



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:39 AM BST

PDB ID : 4CI1
Title : Structure of the DDB1-CRBN E3 ubiquitin ligase bound to thalidomide
Authors : Fischer, E.S.; Boehm, K.; Thoma, N.H.
Deposited on : 2013-12-05
Resolution : 2.98 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

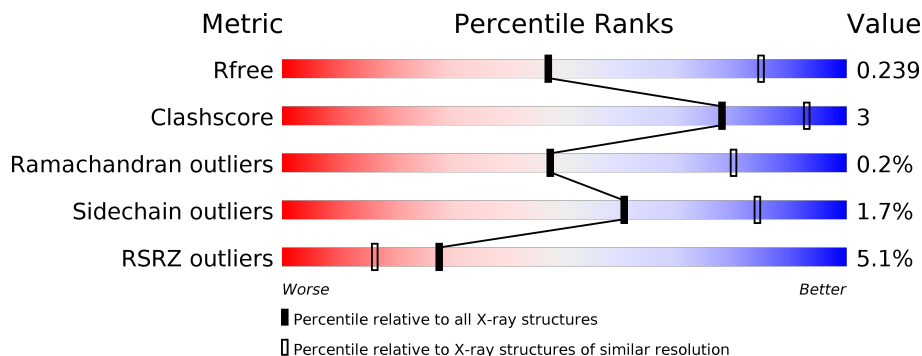
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 on 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	1158	
2	B	469	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11460 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
			Total	As	C	N	O	S			
1	A	1091	8420	2	5352	1412	1609	45	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	HIS	-	expression tag	UNP Q16531
A	-12	HIS	-	expression tag	UNP Q16531
A	-11	HIS	-	expression tag	UNP Q16531
A	-10	ARG	-	expression tag	UNP Q16531
A	-9	ARG	-	expression tag	UNP Q16531
A	-8	LEU	-	expression tag	UNP Q16531
A	-7	VAL	-	expression tag	UNP Q16531
A	-6	PRO	-	expression tag	UNP Q16531
A	-5	ARG	-	expression tag	UNP Q16531
A	-4	GLY	-	expression tag	UNP Q16531
A	-3	SER	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531

- Molecule 2 is a protein called PROTEIN CEREBLON.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
2	B	370	2985	2	1895	522	544	22	0	0	0

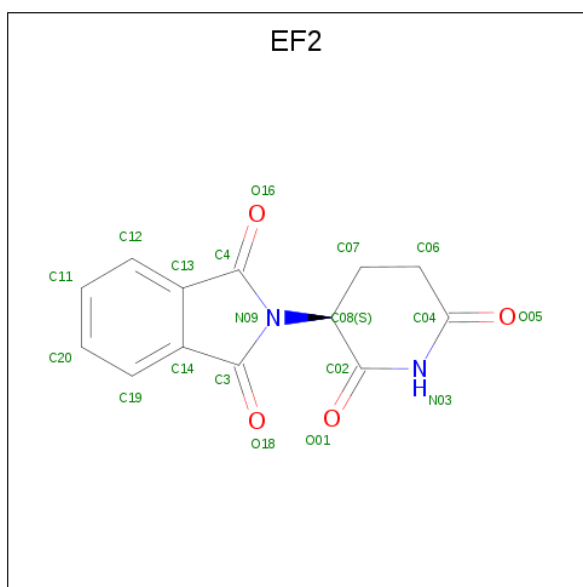
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	expression tag	UNP P0CF65
B	-22	ASP	-	expression tag	UNP P0CF65
B	-21	TRP	-	expression tag	UNP P0CF65
B	-20	SER	-	expression tag	UNP P0CF65
B	-19	HIS	-	expression tag	UNP P0CF65
B	-18	PRO	-	expression tag	UNP P0CF65
B	-17	GLN	-	expression tag	UNP P0CF65
B	-16	PHE	-	expression tag	UNP P0CF65
B	-15	GLU	-	expression tag	UNP P0CF65
B	-14	LYS	-	expression tag	UNP P0CF65
B	-13	SER	-	expression tag	UNP P0CF65
B	-12	ALA	-	expression tag	UNP P0CF65
B	-11	VAL	-	expression tag	UNP P0CF65
B	-10	ASP	-	expression tag	UNP P0CF65
B	-9	GLU	-	expression tag	UNP P0CF65
B	-8	ASN	-	expression tag	UNP P0CF65
B	-7	LEU	-	expression tag	UNP P0CF65
B	-6	TYR	-	expression tag	UNP P0CF65
B	-5	PHE	-	expression tag	UNP P0CF65
B	-4	GLN	-	expression tag	UNP P0CF65
B	-3	GLY	-	expression tag	UNP P0CF65
B	-2	GLY	-	expression tag	UNP P0CF65
B	-1	GLY	-	expression tag	UNP P0CF65
B	0	ARG	-	expression tag	UNP P0CF65

