



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:00 AM UTC

PDB ID : 6Q0R / pdb_00006q0r
Title : Structure of DDB1-DDA1-DCAF15 complex bound to E7820 and RBM39
Authors : Faust, T.; Yoon, H.; Nowak, R.P.; Donovan, K.A.; Li, Z.; Cai, Q.; Eleuteri, N.A.; Zhang, T.; Gray, N.S.; Fischer, E.S.
Deposited on : 2019-08-02
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

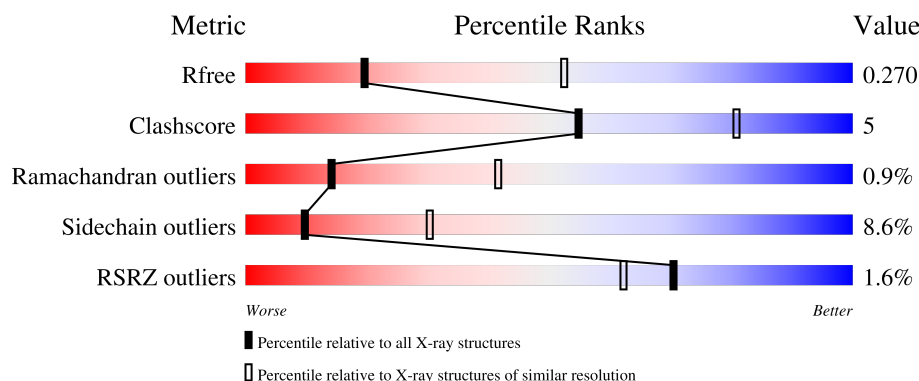
1 Overall quality at a glance

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	864	% 74% 15% • 9%
2	B	276	2% 53% 21% • 25%
3	C	263	2% 55% 13% • 30%
4	D	107	% 65% 10% • 23%
5	E	126	2% 26% 16% • 56%

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
6	OXM	B	301	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10249 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	783	Total	C	N	O	S	0	0	0
			6034	3826	1008	1167	33			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q16531
A	-26	GLY	-	expression tag	UNP Q16531
A	-25	SER	-	expression tag	UNP Q16531
A	-24	SER	-	expression tag	UNP Q16531
A	-23	HIS	-	expression tag	UNP Q16531
A	-22	HIS	-	expression tag	UNP Q16531
A	-21	HIS	-	expression tag	UNP Q16531
A	-20	HIS	-	expression tag	UNP Q16531
A	-19	HIS	-	expression tag	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	SER	-	expression tag	UNP Q16531
A	-16	ALA	-	expression tag	UNP Q16531
A	-15	ALA	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	ILE	-	expression tag	UNP Q16531
A	-12	VAL	-	expression tag	UNP Q16531
A	-11	MET	-	expression tag	UNP Q16531
A	-10	VAL	-	expression tag	UNP Q16531
A	-9	ASP	-	expression tag	UNP Q16531
A	-8	ALA	-	expression tag	UNP Q16531
A	-7	TYR	-	expression tag	UNP Q16531
A	-6	LYS	-	expression tag	UNP Q16531
A	-5	PRO	-	expression tag	UNP Q16531
A	-4	THR	-	expression tag	UNP Q16531
A	-3	LYS	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ARG	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531

- Molecule 2 is a protein called DDB1- and CUL4-associated factor 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1639	1061	280	288	10			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP Q66K64
B	-14	ASP	-	expression tag	UNP Q66K64
B	-13	TRP	-	expression tag	UNP Q66K64
B	-12	SER	-	expression tag	UNP Q66K64
B	-11	HIS	-	expression tag	UNP Q66K64
B	-10	PRO	-	expression tag	UNP Q66K64
B	-9	GLN	-	expression tag	UNP Q66K64
B	-8	PHE	-	expression tag	UNP Q66K64
B	-7	GLU	-	expression tag	UNP Q66K64
B	-6	LYS	-	expression tag	UNP Q66K64
B	-5	SER	-	expression tag	UNP Q66K64
B	-4	ALA	-	expression tag	UNP Q66K64
B	-3	VAL	-	expression tag	UNP Q66K64
B	-2	GLY	-	expression tag	UNP Q66K64
B	-1	LEU	-	expression tag	UNP Q66K64
B	0	ASN	-	expression tag	UNP Q66K64
B	1	ASP	-	expression tag	UNP Q66K64
B	2	ILE	-	expression tag	UNP Q66K64
B	3	PHE	-	expression tag	UNP Q66K64
B	4	GLU	-	expression tag	UNP Q66K64
B	5	ALA	-	expression tag	UNP Q66K64
B	6	GLN	-	expression tag	UNP Q66K64
B	7	LYS	-	expression tag	UNP Q66K64
B	8	ILE	-	expression tag	UNP Q66K64
B	9	GLU	-	expression tag	UNP Q66K64

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	TRP	-	expression tag	UNP Q66K64
B	11	HIS	-	expression tag	UNP Q66K64
B	12	GLU	-	expression tag	UNP Q66K64
B	13	GLY	-	expression tag	UNP Q66K64
B	14	GLY	-	expression tag	UNP Q66K64
B	15	GLY	-	expression tag	UNP Q66K64
B	16	GLY	-	expression tag	UNP Q66K64
B	17	SER	-	expression tag	UNP Q66K64
B	18	GLY	-	expression tag	UNP Q66K64
B	19	GLU	-	expression tag	UNP Q66K64
B	20	ASN	-	expression tag	UNP Q66K64
B	21	LEU	-	expression tag	UNP Q66K64
B	22	TYR	-	expression tag	UNP Q66K64
B	23	PHE	-	expression tag	UNP Q66K64
B	24	GLN	-	expression tag	UNP Q66K64
B	25	GLY	-	expression tag	UNP Q66K64
B	26	GLY	-	expression tag	UNP Q66K64
B	27	GLY	-	expression tag	UNP Q66K64
B	28	ARG	-	expression tag	UNP Q66K64
B	29	MET	-	expression tag	UNP Q66K64
B	30	GLY	-	expression tag	UNP Q66K64
B	31	ARG	-	expression tag	UNP Q66K64
B	32	ARG	-	expression tag	UNP Q66K64
B	33	ARG	-	expression tag	UNP Q66K64

