



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:08 PM UTC

PDB ID : 2B2T / pdb_00002b2t
Title : Tandem chromodomains of human CHD1 complexed with Histone H3 Tail containing trimethyllysine 4 and phosphothreonine 3
Authors : Flanagan IV, J.F.; Mi, L.-Z.; Chruszcz, M.; Cymborowski, M.; Clines, K.L.; Kim, Y.; Minor, W.; Rastinejad, F.; Khorasanizadeh, S.
Deposited on : 2005-09-19
Resolution : 2.45 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

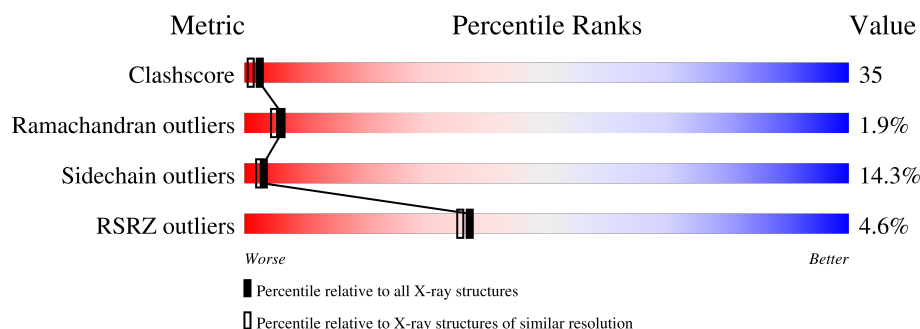
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	187	5% 55% 28% 10% • 6%
1	B	187	2% 52% 30% 11% 7%
2	C	115	5% 37% 22% 14% • 25%
3	D	20	10% 5% 5% 15% 75%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3868 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 Chromodomain-helicase-DNA-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	Se	0	0	0
			1448	914	249	278	4	3			
1	B	174	Total	C	N	O	S	Se	0	0	0
			1410	890	240	273	4	3			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	SEE REMARK 999	UNP O14646
A	2	LYS	-	cloning artifact	UNP O14646
A	3	LYS	-	cloning artifact	UNP O14646
A	4	HIS	-	expression tag	UNP O14646
A	5	HIS	-	expression tag	UNP O14646
A	6	HIS	-	expression tag	UNP O14646
A	7	HIS	-	expression tag	UNP O14646
A	8	HIS	-	expression tag	UNP O14646
A	9	HIS	-	expression tag	UNP O14646
A	20	MSE	MET	modified residue	UNP O14646
A	88	MSE	MET	modified residue	UNP O14646
A	178	MSE	CYS	SEE REMARK 999	UNP O14646
A	186	LYS	-	cloning artifact	UNP O14646
A	187	LYS	-	cloning artifact	UNP O14646
B	1	MSE	-	SEE REMARK 999	UNP O14646
B	2	LYS	-	cloning artifact	UNP O14646
B	3	LYS	-	cloning artifact	UNP O14646
B	4	HIS	-	expression tag	UNP O14646
B	5	HIS	-	expression tag	UNP O14646
B	6	HIS	-	expression tag	UNP O14646
B	7	HIS	-	expression tag	UNP O14646
B	8	HIS	-	expression tag	UNP O14646
B	9	HIS	-	expression tag	UNP O14646
B	20	MSE	MET	modified residue	UNP O14646
B	88	MSE	MET	modified residue	UNP O14646

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Chain	Residue	Modelled	Actual	Comment	Reference
B	178	MSE	CYS	SEE REMARK 999	UNP O14646
B	186	LYS	-	cloning artifact	UNP O14646
B	187	LYS	-	cloning artifact	UNP O14646

- Molecule 2 is a protein called Chromodomain-helicase-DNA-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	86	Total	C	N	O	S	Se	0	0	0
			704	443	124	134	1	2			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	-	SEE REMARK 999	UNP O14646
C	2	LYS	-	cloning artifact	UNP O14646
C	3	LYS	-	cloning artifact	UNP O14646
C	4	HIS	-	expression tag	UNP O14646
C	5	HIS	-	expression tag	UNP O14646
C	6	HIS	-	expression tag	UNP O14646
C	7	HIS	-	expression tag	UNP O14646
C	8	HIS	-	expression tag	UNP O14646
C	9	HIS	-	expression tag	UNP O14646
C	20	MSE	MET	modified residue	UNP O14646
C	88	MSE	MET	modified residue	UNP O14646

- Molecule 3 is a protein called Histone H3 tail.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	P	0	0	0
			48	27	10	10	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	3	TPO	THR	modified residue	UNP P68431
D	4	M3L	LYS	modified residue	UNP P68431
D	20	TYR	-	SEE REMARK 999	UNP P68431