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is S-Thalidomide (three-letter code: EF2) (formula: C₁₃H₁₀N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	19	13	2	4	0	0

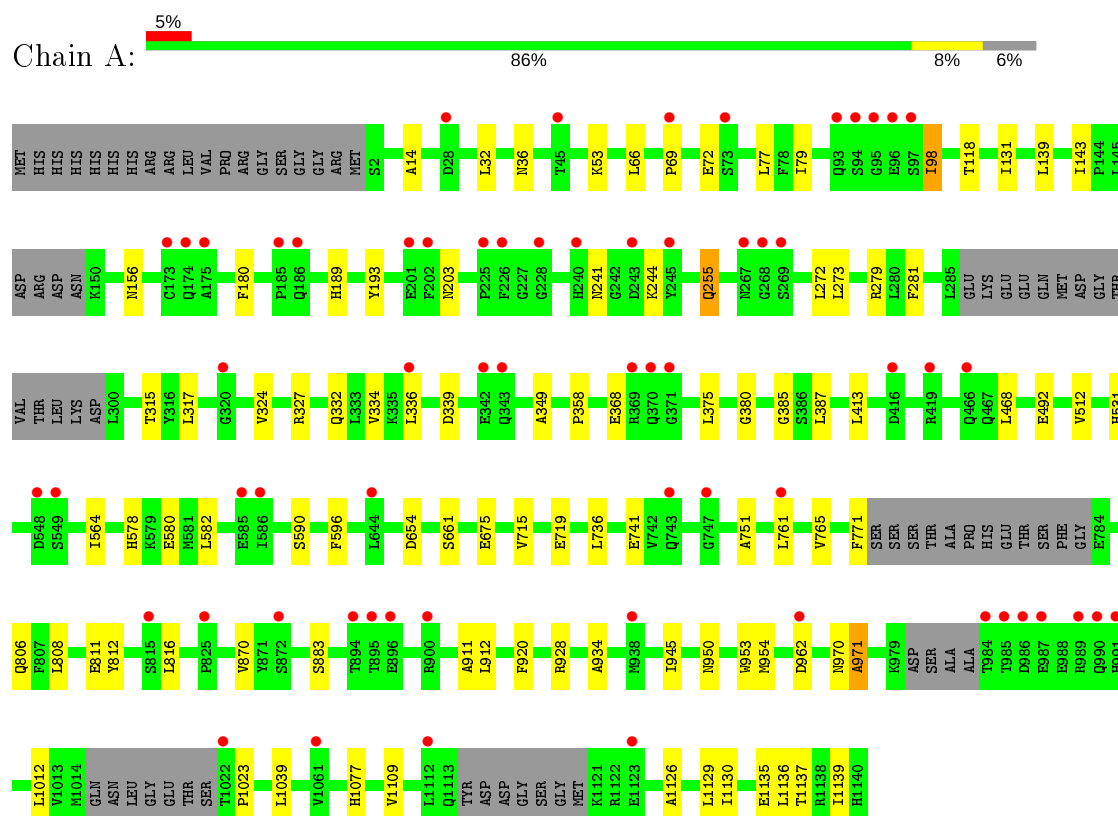
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	13	Total	O	0	0
			13	13		

