



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:12 PM UTC

PDB ID : 4B0J / pdb_00004b0j
Title : Crystal Structure of 3-hydroxydecanoyl-Acyl Carrier Protein Dehydratase (FabA) from Pseudomonas aeruginosa in complex with 5-(2- thienyl)-3-isoxazolyl methanol
Authors : Moynie, L.; McMahon, S.A.; Duthie, F.G.; Naismith, J.H.
Deposited on : 2012-07-02
Resolution : 2.50 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

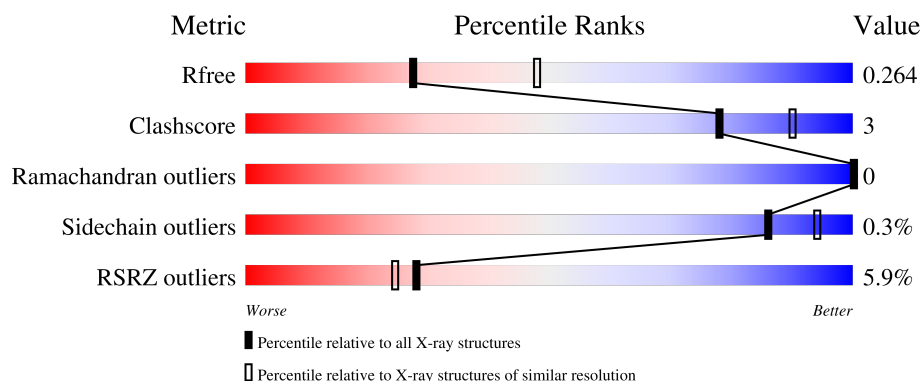
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	171	4% 92% 6%
1	B	171	7% 95% 5%
1	C	171	6% 94% 5%
1	D	171	10% 94% 5%
1	E	171	5% 92% 6%

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Mol	Chain	Length	Quality of chain
1	F	171	
1	G	171	
1	H	171	
1	I	171	
1	J	171	
1	K	171	
1	L	171	
1	M	171	
1	N	171	
1	O	171	
1	P	171	
1	Q	171	
1	R	171	
1	S	171	
1	T	171	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3MQ	L	1172	-	X	-	-
2	3MQ	S	1172	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 27044 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 3-HYDROXYDECANOYL-[ACYL-CARRIER-PROTEIN] DEHYDRATASE.

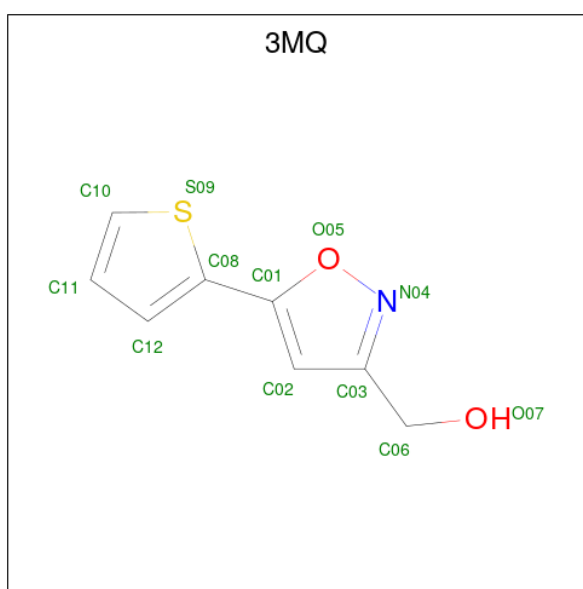
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1287	825	222	233	7			
1	B	170	Total	C	N	O	S	0	0	0
			1312	838	229	238	7			
1	C	168	Total	C	N	O	S	0	0	0
			1295	829	224	235	7			
1	D	170	Total	C	N	O	S	0	0	0
			1312	838	229	238	7			
1	E	168	Total	C	N	O	S	0	0	0
			1295	829	224	235	7			
1	F	169	Total	C	N	O	S	0	0	0
			1306	835	228	236	7			
1	G	166	Total	C	N	O	S	0	0	0
			1279	819	221	232	7			
1	H	167	Total	C	N	O	S	0	0	0
			1287	825	222	233	7			
1	I	169	Total	C	N	O	S	0	0	0
			1306	835	228	236	7			
1	J	168	Total	C	N	O	S	0	0	0
			1295	829	224	235	7			
1	K	169	Total	C	N	O	S	0	0	0
			1306	835	228	236	7			
1	L	170	Total	C	N	O	S	0	0	0
			1312	838	229	238	7			
1	M	168	Total	C	N	O	S	0	0	0
			1295	829	224	235	7			
1	N	168	Total	C	N	O	S	0	0	0
			1298	829	227	235	7			
1	O	170	Total	C	N	O	S	0	0	0
			1312	838	229	238	7			
1	P	170	Total	C	N	O	S	0	0	0
			1312	838	229	238	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	168	Total	C	N	O	S	0	0	0
			1295	829	224	235	7			
1	R	167	Total	C	N	O	S	0	0	0
			1287	825	222	233	7			
1	S	167	Total	C	N	O	S	0	0	0
			1287	825	222	233	7			
1	T	167	Total	C	N	O	S	0	0	0
			1287	825	222	233	7			

- Molecule 2 is (5-thiophen-2-ylisoxazol-3-yl)methanol (CCD ID: 3MQ) (formula: C₈H₇NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	C	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	D	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	E	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	F	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	G	1	Total	C	N	O	S	0	0
			12	8	1	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	I	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	J	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	K	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	L	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	M	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	N	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	O	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	P	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	Q	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	R	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	S	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	T	1	Total	C	N	O	S	0	0
			12	8	1	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	B	41	Total	O	0	0
			41	41		
3	C	60	Total	O	0	0
			60	60		
3	D	35	Total	O	0	0
			35	35		
3	E	41	Total	O	0	0
			41	41		
3	F	35	Total	O	0	0
			35	35		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	42	Total 42	O 42	0	0
3	H	40	Total 40	O 40	0	0
3	I	68	Total 68	O 68	0	0
3	J	54	Total 54	O 54	0	0
3	K	43	Total 43	O 43	0	0
3	L	43	Total 43	O 43	0	0
3	M	51	Total 51	O 51	0	0
3	N	41	Total 41	O 41	0	0
3	O	44	Total 44	O 44	0	0
3	P	33	Total 33	O 33	0	0
3	Q	30	Total 30	O 30	0	0
3	R	29	Total 29	O 29	0	0
3	S	30	Total 30	O 30	0	0
3	T	22	Total 22	O 22	0	0

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.

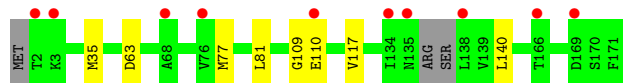
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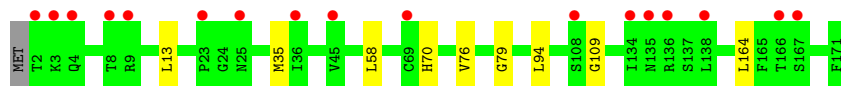
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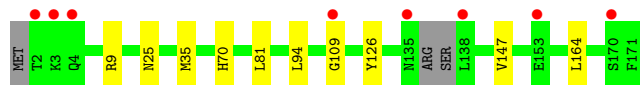
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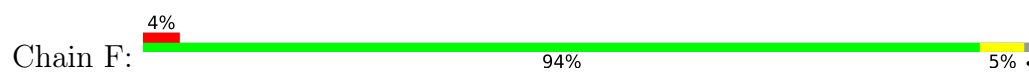
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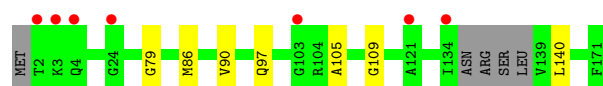
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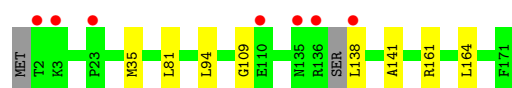
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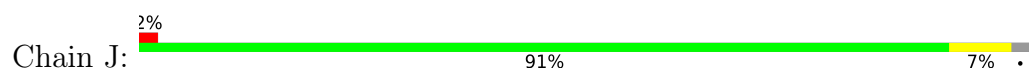
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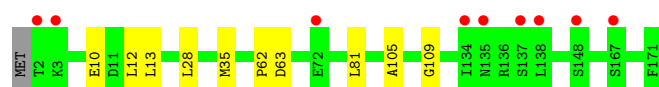
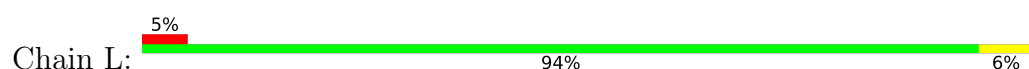
• Molecule 1: 3-HYDROXYDECANOYL-[ACYL-CARRIER-PROTEIN] DEHYDRATASE



