



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 04:15 pm BST

PDB ID : 6H0F / pdb_00006h0f
Title : Structure of DDB1-CRBN-pomalidomide complex bound to IKZF1(ZF2)
Authors : Petzold, G.; Bunker, R.D.; Thoma, N.H.
Deposited on : 2018-07-09
Resolution : 3.25 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

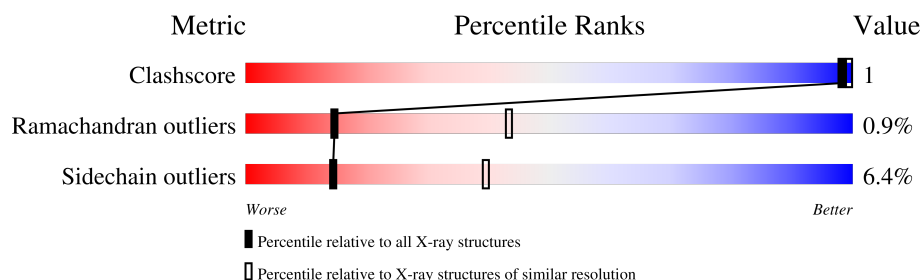
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1546 (3.30-3.22)
Ramachandran outliers	177936	1536 (3.30-3.22)
Sidechain outliers	177891	1535 (3.30-3.22)





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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	856	90% 6% .
1	D	856	90% 5% . .
1	G	856	89% 7% .
1	J	856	91% 7% .
2	B	426	77% 10% . 12%
2	E	426	78% 10% 12%
2	H	426	77% 10% 12%
2	K	426	77% 10% 12%

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Mol	Chain	Length	Quality of chain
3	C	38	 82% • 16%
3	F	38	 82% • 16%
3	I	38	 84% 16%
3	L	38	 82% • 16%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 77598 atoms, of which 38594 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,DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	826	Total	C	H	N	O	S	6417	0	0
			12887	4099	6417	1093	1242	36			
1	D	821	Total	C	H	N	O	S	6381	0	0
			12814	4078	6381	1087	1232	36			
1	G	826	Total	C	H	N	O	S	6418	0	0
			12888	4099	6418	1093	1242	36			
1	J	843	Total	C	H	N	O	S	6526	0	0
			13119	4174	6526	1116	1267	36			

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	374	Total	C	H	N	O	S	2967	2	0
			5955	1905	2967	512	547	24			
2	E	374	Total	C	H	N	O	S	2967	2	0
			5955	1905	2967	512	547	24			
2	H	374	Total	C	H	N	O	S	2959	0	0
			5937	1899	2959	509	546	24			
2	K	374	Total	C	H	N	O	S	2967	2	0
			5955	1905	2967	512	547	24			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	-	initiating methionine	UNP Q96SW2
B	18	ASP	-	expression tag	UNP Q96SW2
B	19	TRP	-	expression tag	UNP Q96SW2
B	20	SER	-	expression tag	UNP Q96SW2
B	21	HIS	-	expression tag	UNP Q96SW2
B	22	PRO	-	expression tag	UNP Q96SW2
B	23	GLN	-	expression tag	UNP Q96SW2
B	24	PHE	-	expression tag	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	25	GLU	-	expression tag	UNP Q96SW2
B	26	LYS	-	expression tag	UNP Q96SW2
B	27	SER	-	expression tag	UNP Q96SW2
B	28	ALA	-	expression tag	UNP Q96SW2
B	29	VAL	-	expression tag	UNP Q96SW2
B	30	ASP	-	expression tag	UNP Q96SW2
B	31	GLU	-	expression tag	UNP Q96SW2
B	32	ASN	-	expression tag	UNP Q96SW2
B	33	LEU	-	expression tag	UNP Q96SW2
B	34	TYR	-	expression tag	UNP Q96SW2
B	35	PHE	-	expression tag	UNP Q96SW2
B	37	GLY	ASP	conflict	UNP Q96SW2
B	38	GLY	SER	conflict	UNP Q96SW2
B	39	GLY	LYS	conflict	UNP Q96SW2
B	40	ARG	GLU	conflict	UNP Q96SW2
E	17	MET	-	initiating methionine	UNP Q96SW2
E	18	ASP	-	expression tag	UNP Q96SW2
E	19	TRP	-	expression tag	UNP Q96SW2
E	20	SER	-	expression tag	UNP Q96SW2
E	21	HIS	-	expression tag	UNP Q96SW2
E	22	PRO	-	expression tag	UNP Q96SW2
E	23	GLN	-	expression tag	UNP Q96SW2
E	24	PHE	-	expression tag	UNP Q96SW2
E	25	GLU	-	expression tag	UNP Q96SW2
E	26	LYS	-	expression tag	UNP Q96SW2
E	27	SER	-	expression tag	UNP Q96SW2
E	28	ALA	-	expression tag	UNP Q96SW2
E	29	VAL	-	expression tag	UNP Q96SW2
E	30	ASP	-	expression tag	UNP Q96SW2
E	31	GLU	-	expression tag	UNP Q96SW2
E	32	ASN	-	expression tag	UNP Q96SW2
E	33	LEU	-	expression tag	UNP Q96SW2
E	34	TYR	-	expression tag	UNP Q96SW2
E	35	PHE	-	expression tag	UNP Q96SW2
E	37	GLY	ASP	conflict	UNP Q96SW2
E	38	GLY	SER	conflict	UNP Q96SW2
E	39	GLY	LYS	conflict	UNP Q96SW2
E	40	ARG	GLU	conflict	UNP Q96SW2
H	17	MET	-	initiating methionine	UNP Q96SW2
H	18	ASP	-	expression tag	UNP Q96SW2
H	19	TRP	-	expression tag	UNP Q96SW2
H	20	SER	-	expression tag	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	21	HIS	-	expression tag	UNP Q96SW2
H	22	PRO	-	expression tag	UNP Q96SW2
H	23	GLN	-	expression tag	UNP Q96SW2
H	24	PHE	-	expression tag	UNP Q96SW2
H	25	GLU	-	expression tag	UNP Q96SW2
H	26	LYS	-	expression tag	UNP Q96SW2
H	27	SER	-	expression tag	UNP Q96SW2
H	28	ALA	-	expression tag	UNP Q96SW2
H	29	VAL	-	expression tag	UNP Q96SW2
H	30	ASP	-	expression tag	UNP Q96SW2
H	31	GLU	-	expression tag	UNP Q96SW2
H	32	ASN	-	expression tag	UNP Q96SW2
H	33	LEU	-	expression tag	UNP Q96SW2
H	34	TYR	-	expression tag	UNP Q96SW2
H	35	PHE	-	expression tag	UNP Q96SW2
H	37	GLY	ASP	conflict	UNP Q96SW2
H	38	GLY	SER	conflict	UNP Q96SW2
H	39	GLY	LYS	conflict	UNP Q96SW2
H	40	ARG	GLU	conflict	UNP Q96SW2
K	17	MET	-	initiating methionine	UNP Q96SW2
K	18	ASP	-	expression tag	UNP Q96SW2
K	19	TRP	-	expression tag	UNP Q96SW2
K	20	SER	-	expression tag	UNP Q96SW2
K	21	HIS	-	expression tag	UNP Q96SW2
K	22	PRO	-	expression tag	UNP Q96SW2
K	23	GLN	-	expression tag	UNP Q96SW2
K	24	PHE	-	expression tag	UNP Q96SW2
K	25	GLU	-	expression tag	UNP Q96SW2
K	26	LYS	-	expression tag	UNP Q96SW2
K	27	SER	-	expression tag	UNP Q96SW2
K	28	ALA	-	expression tag	UNP Q96SW2
K	29	VAL	-	expression tag	UNP Q96SW2
K	30	ASP	-	expression tag	UNP Q96SW2
K	31	GLU	-	expression tag	UNP Q96SW2
K	32	ASN	-	expression tag	UNP Q96SW2
K	33	LEU	-	expression tag	UNP Q96SW2
K	34	TYR	-	expression tag	UNP Q96SW2
K	35	PHE	-	expression tag	UNP Q96SW2
K	37	GLY	ASP	conflict	UNP Q96SW2
K	38	GLY	SER	conflict	UNP Q96SW2
K	39	GLY	LYS	conflict	UNP Q96SW2
K	40	ARG	GLU	conflict	UNP Q96SW2