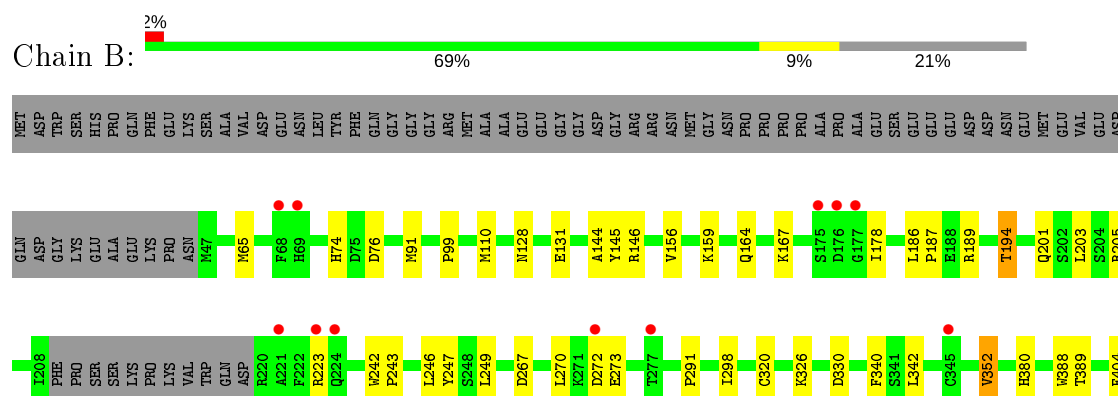
3 Residue-property plots [i](#)

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: PROTEIN CEREBLON



L425	ILE
P426	PRO
R427	GLU
	ALA
	GLU
	ASP
	GLU
	LEU
	GLY
	HIS
	ASP
	ARG
	SER
	PRO
	LEU
	LEU
	CYS
	LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	172.18Å 172.18Å 140.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.82 – 2.98 29.82 – 2.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.82-2.98) 100.0 (29.82-2.98)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.00Å)	Xtrriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.197 , 0.233 0.205 , 0.239	Depositor DCC
R_{free} test set	2461 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11460	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, EF2, CAF

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	0.41	0/8553	0.67	0/11605
2	B	0.42	0/3037	0.67	0/4119
All	All	0.41	0/11590	0.67	0/15724