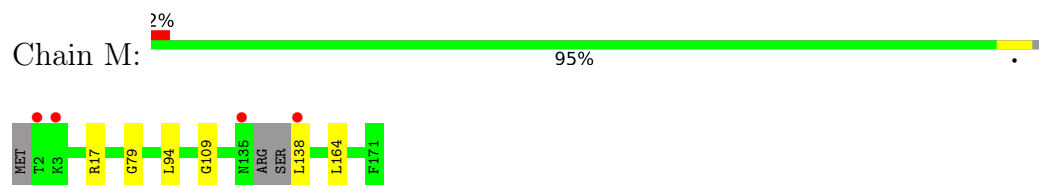
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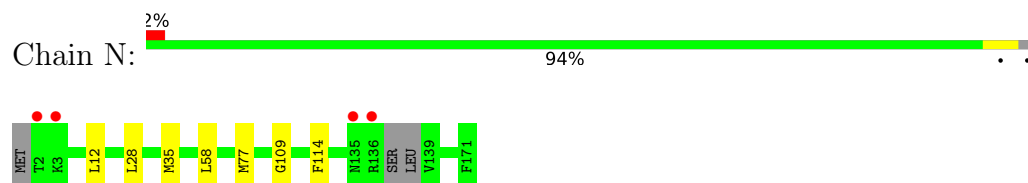
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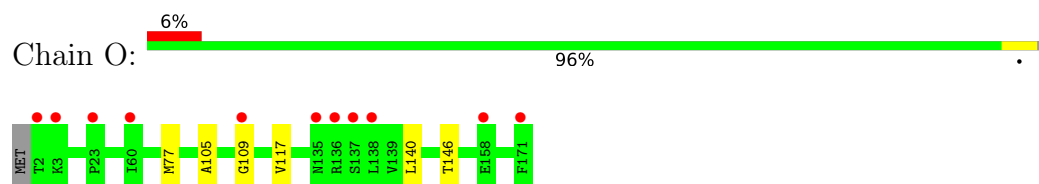
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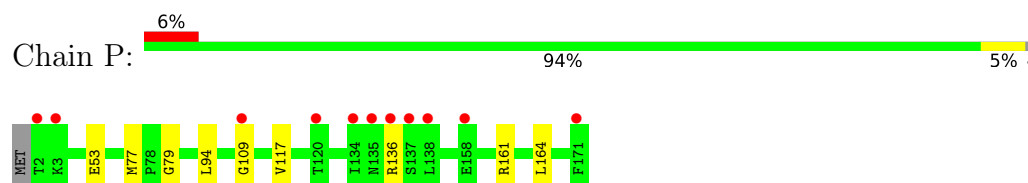
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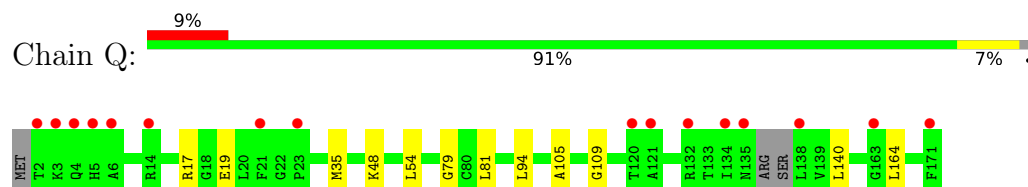
- Molecule 1: 3-HYDROXYDECANOYL-[ACYL-CARRIER-PROTEIN] DEHYDRATASE



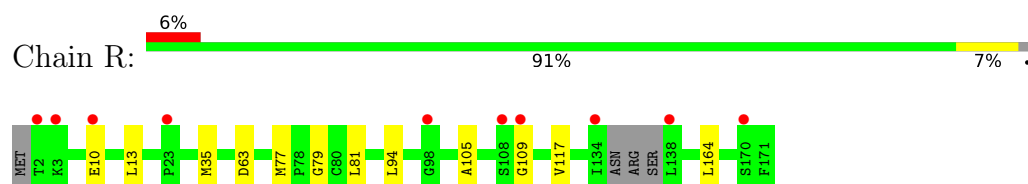
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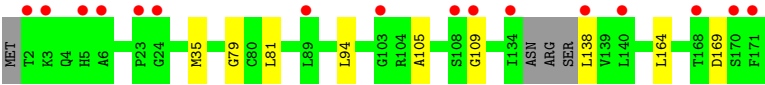
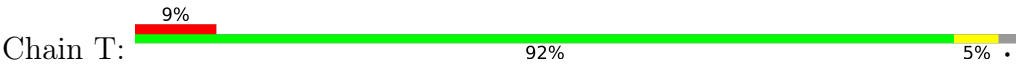


- Molecule 1: 3-HYDROXYDECANOYL-[ACYL-CARRIER-PROTEIN] DEHYDRATASE





● Molecule 1: 3-HYDROXYDECANOYL-[ACYL-CARRIER-PROTEIN] DEHYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.75Å 108.17Å 201.77Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	23.95 – 2.50 23.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.9 (23.95-2.50) 97.2 (23.95-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.233 , 0.265 0.235 , 0.264	Depositor DCC
R_{free} test set	7799 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27044	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2281e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3MQ

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	0.72	0/1317	0.75	0/1779
1	B	0.73	0/1343	0.74	0/1815
1	C	0.68	0/1325	0.72	0/1790
1	D	0.71	1/1343 (0.1%)	0.73	0/1815
1	E	0.74	1/1325 (0.1%)	0.72	0/1790
1	F	0.70	0/1336	0.73	0/1804
1	G	0.70	0/1309	0.70	0/1768
1	H	0.67	0/1317	0.71	0/1779
1	I	0.76	0/1336	0.74	0/1804
1	J	0.72	0/1325	0.75	0/1790
1	K	0.73	0/1336	0.75	0/1804
1	L	0.73	0/1343	0.76	1/1815 (0.1%)
1	M	0.74	0/1325	0.74	0/1790
1	N	0.72	0/1328	0.72	0/1793
1	O	0.68	0/1343	0.71	0/1815
1	P	0.71	0/1343	0.72	0/1815
1	Q	0.71	0/1325	0.72	0/1790
1	R	0.70	0/1317	0.72	0/1779
1	S	0.66	0/1317	0.71	0/1779
1	T	0.69	0/1317	0.73	0/1779
All	All	0.71	2/26570 (0.0%)	0.73	1/35893 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	70	HIS	CG-CD2	5.13	1.41	1.35
1	D	70	HIS	CG-CD2	5.12	1.41	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	10	GLU	CB-CA-C	-8.40	97.69	110.88

