



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:40 AM UTC

PDB ID : 5TNC / pdb_00005tnc
Title : REFINED CRYSTAL STRUCTURE OF TROPONIN C FROM TURKEY
SKELETAL MUSCLE AT 2.0 ANGSTROMS RESOLUTION
Authors : Herzberg, O.; James, M.N.G.
Deposited on : 1988-05-27
Resolution : 2.00 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

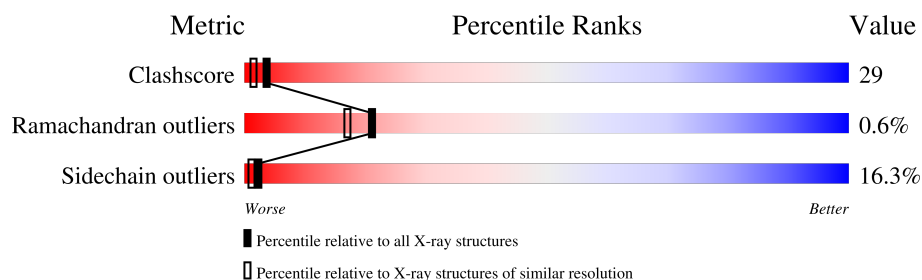
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	162	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1421 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 TROPONIN-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	1	0
			1262	775	199	275	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	GLU	ALA	conflict	UNP P10246
A	100	ASP	ASN	conflict	UNP P10246
A	133	ASP	GLU	conflict	UNP P10246

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

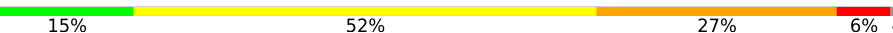
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	157	Total	O	0	0
			157	157		

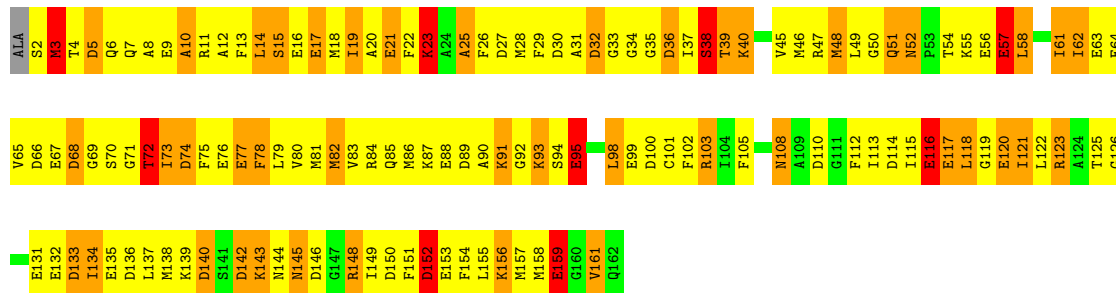
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: TROPONIN-C

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	66.55Å 66.55Å 60.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1421	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.48	8/1279 (0.6%)	2.48	84/1706 (4.9%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ASN	CG-OD1	6.55	1.35	1.23
1	A	26	PHE	CA-CB	6.48	1.64	1.53
1	A	15	SER	N-CA	5.76	1.52	1.45
1	A	145	ASN	C-O	5.57	1.30	1.23
1	A	51	GLN	CD-OE1	5.48	1.33	1.23
1	A	51	GLN	CD-NE2	-5.18	1.22	1.33
1	A	134	ILE	N-CA	5.04	1.52	1.46
1	A	19	ILE	N-CA	5.01	1.52	1.46

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	THR	N-CA-CB	-9.78	94.67	111.69
1	A	133	ASP	CA-CB-CG	9.23	121.83	112.60
1	A	152	ASP	CA-CB-CG	-8.98	103.62	112.60
1	A	36	ASP	CA-CB-CG	8.79	121.39	112.60
1	A	62	ILE	CA-C-N	8.63	138.03	121.54
1	A	62	ILE	C-N-CA	8.63	138.03	121.54
1	A	85	GLN	OE1-CD-NE2	-8.29	114.31	122.60
1	A	145	ASN	CA-C-O	-7.55	112.78	121.54
1	A	140	ASP	CA-CB-CG	-7.47	105.13	112.60
1	A	57	GLU	N-CA-CB	7.35	121.67	110.28
1	A	123	ARG	NE-CZ-NH1	-7.30	114.20	121.50
1	A	118	LEU	CA-C-N	7.10	127.82	119.94
1	A	118	LEU	C-N-CA	7.10	127.82	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ILE	CA-C-O	-6.92	112.72	120.74
1	A	46	MET	O-C-N	6.90	129.18	122.07
1	A	145	ASN	O-C-N	6.83	131.35	122.40
1	A	137	LEU	CA-C-O	-6.73	113.42	120.55
1	A	126	GLY	N-CA-C	-6.71	105.81	115.27
1	A	159	GLU	CA-CB-CG	6.70	127.51	114.10
1	A	39	THR	CA-CB-OG1	-6.64	99.64	109.60
1	A	47	ARG	NE-CZ-NH1	6.61	128.11	121.50
1	A	10	ALA	CB-CA-C	6.61	122.09	110.85
1	A	52	ASN	O-C-N	6.60	126.01	121.19
1	A	120	GLU	CA-C-O	-6.45	114.23	121.00
1	A	158	MET	CA-C-O	-6.38	114.13	120.70
1	A	149	ILE	CA-C-O	-6.33	113.76	120.53
1	A	131	GLU	CB-CG-CD	6.21	123.16	112.60
1	A	152	ASP	N-CA-CB	-6.21	100.38	109.82
1	A	94	SER	CA-C-O	-6.06	114.12	120.55
1	A	95	GLU	CB-CA-C	-5.99	100.50	110.68
1	A	74	ASP	CA-CB-CG	-5.91	106.69	112.60
1	A	125	THR	CA-CB-OG1	-5.91	100.73	109.60
1	A	14	LEU	O-C-N	5.91	130.72	123.10
1	A	45	VAL	CA-C-O	-5.87	114.84	120.95
1	A	117	GLU	O-C-N	5.85	128.10	122.07
1	A	50	GLY	N-CA-C	5.83	124.17	114.48
1	A	121	ILE	CA-CB-CG2	5.83	120.41	110.50
1	A	137	LEU	O-C-N	5.82	128.29	122.12
1	A	57	GLU	CB-CG-CD	5.76	122.39	112.60
1	A	136	ASP	CA-C-N	5.75	127.99	120.28
1	A	136	ASP	C-N-CA	5.75	127.99	120.28
1	A	157	MET	CA-CB-CG	-5.75	102.60	114.10
1	A	58	LEU	N-CA-CB	-5.74	101.67	110.16
1	A	3	MET	CA-C-O	5.65	126.45	119.79
1	A	159	GLU	N-CA-C	5.62	120.00	113.20
1	A	61	ILE	N-CA-C	5.56	116.29	110.62
1	A	57	GLU	CG-CD-OE1	5.53	131.12	118.40
1	A	117	GLU	CB-CA-C	-5.44	102.34	110.88
1	A	39	THR	N-CA-C	-5.43	106.50	113.01
1	A	47	ARG	CD-NE-CZ	5.42	131.98	124.40
1	A	142	ASP	CA-C-N	5.41	128.53	120.31
1	A	142	ASP	C-N-CA	5.41	128.53	120.31
1	A	38	SER	N-CA-C	-5.40	101.67	110.20
1	A	57	GLU	CG-CD-OE2	-5.40	105.99	118.40
1	A	25	ALA	CA-C-N	5.38	129.75	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ALA	C-N-CA	5.38	129.75	121.19
1	A	73	ILE	CA-C-O	-5.37	114.67	120.36
1	A	48	MET	CB-CA-C	5.36	120.97	110.67
1	A	17	GLU	CA-CB-CG	5.34	124.77	114.10
1	A	100	ASP	O-C-N	5.29	127.52	122.07
1	A	120	GLU	N-CA-CB	5.28	117.61	109.91
1	A	23	LYS	CA-C-N	5.25	127.57	120.38
1	A	23	LYS	C-N-CA	5.25	127.57	120.38
1	A	5	ASP	O-C-N	5.23	127.74	122.09
1	A	158	MET	O-C-N	5.23	127.74	122.09
1	A	78	PHE	CA-C-O	-5.21	114.89	120.42
1	A	57	GLU	CA-CB-CG	5.19	124.47	114.10
1	A	123	ARG	NH1-CZ-NH2	5.18	126.03	119.30
1	A	21	GLU	O-C-N	5.17	128.05	122.15
1	A	93	LYS	O-C-N	5.17	127.47	122.09
1	A	54	THR	N-CA-C	-5.17	103.70	110.53
1	A	143	LYS	N-CA-C	5.17	117.81	111.82
1	A	114	ASP	CB-CA-C	5.15	120.25	110.51
1	A	108	ASN	N-CA-C	-5.15	106.40	113.30
1	A	123	ARG	O-C-N	5.15	128.25	122.22
1	A	27	ASP	N-CA-CB	5.15	119.07	110.32
1	A	25	ALA	CA-C-O	5.10	126.16	120.90
1	A	159	GLU	CB-CA-C	-5.10	100.42	110.11
1	A	82	MET	CA-C-O	-5.10	115.47	120.82
1	A	68	ASP	N-CA-C	5.07	119.47	113.28
1	A	98	LEU	O-C-N	5.05	127.91	122.15
1	A	116	GLU	N-CA-CB	5.03	117.36	110.07
1	A	58	LEU	CB-CA-C	5.01	119.37	110.85
1	A	39	THR	CA-C-O	5.01	125.56	119.05

