE:O	2.15	0.46
2:E:101:ILE:HG22	2:E:102:SER:O	2.15	0.46
2:E:142:ILE:HG22	2:E:232:LYS:CD	2.45	0.46
3:F:125:PRO:HB2	3:F:148:VAL:CG1	2.46	0.46
2:B:41:MET:CE	2:B:99:LEU:HD23	2.46	0.46
2:B:85:PRO:HB2	2:B:87:ARG:HG2	1.98	0.46
2:B:226:SER:C	2:B:228:SER:H	2.24	0.46
3:C:190:THR:HB	3:C:193:THR:HG23	1.97	0.46
3:C:97:ALA:HB1	3:C:106:MET:HB3	1.98	0.46
2:E:58:TYR:HD2	2:E:58:TYR:HA	1.47	0.46
3:F:27:PHE:C	3:F:29:PHE:H	2.24	0.46
2:B:138:PRO:HA	2:B:164:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:ARG:HA	3:C:93:MET:O	2.16	0.46
1:D:12:ARG:H	1:D:65:PRO:HG3	1.81	0.46
2:E:121:TYR:CE1	3:F:106:MET:HE3	2.50	0.46
3:F:136:ASP:OD1	3:F:136:ASP:N	2.49	0.46
3:F:158:LEU:HG	3:F:203:VAL:HG22	1.97	0.46
1:A:67:THR:HA	1:A:70:ARG:HD2	1.97	0.46
2:E:146:SER:OG	3:F:128:TYR:HB3	2.15	0.46
2:B:81:GLU:O	2:B:84:VAL:HG23	2.16	0.45
3:F:101:TYR:N	3:F:101:TYR:HD2	2.13	0.45
3:F:162:SER:H	3:F:202:ASN:HD21	1.60	0.45
1:A:13:GLY:C	1:A:15:TRP:N	2.74	0.45
1:A:23:LEU:C	1:A:25:LEU:H	2.24	0.45
1:D:55:LEU:O	1:D:56:GLY:C	2.59	0.45
1:D:118:LYS:HD2	1:D:118:LYS:N	2.31	0.45
3:F:39:GLN:HA	3:F:44:ARG:O	2.15	0.45
1:A:33:GLN:HB3	1:A:34:HIS:CE1	2.52	0.45
1:A:147:LEU:O	1:A:151:ILE:HG13	2.16	0.45
1:D:32:PHE:O	1:D:38:LEU:HB3	2.17	0.45
1:D:138:LEU:O	1:D:138:LEU:HG	2.17	0.45
1:A:74:MET:CE	1:A:161:VAL:HG11	2.37	0.45
2:B:131:ILE:HB	2:B:191:GLN:NE2	2.32	0.45
3:F:103:SER:C	3:F:105:ALA:N	2.74	0.45
3:F:198:SER:HB3	3:F:215:LYS:HE3	1.98	0.45
2:B:56:LYS:HA	2:B:56:LYS:HD3	1.78	0.45
3:C:159:THR:CG2	3:C:202:ASN:HB2	2.34	0.45
2:E:142:ILE:HG22	2:E:232:LYS:HD3	1.98	0.45
1:A:96:LEU:C	1:A:97:TYR:CD1	2.95	0.44
2:B:23:VAL:HG23	2:B:46:SER:HB3	1.98	0.44
3:F:152:PHE:CE2	3:F:153:PRO:HB3	2.53	0.44
3:F:98:ARG:HA	3:F:99:PRO:HD3	1.79	0.44
1:A:37:LEU:HA	1:A:38:LEU:C	2.42	0.44
2:B:33:VAL:HG11	2:B:104:VAL:HG21	1.98	0.44
3:F:12:VAL:HG13	3:F:117:VAL:HG13	1.98	0.44
2:B:176:ASP:OD1	2:B:214:HIS:HB3	2.18	0.44
3:C:54:GLY:O	3:C:56:GLY:N	2.50	0.44
3:C:158:LEU:HG	3:C:203:VAL:HG22	1.99	0.44
3:F:35:SER:OG	3:F:106:MET:HE2	2.18	0.44
2:B:40:THR:CG2	2:B:100:THR:HB	2.17	0.44
2:B:76:TRP:O	2:B:77:ALA:CB	2.66	0.44
1:D:37:LEU:N	1:D:38:LEU:HB2	2.33	0.44
1:D:58:ALA:O	1:D:62:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:29:PHE:C	3:F:31:SER:N	2.75	0.44
1:A:103:THR:O	1:A:104:CYS:CB	2.65	0.44
1:D:18:MET:O	1:D:21:THR:N	2.51	0.44
3:F:4:LEU:HD22	3:F:96:CYS:SG	2.57	0.44
3:C:130:LEU:HB2	3:C:145:GLY:C	2.43	0.44
1:D:19:ALA:HB1	1:D:59:LEU:HD12	2.00	0.43
2:E:33:VAL:HG22	2:E:34:SER:H	1.83	0.43
2:E:92:GLY:HA3	2:E:96:ASP:O	2.18	0.43
1:A:13:GLY:O	1:A:15:TRP:N	2.51	0.43
1:A:99:SER:C	1:A:101:PHE:N	2.75	0.43
2:B:138:PRO:HG3	2:B:223:HIS:HB3	1.99	0.43
3:F:28:ALA:HB3	3:F:31:SER:HB3	2.00	0.43
1:A:146:LEU:O	1:A:150:PHE:HD1	2.00	0.43
1:A:123:VAL:HG13	1:A:124:PHE:HD1	1.83	0.43
2:B:39:VAL:HG23	2:B:101:ILE:HB	1.99	0.43
3:C:127:VAL:HB	3:C:212:VAL:HG11	1.99	0.43
3:C:160:TRP:CD1	3:C:169:VAL:HG21	2.54	0.43
2:E:23:VAL:CG2	2:E:46:SER:HB3	2.48	0.43
2:B:218:THR:HB	2:B:233:SER:CB	2.49	0.43
3:C:84:SER:O	3:C:86:LEU:N	2.52	0.43
2:E:158:VAL:HG21	3:F:130:LEU:HD21	2.01	0.43
2:E:172:LYS:O	2:E:220:GLU:HG3	2.18	0.43
2:B:47:GLN:O	2:B:49:LEU:HD13	2.18	0.43
1:D:36:MET:HB3	1:D:38:LEU:CD1	2.49	0.43
1:A:15:TRP:CD2	1:A:61:GLY:HA3	2.54	0.43
1:A:31:TRP:O	1:A:35:VAL:HG22	2.19	0.43
2:B:111:VAL:HG22	2:B:128:LYS:HA	2.01	0.43
1:D:120:VAL:O	1:D:124:PHE:HB2	2.19	0.43
2:E:131:ILE:H	2:E:191:GLN:NE2	2.16	0.43
2:E:226:SER:O	2:E:228:SER:N	2.50	0.43
3:F:6:GLU:CD	3:F:96:CYS:H	2.27	0.43
3:F:6:GLU:HG2	3:F:111:GLN:NE2	2.32	0.42
3:C:76:LYS:O	3:C:78:THR:HG23	2.19	0.42
3:C:134:CYS:HB3	3:C:219:ARG:HB2	2.01	0.42
1:A:18:MET:C	1:A:21:THR:HG22	2.45	0.42
2:E:54:THR:O	2:E:56:LYS:N	2.52	0.42
1:D:120:VAL:HA	1:D:121:PRO:HD3	1.85	0.42
