



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:07 AM UTC

PDB ID : 6UD7 / pdb_00006ud7
Title : Crystal structure of full-length human DCAF15-DDB1(deltaBPB)-DDA1-RB M39 in complex with indisulam
Authors : Bussiere, D.E.; Shu, W.; Xie, L.; Knapp, M.
Deposited on : 2019-09-18
Resolution : 2.30 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

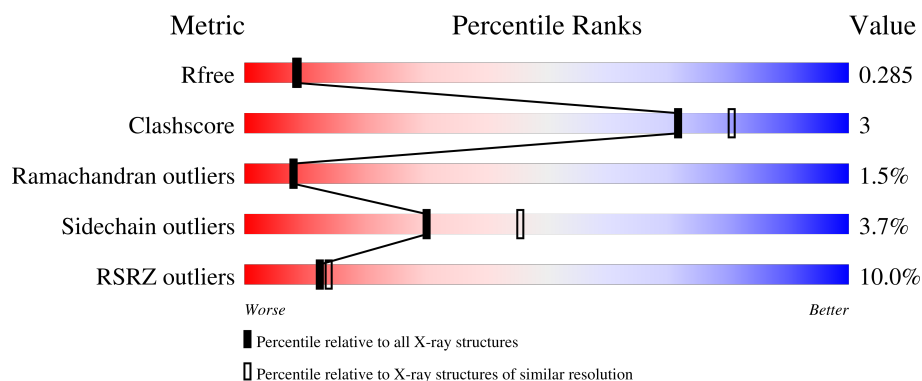
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	601	
2	B	836	
3	C	81	
4	D	101	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11635 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 DDB1- and CUL4-associated factor 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	3	0
			3392	2184	568	618	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q66K64
A	1	PRO	-	expression tag	UNP Q66K64

- Molecule 2 is a protein called DNA damage-binding protein 1,DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	806	Total	C	N	O	S	0	2	0
			6237	3962	1047	1194	34			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	700	GLY	-	linker	UNP Q16531
B	701	ASN	-	linker	UNP Q16531
B	702	GLY	-	linker	UNP Q16531
B	703	ASN	-	linker	UNP Q16531
B	704	SER	-	linker	UNP Q16531
B	705	GLY	-	linker	UNP Q16531

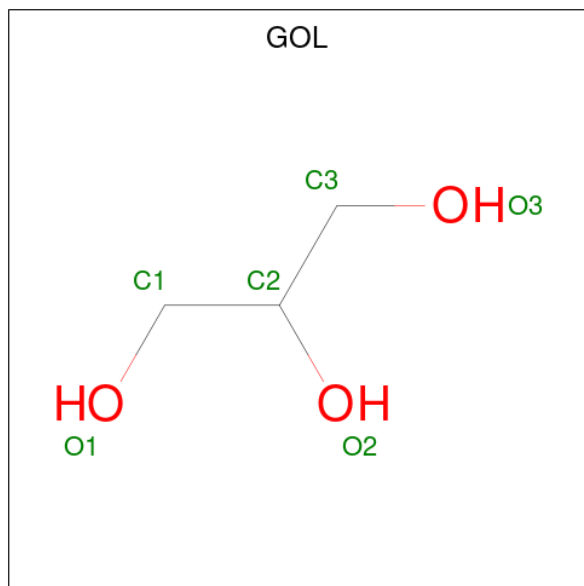
- Molecule 3 is a protein called RNA-binding motif protein 39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	81	Total	C	N	O	S	0	0	0
			626	397	108	115	6			

- Molecule 4 is a protein called DET1- and DDB1-associated protein 1.