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	1287	0	1272	9	0
1	B	1312	0	1297	8	0
1	C	1295	0	1278	6	0
1	D	1312	0	1297	7	0
1	E	1295	0	1278	7	0
1	F	1306	0	1291	8	0
1	G	1279	0	1261	6	0
1	H	1287	0	1272	10	0
1	I	1306	0	1291	5	0
1	J	1295	0	1278	7	0
1	K	1306	0	1291	8	0
1	L	1312	0	1297	18	0
1	M	1295	0	1278	4	0
1	N	1298	0	1280	9	0
1	O	1312	0	1297	7	0
1	P	1312	0	1297	8	0
1	Q	1295	0	1278	10	1
1	R	1287	0	1272	20	0
1	S	1287	0	1272	5	0
1	T	1287	0	1272	8	1
2	A	12	0	7	3	0
2	B	12	0	7	0	0
2	C	12	0	7	0	0
2	D	12	0	7	1	0
2	E	12	0	7	0	0
2	F	12	0	7	0	0
2	G	12	0	7	2	0
2	H	12	0	7	1	0
2	I	12	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	12	0	7	0	0
2	K	12	0	7	1	0
2	L	12	0	7	0	0
2	M	12	0	7	1	0
2	N	12	0	7	0	0
2	O	12	0	7	0	0
2	P	12	0	7	3	0
2	Q	12	0	7	2	0
2	R	12	0	7	3	0
2	S	12	0	7	3	0
2	T	12	0	7	2	0
3	A	57	0	0	0	0
3	B	41	0	0	3	0
3	C	60	0	0	1	0
3	D	35	0	0	1	0
3	E	41	0	0	2	0
3	F	35	0	0	2	0
3	G	42	0	0	1	0
3	H	40	0	0	2	0
3	I	68	0	0	1	0
3	J	54	0	0	0	0
3	K	43	0	0	0	0
3	L	43	0	0	0	0
3	M	51	0	0	1	0
3	N	41	0	0	0	0
3	O	44	0	0	1	0
3	P	33	0	0	3	0
3	Q	30	0	0	1	0
3	R	29	0	0	0	0
3	S	30	0	0	0	0
3	T	22	0	0	0	0
All	All	27044	0	25789	144	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (144) 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:B:2:THR:HG21	3:B:2013:HOH:O	1.52	1.07
1:L:63:ASP:OD2	1:R:13:LEU:HD12	1.52	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:35:MET:HE2	1:N:77:MET:HE3	1.44	0.99
1:L:13:LEU:HD12	1:R:63:ASP:OD2	1.65	0.96
1:B:2:THR:CG2	3:B:2013:HOH:O	2.08	0.95
1:T:35:MET:HE2	1:T:81:LEU:HB3	1.53	0.90
1:L:63:ASP:CG	1:R:10:GLU:OE2	2.15	0.89
1:S:109:GLY:O	1:T:109:GLY:O	1.95	0.84
1:Q:109:GLY:O	1:R:109:GLY:O	1.96	0.83
1:F:77:MET:HE2	1:F:117:VAL:HG21	1.62	0.82
1:F:35:MET:HE2	1:F:81:LEU:HB3	1.63	0.81
1:L:63:ASP:OD2	1:R:10:GLU:OE2	1.98	0.80
1:L:35:MET:HE2	1:L:81:LEU:HB3	1.61	0.80
1:I:109:GLY:O	1:J:109:GLY:O	2.00	0.80
1:N:35:MET:HE2	1:N:77:MET:CE	2.12	0.79
1:L:63:ASP:OD2	1:R:10:GLU:CD	2.27	0.77
1:K:109:GLY:O	1:L:109:GLY:O	2.04	0.76
1:C:109:GLY:O	1:D:109:GLY:O	2.03	0.76
1:G:97:GLN:NE2	3:G:2025:HOH:O	2.18	0.75
1:M:109:GLY:O	1:N:109:GLY:O	2.04	0.75
1:N:35:MET:CE	1:N:77:MET:HE3	2.15	0.75
1:K:35:MET:HE2	1:K:81:LEU:HB3	1.70	0.74
1:G:109:GLY:O	1:H:109:GLY:O	2.06	0.73
1:E:109:GLY:O	1:F:109:GLY:O	2.06	0.73
1:A:109:GLY:O	1:B:109:GLY:O	2.07	0.72
1:K:77:MET:HE2	1:K:117:VAL:HG21	1.72	0.72
1:L:62:PRO:HG2	1:R:10:GLU:HG3	1.71	0.71
1:B:9:ARG:NH1	3:B:2001:HOH:O	2.23	0.71
1:B:35:MET:HE2	1:B:81:LEU:HB3	1.73	0.70
1:F:77:MET:CE	1:F:117:VAL:HG21	2.21	0.70
1:O:109:GLY:O	1:P:109:GLY:O	2.10	0.69
1:F:77:MET:HE2	1:F:117:VAL:CG2	2.25	0.67
1:D:35:MET:HE3	1:D:58:LEU:HD22	1.75	0.67
1:E:25:ASN:OD1	3:E:2008:HOH:O	2.12	0.67
1:P:79:GLY:H	2:P:1172:3MQ:H06A	1.59	0.67
1:G:140:LEU:C	1:G:140:LEU:HD12	2.19	0.67
1:H:77:MET:HE2	1:H:117:VAL:HG21	1.76	0.66
1:N:35:MET:HE3	1:N:58:LEU:HD22	1.78	0.66
1:C:140:LEU:C	1:C:140:LEU:HD12	2.21	0.65
1:O:77:MET:HE2	1:O:117:VAL:HG21	1.77	0.65
1:L:63:ASP:OD2	1:R:13:LEU:CD1	2.39	0.64
1:P:53:GLU:OE2	3:P:2012:HOH:O	2.15	0.63
1:A:77:MET:HE2	1:A:117:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:35:MET:HE2	1:Q:81:LEU:HB3	1.82	0.61
1:R:79:GLY:H	2:R:1172:3MQ:H06A	1.64	0.61
1:T:35:MET:HE2	1:T:81:LEU:CB	2.29	0.60
1:P:161:ARG:NE	3:P:2031:HOH:O	2.28	0.59
1:Q:17:ARG:NH1	3:Q:2004:HOH:O	2.31	0.59
1:D:79:GLY:H	2:D:1172:3MQ:H06A	1.66	0.59
2:S:1172:3MQ:H06	1:T:105:ALA:HB3	1.86	0.58
1:L:63:ASP:CG	1:R:10:GLU:CD	2.71	0.58
1:A:79:GLY:H	2:A:1172:3MQ:H06A	1.67	0.58
1:H:35:MET:HE2	1:H:81:LEU:HB3	1.86	0.58
1:Q:105:ALA:O	2:R:1172:3MQ:H02	2.04	0.57
1:E:9:ARG:NH1	3:E:2003:HOH:O	2.38	0.56
1:Q:79:GLY:H	2:Q:1172:3MQ:H06A	1.69	0.56
1:E:94:LEU:HB3	1:E:164:LEU:HD11	1.87	0.56
1:O:146:THR:HB	3:O:2039:HOH:O	2.05	0.56
1:L:62:PRO:HD2	1:R:10:GLU:CG	2.35	0.56
1:P:77:MET:HE2	1:P:117:VAL:HG21	1.88	0.55
1:C:63:ASP:HB2	3:C:2025:HOH:O	2.07	0.55
1:H:94:LEU:HB3	1:H:164:LEU:HD11	1.88	0.55
1:L:62:PRO:CG	1:R:10:GLU:HG3	2.37	0.54
1:S:79:GLY:H	2:S:1172:3MQ:H06A	1.72	0.54
1:L:13:LEU:HD12	1:R:63:ASP:CG	2.32	0.54
1:I:35:MET:HE2	1:I:81:LEU:HB3	1.90	0.54
2:S:1172:3MQ:H02	1:T:105:ALA:O	2.08	0.53
1:H:166:THR:CG2	3:H:2040:HOH:O	2.56	0.53
1:T:79:GLY:H	2:T:1172:3MQ:H06A	1.74	0.51
1:L:35:MET:HE2	1:L:81:LEU:CB	2.35	0.51
1:O:105:ALA:O	2:P:1172:3MQ:H02	2.11	0.51
1:R:35:MET:HE2	1:R:81:LEU:HB3	1.93	0.51
1:F:35:MET:HE2	1:F:81:LEU:CB	2.39	0.51
1:H:77:MET:HE2	1:H:117:VAL:CG2	2.41	0.50
1:E:126:TYR:HD1	1:E:147:VAL:HG22	1.77	0.50
1:H:77:MET:CE	1:H:117:VAL:HG21	2.41	0.49
1:O:77:MET:HE2	1:O:117:VAL:CG2	2.42	0.49
2:K:1172:3MQ:H02	1:L:105:ALA:O	2.11	0.49
1:H:166:THR:HG21	3:H:2040:HOH:O	2.12	0.49
1:K:77:MET:HE2	1:K:117:VAL:CG2	2.42	0.49
1:O:77:MET:CE	1:O:117:VAL:HG21	2.42	0.49
2:G:1172:3MQ:H02	1:H:105:ALA:O	2.12	0.49
1:A:77:MET:HE2	1:A:117:VAL:CG2	2.42	0.49
1:C:35:MET:HE2	1:C:81:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1172:3MQ:H02	1:J:105:ALA:O	2.13	0.48
1:R:77:MET:HE2	1:R:117:VAL:HG21	1.94	0.48
1:K:77:MET:CE	1:K:117:VAL:HG21	2.42	0.48
2:A:1172:3MQ:H02	1:B:105:ALA:O	2.13	0.48
1:F:61:ASN:HA	3:F:2020:HOH:O	2.13	0.47
1:E:126:TYR:CD1	1:E:147:VAL:HG22	2.49	0.47
1:F:51:LYS:NZ	3:F:2017:HOH:O	2.42	0.47
1:B:94:LEU:HB3	1:B:164:LEU:HD11	1.97	0.46
1:A:79:GLY:N	2:A:1172:3MQ:H06A	2.30	0.46
1:Q:140:LEU:C	1:Q:140:LEU:HD12	2.41	0.46
1:L:12:LEU:HD22	1:L:28:LEU:HD11	1.98	0.46
1:H:86:MET:O	1:H:90:VAL:HG23	2.16	0.46
1:A:94:LEU:HD21	1:A:141:ALA:HB2	1.99	0.45
1:N:35:MET:HE3	1:N:58:LEU:CD2	2.46	0.45
1:Q:94:LEU:HB3	1:Q:164:LEU:HD11	1.98	0.45
1:P:161:ARG:NH2	3:P:2031:HOH:O	2.49	0.45
1:A:77:MET:CE	1:A:117:VAL:HG21	2.44	0.45
1:L:62:PRO:HD2	1:R:10:GLU:HG3	1.98	0.44
1:N:35:MET:CE	1:N:77:MET:CE	2.84	0.44
1:S:110:GLU:HA	1:T:109:GLY:O	2.17	0.44
1:E:35:MET:HE2	1:E:81:LEU:HB3	2.00	0.44
1:R:94:LEU:HB3	1:R:164:LEU:HD11	2.00	0.44
1:A:35:MET:HE2	1:A:81:LEU:HB3	1.98	0.44
1:O:140:LEU:C	1:O:140:LEU:HD12	2.43	0.44
1:J:35:MET:HE2	1:J:81:LEU:HB3	1.99	0.44
1:D:13:LEU:HD23	1:D:13:LEU:HA	1.74	0.43
1:A:94:LEU:HB3	1:A:164:LEU:HD11	2.01	0.43
1:J:126:TYR:HD1	1:J:147:VAL:HG22	1.84	0.43
1:Q:54:LEU:HD12	1:Q:54:LEU:N	2.33	0.43
1:I:94:LEU:HB3	1:I:164:LEU:HD11	2.01	0.43
1:M:79:GLY:H	2:M:1172:3MQ:H06A	1.84	0.43
1:K:126:TYR:HD1	1:K:147:VAL:HG22	1.84	0.43
1:G:79:GLY:H	2:G:1172:3MQ:H06A	1.84	0.42
1:J:94:LEU:HB3	1:J:164:LEU:HD11	2.01	0.42
1:P:94:LEU:HB3	1:P:164:LEU:HD11	2.01	0.42
1:I:94:LEU:HD21	1:I:141:ALA:HB2	2.01	0.42
1:R:94:LEU:HD13	1:R:164:LEU:HG	2.01	0.42
1:N:12:LEU:HD22	1:N:28:LEU:HD11	2.01	0.42
2:Q:1172:3MQ:H02	1:R:105:ALA:O	2.19	0.42
1:M:94:LEU:HB3	1:M:164:LEU:HD11	2.01	0.42
1:K:35:MET:HE2	1:K:81:LEU:CB	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:MET:O	1:G:90:VAL:HG23	2.20	0.42
1:I:161:ARG:NH2	3:I:2067:HOH:O	2.38	0.41
1:D:94:LEU:HB3	1:D:164:LEU:HD11	2.01	0.41
1:M:17:ARG:NH1	3:M:2003:HOH:O	2.31	0.41
1:J:94:LEU:HD21	1:J:141:ALA:HB2	2.03	0.41
1:C:77:MET:HE2	1:C:117:VAL:HG21	2.03	0.41
1:C:110:GLU:HA	1:D:109:GLY:O	2.20	0.41
1:G:105:ALA:O	2:H:1172:3MQ:H02	2.20	0.41
1:J:115:GLY:HA3	1:J:154:ILE:HG22	2.03	0.41
1:L:63:ASP:OD1	1:R:10:GLU:OE1	2.39	0.41
1:K:94:LEU:HB3	1:K:164:LEU:HD11	2.02	0.41
1:Q:105:ALA:HB3	2:R:1172:3MQ:H06	2.02	0.41
1:S:126:TYR:HD1	1:S:147:VAL:HG22	1.86	0.40
1:S:105:ALA:O	2:T:1172:3MQ:H02	2.21	0.40
1:T:94:LEU:HD13	1:T:164:LEU:HG	2.04	0.40
1:D:76:VAL:HG22	3:D:2019:HOH:O	2.20	0.40
1:N:114:PHE:CG	1:Q:48:LYS:HA	2.57	0.40
1:B:2:THR:O	1:B:2:THR:HG22	2.22	0.40
1:P:79:GLY:N	2:P:1172:3MQ:H06A	2.32	0.40

