



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:08 PM UTC

PDB ID : 7F4L / pdb_00007f4l
Title : Crystal structure of MTA1-p1-p2 complex
Authors : Chen, J.; Liu, L.
Deposited on : 2021-06-21
Resolution : 2.72 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:

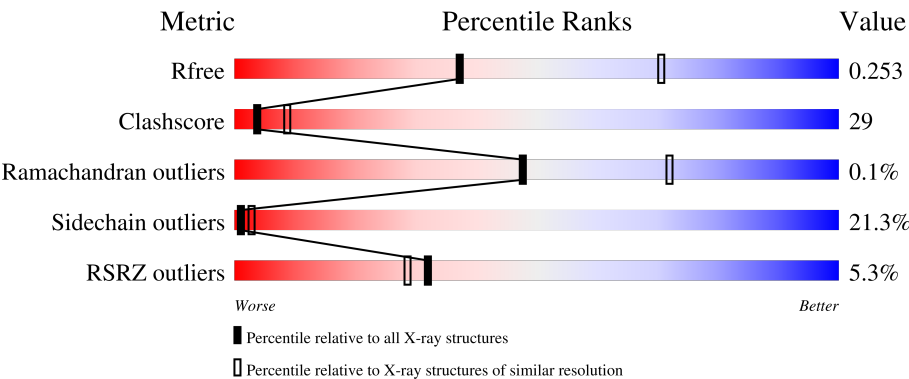
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	142	4% 42%38%10%9%
1	B	142	2% 46%35%10%8%
2	C	247	5% 41%33%12%13%
2	D	247	7% 37%34%15%13%
3	E	309	8% 88%

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Mol	Chain	Length	Quality of chain
3	F	309	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6142 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 Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	130	Total	C	N	O	S	Se	0	0	0
			1055	669	177	205	2	2			
1	A	129	Total	C	N	O	S	Se	0	0	0
			1053	667	177	205	2	2			

- Molecule 2 is a protein called MT-a70 family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	215	Total	C	N	O	S	Se	0	0	0
			1721	1094	298	319	3	7			
2	D	216	Total	C	N	O	S	Se	0	0	0
			1739	1108	299	322	3	7			

- Molecule 3 is a protein called p1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	37	Total	C	N	O	Se	0	0	0
			308	196	51	60	1			
3	F	25	Total	C	N	O		0	0	0
			208	134	37	37				

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	13	Total	O	0	0
			13	13		
4	C	11	Total	O	0	0
			11	11		
4	D	14	Total	O	0	0
			14	14		
4	E	3	Total	O	0	0
			3	3		

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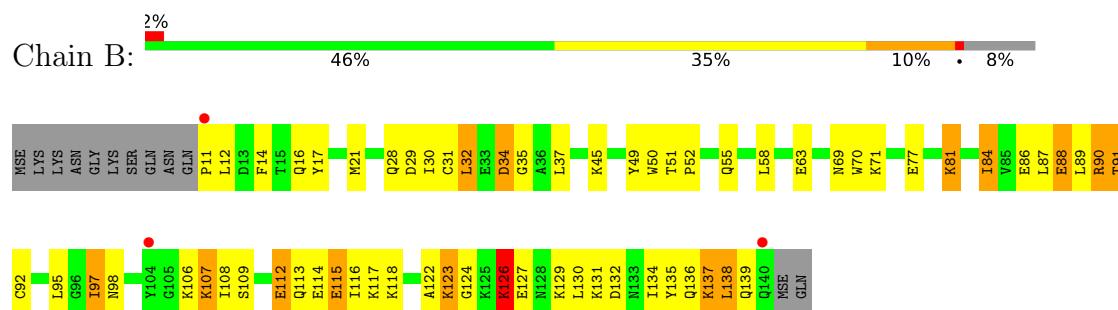
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	3	Total	O	0	0
			3	3		
4	A	14	Total	O	0	0
			14	14		

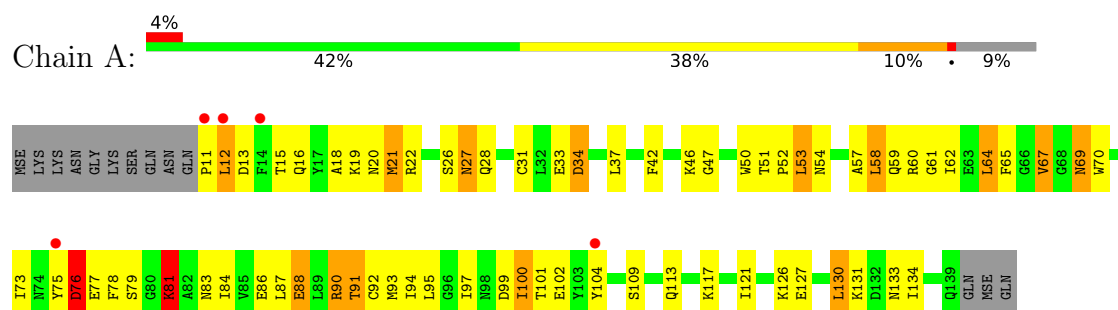
3 Residue-property plots [i](#)

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.

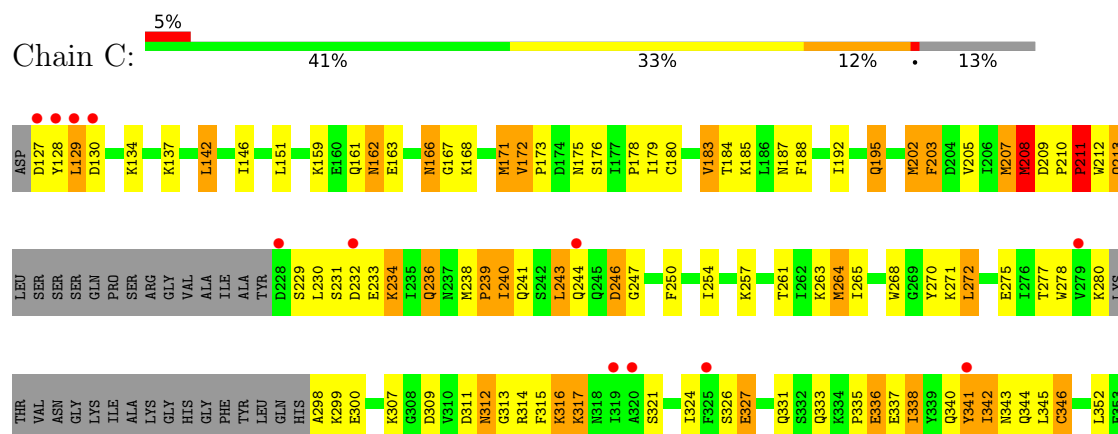
- Molecule 1: Transmembrane protein, putative