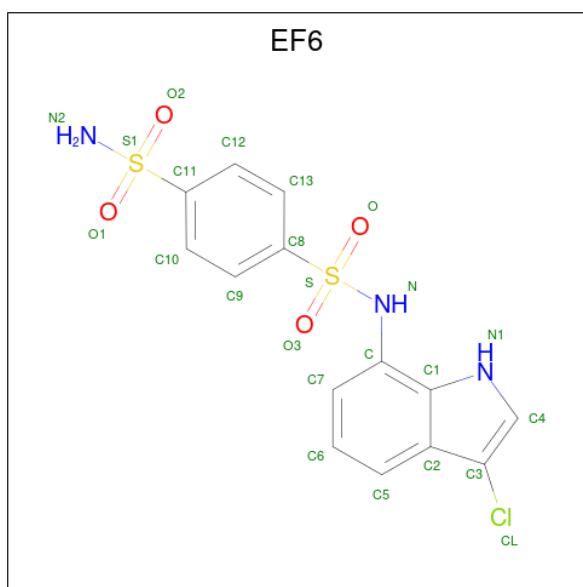
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	73	Total	C	N	O	S	0	2	0
			600	384	107	108	1			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

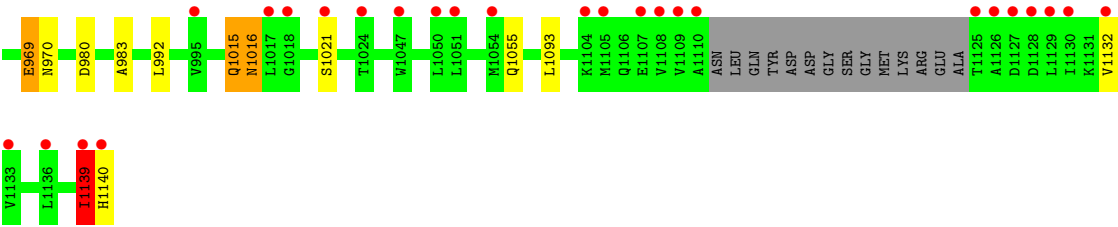
- Molecule 6 is N 1 -(3-chloro-1H-indol-7-yl)benzene-1,4-disulfonamide (CCD ID: EF6) (formula: $C_{14}H_{12}ClN_3O_4S_2$) (labeled as "Ligand of Interest" by depositor).



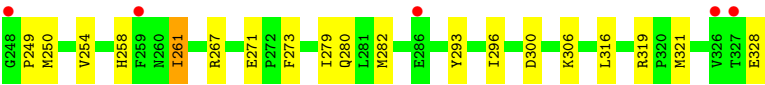
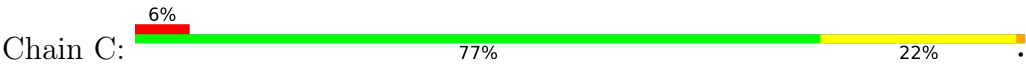
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	S	
			24	14	1	3	4	2	
								0	0

- Molecule 7 is water.

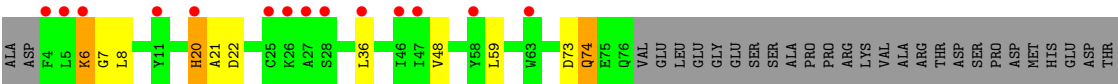
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	199	Total	O		
			199	199	0	0
7	B	441	Total	O		
			441	441	0	0
7	C	48	Total	O		
			48	48	0	0
7	D	56	Total	O		
			56	56	0	0



• Molecule 3: RNA-binding motif protein 39



• Molecule 4: 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	81.03Å 93.78Å 264.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.10 – 2.30 69.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (69.10-2.30) 99.9 (69.10-2.30)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.205 , 0.248 (Not available) , 0.285	Depositor DCC
R_{free} test set	4576 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 83.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11635	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: GOL, EF6

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	0.75	0/3484	1.25	11/4735 (0.2%)
2	B	0.71	1/6356 (0.0%)	1.17	11/8612 (0.1%)
3	C	0.73	0/638	1.27	2/853 (0.2%)
4	D	0.76	0/622	1.52	8/843 (0.9%)
All	All	0.73	1/11100 (0.0%)	1.22	32/15043 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	873	MET	SD-CE	-6.66	1.62	1.79

