Full wwPDB X-ray Structure Validation Report (i)

Apr 14, 2025 – 07:08 pm BST

PDB ID	:	9QE5 / pdb_00009qe5
Title	:	VCB in complex with VHL-binding compound 82
Authors	:	Braun, M.B.; Dierlamm, N.; Hartmann, M.D.
Deposited on	:	2025-03-07
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

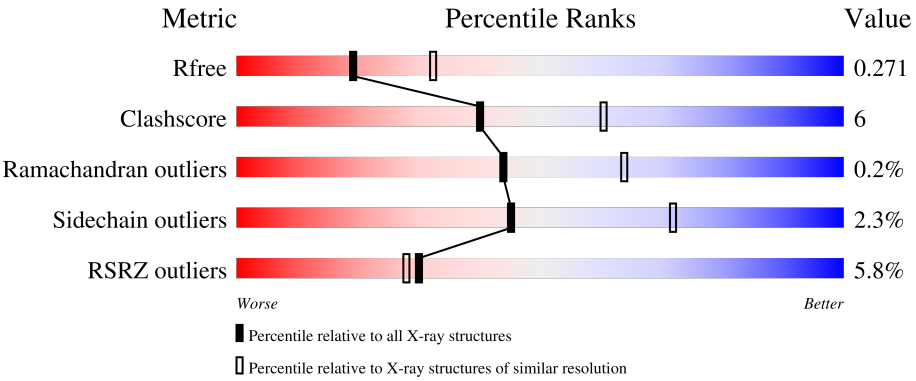
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 <=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	129	3% 72% 9% 19%
1	D	129	7% 53% 23% · 22%
1	G	129	3% 67% 12% 20%
1	J	129	4% 67% 13% 19%
2	B	97	3% 74% 18% 8%

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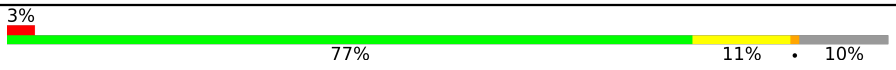
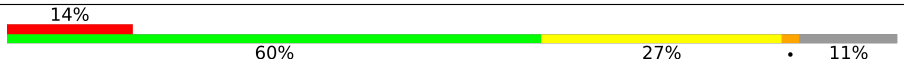
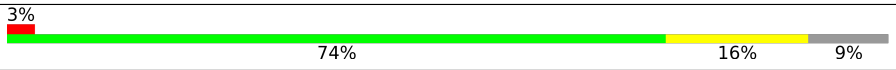
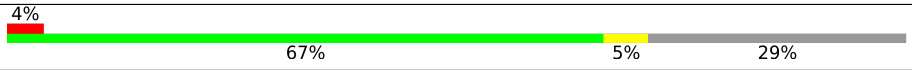
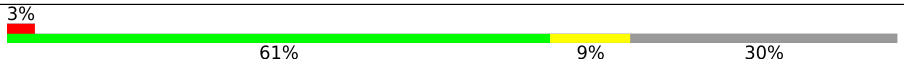
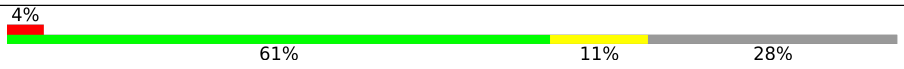
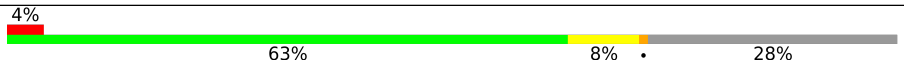
Mol	Chain	Length	Quality of chain
2	E	97	
2	H	97	
2	K	97	
3	C	203	
3	F	203	
3	I	203	
3	L	203	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10783 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 Elongin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	104	Total	As	C	N	O	S	0	0	0
			816	1	517	137	156	5			
1	D	101	Total	As	C	N	O	S	0	0	0
			784	1	500	128	150	5			
1	G	103	Total	As	C	N	O	S	0	0	0
			809	1	513	135	155	5			
1	J	104	Total	As	C	N	O	S	0	0	0
			823	1	520	138	160	4			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP Q15370
A	-23	LYS	-	expression tag	UNP Q15370
A	-22	HIS	-	expression tag	UNP Q15370
A	-21	HIS	-	expression tag	UNP Q15370
A	-20	HIS	-	expression tag	UNP Q15370
A	-19	HIS	-	expression tag	UNP Q15370
A	-18	HIS	-	expression tag	UNP Q15370
A	-17	HIS	-	expression tag	UNP Q15370
A	-16	PRO	-	expression tag	UNP Q15370
A	-15	MET	-	expression tag	UNP Q15370
A	-14	SER	-	expression tag	UNP Q15370
A	-13	ASP	-	expression tag	UNP Q15370
A	-12	TYR	-	expression tag	UNP Q15370
A	-11	ASP	-	expression tag	UNP Q15370
A	-10	ILE	-	expression tag	UNP Q15370
A	-9	PRO	-	expression tag	UNP Q15370
A	-8	THR	-	expression tag	UNP Q15370
A	-7	THR	-	expression tag	UNP Q15370
A	-6	GLU	-	expression tag	UNP Q15370
A	-5	ASN	-	expression tag	UNP Q15370
A	-4	LEU	-	expression tag	UNP Q15370