- Molecule 3 is a protein called DDB1- and CUL4-associated factor 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	183	Total	C	N	O	S	0	0	0
			1460	941	238	274	7			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	338	MET	-	initiating methionine	UNP Q66K64
C	339	ASP	-	expression tag	UNP Q66K64
C	340	TRP	-	expression tag	UNP Q66K64
C	341	SER	-	expression tag	UNP Q66K64
C	342	HIS	-	expression tag	UNP Q66K64
C	343	PRO	-	expression tag	UNP Q66K64
C	344	GLN	-	expression tag	UNP Q66K64
C	345	PHE	-	expression tag	UNP Q66K64

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Chain	Residue	Modelled	Actual	Comment	Reference
C	346	GLU	-	expression tag	UNP Q66K64
C	347	LYS	-	expression tag	UNP Q66K64
C	348	SER	-	expression tag	UNP Q66K64
C	349	ALA	-	expression tag	UNP Q66K64
C	350	VAL	-	expression tag	UNP Q66K64
C	351	GLY	-	expression tag	UNP Q66K64
C	352	LEU	-	expression tag	UNP Q66K64
C	353	ASN	-	expression tag	UNP Q66K64
C	354	ASP	-	expression tag	UNP Q66K64
C	355	ILE	-	expression tag	UNP Q66K64
C	356	PHE	-	expression tag	UNP Q66K64
C	357	GLU	-	expression tag	UNP Q66K64
C	358	ALA	-	expression tag	UNP Q66K64
C	359	GLN	-	expression tag	UNP Q66K64
C	360	LYS	-	expression tag	UNP Q66K64
C	361	ILE	-	expression tag	UNP Q66K64
C	362	GLU	-	expression tag	UNP Q66K64
C	363	TRP	-	expression tag	UNP Q66K64
C	364	HIS	-	expression tag	UNP Q66K64
C	365	GLU	-	expression tag	UNP Q66K64
C	366	GLY	-	expression tag	UNP Q66K64
C	367	GLY	-	expression tag	UNP Q66K64
C	368	GLY	-	expression tag	UNP Q66K64
C	369	GLY	-	expression tag	UNP Q66K64
C	370	SER	-	expression tag	UNP Q66K64
C	371	GLY	-	expression tag	UNP Q66K64
C	372	GLU	-	expression tag	UNP Q66K64
C	373	ASN	-	expression tag	UNP Q66K64
C	374	LEU	-	expression tag	UNP Q66K64
C	375	TYR	-	expression tag	UNP Q66K64
C	376	PHE	-	expression tag	UNP Q66K64
C	377	GLN	-	expression tag	UNP Q66K64
C	378	GLY	-	expression tag	UNP Q66K64
C	379	GLY	-	expression tag	UNP Q66K64
C	380	GLY	-	expression tag	UNP Q66K64
C	381	ARG	-	expression tag	UNP Q66K64
C	382	MET	-	expression tag	UNP Q66K64

- Molecule 4 is a protein called RNA-binding protein 39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	82	Total	C	N	O	S	0	0	0
			612	386	103	118	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	226	MET	-	initiating methionine	UNP Q14498
D	227	GLY	-	expression tag	UNP Q14498
D	228	SER	-	expression tag	UNP Q14498
D	229	SER	-	expression tag	UNP Q14498
D	230	HIS	-	expression tag	UNP Q14498
D	231	HIS	-	expression tag	UNP Q14498
D	232	HIS	-	expression tag	UNP Q14498
D	233	HIS	-	expression tag	UNP Q14498
D	234	HIS	-	expression tag	UNP Q14498
D	235	HIS	-	expression tag	UNP Q14498
D	236	SER	-	expression tag	UNP Q14498
D	237	ALA	-	expression tag	UNP Q14498
D	238	VAL	-	expression tag	UNP Q14498
D	239	ASP	-	expression tag	UNP Q14498
D	240	GLU	-	expression tag	UNP Q14498
D	241	ASN	-	expression tag	UNP Q14498
D	242	LEU	-	expression tag	UNP Q14498
D	243	TYR	-	expression tag	UNP Q14498
D	244	PHE	-	expression tag	UNP Q14498
D	245	GLN	-	expression tag	UNP Q14498
D	246	GLY	-	expression tag	UNP Q14498
D	247	GLY	-	expression tag	UNP Q14498
D	248	GLY	-	expression tag	UNP Q14498
D	249	ARG	-	expression tag	UNP Q14498

- Molecule 5 is a protein called DET1- and DDB1-associated protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	56	Total	C	N	O	0	0	0
			457	299	76	82			

There are 24 discrepancies between the modelled and reference sequences:

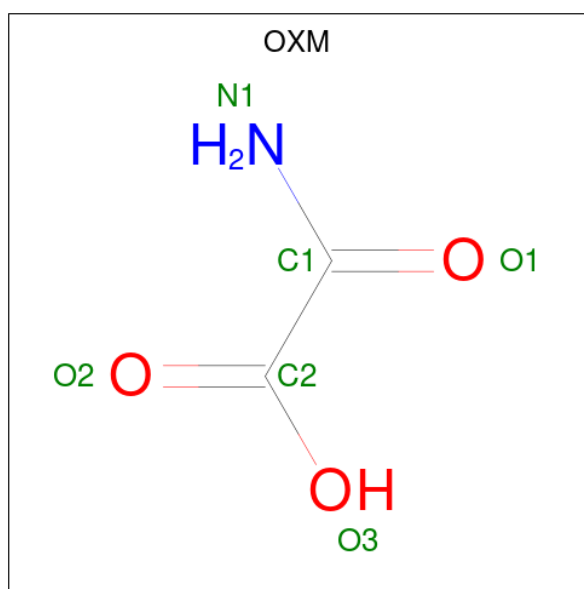
Chain	Residue	Modelled	Actual	Comment	Reference
E	-23	MET	-	initiating methionine	UNP Q9BW61
E	-22	GLY	-	expression tag	UNP Q9BW61
E	-21	SER	-	expression tag	UNP Q9BW61
E	-20	SER	-	expression tag	UNP Q9BW61
E	-19	HIS	-	expression tag	UNP Q9BW61
E	-18	HIS	-	expression tag	UNP Q9BW61
E	-17	HIS	-	expression tag	UNP Q9BW61

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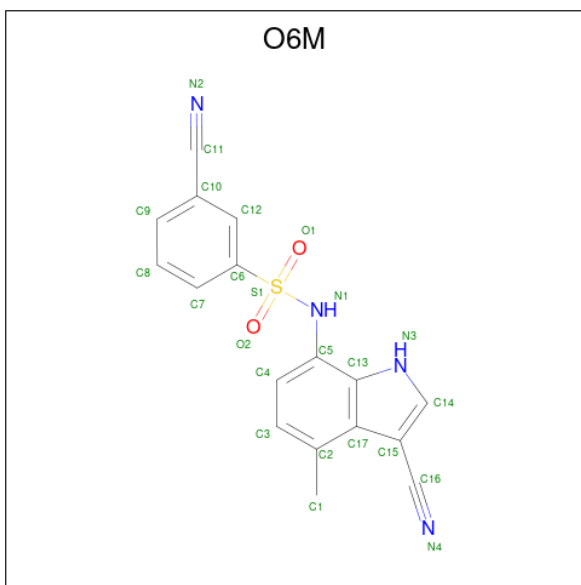
Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	HIS	-	expression tag	UNP Q9BW61
E	-15	HIS	-	expression tag	UNP Q9BW61
E	-14	HIS	-	expression tag	UNP Q9BW61
E	-13	SER	-	expression tag	UNP Q9BW61
E	-12	ALA	-	expression tag	UNP Q9BW61
E	-11	VAL	-	expression tag	UNP Q9BW61
E	-10	ASP	-	expression tag	UNP Q9BW61
E	-9	GLU	-	expression tag	UNP Q9BW61
E	-8	ASN	-	expression tag	UNP Q9BW61
E	-7	LEU	-	expression tag	UNP Q9BW61
E	-6	TYR	-	expression tag	UNP Q9BW61
E	-5	PHE	-	expression tag	UNP Q9BW61
E	-4	GLN	-	expression tag	UNP Q9BW61
E	-3	GLY	-	expression tag	UNP Q9BW61
E	-2	GLY	-	expression tag	UNP Q9BW61
E	-1	GLY	-	expression tag	UNP Q9BW61
E	0	ARG	-	expression tag	UNP Q9BW61

- Molecule 6 is OXAMIC ACID (CCD ID: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	N	O	
			6	2	1	3	

- Molecule 7 is 3-cyano-N-(3-cyano-4-methyl-1H-indol-7-yl)benzene-1-sulfonamide (CCD ID: O6M) (formula: $C_{17}H_{12}N_4O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			24	17	4	2	1		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Zn	0	0
			1	1		

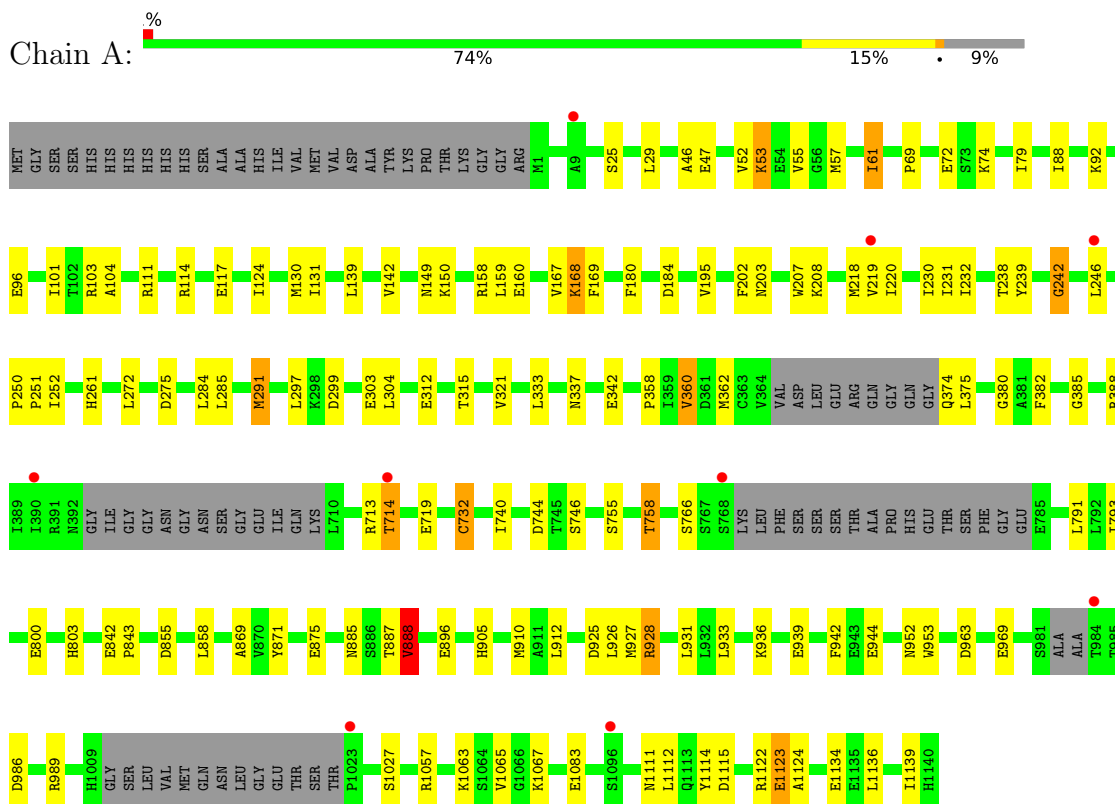
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	8	Total	O	0	0
			8	8		
9	B	3	Total	O	0	0
			3	3		
9	D	3	Total	O	0	0
			3	3		
9	E	2	Total	O	0	0
			2	2		