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	7	GLY	CA-C-N	6.91	130.00	120.39
4	D	7	GLY	C-N-CA	6.91	130.00	120.39
1	A	70	ASP	CA-CB-CG	6.45	119.05	112.60
2	B	961	ASP	CA-CB-CG	6.38	118.98	112.60
2	B	312	GLU	N-CA-C	-6.32	105.22	113.12
1	A	262	GLY	N-CA-C	-6.27	98.32	113.18
2	B	184	ASP	CA-CB-CG	6.08	118.68	112.60
4	D	73	ASP	N-CA-C	5.63	117.96	110.53
2	B	771	PHE	CA-C-N	5.47	127.62	120.28
2	B	771	PHE	C-N-CA	5.47	127.62	120.28
2	B	942	PHE	CA-CB-CG	5.43	119.23	113.80
4	D	6	LYS	CA-C-N	5.39	131.98	121.41
4	D	6	LYS	C-N-CA	5.39	131.98	121.41
1	A	475	ASP	CA-CB-CG	5.37	117.97	112.60
4	D	21	ALA	CA-C-N	5.37	131.79	121.54
4	D	21	ALA	C-N-CA	5.37	131.79	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	267	ASN	CA-CB-CG	5.36	117.96	112.60
1	A	387	VAL	CA-C-N	5.33	129.88	121.56
1	A	387	VAL	C-N-CA	5.33	129.88	121.56
4	D	8	LEU	N-CA-C	5.33	116.41	109.64
2	B	838	PRO	CA-C-N	5.28	127.30	120.44
2	B	838	PRO	C-N-CA	5.28	127.30	120.44
2	B	202	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	583	GLY	CA-C-N	5.23	131.53	121.54
1	A	583	GLY	C-N-CA	5.23	131.53	121.54
1	A	72	ASP	CA-C-N	5.19	131.45	121.54
1	A	72	ASP	C-N-CA	5.19	131.45	121.54
1	A	192	ARG	CA-C-N	5.17	131.41	121.54
1	A	192	ARG	C-N-CA	5.17	131.41	121.54
3	C	250	MET	N-CA-C	5.15	116.81	108.26
3	C	300	ASP	CA-CB-CG	5.10	117.70	112.60
2	B	333	LEU	N-CA-C	-5.07	100.25	108.52

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	3392	0	3295	26	0
2	B	6237	0	6134	38	0
3	C	626	0	615	7	0
4	D	600	0	573	2	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	24	0	0	1	0
7	A	199	0	0	1	0
7	B	441	0	0	1	0
7	C	48	0	0	0	0
7	D	56	0	0	0	0
All	All	11635	0	10633	70	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 3.