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP Q15370
A	-2	PHE	-	expression tag	UNP Q15370
A	-1	GLN	-	expression tag	UNP Q15370
A	0	GLY	-	expression tag	UNP Q15370
D	-24	MET	-	initiating methionine	UNP Q15370
D	-23	LYS	-	expression tag	UNP Q15370
D	-22	HIS	-	expression tag	UNP Q15370
D	-21	HIS	-	expression tag	UNP Q15370
D	-20	HIS	-	expression tag	UNP Q15370
D	-19	HIS	-	expression tag	UNP Q15370
D	-18	HIS	-	expression tag	UNP Q15370
D	-17	HIS	-	expression tag	UNP Q15370
D	-16	PRO	-	expression tag	UNP Q15370
D	-15	MET	-	expression tag	UNP Q15370
D	-14	SER	-	expression tag	UNP Q15370
D	-13	ASP	-	expression tag	UNP Q15370
D	-12	TYR	-	expression tag	UNP Q15370
D	-11	ASP	-	expression tag	UNP Q15370
D	-10	ILE	-	expression tag	UNP Q15370
D	-9	PRO	-	expression tag	UNP Q15370
D	-8	THR	-	expression tag	UNP Q15370
D	-7	THR	-	expression tag	UNP Q15370
D	-6	GLU	-	expression tag	UNP Q15370
D	-5	ASN	-	expression tag	UNP Q15370
D	-4	LEU	-	expression tag	UNP Q15370
D	-3	TYR	-	expression tag	UNP Q15370
D	-2	PHE	-	expression tag	UNP Q15370
D	-1	GLN	-	expression tag	UNP Q15370
D	0	GLY	-	expression tag	UNP Q15370
G	-24	MET	-	initiating methionine	UNP Q15370
G	-23	LYS	-	expression tag	UNP Q15370
G	-22	HIS	-	expression tag	UNP Q15370
G	-21	HIS	-	expression tag	UNP Q15370
G	-20	HIS	-	expression tag	UNP Q15370
G	-19	HIS	-	expression tag	UNP Q15370
G	-18	HIS	-	expression tag	UNP Q15370
G	-17	HIS	-	expression tag	UNP Q15370
G	-16	PRO	-	expression tag	UNP Q15370
G	-15	MET	-	expression tag	UNP Q15370
G	-14	SER	-	expression tag	UNP Q15370
G	-13	ASP	-	expression tag	UNP Q15370
G	-12	TYR	-	expression tag	UNP Q15370

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-11	ASP	-	expression tag	UNP Q15370
G	-10	ILE	-	expression tag	UNP Q15370
G	-9	PRO	-	expression tag	UNP Q15370
G	-8	THR	-	expression tag	UNP Q15370
G	-7	THR	-	expression tag	UNP Q15370
G	-6	GLU	-	expression tag	UNP Q15370
G	-5	ASN	-	expression tag	UNP Q15370
G	-4	LEU	-	expression tag	UNP Q15370
G	-3	TYR	-	expression tag	UNP Q15370
G	-2	PHE	-	expression tag	UNP Q15370
G	-1	GLN	-	expression tag	UNP Q15370
G	0	GLY	-	expression tag	UNP Q15370
J	-24	MET	-	initiating methionine	UNP Q15370
J	-23	LYS	-	expression tag	UNP Q15370
J	-22	HIS	-	expression tag	UNP Q15370
J	-21	HIS	-	expression tag	UNP Q15370
J	-20	HIS	-	expression tag	UNP Q15370
J	-19	HIS	-	expression tag	UNP Q15370
J	-18	HIS	-	expression tag	UNP Q15370
J	-17	HIS	-	expression tag	UNP Q15370
J	-16	PRO	-	expression tag	UNP Q15370
J	-15	MET	-	expression tag	UNP Q15370
J	-14	SER	-	expression tag	UNP Q15370
J	-13	ASP	-	expression tag	UNP Q15370
J	-12	TYR	-	expression tag	UNP Q15370
J	-11	ASP	-	expression tag	UNP Q15370
J	-10	ILE	-	expression tag	UNP Q15370
J	-9	PRO	-	expression tag	UNP Q15370
J	-8	THR	-	expression tag	UNP Q15370
J	-7	THR	-	expression tag	UNP Q15370
J	-6	GLU	-	expression tag	UNP Q15370
J	-5	ASN	-	expression tag	UNP Q15370
J	-4	LEU	-	expression tag	UNP Q15370
J	-3	TYR	-	expression tag	UNP Q15370
J	-2	PHE	-	expression tag	UNP Q15370
J	-1	GLN	-	expression tag	UNP Q15370
J	0	GLY	-	expression tag	UNP Q15370

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	89	Total	C	N	O	S	0	0	0
			693	447	110	130	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	87	Total	C	N	O	S	0	0	0
			681	438	110	127	6			
2	H	86	Total	C	N	O	S	0	0	0
			678	436	110	126	6			
2	K	88	Total	C	N	O	S	0	0	0
			689	447	109	127	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP Q15369
E	16	MET	-	initiating methionine	UNP Q15369
H	16	MET	-	initiating methionine	UNP Q15369
K	16	MET	-	initiating methionine	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	145	Total	As	C	N	O	S	0	0	0
			1151	1	736	206	206	2			
3	F	143	Total	As	C	N	O	S	0	0	0
			1159	1	737	208	211	2			
3	I	147	Total	As	C	N	O	S	0	0	0
			1183	1	753	214	213	2			
3	L	146	Total	As	C	N	O	S	0	0	0
			1165	1	740	211	211	2			

There are 172 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	MET	-	initiating methionine	UNP P40337
C	12	ALA	-	expression tag	UNP P40337
C	13	SER	-	expression tag	UNP P40337
C	14	ALA	-	expression tag	UNP P40337
C	15	TRP	-	expression tag	UNP P40337
C	16	SER	-	expression tag	UNP P40337
C	17	HIS	-	expression tag	UNP P40337
C	18	PRO	-	expression tag	UNP P40337
C	19	GLN	-	expression tag	UNP P40337
C	20	PHE	-	expression tag	UNP P40337
C	21	GLU	-	expression tag	UNP P40337
C	22	LYS	-	expression tag	UNP P40337

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Chain	Residue	Modelled	Actual	Comment	Reference
C	23	GLY	-	expression tag	UNP P40337
C	24	GLY	-	expression tag	UNP P40337
C	25	GLY	-	expression tag	UNP P40337
C	26	SER	-	expression tag	UNP P40337
C	27	GLY	-	expression tag	UNP P40337
C	28	GLY	-	expression tag	UNP P40337
C	29	GLY	-	expression tag	UNP P40337
C	30	SER	-	expression tag	UNP P40337
C	31	GLY	-	expression tag	UNP P40337
C	32	GLY	-	expression tag	UNP P40337
C	33	SER	-	expression tag	UNP P40337
C	34	ALA	-	expression tag	UNP P40337
C	35	TRP	-	expression tag	UNP P40337
C	36	SER	-	expression tag	UNP P40337
C	37	HIS	-	expression tag	UNP P40337
C	38	PRO	-	expression tag	UNP P40337
C	39	GLN	-	expression tag	UNP P40337
C	40	PHE	-	expression tag	UNP P40337
C	41	GLU	-	expression tag	UNP P40337
C	42	LYS	-	expression tag	UNP P40337
C	43	SER	-	expression tag	UNP P40337
C	44	GLY	-	expression tag	UNP P40337
C	45	GLU	-	expression tag	UNP P40337
C	46	ASN	-	expression tag	UNP P40337
C	47	LEU	-	expression tag	UNP P40337
C	48	TYR	-	expression tag	UNP P40337
C	49	PHE	-	expression tag	UNP P40337
C	50	GLN	-	expression tag	UNP P40337
C	51	GLY	-	expression tag	UNP P40337
C	52	SER	-	expression tag	UNP P40337
C	53	HIS	-	expression tag	UNP P40337
F	11	MET	-	initiating methionine	UNP P40337
F	12	ALA	-	expression tag	UNP P40337
F	13	SER	-	expression tag	UNP P40337
F	14	ALA	-	expression tag	UNP P40337
F	15	TRP	-	expression tag	UNP P40337
F	16	SER	-	expression tag	UNP P40337
F	17	HIS	-	expression tag	UNP P40337
F	18	PRO	-	expression tag	UNP P40337
F	19	GLN	-	expression tag	UNP P40337
F	20	PHE	-	expression tag	UNP P40337
F	21	GLU	-	expression tag	UNP P40337