- Molecule 3 is a protein called DNA-binding protein Ikaros.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	32	Total	C	H	N	O	S	237	0	0
			481	148	237	52	42	2			
3	F	32	Total	C	H	N	O	S	237	0	0
			481	148	237	52	42	2			
3	I	32	Total	C	H	N	O	S	237	0	0
			481	148	237	52	42	2			
3	L	32	Total	C	H	N	O	S	237	0	0
			481	148	237	52	42	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	137	GLY	-	expression tag	UNP Q13422
C	138	GLY	-	expression tag	UNP Q13422
C	139	GLY	-	expression tag	UNP Q13422
C	140	ARG	-	expression tag	UNP Q13422
F	137	GLY	-	expression tag	UNP Q13422
F	138	GLY	-	expression tag	UNP Q13422
F	139	GLY	-	expression tag	UNP Q13422
F	140	ARG	-	expression tag	UNP Q13422
I	137	GLY	-	expression tag	UNP Q13422
I	138	GLY	-	expression tag	UNP Q13422
I	139	GLY	-	expression tag	UNP Q13422
I	140	ARG	-	expression tag	UNP Q13422
L	137	GLY	-	expression tag	UNP Q13422
L	138	GLY	-	expression tag	UNP Q13422
L	139	GLY	-	expression tag	UNP Q13422
L	140	ARG	-	expression tag	UNP Q13422

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

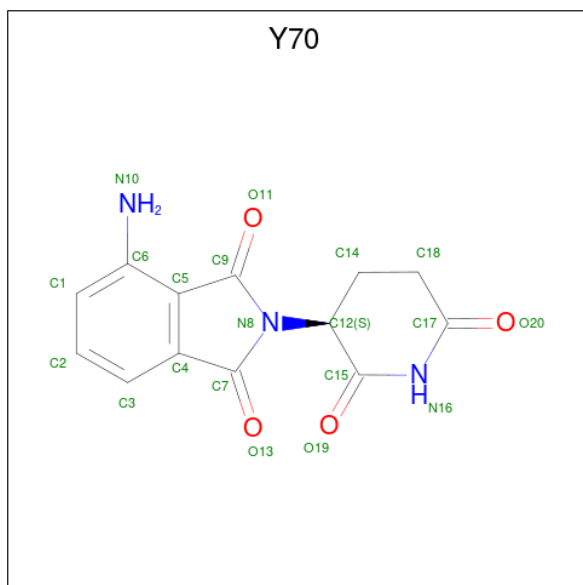
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		

- Molecule 5 is S-Pomalidomide (CCD ID: Y70) (formula: $C_{13}H_{11}N_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	11	0
			31	13	11	3	4		
5	E	1	Total	C	H	N	O	11	0
			31	13	11	3	4		
5	H	1	Total	C	H	N	O	11	0
			31	13	11	3	4		
5	K	1	Total	C	H	N	O	11	0
			31	13	11	3	4		

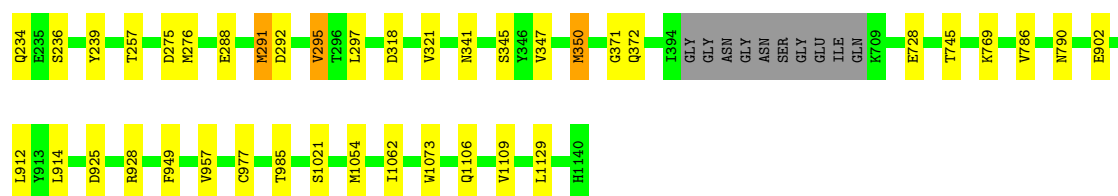
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	3	Total	O	0	0
			3	3		

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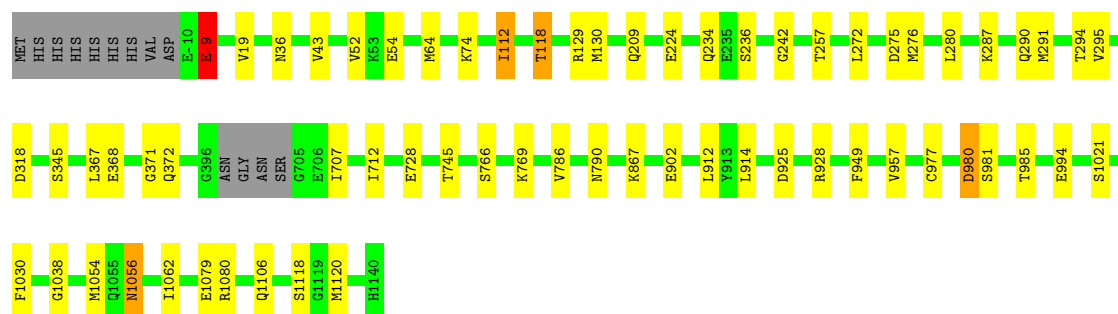
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	3	Total 3	O 3	0	0
6	E	4	Total 4	O 4	0	0
6	G	3	Total 3	O 3	0	0
6	H	5	Total 5	O 5	0	0
6	J	6	Total 6	O 6	0	0



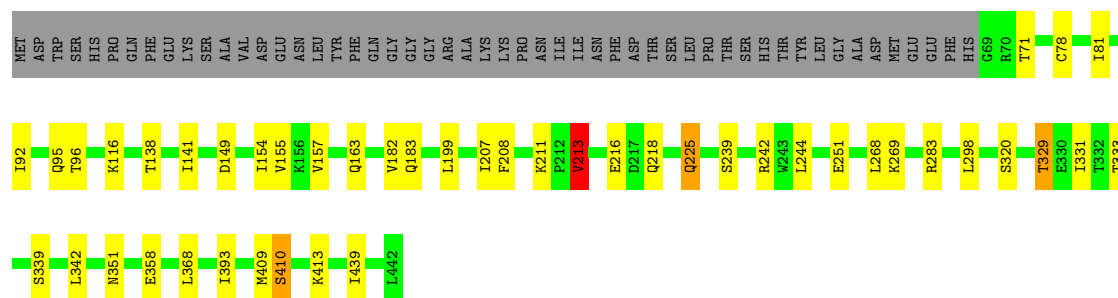
- Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1

Chain J: 91% 7% .