2:E:192:ASP:OD1	2:E:195:ASP:HB3	2.20	0.42
1:A:131:ALA:C	1:A:133:ARG:H	2.28	0.42
3:C:6:GLU:CD	3:C:112:GLY:H	2.28	0.42
3:F:204:ALA:HA	3:F:210:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:GLN:NE2	2:B:118:TYR:H	2.18	0.42
2:B:192:ASP:HB3	2:B:197:THR:H	1.85	0.42
3:C:76:LYS:HD2	3:C:76:LYS:HA	1.83	0.42
3:C:150:GLY:HA2	3:C:180:LEU:HB3	2.00	0.42
1:D:15:TRP:HE3	1:D:58:ALA:HA	1.85	0.42
1:A:115:PRO:HB2	1:A:118:LYS:HB2	2.01	0.42
2:E:61:TRP:CE2	2:E:99:LEU:HB2	2.55	0.42
2:E:123:PHE:HE1	3:F:37:VAL:CG1	2.33	0.42
2:E:131:ILE:N	2:E:191:GLN:HE22	2.15	0.42
3:F:6:GLU:OE1	3:F:111:GLN:N	2.51	0.42
3:F:53:SER:O	3:F:72:ARG:NH1	2.53	0.42
3:F:121:LYS:HG2	3:F:121:LYS:O	2.20	0.42
1:D:79:TYR:O	1:D:80:SER:C	2.61	0.42
2:B:188:TRP:HE3	2:B:188:TRP:H	1.68	0.42
3:C:40:THR:CG2	3:C:44:ARG:HB3	2.50	0.42
3:C:159:THR:HG23	3:C:202:ASN:HD22	1.84	0.42
3:C:188:THR:HG22	3:C:189:VAL:N	2.35	0.42
1:D:155:ILE:O	1:D:157:ALA:N	2.53	0.42
2:E:97:PHE:CD1	2:E:97:PHE:N	2.88	0.42
3:F:11:LEU:HG	3:F:12:VAL:N	2.34	0.42
3:F:100:ASP:HB2	3:F:105:ALA:O	2.20	0.42
2:B:51:ASN:OD1	2:B:58:TYR:CE1	2.69	0.41
3:C:27:PHE:O	3:C:29:PHE:N	2.53	0.41
2:B:212:GLU:CG	2:B:236:ARG:HD2	2.51	0.41
3:C:100:ASP:OD2	3:C:100:ASP:N	2.51	0.41
3:C:161:ASN:HD21	3:C:200:THR:H	1.62	0.41
1:D:11:GLY:O	1:D:13:GLY:N	2.53	0.41
2:E:210:GLU:CG	2:E:213:ARG:HH12	2.32	0.41
2:B:60:ALA:HB3	2:B:115:LYS:HG2	2.03	0.41
3:F:63:THR:O	3:F:67:ARG:NH1	2.53	0.41
1:D:129:ASP:O	1:D:130:CYS:HB2	2.21	0.41
1:A:18:MET:CB	1:A:77:TRP:CH2	3.03	0.41
2:B:167:LYS:HB2	2:B:198:TYR:CZ	2.56	0.41
2:B:105:GLN:HE21	2:B:106:ALA:H	1.68	0.41
2:E:26:GLN:HE21	2:E:124:GLY:HA3	1.85	0.41
2:B:116:GLN:HE21	2:B:116:GLN:HB2	1.59	0.41
3:C:36:TRP:CE2	3:C:81:LEU:HB2	2.55	0.41
3:C:151:TYR:CE1	3:C:181:TYR:HB2	2.56	0.41
1:D:15:TRP:CE3	1:D:61:GLY:HA3	2.56	0.41
2:B:24:MET:SD	2:B:45:SER:CB	3.06	0.41
2:B:105:GLN:NE2	2:B:106:ALA:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:VAL:HA	2:B:160:PHE:O	2.20	0.41
3:F:36:TRP:CE2	3:F:81:LEU:HB2	2.55	0.41
2:B:175:ILE:O	2:B:177:GLY:N	2.48	0.41
3:C:39:GLN:O	3:C:92:ALA:HB1	2.20	0.41
3:C:175:VAL:CG1	3:C:176:LEU:N	2.83	0.41
1:D:62:ALA:O	1:D:65:PRO:HD3	2.20	0.41
1:D:82:PHE:CD1	1:D:82:PHE:C	2.99	0.41
2:E:165:TYR:CD2	2:E:165:TYR:C	2.99	0.41
2:E:218:THR:HB	2:E:233:SER:OG	2.21	0.41
3:F:121:LYS:O	3:F:122:THR:C	2.64	0.41
3:F:127:VAL:HG11	3:F:203:VAL:HG21	2.02	0.41
1:A:146:LEU:HD22	1:A:149:ILE:HG12	2.02	0.41
3:F:64:VAL:HA	3:F:67:ARG:NH1	2.36	0.41
2:B:150:LEU:HA	2:B:154:GLY:O	2.22	0.40
2:B:164:PHE:CE2	2:B:200:MET:HB2	2.56	0.40
1:D:67:THR:H	1:D:68:PRO:CD	2.33	0.40
2:B:169:ILE:HG12	2:B:171:VAL:HG23	2.01	0.40
3:C:144:LEU:HD13	3:C:216:ILE:HG21	2.03	0.40
2:E:59:LEU:HA	2:E:115:LYS:O	2.21	0.40
2:E:215:ASN:HA	2:E:236:ARG:HB2	2.02	0.40
3:F:161:ASN:HD22	3:F:161:ASN:HA	1.71	0.40
2:B:140:VAL:HG22	2:B:141:SER:H	1.85	0.40
1:D:55:LEU:HD23	1:D:55:LEU:HA	1.92	0.40
2:E:211:TYR:CE1	2:E:217:TYR:HE2	2.36	0.40
3:F:30:SER:HB3	3:F:74:ASN:ND2	2.37	0.40
3:F:159:THR:C	3:F:202:ASN:HD22	2.29	0.40
1:A:39:LYS:H	1:A:40:PRO:CD	2.29	0.40
1:A:146:LEU:HD22	1:A:146:LEU:HA	1.92	0.40
1:D:32:PHE:HD2	1:D:38:LEU:HD13	1.87	0.40
2:B:81:GLU:O	2:B:82:SER:C	2.65	0.40
2:B:85:PRO:O	2:B:87:ARG:N	2.54	0.40
1:D:15:TRP:CE3	1:D:58:ALA:HA	2.56	0.40
1:D:66:LYS:O	1:D:70:ARG:NH2	2.54	0.40
3:F:118:SER:OG	3:F:121:LYS:HE2	2.21	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	144/176 (82%)	89 (62%)	36 (25%)	19 (13%)	0	1
1	D	144/176 (82%)	95 (66%)	31 (22%)	18 (12%)	0	1
2	B	214/239 (90%)	171 (80%)	28 (13%)	15 (7%)	1	7
2	E	214/239 (90%)	177 (83%)	26 (12%)	11 (5%)	1	11
3	C	210/221 (95%)	165 (79%)	32 (15%)	13 (6%)	1	9
3	F	210/221 (95%)	160 (76%)	29 (14%)	21 (10%)	0	3
All	All	1136/1272 (89%)	857 (75%)	182 (16%)	97 (8%)	0	4