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	1262	0	1176	71	429
2	A	2	0	0	0	0
3	A	157	0	0	24	45
All	All	1421	0	1176	71	433

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 (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:HB2	3:A:260:HOH:O	1.50	1.10
1:A:3:MET:HE2	3:A:196:HOH:O	1.67	0.94
1:A:133:ASP:OD2	3:A:291:HOH:O	1.83	0.94
1:A:103:ARG:HH11	1:A:103:ARG:HG2	1.32	0.93
1:A:75:PHE:CZ	1:A:79:LEU:HD21	2.06	0.91
1:A:23:LYS:HG2	1:A:75:PHE:CZ	2.11	0.85
1:A:118:LEU:HD22	1:A:138:MET:HE2	1.62	0.82
1:A:35:GLY:HA2	3:A:258:HOH:O	1.81	0.79
1:A:30:ASP:HA	3:A:232:HOH:O	1.88	0.74
1:A:30:ASP:OD1	3:A:232:HOH:O	2.06	0.74
1:A:119:GLY:HA2	1:A:134:ILE:HD13	1.70	0.73
1:A:3:MET:HE1	1:A:77:GLU:HA	1.68	0.72
1:A:103:ARG:HG2	1:A:103:ARG:NH1	2.04	0.70
1:A:72:THR:CG2	3:A:247:HOH:O	2.41	0.67
1:A:135:GLU:O	1:A:139:LYS:HG3	1.95	0.66
1:A:118:LEU:CD2	1:A:138:MET:HE2	2.27	0.65
1:A:122:LEU:HD12	1:A:134:ILE:HG12	1.77	0.65
1:A:23:LYS:HG2	1:A:75:PHE:CE2	2.33	0.63
1:A:74:ASP:OD1	1:A:77:GLU:HG2	1.99	0.63
1:A:108:ASN:HB2	3:A:273:HOH:O	2.01	0.60
1:A:116:GLU:CG	3:A:280:HOH:O	2.52	0.58
1:A:3:MET:SD	1:A:7:GLN:HG3	2.44	0.57
1:A:31:ALA:HB3	3:A:282:HOH:O	2.05	0.57
1:A:31:ALA:C	1:A:33:GLY:H	2.12	0.57
1:A:57:GLU:O	1:A:61:ILE:HG13	2.05	0.56
1:A:25:ALA:O	1:A:28:MET:HB2	2.06	0.55
1:A:3:MET:CE	3:A:196:HOH:O	2.39	0.55
1:A:112:PHE:CD2	1:A:148:ARG:HG3	2.42	0.54
1:A:119:GLY:O	1:A:123:ARG:HG3	2.08	0.54
1:A:98:LEU:HD11	1:A:159:GLU:OE1	2.07	0.54
1:A:64:GLU:OE2	3:A:321:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLU:CD	3:A:280:HOH:O	2.51	0.54
1:A:101[A]:CYS:SG	1:A:105:PHE:CE2	3.01	0.53
1:A:23:LYS:HG2	1:A:75:PHE:CE1	2.43	0.53
1:A:101[A]:CYS:SG	1:A:105:PHE:CZ	3.02	0.53
1:A:52:ASN:HB2	3:A:297:HOH:O	2.09	0.52
1:A:108:ASN:CG	3:A:273:HOH:O	2.53	0.52
1:A:75:PHE:CE1	1:A:79:LEU:HD21	2.45	0.52
1:A:56:GLU:HG3	3:A:281:HOH:O	2.09	0.52
1:A:103:ARG:NH1	1:A:103:ARG:CG	2.71	0.51
1:A:37:ILE:O	1:A:72:THR:HA	2.11	0.51
1:A:2:SER:HA	1:A:5:ASP:OD1	2.11	0.50
1:A:61:ILE:O	1:A:65:VAL:HG22	2.11	0.50
1:A:38:SER:OG	1:A:40:LYS:HB2	2.11	0.49
1:A:116:GLU:HG3	3:A:280:HOH:O	2.12	0.49
1:A:123:ARG:HD2	3:A:199:HOH:O	2.13	0.47
1:A:31:ALA:C	1:A:33:GLY:N	2.73	0.46
1:A:72:THR:HG22	3:A:247:HOH:O	2.13	0.46
1:A:83:VAL:O	1:A:87:LYS:HG3	2.15	0.46
1:A:108:ASN:ND2	3:A:273:HOH:O	2.47	0.46
1:A:39:THR:HB	1:A:62:ILE:HG12	1.97	0.45
1:A:72:THR:HG21	3:A:247:HOH:O	2.11	0.45
1:A:95:GLU:OE1	1:A:95:GLU:CA	2.65	0.45
1:A:70:SER:HB2	3:A:190:HOH:O	2.16	0.44
1:A:77:GLU:O	1:A:81:MET:HG2	2.16	0.44
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.78	0.44
1:A:112:PHE:HB3	1:A:148:ARG:HB2	1.99	0.44
1:A:84:ARG:HB2	3:A:218:HOH:O	2.17	0.44
1:A:36:ASP:HB2	1:A:73:ILE:O	2.18	0.43
1:A:161:VAL:HG22	1:A:161:VAL:O	2.18	0.42
1:A:36:ASP:OD2	1:A:72:THR:HG23	2.17	0.42
1:A:51:GLN:HG2	1:A:82:MET:HE1	2.02	0.42
1:A:3:MET:HA	1:A:6:GLN:HE21	1.84	0.42
1:A:108:ASN:CB	3:A:273:HOH:O	2.63	0.41
1:A:117:GLU:O	1:A:121:ILE:HD12	2.20	0.41
1:A:155:LEU:O	1:A:159:GLU:HG2	2.20	0.41
1:A:30:ASP:OD1	1:A:30:ASP:C	2.60	0.41
1:A:95:GLU:OE1	1:A:95:GLU:HA	2.21	0.41
1:A:38:SER:C	1:A:40:LYS:N	2.78	0.40