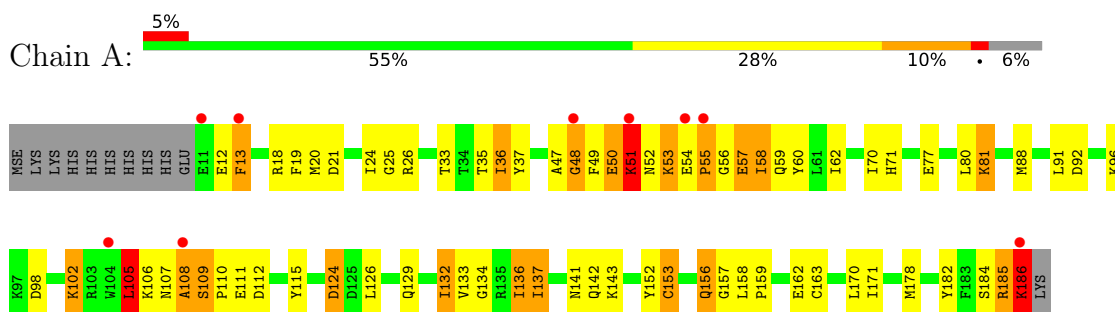
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total 130	O 130	0	0
4	B	80	Total 80	O 80	0	0
4	C	45	Total 45	O 45	0	0
4	D	3	Total 3	O 3	0	0

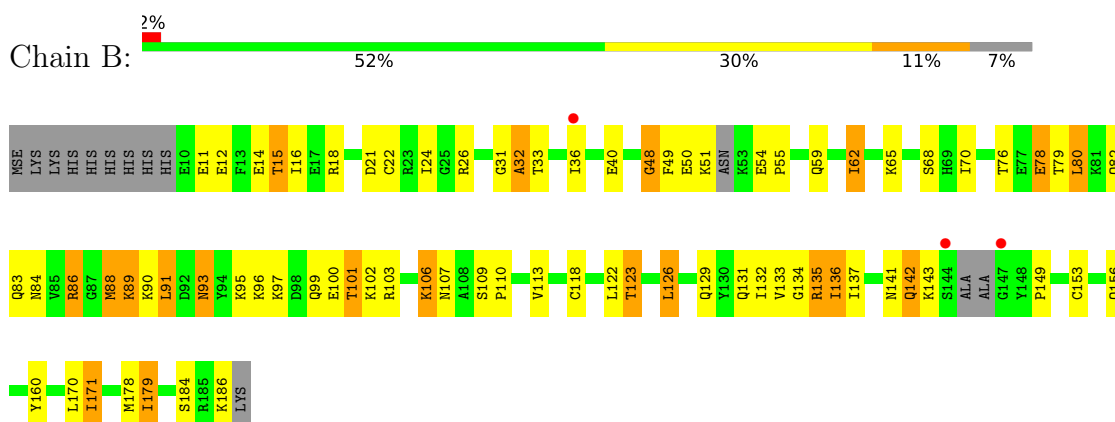
3 Residue-property plots

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 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.

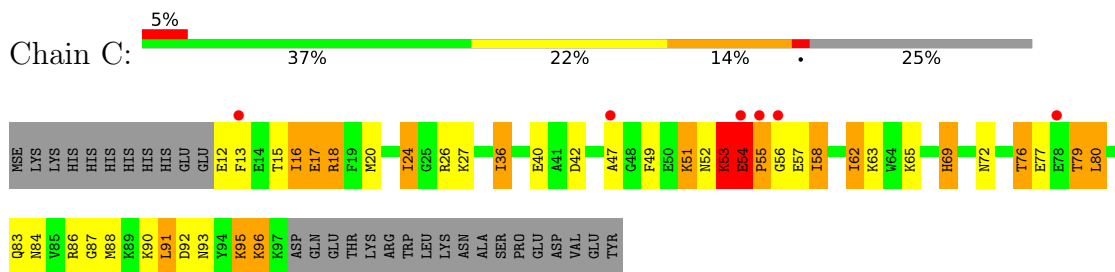
- Molecule 1: Chromodomain-helicase-DNA-binding protein 1



- Molecule 1: Chromodomain-helicase-DNA-binding protein 1



- Molecule 2: Chromodomain-helicase-DNA-binding protein 1



- Molecule 3: Histone H3 tail



L1	R2	T3	K4	Q5	THR	ALA	ARG	LYS	SER	THR	GLY	GLY	LYS	ALA	PRO	ARG	LYS	GLN	TYR
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.99Å 54.69Å 100.99Å 90.00° 112.15° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 20.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.45) 92.1 (20.00-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.266 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3868	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: M3L, TPO

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	0.49	0/1481	1.22	15/1990 (0.8%)
1	B	0.42	0/1440	1.12	14/1936 (0.7%)
2	C	0.45	0/717	1.08	6/958 (0.6%)
3	D	0.08	0/24	0.42	0/30
All	All	0.45	0/3662	1.15	35/4914 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	C	0	2
All	All	0	4