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	8420	0	8287	44	0
2	B	2985	0	2916	25	0
3	B	1	0	0	0	0
4	B	19	0	10	1	0
5	A	22	0	0	0	0
5	B	13	0	0	1	0
All	All	11460	0	11213	66	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 (66) 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:255:GLN:HB2	1:A:279:ARG:HH22	1.57	0.69
1:A:596:PHE:HB3	1:A:661:SER:HB2	1.79	0.63
2:B:110:MET:HG3	2:B:178:ILE:HG21	1.80	0.63
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.80	0.62
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.85	0.58
1:A:765:VAL:HG12	1:A:806:GLN:HB3	1.86	0.57
1:A:385:GLY:HA3	1:A:719:GLU:O	2.06	0.56
1:A:934:ALA:HB2	1:A:945:ILE:HD11	1.89	0.55
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.89	0.55
4:B:1429:EF2:H19	5:B:2006:HOH:O	2.06	0.54
2:B:242:TRP:HB3	2:B:246:LEU:HD23	1.89	0.54
1:A:1109:VAL:HG12	1:A:1129:LEU:HD22	1.89	0.54
1:A:1126:ALA:O	1:A:1130:ILE:HG12	2.09	0.53
1:A:413:LEU:HD22	1:A:468:LEU:HD22	1.91	0.53
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	1.91	0.53
1:A:1039:LEU:HD22	1:A:1139:ILE:HD12	1.91	0.53
1:A:14:ALA:HB1	1:A:327:ARG:HG3	1.91	0.53
1:A:492:GLU:HG3	1:A:512:VAL:HG11	1.90	0.52
2:B:326:LYS:HG3	2:B:425:LEU:HD13	1.92	0.52
2:B:65:MET:HG2	2:B:146:ARG:HB2	1.90	0.52
1:A:32:LEU:HD13	1:A:66:LEU:HD11	1.93	0.51
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.92	0.50
2:B:201:GLN:HE21	2:B:203:LEU:HB2	1.77	0.50
2:B:74:HIS:HB2	2:B:164:GLN:HE22	1.77	0.50
1:A:131:ILE:HB	1:A:143:ILE:HB	1.93	0.49
1:A:928:ARG:HA	1:A:954:MET:HE3	1.94	0.49
2:B:144:ALA:HB3	2:B:159:LYS:HB2	1.94	0.49
1:A:53:LYS:HD3	1:A:98:ILE:HD13	1.93	0.49
2:B:145:TYR:CE1	2:B:156:VAL:HG21	2.47	0.49
1:A:578:HIS:NE2	1:A:580:GLU:HG2	2.28	0.49
1:A:139:LEU:HD22	1:A:156:ASN:HB3	1.96	0.48
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.95	0.48
1:A:1136:LEU:O	1:A:1139:ILE:HG12	2.15	0.47
1:A:241:ASN:HB3	1:A:244:LYS:HB3	1.98	0.46
2:B:267:ASP:HB3	2:B:270:LEU:HB2	1.99	0.45
1:A:358:PRO:HD2	1:A:380:GLY:CA	2.45	0.45
1:A:883:SER:HB2	1:A:911:ALA:HB3	1.99	0.45
2:B:246:LEU:HD12	2:B:249:LEU:HD12	1.99	0.45
1:A:736:LEU:HG	1:A:816:LEU:HD22	1.99	0.45
1:A:77:LEU:HD21	1:A:79:ILE:HD11	1.97	0.44
1:A:971:ALA:HB3	1:A:1077:HIS:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ILE:HG22	1:A:582:LEU:HB2	2.00	0.44
2:B:76:ASP:HB3	2:B:187:PRO:HG3	2.00	0.44
1:A:812:TYR:CZ	2:B:243:PRO:HB3	2.53	0.44
1:A:1023:PRO:HG3	1:A:1135:GLU:CG	2.48	0.43
1:A:808:LEU:HB2	1:A:811:GLU:HB2	1.99	0.42
1:A:741:GLU:HG2	1:A:751:ALA:HA	2.00	0.42
2:B:167:LYS:HB2	2:B:186:LEU:HD21	2.00	0.42
1:A:870:VAL:HA	1:A:883:SER:O	2.20	0.42
2:B:388:TRP:HB3	2:B:404:PHE:CE2	2.54	0.42
1:A:334:VAL:HG12	1:A:349:ALA:HA	2.01	0.42
1:A:950:ASN:HB3	2:B:189:ARG:HH12	1.84	0.42
1:A:387:LEU:HB2	1:A:715:VAL:HB	2.01	0.42
1:A:118:THR:HG22	2:B:205:ARG:HA	2.01	0.41
2:B:267:ASP:HB3	2:B:270:LEU:HD12	2.01	0.41
2:B:352:VAL:O	2:B:380:HIS:HE1	2.04	0.41
2:B:340:PHE:HE2	2:B:342:LEU:HD13	1.85	0.41
2:B:194:THR:HG21	2:B:247:TYR:HD1	1.86	0.41
1:A:272:LEU:HD21	1:A:336:LEU:HD11	2.01	0.41
2:B:128:ASN:ND2	2:B:131:GLU:HB2	2.35	0.41
2:B:99:PRO:HB2	2:B:352:VAL:HG22	2.03	0.41
2:B:91:MET:HE1	2:B:298:ILE:HG13	2.03	0.40
1:A:180:PHE:HE1	1:A:193:TYR:HD2	1.70	0.40
1:A:324:VAL:HB	1:A:332:GLN:HB2	2.03	0.40
1:A:912:LEU:HD21	2:B:246:LEU:HD11	2.03	0.40
2:B:291:PRO:HG2	2:B:320:CAF:O1	2.22	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	1075/1158 (93%)	1011 (94%)	61 (6%)	3 (0%)	41 74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	364/469 (78%)	348 (96%)	16 (4%)	0	100	100
All	All	1439/1627 (88%)	1359 (94%)	77 (5%)	3 (0%)	47	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	368	GLU
1	A	971	ALA