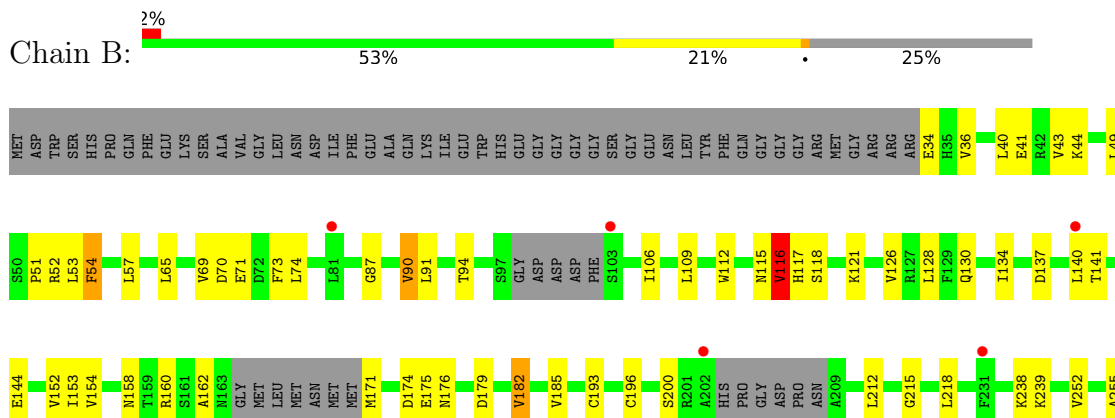
3 Residue-property plots [i](#)

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: DNA damage-binding protein 1

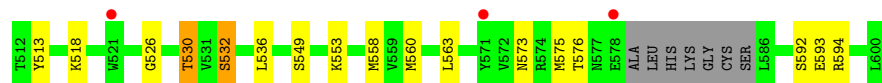
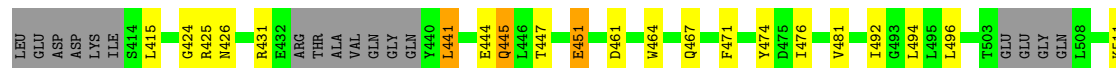
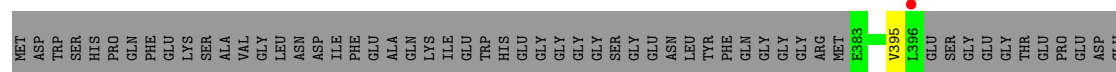


• Molecule 2: DDB1- and CUL4-associated factor 15

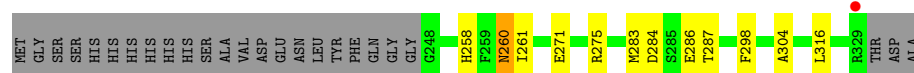




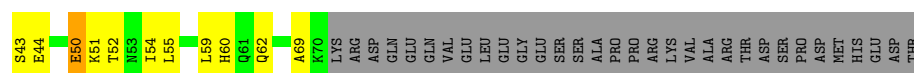
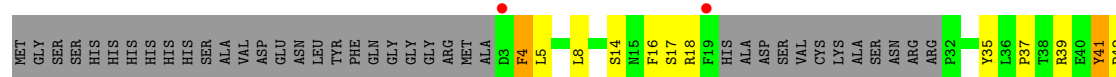
- Molecule 3: DDB1- and CUL4-associated factor 15



- Molecule 4: RNA-binding protein 39



- Molecule 5: DET1- and DDB1-associated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.11Å 93.60Å 258.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.05 – 2.90 46.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.05-2.90) 99.9 (46.05-2.90)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.205 , 0.251 0.224 , 0.270	Depositor DCC
R_{free} test set	2210 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	97.1	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 101.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10249	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: ZN, O6M, OXM