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	LYS	N-CA-C	-14.04	83.72	109.56
1	B	142	GLN	N-CA-C	-12.40	94.82	110.19
1	B	33	THR	N-CA-C	-11.65	95.65	113.02
2	C	52	ASN	N-CA-C	-11.49	98.91	113.16
1	A	108	ALA	CB-CA-C	10.73	131.77	110.42
1	B	32	ALA	CB-CA-C	-10.62	89.29	110.42
1	A	105	LEU	N-CA-C	-10.26	96.57	113.50
1	A	109	SER	N-CA-C	-10.14	97.12	110.40
1	A	53	LYS	N-CA-C	9.38	124.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	LYS	CB-CA-C	8.81	126.84	110.10
1	A	57	GLU	N-CA-C	-8.47	94.43	108.32
1	A	62	ILE	N-CA-C	7.70	118.95	108.17
1	A	56	GLY	N-CA-C	-7.50	95.39	113.18
1	B	14	GLU	N-CA-C	-7.35	97.84	109.23
1	B	49	PHE	CB-CA-C	-6.94	99.43	109.84
1	A	108	ALA	N-CA-C	-6.94	96.03	110.80
1	B	62	ILE	N-CA-C	6.57	117.31	108.11
1	A	110	PRO	N-CA-C	-6.49	105.74	113.86
2	C	62	ILE	N-CA-C	6.42	118.28	108.71
1	A	21	ASP	N-CA-C	6.39	119.17	110.35
1	B	102	LYS	N-CA-C	-6.31	104.50	111.82
1	B	11	GLU	CB-CA-C	6.27	122.91	110.42
2	C	18	ARG	N-CA-C	6.15	117.86	108.52
2	C	16	ILE	CB-CA-C	-5.69	104.08	110.96
1	A	153	CYS	N-CA-C	5.66	118.70	109.59
1	A	136	ILE	N-CA-C	-5.59	101.61	109.21
1	B	32	ALA	N-CA-C	5.48	122.48	110.80
1	B	49	PHE	N-CA-C	5.35	118.11	110.24
1	B	110	PRO	N-CA-C	-5.35	106.56	113.57
1	B	33	THR	N-CA-CB	5.31	120.08	111.27
1	A	185	ARG	N-CA-C	-5.29	106.90	113.19
1	B	184	SER	N-CA-C	-5.29	106.09	112.54
1	B	24	ILE	N-CA-C	-5.24	100.83	108.17
2	C	58	ILE	N-CA-C	-5.24	100.22	108.23
2	C	69	HIS	N-CA-C	5.05	118.54	112.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	GLY	Peptide
1	B	48	GLY	Peptide
2	C	53	LYS	Peptide
2	C	54	GLU	Peptide

5.2 Too-close contacts [i](#)

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	1448	0	1377	82	1
1	B	1410	0	1312	74	0
2	C	704	0	686	85	0
3	D	48	0	52	10	0
4	A	130	0	0	22	0
4	B	80	0	0	4	0
4	C	45	0	0	2	0
4	D	3	0	0	0	0
All	All	3868	0	3427	243	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 35.