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	921/1012 (91%)	907 (98%)	14 (2%)	65	86
2	B	324/414 (78%)	317 (98%)	7 (2%)	52	80
All	All	1245/1426 (87%)	1224 (98%)	21 (2%)	60	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ILE
1	A	189	HIS
1	A	203	ASN
1	A	255	GLN
1	A	315	THR
1	A	317	LEU
1	A	339	ASP
1	A	531	HIS
1	A	590	SER
1	A	761	LEU
1	A	771	PHE
1	A	920	PHE
1	A	962	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1137	THR
2	B	194	THR
2	B	223	ARG
2	B	272	ASP
2	B	273	GLU
2	B	330	ASP
2	B	352	VAL
2	B	389	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	201	GLN
2	B	299	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](#)

4 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	$\# Z > 2$
2	CAF	B	312	2	3,9,10	0.60	0	1,12,14	1.57	0
2	CAF	B	320	2	3,9,10	0.76	0	1,12,14	1.28	0
1	CAF	A	87	1	3,9,10	0.69	0	1,12,14	0.05	0
1	CAF	A	977	1	3,9,10	0.66	0	1,12,14	1.01	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
2	CAF	B	312	2	-	0/0/8/10	-
2	CAF	B	320	2	-	0/0/8/10	-
1	CAF	A	87	1	-	0/0/8/10	-
1	CAF	A	977	1	-	0/0/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	320	CAF	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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
4	EF2	B	1429	-	21,21,21	1.10	2 (9%)	31,31,31	1.96	11 (35%)

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
4	EF2	B	1429	-	-	0/4/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1429	EF2	C3-N09	-2.10	1.36	1.40
4	B	1429	EF2	C13-C4	2.09	1.52	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1429	EF2	C14-C3-N09	3.73	110.02	105.96
4	B	1429	EF2	C06-C04-N03	3.71	120.82	116.65
4	B	1429	EF2	C13-C14-C3	-3.40	105.31	108.26
4	B	1429	EF2	C02-C08-N09	3.32	112.11	109.08
4	B	1429	EF2	O16-C4-C13	-2.99	122.87	128.68
4	B	1429	EF2	O18-C3-C14	-2.94	122.96	128.68
4	B	1429	EF2	C13-C4-N09	2.65	108.84	105.96
4	B	1429	EF2	C07-C06-C04	-2.59	109.54	114.12
4	B	1429	EF2	C14-C13-C4	-2.46	106.13	108.26
4	B	1429	EF2	O16-C4-N09	2.31	128.27	124.97
4	B	1429	EF2	C19-C14-C3	2.17	133.17	129.63

There are no chirality outliers.

There are no torsion outliers.