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Chain	Residue	Modelled	Actual	Comment	Reference
F	22	LYS	-	expression tag	UNP P40337
F	23	GLY	-	expression tag	UNP P40337
F	24	GLY	-	expression tag	UNP P40337
F	25	GLY	-	expression tag	UNP P40337
F	26	SER	-	expression tag	UNP P40337
F	27	GLY	-	expression tag	UNP P40337
F	28	GLY	-	expression tag	UNP P40337
F	29	GLY	-	expression tag	UNP P40337
F	30	SER	-	expression tag	UNP P40337
F	31	GLY	-	expression tag	UNP P40337
F	32	GLY	-	expression tag	UNP P40337
F	33	SER	-	expression tag	UNP P40337
F	34	ALA	-	expression tag	UNP P40337
F	35	TRP	-	expression tag	UNP P40337
F	36	SER	-	expression tag	UNP P40337
F	37	HIS	-	expression tag	UNP P40337
F	38	PRO	-	expression tag	UNP P40337
F	39	GLN	-	expression tag	UNP P40337
F	40	PHE	-	expression tag	UNP P40337
F	41	GLU	-	expression tag	UNP P40337
F	42	LYS	-	expression tag	UNP P40337
F	43	SER	-	expression tag	UNP P40337
F	44	GLY	-	expression tag	UNP P40337
F	45	GLU	-	expression tag	UNP P40337
F	46	ASN	-	expression tag	UNP P40337
F	47	LEU	-	expression tag	UNP P40337
F	48	TYR	-	expression tag	UNP P40337
F	49	PHE	-	expression tag	UNP P40337
F	50	GLN	-	expression tag	UNP P40337
F	51	GLY	-	expression tag	UNP P40337
F	52	SER	-	expression tag	UNP P40337
F	53	HIS	-	expression tag	UNP P40337
I	11	MET	-	initiating methionine	UNP P40337
I	12	ALA	-	expression tag	UNP P40337
I	13	SER	-	expression tag	UNP P40337
I	14	ALA	-	expression tag	UNP P40337
I	15	TRP	-	expression tag	UNP P40337
I	16	SER	-	expression tag	UNP P40337
I	17	HIS	-	expression tag	UNP P40337
I	18	PRO	-	expression tag	UNP P40337
I	19	GLN	-	expression tag	UNP P40337
I	20	PHE	-	expression tag	UNP P40337

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Chain	Residue	Modelled	Actual	Comment	Reference
I	21	GLU	-	expression tag	UNP P40337
I	22	LYS	-	expression tag	UNP P40337
I	23	GLY	-	expression tag	UNP P40337
I	24	GLY	-	expression tag	UNP P40337
I	25	GLY	-	expression tag	UNP P40337
I	26	SER	-	expression tag	UNP P40337
I	27	GLY	-	expression tag	UNP P40337
I	28	GLY	-	expression tag	UNP P40337
I	29	GLY	-	expression tag	UNP P40337
I	30	SER	-	expression tag	UNP P40337
I	31	GLY	-	expression tag	UNP P40337
I	32	GLY	-	expression tag	UNP P40337
I	33	SER	-	expression tag	UNP P40337
I	34	ALA	-	expression tag	UNP P40337
I	35	TRP	-	expression tag	UNP P40337
I	36	SER	-	expression tag	UNP P40337
I	37	HIS	-	expression tag	UNP P40337
I	38	PRO	-	expression tag	UNP P40337
I	39	GLN	-	expression tag	UNP P40337
I	40	PHE	-	expression tag	UNP P40337
I	41	GLU	-	expression tag	UNP P40337
I	42	LYS	-	expression tag	UNP P40337
I	43	SER	-	expression tag	UNP P40337
I	44	GLY	-	expression tag	UNP P40337
I	45	GLU	-	expression tag	UNP P40337
I	46	ASN	-	expression tag	UNP P40337
I	47	LEU	-	expression tag	UNP P40337
I	48	TYR	-	expression tag	UNP P40337
I	49	PHE	-	expression tag	UNP P40337
I	50	GLN	-	expression tag	UNP P40337
I	51	GLY	-	expression tag	UNP P40337
I	52	SER	-	expression tag	UNP P40337
I	53	HIS	-	expression tag	UNP P40337
L	11	MET	-	initiating methionine	UNP P40337
L	12	ALA	-	expression tag	UNP P40337
L	13	SER	-	expression tag	UNP P40337
L	14	ALA	-	expression tag	UNP P40337
L	15	TRP	-	expression tag	UNP P40337
L	16	SER	-	expression tag	UNP P40337
L	17	HIS	-	expression tag	UNP P40337
L	18	PRO	-	expression tag	UNP P40337
L	19	GLN	-	expression tag	UNP P40337