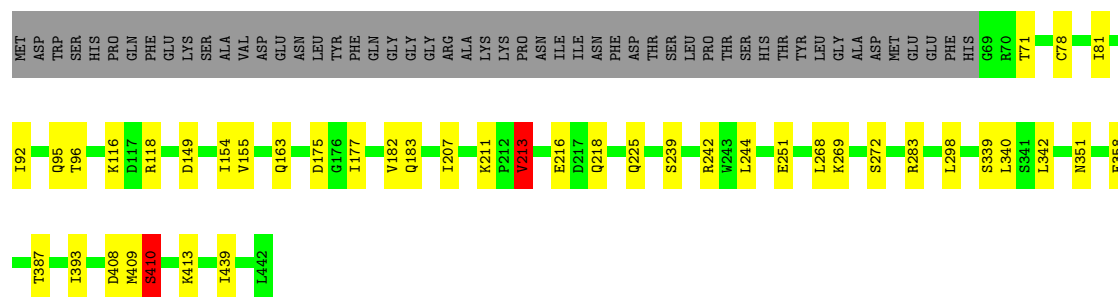
- Molecule 2: Protein cereblon

Chain B: 77% 10% 12% .




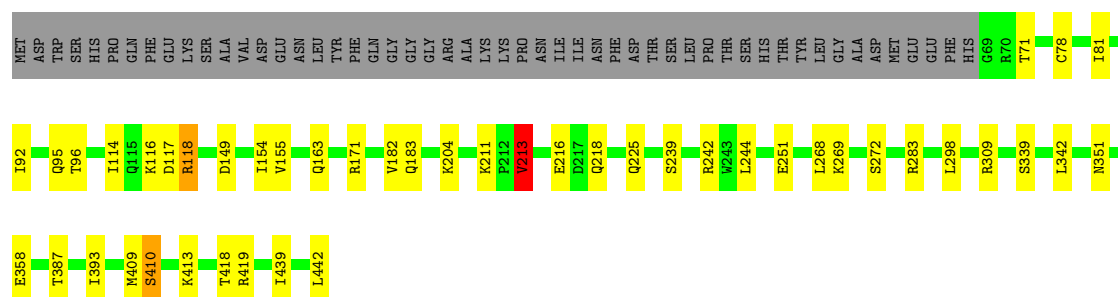
- Molecule 2: Protein cereblon

Chain E: 78% 10% 12% .




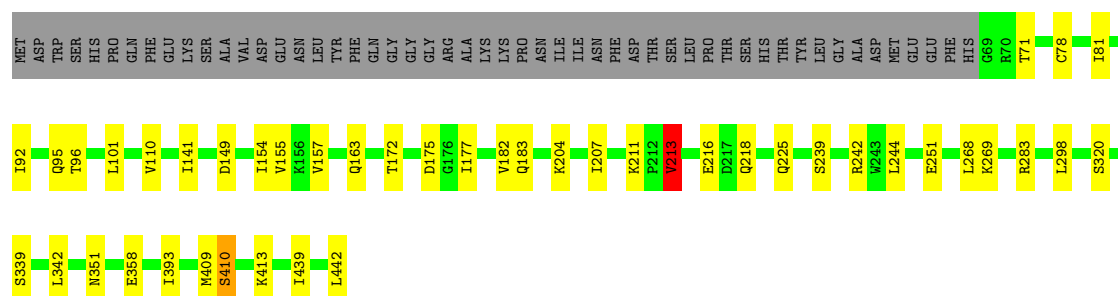
- Molecule 2: Protein cereblon

Chain H:  77% 10% 12%




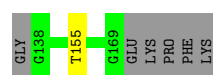
• Molecule 2: Protein cereblon

Chain K:  77% 10% 12%




• Molecule 3: DNA-binding protein Ikaros

Chain C:  82% 16%




• Molecule 3: DNA-binding protein Ikaros

Chain F:  82% 16%




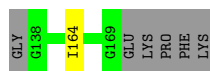
• Molecule 3: DNA-binding protein Ikaros

Chain I:  84% 16%



• Molecule 3: DNA-binding protein Ikaros

Chain L:  82% 16%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	161.45Å 177.86Å 242.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.85 – 3.25	Depositor
% Data completeness (in resolution range)	93.2 (39.85-3.25)	Depositor
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.212 , 0.234	Depositor
Wilson B-factor (Å ²)	76.2	Xtriage
Anisotropy	0.003	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	77598	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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: Y70, ZN

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	0.71	0/6587	0.99	9/8909 (0.1%)
1	D	0.69	1/6549 (0.0%)	0.97	5/8856 (0.1%)
1	G	0.70	1/6587 (0.0%)	0.98	6/8909 (0.1%)
1	J	0.70	1/6712 (0.0%)	0.99	9/9075 (0.1%)
2	B	0.78	1/3063 (0.0%)	1.00	3/4157 (0.1%)
2	E	0.75	1/3064 (0.0%)	1.01	4/4160 (0.1%)
2	H	0.74	0/3047	1.01	7/4137 (0.2%)
2	K	0.74	0/3064	0.99	2/4160 (0.0%)
3	C	0.71	0/248	1.08	0/328
3	F	0.69	0/248	1.13	2/328 (0.6%)
3	I	0.72	0/248	1.04	0/328
3	L	0.75	0/248	1.13	0/328
All	All	0.72	5/39665 (0.0%)	0.99	47/53675 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	225	GLN	C-N	14.29	1.52	1.33
1	D	350	MET	SD-CE	-6.52	1.63	1.79
1	G	350	MET	SD-CE	-6.43	1.63	1.79
2	E	116	LYS	CA-C	6.11	1.57	1.53
1	J	130	MET	SD-CE	-5.88	1.64	1.79