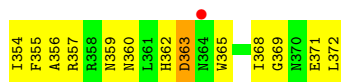


- Molecule 1: Transmembrane protein, putative

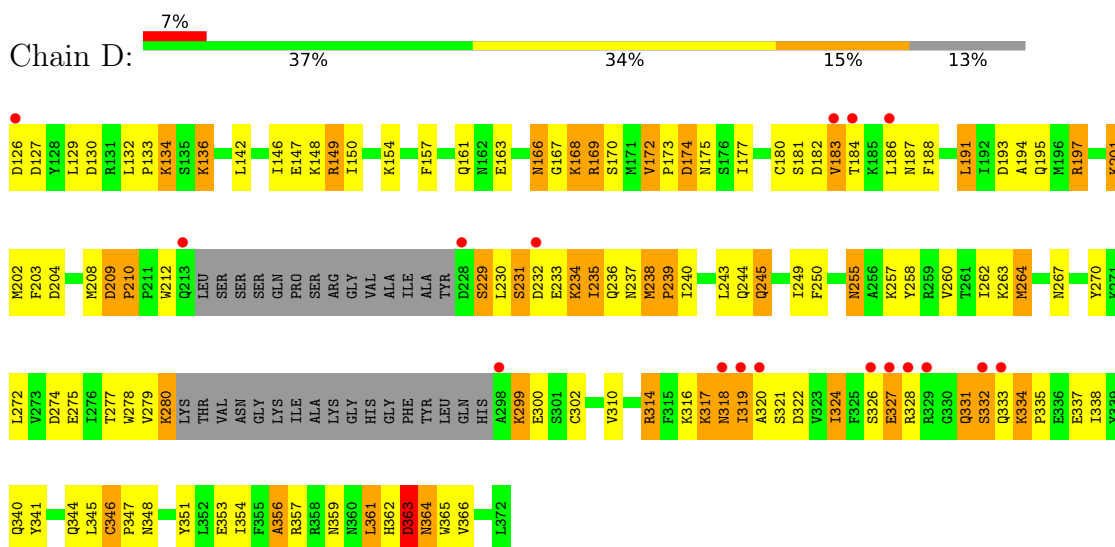


- Molecule 2: MT-a70 family protein

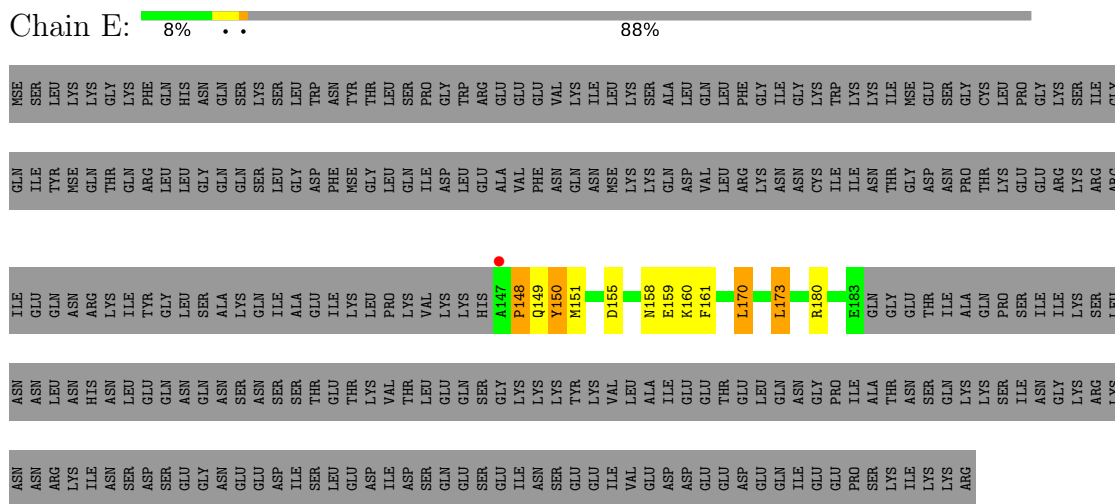




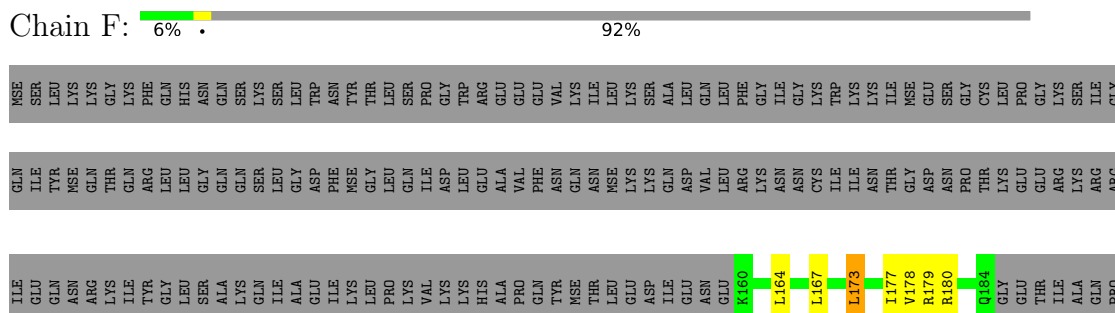
- Molecule 2: MT-a70 family protein



- Molecule 3: p1 protein



- Molecule 3: p1 protein



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.77Å 86.49Å 160.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.72 48.00 – 2.72	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.00-2.72) 98.1 (48.00-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.50 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.240 , 0.254 0.237 , 0.253	Depositor DCC
R_{free} test set	1554 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.032 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6142	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

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	1.19	4/1067 (0.4%)	1.20	11/1426 (0.8%)
1	B	0.95	0/1069	1.01	5/1429 (0.3%)
2	C	1.08	5/1747 (0.3%)	1.18	17/2343 (0.7%)
2	D	1.17	8/1766 (0.5%)	1.32	30/2368 (1.3%)
3	E	1.07	0/310	1.08	3/416 (0.7%)
3	F	0.85	0/210	0.72	0/283
All	All	1.10	17/6169 (0.3%)	1.18	66/8265 (0.8%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	209	ASP	C-N	8.14	1.40	1.33
2	D	238	MSE	CA-C	-5.99	1.47	1.53
2	C	209	ASP	C-N	5.86	1.40	1.33
2	C	172	VAL	C-N	5.72	1.41	1.33
2	D	132	LEU	C-N	5.57	1.40	1.33
2	D	334	LYS	C-N	5.57	1.40	1.33
2	D	172	VAL	C-N	5.57	1.40	1.33
1	A	60	ARG	C-O	-5.48	1.17	1.24
2	D	133	PRO	N-CD	5.43	1.55	1.47
2	C	239	PRO	N-CD	5.30	1.55	1.47
1	A	19	LYS	C-O	-5.25	1.18	1.24
1	A	52	PRO	N-CD	5.24	1.55	1.47
2	D	346	CYS	C-N	5.21	1.40	1.33
2	C	211	PRO	N-CD	5.16	1.54	1.47
2	C	173	PRO	N-CD	5.14	1.54	1.47
2	D	210	PRO	N-CD	5.08	1.54	1.47
1	A	84	ILE	C-O	-5.02	1.17	1.24