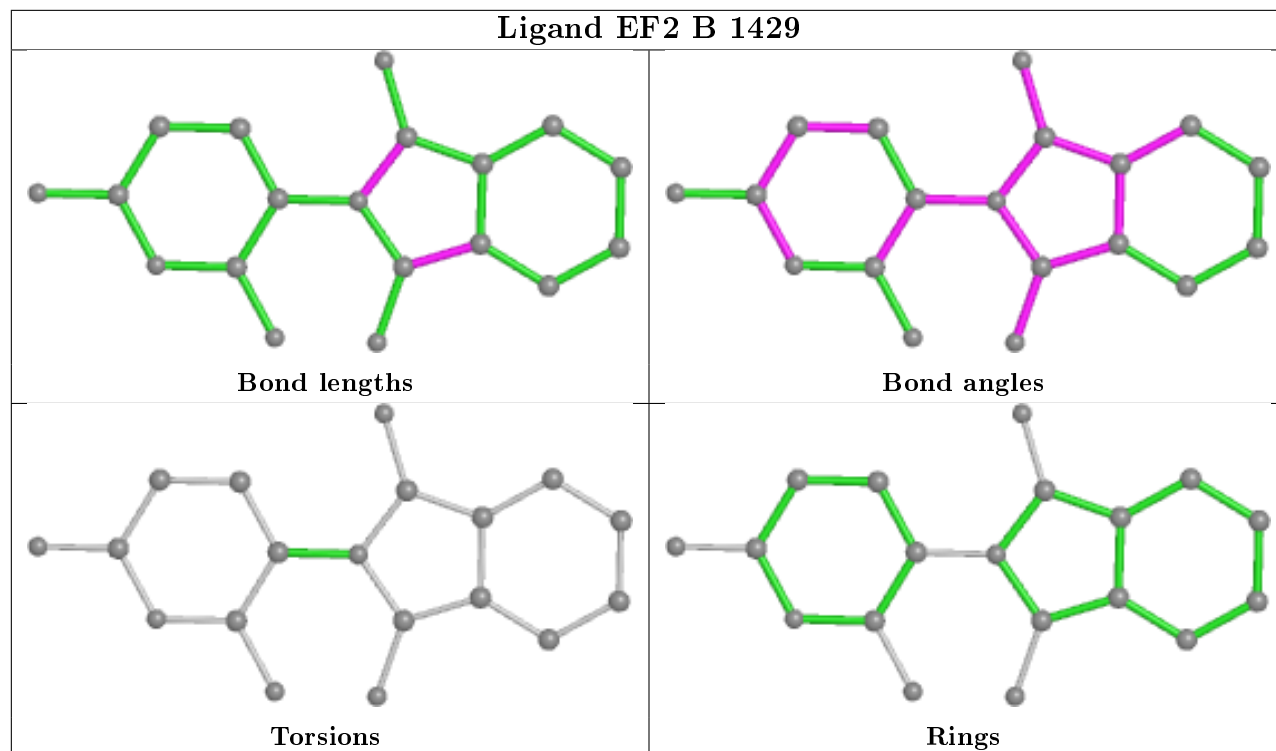
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1429	EF2	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	1089/1158 (94%)	0.25	63 (5%) 23 12	48, 91, 131, 156	0
2	B	368/469 (78%)	0.05	11 (2%) 50 31	40, 65, 111, 140	0
All	All	1457/1627 (89%)	0.20	74 (5%) 28 16	40, 86, 128, 156	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	GLN	4.8
1	A	268	GLY	4.2
1	A	872	SER	4.1
1	A	225	PRO	4.1
1	A	175	ALA	3.9
1	A	990	GLN	3.8
1	A	644	LEU	3.5
1	A	93	GLN	3.4
1	A	73	SER	3.4
2	B	224	GLN	3.3
2	B	69	HIS	3.3
1	A	900	ARG	3.2
1	A	548	ASP	3.2
1	A	173	CYS	3.2
1	A	991	HIS	3.2
1	A	174	GLN	3.1
1	A	466	GLN	3.1
1	A	243	ASP	3.1
1	A	419	ARG	3.0
1	A	336	LEU	2.9
1	A	371	GLY	2.9
1	A	69	PRO	2.9
1	A	240	HIS	2.9
1	A	226	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1112	LEU	2.8
1	A	95	GLY	2.8
1	A	986	ASP	2.7
1	A	94	SER	2.7
1	A	815	SER	2.7
1	A	1123	GLU	2.7
1	A	585	GLU	2.7
1	A	269	SER	2.6
1	A	202	PHE	2.6
1	A	586	ILE	2.5
1	A	895	THR	2.5
1	A	989	ARG	2.5
1	A	761	LEU	2.5
1	A	962	ASP	2.5
2	B	223	ARG	2.5
2	B	176	ASP	2.5
1	A	369	ARG	2.5
1	A	185	PRO	2.4
2	B	175	SER	2.4
2	B	277	THR	2.4
1	A	97	SER	2.4
1	A	267	ASN	2.4
1	A	984	THR	2.3
1	A	45	THR	2.3
1	A	245	TYR	2.3
1	A	985	THR	2.3
1	A	747	GLY	2.3
1	A	938	MET	2.3
1	A	228	GLY	2.3
1	A	186	GLN	2.3
2	B	345	CYS	2.3
1	A	28	ASP	2.2
1	A	1022	THR	2.2
2	B	68	PHE	2.2
1	A	342	GLU	2.2
1	A	96	GLU	2.2
1	A	987	GLU	2.1
2	B	272	ASP	2.1
1	A	1061	VAL	2.1
1	A	549	SER	2.1
1	A	894	THR	2.1
1	A	896	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	177	GLY	2.1
1	A	416	ASP	2.1
1	A	320	GLY	2.1
1	A	343	GLN	2.0
1	A	743	GLN	2.0
1	A	201	GLU	2.0
2	B	221	ALA	2.0
1	A	825	PRO	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
1	CAF	A	87	10/11	0.96	0.18	81,84,86,87	4
2	CAF	B	320	10/11	0.97	0.20	65,66,69,69	4
1	CAF	A	977	10/11	0.97	0.17	74,82,86,88	4
2	CAF	B	312	10/11	0.98	0.14	55,62,67,68	4