All (243) 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:54:GLU:HG3	2:C:56:GLY:CA	1.55	1.36
1:A:55:PRO:HB3	4:A:311:HOH:O	1.28	1.27
2:C:54:GLU:HA	2:C:55:PRO:C	1.66	1.18
2:C:54:GLU:CG	2:C:56:GLY:HA3	1.75	1.17
2:C:54:GLU:HG3	2:C:56:GLY:N	1.61	1.14
2:C:26:ARG:HA	2:C:55:PRO:HB2	1.29	1.12
2:C:54:GLU:HG3	2:C:56:GLY:HA3	1.09	1.07
1:A:54:GLU:HG3	1:A:55:PRO:CD	1.86	1.05
1:A:54:GLU:HG3	1:A:55:PRO:HD2	1.34	1.04
1:A:54:GLU:CG	1:A:55:PRO:HD2	1.92	0.99
2:C:54:GLU:CG	2:C:56:GLY:CA	2.35	0.99
2:C:27:LYS:H	2:C:55:PRO:CB	1.77	0.97
1:B:103:ARG:O	1:B:106:LYS:HD2	1.65	0.95
2:C:24:ILE:HD13	2:C:51:LYS:HE3	1.44	0.95
2:C:54:GLU:CG	2:C:56:GLY:N	2.30	0.93
4:A:313:HOH:O	1:B:18:ARG:HD2	1.72	0.89
2:C:24:ILE:O	2:C:24:ILE:HD12	1.70	0.89
2:C:27:LYS:H	2:C:55:PRO:HB3	1.37	0.86
2:C:15:THR:HG23	2:C:86:ARG:HB2	1.59	0.83
1:A:185:ARG:O	1:A:186:LYS:HB2	1.79	0.80
1:B:135:ARG:HA	1:B:178:MSE:CE	2.11	0.80
2:C:54:GLU:HA	2:C:56:GLY:N	1.95	0.80
1:A:26:ARG:HH21	1:A:53:LYS:HD2	1.46	0.80
2:C:54:GLU:CA	2:C:55:PRO:C	2.49	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:92:ASP:O	2:C:96:LYS:HD2	1.85	0.77
3:D:4:M3L:O	3:D:5:GLN:CB	2.34	0.76
1:A:51:LYS:O	1:A:52:ASN:HB3	1.85	0.76
1:A:54:GLU:HG3	1:A:55:PRO:HD3	1.68	0.74
2:C:16:ILE:HD12	2:C:62:ILE:HD13	1.69	0.74
2:C:49:PHE:HE2	2:C:55:PRO:O	1.70	0.74
1:B:135:ARG:HA	1:B:178:MSE:HE3	1.70	0.74
1:A:12:GLU:O	1:A:13:PHE:HB2	1.89	0.72
2:C:13:PHE:HB2	2:C:86:ARG:HH11	1.52	0.72
1:B:91:LEU:HD22	1:B:95:LYS:HD2	1.69	0.72
1:B:86:ARG:HD3	4:B:246:HOH:O	1.89	0.72
1:A:55:PRO:CB	4:A:311:HOH:O	2.03	0.72
3:D:3:TPO:O2P	3:D:3:TPO:HG21	1.89	0.71
2:C:13:PHE:HB2	2:C:86:ARG:NH1	2.05	0.71
1:B:137:ILE:CD1	1:B:160:TYR:HE2	2.04	0.71
2:C:24:ILE:CD1	2:C:51:LYS:HE3	2.20	0.70
2:C:49:PHE:CE2	2:C:55:PRO:O	2.44	0.70
2:C:26:ARG:HH21	2:C:53:LYS:HE2	1.56	0.68
2:C:27:LYS:HG3	2:C:55:PRO:HA	1.76	0.68
2:C:36:ILE:HD13	2:C:36:ILE:O	1.94	0.68
1:B:76:THR:HG23	1:B:79:THR:H	1.58	0.68
2:C:26:ARG:CA	2:C:55:PRO:HB2	2.16	0.68
2:C:27:LYS:HG2	2:C:57:GLU:CG	2.24	0.68
1:A:55:PRO:CA	4:A:311:HOH:O	2.38	0.67
1:B:153:CYS:SG	1:B:171:ILE:HD12	2.34	0.67
1:B:91:LEU:CD2	1:B:95:LYS:HD2	2.25	0.67
2:C:91:LEU:HD22	2:C:95:LYS:HD3	1.77	0.67
2:C:27:LYS:HG2	2:C:57:GLU:HG3	1.78	0.66
1:B:134:GLY:C	1:B:178:MSE:HE2	2.21	0.66
1:A:35:THR:HG21	3:D:4:M3L:HG2	1.78	0.65
1:B:36:ILE:O	1:B:40:GLU:HG3	1.96	0.65
1:A:51:LYS:O	1:A:51:LYS:CG	2.44	0.65
2:C:87:GLY:O	2:C:90:LYS:HG2	1.97	0.65
1:B:136:ILE:CD1	1:B:179:ILE:HG22	2.27	0.65
1:A:137:ILE:CG2	1:A:152:TYR:HD2	2.10	0.65
2:C:13:PHE:HB3	2:C:86:ARG:NE	2.11	0.65