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	157	ALA
2	B	77	ALA
2	B	176	ASP
2	B	236	ARG
2	B	237	ASN
3	C	85	SER
3	C	137	THR
3	C	194	TRP
1	D	12	ARG
1	D	67	THR
1	D	107	MET
1	D	121	PRO
2	E	104	VAL
2	E	237	ASN
3	F	29	PHE
3	F	55	GLY
3	F	138	THR
3	F	167	SER
3	F	194	TRP

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Mol	Chain	Res	Type
3	F	195	PRO
3	F	196	SER
1	A	14	ALA
1	A	40	PRO
1	A	103	THR
1	A	156	VAL
2	B	35	ALA
2	B	54	THR
2	B	86	ASP
2	B	191	GLN
3	C	18	LEU
3	C	28	ALA
3	C	195	PRO
1	D	42	VAL
1	D	44	CYS
1	D	68	PRO
1	D	156	VAL
2	E	55	ARG
2	E	168	ASP
2	E	176	ASP
2	E	191	GLN
3	F	101	TYR
3	F	209	SER
1	A	37	LEU
1	A	55	LEU
1	A	65	PRO
1	A	94	LEU
1	A	100	PRO
1	A	107	MET
1	A	121	PRO
2	B	82	SER
2	B	182	ASN
2	B	198	TYR
3	C	91	THR
3	C	209	SER
3	C	218	PRO
1	D	76	ILE
2	E	58	TYR
2	E	147	SER
3	F	28	ALA
3	F	30	SER
3	F	65	LYS