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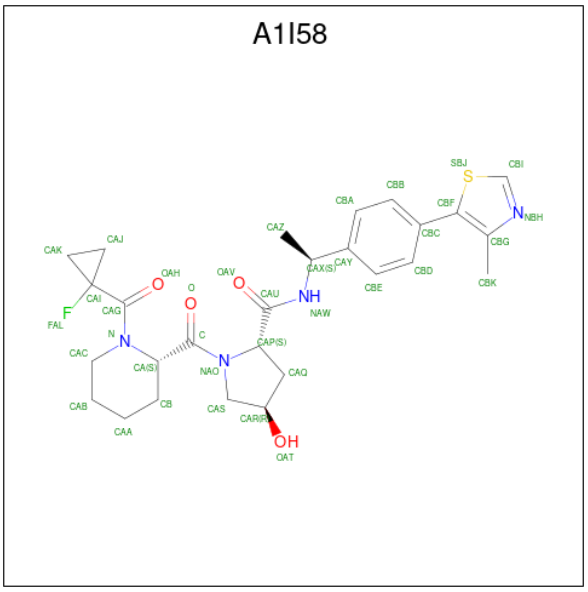
Chain	Residue	Modelled	Actual	Comment	Reference
L	20	PHE	-	expression tag	UNP P40337
L	21	GLU	-	expression tag	UNP P40337
L	22	LYS	-	expression tag	UNP P40337
L	23	GLY	-	expression tag	UNP P40337
L	24	GLY	-	expression tag	UNP P40337
L	25	GLY	-	expression tag	UNP P40337
L	26	SER	-	expression tag	UNP P40337
L	27	GLY	-	expression tag	UNP P40337
L	28	GLY	-	expression tag	UNP P40337
L	29	GLY	-	expression tag	UNP P40337
L	30	SER	-	expression tag	UNP P40337
L	31	GLY	-	expression tag	UNP P40337
L	32	GLY	-	expression tag	UNP P40337
L	33	SER	-	expression tag	UNP P40337
L	34	ALA	-	expression tag	UNP P40337
L	35	TRP	-	expression tag	UNP P40337
L	36	SER	-	expression tag	UNP P40337
L	37	HIS	-	expression tag	UNP P40337
L	38	PRO	-	expression tag	UNP P40337
L	39	GLN	-	expression tag	UNP P40337
L	40	PHE	-	expression tag	UNP P40337
L	41	GLU	-	expression tag	UNP P40337
L	42	LYS	-	expression tag	UNP P40337
L	43	SER	-	expression tag	UNP P40337
L	44	GLY	-	expression tag	UNP P40337
L	45	GLU	-	expression tag	UNP P40337
L	46	ASN	-	expression tag	UNP P40337
L	47	LEU	-	expression tag	UNP P40337
L	48	TYR	-	expression tag	UNP P40337
L	49	PHE	-	expression tag	UNP P40337
L	50	GLN	-	expression tag	UNP P40337
L	51	GLY	-	expression tag	UNP P40337
L	52	SER	-	expression tag	UNP P40337
L	53	HIS	-	expression tag	UNP P40337

- Molecule 4 is (2 {S},4 {R})-1-[(2 {S})-1-(1-fluoranylcyclopropyl)carbonylpiperidin-2-yl]carbonyl- {N}-[(1 {S})-1-[4-(4-methyl-1,3-thiazol-5-yl)phenyl]ethyl]-4-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: A1I58) (formula: $C_{27}H_{33}FN_4O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C F N O S 37 27 1 4 4 1	0	0
4	F	1	Total C F N O S 37 27 1 4 4 1	0	0
4	I	1	Total C F N O S 37 27 1 4 4 1	0	0
4	L	1	Total C F N O S 37 27 1 4 4 1	0	0

- Molecule 5 is water.

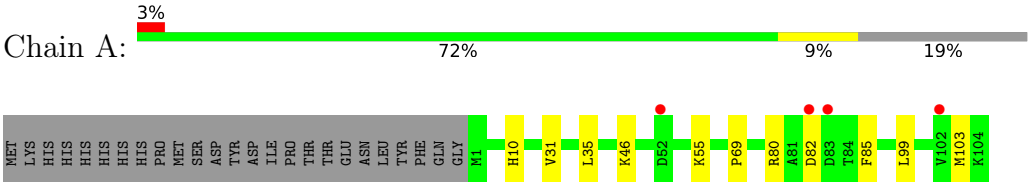
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	G	1	Total O 1 1	0	0
5	J	1	Total O 1 1	0	0

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.

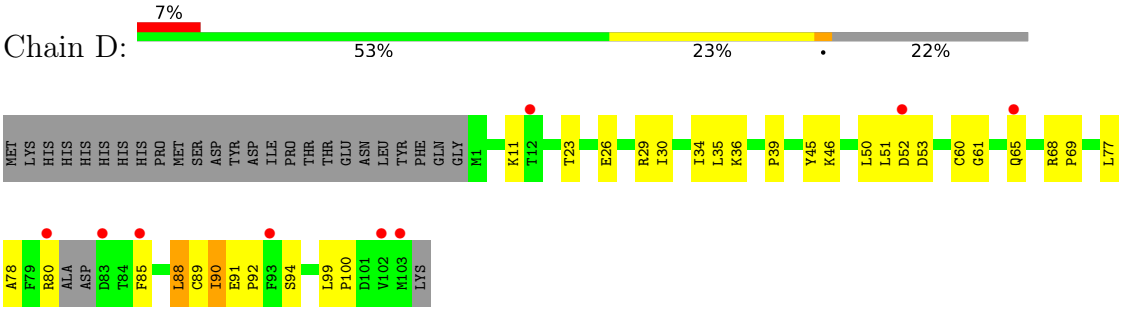
• Molecule 1: Elongin-B

Chain A:



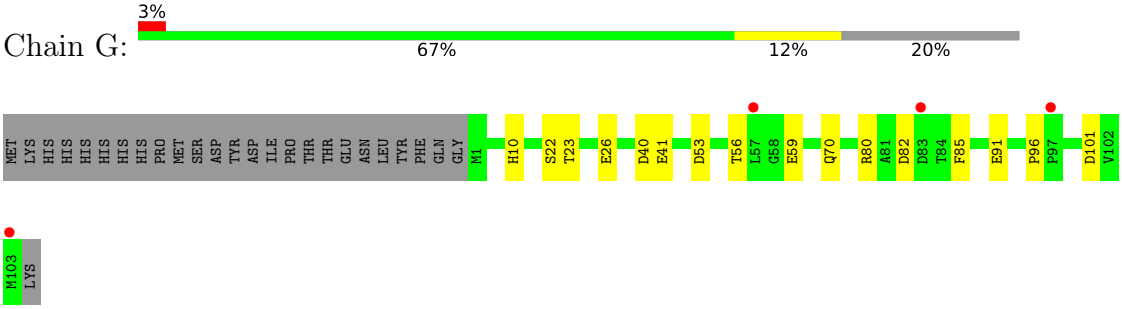
• Molecule 1: Elongin-B

Chain D:



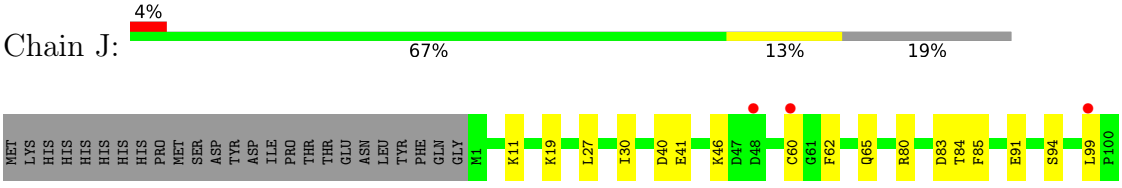
• Molecule 1: Elongin-B

Chain G:



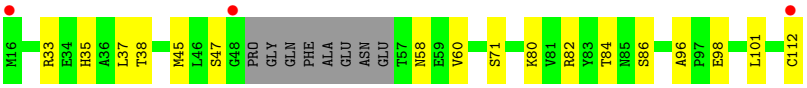
• Molecule 1: Elongin-B

Chain J:



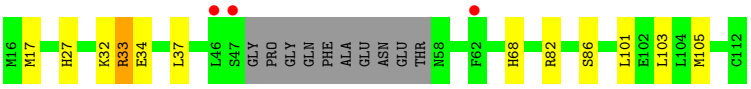
• Molecule 2: Elongin-C

Chain B:



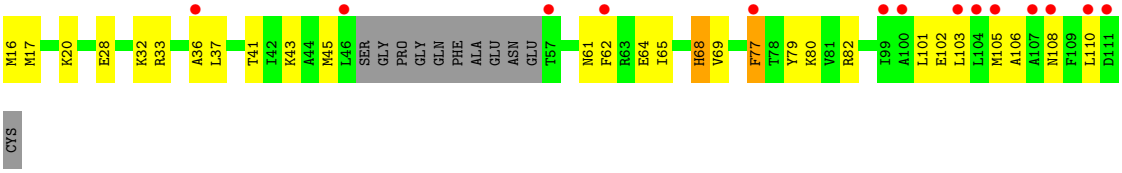
• Molecule 2: Elongin-C

Chain E:



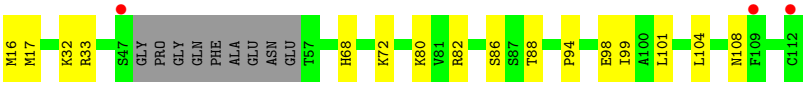
• Molecule 2: Elongin-C

Chain H:



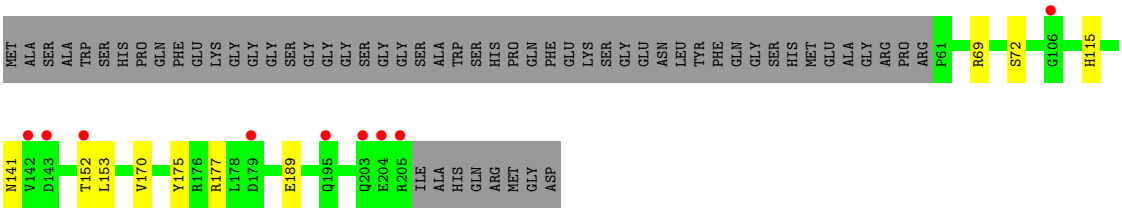
• Molecule 2: Elongin-C

Chain K:



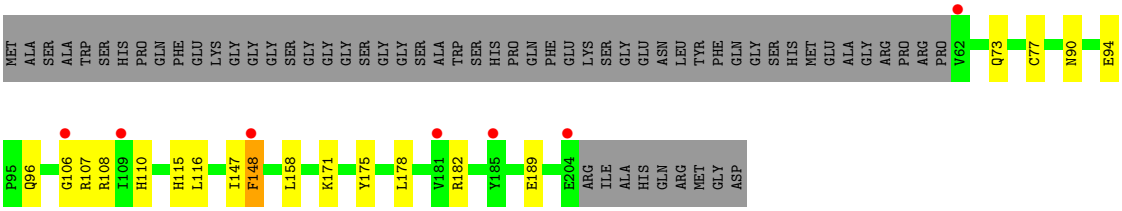
• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain C:

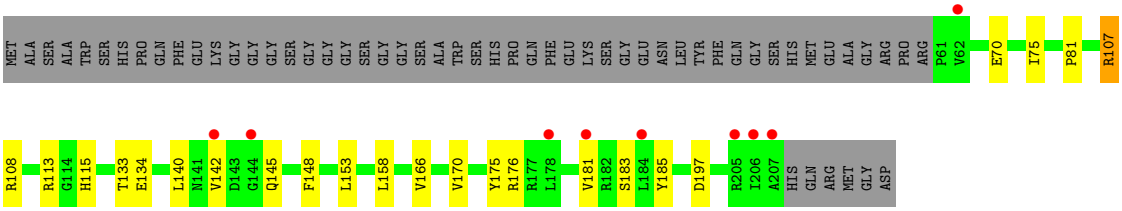


• Molecule 3: von Hippel-Lindau disease tumor suppressor

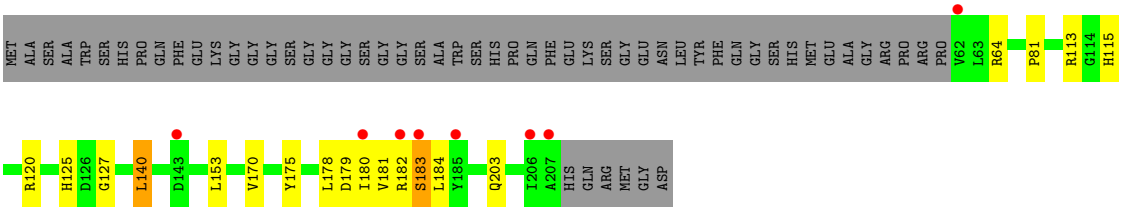
Chain F:



• Molecule 3: von Hippel-Lindau disease tumor suppressor



• Molecule 3: von Hippel-Lindau disease tumor suppressor



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	94.22Å 94.22Å 366.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.72 – 2.50 45.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.72-2.50) 99.7 (45.72-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.245 , 0.273 0.244 , 0.271	Depositor DCC
R_{free} test set	1569 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å^2)	64.5	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10783	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0555e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: A1I58, CAS

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	0.39	0/822	0.70	1/1109 (0.1%)
1	D	0.45	0/789	0.87	3/1066 (0.3%)
1	G	0.35	0/815	0.66	0/1101
1	J	0.36	0/829	0.72	1/1118 (0.1%)
2	B	0.42	0/707	0.67	0/955
2	E	0.39	0/695	0.65	0/939
2	H	0.38	0/691	0.74	0/933
2	K	0.38	0/703	0.64	1/951 (0.1%)
3	C	0.34	0/1171	0.66	0/1601
3	F	0.35	0/1179	0.72	0/1610
3	I	0.35	0/1204	0.71	1/1646 (0.1%)
3	L	0.35	0/1184	0.69	1/1618 (0.1%)
All	All	0.37	0/10789	0.71	8/14647 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	88	LEU	CA-CB-CG	-9.22	94.08	115.30
1	J	99	LEU	CA-CB-CG	6.53	130.32	115.30
1	D	90	ILE	CG1-CB-CG2	-6.39	97.34	111.40
2	K	80	LYS	CB-CG-CD	5.86	126.84	111.60
1	D	51	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	46	LYS	CA-CB-CG	-5.61	101.06	113.40
3	L	140	LEU	CA-CB-CG	5.06	126.94	115.30
3	I	140	LEU	CB-CG-CD1	-5.02	102.46	111.00

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	816	0	807	6	0
1	D	784	0	771	24	0
1	G	809	0	801	17	0
1	J	823	0	815	10	0
2	B	693	0	685	8	0
2	E	681	0	666	13	0
2	H	678	0	673	21	0
2	K	689	0	683	12	0
3	C	1151	0	1116	7	0
3	F	1159	0	1134	13	0
3	I	1183	0	1160	17	0
3	L	1165	0	1138	12	0
4	C	37	0	0	1	0
4	F	37	0	0	2	0
4	I	37	0	0	2	0
4	L	37	0	0	1	0
5	A	2	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
All	All	10783	0	10449	138	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 6.