All (433) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLN:O	1:A:21:GLU:OE1[4_555]	0.26	1.94
1:A:68:ASP:C	1:A:155:LEU:CD2[2_664]	0.29	1.91
1:A:150:ASP:C	3:A:247:HOH:O[3_565]	0.36	1.84
1:A:17:GLU:CD	1:A:77:GLU:N[4_555]	0.41	1.79
1:A:70:SER:CA	1:A:151:PHE:CG[2_664]	0.48	1.72
1:A:69:GLY:O	1:A:151:PHE:CE2[2_664]	0.53	1.67
1:A:72:THR:O	1:A:152:ASP:CB[2_664]	0.57	1.63
1:A:65:VAL:CA	1:A:156:LYS:NZ[2_664]	0.62	1.58
1:A:75:PHE:N	1:A:144:ASN:ND2[2_664]	0.63	1.57
1:A:146:ASP:CB	3:A:276:HOH:O[3_565]	0.66	1.54
1:A:74:ASP:OD2	1:A:153:GLU:OE2[2_664]	0.67	1.53
1:A:108:ASN:CB	1:A:116:GLU:OE1[5_555]	0.69	1.51
1:A:7:GLN:O	1:A:21:GLU:CB[4_555]	0.75	1.45
1:A:17:GLU:CG	1:A:143:LYS:O[5_665]	0.79	1.41
1:A:17:GLU:N	1:A:76:GLU:CA[4_555]	0.79	1.41
1:A:89:ASP:O	1:A:91:LYS:N[4_555]	0.82	1.38
1:A:68:ASP:N	1:A:155:LEU:CB[2_664]	0.83	1.37
1:A:86:MET:O	1:A:86:MET:O[4_555]	0.83	1.37
1:A:10:ALA:O	1:A:22:PHE:CD2[4_555]	0.85	1.35
1:A:74:ASP:OD2	1:A:153:GLU:CD[2_664]	0.85	1.35
1:A:89:ASP:N	1:A:90:ALA:CB[4_555]	0.86	1.34
1:A:11:ARG:C	1:A:22:PHE:CA[4_555]	0.87	1.33
1:A:76:GLU:CA	1:A:144:ASN:CA[2_664]	0.88	1.32
1:A:11:ARG:C	1:A:22:PHE:CB[4_555]	0.90	1.30
1:A:76:GLU:CG	1:A:145:ASN:N[2_664]	0.90	1.30
1:A:152:ASP:CA	3:A:190:HOH:O[3_565]	0.92	1.28
1:A:153:GLU:N	3:A:220:HOH:O[3_565]	0.93	1.27
3:A:296:HOH:O	3:A:296:HOH:O[4_555]	0.93	1.27
1:A:8:ALA:O	1:A:21:GLU:O[4_555]	0.95	1.25
1:A:11:ARG:CD	1:A:20:ALA:CA[4_555]	0.96	1.24
1:A:17:GLU:OE1	1:A:77:GLU:CB[4_555]	0.96	1.24
1:A:10:ALA:O	1:A:22:PHE:CG[4_555]	0.97	1.23
1:A:15:SER:CB	1:A:78:PHE:CA[4_555]	0.98	1.22
1:A:17:GLU:OE1	1:A:77:GLU:CA[4_555]	0.99	1.21
1:A:70:SER:CB	1:A:151:PHE:CB[2_664]	0.99	1.21
1:A:13:PHE:CZ	1:A:51:GLN:CG[4_555]	1.01	1.19
1:A:68:ASP:N	1:A:155:LEU:CA[2_664]	1.01	1.19
1:A:76:GLU:CB	1:A:144:ASN:C[2_664]	1.01	1.19
1:A:69:GLY:N	1:A:155:LEU:CG[2_664]	1.02	1.18
1:A:92:GLY:N	1:A:93:LYS:N[4_555]	1.02	1.18
1:A:76:GLU:N	1:A:144:ASN:CB[2_664]	1.03	1.17
1:A:12:ALA:N	1:A:22:PHE:CA[4_555]	1.07	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:CB	1:A:151:PHE:CA[2_664]	1.08	1.12
1:A:74:ASP:N	3:A:204:HOH:O[2_664]	1.08	1.12
1:A:10:ALA:C	1:A:22:PHE:CD2[4_555]	1.09	1.11
1:A:15:SER:OG	1:A:79:LEU:N[4_555]	1.09	1.11
1:A:25:ALA:CA	3:A:301:HOH:O[4_555]	1.09	1.11
1:A:89:ASP:CA	1:A:90:ALA:CB[4_555]	1.09	1.11
1:A:90:ALA:N	1:A:90:ALA:N[4_555]	1.09	1.11
1:A:36:ASP:OD2	1:A:150:ASP:CB[2_664]	1.10	1.10
1:A:64:GLU:C	1:A:156:LYS:CE[2_664]	1.10	1.10
1:A:69:GLY:N	1:A:155:LEU:CD1[2_664]	1.10	1.10
1:A:13:PHE:O	1:A:82:MET:SD[4_555]	1.11	1.09
1:A:102:PHE:CG	3:A:195:HOH:O[3_565]	1.11	1.09
1:A:74:ASP:CG	1:A:153:GLU:OE2[2_664]	1.13	1.07
1:A:11:ARG:NE	1:A:20:ALA:CA[4_555]	1.14	1.06
1:A:68:ASP:O	1:A:155:LEU:CD2[2_664]	1.14	1.06
1:A:76:GLU:CB	1:A:145:ASN:N[2_664]	1.14	1.06
1:A:13:PHE:CD2	1:A:82:MET:CE[4_555]	1.15	1.05
1:A:65:VAL:C	1:A:156:LYS:NZ[2_664]	1.15	1.05
1:A:10:ALA:N	1:A:21:GLU:OE2[4_555]	1.16	1.04
1:A:64:GLU:O	1:A:156:LYS:CE[2_664]	1.16	1.04
1:A:70:SER:CA	1:A:151:PHE:CD2[2_664]	1.16	1.04
1:A:108:ASN:CB	1:A:116:GLU:CD[5_555]	1.16	1.04
1:A:13:PHE:O	1:A:82:MET:CG[4_555]	1.17	1.03
1:A:14:LEU:O	1:A:78:PHE:CE2[4_555]	1.17	1.03
1:A:70:SER:C	1:A:151:PHE:CD2[2_664]	1.17	1.03
1:A:76:GLU:CG	1:A:144:ASN:C[2_664]	1.17	1.03
1:A:16:GLU:N	1:A:75:PHE:O[4_555]	1.18	1.02
1:A:64:GLU:O	1:A:156:LYS:CD[2_664]	1.18	1.02
1:A:6:GLN:C	1:A:21:GLU:OE1[4_555]	1.19	1.01
1:A:7:GLN:CG	3:A:261:HOH:O[2_664]	1.19	1.01
1:A:18:MET:SD	1:A:79:LEU:O[4_555]	1.20	1.00
1:A:68:ASP:OD1	1:A:154:PHE:CB[2_664]	1.20	1.00