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	0.88	2/6142 (0.0%)	1.24	20/8328 (0.2%)
2	B	0.92	0/1682	1.29	7/2287 (0.3%)
3	C	0.90	0/1493	1.25	5/2035 (0.2%)
4	D	0.89	0/623	1.37	1/838 (0.1%)
5	E	0.92	0/469	1.46	7/636 (1.1%)
All	All	0.89	2/10409 (0.0%)	1.27	40/14124 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	ILE	CA-C	5.60	1.59	1.53
1	A	374	GLN	CA-C	5.21	1.63	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	ALA	CA-C-N	8.43	136.87	121.70
2	B	162	ALA	C-N-CA	8.43	136.87	121.70
1	A	888	VAL	N-CA-CB	7.25	119.69	110.99
3	C	592	SER	CA-C-N	7.19	130.64	120.28
3	C	592	SER	C-N-CA	7.19	130.64	120.28
1	A	312	GLU	N-CA-C	-7.03	103.69	112.90
3	C	526	GLY	CA-C-N	7.02	130.52	120.98
3	C	526	GLY	C-N-CA	7.02	130.52	120.98
1	A	362	MET	CA-C-N	6.91	133.39	122.62
1	A	362	MET	C-N-CA	6.91	133.39	122.62
4	D	260	ASN	CA-CB-CG	6.71	119.31	112.60
1	A	875	GLU	CB-CG-CD	6.61	123.83	112.60
3	C	593	GLU	CB-CG-CD	6.52	123.68	112.60
1	A	299	ASP	CA-CB-CG	6.43	119.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	PHE	CA-C-N	6.16	130.07	120.82
2	B	54	PHE	C-N-CA	6.16	130.07	120.82
5	E	4	PHE	CA-C-N	6.09	133.18	121.54
5	E	4	PHE	C-N-CA	6.09	133.18	121.54
1	A	952	ASN	CA-CB-CG	5.99	118.59	112.60
1	A	184	ASP	CA-CB-CG	5.92	118.52	112.60
5	E	52	THR	CA-C-N	5.74	129.26	120.82
5	E	52	THR	C-N-CA	5.74	129.26	120.82
1	A	275	ASP	CA-C-N	5.58	128.31	120.28
1	A	275	ASP	C-N-CA	5.58	128.31	120.28
5	E	50	GLU	CA-C-N	5.55	127.66	120.44
5	E	50	GLU	C-N-CA	5.55	127.66	120.44
1	A	203	ASN	CA-CB-CG	5.38	117.98	112.60
1	A	875	GLU	N-CA-C	-5.33	101.97	109.96
1	A	942	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	149	ASN	CA-C-N	5.30	127.64	120.38
1	A	149	ASN	C-N-CA	5.30	127.64	120.38
1	A	275	ASP	CA-CB-CG	5.28	117.88	112.60
5	E	41	TYR	N-CA-C	5.26	117.70	108.75
1	A	333	LEU	N-CA-C	-5.15	100.01	108.41
1	A	29	LEU	N-CA-C	-5.14	100.36	108.73
1	A	202	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	1124	ALA	N-CA-C	5.03	117.50	109.96
2	B	69	VAL	CA-C-N	5.02	127.90	120.82
2	B	69	VAL	C-N-CA	5.02	127.90	120.82
2	B	137	ASP	CA-CB-CG	5.01	117.61	112.60