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1016	ASN	CA-CB-CG	7.35	119.95	112.60
1	J	-9	GLU	N-CA-CB	6.95	122.24	110.49
2	H	213	VAL	N-CA-CB	6.55	122.04	111.23
2	B	213	VAL	N-CA-CB	6.51	121.96	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	213	VAL	N-CA-CB	6.47	121.91	111.23
1	G	275	ASP	CA-CB-CG	6.45	119.05	112.60
2	E	213	VAL	N-CA-CB	6.43	121.85	111.23
2	H	351	ASN	CA-CB-CG	6.18	118.78	112.60
2	B	351	ASN	CA-CB-CG	6.07	118.67	112.60
2	K	351	ASN	CA-CB-CG	6.03	118.63	112.60
2	E	351	ASN	CA-CB-CG	5.98	118.58	112.60
1	D	949	PHE	CA-CB-CG	5.93	119.73	113.80
1	J	949	PHE	CA-CB-CG	5.90	119.70	113.80
1	A	949	PHE	CA-CB-CG	5.89	119.69	113.80
2	H	309	ARG	CD-NE-CZ	5.83	132.56	124.40
3	F	154	PHE	CA-C-N	5.82	128.55	120.29
3	F	154	PHE	C-N-CA	5.82	128.55	120.29
1	G	949	PHE	CA-CB-CG	5.79	119.59	113.80
1	A	236	SER	N-CA-C	5.62	117.95	109.41
2	H	117	ASP	CA-CB-CG	5.59	118.19	112.60
1	J	290	GLN	CA-C-N	5.59	132.22	121.54
1	J	290	GLN	C-N-CA	5.59	132.22	121.54
1	G	236	SER	N-CA-C	5.55	117.85	109.41
1	G	925	ASP	CA-CB-CG	5.51	118.11	112.60
1	J	925	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	925	ASP	CA-CB-CG	5.46	118.06	112.60
1	D	925	ASP	CA-CB-CG	5.42	118.02	112.60
1	J	236	SER	N-CA-C	5.41	117.91	109.52
1	J	275	ASP	CA-CB-CG	5.40	118.00	112.60
1	J	980	ASP	CA-CB-CG	5.38	117.97	112.60
1	D	236	SER	N-CA-C	5.35	117.82	109.52
1	J	1056	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	1104	LYS	N-CA-C	-5.33	105.64	111.82
1	A	275	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	1056	ASN	CA-CB-CG	5.25	117.85	112.60
2	B	329	THR	N-CA-CB	-5.18	102.96	110.84
2	H	272	SER	N-CA-C	5.15	116.89	111.28
2	E	272	SER	N-CA-C	5.15	116.89	111.28
1	G	184	ASP	CA-CB-CG	5.13	117.73	112.60
2	H	418	THR	CB-CA-C	5.13	117.96	110.26
1	D	275	ASP	CA-CB-CG	5.11	117.71	112.60
2	H	309	ARG	CG-CD-NE	-5.06	100.87	112.00
1	A	769	LYS	CA-C-N	5.06	127.32	120.44
1	A	769	LYS	C-N-CA	5.06	127.32	120.44
2	E	116	LYS	N-CA-C	5.05	112.92	108.78
1	G	28	ASP	CA-CB-CG	5.02	117.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	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	6470	6417	6421	11	0
1	D	6433	6381	6384	10	0
1	G	6470	6418	6421	12	0
1	J	6593	6526	6528	8	0
2	B	2988	2967	2960	9	0
2	E	2988	2967	2961	5	0
2	H	2978	2959	2959	2	0
2	K	2988	2967	2961	5	0
3	C	244	237	237	0	0
3	F	244	237	237	0	0
3	I	244	237	237	0	0
3	L	244	237	237	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	B	20	11	11	0	0
5	E	20	11	11	0	0
5	H	20	11	11	0	0
5	K	20	11	11	0	0
6	A	8	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	E	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	3	0	0	0	0
6	H	5	0	0	0	0
6	J	6	0	0	0	0
All	All	39004	38594	38587	50	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 1.

All (50) 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:B:207:ILE:C	2:B:208:PHE:N	2.27	0.93
1:A:1103:PRO:HG3	1:D:774:SER:HA	1.71	0.72
1:G:43:VAL:HG23	1:G:52:VAL:HG21	1.77	0.66
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.77	0.66
1:D:43:VAL:HG23	1:D:52:VAL:HG21	1.77	0.66
1:J:43:VAL:HG23	1:J:52:VAL:HG21	1.77	0.66
1:J:272:LEU:HD22	1:J:280:LEU:HD11	1.78	0.64
1:D:130:MET:HE2	1:D:197:LEU:HD21	1.84	0.60
1:D:19:VAL:HG22	1:D:64:MET:HE3	1.85	0.59
1:A:130:MET:HE2	1:A:197:LEU:HD21	1.84	0.59
1:A:19:VAL:HG22	1:A:64:MET:HE3	1.85	0.58
1:G:19:VAL:HG22	1:G:64:MET:HE3	1.84	0.58
1:J:19:VAL:HG22	1:J:64:MET:HE3	1.85	0.58
1:A:1056:ASN:ND2	2:E:410:SER:HB3	2.18	0.57
1:G:912:LEU:HD21	2:H:244:LEU:HD11	1.87	0.57
1:A:912:LEU:HD21	2:B:244:LEU:HD11	1.85	0.57
1:G:130:MET:HE2	1:G:197:LEU:HD21	1.88	0.54
1:D:912:LEU:HD21	2:E:244:LEU:HD11	1.93	0.51
1:J:118:THR:CG2	2:K:204:LYS:HA	2.40	0.51
1:G:1054:MET:HE2	1:G:1129:LEU:HD11	1.94	0.50
2:B:207:ILE:C	2:B:208:PHE:CA	2.85	0.49
1:G:321:VAL:HG13	1:G:350:MET:HE1	1.95	0.47
2:H:118:ARG:CG	2:H:118:ARG:HH11	2.28	0.47
1:J:912:LEU:HD21	2:K:244:LEU:HD11	1.95	0.47
1:A:1086:THR:HG22	2:E:408:ASP:OD2	2.15	0.47
1:D:321:VAL:HG13	1:D:350:MET:HE1	1.97	0.46
1:J:118:THR:HG23	2:K:207:ILE:CD1	2.47	0.45
2:B:81:ILE:HD11	2:B:138:THR:HG22	1.98	0.44
1:D:1109:VAL:HG12	1:D:1129:LEU:HD22	1.99	0.44
1:D:1120:MET:HA	1:D:1120:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:THR:HB	1:A:276:MET:HE3	2.00	0.44
1:A:282:MET:HE2	1:A:305:LEU:HD11	1.98	0.44
1:G:59:GLY:HA2	1:G:1073:TRP:CZ3	2.53	0.44
1:G:257:THR:HB	1:G:276:MET:HE3	2.00	0.44
1:A:1056:ASN:HD21	2:E:410:SER:HB3	1.83	0.43
1:D:118:THR:HG23	2:E:207:ILE:CD1	2.48	0.43
1:G:239:TYR:CD2	1:G:297:LEU:HD23	2.54	0.43
1:J:257:THR:HB	1:J:276:MET:HE3	2.01	0.42
2:K:141:ILE:HG23	2:K:157:VAL:HG13	2.00	0.42
2:B:331:ILE:HD12	2:B:368:LEU:HD21	2.02	0.41
1:A:912:LEU:HD21	2:B:244:LEU:CD1	2.49	0.41
1:D:257:THR:HB	1:D:276:MET:HE3	2.02	0.41
1:G:321:VAL:HG22	1:G:350:MET:HE1	2.02	0.41
2:B:320:SER:OG	2:B:333:THR:HG22	2.21	0.41
1:G:181:VAL:HG23	1:G:219:VAL:CG2	2.51	0.41
2:B:81:ILE:CD1	2:B:138:THR:HG22	2.51	0.41
2:B:141:ILE:HG23	2:B:157:VAL:HG13	2.03	0.41
2:K:110:VAL:HG11	2:K:157:VAL:HG21	2.02	0.40
1:J:1030:PHE:CZ	1:J:1038:GLY:HA3	2.56	0.40
1:G:1109:VAL:HG12	1:G:1129:LEU:HD22	2.04	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	822/856 (96%)	762 (93%)	52 (6%)	8 (1%)	13	41
1	D	815/856 (95%)	757 (93%)	51 (6%)	7 (1%)	14	43
1	G	822/856 (96%)	769 (94%)	47 (6%)	6 (1%)	19	49
1	J	839/856 (98%)	775 (92%)	52 (6%)	12 (1%)	9	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	372/426 (87%)	354 (95%)	15 (4%)	3 (1%)	16	45
2	E	374/426 (88%)	354 (95%)	17 (4%)	3 (1%)	16	45
2	H	372/426 (87%)	355 (95%)	14 (4%)	3 (1%)	16	45
2	K	374/426 (88%)	356 (95%)	15 (4%)	3 (1%)	16	45
3	C	30/38 (79%)	28 (93%)	2 (7%)	0	100	100
3	F	30/38 (79%)	28 (93%)	2 (7%)	0	100	100
3	I	30/38 (79%)	28 (93%)	2 (7%)	0	100	100
3	L	30/38 (79%)	27 (90%)	3 (10%)	0	100	100
All	All	4910/5280 (93%)	4593 (94%)	272 (6%)	45 (1%)	14	43