All (70) 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)
3:C:258:HIS:HB3	3:C:261:ILE:HD12	1.58	0.85
2:B:130:MET:HE2	2:B:169:PHE:HZ	1.44	0.80
1:A:36:VAL:HG22	1:A:57:LEU:HD11	1.70	0.73
1:A:583:GLY:HA2	3:C:280:GLN:HG2	1.68	0.73
2:B:130:MET:HE2	2:B:169:PHE:CZ	2.24	0.72
2:B:848:ILE:HG23	2:B:873:MET:HE1	1.74	0.70
2:B:174:GLN:H	2:B:174:GLN:CD	2.02	0.68
2:B:358:PRO:HD2	2:B:380:GLY:HA2	1.76	0.66
3:C:273:PHE:HD1	3:C:306:LYS:HE3	1.59	0.65
2:B:1015:GLN:HG3	2:B:1016:ASN:H	1.61	0.65
2:B:854:SER:OG	2:B:859:GLN:NE2	2.23	0.65
2:B:119:GLY:O	2:B:134:ARG:NH1	2.29	0.65
2:B:69:PRO:HD2	2:B:72:GLU:HG3	1.81	0.63
1:A:213:ARG:HD3	1:A:214:HIS:H	1.63	0.62
2:B:37:THR:HG23	2:B:38:ARG:HD2	1.81	0.61
2:B:870:VAL:HG11	2:B:873:MET:HE3	1.82	0.61
1:A:65:LEU:HD22	1:A:600:LEU:HD23	1.82	0.60
1:A:107:TYR:HE2	1:A:134:ILE:HG21	1.67	0.60
4:D:74:GLN:O	4:D:74:GLN:HG3	2.03	0.59
1:A:213:ARG:HD2	1:A:213:ARG:H	1.68	0.58
1:A:144:GLU:HB2	1:A:573:ASN:HB3	1.88	0.55
1:A:263:ASP:N	1:A:263:ASP:OD1	2.40	0.55
3:C:267:ARG:O	3:C:271:GLU:HB2	2.06	0.54
2:B:938:MET:HA	2:B:938:MET:HE2	1.89	0.54
2:B:113:GLY:HA2	7:B:1301:HOH:O	2.08	0.53
2:B:134:ARG:HD2	2:B:134:ARG:C	2.36	0.51
2:B:174:GLN:CD	2:B:174:GLN:N	2.69	0.51
2:B:63:VAL:HB	2:B:80:LEU:HB3	1.93	0.50
2:B:230:ILE:HD11	2:B:285:LEU:HD21	1.94	0.49
2:B:840:GLU:HG3	2:B:842:GLU:H	1.77	0.48
2:B:910:MET:HE2	2:B:912:LEU:HD21	1.95	0.48
2:B:289:GLU:HA	2:B:295:VAL:HG12	1.97	0.47
1:A:220:THR:HB	1:A:420:THR:HG22	1.97	0.47
1:A:80:PHE:HB3	1:A:589:LEU:HD11	1.96	0.46
1:A:145:TRP:CD1	1:A:240:ASP:HA	2.50	0.46
2:B:946:ALA:HB1	2:B:992:LEU:HG	1.98	0.46
2:B:57:MET:HE2	2:B:79:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:316:LEU:HD22	3:C:321:MET:HE2	1.98	0.45
1:A:391:LYS:HG3	1:A:444:GLU:HG2	1.99	0.45
1:A:518:LYS:HB2	1:A:532:SER:HB3	1.98	0.45
2:B:130:MET:HE1	2:B:195:VAL:HG11	1.99	0.44
2:B:207:TRP:HB3	2:B:242:GLY:HA2	1.98	0.44
2:B:271:TYR:HB2	2:B:283:LEU:HB3	1.99	0.44
1:A:422:LEU:HD11	1:A:443:VAL:HG21	2.00	0.43
1:A:61:VAL:HG13	1:A:596:THR:HG23	2.00	0.43
3:C:254:VAL:HG21	3:C:296:ILE:HD12	2.01	0.43
1:A:126:VAL:HG11	1:A:185:VAL:HG11	1.99	0.43
2:B:286:GLU:HB2	2:B:299:ASP:H	1.85	0.42
1:A:518:LYS:HD3	4:D:59:LEU:HD13	2.02	0.42
1:A:232:GLN:HG2	6:A:702:EF6:C1	2.50	0.42
1:A:256:VAL:HG23	1:A:441:LEU:HD21	2.00	0.42
1:A:264:ARG:H	1:A:264:ARG:HG3	1.58	0.42
2:B:1139:ILE:O	2:B:1140:HIS:HB2	2.20	0.42
1:A:40:LEU:HD11	2:B:910:MET:HE1	2.02	0.42
2:B:385:GLY:HA3	2:B:719:GLU:O	2.20	0.42
3:C:282:MET:HG3	3:C:293:TYR:CE2	2.55	0.42
2:B:1055:GLN:HG3	2:B:1093:LEU:HD23	2.02	0.41
2:B:980:ASP:HB3	2:B:983:ALA:HB2	2.02	0.41
1:A:213:ARG:CD	1:A:214:HIS:H	2.31	0.41
1:A:492:ILE:O	1:A:516:SER:HA	2.21	0.41
2:B:134:ARG:HD2	2:B:134:ARG:O	2.21	0.41
2:B:312:GLU:HB2	2:B:327:ARG:HG2	2.03	0.41
2:B:1139:ILE:HB	2:B:1140:HIS:H	1.65	0.41
1:A:391:LYS:HE2	1:A:442:THR:HG21	2.04	0.40
1:A:543:THR:HG22	1:A:545:GLY:H	1.87	0.40
2:B:118:THR:OG1	2:B:134:ARG:NH2	2.55	0.40
2:B:292:ASP:HB3	2:B:294:THR:HG22	2.04	0.40
2:B:969:GLU:HG2	2:B:970:ASN:N	2.36	0.40
1:A:214:HIS:HB2	7:A:805:HOH:O	2.20	0.40
2:B:124:ILE:HG12	2:B:131:ILE:HG12	2.03	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	421/601 (70%)	376 (89%)	33 (8%)	12 (3%)	3	2
2	B	800/836 (96%)	753 (94%)	43 (5%)	4 (0%)	24	31
3	C	79/81 (98%)	76 (96%)	2 (2%)	1 (1%)	9	10
4	D	73/101 (72%)	60 (82%)	9 (12%)	4 (6%)	1	0
All	All	1373/1619 (85%)	1265 (92%)	87 (6%)	21 (2%)	8	8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	PHE
1	A	267	CYS
1	A	434	THR
2	B	1139	ILE
1	A	103	SER
1	A	116	VAL
1	A	163	ASN
1	A	168	ASN
1	A	435	ALA
2	B	1015	GLN
4	D	20[A]	HIS
4	D	20[B]	HIS
2	B	36	ASN
2	B	1021	SER
4	D	22	ASP
1	A	72	ASP
1	A	75	TYR
4	D	74	GLN
1	A	428	ARG
3	C	249	PRO
1	A	98	GLY