All (1) 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:Q:19:GLU:O	1:T:169:ASP:OD2[2_647]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	163/171 (95%)	159 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	168/171 (98%)	161 (96%)	7 (4%)	0	100	100
1	C	164/171 (96%)	160 (98%)	4 (2%)	0	100	100
1	D	168/171 (98%)	162 (96%)	6 (4%)	0	100	100
1	E	164/171 (96%)	160 (98%)	4 (2%)	0	100	100
1	F	165/171 (96%)	161 (98%)	4 (2%)	0	100	100
1	G	162/171 (95%)	157 (97%)	5 (3%)	0	100	100
1	H	163/171 (95%)	159 (98%)	4 (2%)	0	100	100
1	I	165/171 (96%)	160 (97%)	5 (3%)	0	100	100
1	J	164/171 (96%)	160 (98%)	4 (2%)	0	100	100
1	K	165/171 (96%)	161 (98%)	4 (2%)	0	100	100
1	L	168/171 (98%)	161 (96%)	7 (4%)	0	100	100
1	M	164/171 (96%)	159 (97%)	5 (3%)	0	100	100
1	N	164/171 (96%)	159 (97%)	5 (3%)	0	100	100
1	O	168/171 (98%)	161 (96%)	7 (4%)	0	100	100
1	P	168/171 (98%)	161 (96%)	7 (4%)	0	100	100
1	Q	164/171 (96%)	159 (97%)	5 (3%)	0	100	100
1	R	163/171 (95%)	159 (98%)	4 (2%)	0	100	100
1	S	163/171 (95%)	159 (98%)	4 (2%)	0	100	100
1	T	163/171 (95%)	159 (98%)	4 (2%)	0	100	100
All	All	3296/3420 (96%)	3197 (97%)	99 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/138 (97%)	133 (99%)	1 (1%)	76	89
1	B	137/138 (99%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	135/138 (98%)	135 (100%)	0	100	100
1	D	137/138 (99%)	137 (100%)	0	100	100
1	E	135/138 (98%)	135 (100%)	0	100	100
1	F	136/138 (99%)	135 (99%)	1 (1%)	76	89
1	G	133/138 (96%)	133 (100%)	0	100	100
1	H	134/138 (97%)	134 (100%)	0	100	100
1	I	136/138 (99%)	135 (99%)	1 (1%)	76	89
1	J	135/138 (98%)	134 (99%)	1 (1%)	76	89
1	K	136/138 (99%)	136 (100%)	0	100	100
1	L	137/138 (99%)	137 (100%)	0	100	100
1	M	135/138 (98%)	134 (99%)	1 (1%)	76	89
1	N	135/138 (98%)	135 (100%)	0	100	100
1	O	137/138 (99%)	137 (100%)	0	100	100
1	P	137/138 (99%)	136 (99%)	1 (1%)	76	89
1	Q	135/138 (98%)	135 (100%)	0	100	100
1	R	134/138 (97%)	134 (100%)	0	100	100
1	S	134/138 (97%)	133 (99%)	1 (1%)	76	89
1	T	134/138 (97%)	133 (99%)	1 (1%)	76	89
All	All	2706/2760 (98%)	2698 (100%)	8 (0%)	86	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	F	140	LEU
1	I	138	LEU
1	J	140	LEU
1	M	138	LEU
1	P	136	ARG
1	S	3	LYS
1	T	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	B	97	GLN
1	C	97	GLN
1	D	97	GLN
1	F	97	GLN
1	F	99	ASN
1	G	97	GLN
1	H	97	GLN
1	I	97	GLN
1	J	97	GLN
1	J	135	ASN
1	K	97	GLN
1	K	135	ASN
1	M	97	GLN
1	N	97	GLN
1	P	97	GLN
1	Q	97	GLN
1	R	97	GLN
1	S	97	GLN
1	T	97	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 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
2	3MQ	R	1172	-	13,13,13	3.60	3 (23%)	14,17,17	3.33	7 (50%)
2	3MQ	M	1172	-	13,13,13	3.15	6 (46%)	14,17,17	2.80	8 (57%)
2	3MQ	C	1172	-	13,13,13	2.08	4 (30%)	14,17,17	2.37	7 (50%)
2	3MQ	H	1172	-	13,13,13	2.00	4 (30%)	14,17,17	2.05	6 (42%)
2	3MQ	K	1172	-	13,13,13	1.78	3 (23%)	14,17,17	2.05	6 (42%)
2	3MQ	A	1172	-	13,13,13	3.27	5 (38%)	14,17,17	2.72	8 (57%)
2	3MQ	F	1172	-	13,13,13	2.11	3 (23%)	14,17,17	2.42	7 (50%)
2	3MQ	S	1172	-	13,13,13	4.08	5 (38%)	14,17,17	3.55	9 (64%)
2	3MQ	B	1172	-	13,13,13	2.32	4 (30%)	14,17,17	2.67	7 (50%)
2	3MQ	G	1172	-	13,13,13	3.58	3 (23%)	14,17,17	2.90	8 (57%)
2	3MQ	P	1172	-	13,13,13	2.78	4 (30%)	14,17,17	2.43	8 (57%)
2	3MQ	T	1172	-	13,13,13	3.04	4 (30%)	14,17,17	2.92	9 (64%)
2	3MQ	N	1172	-	13,13,13	2.63	4 (30%)	14,17,17	2.67	7 (50%)
2	3MQ	E	1172	-	13,13,13	1.68	3 (23%)	14,17,17	1.78	4 (28%)
2	3MQ	I	1172	-	13,13,13	2.26	3 (23%)	14,17,17	2.88	9 (64%)
2	3MQ	D	1172	-	13,13,13	3.78	4 (30%)	14,17,17	3.21	9 (64%)
2	3MQ	Q	1172	-	13,13,13	3.62	2 (15%)	14,17,17	2.83	9 (64%)
2	3MQ	J	1172	-	13,13,13	3.87	4 (30%)	14,17,17	2.88	8 (57%)
2	3MQ	O	1172	-	13,13,13	1.75	3 (23%)	14,17,17	1.66	4 (28%)
2	3MQ	L	1172	-	13,13,13	2.56	6 (46%)	14,17,17	2.36	9 (64%)