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	6034	0	5865	57	0
2	B	1639	0	1578	27	0
3	C	1460	0	1407	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	612	0	565	5	0
5	E	457	0	443	12	0
6	B	6	0	2	0	0
7	B	24	0	0	0	0
8	B	1	0	0	0	0
9	A	8	0	0	0	0
9	B	3	0	0	0	0
9	D	3	0	0	0	0
9	E	2	0	0	0	0
All	All	10249	0	9860	97	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 5.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:TRP:HB3	1:A:242:GLY:HA2	1.63	0.80
1:A:130:MET:HE2	1:A:169:PHE:HZ	1.58	0.67
1:A:732:CYS:SG	1:A:793:ILE:HG23	2.33	0.67
1:A:55:VAL:HG21	1:A:1065:VAL:HG21	1.77	0.65
1:A:53:LYS:HG2	5:E:35:TYR:HB2	1.81	0.63
2:B:126:VAL:HG21	2:B:185:VAL:HG11	1.80	0.62
3:C:558:MET:HE2	5:E:55:LEU:HD11	1.81	0.62
1:A:130:MET:HE2	1:A:169:PHE:CZ	2.37	0.60
3:C:518:LYS:HB2	3:C:532:SER:HB3	1.84	0.59
4:D:284:ASP:HB3	4:D:287:THR:OG1	2.03	0.58
2:B:70:ASP:HB3	2:B:73:PHE:HD2	1.69	0.57
1:A:231:ILE:HG13	1:A:238:THR:OG1	2.05	0.57
1:A:755:SER:H	1:A:758:THR:HG22	1.69	0.57
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.87	0.56
1:A:284:LEU:CD2	5:E:4:PHE:HB2	2.35	0.56
2:B:71:GLU:HA	2:B:74:LEU:HD13	1.86	0.56
1:A:793:ILE:HD13	1:A:803:HIS:HB3	1.91	0.53
1:A:130:MET:HE1	1:A:195:VAL:HG11	1.90	0.52
1:A:219:VAL:HG12	1:A:231:ILE:HG22	1.90	0.52
1:A:910:MET:HE2	1:A:912:LEU:HD21	1.90	0.52
5:E:35:TYR:CE2	5:E:37:PRO:HG3	2.45	0.52
3:C:464:TRP:O	3:C:467:GLN:HG2	2.09	0.52
1:A:791:LEU:HD23	1:A:858:LEU:HD21	1.91	0.52
1:A:284:LEU:HD21	5:E:4:PHE:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:ASP:HB3	1:A:928:ARG:H	1.77	0.50
1:A:936:LYS:HB2	1:A:939:GLU:HB2	1.93	0.50
1:A:382:PHE:HD1	1:A:740:ILE:HD11	1.75	0.50
2:B:193:CYS:HB3	2:B:196:CYS:HB2	1.93	0.50
3:C:494:LEU:HD23	3:C:496:LEU:HD23	1.94	0.50
2:B:238:LYS:HD3	3:C:481:VAL:O	2.12	0.50
1:A:88:ILE:HD12	1:A:104:ALA:HB3	1.93	0.49
1:A:261:HIS:HA	1:A:272:LEU:O	2.12	0.49
2:B:212:LEU:HD21	3:C:441:LEU:HB2	1.95	0.48
1:A:25:SER:HA	1:A:74:LYS:HE3	1.95	0.48
1:A:167:VAL:HG23	1:A:180:PHE:HB3	1.95	0.48
1:A:360:VAL:HG23	2:B:44:LYS:HB3	1.96	0.48
3:C:476:ILE:HD12	3:C:492:ILE:HG12	1.96	0.48
1:A:385:GLY:HA3	1:A:719:GLU:O	2.14	0.47
2:B:54:PHE:CD2	2:B:57:LEU:HD21	2.50	0.47
2:B:54:PHE:O	2:B:57:LEU:HG	2.13	0.47
1:A:1067:LYS:NZ	5:E:43:SER:HB2	2.28	0.47
1:A:910:MET:HE1	2:B:40:LEU:HD11	1.95	0.47
2:B:109:LEU:HB2	2:B:128:LEU:HD11	1.96	0.47
1:A:239:TYR:HB3	1:A:246:LEU:HB2	1.96	0.46
4:D:258:HIS:HB3	4:D:261:ILE:HG12	1.97	0.46
1:A:321:VAL:HG21	5:E:16:PHE:CG	2.50	0.46
1:A:793:ILE:HD11	1:A:858:LEU:HD22	1.97	0.46
2:B:144:GLU:HG2	2:B:152:VAL:HG12	1.98	0.46
1:A:843:PRO:HG2	1:A:869:ALA:HB2	1.98	0.45
2:B:90:VAL:HG13	2:B:112:TRP:HB2	1.99	0.45
1:A:230:ILE:HD11	1:A:285:LEU:HD21	1.99	0.45
1:A:103:ARG:O	5:E:44:GLU:HB3	2.17	0.45
1:A:158:ARG:HB2	5:E:54:ILE:HD12	1.99	0.45
1:A:168:LYS:HD3	1:A:219:VAL:HG23	1.98	0.44
3:C:461:ASP:CG	3:C:530:THR:HG21	2.42	0.44
1:A:888:VAL:HG22	1:A:905:HIS:HB3	1.99	0.44
2:B:255:ALA:HB3	3:C:444:GLU:HB2	1.99	0.44
2:B:158:ASN:HD21	2:B:179:ASP:HB2	1.82	0.44
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.96	0.44
1:A:1063:LYS:HB2	5:E:37:PRO:HB2	2.00	0.43
1:A:57:MET:HE2	1:A:79:ILE:HG21	2.00	0.43
1:A:220:ILE:HB	1:A:230:ILE:HB	2.00	0.43
2:B:141:THR:HG23	3:C:576:THR:HB	2.00	0.43
1:A:239:TYR:CG	1:A:297:LEU:HD23	2.54	0.43
1:A:926:LEU:HD22	2:B:40:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:474:TYR:HB3	3:C:494:LEU:HD12	1.99	0.43
2:B:51:PRO:C	2:B:53:LEU:H	2.27	0.43
1:A:69:PRO:HD2	1:A:72:GLU:HG3	2.00	0.43
2:B:70:ASP:HB3	2:B:73:PHE:CD2	2.52	0.43
3:C:415:LEU:H	3:C:445:GLN:HE22	1.64	0.43
1:A:927:MET:HG2	1:A:953:TRP:CZ2	2.54	0.43
2:B:91:LEU:HB2	3:C:575:MET:HE1	2.00	0.43
2:B:116:VAL:HG22	2:B:117:HIS:N	2.34	0.42
2:B:43:VAL:HG13	2:B:49:LEU:HB2	2.00	0.42
3:C:511:LYS:HB2	3:C:513:TYR:CE1	2.55	0.42
1:A:291:MET:HE3	1:A:291:MET:HB2	1.94	0.42
1:A:871:TYR:HE2	1:A:885:ASN:HA	1.84	0.42
3:C:553:LYS:HG2	4:D:316:LEU:HD13	2.02	0.42
3:C:560:MET:HE1	4:D:260:ASN:CB	2.50	0.42
1:A:218:MET:HG2	1:A:232:ILE:HB	2.00	0.42
1:A:933:LEU:HD23	1:A:944:GLU:HA	2.02	0.42
2:B:160:ARG:HG3	2:B:174:ASP:O	2.19	0.42
3:C:558:MET:HE1	5:E:59:LEU:HD21	2.02	0.41
4:D:298:PHE:HB2	4:D:304:ALA:HB2	2.01	0.41
1:A:358:PRO:HD2	1:A:380:GLY:CA	2.48	0.41
2:B:154:VAL:O	2:B:182:VAL:HA	2.21	0.41
1:A:388:ARG:HD3	1:A:714:THR:HB	2.03	0.41
2:B:115:ASN:HB3	2:B:118:SER:HB2	2.03	0.41
1:A:57:MET:HG3	1:A:61:ILE:HD11	2.03	0.41
1:A:1057:ARG:CZ	1:A:1112:LEU:HB2	2.50	0.41
3:C:451:GLU:HG3	3:C:471:PHE:HZ	1.85	0.41
1:A:124:ILE:HG12	1:A:131:ILE:HG12	2.02	0.40
2:B:144:GLU:HB2	3:C:573:ASN:HB3	2.03	0.40
1:A:46:ALA:O	5:E:18:ARG:HB2	2.21	0.40
1:A:1122:ARG:HB3	1:A:1123:GLU:H	1.66	0.40
1:A:1136:LEU:O	1:A:1139:ILE:HG12	2.20	0.40
1:A:843:PRO:HD3	2:B:36:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	771/864 (89%)	728 (94%)	39 (5%)	4 (0%)	24 54
2	B	200/276 (72%)	191 (96%)	6 (3%)	3 (2%)	8 28
3	C	173/263 (66%)	163 (94%)	8 (5%)	2 (1%)	10 34
4	D	80/107 (75%)	79 (99%)	1 (1%)	0	100 100
5	E	52/126 (41%)	41 (79%)	8 (15%)	3 (6%)	1 4
All	All	1276/1636 (78%)	1202 (94%)	62 (5%)	12 (1%)	14 41