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	371/514 (72%)	353 (95%)	18 (5%)	22	34
2	B	680/727 (94%)	663 (98%)	17 (2%)	42	60
3	C	66/68 (97%)	62 (94%)	4 (6%)	17	24
4	D	63/92 (68%)	58 (92%)	5 (8%)	11	15
All	All	1180/1401 (84%)	1136 (96%)	44 (4%)	30	45

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	PHE
1	A	126	VAL
1	A	129	PHE
1	A	131	ASP
1	A	212	LEU
1	A	213	ARG
1	A	219	HIS
1	A	237	LEU
1	A	263	ASP
1	A	267	CYS
1	A	268	GLN
1	A	387	VAL
1	A	434	THR
1	A	442	THR
1	A	472	SER
1	A	519	VAL
1	A	531	VAL
1	A	584	CYS
2	B	60	LYS
2	B	117	GLU
2	B	134	ARG
2	B	207	TRP
2	B	209	GLN
2	B	253	ILE

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Mol	Chain	Res	Type
2	B	275	ASP
2	B	291	MET
2	B	299	ASP
2	B	338	VAL
2	B	770	LEU
2	B	896	GLU
2	B	931	LEU
2	B	969	GLU
2	B	1016	ASN
2	B	1132	VAL
2	B	1139	ILE
3	C	261	ILE
3	C	279	ILE
3	C	319	ARG
3	C	328	GLU
4	D	6	LYS
4	D	20[A]	HIS
4	D	20[B]	HIS
4	D	36	LEU
4	D	48	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	223	GLN
1	A	246	ASN
1	A	388	ASN
1	A	467	GLN
1	A	486	ASN
1	A	491	ASN
1	A	577	ASN
2	B	105	HIS
2	B	209	GLN
2	B	211	ASN
2	B	337	ASN
2	B	392	ASN
2	B	731	GLN
2	B	759	GLN
2	B	796	GLN
2	B	810	ASN
2	B	877	ASN

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Mol	Chain	Res	Type
2	B	908	ASN
2	B	941	ASN
2	B	970	ASN
2	B	1009	HIS
2	B	1056	ASN
4	D	12	ASN
4	D	53	ASN
4	D	61	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
5	GOL	B	1201	-	5,5,5	0.06	0	5,5,5	0.20	0
6	EF6	A	702	-	26,26,26	0.84	2 (7%)	38,40,40	1.98	5 (13%)
5	GOL	A	701	-	5,5,5	0.04	0	5,5,5	0.21	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	GOL	B	1201	-	-	2/4/4/4	-
6	EF6	A	702	-	-	4/17/17/17	0/3/3/3
5	GOL	A	701	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	702	EF6	C-N	-2.19	1.39	1.42
6	A	702	EF6	C1-C	2.19	1.42	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	702	EF6	C1-C-N	-9.29	110.33	119.97
6	A	702	EF6	C7-C-N	5.66	131.85	120.92
6	A	702	EF6	O3-S-O	-2.65	116.30	119.52
6	A	702	EF6	C3-C4-N1	2.43	110.67	107.28
6	A	702	EF6	C2-C1-C	-2.00	120.70	122.06