1:B:133:VAL:HG21	1:B:171:ILE:HD13	1.78	0.64
1:B:136:ILE:HD12	1:B:179:ILE:HG22	1.78	0.64
2:C:54:GLU:CA	2:C:56:GLY:N	2.59	0.64
1:A:105:LEU:O	1:A:106:LYS:C	2.39	0.64
2:C:13:PHE:CB	2:C:86:ARG:NE	2.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:HD11	1:A:156:GLN:NE2	2.13	0.63
2:C:13:PHE:CB	2:C:86:ARG:HE	2.11	0.63
2:C:27:LYS:N	2:C:55:PRO:HB3	2.11	0.63
1:A:137:ILE:HG22	1:A:152:TYR:HD2	1.64	0.63
3:D:4:M3L:O	3:D:5:GLN:HB3	1.97	0.63
2:C:16:ILE:CD1	2:C:62:ILE:HD13	2.29	0.63
1:A:134:GLY:O	1:A:178:MSE:HE2	2.00	0.62
1:B:22:CYS:HA	1:B:59:GLN:O	2.00	0.62
1:A:132:ILE:HG12	1:A:156:GLN:HG3	1.82	0.61
1:A:33:THR:HG23	4:A:191:HOH:O	1.99	0.61
1:B:118:CYS:O	1:B:122:LEU:HG	1.99	0.61
1:A:49:PHE:CG	1:A:50:GLU:N	2.69	0.61
1:A:54:GLU:O	1:A:55:PRO:C	2.44	0.61
1:B:122:LEU:O	1:B:126:LEU:HD22	2.01	0.61
2:C:76:THR:HG21	4:C:153:HOH:O	2.01	0.61
1:A:132:ILE:CG1	1:A:156:GLN:HG3	2.31	0.60
2:C:27:LYS:N	2:C:55:PRO:CB	2.57	0.60
2:C:54:GLU:CG	2:C:56:GLY:H	2.14	0.60
1:B:15:THR:HG21	1:B:65:LYS:HE2	1.84	0.60
1:B:137:ILE:HD12	1:B:160:TYR:HE2	1.64	0.60
1:B:79:THR:O	1:B:83:GLN:NE2	2.34	0.59
1:A:159:PRO:HB3	1:B:123:THR:HG21	1.82	0.59
1:B:79:THR:O	1:B:82:GLN:HG2	2.02	0.59
1:A:51:LYS:O	1:A:52:ASN:CB	2.51	0.59
2:C:51:LYS:HD3	2:C:51:LYS:N	2.17	0.59
1:B:106:LYS:HD3	1:B:107:ASN:H	1.68	0.58
2:C:95:LYS:C	2:C:96:LYS:HG3	2.27	0.58
2:C:27:LYS:H	2:C:55:PRO:CA	2.17	0.58
2:C:49:PHE:CD2	2:C:53:LYS:HD2	2.39	0.57
1:B:97:LYS:O	1:B:101:THR:HG23	2.04	0.57
1:A:152:TYR:OH	1:B:97:LYS:HE2	2.06	0.56
2:C:54:GLU:HA	2:C:55:PRO:O	2.01	0.56
1:B:153:CYS:SG	1:B:171:ILE:CD1	2.94	0.56
1:A:54:GLU:HG2	1:A:55:PRO:HD2	1.84	0.56
2:C:53:LYS:HB2	2:C:55:PRO:HG2	1.88	0.56
1:B:103:ARG:C	1:B:106:LYS:HD2	2.31	0.55
1:B:50:GLU:O	1:B:51:LYS:C	2.48	0.55
1:A:53:LYS:O	1:A:54:GLU:C	2.49	0.55
1:B:103:ARG:O	1:B:106:LYS:CD	2.46	0.55
1:B:31:GLY:O	1:B:32:ALA:HB3	2.07	0.54
2:C:49:PHE:HD2	2:C:53:LYS:HD2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:63:LYS:HA	2:C:72:ASN:OD1	2.08	0.54
1:A:105:LEU:O	1:A:105:LEU:HD12	2.08	0.54
3:D:3:TPO:C	3:D:5:GLN:N	2.68	0.53
1:A:51:LYS:O	1:A:51:LYS:HG3	2.08	0.53
1:B:137:ILE:HD12	1:B:160:TYR:CE2	2.44	0.53
1:B:179:ILE:HD12	1:B:179:ILE:C	2.33	0.53
1:A:12:GLU:O	1:A:13:PHE:CB	2.57	0.53
1:B:134:GLY:O	1:B:135:ARG:HB2	2.08	0.53
2:C:27:LYS:CG	2:C:57:GLU:HG3	2.39	0.52
1:A:184:SER:C	1:A:186:LYS:H	2.18	0.52
1:A:136:ILE:HG12	1:A:178:MSE:HB3	1.91	0.52
1:B:26:ARG:HH22	1:B:48:GLY:HA3	1.75	0.52
3:D:3:TPO:O	3:D:5:GLN:N	2.43	0.52
1:B:137:ILE:CD1	1:B:160:TYR:CE2	2.90	0.51
1:B:12:GLU:CB	4:B:264:HOH:O	2.58	0.51
2:C:54:GLU:CD	2:C:56:GLY:HA3	2.33	0.51