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1114	TYR
1	A	1115	ASP
2	B	116	VAL
5	E	39	ARG
1	A	1123	GLU
5	E	69	ALA
3	C	424	GLY
3	C	426	ASN
1	A	242	GLY
2	B	215	GLY
2	B	87	GLY
5	E	42	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	653/749 (87%)	605 (93%)	48 (7%)	13 38
2	B	177/242 (73%)	156 (88%)	21 (12%)	5 16
3	C	162/232 (70%)	149 (92%)	13 (8%)	11 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	61/89 (68%)	57 (93%)	4 (7%)	15	43
5	E	49/112 (44%)	40 (82%)	9 (18%)	1	6
All	All	1102/1424 (77%)	1007 (91%)	95 (9%)	10	30

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	52	VAL
1	A	53	LYS
1	A	92	LYS
1	A	96	GLU
1	A	101	ILE
1	A	111	ARG
1	A	114	ARG
1	A	117	GLU
1	A	139	LEU
1	A	142	VAL
1	A	150	LYS
1	A	159	LEU
1	A	160	GLU
1	A	168	LYS
1	A	208	LYS
1	A	252	ILE
1	A	291	MET
1	A	303	GLU
1	A	304	LEU
1	A	315	THR
1	A	337	ASN
1	A	342	GLU
1	A	360	VAL
1	A	375	LEU
1	A	713	ARG
1	A	714	THR
1	A	732	CYS
1	A	744	ASP
1	A	746	SER
1	A	758	THR
1	A	766	SER
1	A	800	GLU
1	A	842	GLU

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Mol	Chain	Res	Type
1	A	855	ASP
1	A	887	THR
1	A	888	VAL
1	A	896	GLU
1	A	928	ARG
1	A	931	LEU
1	A	963	ASP
1	A	969	GLU
1	A	986	ASP
1	A	989	ARG
1	A	1027	SER
1	A	1083	GLU
1	A	1111	ASN
1	A	1134	GLU
2	B	34	GLU
2	B	41	GLU
2	B	52	ARG
2	B	65	LEU
2	B	90	VAL
2	B	94	THR
2	B	106	ILE
2	B	116	VAL
2	B	121	LYS
2	B	130	GLN
2	B	134	ILE
2	B	140	LEU
2	B	153	ILE
2	B	171	MET
2	B	175	GLU
2	B	176	ASN
2	B	182	VAL
2	B	200	SER
2	B	218	LEU
2	B	239	LYS
2	B	252	VAL
3	C	395	VAL
3	C	425	ARG
3	C	431	ARG
3	C	441	LEU
3	C	445	GLN
3	C	447	THR
3	C	451	GLU

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Mol	Chain	Res	Type
3	C	530	THR
3	C	532	SER
3	C	536	LEU
3	C	549	SER
3	C	563	LEU
3	C	594	ARG
4	D	271	GLU
4	D	275	ARG
4	D	283	MET
4	D	286	GLU
5	E	5	LEU
5	E	8	LEU
5	E	14	SER
5	E	17	SER
5	E	41	TYR
5	E	50	GLU
5	E	51	LYS
5	E	60	HIS
5	E	62	GLN

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

Mol	Chain	Res	Type
1	A	4	ASN
1	A	149	ASN
1	A	156	ASN
1	A	163	HIS
1	A	203	ASN
1	A	234	GLN
1	A	241	ASN
1	A	290	GLN
1	A	337	ASN
1	A	731	GLN
1	A	759	GLN
1	A	797	HIS
1	A	810	ASN
1	A	950	ASN
1	A	978	GLN
2	B	130	GLN
2	B	197	GLN
2	B	241	GLN
3	C	455	ASN

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Mol	Chain	Res	Type
4	D	310	GLN
4	D	312	ASN

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
6	OXM	B	301	-	5,5,5	2.27	2 (40%)	2,6,6	0.42	0
7	O6M	B	302	-	25,26,26	0.24	0	34,38,38	0.74	2 (5%)

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
6	OXM	B	301	-	-	4/4/4/4	-
7	O6M	B	302	-	-	0/13/15/15	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	301	OXM	O2-C2	4.17	1.32	1.22
6	B	301	OXM	O3-C2	-2.86	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	302	O6M	C15-C14-N3	2.59	110.33	107.45
7	B	302	O6M	C5-N1-S1	2.05	129.92	123.34

There are no chirality outliers.