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	EF6	C10-C11-S1-N2
6	A	702	EF6	C12-C11-S1-O2
6	A	702	EF6	C12-C11-S1-N2
6	A	702	EF6	C10-C11-S1-O2
5	B	1201	GOL	C1-C2-C3-O3
5	B	1201	GOL	O2-C2-C3-O3

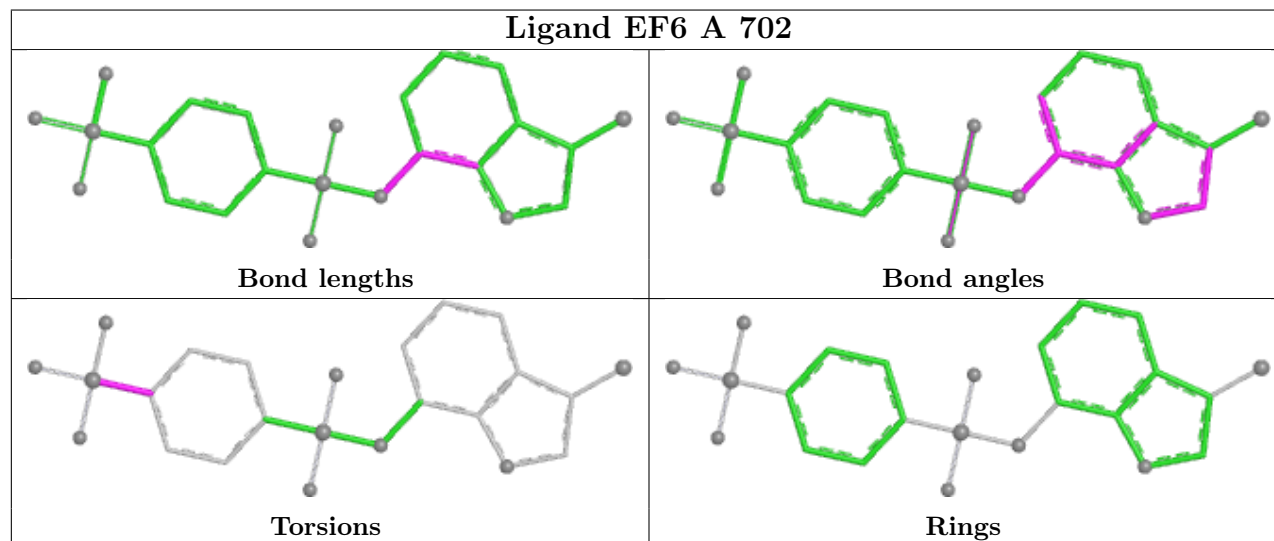
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	702	EF6	1	0