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
2	3MQ	R	1172	-	-	3/6/6/6	0/2/2/2
2	3MQ	M	1172	-	-	0/6/6/6	0/2/2/2
2	3MQ	C	1172	-	-	1/6/6/6	0/2/2/2
2	3MQ	H	1172	-	-	1/6/6/6	0/2/2/2
2	3MQ	K	1172	-	-	2/6/6/6	0/2/2/2
2	3MQ	A	1172	-	-	0/6/6/6	0/2/2/2
2	3MQ	F	1172	-	-	0/6/6/6	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3MQ	S	1172	-	-	4/6/6/6	0/2/2/2
2	3MQ	B	1172	-	-	0/6/6/6	0/2/2/2
2	3MQ	G	1172	-	-	4/6/6/6	0/2/2/2
2	3MQ	P	1172	-	-	0/6/6/6	0/2/2/2
2	3MQ	T	1172	-	-	2/6/6/6	0/2/2/2
2	3MQ	N	1172	-	-	0/6/6/6	0/2/2/2
2	3MQ	E	1172	-	-	1/6/6/6	0/2/2/2
2	3MQ	I	1172	-	-	0/6/6/6	0/2/2/2
2	3MQ	D	1172	-	-	0/6/6/6	0/2/2/2
2	3MQ	Q	1172	-	-	3/6/6/6	0/2/2/2
2	3MQ	J	1172	-	-	0/6/6/6	0/2/2/2
2	3MQ	O	1172	-	-	0/6/6/6	0/2/2/2
2	3MQ	L	1172	-	-	1/6/6/6	0/2/2/2

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1172	3MQ	C06-C03	13.52	1.60	1.50
2	D	1172	3MQ	C06-C03	12.33	1.59	1.50
2	J	1172	3MQ	C06-C03	12.24	1.59	1.50
2	Q	1172	3MQ	C06-C03	11.98	1.59	1.50
2	R	1172	3MQ	C06-C03	11.78	1.59	1.50
2	G	1172	3MQ	C06-C03	11.69	1.59	1.50
2	A	1172	3MQ	C06-C03	10.14	1.58	1.50
2	T	1172	3MQ	C06-C03	9.46	1.57	1.50
2	M	1172	3MQ	C06-C03	9.38	1.57	1.50
2	P	1172	3MQ	C06-C03	8.66	1.56	1.50
2	N	1172	3MQ	C06-C03	7.85	1.56	1.50
2	L	1172	3MQ	C06-C03	6.64	1.55	1.50
2	I	1172	3MQ	C06-C03	6.59	1.55	1.50
2	B	1172	3MQ	C06-C03	6.27	1.55	1.50
2	F	1172	3MQ	C06-C03	5.05	1.54	1.50
2	C	1172	3MQ	C06-C03	4.67	1.53	1.50
2	H	1172	3MQ	C06-C03	4.46	1.53	1.50
2	M	1172	3MQ	O05-N04	4.08	1.49	1.42
2	J	1172	3MQ	O05-N04	3.88	1.49	1.42
2	E	1172	3MQ	C06-C03	3.65	1.53	1.50
2	O	1172	3MQ	C06-C03	3.63	1.52	1.50
2	G	1172	3MQ	O07-C06	3.57	1.53	1.41
2	K	1172	3MQ	C02-C03	-3.44	1.33	1.40
2	J	1172	3MQ	O07-C06	3.37	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1172	3MQ	C02-C03	-3.36	1.33	1.40
2	O	1172	3MQ	C01-C08	-3.31	1.38	1.46
2	A	1172	3MQ	O05-N04	3.24	1.48	1.42
2	E	1172	3MQ	C01-C08	-3.23	1.38	1.46
2	B	1172	3MQ	C02-C03	-3.16	1.33	1.40
2	H	1172	3MQ	C02-C03	-3.14	1.33	1.40
2	K	1172	3MQ	C06-C03	3.08	1.52	1.50
2	L	1172	3MQ	O05-N04	3.03	1.47	1.42
2	K	1172	3MQ	C01-C08	-3.02	1.39	1.46
2	S	1172	3MQ	O07-C06	2.99	1.51	1.41
2	Q	1172	3MQ	O07-C06	2.99	1.51	1.41
2	D	1172	3MQ	O07-C06	2.88	1.51	1.41
2	C	1172	3MQ	O05-N04	2.88	1.47	1.42
2	T	1172	3MQ	O05-N04	2.85	1.47	1.42
2	F	1172	3MQ	C02-C03	-2.81	1.34	1.40
2	L	1172	3MQ	C01-C08	-2.79	1.39	1.46
2	F	1172	3MQ	C01-C08	-2.79	1.39	1.46
2	N	1172	3MQ	C02-C03	-2.79	1.34	1.40
2	R	1172	3MQ	O07-C06	2.78	1.50	1.41
2	R	1172	3MQ	O05-N04	2.73	1.47	1.42
2	H	1172	3MQ	C01-C08	-2.70	1.40	1.46
2	C	1172	3MQ	C01-C08	-2.67	1.40	1.46
2	L	1172	3MQ	C02-C03	-2.67	1.34	1.40
2	M	1172	3MQ	C01-C08	-2.64	1.40	1.46
2	N	1172	3MQ	O05-N04	2.62	1.47	1.42
2	B	1172	3MQ	C01-C08	-2.57	1.40	1.46
2	S	1172	3MQ	O05-N04	2.54	1.47	1.42
2	I	1172	3MQ	C02-C03	-2.50	1.35	1.40
2	O	1172	3MQ	C02-C03	-2.46	1.35	1.40
2	D	1172	3MQ	C02-C03	-2.44	1.35	1.40
2	N	1172	3MQ	C01-C08	-2.42	1.40	1.46
2	P	1172	3MQ	C01-C08	-2.41	1.40	1.46
2	A	1172	3MQ	O07-C06	2.40	1.49	1.41
2	P	1172	3MQ	C02-C03	-2.39	1.35	1.40
2	E	1172	3MQ	C02-C03	-2.36	1.35	1.40
2	L	1172	3MQ	C03-N04	2.32	1.36	1.29
2	A	1172	3MQ	C02-C03	-2.32	1.35	1.40
2	B	1172	3MQ	O05-N04	2.31	1.46	1.42
2	G	1172	3MQ	O05-N04	2.29	1.46	1.42
2	J	1172	3MQ	C03-N04	2.29	1.36	1.29
2	S	1172	3MQ	C02-C03	-2.24	1.35	1.40
2	I	1172	3MQ	C01-C08	-2.24	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	1172	3MQ	C02-C03	-2.22	1.35	1.40
2	T	1172	3MQ	O07-C06	2.21	1.48	1.41
2	P	1172	3MQ	O07-C06	2.17	1.48	1.41
2	D	1172	3MQ	O05-N04	2.14	1.46	1.42
2	M	1172	3MQ	C03-N04	2.11	1.35	1.29
2	M	1172	3MQ	C02-C03	-2.11	1.35	1.40
2	M	1172	3MQ	O07-C06	2.08	1.48	1.41
2	H	1172	3MQ	O05-N04	2.08	1.46	1.42
2	L	1172	3MQ	C08-S09	-2.06	1.65	1.71
2	A	1172	3MQ	C03-N04	2.05	1.35	1.29
2	S	1172	3MQ	C03-N04	2.01	1.35	1.29