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	203	PHE	N-CA-CB	-14.99	87.66	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	150	TYR	N-CA-CB	-11.73	89.78	110.42
2	D	209	ASP	CA-C-N	-9.44	112.77	119.66
2	D	209	ASP	C-N-CA	-9.44	112.77	119.66
1	A	76	ASP	N-CA-C	8.82	120.67	111.14
2	D	321	SER	N-CA-C	8.46	121.37	108.52
2	C	209	ASP	CA-C-N	-8.33	113.66	119.66
2	C	209	ASP	C-N-CA	-8.33	113.66	119.66
2	C	234	LYS	N-CA-C	-8.00	103.66	113.50
2	D	322	ASP	N-CA-C	7.75	119.81	111.36
1	A	97	ILE	N-CA-C	7.65	118.86	110.21
2	C	317	LYS	N-CA-C	7.63	119.59	111.28
1	A	67	VAL	N-CA-C	7.29	118.05	110.62
2	C	208	MSE	N-CA-CB	-7.27	98.59	110.81
1	A	81	LYS	N-CA-C	7.15	119.15	111.36
2	D	243	LEU	N-CA-C	7.05	119.05	111.36
2	D	346	CYS	CA-C-N	-7.02	112.74	119.76
2	D	346	CYS	C-N-CA	-7.02	112.74	119.76
2	D	210	PRO	O-C-N	6.97	124.52	121.31
1	B	123	LYS	N-CA-C	-6.80	103.87	111.28
1	A	11	PRO	N-CA-CB	6.75	110.43	103.00
1	B	11	PRO	N-CA-CB	6.71	110.38	103.00
1	A	130	LEU	N-CA-C	6.71	119.39	108.26
2	D	172	VAL	CA-C-N	-6.64	113.14	119.85
2	D	172	VAL	C-N-CA	-6.64	113.14	119.85
2	D	334	LYS	CA-C-N	-6.53	113.56	120.03
2	D	334	LYS	C-N-CA	-6.53	113.56	120.03
2	D	317	LYS	N-CA-C	6.41	118.35	111.36
2	C	172	VAL	CA-C-N	-6.35	113.43	119.85
2	C	172	VAL	C-N-CA	-6.35	113.43	119.85
3	E	158	ASN	N-CA-C	6.33	119.17	111.82
1	A	64	LEU	N-CA-C	6.32	117.97	111.14
2	C	243	LEU	N-CA-C	6.26	118.11	111.28
2	C	202	MSE	N-CA-C	-6.21	101.78	110.35
2	D	356	ALA	N-CA-C	6.17	118.88	110.55
2	D	364	ASN	N-CA-C	-6.16	103.61	113.28
2	D	132	LEU	CA-C-N	-6.16	113.63	119.85
2	D	132	LEU	C-N-CA	-6.16	113.63	119.85
1	B	126	LYS	N-CA-C	6.13	117.76	111.14
1	A	65	PHE	N-CA-C	6.11	120.90	113.38
2	D	363	ASP	N-CA-CB	6.03	118.86	110.17
2	D	320	ALA	N-CA-C	6.00	117.62	111.14
2	D	235	ILE	CB-CA-C	-5.93	104.13	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	ILE	N-CA-C	5.79	116.56	110.72
1	A	12	LEU	N-CA-C	5.74	117.54	111.28
2	D	210	PRO	CA-C-N	-5.73	112.68	119.84
2	D	210	PRO	C-N-CA	-5.73	112.68	119.84
2	D	231	SER	N-CA-C	-5.70	102.47	110.50
3	E	148	PRO	N-CA-CB	5.70	109.23	103.25
2	D	186	LEU	N-CA-C	5.69	118.08	110.35
1	A	69	ASN	N-CA-C	5.58	118.26	108.56
2	C	162	ASN	N-CA-C	5.52	117.38	111.36
2	D	172	VAL	N-CA-C	5.51	114.35	108.95
2	D	264	MSE	CB-CA-C	-5.43	102.36	110.88
2	C	167	GLY	N-CA-C	5.41	123.49	113.76
2	C	203	PHE	N-CA-C	5.31	117.71	110.55
1	B	34	ASP	N-CA-C	-5.27	104.95	111.33
2	D	204	ASP	N-CA-C	5.27	117.11	111.36
2	C	346	CYS	CA-C-N	-5.24	113.29	119.84
2	C	346	CYS	C-N-CA	-5.24	113.29	119.84
2	D	233	GLU	CA-C-N	-5.24	111.63	120.58
2	D	233	GLU	C-N-CA	-5.24	111.63	120.58
2	C	240	ILE	N-CA-C	5.22	115.99	110.72
2	C	233	GLU	N-CA-C	5.17	116.91	111.28
2	D	239	PRO	CA-N-CD	-5.15	104.79	112.00
1	A	31	CYS	N-CA-C	5.06	116.88	109.24