1:B:141:ASN:C	1:B:142:GLN:O	2.50	0.51
2:C:62:ILE:HD11	2:C:80:LEU:HD21	1.92	0.51
1:A:77:GLU:HG3	1:A:91:LEU:CD2	2.39	0.51
1:A:132:ILE:HD11	1:A:156:GLN:CD	2.35	0.51
1:A:133:VAL:HG11	1:A:136:ILE:HD13	1.93	0.51
1:A:170:LEU:HD13	1:A:170:LEU:C	2.36	0.51
1:B:15:THR:CG2	1:B:65:LYS:HE2	2.41	0.50
1:B:132:ILE:HB	1:B:156:GLN:HG3	1.93	0.50
1:B:142:GLN:O	1:B:143:LYS:HB2	2.10	0.50
2:C:36:ILE:O	2:C:40:GLU:HG3	2.11	0.50
1:A:18:ARG:HG3	1:A:19:PHE:N	2.26	0.50
1:B:89:LYS:H	1:B:89:LYS:HD3	1.76	0.50
1:A:178:MSE:HE1	4:A:211:HOH:O	2.11	0.50
1:A:158:LEU:HB3	1:A:162:GLU:HG3	1.93	0.50
2:C:20:MSE:HE2	2:C:69:HIS:HE1	1.76	0.50
2:C:77:GLU:HG2	2:C:91:LEU:HD11	1.94	0.50
1:A:48:GLY:O	1:A:49:PHE:O	2.30	0.49
1:B:143:LYS:HE2	1:B:149:PRO:HB3	1.94	0.49
1:A:49:PHE:O	1:A:50:GLU:C	2.55	0.49
1:A:49:PHE:CE2	1:A:50:GLU:HB2	2.48	0.49
2:C:27:LYS:HG2	2:C:57:GLU:CD	2.36	0.49
1:A:54:GLU:O	1:A:55:PRO:O	2.30	0.49
1:B:179:ILE:HD12	1:B:179:ILE:O	2.13	0.49
1:A:53:LYS:HB3	4:A:312:HOH:O	2.11	0.48
1:A:107:ASN:C	1:A:108:ALA:O	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:HA	4:A:259:HOH:O	2.12	0.48
2:C:26:ARG:HA	2:C:55:PRO:CB	2.21	0.48
1:A:58:ILE:HD11	4:A:231:HOH:O	2.13	0.48
1:A:53:LYS:CE	4:A:265:HOH:O	2.61	0.48
1:A:51:LYS:N	4:A:265:HOH:O	2.45	0.48
2:C:51:LYS:C	2:C:53:LYS:H	2.19	0.48
2:C:53:LYS:HD3	2:C:55:PRO:HG2	1.96	0.48
2:C:20:MSE:HE2	2:C:69:HIS:CE1	2.48	0.48
2:C:36:ILE:HD13	2:C:36:ILE:C	2.39	0.47
1:A:98:ASP:O	1:A:102:LYS:HD2	2.14	0.47
1:B:76:THR:CG2	1:B:79:THR:H	2.27	0.47
1:B:21:ASP:OD1	1:B:22:CYS:N	2.45	0.47
1:B:76:THR:HG21	4:B:196:HOH:O	2.13	0.47
1:A:25:GLY:HA2	1:A:49:PHE:CE2	2.49	0.47
1:B:82:GLN:HG3	1:B:83:GLN:N	2.28	0.47
3:D:4:M3L:O	3:D:5:GLN:HB2	2.11	0.47
2:C:24:ILE:O	2:C:24:ILE:CD1	2.55	0.47
1:A:52:ASN:OD1	1:A:52:ASN:O	2.31	0.47
1:A:54:GLU:CG	1:A:55:PRO:CD	2.65	0.47
2:C:27:LYS:CG	2:C:55:PRO:HA	2.43	0.47
2:C:54:GLU:CB	2:C:56:GLY:N	2.78	0.47
1:B:80:LEU:HB3	1:B:88:MSE:SE	2.65	0.47
1:B:16:ILE:CD1	1:B:62:ILE:HG21	2.45	0.46
1:B:88:MSE:C	1:B:90:LYS:N	2.72	0.46
2:C:17:GLU:HG2	2:C:63:LYS:HG3	1.98	0.46
2:C:24:ILE:HA	2:C:57:GLU:O	2.16	0.46
1:A:157:GLY:HA3	4:A:269:HOH:O	2.15	0.45
2:C:24:ILE:HD13	2:C:51:LYS:CE	2.31	0.45
1:A:141:ASN:HA	2:C:42:ASP:O	2.17	0.45
2:C:26:ARG:HG3	2:C:55:PRO:CB	2.46	0.45
2:C:83:GLN:O	2:C:84:ASN:HB2	2.16	0.45
1:B:107:ASN:CB	2:C:36:ILE:HG13	2.46	0.45
1:B:135:ARG:N	1:B:178:MSE:HE2	2.32	0.45
2:C:88:MSE:CE	2:C:91:LEU:HD12	2.47	0.45
1:B:93:ASN:OD1	1:B:93:ASN:N	2.49	0.45
2:C:53:LYS:HD3	2:C:55:PRO:CG	2.47	0.45
1:A:81:LYS:NZ	4:A:250:HOH:O	2.46	0.45