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	1172	3MQ	O05-C01-C02	-7.34	105.01	109.86
2	S	1172	3MQ	C02-C03-N04	-6.73	104.95	111.41
2	D	1172	3MQ	C02-C03-N04	-6.27	105.39	111.41
2	N	1172	3MQ	C02-C03-N04	-6.08	105.57	111.41
2	G	1172	3MQ	C02-C03-N04	-5.91	105.74	111.41
2	I	1172	3MQ	C02-C03-N04	-5.89	105.76	111.41
2	B	1172	3MQ	C02-C03-N04	-5.82	105.83	111.41
2	T	1172	3MQ	C02-C03-N04	-5.81	105.83	111.41
2	S	1172	3MQ	O05-C01-C02	-5.79	106.04	109.86
2	Q	1172	3MQ	C02-C03-N04	-5.70	105.94	111.41
2	J	1172	3MQ	C02-C03-N04	-5.68	105.96	111.41
2	M	1172	3MQ	C01-O05-N04	-5.48	102.31	108.38
2	S	1172	3MQ	O07-C06-C03	5.35	122.92	111.79
2	R	1172	3MQ	C02-C03-N04	-5.25	106.37	111.41
2	D	1172	3MQ	O05-C01-C02	-5.18	106.44	109.86
2	A	1172	3MQ	C02-C03-N04	-5.06	106.55	111.41
2	G	1172	3MQ	O05-C01-C02	-5.02	106.55	109.86
2	F	1172	3MQ	C01-O05-N04	-5.00	102.83	108.38
2	M	1172	3MQ	C02-C03-N04	-5.00	106.61	111.41
2	P	1172	3MQ	C02-C03-N04	-4.98	106.63	111.41
2	J	1172	3MQ	O05-C01-C02	-4.96	106.59	109.86
2	S	1172	3MQ	C01-C08-S09	4.81	131.10	119.15
2	D	1172	3MQ	C01-C08-S09	4.77	130.99	119.15
2	N	1172	3MQ	C01-O05-N04	-4.36	103.55	108.38
2	R	1172	3MQ	C01-C08-S09	4.36	129.97	119.15
2	F	1172	3MQ	C02-C03-N04	-4.30	107.28	111.41
2	E	1172	3MQ	C01-O05-N04	-4.27	103.65	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1172	3MQ	C02-C03-N04	-4.08	107.49	111.41
2	I	1172	3MQ	C01-O05-N04	-4.06	103.87	108.38
2	J	1172	3MQ	C01-C08-S09	3.98	129.03	119.15
2	A	1172	3MQ	C01-C08-S09	3.91	128.86	119.15
2	A	1172	3MQ	O05-C01-C02	-3.89	107.29	109.86
2	R	1172	3MQ	C12-C08-S09	-3.83	102.30	111.23
2	C	1172	3MQ	C01-O05-N04	-3.80	104.16	108.38
2	T	1172	3MQ	C01-O05-N04	-3.72	104.26	108.38
2	L	1172	3MQ	C01-O05-N04	-3.69	104.29	108.38
2	I	1172	3MQ	O05-N04-C03	3.68	110.42	105.74
2	B	1172	3MQ	C01-O05-N04	-3.67	104.31	108.38
2	P	1172	3MQ	C01-O05-N04	-3.67	104.31	108.38
2	K	1172	3MQ	C01-O05-N04	-3.62	104.36	108.38
2	I	1172	3MQ	C01-C08-S09	3.59	128.07	119.15
2	Q	1172	3MQ	C01-O05-N04	-3.58	104.41	108.38
2	R	1172	3MQ	O07-C06-C03	3.48	119.02	111.79
2	Q	1172	3MQ	O05-C01-C02	-3.42	107.60	109.86
2	Q	1172	3MQ	O05-N04-C03	3.41	110.08	105.74
2	D	1172	3MQ	O05-N04-C03	3.41	110.08	105.74
2	Q	1172	3MQ	O07-C06-C03	3.39	118.85	111.79
2	H	1172	3MQ	C02-C03-N04	-3.38	108.17	111.41
2	H	1172	3MQ	C01-O05-N04	-3.37	104.65	108.38
2	A	1172	3MQ	C01-O05-N04	-3.36	104.65	108.38
2	T	1172	3MQ	C11-C10-S09	-3.35	104.83	113.02
2	D	1172	3MQ	C01-O05-N04	-3.34	104.67	108.38
2	S	1172	3MQ	C12-C08-S09	-3.33	103.47	111.23
2	G	1172	3MQ	C11-C10-S09	-3.32	104.91	113.02
2	T	1172	3MQ	O07-C06-C03	3.31	118.68	111.79
2	L	1172	3MQ	C02-C03-N04	-3.31	108.23	111.41
2	N	1172	3MQ	O05-N04-C03	3.28	109.92	105.74
2	M	1172	3MQ	O07-C06-C03	3.27	118.59	111.79
2	G	1172	3MQ	C01-C08-S09	3.25	127.22	119.15
2	B	1172	3MQ	C01-C08-S09	3.24	127.19	119.15
2	T	1172	3MQ	C01-C08-S09	3.23	127.17	119.15
2	J	1172	3MQ	C12-C08-S09	-3.21	103.76	111.23
2	T	1172	3MQ	O05-C01-C02	-3.19	107.75	109.86
2	M	1172	3MQ	C11-C10-S09	-3.15	105.32	113.02
2	O	1172	3MQ	C01-O05-N04	-3.14	104.90	108.38
2	G	1172	3MQ	C10-S09-C08	3.14	97.97	92.33
2	M	1172	3MQ	O05-N04-C03	3.11	109.70	105.74
2	B	1172	3MQ	O05-C01-C02	-3.10	107.81	109.86
2	O	1172	3MQ	C11-C10-S09	-3.07	105.51	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1172	3MQ	C11-C10-S09	-3.06	105.54	113.02
2	G	1172	3MQ	C12-C08-S09	-3.05	104.12	111.23
2	I	1172	3MQ	C11-C10-S09	-3.05	105.56	113.02
2	A	1172	3MQ	C12-C08-S09	-3.02	104.19	111.23
2	C	1172	3MQ	C01-C08-S09	3.02	126.64	119.15
2	R	1172	3MQ	C11-C10-S09	-3.01	105.66	113.02
2	T	1172	3MQ	C10-S09-C08	3.00	97.71	92.33
2	P	1172	3MQ	C11-C10-S09	-2.97	105.76	113.02
2	K	1172	3MQ	C02-C03-N04	-2.95	108.57	111.41
2	T	1172	3MQ	O05-N04-C03	2.94	109.48	105.74
2	Q	1172	3MQ	C12-C08-S09	-2.94	104.39	111.23
2	F	1172	3MQ	C11-C10-S09	-2.90	105.94	113.02
2	S	1172	3MQ	O05-N04-C03	2.88	109.41	105.74
2	C	1172	3MQ	C02-C01-C08	-2.85	124.37	131.64
2	R	1172	3MQ	C10-S09-C08	2.85	97.45	92.33
2	F	1172	3MQ	O05-N04-C03	2.85	109.37	105.74
2	L	1172	3MQ	C10-S09-C08	2.85	97.44	92.33
2	J	1172	3MQ	C01-O05-N04	-2.84	105.23	108.38
2	B	1172	3MQ	O07-C06-C03	2.83	117.67	111.79
2	C	1172	3MQ	O05-C01-C02	-2.80	108.01	109.86
2	T	1172	3MQ	C12-C08-S09	-2.79	104.73	111.23
2	B	1172	3MQ	O05-N04-C03	2.78	109.28	105.74
2	Q	1172	3MQ	C01-C08-S09	2.78	126.06	119.15
2	S	1172	3MQ	C01-O05-N04	-2.76	105.32	108.38
2	A	1172	3MQ	O07-C06-C03	2.74	117.50	111.79
2	L	1172	3MQ	C06-C03-C02	-2.71	122.20	128.84
2	N	1172	3MQ	C11-C10-S09	-2.70	106.43	113.02
2	C	1172	3MQ	C06-C03-C02	-2.68	122.27	128.84
2	P	1172	3MQ	O05-N04-C03	2.67	109.13	105.74
2	M	1172	3MQ	C10-S09-C08	2.66	97.11	92.33
2	Q	1172	3MQ	C11-C10-S09	-2.65	106.55	113.02
2	D	1172	3MQ	C12-C08-S09	-2.64	105.08	111.23
2	H	1172	3MQ	C06-C03-C02	-2.63	122.40	128.84
2	I	1172	3MQ	C12-C08-S09	-2.62	105.14	111.23
2	E	1172	3MQ	C11-C10-S09	-2.62	106.63	113.02
2	G	1172	3MQ	O05-N04-C03	2.60	109.05	105.74
2	I	1172	3MQ	O05-C01-C02	-2.59	108.15	109.86
2	K	1172	3MQ	C11-C10-S09	-2.59	106.70	113.02
2	S	1172	3MQ	C11-C10-S09	-2.58	106.72	113.02
2	H	1172	3MQ	C02-C01-C08	-2.56	125.11	131.64
2	M	1172	3MQ	C01-C08-S09	2.53	125.44	119.15
2	D	1172	3MQ	O07-C06-C03	2.52	117.02	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1172	3MQ	C11-C10-S09	-2.51	106.88	113.02
2	M	1172	3MQ	C12-C08-S09	-2.51	105.39	111.23
2	L	1172	3MQ	C01-C08-S09	2.51	125.38	119.15
2	L	1172	3MQ	C02-C01-C08	-2.50	125.27	131.64
2	E	1172	3MQ	O05-N04-C03	2.49	108.90	105.74
2	J	1172	3MQ	C11-C10-S09	-2.48	106.97	113.02
2	N	1172	3MQ	C10-S09-C08	2.46	96.74	92.33
2	K	1172	3MQ	C01-C08-S09	2.45	125.23	119.15
2	I	1172	3MQ	C10-S09-C08	2.45	96.72	92.33
2	K	1172	3MQ	C02-C01-C08	-2.43	125.45	131.64
2	E	1172	3MQ	C02-C03-N04	-2.40	109.11	111.41
2	H	1172	3MQ	C01-C08-S09	2.40	125.10	119.15
2	A	1172	3MQ	C11-C10-S09	-2.39	107.18	113.02
2	A	1172	3MQ	O05-N04-C03	2.39	108.78	105.74
2	P	1172	3MQ	C10-S09-C08	2.34	96.53	92.33
2	P	1172	3MQ	C12-C08-S09	-2.32	105.82	111.23
2	L	1172	3MQ	C12-C08-S09	-2.29	105.90	111.23
2	O	1172	3MQ	C10-S09-C08	2.28	96.42	92.33
2	B	1172	3MQ	C11-C10-S09	-2.27	107.47	113.02
2	O	1172	3MQ	C02-C03-N04	-2.27	109.23	111.41
2	F	1172	3MQ	C02-C01-C08	-2.27	125.87	131.64
2	P	1172	3MQ	O05-C01-C02	-2.25	108.38	109.86
2	G	1172	3MQ	C01-O05-N04	-2.23	105.91	108.38
2	Q	1172	3MQ	C10-S09-C08	2.22	96.32	92.33
2	J	1172	3MQ	C10-S09-C08	2.22	96.32	92.33
2	I	1172	3MQ	O07-C06-C03	2.22	116.41	111.79
2	L	1172	3MQ	O07-C06-C03	2.22	116.41	111.79
2	H	1172	3MQ	C11-C10-S09	-2.22	107.60	113.02
2	N	1172	3MQ	O07-C06-C03	2.19	116.35	111.79
2	C	1172	3MQ	C11-C10-S09	-2.18	107.68	113.02
2	P	1172	3MQ	O07-C06-C03	2.18	116.33	111.79
2	F	1172	3MQ	C01-C08-S09	2.17	124.55	119.15
2	N	1172	3MQ	C12-C08-S09	-2.14	106.24	111.23
2	D	1172	3MQ	C02-C01-C08	-2.11	126.25	131.64
2	J	1172	3MQ	O05-N04-C03	2.08	108.39	105.74
2	F	1172	3MQ	C10-S09-C08	2.04	95.99	92.33
2	K	1172	3MQ	C06-C03-C02	-2.03	123.85	128.84
2	S	1172	3MQ	C10-S09-C08	2.03	95.98	92.33