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	1053	0	1041	54	0
1	B	1055	0	1039	54	0
2	C	1721	0	1681	105	0
2	D	1739	0	1706	140	0
3	E	308	0	305	14	0
3	F	208	0	213	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	0	1	0
4	B	13	0	0	1	0
4	C	11	0	0	2	0
4	D	14	0	0	4	0
4	E	3	0	0	1	0
4	F	3	0	0	0	0
All	All	6142	0	5985	347	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 (347) 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:C:192:ILE:HG23	2:C:202:MSE:CE	1.37	1.51
2:C:213:GLN:HG3	2:C:229:SER:OG	1.30	1.28
1:B:131:LYS:HD2	1:B:136:GLN:OE1	1.25	1.27
2:C:336:GLU:OE2	2:C:362:HIS:CE1	1.95	1.19
1:B:131:LYS:CD	1:B:136:GLN:OE1	1.92	1.17
2:D:188:PHE:CE1	2:D:239:PRO:HD2	1.81	1.16
2:C:213:GLN:CG	2:C:229:SER:OG	1.94	1.15
2:D:244:GLN:OE1	2:D:270:TYR:OH	1.65	1.13
2:C:192:ILE:CG2	2:C:202:MSE:HE1	1.77	1.13
2:D:126:ASP:N	3:E:180:ARG:HH12	1.47	1.13
2:C:159:LYS:NZ	2:C:163:GLU:OE2	1.84	1.10
3:E:151:MSE:HE1	3:E:159:GLU:HG3	1.28	1.09
2:C:236:GLN:HA	2:C:264:MSE:HE3	1.32	1.07
1:B:17:TYR:OH	2:C:195:GLN:NE2	1.87	1.06
2:D:175:ASN:HB2	2:D:363:ASP:CB	1.85	1.06
2:D:201:LYS:NZ	2:D:202:MSE:O	1.88	1.06
2:D:324:ILE:HD11	2:D:335:PRO:HG2	1.38	1.04
2:C:192:ILE:CG2	2:C:202:MSE:CE	2.33	1.04
3:E:151:MSE:HE1	3:E:159:GLU:CG	1.89	1.02
2:D:175:ASN:HB2	2:D:363:ASP:HB3	1.33	1.02
2:D:183:VAL:HG21	2:D:230:LEU:HD11	1.38	1.01
2:C:192:ILE:HG23	2:C:202:MSE:HE1	0.99	0.98
2:C:162:ASN:O	2:C:166:ASN:OD1	1.80	0.97
2:C:213:GLN:HG3	2:C:229:SER:HG	1.25	0.96
2:C:336:GLU:OE2	2:C:362:HIS:HE1	1.36	0.96
2:C:313:GLY:O	2:C:316:LYS:NZ	1.99	0.94
1:B:98:ASN:HD21	1:B:138:LEU:H	1.14	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:PHE:CD1	2:D:239:PRO:HD2	2.03	0.94
2:D:174:ASP:O	1:A:22:ARG:NH2	2.01	0.93
2:D:236:GLN:O	2:D:236:GLN:NE2	2.01	0.93
1:B:112:GLU:OE1	1:B:115:GLU:HG2	1.70	0.92
2:D:327:GLU:OE1	2:D:331:GLN:HG3	1.71	0.90
2:C:192:ILE:HG23	2:C:202:MSE:HE2	1.51	0.90
2:C:129:LEU:HD13	2:C:130:ASP:N	1.87	0.89
2:D:188:PHE:CE1	2:D:239:PRO:CD	2.55	0.88
2:D:212:TRP:CE3	2:D:257:LYS:HE3	2.09	0.88
2:D:175:ASN:CB	2:D:363:ASP:HB3	2.01	0.88
1:A:16:GLN:O	1:A:20:ASN:ND2	2.09	0.86
2:D:346:CYS:O	2:D:351:TYR:OH	1.94	0.84
1:A:77:GLU:OE1	1:A:77:GLU:N	2.11	0.83
2:D:236:GLN:HB2	2:D:264:MSE:HE2	1.60	0.83
1:B:138:LEU:HD22	2:C:151:LEU:HD11	1.59	0.82
2:D:134:LYS:O	2:D:134:LYS:HD3	1.78	0.82
2:D:163:GLU:O	2:D:166:ASN:O	1.98	0.81
2:D:126:ASP:N	3:E:180:ARG:NH1	2.28	0.81
2:D:180:CYS:SG	1:A:46:LYS:NZ	2.53	0.81
2:D:327:GLU:OE1	2:D:331:GLN:CG	2.28	0.81
2:D:357:ARG:HG3	2:D:357:ARG:HH11	1.46	0.81
2:C:207:MSE:HG2	2:C:250:PHE:HB2	1.63	0.80
2:C:246:ASP:OD1	2:C:309:ASP:N	2.15	0.79
2:D:324:ILE:CD1	2:D:335:PRO:HG2	2.11	0.78
2:C:142:LEU:HD13	3:F:177:ILE:HD11	1.64	0.78
2:C:337:GLU:OE1	2:C:337:GLU:N	2.17	0.78
2:D:188:PHE:HE1	2:D:239:PRO:HD2	1.45	0.78
1:A:79:SER:HB2	1:A:81:LYS:HG2	1.65	0.77
2:C:203:PHE:O	2:C:244:GLN:HG3	1.85	0.77
1:A:76:ASP:HB3	1:A:77:GLU:OE1	1.84	0.76
2:C:205:VAL:HG11	2:C:342:ILE:HD13	1.67	0.76
2:D:173:PRO:HG3	2:D:362:HIS:HA	1.68	0.76
2:D:331:GLN:OE1	2:D:332:SER:N	2.20	0.75
2:C:213:GLN:HG2	2:C:229:SER:OG	1.85	0.75
2:D:230:LEU:HB2	2:D:235:ILE:CG1	2.17	0.74
2:D:255:ASN:HA	2:D:258:TYR:CE2	2.22	0.74
1:A:86:GLU:OE2	1:A:90:ARG:NH1	2.22	0.73
2:D:327:GLU:OE2	2:D:328:ARG:N	2.21	0.73
2:D:175:ASN:CB	2:D:363:ASP:CB	2.66	0.72
2:D:353:GLU:HG2	2:D:356:ALA:HB2	1.71	0.72
2:D:232:ASP:OD2	2:D:257:LYS:NZ	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:HE3	1:A:81:LYS:HA	1.70	0.72
1:B:131:LYS:HD3	1:B:136:GLN:OE1	1.89	0.72
2:D:327:GLU:OE2	2:D:327:GLU:N	2.22	0.72
2:D:274:ASP:OD1	2:D:275:GLU:N	2.22	0.71
2:C:213:GLN:CG	2:C:229:SER:HG	1.89	0.71
2:C:236:GLN:HA	2:C:264:MSE:CE	2.14	0.71
2:D:324:ILE:C	2:D:324:ILE:HD12	2.15	0.71
2:C:331:GLN:HE21	2:C:333:GLN:H	1.36	0.71
3:E:151:MSE:CE	3:E:159:GLU:CG	2.69	0.71
2:C:244:GLN:NE2	2:C:247:GLY:HA3	2.04	0.70
2:D:175:ASN:HB2	2:D:363:ASP:HB2	1.71	0.70
2:D:255:ASN:HB3	4:D:410:HOH:O	1.90	0.70
2:D:326:SER:HB3	2:D:327:GLU:HA	1.73	0.70
2:D:314:ARG:HG2	2:D:314:ARG:HH11	1.57	0.69
2:D:314:ARG:HG2	2:D:314:ARG:NH1	2.07	0.69
2:D:326:SER:OG	2:D:337:GLU:OE2	2.10	0.69
1:B:97:ILE:HD11	1:B:137:LYS:HB3	1.74	0.69
2:D:210:PRO:HG2	2:D:212:TRP:CZ2	2.28	0.69
2:C:264:MSE:HE2	2:C:268:TRP:CH2	2.27	0.69
1:B:98:ASN:ND2	1:B:136:GLN:HA	2.09	0.68
2:D:333:GLN:CD	2:D:359:ASN:ND2	2.52	0.67
1:B:21:MSE:HE1	2:C:195:GLN:HG2	1.77	0.67
2:C:188:PHE:HZ	2:C:238:MSE:HE3	1.59	0.66
2:D:262:ILE:HD12	2:D:272:LEU:HD22	1.78	0.66
2:D:230:LEU:HB2	2:D:235:ILE:HG12	1.76	0.66
2:C:327:GLU:OE1	2:C:331:GLN:HG2	1.95	0.66
2:C:129:LEU:HD22	2:C:129:LEU:O	1.96	0.66
2:C:192:ILE:HG23	2:C:202:MSE:HE3	1.67	0.65
2:C:171:MSE:HE3	2:C:171:MSE:HA	1.76	0.65
2:C:175:ASN:HB2	2:C:363:ASP:HB2	1.77	0.65
2:D:236:GLN:HG2	2:D:264:MSE:HG3	1.77	0.65
2:C:277:THR:HG21	2:D:277:THR:HG21	1.78	0.65
1:A:79:SER:HB2	1:A:81:LYS:CG	2.26	0.65
2:D:255:ASN:CB	4:D:410:HOH:O	2.45	0.64
2:C:254:ILE:HG12	2:C:257:LYS:HG2	1.79	0.64
2:C:265:ILE:HD11	2:C:272:LEU:CD2	2.27	0.64
2:D:318:ASN:H	2:D:318:ASN:HD22	1.46	0.64
2:D:326:SER:OG	2:D:337:GLU:CG	2.46	0.64
2:C:244:GLN:HE21	2:C:247:GLY:HA3	1.61	0.64
2:D:146:ILE:HD11	3:E:173:LEU:HD13	1.80	0.64
2:C:127:ASP:CB	2:C:128:TYR:HA	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:340:GLN:O	2:C:343:ASN:HB2	1.98	0.63
1:B:32:LEU:O	1:B:35:GLY:N	2.30	0.63
2:D:210:PRO:HB2	2:D:235:ILE:HD13	1.81	0.62
2:D:177:ILE:HD12	2:D:366:VAL:HG22	1.81	0.62