1:B:109:SER:O	1:B:113:VAL:HG23	2.17	0.45
1:A:129:GLN:HB2	4:A:269:HOH:O	2.17	0.45
1:A:24:ILE:O	1:A:49:PHE:CE2	2.71	0.44
1:A:134:GLY:C	1:A:178:MSE:HE2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:SER:H	1:A:112:ASP:HB2	1.81	0.44
1:B:99:GLN:HB2	4:B:225:HOH:O	2.15	0.44
1:A:37:TYR:CG	1:A:170:LEU:HD21	2.52	0.44
2:C:92:ASP:HA	2:C:95:LYS:HB2	1.98	0.44
1:A:115:TYR:CE2	1:B:135:ARG:HD2	2.53	0.44
1:B:54:GLU:HB2	1:B:55:PRO:HD2	2.00	0.44
1:B:78:GLU:OE2	1:B:78:GLU:HA	2.16	0.44
1:A:58:ILE:HD11	1:A:60:TYR:OH	2.18	0.43
1:A:81:LYS:HG3	1:A:88:MSE:HE2	2.00	0.43
1:A:55:PRO:HA	4:A:311:HOH:O	2.12	0.43
1:A:77:GLU:HG3	1:A:91:LEU:HD21	2.00	0.43
1:B:83:GLN:O	1:B:84:ASN:HB2	2.18	0.43
1:A:51:LYS:HB3	4:A:265:HOH:O	2.18	0.43
1:B:137:ILE:O	1:B:137:ILE:CG2	2.66	0.43
2:C:76:THR:HB	2:C:79:THR:OG1	2.19	0.43
1:A:18:ARG:HG2	1:A:20:MSE:SE	2.68	0.43
2:C:13:PHE:HB2	2:C:86:ARG:CZ	2.49	0.43
2:C:76:THR:CG2	2:C:77:GLU:N	2.81	0.43
1:A:115:TYR:CD2	1:B:135:ARG:HD2	2.54	0.43
1:B:99:GLN:O	1:B:103:ARG:HB2	2.18	0.43
1:A:53:LYS:HE2	4:A:265:HOH:O	2.18	0.43
1:B:95:LYS:O	1:B:96:LYS:C	2.62	0.42
3:D:3:TPO:O	3:D:4:M3L:C	2.63	0.42
1:B:79:THR:HA	1:B:82:GLN:HG2	2.00	0.42
1:A:153:CYS:O	1:A:163:CYS:HA	2.20	0.42
1:B:70:ILE:HG22	1:B:131:GLN:HB3	2.01	0.42
1:B:107:ASN:OD1	2:C:36:ILE:HG13	2.20	0.42
1:B:129:GLN:HA	1:B:132:ILE:HD12	2.02	0.42
1:A:137:ILE:HD11	4:A:230:HOH:O	2.20	0.41
1:B:68:SER:OG	1:B:70:ILE:HG12	2.20	0.41
2:C:54:GLU:HG2	2:C:56:GLY:CA	2.41	0.41
1:A:178:MSE:CE	4:A:211:HOH:O	2.66	0.41
1:A:182:TYR:O	1:A:186:LYS:O	2.38	0.41
4:A:195:HOH:O	3:D:4:M3L:HB3	2.21	0.41
2:C:91:LEU:CD2	2:C:95:LYS:HD3	2.48	0.41
1:A:36:ILE:HG23	1:A:37:TYR:N	2.34	0.41
4:A:246:HOH:O	1:B:137:ILE:HG23	2.19	0.41
2:C:20:MSE:CE	2:C:69:HIS:HE1	2.33	0.41
1:A:159:PRO:HG2	1:A:162:GLU:HG2	2.02	0.41
1:B:143:LYS:HB2	1:B:143:LYS:HE3	1.76	0.41
2:C:15:THR:HB	2:C:65:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLU:HB2	1:B:55:PRO:CD	2.51	0.41
1:B:170:LEU:HD12	1:B:170:LEU:O	2.21	0.41
2:C:90:LYS:HA	2:C:93:ASN:HB2	2.01	0.41
1:A:51:LYS:CB	4:A:265:HOH:O	2.68	0.41
1:A:92:ASP:O	1:A:96:LYS:HG3	2.20	0.40
2:C:80:LEU:HD12	2:C:80:LEU:HA	1.81	0.40
3:D:3:TPO:C	3:D:5:GLN:H	2.34	0.40
1:A:57:GLU:O	1:A:59:GLN:HG3	2.21	0.40
1:A:70:ILE:HG13	1:A:71:HIS:CD2	2.57	0.40
1:B:26:ARG:NH2	1:B:54:GLU:OE1	2.55	0.40
2:C:24:ILE:HG13	4:C:127:HOH:O	2.20	0.40
2:C:27:LYS:CB	2:C:55:PRO:HA	2.51	0.40
1:A:70:ILE:HG13	1:A:71:HIS:N	2.37	0.40
2:C:53:LYS:CD	2:C:55:PRO:HG2	2.52	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:A:50:GLU:OE1	1:A:50:GLU:OE1[2_555]	2.04	0.16