All (138) 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:F:108:ARG:HD2	2:H:41:THR:HG22	1.60	0.82
3:C:72:SER:HA	3:C:141:ASN:HD21	1.48	0.79
3:F:115:HIS:ND1	4:F:301:A1I58:OAT	2.23	0.72
2:K:101:LEU:HD22	3:L:180:ILE:HD11	1.69	0.71
2:B:80:LYS:O	2:B:84:THR:HG23	1.90	0.71
2:E:32:LYS:HD2	2:E:34:GLU:H	1.58	0.69
1:D:78:ALA:HB2	1:D:88:LEU:HD13	1.75	0.67
2:H:82:ARG:O	2:H:82:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:MET:HE3	2:H:33:ARG:HD2	1.76	0.66
2:K:82:ARG:HH22	2:K:88:THR:HG21	1.60	0.65
1:D:77:LEU:O	1:D:88:LEU:HD11	1.96	0.65
2:K:98:GLU:N	2:K:98:GLU:OE1	2.29	0.65
1:G:56:THR:N	1:G:59:GLU:OE2	2.19	0.64
1:D:65:GLN:O	1:D:68:ARG:HD2	1.98	0.64
3:I:133:THR:HG22	3:I:134:GLU:H	1.63	0.63
2:H:20:LYS:HD3	2:H:28:GLU:HB3	1.80	0.62
1:G:56:THR:OG1	1:G:59:GLU:HG3	2.00	0.62
2:B:35:HIS:O	2:B:38:THR:OG1	2.17	0.61
3:L:179:ASP:O	3:L:180:ILE:HD13	2.00	0.61
1:D:29:ARG:HH21	1:D:39:PRO:HG2	1.67	0.60
3:C:177:ARG:O	3:C:177:ARG:NE	2.35	0.59
3:I:166:VAL:O	3:I:170:VAL:HG22	2.03	0.59
2:K:101:LEU:CD2	3:L:180:ILE:HD11	2.33	0.58
3:I:115:HIS:ND1	4:I:301:A1I58:OAT	2.34	0.58
1:D:34:ILE:HG22	1:D:35:LEU:HD23	1.85	0.58
1:J:11:LYS:HG3	1:J:91:GLU:HG3	1.86	0.58
3:C:115:HIS:ND1	4:C:301:A1I58:OAT	2.37	0.58
3:L:115:HIS:ND1	4:L:301:A1I58:OAT	2.32	0.57
1:D:23:THR:OG1	1:D:26:GLU:HG3	2.04	0.57
2:H:103:LEU:HD21	3:I:158:LEU:HD11	1.87	0.57
2:K:86:SER:OG	2:K:88:THR:HG22	2.04	0.57
3:C:152:THR:HG22	3:C:153:LEU:O	2.04	0.56
1:D:94:SER:CB	2:E:68:HIS:HD1	2.18	0.56
2:H:64:GLU:OE1	2:H:64:GLU:N	2.39	0.56
2:H:101:LEU:O	2:H:105:MET:HG3	2.06	0.55
1:G:80:ARG:HA	1:G:85:PHE:HA	1.89	0.55
3:C:175:TYR:HD2	3:C:189:GLU:HG3	1.71	0.55
3:I:133:THR:HG22	3:I:134:GLU:N	2.22	0.55
1:D:11:LYS:HG3	1:D:91:GLU:HG3	1.89	0.54
1:G:23:THR:CG2	1:G:26:GLU:HG3	2.36	0.54
3:L:120:ARG:HD2	3:L:125:HIS:O	2.07	0.54
1:A:80:ARG:HA	1:A:85:PHE:HA	1.90	0.54
3:L:81:PRO:HD2	3:L:153:LEU:HG	1.89	0.54
2:H:37:LEU:HD22	2:H:43:LYS:HG3	1.89	0.54
3:F:175:TYR:HA	3:F:178:LEU:HD23	1.90	0.53
1:G:82:ASP:OD2	1:J:19:LYS:NZ	2.42	0.53
3:I:176:ARG:HH11	3:I:185:TYR:HB3	1.74	0.53
1:D:45:TYR:CD1	1:D:88:LEU:HD22	2.44	0.53
2:H:62:PHE:CD1	2:H:65:ILE:HD12	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:LYS:HD2	2:E:34:GLU:N	2.23	0.52
2:H:68:HIS:CD2	2:H:69:VAL:HG23	2.45	0.52
1:D:45:TYR:CZ	1:D:50:LEU:HD12	2.45	0.52
1:D:99:LEU:HD12	1:D:100:PRO:HD2	1.91	0.52
1:G:41:GLU:HG2	1:G:80:ARG:HH21	1.74	0.51
2:K:16:MET:SD	2:K:32:LYS:HD3	2.50	0.51
1:G:101:ASP:OD2	1:G:101:ASP:N	2.44	0.51
1:J:27:LEU:HD12	1:J:30:ILE:HD12	1.92	0.51
1:G:23:THR:OG1	1:G:53:ASP:O	2.29	0.51
2:E:17:MET:HB2	2:E:33:ARG:HD2	1.94	0.50
1:D:92:PRO:O	2:E:27:HIS:NE2	2.46	0.49
1:D:46:LYS:NZ	1:D:61:GLY:HA3	2.28	0.49
1:A:69:PRO:HG2	2:B:82:ARG:HG2	1.95	0.49
3:I:170:VAL:HG23	3:I:175:TYR:CE1	2.48	0.48
1:D:89:CAS:C	1:D:90:ILE:HG13	2.44	0.48
1:G:70:GLN:HB3	2:H:79:TYR:HD2	1.78	0.48
1:A:31:VAL:HG13	1:A:35:LEU:HD12	1.96	0.48
2:B:33:ARG:O	2:B:37:LEU:HD13	2.14	0.47
1:G:23:THR:HG22	1:G:26:GLU:HG3	1.96	0.47
3:L:181:VAL:O	3:L:183:SER:N	2.48	0.47
2:E:103:LEU:HD21	3:F:158:LEU:HD11	1.95	0.47
1:G:23:THR:HA	1:G:56:THR:HA	1.97	0.47
3:I:70:GLU:OE1	3:I:113:ARG:HD3	2.14	0.47
2:K:101:LEU:HD21	3:L:178:LEU:HD22	1.95	0.47
1:D:26:GLU:O	1:D:30:ILE:HD12	2.15	0.47
2:H:36:ALA:HA	2:H:77:PHE:CE1	2.50	0.47
1:J:46:LYS:HD3	1:J:62:PHE:CZ	2.50	0.47
2:B:96:ALA:HB1	2:B:98:GLU:OE1	2.15	0.46
1:G:22:SER:HB2	1:G:26:GLU:OE2	2.14	0.46
1:D:88:LEU:HA	1:D:88:LEU:HD12	1.40	0.46
2:H:16:MET:SD	2:H:32:LYS:HG2	2.55	0.46
1:A:99:LEU:HD22	1:A:103:MET:HB3	1.97	0.46
1:D:46:LYS:HZ2	1:D:61:GLY:HA3	1.81	0.46
1:A:55:LYS:HD3	1:A:55:LYS:HA	1.55	0.46
2:K:72:LYS:NZ	2:K:94:PRO:O	2.49	0.46
1:J:94:SER:O	2:K:68:HIS:HB3	2.16	0.45
3:L:120:ARG:HD3	3:L:127:GLY:HA2	1.99	0.45
1:D:78:ALA:HB2	1:D:88:LEU:CD1	2.45	0.45
3:I:81:PRO:HD2	3:I:153:LEU:HG	1.99	0.45
1:D:94:SER:OG	2:E:68:HIS:ND1	2.12	0.45
3:I:133:THR:CG2	3:I:134:GLU:H	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:ARG:NH1	2:B:58:ASN:OD1	2.48	0.45
2:H:77:PHE:H	2:H:77:PHE:HD2	1.65	0.45
3:F:106:GLY:O	3:F:107:ARG:HG2	2.17	0.44
1:G:96:PRO:HA	2:H:68:HIS:HE1	1.81	0.44
1:D:69:PRO:HG2	2:E:82:ARG:HG2	2.00	0.44
3:I:142:VAL:O	3:I:145:GLN:HB2	2.17	0.44
1:G:40:ASP:OD1	1:G:41:GLU:HG3	2.16	0.44
2:H:106:ALA:O	2:H:110:LEU:HD12	2.17	0.44
2:B:45:MET:CE	2:B:60:VAL:HG11	2.48	0.44
1:J:40:ASP:OD2	1:J:41:GLU:HG3	2.18	0.44
2:E:32:LYS:HD3	2:E:33:ARG:N	2.33	0.43
3:F:115:HIS:HE1	4:F:301:A1I58:OAH	2.01	0.43
1:G:96:PRO:HA	2:H:68:HIS:CE1	2.53	0.43
2:E:101:LEU:O	2:E:105:MET:HG3	2.18	0.43
3:F:77:CAS:CE2	3:F:106:GLY:HA3	2.48	0.43
3:I:75:ILE:HD13	3:I:108:ARG:HG3	2.00	0.43
2:K:17:MET:HE2	2:K:33:ARG:HD3	2.00	0.43
3:F:148:PHE:CE1	2:H:45:MET:HA	2.54	0.43
1:D:80:ARG:HA	1:D:85:PHE:HD2	1.84	0.43
3:F:90:ASN:HD21	3:F:94:GLU:HB2	1.84	0.43
3:L:170:VAL:HG23	3:L:175:TYR:CE1	2.53	0.43
2:K:72:LYS:HG3	2:K:99:ILE:CD1	2.49	0.43
2:K:104:LEU:HG	3:L:184:LEU:HD13	1.99	0.43
3:I:181:VAL:HG12	3:I:183:SER:H	1.84	0.43
1:D:60:CYS:HA	1:J:65:GLN:OE1	2.20	0.42
2:E:103:LEU:HD12	2:E:103:LEU:HA	1.87	0.42
3:C:69:ARG:HB2	3:C:69:ARG:HH11	1.84	0.42
3:F:171:LYS:HD3	3:F:171:LYS:HA	1.85	0.42
2:H:103:LEU:HD11	3:I:158:LEU:HD21	2.02	0.42
2:E:33:ARG:O	2:E:37:LEU:HG	2.20	0.42
1:G:10:HIS:O	1:G:91:GLU:HB2	2.20	0.42
2:H:69:VAL:HG21	2:H:102:GLU:HB3	2.01	0.42
3:I:170:VAL:HG23	3:I:175:TYR:HE1	1.84	0.42
1:J:83:ASP:OD2	1:J:84:THR:HG23	2.20	0.42
1:G:23:THR:HG23	1:G:26:GLU:HG3	2.01	0.41
3:F:90:ASN:ND2	3:F:94:GLU:HB2	2.36	0.41
1:D:77:LEU:C	1:D:88:LEU:HD11	2.41	0.41
3:I:107:ARG:HD2	4:I:301:A1I58:NBH	2.36	0.41
1:D:65:GLN:OE1	1:J:60:CYS:HA	2.20	0.41
3:F:175:TYR:HD2	3:F:189:GLU:HG3	1.86	0.41
2:E:33:ARG:HE	2:E:33:ARG:HB2	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:MET:HG3	3:C:170:VAL:HG22	2.03	0.41
3:I:75:ILE:CD1	3:I:108:ARG:HG3	2.51	0.41
2:B:98:GLU:H	2:B:98:GLU:CD	2.25	0.40
1:J:80:ARG:HA	1:J:85:PHE:HA	2.04	0.40
2:H:64:GLU:H	2:H:64:GLU:CD	2.24	0.40
3:L:113:ARG:HD3	3:L:140:LEU:N	2.36	0.40
3:F:73:GLN:OE1	3:F:110:HIS:HD2	2.03	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	101/129 (78%)	97 (96%)	3 (3%)	1 (1%)	13 25
1	D	96/129 (74%)	92 (96%)	4 (4%)	0	100 100
1	G	100/129 (78%)	94 (94%)	6 (6%)	0	100 100
1	J	101/129 (78%)	98 (97%)	3 (3%)	0	100 100
2	B	85/97 (88%)	85 (100%)	0	0	100 100
2	E	83/97 (86%)	83 (100%)	0	0	100 100
2	H	82/97 (84%)	82 (100%)	0	0	100 100
2	K	84/97 (87%)	84 (100%)	0	0	100 100
3	C	142/203 (70%)	139 (98%)	3 (2%)	0	100 100
3	F	140/203 (69%)	136 (97%)	4 (3%)	0	100 100
3	I	144/203 (71%)	138 (96%)	6 (4%)	0	100 100
3	L	143/203 (70%)	135 (94%)	6 (4%)	2 (1%)	9 17
All	All	1301/1716 (76%)	1263 (97%)	35 (3%)	3 (0%)	44 64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
3	L	183	SER
3	L	182	ARG