2:D:232:ASP:O	2:D:236:GLN:HB2	2.00	0.62
1:A:18:ALA:O	1:A:22:ARG:HB2	2.00	0.61
1:A:50:TRP:HA	1:A:54:ASN:HD22	1.64	0.61
1:B:70:TRP:CZ3	1:B:91:THR:HG21	2.37	0.60
2:C:263:LYS:HB3	4:C:401:HOH:O	2.01	0.60
2:D:319:ILE:HG13	2:D:341:TYR:CE2	2.36	0.60
2:D:340:GLN:O	2:D:344:GLN:HG2	2.01	0.60
2:D:314:ARG:HH11	2:D:314:ARG:CG	2.13	0.60
1:B:37:LEU:HD21	2:C:172:VAL:HG12	1.84	0.60
2:D:232:ASP:O	2:D:236:GLN:CB	2.50	0.60
1:B:112:GLU:OE1	1:B:112:GLU:HA	2.01	0.59
2:C:129:LEU:HD13	2:C:130:ASP:CA	2.30	0.59
2:C:240:ILE:HD12	2:C:268:TRP:CH2	2.37	0.59
2:D:238:MSE:HE1	2:D:354:ILE:HG21	1.84	0.59
1:B:98:ASN:ND2	1:B:137:LYS:N	2.51	0.59
2:C:244:GLN:NE2	2:C:247:GLY:CA	2.65	0.59
1:B:98:ASN:HD22	1:B:136:GLN:HA	1.68	0.58
2:D:333:GLN:NE2	2:D:359:ASN:HD21	2.00	0.58
2:C:261:THR:O	2:C:265:ILE:HG23	2.04	0.58
2:D:267:ASN:HB2	4:D:404:HOH:O	2.04	0.58
3:F:177:ILE:O	3:F:180:ARG:N	2.37	0.58
1:B:21:MSE:CE	2:C:195:GLN:HG2	2.34	0.57
1:A:70:TRP:CZ2	1:A:88:GLU:HG3	2.39	0.57
2:D:175:ASN:CA	2:D:363:ASP:HB3	2.33	0.57
2:D:357:ARG:HG3	2:D:357:ARG:NH1	2.13	0.57
1:A:81:LYS:HE3	1:A:81:LYS:CA	2.34	0.57
1:B:97:ILE:HG13	1:B:98:ASN:N	2.20	0.57
1:B:70:TRP:CH2	1:B:91:THR:HG21	2.39	0.57
1:A:92:CYS:O	1:A:95:LEU:O	2.22	0.57
2:D:188:PHE:CD2	2:D:188:PHE:N	2.73	0.56
1:A:27:ASN:OD1	1:A:27:ASN:N	2.36	0.56
2:C:265:ILE:HD11	2:C:272:LEU:HD22	1.86	0.56
1:A:16:GLN:HE21	1:A:20:ASN:HD21	1.53	0.56
1:A:16:GLN:HE21	1:A:20:ASN:ND2	2.03	0.56
2:D:150:ILE:O	2:D:154:LYS:HB2	2.05	0.56
2:C:263:LYS:CB	4:C:401:HOH:O	2.54	0.56
2:D:172:VAL:CG1	1:A:37:LEU:HD21	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:ASP:O	2:D:197:ARG:HG2	2.06	0.56
1:A:76:ASP:HB3	1:A:77:GLU:CD	2.31	0.56
2:D:232:ASP:CG	2:D:257:LYS:HZ1	2.14	0.56
2:C:188:PHE:CE2	2:C:239:PRO:HD2	2.41	0.55
2:C:238:MSE:HE1	2:C:354:ILE:HD13	1.88	0.55
2:D:172:VAL:HG11	1:A:37:LEU:HD21	1.88	0.55
1:A:91:THR:HA	1:A:94:ILE:HB	1.88	0.55
2:D:232:ASP:CG	2:D:257:LYS:NZ	2.64	0.55
2:C:179:ILE:HB	2:C:368:ILE:HG12	1.89	0.55
1:A:69:ASN:O	1:A:73:ILE:HG13	2.07	0.55
2:C:356:ALA:HB3	2:C:372:LEU:HD11	1.89	0.55
2:C:207:MSE:CG	2:C:250:PHE:HB2	2.36	0.55
3:E:151:MSE:HG2	3:E:155:ASP:CB	2.37	0.55
1:B:112:GLU:O	1:B:116:ILE:HG12	2.07	0.55
2:C:341:TYR:C	2:C:341:TYR:CD2	2.85	0.54
1:A:13:ASP:OD1	1:A:16:GLN:HB2	2.07	0.54
1:A:83:ASN:HA	4:A:202:HOH:O	2.06	0.54
2:D:194:ALA:HB1	1:A:21:MSE:HE1	1.89	0.54
1:A:117:LYS:O	1:A:121:ILE:HG13	2.07	0.54
1:B:87:LEU:O	1:B:91:THR:HG23	2.07	0.54
1:B:14:PHE:O	1:B:17:TYR:HB3	2.08	0.54
2:C:280:LYS:HD2	2:C:298:ALA:HB1	1.90	0.54
2:C:146:ILE:HD11	3:F:173:LEU:HD13	1.90	0.54
1:B:52:PRO:HG2	4:B:204:HOH:O	2.08	0.54
2:C:183:VAL:HG21	2:C:355:PHE:CE1	2.42	0.54
1:A:78:PHE:O	1:A:79:SER:HB2	2.07	0.53
1:B:63:GLU:HG2	1:B:108:ILE:O	2.08	0.53
2:C:270:TYR:CE1	2:C:307:LYS:HE3	2.43	0.53
1:B:97:ILE:HG13	1:B:98:ASN:H	1.74	0.53
1:A:33:GLU:HA	1:A:33:GLU:OE2	2.07	0.53
2:D:194:ALA:HA	2:D:197:ARG:HG3	1.90	0.53
2:D:149:ARG:HD3	4:E:402:HOH:O	2.08	0.53
2:D:278:TRP:CD1	2:D:324:ILE:HD11	2.43	0.53
2:D:333:GLN:NE2	2:D:359:ASN:ND2	2.56	0.53
2:D:278:TRP:CE2	2:D:335:PRO:HG3	2.44	0.52
2:C:299:LYS:NZ	2:D:275:GLU:O	2.43	0.52
2:C:324:ILE:HD13	2:C:335:PRO:HG2	1.91	0.52
3:E:151:MSE:HG2	3:E:155:ASP:HB3	1.90	0.52
2:C:175:ASN:HB2	2:C:363:ASP:CB	2.38	0.52
2:D:232:ASP:OD1	2:D:257:LYS:NZ	2.42	0.52
1:A:88:GLU:HG2	1:A:100:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HD11	1:A:91:THR:HB	1.90	0.52
2:D:319:ILE:HG13	2:D:341:TYR:HE2	1.73	0.52
2:C:129:LEU:HD13	2:C:129:LEU:C	2.35	0.52
2:C:211:PRO:O	2:C:211:PRO:HG2	2.09	0.51
2:D:324:ILE:HD12	2:D:324:ILE:O	2.10	0.51
2:C:244:GLN:HE21	2:C:247:GLY:CA	2.22	0.51
1:B:37:LEU:HD21	2:C:172:VAL:CG1	2.39	0.51
2:D:319:ILE:HG13	2:D:341:TYR:OH	2.10	0.51
2:D:194:ALA:CB	1:A:21:MSE:HE1	2.40	0.51
2:D:326:SER:CB	2:D:327:GLU:HA	2.35	0.51
1:A:51:THR:O	1:A:54:ASN:HB2	2.10	0.51
2:D:229:SER:C	2:D:230:LEU:HG	2.35	0.51
2:C:362:HIS:O	2:C:365:TRP:HB2	2.10	0.51
1:B:109:SER:O	1:B:113:GLN:HG3	2.10	0.51
1:B:95:LEU:HA	1:B:117:LYS:HB2	1.93	0.51
2:D:250:PHE:HB3	2:D:302:CYS:SG	2.52	0.50
2:D:279:VAL:HG23	2:D:279:VAL:O	2.11	0.50
2:D:163:GLU:O	2:D:168:LYS:HB3	2.11	0.50
2:D:194:ALA:HA	2:D:197:ARG:HD2	1.92	0.50
2:D:188:PHE:HE1	2:D:239:PRO:CD	2.13	0.50
2:C:212:TRP:CG	2:C:257:LYS:HG3	2.47	0.50
2:C:312:ASN:HB3	2:C:314:ARG:H	1.77	0.50
2:C:341:TYR:C	2:C:341:TYR:HD2	2.20	0.50
1:A:87:LEU:O	1:A:91:THR:HG23	2.12	0.50
2:D:318:ASN:HD22	2:D:318:ASN:N	2.10	0.49
2:D:326:SER:OG	2:D:337:GLU:HG3	2.12	0.49
2:D:318:ASN:N	2:D:318:ASN:ND2	2.60	0.49
2:C:357:ARG:O	2:C:360:ASN:HB2	2.12	0.49
2:C:129:LEU:HD22	2:C:129:LEU:C	2.38	0.49
2:D:244:GLN:OE1	2:D:270:TYR:CZ	2.61	0.49
2:D:347:PRO:O	2:D:348:ASN:HB2	2.13	0.49
1:A:51:THR:H	1:A:54:ASN:HD22	1.61	0.49
2:D:202:MSE:HG3	2:D:245:GLN:NE2	2.28	0.48
2:D:210:PRO:HG2	2:D:212:TRP:CE2	2.48	0.48
2:C:278:TRP:O	2:C:299:LYS:HA	2.13	0.48
2:C:188:PHE:HZ	2:C:238:MSE:CE	2.26	0.48
2:D:236:GLN:CG	2:D:264:MSE:HG3	2.44	0.48
2:D:319:ILE:CG1	2:D:341:TYR:HE2	2.27	0.48
1:B:63:GLU:O	1:B:107:LYS:HG2	2.13	0.48
2:C:312:ASN:CG	2:C:314:ARG:HH21	2.22	0.48
2:D:262:ILE:CD1	2:D:272:LEU:HD22	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLU:OE2	1:B:90:ARG:NH1	2.48	0.47
1:B:122:ALA:O	1:B:123:LYS:C	2.58	0.47
1:A:22:ARG:O	1:A:26:SER:HB2	2.14	0.47
2:C:324:ILE:HD11	2:C:337:GLU:HB2	1.96	0.47
2:C:264:MSE:HE2	2:C:268:TRP:CZ2	2.49	0.47
2:D:188:PHE:N	2:D:188:PHE:HD2	2.11	0.47
2:D:129:LEU:HD11	3:E:150:TYR:CD1	2.49	0.47