1:A:73:ILE:C	3:A:204:HOH:O[2_664]	1.20	1.00
1:A:92:GLY:CA	1:A:92:GLY:C[4_555]	1.20	1.00
1:A:17:GLU:OE2	1:A:77:GLU:N[4_555]	1.21	0.99
1:A:152:ASP:N	3:A:190:HOH:O[3_565]	1.21	0.99
1:A:13:PHE:CG	1:A:82:MET:CE[4_555]	1.22	0.98
1:A:15:SER:OG	1:A:78:PHE:C[4_555]	1.22	0.98
1:A:13:PHE:CZ	1:A:51:GLN:CD[4_555]	1.23	0.97
1:A:89:ASP:N	1:A:90:ALA:CA[4_555]	1.23	0.97
1:A:6:GLN:O	1:A:21:GLU:CD[4_555]	1.24	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLU:N	1:A:21:GLU:CG[4_555]	1.24	0.96
1:A:151:PHE:N	3:A:247:HOH:O[3_565]	1.24	0.96
1:A:14:LEU:O	1:A:78:PHE:CD2[4_555]	1.25	0.95
1:A:19:ILE:N	1:A:79:LEU:CD1[4_555]	1.25	0.95
1:A:69:GLY:O	1:A:151:PHE:CZ[2_664]	1.25	0.95
1:A:69:GLY:C	1:A:151:PHE:CE2[2_664]	1.25	0.95
1:A:70:SER:OG	1:A:151:PHE:CA[2_664]	1.25	0.95
1:A:13:PHE:N	1:A:49:LEU:CD1[4_555]	1.27	0.93
1:A:17:GLU:CA	1:A:76:GLU:CB[4_555]	1.27	0.93
1:A:7:GLN:C	1:A:21:GLU:CB[4_555]	1.28	0.92
1:A:17:GLU:CG	1:A:77:GLU:N[4_555]	1.28	0.92
1:A:34:GLY:CA	1:A:112:PHE:CE1[2_664]	1.29	0.91
1:A:17:GLU:CB	1:A:143:LYS:O[5_665]	1.30	0.90
1:A:68:ASP:C	1:A:155:LEU:CG[2_664]	1.30	0.90
1:A:15:SER:C	1:A:75:PHE:O[4_555]	1.31	0.89
1:A:17:GLU:CG	1:A:76:GLU:C[4_555]	1.31	0.89
1:A:17:GLU:CA	1:A:76:GLU:CA[4_555]	1.32	0.88
1:A:17:GLU:CD	1:A:77:GLU:CA[4_555]	1.32	0.88
1:A:150:ASP:CA	3:A:247:HOH:O[3_565]	1.32	0.88
1:A:7:GLN:OE1	1:A:143:LYS:CA[2_664]	1.34	0.86
1:A:15:SER:O	1:A:79:LEU:CG[4_555]	1.34	0.86
1:A:15:SER:CB	1:A:78:PHE:C[4_555]	1.34	0.86
1:A:17:GLU:OE2	1:A:144:ASN:CB[5_665]	1.34	0.86
1:A:89:ASP:C	1:A:91:LYS:N[4_555]	1.34	0.86
1:A:76:GLU:CG	1:A:145:ASN:CA[2_664]	1.35	0.85
1:A:65:VAL:N	1:A:156:LYS:CE[2_664]	1.36	0.84
1:A:12:ALA:C	1:A:49:LEU:CD1[4_555]	1.37	0.83
1:A:19:ILE:CA	1:A:79:LEU:CD1[4_555]	1.38	0.82
1:A:68:ASP:OD2	1:A:151:PHE:O[2_664]	1.38	0.82
1:A:86:MET:CB	1:A:86:MET:CB[4_555]	1.38	0.82
1:A:11:ARG:CA	1:A:22:PHE:CB[4_555]	1.39	0.81
1:A:16:GLU:OE1	1:A:75:PHE:CD2[4_555]	1.39	0.81
1:A:102:PHE:CD1	3:A:195:HOH:O[3_565]	1.40	0.80
1:A:11:ARG:NE	1:A:20:ALA:N[4_555]	1.41	0.79
1:A:99:GLU:OE2	1:A:99:GLU:OE2[4_555]	1.41	0.79
1:A:76:GLU:N	1:A:144:ASN:CA[2_664]	1.42	0.78
1:A:11:ARG:CG	1:A:19:ILE:C[4_555]	1.43	0.77
1:A:16:GLU:C	1:A:144:ASN:O[5_665]	1.43	0.77
1:A:11:ARG:O	1:A:22:PHE:CB[4_555]	1.44	0.76
1:A:68:ASP:OD1	1:A:154:PHE:CA[2_664]	1.44	0.76
1:A:69:GLY:N	1:A:155:LEU:CD2[2_664]	1.44	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:CA	1:A:22:PHE:CA[4_555]	1.45	0.75
3:A:192:HOH:O	3:A:210:HOH:O[3_565]	1.45	0.75
1:A:19:ILE:CB	1:A:79:LEU:CD1[4_555]	1.47	0.73
1:A:75:PHE:C	1:A:144:ASN:CB[2_664]	1.47	0.73
1:A:76:GLU:CA	1:A:144:ASN:C[2_664]	1.47	0.73
1:A:11:ARG:CA	1:A:22:PHE:N[4_555]	1.48	0.72
1:A:13:PHE:CE1	1:A:51:GLN:CG[4_555]	1.48	0.72
1:A:17:GLU:CG	1:A:143:LYS:C[5_665]	1.48	0.72
1:A:65:VAL:N	1:A:156:LYS:NZ[2_664]	1.48	0.72
1:A:89:ASP:CA	1:A:90:ALA:CA[4_555]	1.48	0.72
1:A:11:ARG:CD	1:A:20:ALA:C[4_555]	1.49	0.71
1:A:17:GLU:CB	1:A:143:LYS:C[5_665]	1.49	0.71
1:A:68:ASP:CA	1:A:155:LEU:CA[2_664]	1.49	0.71
1:A:74:ASP:OD2	1:A:153:GLU:OE1[2_664]	1.49	0.71
1:A:92:GLY:N	1:A:92:GLY:C[4_555]	1.50	0.70
1:A:17:GLU:N	1:A:76:GLU:N[4_555]	1.51	0.69
1:A:68:ASP:CG	1:A:155:LEU:N[2_664]	1.51	0.69
1:A:103:ARG:NH1	3:A:300:HOH:O[4_555]	1.51	0.69
1:A:17:GLU:N	1:A:144:ASN:C[5_665]	1.52	0.68
1:A:76:GLU:CB	1:A:144:ASN:CA[2_664]	1.52	0.68
1:A:16:GLU:CB	1:A:75:PHE:CB[4_555]	1.53	0.67
1:A:4:THR:CA	3:A:253:HOH:O[2_664]	1.54	0.66
1:A:10:ALA:O	1:A:22:PHE:CE2[4_555]	1.54	0.66
1:A:15:SER:CB	1:A:78:PHE:N[4_555]	1.54	0.66
1:A:72:THR:O	1:A:152:ASP:CG[2_664]	1.54	0.66