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	209	GLN
2	E	71	THR
2	H	116	LYS
1	J	291	MET
1	A	291	MET
1	A	1021	SER
1	D	291	MET
1	G	291	MET
1	G	295	VAL
1	G	1021	SER
1	J	112	ILE
1	J	209	GLN
1	J	295	VAL
1	J	371	GLY
1	J	1021	SER
1	A	112	ILE
1	A	208	LYS
1	A	295	VAL
1	A	371	GLY
1	D	112	ILE
1	D	295	VAL
1	G	112	ILE
1	G	371	GLY
1	J	-9	GLU
1	A	36	ASN
1	A	367	LEU

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Mol	Chain	Res	Type
1	D	36	ASN
1	D	371	GLY
1	G	36	ASN
1	J	36	ASN
1	J	1118	SER
1	J	1120	MET
2	B	116	LYS
2	B	410	SER
2	E	410	SER
2	H	410	SER
1	J	367	LEU
2	K	410	SER
2	K	175	ASP
1	J	242	GLY
1	D	242	GLY
2	B	213	VAL
2	E	213	VAL
2	H	213	VAL
2	K	213	VAL

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	713/744 (96%)	683 (96%)	30 (4%)	25	52
1	D	708/744 (95%)	680 (96%)	28 (4%)	27	53
1	G	713/744 (96%)	682 (96%)	31 (4%)	25	51
1	J	723/744 (97%)	685 (95%)	38 (5%)	19	45
2	B	332/385 (86%)	299 (90%)	33 (10%)	6	23
2	E	332/385 (86%)	296 (89%)	36 (11%)	5	20
2	H	330/385 (86%)	291 (88%)	39 (12%)	4	17
2	K	332/385 (86%)	295 (89%)	37 (11%)	5	19
3	C	25/30 (83%)	24 (96%)	1 (4%)	27	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	25/30 (83%)	25 (100%)	0	100	100
3	I	25/30 (83%)	25 (100%)	0	100	100
3	L	25/30 (83%)	24 (96%)	1 (4%)	27	53
All	All	4283/4636 (92%)	4009 (94%)	274 (6%)	14	39

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	74	LYS
1	A	112	ILE
1	A	118	THR
1	A	208	LYS
1	A	224	GLU
1	A	234	GLN
1	A	287	LYS
1	A	288	GLU
1	A	294	THR
1	A	295	VAL
1	A	318	ASP
1	A	345	SER
1	A	368	GLU
1	A	372	GLN
1	A	728	GLU
1	A	745	THR
1	A	786	VAL
1	A	902	GLU
1	A	914	LEU
1	A	928	ARG
1	A	957	VAL
1	A	977	CYS
1	A	985	THR
1	A	1016	ASN
1	A	1054	MET
1	A	1062	ILE
1	A	1078	THR
1	A	1106	GLN
1	A	1120	MET
2	B	71	THR
2	B	78	CYS
2	B	92	ILE

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Mol	Chain	Res	Type
2	B	95	GLN
2	B	96	THR
2	B	149	ASP
2	B	154	ILE
2	B	155	VAL
2	B	163	GLN
2	B	182	VAL
2	B	183	GLN
2	B	199	LEU
2	B	211	LYS
2	B	213	VAL
2	B	216	GLU
2	B	218	GLN
2	B	225	GLN
2	B	239	SER
2	B	242	ARG
2	B	251	GLU
2	B	268	LEU
2	B	269	LYS
2	B	283	ARG
2	B	298	LEU
2	B	329	THR
2	B	339	SER
2	B	342	LEU
2	B	358	GLU
2	B	393	ILE
2	B	409	MET
2	B	410	SER
2	B	413	LYS
2	B	439	ILE
3	C	155	THR
1	D	54	GLU
1	D	74	LYS
1	D	112	ILE
1	D	118	THR
1	D	234	GLN
1	D	288	GLU
1	D	294	THR
1	D	295	VAL
1	D	318	ASP
1	D	345	SER
1	D	347	VAL

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Mol	Chain	Res	Type
1	D	368	GLU
1	D	372	GLN
1	D	728	GLU
1	D	745	THR
1	D	786	VAL
1	D	815	SER
1	D	902	GLU
1	D	914	LEU
1	D	928	ARG
1	D	957	VAL
1	D	977	CYS
1	D	985	THR
1	D	1056	ASN
1	D	1062	ILE
1	D	1079	GLU
1	D	1080	ARG
1	D	1106	GLN
2	E	78	CYS
2	E	81	ILE
2	E	92	ILE
2	E	95	GLN
2	E	96	THR
2	E	118	ARG
2	E	149	ASP
2	E	154	ILE
2	E	155	VAL
2	E	163	GLN
2	E	175	ASP
2	E	177	ILE
2	E	182	VAL
2	E	183	GLN
2	E	211	LYS
2	E	213	VAL
2	E	216	GLU
2	E	218	GLN
2	E	225	GLN
2	E	239	SER
2	E	242	ARG
2	E	251	GLU
2	E	268	LEU
2	E	269	LYS
2	E	283	ARG