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1172	3MQ	N04-C03-C06-O07
2	E	1172	3MQ	N04-C03-C06-O07
2	G	1172	3MQ	C02-C01-C08-S09
2	G	1172	3MQ	C02-C01-C08-C12
2	H	1172	3MQ	N04-C03-C06-O07
2	K	1172	3MQ	N04-C03-C06-O07
2	L	1172	3MQ	N04-C03-C06-O07
2	S	1172	3MQ	C02-C01-C08-S09
2	S	1172	3MQ	C02-C01-C08-C12
2	S	1172	3MQ	O05-C01-C08-S09
2	S	1172	3MQ	O05-C01-C08-C12
2	Q	1172	3MQ	C02-C01-C08-S09
2	Q	1172	3MQ	C02-C01-C08-C12
2	R	1172	3MQ	C02-C01-C08-C12
2	G	1172	3MQ	O05-C01-C08-C12
2	R	1172	3MQ	O05-C01-C08-C12
2	K	1172	3MQ	C02-C03-C06-O07
2	T	1172	3MQ	C02-C01-C08-C12
2	G	1172	3MQ	O05-C01-C08-S09
2	R	1172	3MQ	O05-C01-C08-S09
2	Q	1172	3MQ	O05-C01-C08-C12
2	T	1172	3MQ	O05-C01-C08-C12

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	1172	3MQ	3	0
2	M	1172	3MQ	1	0
2	H	1172	3MQ	1	0
2	K	1172	3MQ	1	0
2	A	1172	3MQ	3	0
2	S	1172	3MQ	3	0
2	G	1172	3MQ	2	0
2	P	1172	3MQ	3	0
2	T	1172	3MQ	2	0
2	I	1172	3MQ	1	0
2	D	1172	3MQ	1	0
2	Q	1172	3MQ	2	0

