



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:02 PM UTC

PDB ID : 4AUW / pdb_00004auw
Title : CRYSTAL STRUCTURE OF THE BZIP HOMODIMERIC MAFB IN COM-
PLEX WITH THE C- MARE BINDING SITE
Authors : Textor, L.C.; Holton, S.; Wilmanns, M.
Deposited on : 2012-05-22
Resolution : 2.90 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

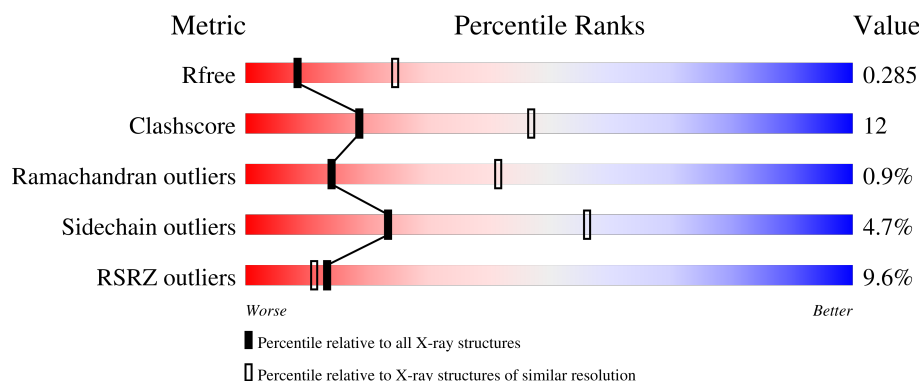
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	96	11% 67% 23% 8%
1	B	96	10% 68% 20% 10%
1	E	96	14% 66% 25% 5%
1	F	96	7% 71% 22% 6%
2	C	21	71% 29%

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Mol	Chain	Length	Quality of chain
2	H	21	
3	D	21	
3	G	21	

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
5	DTU	B	1299	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4665 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 TRANSCRIPTION FACTOR MAFB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	88	Total	C	N	O	S	0	0	1
			723	443	146	132	2			
1	B	86	Total	C	N	O	S	0	0	1
			718	439	147	130	2			
1	E	91	Total	C	N	O	S	0	1	1
			750	455	152	140	3			
1	F	90	Total	C	N	O	S	0	0	1
			752	458	155	136	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	MET	-	expression tag	UNP P54841
A	298	SER	CYS	engineered mutation	UNP P54841
B	210	MET	-	expression tag	UNP P54841
B	298	SER	CYS	engineered mutation	UNP P54841
E	210	MET	-	expression tag	UNP P54841
E	298	SER	CYS	engineered mutation	UNP P54841
F	210	MET	-	expression tag	UNP P54841
F	298	SER	CYS	engineered mutation	UNP P54841

- Molecule 2 is a DNA chain called C-MARE BINDING SITE (5'-D(*AP*TP*AP*AP*TP*GP*CP*TP* GP*AP*CP*GP*TP*CP*AP*GP*CP*AP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	P	0	0	0
			427	206	76	125	20			
2	H	21	Total	C	N	O	P	0	0	0
			427	206	76	125	20			

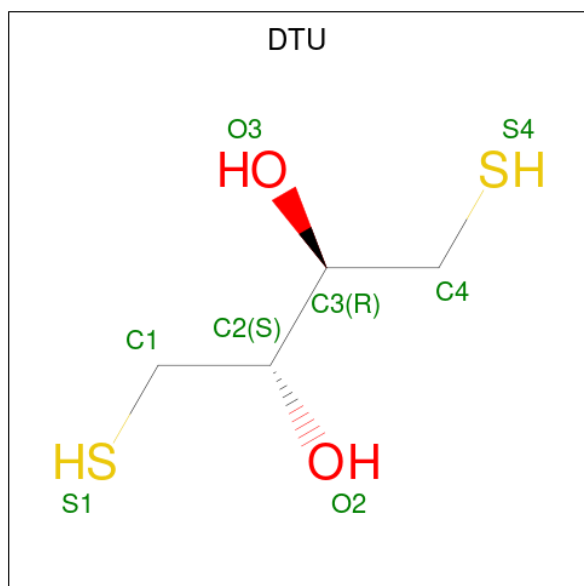
- Molecule 3 is a DNA chain called C-MARE BINDING SITE (5'-D(*AP*TP*AP*AP*TP*GP*CP*TP* GP*AP*CP*GP*TP*CP*AP*GP*CP*AP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	21	Total	C	N	O	P	0	0	0
			428	206	79	123	20			
3	G	21	Total	C	N	O	P	0	0	0
			428	206	79	123	20			