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Mol	Chain	Res	Type
2	E	298	LEU
2	E	339	SER
2	E	340	LEU
2	E	342	LEU
2	E	358	GLU
2	E	387	THR
2	E	393	ILE
2	E	409	MET
2	E	410	SER
2	E	413	LYS
2	E	439	ILE
1	G	1	MET
1	G	54	GLU
1	G	74	LYS
1	G	112	ILE
1	G	118	THR
1	G	207	TRP
1	G	210	GLU
1	G	224	GLU
1	G	234	GLN
1	G	288	GLU
1	G	291	MET
1	G	292	ASP
1	G	295	VAL
1	G	318	ASP
1	G	341	ASN
1	G	345	SER
1	G	347	VAL
1	G	372	GLN
1	G	728	GLU
1	G	745	THR
1	G	769	LYS
1	G	786	VAL
1	G	790	ASN
1	G	902	GLU
1	G	914	LEU
1	G	928	ARG
1	G	957	VAL
1	G	977	CYS
1	G	985	THR
1	G	1062	ILE
1	G	1106	GLN

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Mol	Chain	Res	Type
2	H	71	THR
2	H	78	CYS
2	H	81	ILE
2	H	92	ILE
2	H	95	GLN
2	H	96	THR
2	H	114	ILE
2	H	118	ARG
2	H	149	ASP
2	H	154	ILE
2	H	155	VAL
2	H	163	GLN
2	H	171	ARG
2	H	182	VAL
2	H	183	GLN
2	H	204	LYS
2	H	211	LYS
2	H	213	VAL
2	H	216	GLU
2	H	218	GLN
2	H	225	GLN
2	H	239	SER
2	H	242	ARG
2	H	251	GLU
2	H	268	LEU
2	H	269	LYS
2	H	283	ARG
2	H	298	LEU
2	H	339	SER
2	H	342	LEU
2	H	358	GLU
2	H	387	THR
2	H	393	ILE
2	H	409	MET
2	H	410	SER
2	H	413	LYS
2	H	419	ARG
2	H	439	ILE
2	H	442	LEU
1	J	-9	GLU
1	J	54	GLU
1	J	74	LYS

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Mol	Chain	Res	Type
1	J	112	ILE
1	J	118	THR
1	J	129	ARG
1	J	224	GLU
1	J	234	GLN
1	J	287	LYS
1	J	294	THR
1	J	318	ASP
1	J	345	SER
1	J	368	GLU
1	J	372	GLN
1	J	707	ILE
1	J	712	ILE
1	J	728	GLU
1	J	745	THR
1	J	766	SER
1	J	769	LYS
1	J	786	VAL
1	J	790	ASN
1	J	867	LYS
1	J	902	GLU
1	J	914	LEU
1	J	928	ARG
1	J	957	VAL
1	J	977	CYS
1	J	980	ASP
1	J	981	SER
1	J	985	THR
1	J	994	GLU
1	J	1054	MET
1	J	1056	ASN
1	J	1062	ILE
1	J	1079	GLU
1	J	1080	ARG
1	J	1106	GLN
2	K	71	THR
2	K	78	CYS
2	K	81	ILE
2	K	92	ILE
2	K	95	GLN
2	K	96	THR
2	K	101	LEU

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Mol	Chain	Res	Type
2	K	149	ASP
2	K	154	ILE
2	K	155	VAL
2	K	163	GLN
2	K	172	THR
2	K	177	ILE
2	K	182	VAL
2	K	183	GLN
2	K	211	LYS
2	K	213	VAL
2	K	216	GLU
2	K	218	GLN
2	K	225	GLN
2	K	239	SER
2	K	242	ARG
2	K	251	GLU
2	K	268	LEU
2	K	269	LYS
2	K	283	ARG
2	K	298	LEU
2	K	320	SER
2	K	339	SER
2	K	342	LEU
2	K	358	GLU
2	K	393	ILE
2	K	409	MET
2	K	410	SER
2	K	413	LYS
2	K	439	ILE
2	K	442	LEU
3	L	164	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	211	ASN
1	A	255	GLN
1	A	337	ASN
1	A	711	HIS
1	A	790	ASN
1	A	907	ASN

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Mol	Chain	Res	Type
1	A	941	ASN
1	A	950	ASN
1	A	964	ASN
1	A	978	GLN
1	A	1055	GLN
1	A	1056	ASN
1	A	1106	GLN
1	A	1113	GLN
2	B	95	GLN
2	B	112	ASN
2	B	115	GLN
2	B	129	GLN
2	B	134	GLN
2	B	178	GLN
2	B	228	GLN
2	B	267	ASN
2	B	306	GLN
1	D	4	ASN
1	D	337	ASN
1	D	711	HIS
1	D	790	ASN
1	D	907	ASN
1	D	941	ASN
1	D	950	ASN
1	D	1015	GLN
1	D	1049	ASN
2	E	95	GLN
2	E	112	ASN
2	E	129	GLN
2	E	134	GLN
2	E	173	GLN
2	E	178	GLN
2	E	228	GLN
2	E	267	ASN
2	E	306	GLN
1	G	209	GLN
1	G	241	ASN
1	G	711	HIS
1	G	727	GLN
1	G	778	HIS
1	G	790	ASN
1	G	907	ASN

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Mol	Chain	Res	Type
1	G	941	ASN
1	G	950	ASN
1	G	964	ASN
1	G	978	GLN
1	G	1049	ASN
1	G	1113	GLN
2	H	95	GLN
2	H	112	ASN
2	H	129	GLN
2	H	134	GLN
2	H	178	GLN
2	H	228	GLN
2	H	267	ASN
1	J	209	GLN
1	J	241	ASN
1	J	337	ASN
1	J	907	ASN
1	J	941	ASN
1	J	950	ASN
1	J	1049	ASN
1	J	1055	GLN
2	K	112	ASN
2	K	115	GLN
2	K	129	GLN
2	K	134	GLN
2	K	228	GLN
2	K	267	ASN
2	K	335	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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	Y70	H	502	-	22,22,22	0.27	0	31,33,33	0.75	2 (6%)
5	Y70	B	502	-	22,22,22	0.29	0	31,33,33	0.74	2 (6%)
5	Y70	E	502	-	22,22,22	0.26	0	31,33,33	0.73	2 (6%)
5	Y70	K	502	-	22,22,22	0.29	0	31,33,33	0.75	2 (6%)

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	Y70	H	502	-	-	0/4/33/33	0/3/3/3
5	Y70	B	502	-	-	0/4/33/33	0/3/3/3
5	Y70	E	502	-	-	0/4/33/33	0/3/3/3
5	Y70	K	502	-	-	0/4/33/33	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	502	Y70	C14-C12-N8	-2.80	107.07	113.85
5	E	502	Y70	C14-C12-N8	-2.79	107.10	113.85
5	H	502	Y70	C14-C12-N8	-2.73	107.22	113.85
5	B	502	Y70	C14-C12-N8	-2.71	107.28	113.85
5	K	502	Y70	C15-C12-N8	2.25	111.13	109.08
5	H	502	Y70	C15-C12-N8	2.25	111.13	109.08
5	B	502	Y70	C15-C12-N8	2.24	111.12	109.08
5	E	502	Y70	C15-C12-N8	2.02	110.92	109.08