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	167/171 (97%)	0.46	6 (3%) 46 41	37, 49, 65, 106	0
1	B	170/171 (99%)	0.59	12 (7%) 22 19	37, 51, 72, 138	0
1	C	168/171 (98%)	0.71	10 (5%) 27 24	43, 55, 75, 104	0
1	D	170/171 (99%)	0.92	17 (10%) 12 10	43, 58, 92, 133	0
1	E	168/171 (98%)	0.64	8 (4%) 35 31	40, 51, 72, 109	0
1	F	169/171 (98%)	0.58	6 (3%) 46 41	39, 51, 71, 129	0
1	G	166/171 (97%)	0.78	7 (4%) 40 36	45, 57, 76, 125	0
1	H	167/171 (97%)	0.78	9 (5%) 31 27	44, 56, 76, 119	0
1	I	169/171 (98%)	0.51	7 (4%) 41 37	36, 47, 65, 125	0
1	J	168/171 (98%)	0.37	4 (2%) 59 55	35, 46, 64, 103	0
1	K	169/171 (98%)	0.77	13 (7%) 19 17	41, 55, 75, 148	0
1	L	170/171 (99%)	0.62	9 (5%) 32 28	39, 51, 68, 129	0
1	M	168/171 (98%)	0.46	4 (2%) 59 55	38, 48, 67, 107	0
1	N	168/171 (98%)	0.42	4 (2%) 59 55	37, 48, 70, 126	0
1	O	170/171 (99%)	0.80	11 (6%) 25 22	43, 56, 83, 133	0
1	P	170/171 (99%)	0.74	11 (6%) 25 22	46, 55, 75, 125	0
1	Q	168/171 (98%)	0.83	16 (9%) 14 12	39, 55, 80, 138	0
1	R	167/171 (97%)	0.74	10 (5%) 27 24	40, 54, 75, 117	0
1	S	167/171 (97%)	1.13	19 (11%) 10 8	49, 62, 82, 107	0
1	T	167/171 (97%)	0.92	16 (9%) 13 11	44, 59, 88, 140	0
All	All	3366/3420 (98%)	0.69	199 (5%) 28 24	35, 53, 78, 148	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	135	ASN	6.7
1	H	2	THR	6.0
1	M	2	THR	5.9
1	D	138	LEU	5.3
1	T	2	THR	5.2
1	Q	3	LYS	5.2
1	Q	6	ALA	5.2
1	H	3	LYS	5.2
1	R	3	LYS	5.1
1	D	2	THR	5.1
1	M	138	LEU	5.1
1	J	135	ASN	5.0
1	F	138	LEU	5.0
1	E	2	THR	5.0
1	R	138	LEU	5.0
1	F	2	THR	4.9
1	L	2	THR	4.8
1	S	138	LEU	4.8
1	L	138	LEU	4.7
1	B	3	LYS	4.6
1	C	138	LEU	4.6
1	G	2	THR	4.6
1	B	135	ASN	4.6
1	E	138	LEU	4.4
1	A	2	THR	4.3
1	N	136	ARG	4.3
1	R	134	ILE	4.3
1	F	3	LYS	4.2
1	C	135	ASN	4.2
1	K	138	LEU	4.2
1	L	135	ASN	4.0
1	T	3	LYS	4.0
1	J	2	THR	4.0
1	S	2	THR	4.0
1	P	3	LYS	4.0
1	B	23	PRO	3.9
1	H	138	LEU	3.9
1	T	6	ALA	3.9
1	R	2	THR	3.9
1	T	138	LEU	3.8
1	S	134	ILE	3.8
1	E	135	ASN	3.7
1	M	3	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	J	138	LEU	3.7
1	T	171	PHE	3.7
1	T	170	SER	3.6
1	Q	138	LEU	3.6
1	A	3	LYS	3.5
1	N	3	LYS	3.5
1	Q	2	THR	3.5
1	T	134	ILE	3.5
1	D	45	VAL	3.5
1	D	3	LYS	3.5
1	I	2	THR	3.5
1	N	2	THR	3.4
1	S	3	LYS	3.4
1	B	2	THR	3.4
1	G	3	LYS	3.4
1	K	2	THR	3.3
1	O	2	THR	3.3
1	K	3	LYS	3.3
1	P	2	THR	3.3
1	F	136	ARG	3.3
1	A	138	LEU	3.2
1	Q	23	PRO	3.2
1	Q	135	ASN	3.2
1	D	166	THR	3.2
1	I	135	ASN	3.1
1	P	134	ILE	3.1
1	K	136	ARG	3.1
1	B	137	SER	3.1
1	P	158	GLU	3.1
1	C	3	LYS	3.1
1	K	23	PRO	3.1
1	O	136	ARG	3.0
1	K	121	ALA	3.0
1	I	138	LEU	3.0
1	L	137	SER	3.0
1	O	138	LEU	2.9
1	D	135	ASN	2.9
1	G	134	ILE	2.9
1	Q	5	HIS	2.9
1	I	136	ARG	2.9
1	B	138	LEU	2.9
1	C	76	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	4	GLN	2.9
1	F	135	ASN	2.9
1	S	163	GLY	2.9
1	C	2	THR	2.9
1	C	166	THR	2.8
1	R	98	GLY	2.8
1	D	134	ILE	2.8
1	O	137	SER	2.8
1	P	138	LEU	2.8
1	R	10	GLU	2.8
1	S	38	ARG	2.8
1	C	110	GLU	2.8
1	D	9	ARG	2.8
1	E	3	LYS	2.8
1	A	134	ILE	2.8
1	G	4	GLN	2.8
1	D	23	PRO	2.7
1	Q	120	THR	2.7
1	D	136	ARG	2.7
1	E	4	GLN	2.7
1	P	109	GLY	2.7
1	Q	163	GLY	2.7
1	P	120	THR	2.7
1	O	3	LYS	2.6
1	S	76	VAL	2.6
1	P	137	SER	2.6
1	B	134	ILE	2.6
1	C	68	ALA	2.6
1	J	3	LYS	2.6
1	L	3	LYS	2.6
1	T	109	GLY	2.5
1	P	135	ASN	2.5
1	I	3	LYS	2.5
1	B	136	ARG	2.5
1	E	109	GLY	2.5
1	O	171	PHE	2.5
1	S	171	PHE	2.5
1	R	109	GLY	2.5
1	K	110	GLU	2.5
1	T	168	THR	2.5
1	K	171	PHE	2.5
1	N	135	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	23	PRO	2.4
1	H	16	SER	2.4
1	H	134	ILE	2.4
1	K	4	GLN	2.4
1	S	21	PHE	2.4
1	O	23	PRO	2.4
1	C	134	ILE	2.4
1	S	132	ARG	2.4
1	S	152	ARG	2.4
1	O	135	ASN	2.4
1	K	170	SER	2.4
1	S	5	HIS	2.4
1	I	110	GLU	2.4
1	L	148	SER	2.3
1	T	108	SER	2.3
1	Q	14	ARG	2.3
1	A	10	GLU	2.3
1	Q	171	PHE	2.3
1	L	72	GLU	2.3
1	G	24	GLY	2.3
1	Q	4	GLN	2.3
1	T	24	GLY	2.3
1	B	158	GLU	2.3
1	E	153	GLU	2.3
1	S	25	ASN	2.3
1	Q	134	ILE	2.3
1	Q	21	PHE	2.3
1	O	109	GLY	2.2
1	S	91	GLY	2.2
1	S	39	ILE	2.2
1	T	89	LEU	2.2
1	O	158	GLU	2.2
1	P	136	ARG	2.2
1	D	25	ASN	2.2
1	K	135	ASN	2.2
1	L	134	ILE	2.2
1	R	108	SER	2.2
1	R	170	SER	2.2
1	C	169	ASP	2.2
1	D	8	THR	2.2
1	G	103	GLY	2.2
1	T	23	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	97	GLN	2.2
1	T	103	GLY	2.1
1	B	170	SER	2.1
1	P	171	PHE	2.1
1	K	45	VAL	2.1
1	Q	121	ALA	2.1
1	D	108	SER	2.1
1	D	167	SER	2.1
1	S	167	SER	2.1
1	R	23	PRO	2.1
1	B	9	ARG	2.1
1	Q	132	ARG	2.1
1	D	69	CYS	2.1
1	H	170	SER	2.1
1	L	167	SER	2.1
1	S	40	VAL	2.1
1	A	73	GLY	2.1
1	H	161	ARG	2.1
1	T	5	HIS	2.1
1	G	121	ALA	2.0
1	H	17	ARG	2.0
1	H	68	ALA	2.0
1	T	140	LEU	2.0
1	O	60	ILE	2.0
1	S	8	THR	2.0
1	S	139	VAL	2.0
1	B	146	THR	2.0
1	D	36	ILE	2.0
1	F	134	ILE	2.0
1	E	170	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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
2	3MQ	D	1172	12/12	0.83	0.16	53,57,62,67	0
2	3MQ	J	1172	12/12	0.83	0.17	43,51,63,65	0
2	3MQ	P	1172	12/12	0.83	0.16	52,65,70,76	0
2	3MQ	R	1172	12/12	0.83	0.16	58,64,69,72	0
2	3MQ	S	1172	12/12	0.83	0.18	61,73,76,76	0
2	3MQ	T	1172	12/12	0.83	0.17	65,75,77,80	0
2	3MQ	F	1172	12/12	0.87	0.14	53,57,66,69	0
2	3MQ	Q	1172	12/12	0.88	0.15	56,63,68,70	0
2	3MQ	G	1172	12/12	0.88	0.16	49,61,65,66	0
2	3MQ	O	1172	12/12	0.89	0.15	51,60,66,67	0
2	3MQ	M	1172	12/12	0.89	0.14	41,54,63,75	0
2	3MQ	A	1172	12/12	0.90	0.14	39,49,61,73	0
2	3MQ	I	1172	12/12	0.90	0.13	47,52,57,63	0
2	3MQ	N	1172	12/12	0.90	0.14	48,53,60,66	0
2	3MQ	H	1172	12/12	0.91	0.15	57,61,65,65	0
2	3MQ	E	1172	12/12	0.92	0.13	49,58,61,64	0
2	3MQ	L	1172	12/12	0.93	0.12	53,56,60,70	0
2	3MQ	B	1172	12/12	0.94	0.11	49,54,60,75	0
2	3MQ	C	1172	12/12	0.95	0.11	49,60,66,72	0
2	3MQ	K	1172	12/12	0.96	0.09	53,55,58,61	0

6.5 Other polymers

There are no such residues in this entry.