- Molecule 4 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Hg	0	0
			1	1		
4	B	1	Total	Hg	0	0
			1	1		
4	E	1	Total	Hg	0	0
			1	1		
4	F	1	Total	Hg	0	0
			1	1		

- Molecule 5 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (CCD ID: DTU) (formula: C₄H₁₀O₂S₂).

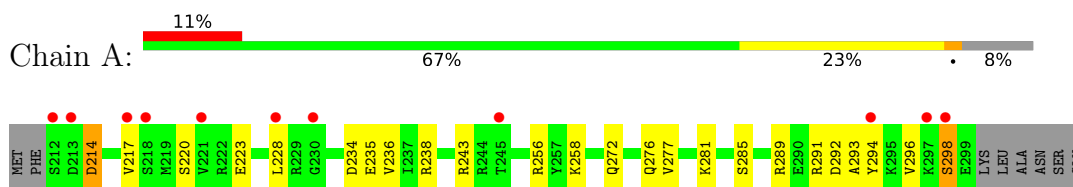


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			8	4	2	2		

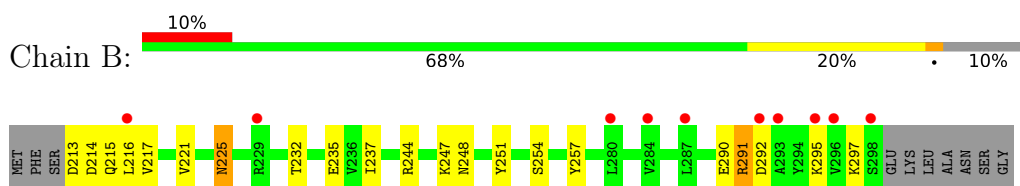
3 Residue-property plots [i](#)

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.