1:B:84:ILE:HD12	1:B:84:ILE:HA	1.72	0.47
2:C:205:VAL:HG11	2:C:342:ILE:CD1	2.43	0.47
1:A:75:TYR:C	1:A:75:TYR:CD2	2.89	0.47
1:B:131:LYS:HB2	1:B:136:GLN:OE1	2.15	0.47
2:D:170:SER:OG	1:A:42:PHE:HB2	2.14	0.47
2:D:280:LYS:CE	2:D:300:GLU:HG3	2.46	0.46
1:B:108:ILE:HG22	1:B:109:SER:N	2.31	0.46
2:C:208:MSE:HE1	2:C:268:TRP:HH2	1.81	0.46
2:D:236:GLN:NE2	4:D:404:HOH:O	2.47	0.46
2:D:230:LEU:HB2	2:D:235:ILE:HG13	1.94	0.46
2:D:257:LYS:O	2:D:260:VAL:HG22	2.15	0.46
2:D:240:ILE:CG2	2:D:270:TYR:HE1	2.28	0.46
2:D:195:GLN:HG3	2:D:203:PHE:CZ	2.51	0.46
2:D:363:ASP:C	2:D:365:TRP:H	2.23	0.46
1:B:114:GLU:O	1:B:118:LYS:HG3	2.15	0.46
2:C:229:SER:C	2:C:230:LEU:HD12	2.41	0.46
2:D:169:ARG:HG2	2:D:169:ARG:HH11	1.80	0.46
2:C:243:LEU:HD13	2:C:352:LEU:CD2	2.46	0.45
2:D:210:PRO:CG	2:D:212:TRP:CZ2	2.99	0.45
1:A:77:GLU:N	1:A:77:GLU:CD	2.74	0.45
1:A:59:GLN:HG2	1:A:113:GLN:OE1	2.16	0.45
1:A:57:ALA:HB1	1:A:77:GLU:HB3	1.99	0.45
2:C:309:ASP:OD2	2:C:311:ASP:HB2	2.16	0.45
2:C:175:ASN:CB	2:C:363:ASP:HB2	2.45	0.45
1:A:67:VAL:HG12	1:A:104:TYR:CD2	2.52	0.45
1:B:32:LEU:HB2	1:B:34:ASP:HB3	1.99	0.45
1:B:108:ILE:CG2	1:B:112:GLU:HB3	2.47	0.45
2:C:184:THR:OG1	2:C:185:LYS:N	2.49	0.45
2:D:357:ARG:NH1	2:D:357:ARG:CG	2.73	0.45
2:C:278:TRP:CZ3	2:C:335:PRO:HD3	2.52	0.44
2:D:194:ALA:HA	2:D:197:ARG:CG	2.46	0.44
2:D:173:PRO:HG3	2:D:362:HIS:CA	2.42	0.44
1:B:97:ILE:CD1	1:B:137:LYS:HB3	2.46	0.44
2:D:195:GLN:OE1	2:D:201:LYS:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:ALA:HB1	1:A:21:MSE:CE	2.46	0.44
2:D:338:ILE:HD12	2:D:338:ILE:HA	1.87	0.44
1:A:90:ARG:HG3	1:A:93:MSE:HE2	1.98	0.44
2:D:201:LYS:HB2	2:D:201:LYS:HE2	1.67	0.44
2:D:326:SER:OG	2:D:337:GLU:CD	2.60	0.44
2:D:193:ASP:O	2:D:197:ARG:CG	2.65	0.44
2:D:172:VAL:HG22	2:D:361:LEU:CD1	2.47	0.43
2:D:194:ALA:O	2:D:197:ARG:HG3	2.18	0.43
2:C:212:TRP:CE3	2:C:257:LYS:HE2	2.53	0.43
2:C:299:LYS:HG2	2:C:300:GLU:N	2.31	0.43
2:D:126:ASP:HA	3:E:180:ARG:HH22	1.83	0.43
1:A:34:ASP:OD1	1:A:34:ASP:N	2.50	0.43
1:A:53:LEU:N	1:A:53:LEU:HD23	2.33	0.43
2:D:194:ALA:HA	2:D:197:ARG:CD	2.48	0.43
2:D:232:ASP:O	2:D:236:GLN:HB3	2.19	0.43
3:E:151:MSE:HE2	3:E:155:ASP:C	2.44	0.43
2:C:321:SER:O	2:C:341:TYR:HE1	2.02	0.43
2:C:180:CYS:HA	2:C:369:GLY:O	2.19	0.43
2:C:192:ILE:CG2	2:C:202:MSE:HE2	2.30	0.43
2:D:234:LYS:HD3	2:D:234:LYS:HA	1.65	0.43
1:A:58:LEU:HD11	1:A:91:THR:HG22	2.01	0.43
1:A:75:TYR:CD2	1:A:75:TYR:O	2.70	0.43
1:A:95:LEU:N	1:A:95:LEU:HD23	2.34	0.43
2:D:157:PHE:O	2:D:161:GLN:HG2	2.18	0.43
2:D:255:ASN:HA	2:D:258:TYR:CD2	2.53	0.43
1:B:70:TRP:HB2	1:B:84:ILE:HG13	2.01	0.42
2:C:275:GLU:O	2:D:299:LYS:NZ	2.50	0.42
1:A:75:TYR:O	1:A:75:TYR:HD2	2.01	0.42
1:B:70:TRP:CZ2	1:B:88:GLU:HG2	2.53	0.42
1:B:14:PHE:HA	1:B:17:TYR:HB3	2.00	0.42
1:B:129:LYS:O	1:B:135:TYR:HD1	2.02	0.42
2:C:232:ASP:O	2:C:236:GLN:HB3	2.19	0.42
2:D:236:GLN:NE2	2:D:236:GLN:C	2.73	0.42
1:B:87:LEU:HA	1:B:87:LEU:HD23	1.81	0.42
2:C:176:SER:C	2:C:178:PRO:HD3	2.45	0.42
2:D:191:LEU:O	2:D:195:GLN:HB2	2.18	0.42
2:D:363:ASP:O	2:D:364:ASN:HB2	2.19	0.42
2:C:183:VAL:HB	2:C:238:MSE:HE3	2.01	0.42
1:B:45:LYS:HE2	1:B:45:LYS:HB3	1.87	0.42
1:B:98:ASN:HD22	1:B:137:LYS:H	1.68	0.42
2:C:188:PHE:O	2:C:192:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:TRP:CE3	2:C:335:PRO:HD3	2.55	0.42
1:B:126:LYS:HD3	1:B:127:GLU:HG3	2.01	0.42
2:C:207:MSE:SE	2:C:338:ILE:HD12	2.69	0.42
1:B:89:LEU:O	1:B:92:CYS:HB2	2.20	0.42
2:C:234:LYS:HB3	2:C:234:LYS:HE3	1.84	0.41
1:B:81:LYS:N	1:B:81:LYS:HD2	2.36	0.41
1:B:98:ASN:ND2	1:B:137:LYS:H	2.17	0.41
2:C:171:MSE:HA	2:C:171:MSE:CE	2.40	0.41
2:C:176:SER:O	2:C:178:PRO:HD3	2.19	0.41
1:A:61:GLY:HA3	1:A:73:ILE:HG23	2.01	0.41
3:E:170:LEU:HD12	3:E:170:LEU:HA	1.86	0.41
1:A:70:TRP:CE2	1:A:88:GLU:HG3	2.55	0.41
3:E:151:MSE:HG2	3:E:155:ASP:HB2	2.02	0.41
3:F:177:ILE:O	3:F:178:VAL:C	2.63	0.41
1:B:70:TRP:CB	1:B:84:ILE:HG13	2.51	0.41
2:D:280:LYS:CE	2:D:300:GLU:CG	2.99	0.41
3:E:161:PHE:HD1	3:E:161:PHE:HA	1.77	0.41
1:B:89:LEU:HD11	3:F:167:LEU:HD13	2.03	0.41
2:D:188:PHE:CE1	2:D:239:PRO:HD3	2.51	0.41
1:B:50:TRP:HE1	1:B:55:GLN:HB2	1.86	0.41
2:C:208:MSE:HG2	2:C:210:PRO:HG3	2.02	0.41
2:C:272:LEU:HD22	2:C:272:LEU:HA	1.89	0.41
2:C:315:PHE:HA	2:C:345:LEU:O	2.21	0.41
2:D:209:ASP:OD2	2:D:334:LYS:NZ	2.50	0.41
2:D:212:TRP:HZ3	2:D:232:ASP:OD1	2.03	0.41
2:D:136:LYS:HE3	2:D:136:LYS:HB2	1.55	0.41
2:D:167:GLY:HA3	2:D:168:LYS:HA	1.86	0.40
2:D:319:ILE:HG13	2:D:341:TYR:CZ	2.56	0.40
1:A:21:MSE:CE	1:A:21:MSE:HA	2.51	0.40
1:A:46:LYS:HG3	1:A:47:GLY:N	2.36	0.40
1:A:67:VAL:HG12	1:A:104:TYR:HD2	1.84	0.40
1:B:49:TYR:CD2	1:B:51:THR:HG22	2.56	0.40
1:B:124:GLY:HA2	1:B:135:TYR:CD1	2.56	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	127/142 (89%)	125 (98%)	2 (2%)	0	100	100
1	B	128/142 (90%)	126 (98%)	2 (2%)	0	100	100
2	C	209/247 (85%)	206 (99%)	3 (1%)	0	100	100
2	D	210/247 (85%)	203 (97%)	7 (3%)	0	100	100
3	E	35/309 (11%)	34 (97%)	0	1 (3%)	3	8
3	F	23/309 (7%)	21 (91%)	2 (9%)	0	100	100
All	All	732/1396 (52%)	715 (98%)	16 (2%)	1 (0%)	48	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	148	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	113/123 (92%)	88 (78%)	25 (22%)	1	2
1	B	112/123 (91%)	85 (76%)	27 (24%)	1	2
2	C	185/212 (87%)	149 (80%)	36 (20%)	1	3
2	D	188/212 (89%)	144 (77%)	44 (23%)	1	2
3	E	33/276 (12%)	29 (88%)	4 (12%)	5	12
3	F	22/276 (8%)	19 (86%)	3 (14%)	3	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	653/1222 (53%)	514 (79%)	139 (21%)	1 3