1:A:16:GLU:OE1	1:A:75:PHE:CE2[4_555]	1.55	0.65
1:A:76:GLU:CD	1:A:145:ASN:CB[2_664]	1.55	0.65
1:A:89:ASP:C	1:A:90:ALA:C[4_555]	1.55	0.65
1:A:89:ASP:O	1:A:90:ALA:C[4_555]	1.55	0.65
1:A:4:THR:N	3:A:253:HOH:O[2_664]	1.56	0.64
1:A:69:GLY:C	1:A:151:PHE:CZ[2_664]	1.56	0.64
1:A:74:ASP:C	1:A:144:ASN:ND2[2_664]	1.56	0.64
1:A:76:GLU:CG	1:A:144:ASN:O[2_664]	1.56	0.64
1:A:9:GLU:C	1:A:21:GLU:OE2[4_555]	1.57	0.63
1:A:17:GLU:N	1:A:144:ASN:CA[5_665]	1.57	0.63
1:A:83:VAL:CG1	3:A:259:HOH:O[4_555]	1.57	0.63
1:A:152:ASP:C	3:A:220:HOH:O[3_565]	1.57	0.63
1:A:11:ARG:N	1:A:22:PHE:N[4_555]	1.58	0.62
1:A:17:GLU:CB	1:A:76:GLU:CB[4_555]	1.58	0.62
1:A:17:GLU:N	1:A:144:ASN:O[5_665]	1.58	0.62
1:A:88:GLU:C	1:A:90:ALA:CA[4_555]	1.58	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:O	1:A:21:GLU:C[4_555]	1.59	0.61
1:A:11:ARG:CG	1:A:20:ALA:N[4_555]	1.59	0.61
1:A:11:ARG:CB	1:A:22:PHE:N[4_555]	1.59	0.61
1:A:14:LEU:C	1:A:78:PHE:CD2[4_555]	1.60	0.60
1:A:16:GLU:N	1:A:75:PHE:C[4_555]	1.60	0.60
1:A:48:MET:CE	1:A:135:GLU:OE2[3_664]	1.60	0.60
1:A:70:SER:CB	1:A:151:PHE:C[2_664]	1.60	0.60
1:A:70:SER:CA	1:A:151:PHE:CB[2_664]	1.60	0.60
1:A:150:ASP:O	3:A:247:HOH:O[3_565]	1.60	0.60
1:A:11:ARG:CG	1:A:19:ILE:O[4_555]	1.61	0.59
1:A:17:GLU:OE1	1:A:77:GLU:N[4_555]	1.61	0.59
1:A:70:SER:CB	1:A:151:PHE:CG[2_664]	1.61	0.59
1:A:70:SER:N	1:A:151:PHE:CD2[2_664]	1.61	0.59
1:A:73:ILE:CA	3:A:204:HOH:O[2_664]	1.61	0.59
1:A:89:ASP:C	1:A:90:ALA:CA[4_555]	1.61	0.59
1:A:108:ASN:CA	1:A:116:GLU:OE1[5_555]	1.61	0.59
1:A:68:ASP:CA	1:A:155:LEU:CD2[2_664]	1.62	0.58
1:A:92:GLY:CA	1:A:93:LYS:N[4_555]	1.62	0.58
1:A:146:ASP:CA	3:A:276:HOH:O[3_565]	1.63	0.57
1:A:11:ARG:C	1:A:22:PHE:C[4_555]	1.64	0.56
1:A:146:ASP:CG	3:A:276:HOH:O[3_565]	1.64	0.56
1:A:76:GLU:C	1:A:144:ASN:CA[2_664]	1.65	0.55
1:A:8:ALA:C	1:A:21:GLU:CG[4_555]	1.66	0.54
1:A:89:ASP:CA	1:A:90:ALA:C[4_555]	1.66	0.54
1:A:18:MET:CB	1:A:79:LEU:C[4_555]	1.67	0.53
1:A:70:SER:OG	1:A:151:PHE:C[2_664]	1.67	0.53
1:A:10:ALA:O	1:A:22:PHE:CD1[4_555]	1.68	0.52
1:A:12:ALA:CB	1:A:25:ALA:CB[4_555]	1.68	0.52
1:A:68:ASP:CB	1:A:155:LEU:N[2_664]	1.68	0.52
1:A:69:GLY:CA	1:A:155:LEU:CD1[2_664]	1.68	0.52
1:A:74:ASP:OD1	1:A:153:GLU:OE2[2_664]	1.68	0.52
1:A:76:GLU:OE1	1:A:145:ASN:CB[2_664]	1.68	0.52
1:A:91:LYS:CD	1:A:93:LYS:CG[4_555]	1.68	0.52
1:A:18:MET:CB	1:A:80:VAL:N[4_555]	1.69	0.51
1:A:39:THR:CG2	1:A:152:ASP:OD2[2_664]	1.69	0.51
1:A:68:ASP:OD1	1:A:154:PHE:C[2_664]	1.69	0.51
1:A:74:ASP:CB	3:A:167:HOH:O[2_664]	1.69	0.51
1:A:89:ASP:C	1:A:90:ALA:N[4_555]	1.69	0.51
1:A:17:GLU:OE1	1:A:77:GLU:CG[4_555]	1.70	0.50
1:A:91:LYS:O	1:A:92:GLY:CA[4_555]	1.70	0.50
1:A:10:ALA:N	1:A:21:GLU:CD[4_555]	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PHE:N	1:A:144:ASN:CG[2_664]	1.71	0.49
1:A:17:GLU:CB	1:A:144:ASN:N[5_665]	1.72	0.48
1:A:17:GLU:CD	1:A:76:GLU:C[4_555]	1.72	0.48
1:A:65:VAL:CA	1:A:156:LYS:CE[2_664]	1.72	0.48
1:A:68:ASP:CB	1:A:155:LEU:CA[2_664]	1.72	0.48
1:A:68:ASP:CA	1:A:155:LEU:CB[2_664]	1.72	0.48
1:A:17:GLU:CB	1:A:76:GLU:C[4_555]	1.73	0.47
1:A:17:GLU:CA	1:A:144:ASN:C[5_665]	1.73	0.47
1:A:70:SER:CA	1:A:151:PHE:CD1[2_664]	1.73	0.47
1:A:88:GLU:O	1:A:90:ALA:O[4_555]	1.73	0.47
1:A:89:ASP:O	1:A:91:LYS:CA[4_555]	1.73	0.47
1:A:11:ARG:CD	1:A:20:ALA:N[4_555]	1.74	0.46
1:A:12:ALA:N	1:A:22:PHE:C[4_555]	1.74	0.46
1:A:13:PHE:CZ	1:A:51:GLN:OE1[4_555]	1.74	0.46
1:A:15:SER:CB	1:A:78:PHE:CB[4_555]	1.74	0.46
1:A:91:LYS:C	1:A:93:LYS:N[4_555]	1.74	0.46
1:A:17:GLU:O	1:A:145:ASN:ND2[5_665]	1.75	0.45
1:A:74:ASP:OD1	1:A:144:ASN:OD1[2_664]	1.75	0.45