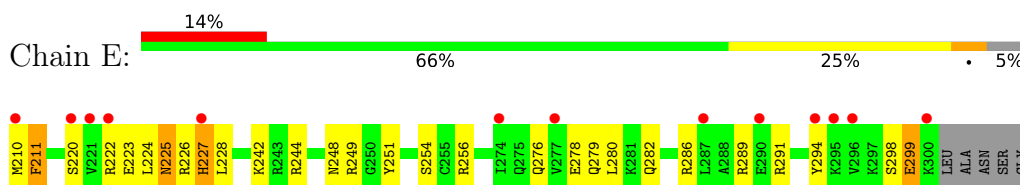
- Molecule 1: TRANSCRIPTION FACTOR MAFB



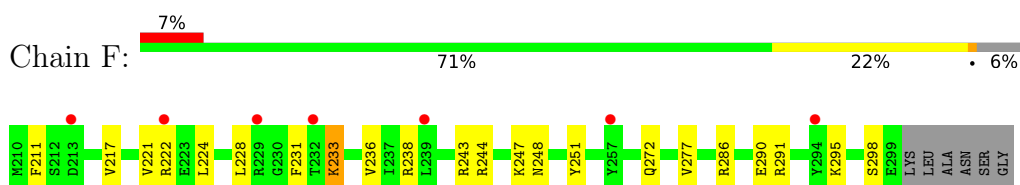
- Molecule 1: TRANSCRIPTION FACTOR MAFB



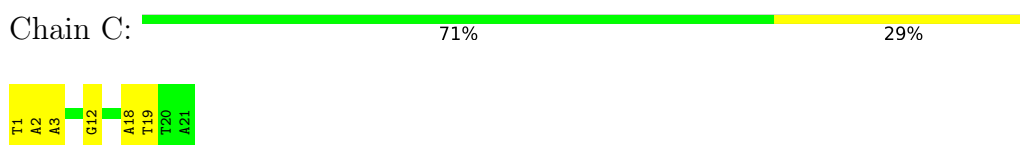
- Molecule 1: TRANSCRIPTION FACTOR MAFB



- Molecule 1: TRANSCRIPTION FACTOR MAFB



- Molecule 2: C-MARE BINDING SITE (5'-D(*AP*TP*AP*AP*TP*GP*CP*TP* GP*AP*CP*GP*TP*CP*AP*GP*CP*AP*AP*TP*T)-3')



- Molecule 2: C-MARE BINDING SITE (5'-D(*AP*TP*AP*AP*TP*GP*CP*TP* GP*AP*CP*GP*TP*CP*AP*GP*CP*AP*AP*TP*T)-3')

Chain H:  38% 62%



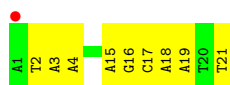
- Molecule 3: C-MARE BINDING SITE (5'-D(*AP*TP*AP*AP*TP*GP*CP*TP* GP*AP*CP*GP*TP*CP*AP*GP*CP*AP*AP*TP*T)-3')

Chain D:  67% 29% 5%



- Molecule 3: C-MARE BINDING SITE (5'-D(*AP*TP*AP*AP*TP*GP*CP*TP* GP*AP*CP*GP*TP*CP*AP*GP*CP*AP*AP*TP*T)-3')

Chain G:  5% 57% 43%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.96Å 94.96Å 200.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.75 – 2.90 85.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (85.75-2.90) 99.7 (85.75-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.255 , 0.290 0.259 , 0.285	Depositor DCC
R_{free} test set	1081 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4665	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.46	1/729 (0.1%)	0.88	0/971
1	B	0.48	1/724 (0.1%)	0.88	0/964
1	E	0.45	1/759 (0.1%)	0.83	0/1011
1	F	0.45	1/758 (0.1%)	0.82	0/1006
2	C	0.30	0/478	0.95	0/736
2	H	0.26	0/478	0.95	0/736
3	D	0.25	0/480	0.90	1/739 (0.1%)
3	G	0.26	0/480	0.97	0/739
All	All	0.40	4/4886 (0.1%)	0.89	1/6902 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	298	SER	C-N	-6.96	1.23	1.33
1	B	297	LYS	C-N	-6.91	1.23	1.33
1	A	298	SER	C-N	-6.85	1.23	1.33
1	E	299	GLU	C-N	-6.80	1.23	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	DA	N9-C1'-C2'	-5.16	105.75	113.50

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	723	0	736	16	0
1	B	718	0	736	21	0
1	E	750	0	749	28	0
1	F	752	0	777	13	0
2	C	427	0	240	7	0
2	H	427	0	240	16	0
3	D	428	0	239	6	0
3	G	428	0	239	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	B	8	0	10	7	0
All	All	4665	0	3966	100	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 12.