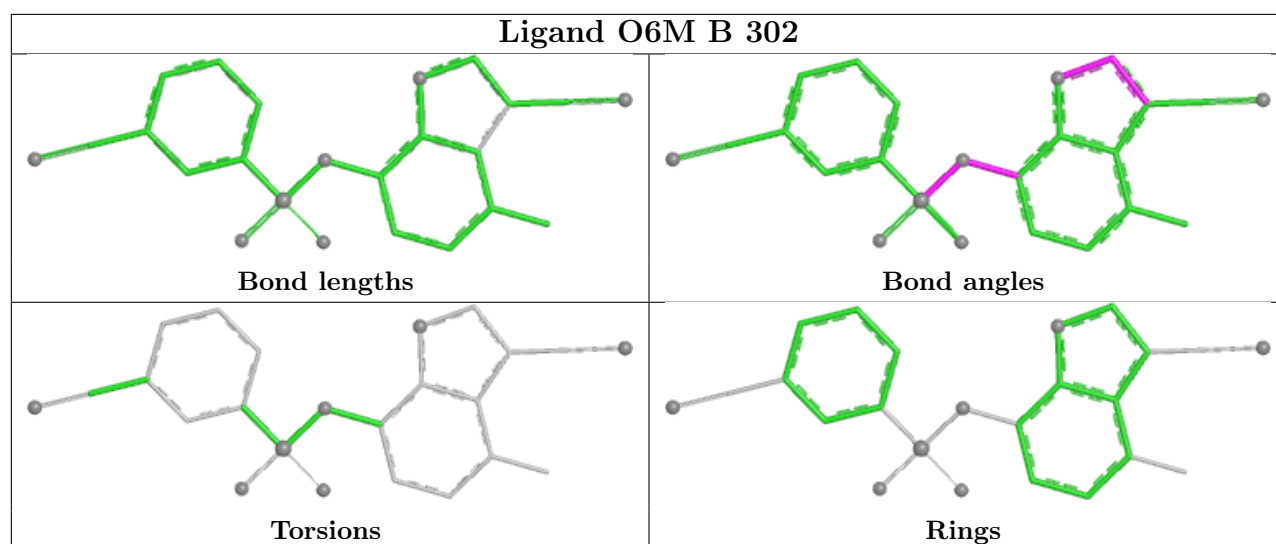
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	301	OXM	N1-C1-C2-O2
6	B	301	OXM	N1-C1-C2-O3
6	B	301	OXM	O1-C1-C2-O2
6	B	301	OXM	O1-C1-C2-O3

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	783/864 (90%)	-0.05	9 (1%) 78 71	80, 137, 186, 209	0
2	B	208/276 (75%)	-0.03	5 (2%) 59 50	84, 117, 166, 205	0
3	C	183/263 (69%)	-0.11	4 (2%) 62 53	83, 114, 171, 224	0
4	D	82/107 (76%)	-0.34	1 (1%) 76 69	96, 119, 148, 185	0
5	E	56/126 (44%)	0.13	2 (3%) 46 38	104, 161, 182, 201	0
All	All	1312/1636 (80%)	-0.07	21 (1%) 70 62	80, 128, 184, 224	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ALA	5.5
3	C	396	LEU	4.0
2	B	81	LEU	3.6
2	B	202	ALA	3.0
1	A	1023	PRO	2.8
1	A	390	ILE	2.6
5	E	19	PHE	2.6
3	C	521	TRP	2.6
4	D	329	ARG	2.6
1	A	1096	SER	2.5
1	A	219	VAL	2.3
1	A	246	LEU	2.2
5	E	3	ASP	2.2
1	A	984	THR	2.2
2	B	140	LEU	2.1
2	B	231	PHE	2.1
3	C	571	TYR	2.1
1	A	714	THR	2.1
2	B	103	SER	2.1
3	C	578	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	768	SER	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](#)

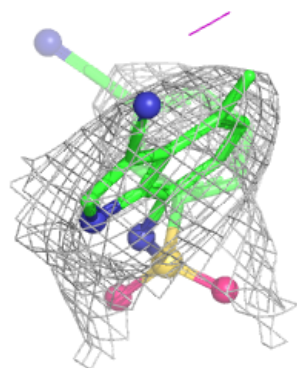
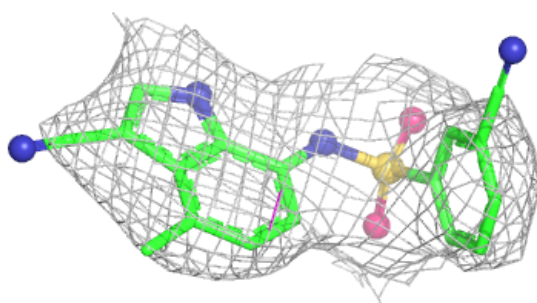
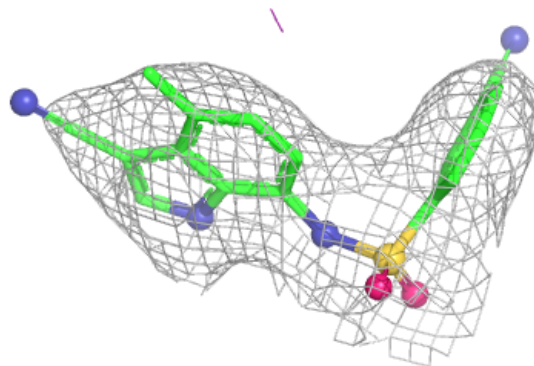
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	OXM	B	301	6/6	0.94	0.09	118,121,126,128	0
7	O6M	B	302	24/24	0.99	0.07	82,97,109,119	0
8	ZN	B	303	1/1	0.99	0.05	155,155,155,155	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around O6M B 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.