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	426/601 (70%)	0.96	62 (14%) 6 6	29, 75, 140, 195	3 (0%)
2	B	806/836 (96%)	0.61	57 (7%) 22 24	42, 73, 130, 222	2 (0%)
3	C	81/81 (100%)	0.58	5 (6%) 26 28	50, 65, 90, 138	0
4	D	73/101 (72%)	1.36	14 (19%) 3 3	41, 95, 127, 148	2 (2%)
All	All	1386/1619 (85%)	0.75	138 (9%) 12 14	29, 74, 134, 222	7 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1129	LEU	5.9
2	B	395	GLY	5.6
1	A	194	ALA	5.3
1	A	387	VAL	4.9
2	B	1110	ALA	4.8
2	B	1126	ALA	4.8
4	D	20[A]	HIS	4.8
2	B	145	LEU	4.8
2	B	1107	GLU	4.5
1	A	271	TYR	4.5
2	B	1109	VAL	4.5
1	A	199	ALA	4.2
1	A	171[A]	MET	4.1
2	B	1132	VAL	4.1
1	A	390	THR	4.0
2	B	1108	VAL	3.9
2	B	1133	VAL	3.8
1	A	508	LEU	3.7
2	B	745	THR	3.6
1	A	418	VAL	3.6
1	A	266	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	1018	GLY	3.6
2	B	1140	HIS	3.5
2	B	1125	THR	3.5
3	C	286	GLU	3.5
1	A	429	PRO	3.4
3	C	248	GLY	3.4
1	A	195	ALA	3.4
2	B	1130	ILE	3.4
1	A	73	PHE	3.4
2	B	394	ILE	3.3
1	A	268	GLN	3.3
4	D	5	LEU	3.3
2	B	1139	ILE	3.3
1	A	507	GLN	3.3
2	B	346	TYR	3.3
2	B	287	LYS	3.2
4	D	25	CYS	3.2
4	D	4	PHE	3.2
1	A	212	LEU	3.2
1	A	213	ARG	3.1
4	D	36	LEU	3.1
2	B	780	THR	3.1
1	A	417	PHE	3.1
2	B	144	PRO	3.1
4	D	27	ALA	3.0
1	A	427	LEU	3.0
1	A	396	LEU	2.9
1	A	394	TYR	2.9
2	B	773	SER	2.9
2	B	294	THR	2.9
1	A	166	LEU	2.9
1	A	134	ILE	2.8
3	C	327	THR	2.8
1	A	74	LEU	2.8
1	A	270	LEU	2.8
2	B	752	LEU	2.8
2	B	1024	THR	2.8
2	B	1127	ASP	2.8
2	B	1136	LEU	2.8
1	A	180	ILE	2.8
2	B	1050	LEU	2.7
2	B	140	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	995	VAL	2.7
1	A	431	ARG	2.7
1	A	101	ASP	2.7
1	A	32	ARG	2.7
3	C	326	VAL	2.6
1	A	269	ILE	2.6
1	A	569	GLY	2.6
1	A	425	ARG	2.6
1	A	528	PHE	2.6
1	A	438	GLY	2.6
2	B	291	MET	2.6
1	A	586	LEU	2.5
1	A	102	PHE	2.5
4	D	6	LYS	2.5
2	B	1017	LEU	2.5
2	B	751	ALA	2.5
2	B	307	GLU	2.4
3	C	259	PHE	2.4
4	D	28	SER	2.4
2	B	1105	MET	2.4
2	B	146	ASP	2.4
1	A	428	ARG	2.4
1	A	214	HIS	2.4
4	D	63	TRP	2.4
2	B	1128	ASP	2.4
1	A	568	SER	2.4
1	A	170	MET	2.4
2	B	744	ASP	2.3
4	D	11[A]	TYR	2.3
1	A	424	GLY	2.3
1	A	543	THR	2.3
2	B	1021	SER	2.3
1	A	600	LEU	2.3
1	A	571	TYR	2.3
1	A	419	VAL	2.3
2	B	226	PHE	2.3
2	B	338	VAL	2.3
2	B	771	PHE	2.3
2	B	246	LEU	2.3
1	A	148	ASP	2.3
1	A	191	GLY	2.3
1	A	215	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	262	GLY	2.3
1	A	585	SER	2.3
2	B	754	PRO	2.3
1	A	506	GLY	2.3
4	D	58	TYR	2.3
2	B	746	SER	2.3
1	A	106	ILE	2.3
1	A	420	THR	2.2
2	B	1047	TRP	2.2
2	B	1051	LEU	2.2
1	A	69	VAL	2.2
4	D	26	LYS	2.2
1	A	162	ALA	2.2
2	B	152	LEU	2.2
1	A	193	CYS	2.2
2	B	88	ILE	2.1
2	B	347	VAL	2.1
1	A	51	PRO	2.1
1	A	77	GLY	2.1
1	A	165	MET	2.1
1	A	172	MET	2.1
2	B	285	LEU	2.1
2	B	858	LEU	2.1
2	B	1054	MET	2.1
4	D	47	ILE	2.1
1	A	592[A]	SER	2.1
2	B	750	THR	2.1
2	B	747	GLY	2.1
2	B	1104	LYS	2.1
1	A	422	LEU	2.1
1	A	386	TYR	2.1
2	B	888	VAL	2.1
4	D	46	ILE	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 ⓘ