All (100) 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:H:1:DT:H2''	2:H:2:DA:H5''	1.22	1.16
1:A:243:ARG:HH12	3:D:5:DT:P	1.87	0.96
2:C:18:DA:H2''	2:C:19:DT:H5'	1.55	0.89
1:E:222:ARG:O	1:E:225:ASN:ND2	2.12	0.83
1:B:254:SER:HA	5:B:1299:DTU:H4C1	1.62	0.82
2:C:18:DA:H2''	2:C:19:DT:C5'	2.10	0.81
2:H:1:DT:C2'	2:H:2:DA:H5''	2.07	0.80
1:B:217:VAL:HG23	1:B:247:LYS:HD2	1.64	0.79
1:F:233:LYS:H	1:F:233:LYS:HD3	1.46	0.79
1:A:243:ARG:NH1	3:D:5:DT:OP2	2.16	0.79
1:E:222:ARG:HG2	1:E:226:ARG:HH21	1.48	0.78
1:B:254:SER:OG	5:B:1299:DTU:H4C2	1.84	0.76
1:A:243:ARG:NH1	3:D:5:DT:P	2.61	0.72
1:B:292:ASP:HA	1:B:295:LYS:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASP:CG	1:B:214:ASP:H	1.98	0.71
1:E:249:ARG:HD2	2:H:12:DG:H3'	1.74	0.70
5:B:1299:DTU:O2	1:E:254:SER:OG	2.10	0.70
1:E:225:ASN:HA	1:E:228:LEU:HB2	1.74	0.69
1:B:221:VAL:O	1:B:225:ASN:OD1	2.10	0.69
1:B:291:ARG:NH1	1:B:292:ASP:OD1	2.28	0.67
1:B:254:SER:HA	5:B:1299:DTU:C4	2.24	0.67
1:E:222:ARG:O	1:E:222:ARG:HG3	1.95	0.66
1:E:210:MET:HG3	1:E:211:PHE:H	1.60	0.66
1:E:244:ARG:O	1:E:248:ASN:HB2	1.95	0.65
3:D:19:DA:H2''	3:D:20:DT:H5''	1.79	0.65
1:F:233:LYS:H	1:F:233:LYS:CD	2.10	0.64
1:A:234:ASP:OD1	1:A:235:GLU:N	2.31	0.64
1:E:220:SER:HB3	1:E:223:GLU:HB3	1.79	0.64
1:B:213:ASP:O	1:B:216:LEU:HB2	1.98	0.63
1:F:217:VAL:HG23	1:F:247:LYS:HG2	1.80	0.63
2:C:18:DA:H4'	2:C:18:DA:OP1	1.99	0.63
1:A:277:VAL:HG12	1:A:281:LYS:HE2	1.82	0.61
2:H:2:DA:C2'	2:H:3:DA:C8	2.87	0.57
1:A:256:ARG:NH2	2:C:12:DG:N7	2.53	0.56
3:G:2:DT:H4'	3:G:3:DA:OP1	2.05	0.56
1:A:214:ASP:O	1:A:217:VAL:HG12	2.06	0.56
2:H:2:DA:H2''	2:H:3:DA:C8	2.41	0.56
1:A:294:TYR:HE2	1:B:295:LYS:HD3	1.71	0.56
1:F:221:VAL:HG23	1:F:222:ARG:HG3	1.88	0.56
1:A:285:SER:O	1:A:289:ARG:HG2	2.07	0.55
1:B:217:VAL:O	1:B:247:LYS:NZ	2.40	0.55
1:F:228:LEU:HA	1:F:231:PHE:CD1	2.42	0.55
1:B:248:ASN:HA	1:B:251:TYR:CD2	2.42	0.54
1:E:224:LEU:HD12	1:E:227:HIS:HE1	1.70	0.54
1:E:248:ASN:HA	1:E:251:TYR:CD2	2.43	0.54
1:E:249:ARG:CD	2:H:12:DG:H3'	2.36	0.54
1:E:276:GLN:O	1:E:279:GLN:HG2	2.08	0.53
1:A:228:LEU:HD23	1:A:236:VAL:HG13	1.91	0.53
5:B:1299:DTU:HA	1:E:254:SER:HG	1.49	0.52