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Mol	Chain	Res	Type
3	F	74	ASN
3	F	132	PRO
1	A	42	VAL
1	A	56	GLY
1	A	119	TRP
2	B	76	TRP
1	D	65	PRO
1	D	130	CYS
2	E	57	ASN
3	F	92	ALA
3	F	125	PRO
1	A	68	PRO
1	A	104	CYS
2	B	104	VAL
1	D	38	LEU
1	D	55	LEU
1	D	63	ILE
3	F	106	MET
3	F	140	SER
1	A	158	VAL
2	B	93	SER
3	C	99	PRO
1	D	41	SER
2	E	85	PRO
2	E	236	ARG
3	F	14	PRO
3	C	206	PRO
1	D	39	LYS
3	C	55	GLY
2	B	229	PRO
3	C	189	VAL
1	D	160	VAL
1	D	161	VAL
3	F	8	GLY
3	F	155	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	122/147 (83%)	92 (75%)	30 (25%)	1	3
1	D	122/147 (83%)	91 (75%)	31 (25%)	0	3
2	B	194/212 (92%)	162 (84%)	32 (16%)	2	11
2	E	194/212 (92%)	159 (82%)	35 (18%)	2	8
3	C	184/188 (98%)	144 (78%)	40 (22%)	1	5
3	F	183/188 (97%)	148 (81%)	35 (19%)	1	7
All	All	999/1094 (91%)	796 (80%)	203 (20%)	1	6

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	30	LEU
1	A	33	GLN
1	A	35	VAL
1	A	39	LYS
1	A	41	SER
1	A	42	VAL
1	A	48	ARG
1	A	55	LEU
1	A	75	VAL
1	A	83	ARG
1	A	87	LEU
1	A	92	THR
1	A	94	LEU
1	A	96	LEU
1	A	108	VAL
1	A	118	LYS
1	A	119	TRP
1	A	120	VAL
1	A	122	GLN
1	A	133	ARG
1	A	134	GLN
1	A	138	LEU
1	A	142	MET
1	A	146	LEU
1	A	147	LEU
1	A	149	ILE
1	A	154	LEU

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Mol	Chain	Res	Type
1	A	159	LEU
1	A	160	VAL
2	B	23	VAL
2	B	33	VAL
2	B	39	VAL
2	B	41	MET
2	B	47	GLN
2	B	49	LEU
2	B	50	LEU
2	B	53	ARG
2	B	57	ASN
2	B	63	GLN
2	B	79	THR
2	B	86	ASP
2	B	89	THR
2	B	96	ASP
2	B	100	THR
2	B	105	GLN
2	B	109	LEU
2	B	115	LYS
2	B	116	GLN
2	B	120	LEU
2	B	127	THR
2	B	135	ASP
2	B	147	SER
2	B	159	CYS
2	B	175	ILE
2	B	176	ASP
2	B	185	LEU
2	B	195	ASP
2	B	222	THR
2	B	225	THR
2	B	228	SER
2	B	237	ASN
3	C	2	VAL
3	C	5	VAL
3	C	6	GLU
3	C	18	LEU
3	C	20	LEU
3	C	21	SER
3	C	25	SER
3	C	40	THR

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Mol	Chain	Res	Type
3	C	42	GLU
3	C	44	ARG
3	C	48	VAL
3	C	69	THR
3	C	74	ASN
3	C	76	LYS
3	C	82	GLN
3	C	86	LEU
3	C	96	CYS
3	C	100	ASP
3	C	106	MET
3	C	113	THR
3	C	116	THR
3	C	118	SER
3	C	121	LYS
3	C	130	LEU
3	C	143	THR
3	C	144	LEU
3	C	156	VAL
3	C	159	THR
3	C	165	LEU
3	C	169	VAL
3	C	176	LEU
3	C	177	GLN
3	C	179	ASP
3	C	186	SER
3	C	190	THR
3	C	192	SER
3	C	193	THR
3	C	200	THR
3	C	214	LYS
3	C	219	ARG
1	D	16	LEU
1	D	18	MET
1	D	27	LEU
1	D	30	LEU
1	D	35	VAL
1	D	37	LEU
1	D	38	LEU
1	D	41	SER
1	D	42	VAL
1	D	45	ILE