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	12	LEU
1	B	16	GLN
1	B	28	GLN
1	B	29	ASP
1	B	31	CYS
1	B	32	LEU
1	B	58	LEU
1	B	69	ASN
1	B	71	LYS
1	B	77	GLU
1	B	81	LYS
1	B	84	ILE
1	B	88	GLU
1	B	90	ARG
1	B	91	THR
1	B	97	ILE
1	B	106	LYS
1	B	107	LYS
1	B	112	GLU
1	B	115	GLU
1	B	126	LYS
1	B	130	LEU
1	B	132	ASP
1	B	134	ILE
1	B	137	LYS
1	B	138	LEU
1	B	139	GLN
2	C	129	LEU
2	C	134	LYS
2	C	137	LYS
2	C	142	LEU
2	C	161	GLN
2	C	166	ASN
2	C	168	LYS
2	C	171	MSE
2	C	183	VAL
2	C	187	ASN

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Mol	Chain	Res	Type
2	C	195	GLN
2	C	207	MSE
2	C	208	MSE
2	C	211	PRO
2	C	213	GLN
2	C	231	SER
2	C	236	GLN
2	C	241	GLN
2	C	246	ASP
2	C	264	MSE
2	C	271	LYS
2	C	272	LEU
2	C	312	ASN
2	C	316	LYS
2	C	317	LYS
2	C	326	SER
2	C	327	GLU
2	C	336	GLU
2	C	338	ILE
2	C	341	TYR
2	C	342	ILE
2	C	344	GLN
2	C	346	CYS
2	C	359	ASN
2	C	363	ASP
2	C	371	GLU
2	D	127	ASP
2	D	130	ASP
2	D	134	LYS
2	D	136	LYS
2	D	142	LEU
2	D	147	GLU
2	D	148	LYS
2	D	149	ARG
2	D	166	ASN
2	D	168	LYS
2	D	169	ARG
2	D	174	ASP
2	D	181	SER
2	D	182	ASP
2	D	183	VAL
2	D	184	THR