1:A:75:PHE:CA	1:A:144:ASN:ND2[2_664]	1.75	0.45
1:A:89:ASP:CB	1:A:90:ALA:CB[4_555]	1.75	0.45
3:A:186:HOH:O	3:A:202:HOH:O[2_664]	1.76	0.44
1:A:11:ARG:NH1	1:A:16:GLU:OE2[4_555]	1.77	0.43
1:A:17:GLU:CG	1:A:76:GLU:O[4_555]	1.77	0.43
1:A:17:GLU:OE2	1:A:144:ASN:CA[5_665]	1.78	0.42
1:A:19:ILE:CD1	1:A:75:PHE:CZ[4_555]	1.78	0.42
1:A:34:GLY:C	1:A:112:PHE:CZ[2_664]	1.78	0.42
1:A:70:SER:N	1:A:151:PHE:CG[2_664]	1.78	0.42
1:A:108:ASN:CG	1:A:116:GLU:OE1[5_555]	1.78	0.42
1:A:7:GLN:CB	3:A:261:HOH:O[2_664]	1.79	0.41
1:A:69:GLY:O	1:A:99:GLU:OE1[6_664]	1.79	0.41
1:A:70:SER:C	1:A:151:PHE:CG[2_664]	1.79	0.41
1:A:92:GLY:CA	1:A:92:GLY:CA[4_555]	1.79	0.41
1:A:7:GLN:O	1:A:21:GLU:CA[4_555]	1.80	0.40
1:A:67:GLU:C	1:A:155:LEU:CB[2_664]	1.80	0.40
1:A:72:THR:C	1:A:152:ASP:CB[2_664]	1.80	0.40
1:A:110:ASP:OD2	3:A:186:HOH:O[3_565]	1.80	0.40
1:A:151:PHE:C	3:A:190:HOH:O[3_565]	1.80	0.40
1:A:10:ALA:C	1:A:22:PHE:CG[4_555]	1.81	0.39
1:A:68:ASP:CA	1:A:155:LEU:CG[2_664]	1.81	0.39
1:A:83:VAL:CA	1:A:86:MET:CE[4_555]	1.81	0.39
1:A:76:GLU:CD	1:A:145:ASN:CA[2_664]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:CB	1:A:116:GLU:OE2[5_555]	1.82	0.38
1:A:15:SER:CB	1:A:79:LEU:N[4_555]	1.83	0.37
1:A:16:GLU:CD	1:A:75:PHE:CD2[4_555]	1.83	0.37
1:A:17:GLU:CB	1:A:144:ASN:CA[5_665]	1.83	0.37
1:A:17:GLU:OE2	1:A:76:GLU:C[4_555]	1.83	0.37
1:A:76:GLU:OE2	1:A:145:ASN:O[2_664]	1.83	0.37
1:A:12:ALA:CA	1:A:22:PHE:O[4_555]	1.84	0.36
1:A:17:GLU:CB	1:A:76:GLU:CA[4_555]	1.84	0.36
1:A:152:ASP:C	3:A:190:HOH:O[3_565]	1.84	0.36
1:A:11:ARG:CB	1:A:19:ILE:O[4_555]	1.85	0.35
1:A:11:ARG:CG	1:A:20:ALA:C[4_555]	1.85	0.35
1:A:18:MET:N	1:A:76:GLU:O[4_555]	1.85	0.35
1:A:19:ILE:CG2	1:A:19:ILE:CG2[4_555]	1.85	0.35
1:A:68:ASP:N	1:A:155:LEU:C[2_664]	1.85	0.35
1:A:74:ASP:C	1:A:144:ASN:CG[2_664]	1.85	0.35
1:A:76:GLU:N	1:A:144:ASN:C[2_664]	1.85	0.35
1:A:14:LEU:C	1:A:78:PHE:CE2[4_555]	1.86	0.34
1:A:14:LEU:CD1	1:A:14:LEU:CD1[4_555]	1.86	0.34
1:A:19:ILE:CG1	1:A:79:LEU:CD2[4_555]	1.87	0.33
1:A:92:GLY:C	1:A:92:GLY:C[4_555]	1.87	0.33
1:A:103:ARG:CZ	3:A:300:HOH:O[4_555]	1.87	0.33
1:A:68:ASP:CG	1:A:154:PHE:C[2_664]	1.88	0.32
1:A:76:GLU:N	1:A:144:ASN:CG[2_664]	1.88	0.32
1:A:89:ASP:CA	1:A:91:LYS:N[4_555]	1.88	0.32
1:A:8:ALA:N	1:A:21:GLU:CB[4_555]	1.89	0.31
1:A:17:GLU:N	1:A:76:GLU:CB[4_555]	1.89	0.31
1:A:65:VAL:O	1:A:152:ASP:O[2_664]	1.89	0.31
1:A:76:GLU:CD	1:A:144:ASN:O[2_664]	1.89	0.31
1:A:10:ALA:C	1:A:22:PHE:CE2[4_555]	1.90	0.30
1:A:13:PHE:CA	1:A:49:LEU:CD1[4_555]	1.90	0.30
1:A:15:SER:N	1:A:79:LEU:N[4_555]	1.90	0.30
1:A:28:MET:CE	1:A:139:LYS:NZ[3_664]	1.90	0.30
1:A:70:SER:OG	1:A:151:PHE:O[2_664]	1.90	0.30
1:A:70:SER:N	1:A:151:PHE:CE2[2_664]	1.90	0.30
1:A:86:MET:C	1:A:86:MET:O[4_555]	1.90	0.30
1:A:92:GLY:N	1:A:92:GLY:CA[4_555]	1.90	0.30
1:A:69:GLY:O	1:A:151:PHE:CD2[2_664]	1.91	0.29
1:A:11:ARG:NE	1:A:20:ALA:CB[4_555]	1.92	0.28
1:A:11:ARG:CG	1:A:21:GLU:N[4_555]	1.92	0.28
1:A:12:ALA:O	1:A:49:LEU:CD1[4_555]	1.92	0.28
1:A:15:SER:O	1:A:79:LEU:CB[4_555]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLU:CA	1:A:144:ASN:CA[5_665]	1.92	0.28
1:A:68:ASP:OD1	1:A:154:PHE:CG[2_664]	1.92	0.28
1:A:16:GLU:CB	1:A:75:PHE:CG[4_555]	1.93	0.27
1:A:34:GLY:C	1:A:112:PHE:CE1[2_664]	1.93	0.27
1:A:76:GLU:C	1:A:143:LYS:O[2_664]	1.93	0.27
1:A:76:GLU:CA	1:A:144:ASN:CB[2_664]	1.93	0.27
1:A:11:ARG:CG	1:A:20:ALA:CA[4_555]	1.94	0.26
1:A:15:SER:OG	1:A:78:PHE:CA[4_555]	1.94	0.26
1:A:16:GLU:CA	1:A:75:PHE:CD2[4_555]	1.94	0.26
1:A:22:PHE:CZ	1:A:83:VAL:CG2[4_555]	1.94	0.26
1:A:74:ASP:CG	1:A:153:GLU:CD[2_664]	1.94	0.26