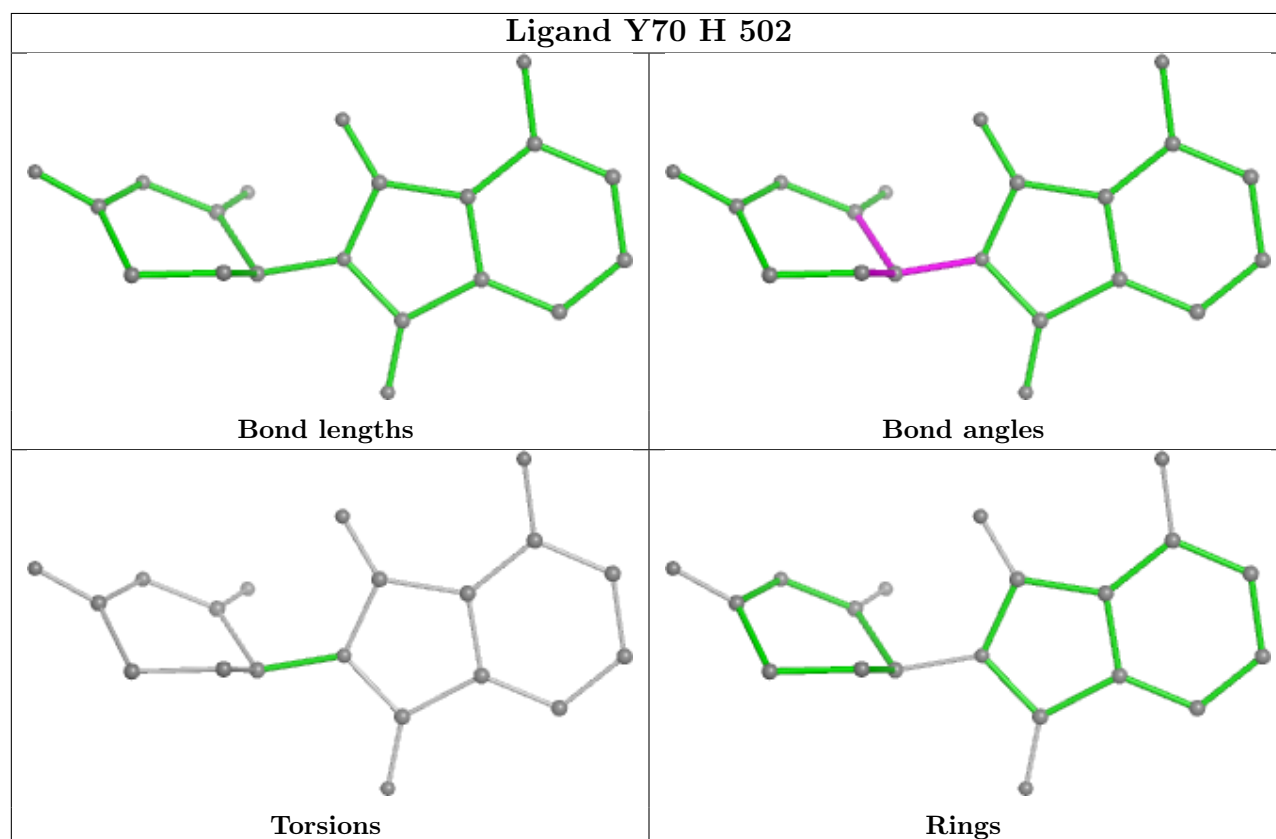
There are no chirality outliers.

There are no torsion outliers.

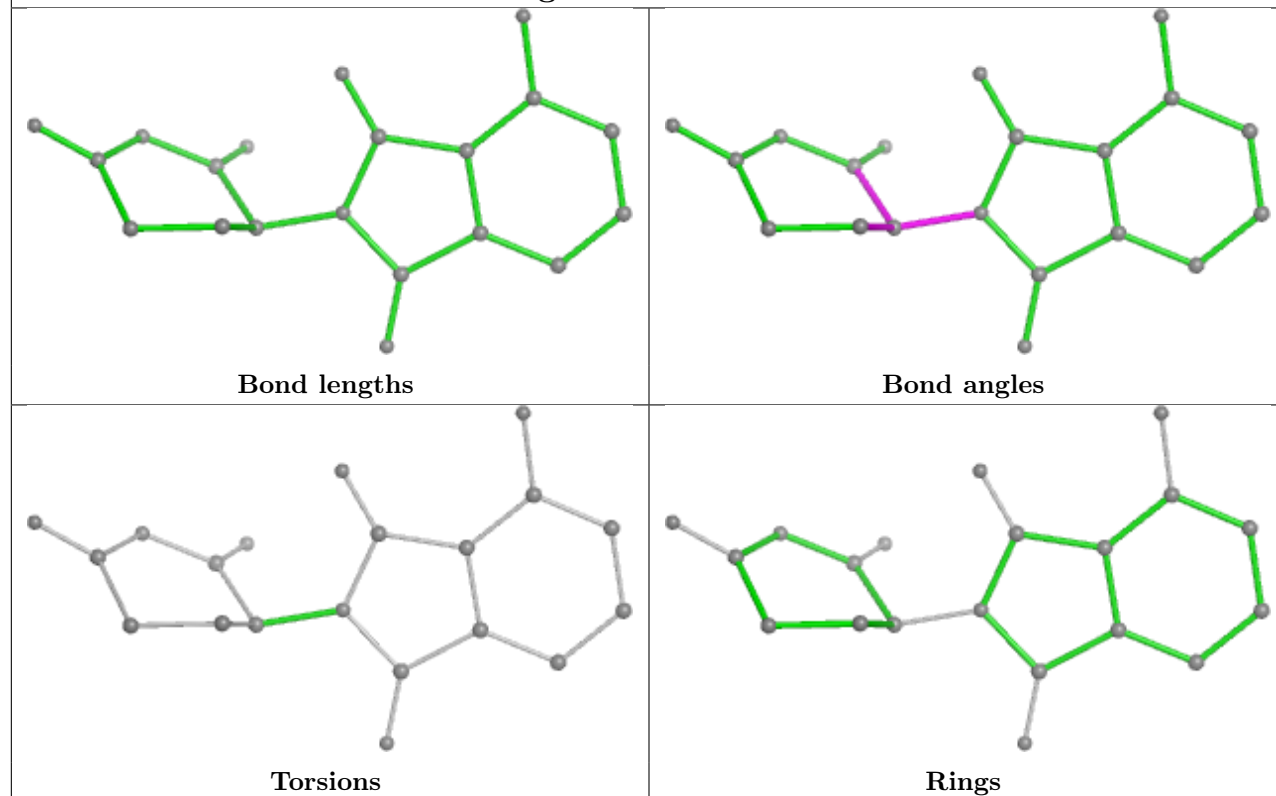
There are no ring outliers.