1:B:213:ASP:CG	1:B:214:ASP:N	2.65	0.52
1:B:257:TYR:OH	1:E:249:ARG:HG2	2.10	0.52
1:E:210:MET:HG3	1:E:211:PHE:N	2.24	0.52
1:B:213:ASP:O	1:B:216:LEU:N	2.42	0.52
1:E:279:GLN:HG3	1:E:280:LEU:N	2.25	0.51
1:E:278:GLU:O	1:E:282:GLN:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:18:DA:H1'	3:G:19:DA:H5'	1.93	0.50
1:A:292:ASP:O	1:A:296:VAL:HG13	2.11	0.50
2:C:18:DA:H2''	2:C:19:DT:H5''	1.89	0.50
3:D:17:DC:H2''	3:D:18:DA:H5'	1.93	0.50
1:A:291:ARG:HD3	1:B:290:GLU:OE1	2.12	0.50
1:E:210:MET:CG	1:E:211:PHE:H	2.25	0.50
1:E:224:LEU:HD12	1:E:227:HIS:CE1	2.46	0.50
1:E:244:ARG:HG2	1:E:244:ARG:HH11	1.77	0.49
1:F:228:LEU:HD23	1:F:236:VAL:HG13	1.93	0.49
1:A:272:GLN:HE22	1:A:276:GLN:HE21	1.60	0.49
3:G:3:DA:H2''	3:G:4:DA:O5'	2.12	0.49
1:B:215:GLN:HA	1:B:215:GLN:OE1	2.13	0.49
1:B:244:ARG:HG2	1:B:244:ARG:HH11	1.77	0.49
3:G:3:DA:H5''	3:G:3:DA:H8	1.78	0.48
2:H:2:DA:H2'	2:H:3:DA:C8	2.48	0.48
2:C:1:DT:H2''	2:C:2:DA:O5'	2.12	0.48
3:G:21:DT:H3	2:H:2:DA:H62	1.61	0.48
1:E:286:ARG:O	1:E:289:ARG:HG2	2.15	0.46
2:H:18:DA:H2''	2:H:19:DT:H5'	1.98	0.46
1:F:248:ASN:HA	1:F:251:TYR:CD2	2.51	0.46
2:H:6:DG:H2''	2:H:7:DC:O5'	2.16	0.46
3:G:17:DC:H2''	3:G:18:DA:O5'	2.17	0.45
3:G:15:DA:H2''	3:G:16:DG:H5'	1.97	0.45
1:A:220:SER:HB3	1:A:223:GLU:HB2	1.99	0.45
2:H:8:DT:H2''	2:H:9:DG:C8	2.52	0.45
3:D:1:DA:H2''	3:D:2:DT:C5'	2.47	0.44
1:E:294:TYR:CE2	1:F:295:LYS:HD3	2.53	0.44
1:F:244:ARG:NH2	2:H:6:DG:O6	2.37	0.44
1:E:298:SER:O	1:E:299:GLU:HG3	2.18	0.44
1:F:243:ARG:NH1	2:H:5:DT:OP2	2.51	0.43
1:F:243:ARG:HH12	2:H:5:DT:P	2.41	0.43
1:B:214:ASP:C	1:B:216:LEU:H	2.27	0.42
1:A:235:GLU:CD	1:A:238:ARG:HH21	2.27	0.42
1:E:291:ARG:NH1	1:F:290:GLU:OE1	2.45	0.42
1:B:225:ASN:OD1	1:B:225:ASN:N	2.54	0.41
1:A:293:ALA:O	1:A:296:VAL:HG22	2.21	0.41
2:H:17:DC:H2''	2:H:18:DA:OP2	2.20	0.41
1:F:238:ARG:HH11	1:F:238:ARG:HB3	1.85	0.41
1:E:222:ARG:HG3	1:E:225:ASN:HD21	1.85	0.41
5:B:1299:DTU:H2	1:E:254:SER:HA	2.03	0.41
1:B:232:THR:HG23	1:B:235:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:ARG:HD3	2:H:13:DT:OP2	2.20	0.40
3:G:3:DA:H5''	3:G:3:DA:C8	2.57	0.40
2:C:2:DA:H2''	2:C:3:DA:C8	2.57	0.40
5:B:1299:DTU:O2	5:B:1299:DTU:S4	2.77	0.40