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Mol	Chain	Res	Type
1	D	51	LEU
1	D	54	VAL
1	D	55	LEU
1	D	59	LEU
1	D	75	VAL
1	D	78	LEU
1	D	90	GLU
1	D	94	LEU
1	D	95	GLN
1	D	116	LEU
1	D	117	ASP
1	D	118	LYS
1	D	132	GLU
1	D	133	ARG
1	D	140	LEU
1	D	146	LEU
1	D	147	LEU
1	D	151	ILE
1	D	153	TYR
1	D	159	LEU
1	D	161	VAL
2	E	30	SER
2	E	39	VAL
2	E	41	MET
2	E	49	LEU
2	E	53	ARG
2	E	55	ARG
2	E	57	ASN
2	E	63	GLN
2	E	73	LEU
2	E	79	THR
2	E	87	ARG
2	E	89	THR
2	E	95	THR
2	E	96	ASP
2	E	100	THR
2	E	102	SER
2	E	103	SER
2	E	115	LYS
2	E	116	GLN
2	E	130	GLU
2	E	132	LYS

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Mol	Chain	Res	Type
2	E	140	VAL
2	E	151	THR
2	E	161	LEU
2	E	168	ASP
2	E	171	VAL
2	E	172	LYS
2	E	175	ILE
2	E	176	ASP
2	E	195	ASP
2	E	207	THR
2	E	218	THR
2	E	220	GLU
2	E	228	SER
2	E	237	ASN
3	F	2	VAL
3	F	4	LEU
3	F	7	SER
3	F	13	LYS
3	F	20	LEU
3	F	30	SER
3	F	37	VAL
3	F	40	THR
3	F	44	ARG
3	F	69	THR
3	F	82	GLN
3	F	84	SER
3	F	101	TYR
3	F	111	GLN
3	F	116	THR
3	F	121	LYS
3	F	122	THR
3	F	126	SER
3	F	130	LEU
3	F	136	ASP
3	F	140	SER
3	F	143	THR
3	F	176	LEU
3	F	177	GLN
3	F	182	THR
3	F	187	VAL
3	F	188	THR
3	F	193	THR

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Mol	Chain	Res	Type
3	F	194	TRP
3	F	198	SER
3	F	200	THR
3	F	202	ASN
3	F	210	THR
3	F	212	VAL
3	F	214	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
2	B	26	GLN
2	B	57	ASN
2	B	64	GLN
2	B	105	GLN
2	B	116	GLN
2	B	191	GLN
2	B	235	ASN
2	B	237	ASN
3	C	39	GLN
3	C	82	GLN
3	C	161	ASN
3	C	170	HIS
3	C	202	ASN
1	D	33	GLN
1	D	34	HIS
1	D	144	GLN
2	E	26	GLN
2	E	51	ASN
2	E	63	GLN
2	E	105	GLN
2	E	116	GLN
2	E	149	GLN
2	E	186	ASN
2	E	191	GLN
2	E	214	HIS
2	E	235	ASN
2	E	237	ASN
3	F	74	ASN
3	F	77	ASN
3	F	161	ASN

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Mol	Chain	Res	Type
3	F	202	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
4	UQ1	A	177	-	18,18,18	2.24	2 (11%)	24,25,25	1.24	3 (12%)
4	UQ1	D	177	-	18,18,18	2.18	2 (11%)	24,25,25	1.18	2 (8%)

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	UQ1	A	177	-	-	0/9/33/33	0/1/1/1
4	UQ1	D	177	-	-	0/9/33/33	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	177	UQ1	C6-C5	8.38	1.50	1.35
4	D	177	UQ1	C6-C5	8.10	1.49	1.35
4	D	177	UQ1	C3-C2	3.59	1.49	1.36
4	A	177	UQ1	C3-C2	3.43	1.48	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	177	UQ1	C7-C6-C5	-2.81	120.08	124.89
4	A	177	UQ1	C7-C6-C5	-2.54	120.54	124.89
4	A	177	UQ1	C11-C9-C10	2.26	119.78	114.59
4	A	177	UQ1	CM5-C5-C6	-2.16	120.90	124.45
4	D	177	UQ1	CM5-C5-C6	-2.09	121.02	124.45

There are no chirality outliers.

There are no torsion outliers.