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Mol	Chain	Res	Type
2	D	187	ASN
2	D	191	LEU
2	D	197	ARG
2	D	201	LYS
2	D	208	MSE
2	D	229	SER
2	D	231	SER
2	D	234	LYS
2	D	237	ASN
2	D	245	GLN
2	D	249	ILE
2	D	255	ASN
2	D	263	LYS
2	D	280	LYS
2	D	299	LYS
2	D	310	VAL
2	D	314	ARG
2	D	316	LYS
2	D	317	LYS
2	D	318	ASN
2	D	319	ILE
2	D	324	ILE
2	D	327	GLU
2	D	331	GLN
2	D	332	SER
2	D	345	LEU
2	D	361	LEU
2	D	363	ASP
3	E	149	GLN
3	E	160	LYS
3	E	170	LEU
3	E	173	LEU
3	F	164	LEU
3	F	173	LEU
3	F	179	ARG
1	A	12	LEU
1	A	15	THR
1	A	21	MSE
1	A	27	ASN
1	A	28	GLN
1	A	34	ASP
1	A	53	LEU

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Mol	Chain	Res	Type
1	A	58	LEU
1	A	64	LEU
1	A	76	ASP
1	A	81	LYS
1	A	88	GLU
1	A	90	ARG
1	A	91	THR
1	A	99	ASP
1	A	100	ILE
1	A	101	THR
1	A	102	GLU
1	A	109	SER
1	A	126	LYS
1	A	127	GLU
1	A	130	LEU
1	A	131	LYS
1	A	133	ASN
1	A	134	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	B	98	ASN
2	C	152	HIS
2	C	195	GLN
2	C	198	HIS
2	C	213	GLN
2	C	244	GLN
2	C	331	GLN
2	C	360	ASN
2	C	362	HIS
2	D	162	ASN
2	D	236	GLN
2	D	245	GLN
2	D	318	ASN
2	D	348	ASN
2	D	359	ASN
2	D	360	ASN
3	F	184	GLN
1	A	16	GLN
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	69	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](#)

There are no ligands in this entry.

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	127/142 (89%)	0.36	5 (3%) 43 39	9, 30, 54, 83	0
1	B	128/142 (90%)	0.30	3 (2%) 61 58	10, 32, 59, 81	0
2	C	208/247 (84%)	0.48	13 (6%) 26 23	11, 34, 65, 80	0
2	D	209/247 (84%)	0.45	17 (8%) 18 16	7, 29, 72, 92	0
3	E	36/309 (11%)	-0.10	1 (2%) 55 52	6, 13, 33, 47	0
3	F	25/309 (8%)	-0.29	0 100 100	7, 14, 39, 52	0
All	All	733/1396 (52%)	0.36	39 (5%) 32 28	6, 30, 64, 92	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	LEU	7.0
2	D	326	SER	6.5
1	A	11	PRO	5.7
2	D	183	VAL	5.1
2	C	228	ASP	4.8
2	C	320	ALA	4.5
2	C	128	TYR	4.1
2	D	320	ALA	4.1
2	D	228	ASP	4.1
1	B	11	PRO	4.0
2	C	341	TYR	4.0
2	D	213	GLN	3.8
2	D	319	ILE	3.8
2	D	327	GLU	3.7
2	D	232	ASP	3.5
2	D	328	ARG	3.4
2	C	244	GLN	3.3
2	D	332	SER	3.3
2	C	319	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	104	TYR	2.9
2	D	329	ARG	2.8
1	B	140	GLN	2.8
2	D	126	ASP	2.7
2	D	184	THR	2.6
2	C	127	ASP	2.5
2	D	186	LEU	2.5
1	A	104	TYR	2.5
2	D	333	GLN	2.5
2	C	232	ASP	2.4
1	A	14	PHE	2.3
2	C	325	PHE	2.3
3	E	147	ALA	2.3
2	C	364	ASN	2.3
1	A	75	TYR	2.2
2	C	129	LEU	2.2
2	C	130	ASP	2.2
2	C	279	VAL	2.1
2	D	298	ALA	2.1
2	D	318	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.