There are no symmetry-related clashes.

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	86/96 (90%)	83 (96%)	2 (2%)	1 (1%)	10	34
1	B	84/96 (88%)	78 (93%)	6 (7%)	0	100	100
1	E	90/96 (94%)	88 (98%)	1 (1%)	1 (1%)	11	36
1	F	88/96 (92%)	85 (97%)	2 (2%)	1 (1%)	11	36
All	All	348/384 (91%)	334 (96%)	11 (3%)	3 (1%)	14	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	211	PHE
1	F	211	PHE
1	A	298	SER

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	78/89 (88%)	76 (97%)	2 (3%)	40	73
1	B	78/89 (88%)	75 (96%)	3 (4%)	29	64
1	E	81/89 (91%)	77 (95%)	4 (5%)	22	54
1	F	83/89 (93%)	77 (93%)	6 (7%)	13	39
All	All	320/356 (90%)	305 (95%)	15 (5%)	23	56

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ASP
1	A	258	LYS
1	B	225	ASN
1	B	237	ILE
1	B	291	ARG
1	E	225	ASN
1	E	227	HIS
1	E	242	LYS
1	E	256	ARG
1	F	224	LEU
1	F	233	LYS
1	F	272	GLN
1	F	277	VAL
1	F	286	ARG
1	F	291	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	268	ASN
1	A	276	GLN
1	A	279	GLN
1	E	215	GLN
1	E	225	ASN
1	E	265	HIS
1	E	276	GLN
1	F	215	GLN
1	F	241	GLN
1	F	272	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 ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	DTU	B	1299	-	7,7,7	0.64	0	4,8,8	0.92	0

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
5	DTU	B	1299	-	-	6/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1299	DTU	S1-C1-C2-O2
5	B	1299	DTU	C1-C2-C3-O3
5	B	1299	DTU	C1-C2-C3-C4
5	B	1299	DTU	O2-C2-C3-O3
5	B	1299	DTU	O2-C2-C3-C4
5	B	1299	DTU	S1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1299	DTU	7	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	88/96 (91%)	0.80	11 (12%) 8 7	28, 54, 85, 88	0
1	B	86/96 (89%)	0.84	10 (11%) 9 8	17, 53, 83, 86	1 (1%)
1	E	91/96 (94%)	0.97	13 (14%) 6 5	16, 54, 85, 87	1 (1%)
1	F	90/96 (93%)	0.88	7 (7%) 19 16	31, 58, 84, 88	0
2	C	21/21 (100%)	-0.09	0 100 100	17, 21, 38, 44	0
2	H	21/21 (100%)	-0.10	0 100 100	12, 26, 38, 39	0
3	D	21/21 (100%)	-0.08	0 100 100	11, 25, 45, 47	0
3	G	21/21 (100%)	0.05	1 (4%) 35 28	13, 31, 44, 54	0
All	All	439/468 (93%)	0.70	42 (9%) 13 11	11, 48, 84, 88	2 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	222	ARG	3.6
1	F	257	TYR	3.4
1	F	229	ARG	3.3
1	E	300	LYS	3.2
1	F	213	ASP	3.2
1	E	210	MET	3.1
3	G	1	DA	2.9
1	F	294	TYR	2.9
1	E	277	VAL	2.8
1	B	296	VAL	2.8
1	E	274	ILE	2.7
1	A	217	VAL	2.7
1	B	216	LEU	2.6
1	B	280	LEU	2.6
1	F	232	THR	2.5
1	E	295	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	229	ARG	2.5
1	E	294	TYR	2.5
1	F	222	ARG	2.4
1	F	239	LEU	2.4
1	A	297	LYS	2.4
1	A	218	SER	2.3
1	E	287	LEU	2.3
1	A	228	LEU	2.3
1	E	221	VAL	2.2
1	E	296	VAL	2.2
1	E	227	HIS	2.2
1	A	298	SER	2.2
1	B	284	VAL	2.2
1	B	298	SER	2.2
1	B	293	ALA	2.2
1	E	290	GLU	2.2
1	A	213	ASP	2.1
1	B	295	LYS	2.1
1	E	220	SER	2.1
1	A	294	TYR	2.1
1	A	212	SER	2.1
1	B	292	ASP	2.1
1	A	221	VAL	2.0
1	B	287	LEU	2.0
1	A	230	GLY	2.0
1	A	245	THR	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](#)

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
5	DTU	B	1299	8/8	0.91	0.22	46,48,48,50	0
4	HG	F	1299	1/1	0.95	0.07	70,70,70,70	0
4	HG	B	1298	1/1	0.95	0.08	56,56,56,56	0
4	HG	A	1299	1/1	0.96	0.05	66,66,66,66	0
4	HG	E	1300	1/1	0.97	0.09	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.