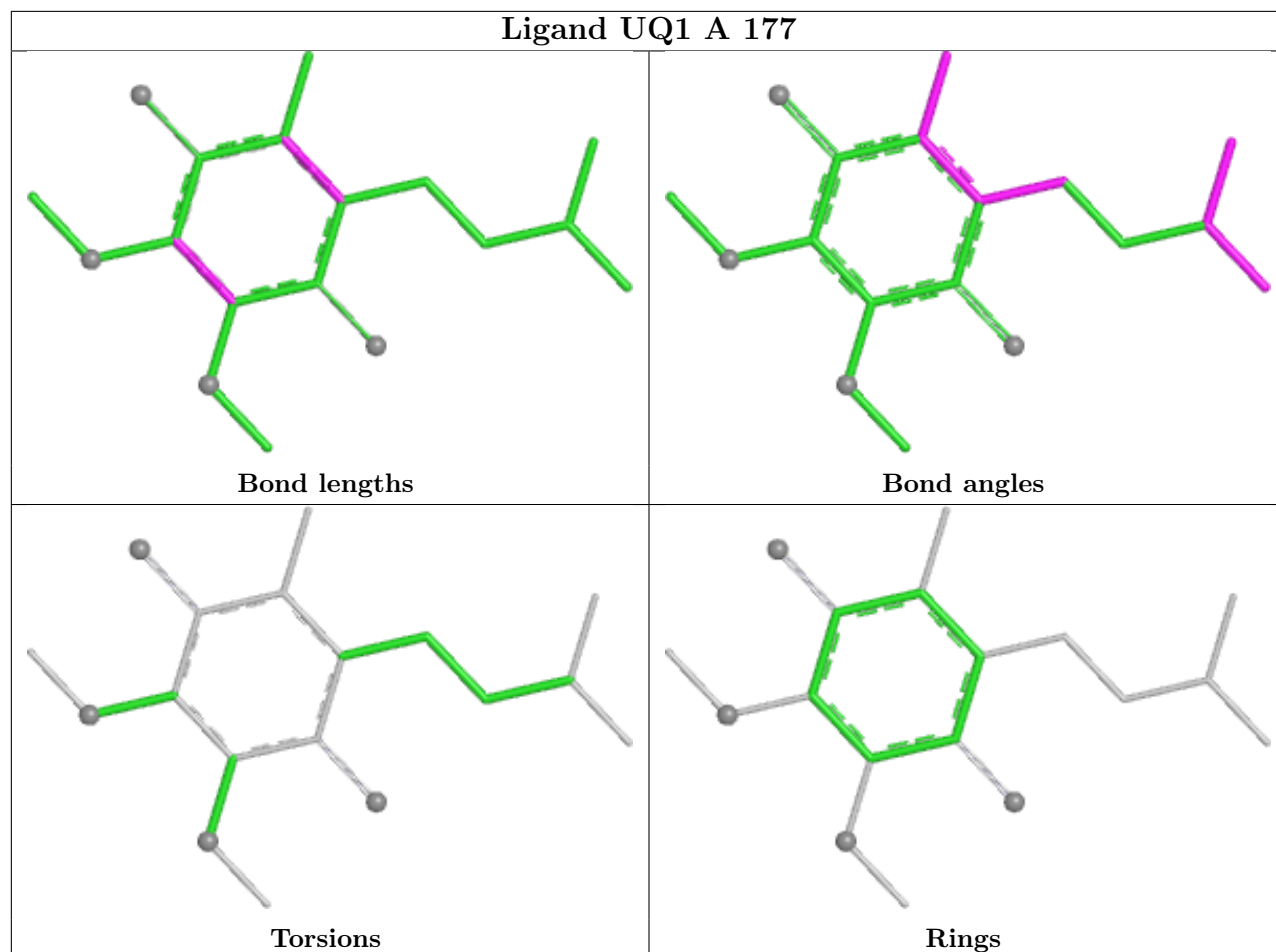
There are no ring outliers.

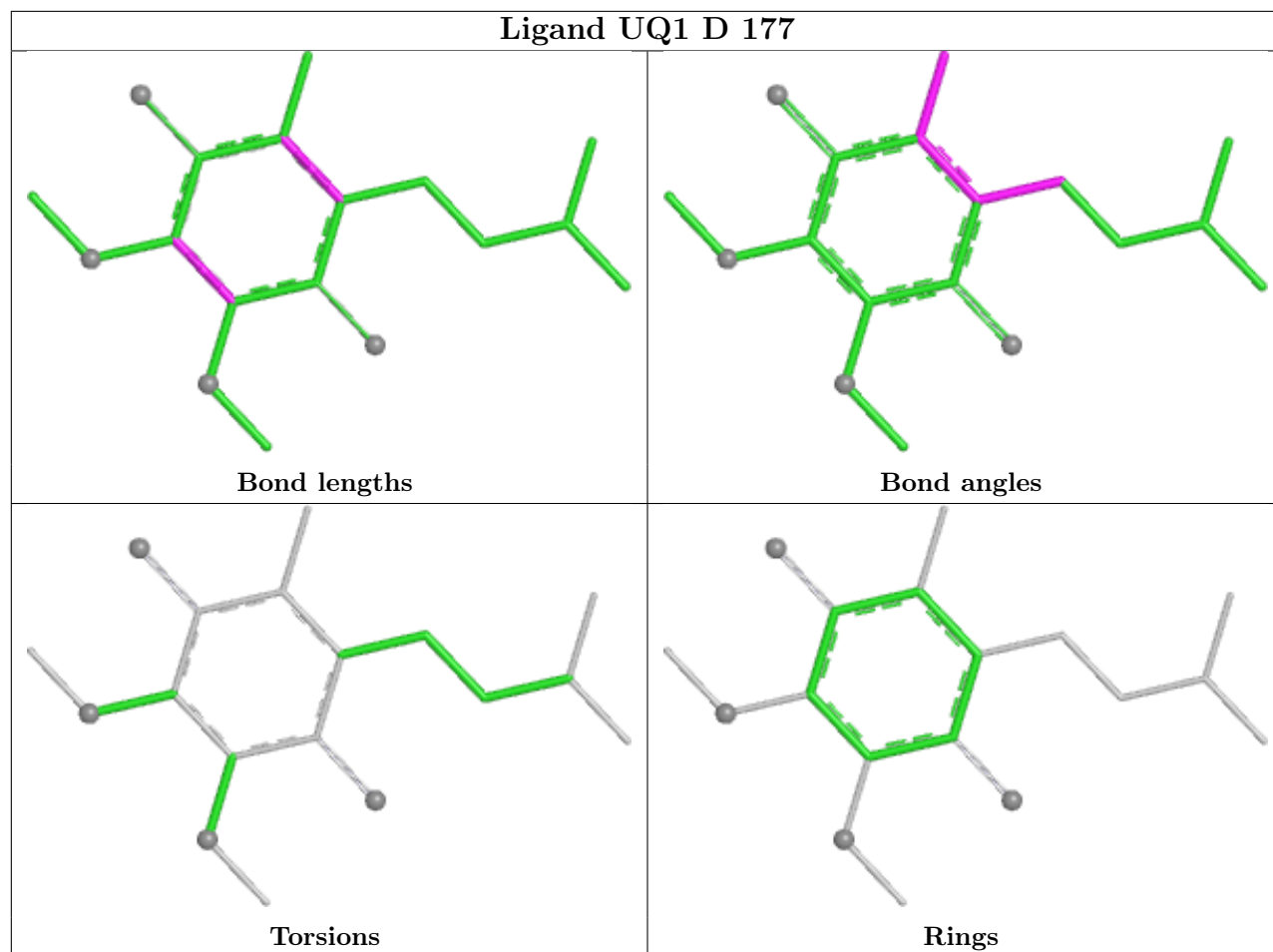
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	177	UQ1	2	0
4	D	177	UQ1	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand UQ1 A 177