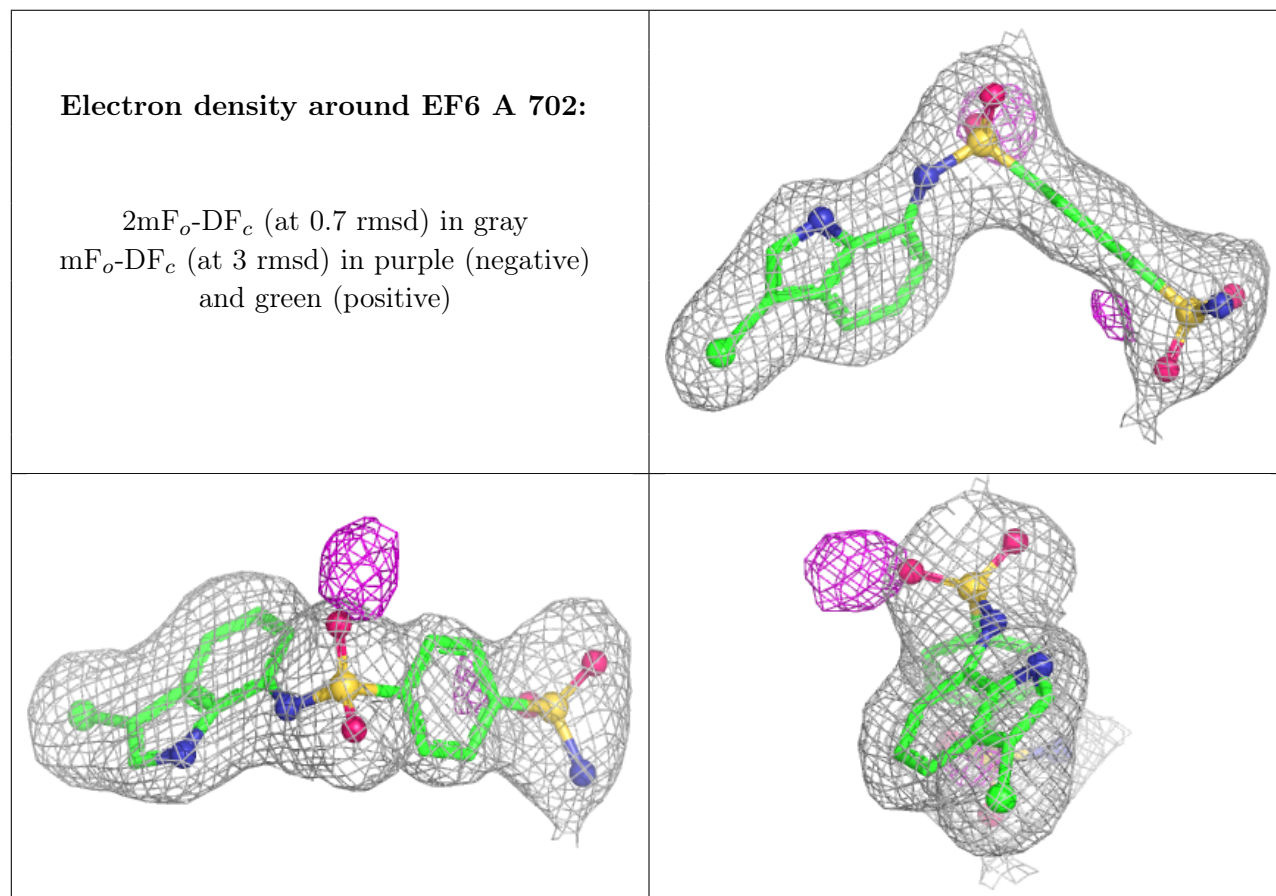
There are no oligosaccharides in this entry.

6.4 Ligands [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	GOL	A	701	6/6	0.88	0.20	95,96,97,98	0
5	GOL	B	1201	6/6	0.94	0.07	62,64,64,64	0
6	EF6	A	702	24/24	0.97	0.07	51,58,73,74	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.