1:A:8:ALA:CA	1:A:21:GLU:CA[4_555]	1.95	0.25
1:A:9:GLU:O	1:A:49:LEU:CD2[4_555]	1.95	0.25
1:A:15:SER:N	1:A:78:PHE:C[4_555]	1.95	0.25
1:A:19:ILE:CG1	1:A:79:LEU:CD1[4_555]	1.95	0.25
1:A:19:ILE:N	1:A:79:LEU:CG[4_555]	1.95	0.25
1:A:76:GLU:N	1:A:144:ASN:O[2_664]	1.95	0.25
1:A:88:GLU:O	1:A:90:ALA:CA[4_555]	1.95	0.25
1:A:7:GLN:NE2	1:A:142:ASP:O[2_664]	1.96	0.24
1:A:10:ALA:CB	1:A:18:MET:CG[4_555]	1.96	0.24
1:A:17:GLU:CG	1:A:77:GLU:CA[4_555]	1.96	0.24
1:A:71:GLY:N	1:A:151:PHE:CD2[2_664]	1.96	0.24
1:A:102:PHE:CB	3:A:195:HOH:O[3_565]	1.96	0.24
1:A:8:ALA:C	1:A:21:GLU:O[4_555]	1.97	0.23
1:A:15:SER:CA	1:A:79:LEU:N[4_555]	1.97	0.23
1:A:16:GLU:O	1:A:144:ASN:O[5_665]	1.97	0.23
1:A:76:GLU:CB	1:A:144:ASN:N[2_664]	1.97	0.23
1:A:153:GLU:CA	3:A:220:HOH:O[3_565]	1.97	0.23
1:A:7:GLN:OE1	1:A:143:LYS:N[2_664]	1.98	0.22
1:A:10:ALA:CA	1:A:22:PHE:CE2[4_555]	1.98	0.22
1:A:15:SER:OG	1:A:78:PHE:N[4_555]	1.98	0.22
1:A:16:GLU:CA	1:A:75:PHE:CG[4_555]	1.98	0.22
1:A:76:GLU:CG	1:A:145:ASN:C[2_664]	1.98	0.22
1:A:11:ARG:N	1:A:18:MET:O[4_555]	1.99	0.21
1:A:69:GLY:C	1:A:151:PHE:CD2[2_664]	1.99	0.21
1:A:7:GLN:CA	3:A:261:HOH:O[2_664]	2.00	0.20
1:A:35:GLY:O	3:A:310:HOH:O[2_664]	2.00	0.20
1:A:92:GLY:CA	1:A:92:GLY:O[4_555]	2.00	0.20
1:A:103:ARG:CD	3:A:300:HOH:O[4_555]	2.00	0.20
1:A:12:ALA:N	1:A:22:PHE:O[4_555]	2.01	0.19
1:A:15:SER:CA	1:A:78:PHE:C[4_555]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:SER:O	1:A:79:LEU:CD2[4_555]	2.01	0.19
1:A:66:ASP:N	1:A:156:LYS:NZ[2_664]	2.01	0.19
1:A:77:GLU:N	1:A:143:LYS:O[2_664]	2.01	0.19
1:A:12:ALA:N	1:A:22:PHE:CB[4_555]	2.02	0.18
1:A:15:SER:CA	1:A:78:PHE:CB[4_555]	2.02	0.18
1:A:16:GLU:CB	1:A:75:PHE:CD2[4_555]	2.02	0.18
1:A:25:ALA:N	3:A:301:HOH:O[4_555]	2.02	0.18
1:A:88:GLU:O	1:A:90:ALA:C[4_555]	2.02	0.18
1:A:68:ASP:CB	1:A:154:PHE:C[2_664]	2.03	0.17
1:A:70:SER:O	1:A:151:PHE:CD2[2_664]	2.03	0.17
1:A:99:GLU:OE1	1:A:151:PHE:CE2[4_555]	2.03	0.17
1:A:17:GLU:OE2	1:A:144:ASN:N[5_665]	2.04	0.16
1:A:67:GLU:C	1:A:155:LEU:C[2_664]	2.04	0.16
1:A:77:GLU:N	1:A:143:LYS:C[2_664]	2.04	0.16
1:A:77:GLU:N	1:A:144:ASN:N[2_664]	2.04	0.16
3:A:258:HOH:O	3:A:310:HOH:O[2_664]	2.04	0.16
1:A:76:GLU:CA	1:A:144:ASN:O[2_664]	2.05	0.15
1:A:6:GLN:O	1:A:21:GLU:OE2[4_555]	2.06	0.14
1:A:10:ALA:O	1:A:22:PHE:CZ[4_555]	2.06	0.14
1:A:13:PHE:CB	1:A:82:MET:CE[4_555]	2.06	0.14
1:A:17:GLU:CD	1:A:143:LYS:C[5_665]	2.06	0.14
1:A:72:THR:O	1:A:152:ASP:CA[2_664]	2.06	0.14
1:A:92:GLY:O	1:A:92:GLY:O[4_555]	2.06	0.14
1:A:102:PHE:CD2	3:A:195:HOH:O[3_565]	2.06	0.14
1:A:103:ARG:NE	3:A:300:HOH:O[4_555]	2.06	0.14
1:A:13:PHE:C	1:A:82:MET:CG[4_555]	2.07	0.13
1:A:16:GLU:CA	1:A:75:PHE:C[4_555]	2.07	0.13
1:A:18:MET:SD	1:A:79:LEU:C[4_555]	2.07	0.13
1:A:151:PHE:O	3:A:190:HOH:O[3_565]	2.07	0.13
1:A:10:ALA:CA	1:A:22:PHE:CD2[4_555]	2.08	0.12
1:A:11:ARG:CD	1:A:19:ILE:O[4_555]	2.08	0.12
1:A:11:ARG:N	1:A:22:PHE:CD2[4_555]	2.08	0.12
1:A:14:LEU:CG	1:A:22:PHE:CE1[4_555]	2.08	0.12
1:A:15:SER:CA	1:A:75:PHE:O[4_555]	2.08	0.12
1:A:15:SER:N	1:A:78:PHE:CD2[4_555]	2.08	0.12
1:A:70:SER:OG	1:A:151:PHE:CB[2_664]	2.08	0.12
1:A:74:ASP:CG	1:A:144:ASN:OD1[2_664]	2.08	0.12
1:A:92:GLY:N	1:A:92:GLY:N[4_555]	2.08	0.12
1:A:7:GLN:N	1:A:21:GLU:OE1[4_555]	2.09	0.11
1:A:8:ALA:N	1:A:21:GLU:CG[4_555]	2.09	0.11
1:A:11:ARG:CD	1:A:20:ALA:O[4_555]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:OE2	1:A:145:ASN:C[2_664]	2.09	0.11
1:A:13:PHE:C	1:A:82:MET:SD[4_555]	2.10	0.10
1:A:15:SER:O	1:A:79:LEU:N[4_555]	2.10	0.10
1:A:17:GLU:CD	1:A:144:ASN:N[5_665]	2.10	0.10