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	A	148/176 (84%)	0.73	17 (11%) 9 8	87, 123, 150, 154	0
1	D	148/176 (84%)	0.80	21 (14%) 6 5	109, 140, 180, 183	0
2	B	218/239 (91%)	0.09	4 (1%) 67 49	60, 99, 137, 141	0
2	E	218/239 (91%)	0.63	27 (12%) 8 6	92, 113, 128, 140	0
3	C	216/221 (97%)	0.19	7 (3%) 50 34	73, 95, 120, 131	0
3	F	214/221 (96%)	0.47	20 (9%) 14 11	98, 118, 133, 136	0
All	All	1162/1272 (91%)	0.45	96 (8%) 17 13	60, 114, 151, 183	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	VAL	10.6
1	D	41	SER	7.3
2	E	182	ASN	6.2
3	F	70	ILE	6.1
1	D	43	LEU	5.9
1	D	42	VAL	5.7
1	D	107	MET	5.7
1	A	89	TYR	5.4
2	B	55	ARG	5.3
1	D	127	SER	5.3
2	B	57	ASN	5.2
1	A	159	LEU	5.2
3	F	50	TYR	5.1
2	E	185	LEU	5.0
2	E	181	GLN	4.9
3	F	71	SER	4.9
2	E	109	LEU	4.8
1	D	45	ILE	4.6
3	F	131	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	106	PHE	4.5
2	E	134	ALA	4.3
1	D	126	ALA	4.3
1	D	152	ALA	4.3
3	F	215	LYS	4.3
2	E	110	ALA	4.2
2	E	184	VAL	4.2
3	F	174	ALA	4.0
2	E	63	GLN	3.9
2	E	186	ASN	3.8
3	C	82	GLN	3.8
1	D	40	PRO	3.7
3	F	177	GLN	3.7
2	E	123	PHE	3.6
1	D	105	ASP	3.6
2	E	62	TYR	3.5
3	F	1	GLU	3.4
2	E	77	ALA	3.3
3	F	80	TYR	3.3
1	A	101	PHE	3.2
3	F	130	LEU	3.2
2	E	190	ASP	3.1
1	D	128	GLY	3.0
1	D	119	TRP	3.0
1	D	137	PHE	3.0
1	D	159	LEU	2.9
3	F	198	SER	2.9
3	F	51	ILE	2.9
1	D	115	PRO	2.9
1	A	80	SER	2.9
2	E	131	ILE	2.9
1	D	138	LEU	2.9
3	F	175	VAL	2.9
3	F	19	LYS	2.8
2	E	187	SER	2.8
1	A	49	VAL	2.8
2	B	237	ASN	2.7
2	E	90	GLY	2.7
3	F	21	SER	2.7
1	A	81	ALA	2.7
2	E	214	HIS	2.7
3	F	129	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	61	TRP	2.6
3	F	173	PRO	2.6
1	A	82	PHE	2.6
3	C	207	ALA	2.6
1	D	125	VAL	2.5
3	F	100	ASP	2.5
3	C	138	THR	2.5
3	F	36	TRP	2.4
2	E	98	THR	2.4
1	A	86	GLN	2.4
1	A	16	LEU	2.4
2	E	179	GLU	2.4
2	E	39	VAL	2.4
3	C	24	ALA	2.4
2	E	188	TRP	2.4
1	D	10	GLN	2.3
1	D	94	LEU	2.3
2	E	66	PRO	2.3
3	C	157	THR	2.2
3	F	22	CYS	2.2
2	E	183	GLY	2.2
1	A	114	LEU	2.2
2	B	190	ASP	2.2
1	A	71	TYR	2.2
1	A	97	TYR	2.2
1	A	50	ALA	2.2
1	A	42	VAL	2.1
2	E	113	TYR	2.1
1	A	155	ILE	2.1
1	D	54	VAL	2.1
3	C	88	SER	2.0
2	E	59	LEU	2.0
2	E	64	GLN	2.0
3	C	89	GLU	2.0
1	A	116	LEU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