No monomer is involved in short contacts.

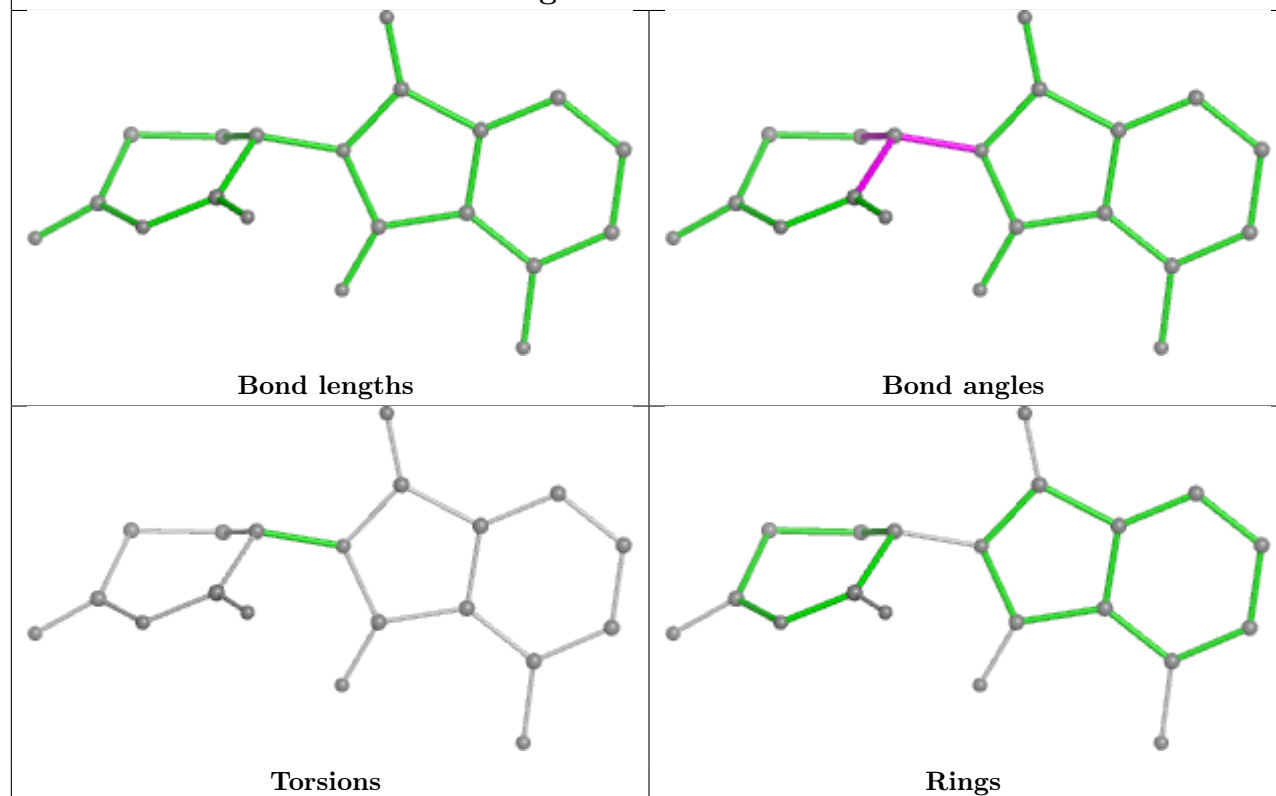
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

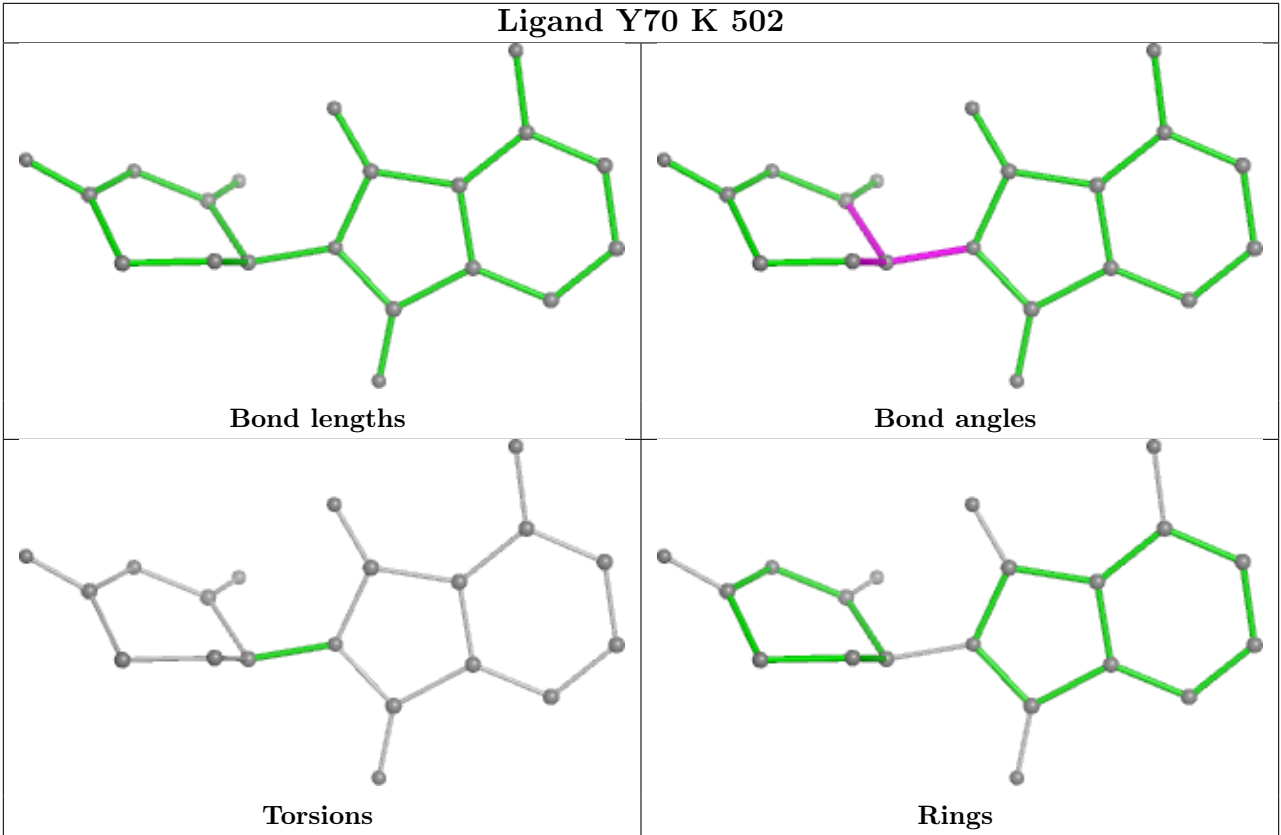


Ligand Y70 B 502



Ligand Y70 E 502





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	207:ILE	C	208:PHE	N	2.27

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.