1:A:17:GLU:N	1:A:76:GLU:C[4_555]	2.10	0.10
1:A:34:GLY:O	1:A:148:ARG:CZ[2_664]	2.10	0.10
1:A:68:ASP:OD1	1:A:155:LEU:N[2_664]	2.10	0.10
1:A:72:THR:CG2	1:A:151:PHE:N[2_664]	2.10	0.10
1:A:90:ALA:N	1:A:90:ALA:CA[4_555]	2.10	0.10
1:A:4:THR:CB	3:A:253:HOH:O[2_664]	2.11	0.09
1:A:7:GLN:C	1:A:21:GLU:CG[4_555]	2.11	0.09
1:A:11:ARG:O	1:A:22:PHE:C[4_555]	2.11	0.09
1:A:16:GLU:C	1:A:76:GLU:CA[4_555]	2.11	0.09
1:A:17:GLU:CG	1:A:144:ASN:N[5_665]	2.11	0.09
1:A:65:VAL:CB	1:A:156:LYS:NZ[2_664]	2.11	0.09
1:A:67:GLU:O	1:A:159:GLU:CG[2_664]	2.11	0.09
1:A:70:SER:C	1:A:151:PHE:CB[2_664]	2.11	0.09
1:A:11:ARG:O	1:A:22:PHE:CA[4_555]	2.12	0.08
1:A:16:GLU:O	1:A:76:GLU:OE1[4_555]	2.12	0.08
1:A:25:ALA:CB	3:A:301:HOH:O[4_555]	2.12	0.08
1:A:29:PHE:CZ	1:A:135:GLU:OE1[3_664]	2.12	0.08
1:A:65:VAL:O	1:A:156:LYS:NZ[2_664]	2.12	0.08
1:A:68:ASP:N	1:A:155:LEU:CG[2_664]	2.12	0.08
1:A:74:ASP:N	1:A:150:ASP:OD2[2_664]	2.12	0.08
1:A:77:GLU:N	1:A:144:ASN:CA[2_664]	2.12	0.08
1:A:3:MET:CG	1:A:143:LYS:CE[2_664]	2.13	0.07
1:A:10:ALA:O	1:A:22:PHE:CE1[4_555]	2.13	0.07
1:A:11:ARG:CD	1:A:19:ILE:C[4_555]	2.13	0.07
1:A:17:GLU:CA	1:A:76:GLU:C[4_555]	2.13	0.07
1:A:10:ALA:N	1:A:21:GLU:CG[4_555]	2.14	0.06
1:A:16:GLU:C	1:A:76:GLU:N[4_555]	2.14	0.06
1:A:18:MET:CB	1:A:79:LEU:CB[4_555]	2.14	0.06
1:A:20:ALA:CB	1:A:76:GLU:OE1[4_555]	2.14	0.06
1:A:34:GLY:CA	1:A:112:PHE:CD1[2_664]	2.14	0.06
1:A:67:GLU:C	1:A:155:LEU:CA[2_664]	2.14	0.06
1:A:73:ILE:C	1:A:150:ASP:OD2[2_664]	2.14	0.06
1:A:74:ASP:OD1	1:A:144:ASN:CG[2_664]	2.14	0.06
1:A:76:GLU:CB	1:A:144:ASN:O[2_664]	2.14	0.06
1:A:9:GLU:CG	1:A:132:GLU:OE1[6_665]	2.15	0.05
1:A:11:ARG:N	1:A:22:PHE:CA[4_555]	2.15	0.05
1:A:16:GLU:N	1:A:75:PHE:CG[4_555]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:MET:CB	1:A:79:LEU:CA[4_555]	2.15	0.05
1:A:11:ARG:CB	1:A:23:LYS:N[4_555]	2.16	0.04
1:A:14:LEU:CG	1:A:22:PHE:CD1[4_555]	2.16	0.04
1:A:68:ASP:OD2	1:A:155:LEU:N[2_664]	2.16	0.04
1:A:103:ARG:CG	3:A:300:HOH:O[4_555]	2.16	0.04
1:A:110:ASP:OD2	3:A:227:HOH:O[3_565]	2.16	0.04
1:A:8:ALA:C	1:A:21:GLU:C[4_555]	2.17	0.03
1:A:70:SER:N	1:A:151:PHE:CD1[2_664]	2.17	0.03
1:A:88:GLU:C	1:A:90:ALA:CB[4_555]	2.17	0.03
1:A:6:GLN:C	1:A:21:GLU:CD[4_555]	2.18	0.02
1:A:7:GLN:OE1	1:A:143:LYS:C[2_664]	2.18	0.02
1:A:9:GLU:CA	1:A:21:GLU:OE2[4_555]	2.18	0.02
1:A:13:PHE:CE2	1:A:82:MET:CE[4_555]	2.18	0.02
1:A:17:GLU:CD	1:A:143:LYS:O[5_665]	2.18	0.02
1:A:76:GLU:OE2	1:A:145:ASN:CB[2_664]	2.18	0.02
1:A:76:GLU:CD	1:A:145:ASN:N[2_664]	2.18	0.02
1:A:7:GLN:O	1:A:21:GLU:CG[4_555]	2.19	0.01
1:A:9:GLU:N	1:A:21:GLU:CD[4_555]	2.19	0.01
1:A:16:GLU:O	1:A:76:GLU:CD[4_555]	2.19	0.01
1:A:16:GLU:N	1:A:75:PHE:CA[4_555]	2.19	0.01
1:A:17:GLU:OE1	1:A:77:GLU:C[4_555]	2.19	0.01
1:A:34:GLY:CA	1:A:112:PHE:CZ[2_664]	2.19	0.01

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	160/162 (99%)	158 (99%)	1 (1%)	1 (1%)	21 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	ASP

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	136/137 (99%)	114 (84%)	22 (16%)	2 1

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	23	LYS
1	A	32	ASP
1	A	38	SER
1	A	40	LYS
1	A	55	LYS
1	A	57	GLU
1	A	58	LEU
1	A	63	GLU
1	A	72	THR
1	A	77	GLU
1	A	91	LYS
1	A	95	GLU
1	A	103	ARG
1	A	115	ILE
1	A	116	GLU
1	A	120	GLU
1	A	148	ARG
1	A	152	ASP
1	A	156	LYS
1	A	159	GLU
1	A	161	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	GLN
1	A	51	GLN

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](#)

Of 2 ligands modelled in this entry, 2 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.