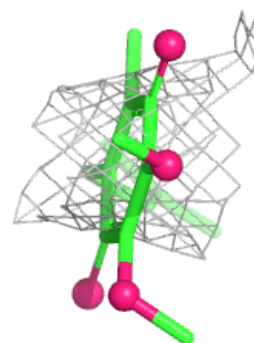
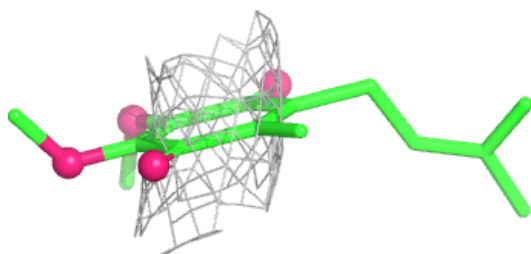
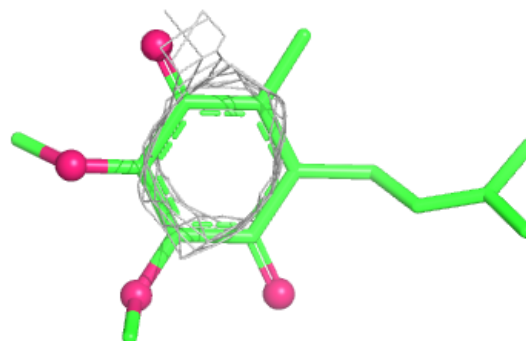
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

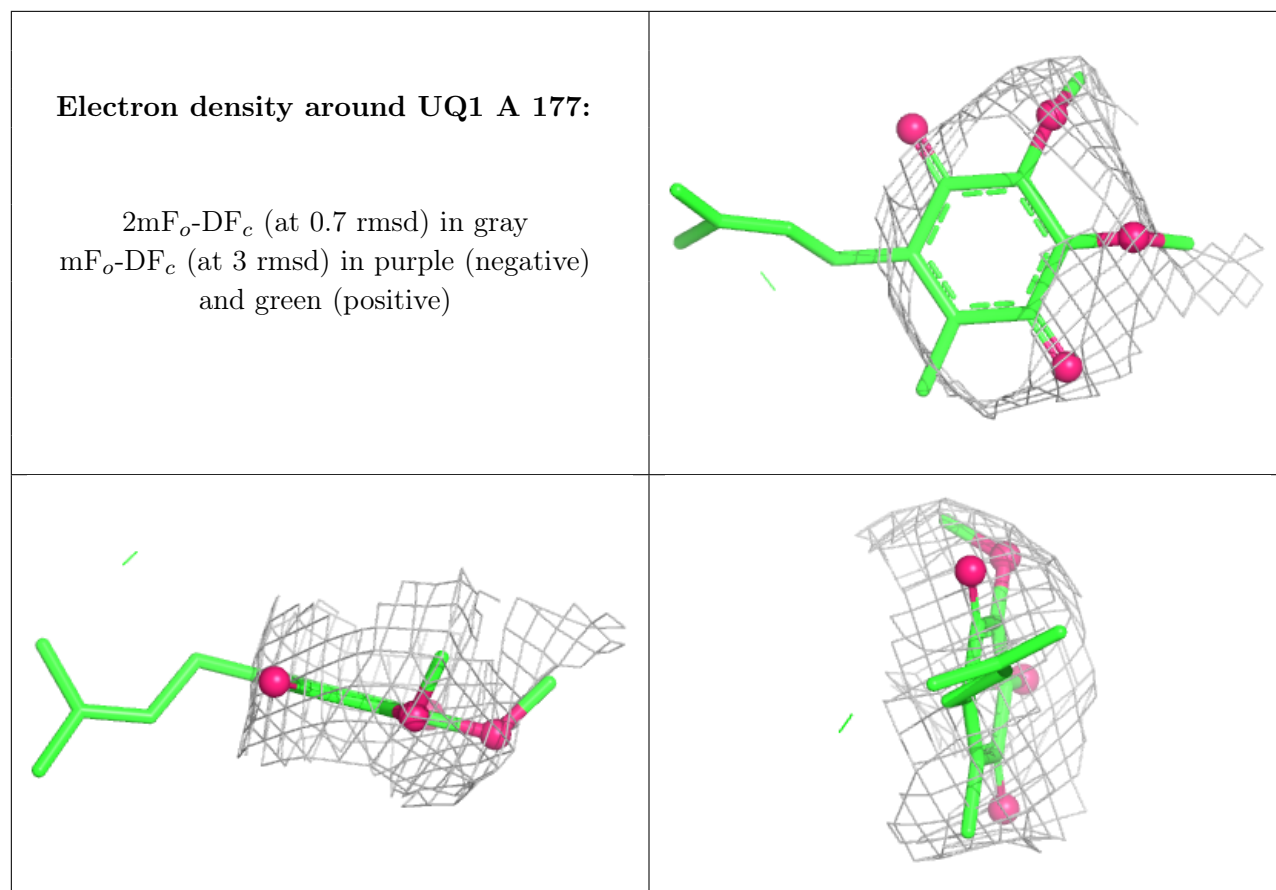
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	UQ1	D	177	18/18	0.82	0.26	267,268,268,268	0
4	UQ1	A	177	18/18	0.83	0.21	167,169,169,169	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UQ1 D 177:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.