6.3 Carbohydrates [i](#)

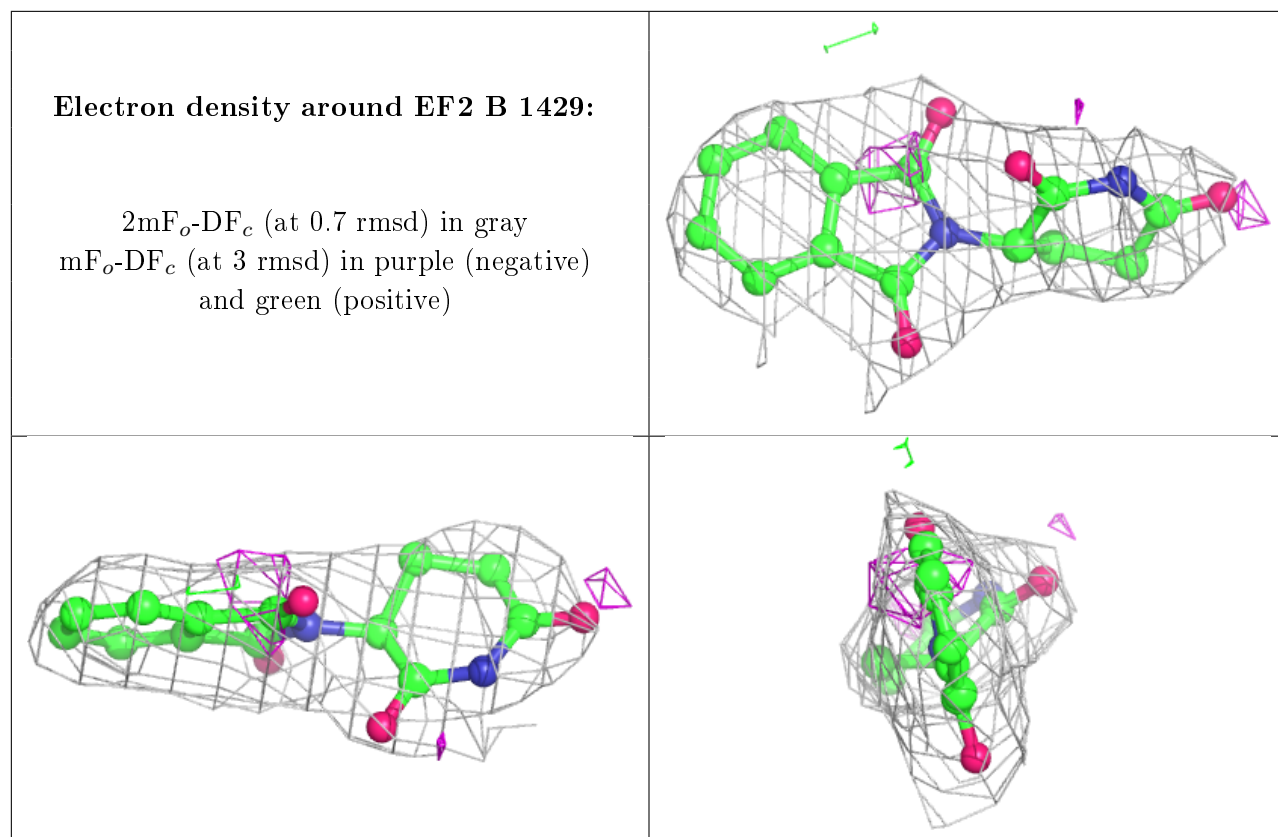
There are no monosaccharides in this entry.

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
4	EF2	B	1429	19/19	0.97	0.17	45,52,60,63	0
3	ZN	B	1428	1/1	1.00	0.14	52,52,52,52	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.