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	174/187 (93%)	153 (88%)	17 (10%)	4 (2%)	5	3
1	B	168/187 (90%)	156 (93%)	11 (6%)	1 (1%)	21	27
2	C	84/115 (73%)	73 (87%)	8 (10%)	3 (4%)	2	1
3	D	1/20 (5%)	1 (100%)	0	0	100	100
All	All	427/509 (84%)	383 (90%)	36 (8%)	8 (2%)	6	5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	PRO
2	C	55	PRO
2	C	47	ALA
1	A	47	ALA
2	C	95	LYS
1	A	50	GLU
1	B	135	ARG
1	A	13	PHE

5.3.2 Protein sidechains [i](#)

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	131/160 (82%)	114 (87%)	17 (13%)	4	3
1	B	144/160 (90%)	127 (88%)	17 (12%)	5	4
2	C	73/98 (74%)	59 (81%)	14 (19%)	1	0
3	D	2/13 (15%)	0	2 (100%)	0	0
All	All	350/431 (81%)	300 (86%)	50 (14%)	3	2

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	51	LYS
1	A	58	ILE
1	A	80	LEU
1	A	81	LYS
1	A	102	LYS
1	A	105	LEU
1	A	111	GLU
1	A	124	ASP
1	A	126	LEU
1	A	132	ILE
1	A	137	ILE

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Mol	Chain	Res	Type
1	A	142	GLN
1	A	143	LYS
1	A	156	GLN
1	A	171	ILE
1	A	186	LYS
1	B	15	THR
1	B	78	GLU
1	B	80	LEU
1	B	86	ARG
1	B	88	MSE
1	B	89	LYS
1	B	91	LEU
1	B	93	ASN
1	B	100	GLU
1	B	101	THR
1	B	106	LYS
1	B	123	THR
1	B	126	LEU
1	B	136	ILE
1	B	171	ILE
1	B	179	ILE
1	B	186	LYS
2	C	12	GLU
2	C	17	GLU
2	C	18	ARG
2	C	24	ILE
2	C	36	ILE
2	C	51	LYS
2	C	53	LYS
2	C	54	GLU
2	C	58	ILE
2	C	76	THR
2	C	79	THR
2	C	80	LEU
2	C	91	LEU
2	C	96	LYS
3	D	2	ARG
3	D	5	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	131	GLN
1	A	141	ASN
1	B	69	HIS
1	B	82	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	M3L	D	4	3	10,11,12	1.71	3 (30%)	9,14,16	1.20	0
3	TPO	D	3	3	8,10,11	2.18	2 (25%)	10,14,16	1.43	3 (30%)

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
3	M3L	D	4	3	-	4/9/10/12	-
3	TPO	D	3	3	-	0/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	TPO	P-OG1	5.35	1.68	1.59
3	D	4	M3L	CG-CB	3.22	1.65	1.52
3	D	4	M3L	CB-CA	-2.80	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	TPO	P-O3P	2.15	1.62	1.54
3	D	4	M3L	CD-CG	2.00	1.61	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	TPO	P-OG1-CB	-3.04	115.07	123.33
3	D	3	TPO	O-C-CA	-2.34	118.75	124.77
3	D	3	TPO	CG2-CB-CA	-2.15	109.07	113.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4	M3L	CD-CE-NZ-CM3
3	D	4	M3L	CD-CE-NZ-CM1
3	D	4	M3L	CD-CE-NZ-CM2
3	D	4	M3L	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4	M3L	6	0
3	D	3	TPO	5	0

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 ⓘ

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	173/187 (92%)	0.01	9 (5%)	33 30	21, 39, 72, 82	0
1	B	171/187 (91%)	0.22	3 (1%)	67 69	24, 50, 77, 83	0
2	C	84/115 (73%)	0.38	6 (7%)	22 19	29, 47, 76, 80	0
3	D	3/20 (15%)	2.40	2 (66%)	0 0	107, 107, 117, 120	0
All	All	431/509 (84%)	0.18	20 (4%)	37 36	21, 45, 76, 120	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	55	PRO	5.2
3	D	1	ALA	4.0
1	A	13	PHE	3.8
2	C	56	GLY	3.3
1	A	55	PRO	3.1
1	A	11	GLU	2.9
2	C	13	PHE	2.8
1	B	144	SER	2.7
1	A	108	ALA	2.6
1	A	104	TRP	2.6
2	C	54	GLU	2.5
1	A	186	LYS	2.5
1	B	147	GLY	2.4
2	C	47	ALA	2.4
1	A	51	LYS	2.3
2	C	78	GLU	2.2
3	D	2	ARG	2.2
1	A	54	GLU	2.0
1	A	48	GLY	2.0
1	B	36	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TPO	D	3	11/12	0.76	0.17	110,114,118,118	0
3	M3L	D	4	12/13	0.82	0.25	93,98,107,108	0

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.