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	88/115 (76%)	87 (99%)	1 (1%)	70 87
1	D	85/115 (74%)	82 (96%)	3 (4%)	31 57
1	G	88/115 (76%)	88 (100%)	0	100 100
1	J	90/115 (78%)	90 (100%)	0	100 100
2	B	77/86 (90%)	72 (94%)	5 (6%)	14 29
2	E	75/86 (87%)	73 (97%)	2 (3%)	40 67
2	H	75/86 (87%)	70 (93%)	5 (7%)	13 28
2	K	76/86 (88%)	75 (99%)	1 (1%)	65 85
3	C	124/176 (70%)	124 (100%)	0	100 100
3	F	129/176 (73%)	124 (96%)	5 (4%)	27 52
3	I	131/176 (74%)	128 (98%)	3 (2%)	45 72
3	L	128/176 (73%)	126 (98%)	2 (2%)	58 80
All	All	1166/1508 (77%)	1139 (98%)	27 (2%)	45 72

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
2	B	47	SER
2	B	71	SER
2	B	86	SER
2	B	101	LEU
2	B	112	CYS
1	D	36	LYS
1	D	52	ASP

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Mol	Chain	Res	Type
1	D	53	ASP
2	E	33	ARG
2	E	86	SER
3	F	96	GLN
3	F	116	LEU
3	F	147	ILE
3	F	148	PHE
3	F	182	ARG
2	H	61	ASN
2	H	68	HIS
2	H	77	PHE
2	H	80	LYS
2	H	108	ASN
3	I	107	ARG
3	I	148	PHE
3	I	197	ASP
2	K	108	ASN
3	L	64	ARG
3	L	203	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	85	ASN
3	C	141	ASN
3	C	191	HIS
3	F	110	HIS
3	F	132	GLN
3	F	174	ASN
2	H	68	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 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	$\#\|Z\| > 2$
1	CAS	J	89	1	5,8,9	1.29	0	1,9,11	1.28	0
3	CAS	C	77	3	5,8,9	0.88	0	1,9,11	1.66	0
1	CAS	D	89	1	5,8,9	1.17	0	1,9,11	1.78	0
1	CAS	A	89	1	5,8,9	1.11	0	1,9,11	1.54	0
1	CAS	G	89	1	5,8,9	1.29	0	1,9,11	1.12	0
3	CAS	I	77	3	5,8,9	1.03	0	1,9,11	0.37	0
3	CAS	L	77	3	5,8,9	1.10	0	1,9,11	0.29	0
3	CAS	F	77	3	5,8,9	1.33	0	1,9,11	1.94	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
1	CAS	J	89	1	-	0/0/7/9	-
3	CAS	C	77	3	-	0/0/7/9	-
1	CAS	D	89	1	-	0/0/7/9	-
1	CAS	A	89	1	-	0/0/7/9	-
1	CAS	G	89	1	-	0/0/7/9	-
3	CAS	I	77	3	-	0/0/7/9	-
3	CAS	L	77	3	-	0/0/7/9	-
3	CAS	F	77	3	-	0/0/7/9	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	89	CAS	1	0
3	F	77	CAS	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
4	A1I58	F	301	-	34,41,41	2.81	9 (26%)	42,61,61	2.52	13 (30%)
4	A1I58	C	301	-	34,41,41	3.15	13 (38%)	42,61,61	2.50	11 (26%)
4	A1I58	L	301	-	34,41,41	3.02	11 (32%)	42,61,61	2.61	14 (33%)
4	A1I58	I	301	-	34,41,41	3.06	14 (41%)	42,61,61	2.48	11 (26%)

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	A1I58	F	301	-	-	2/32/61/61	0/5/5/5
4	A1I58	C	301	-	-	3/32/61/61	0/5/5/5
4	A1I58	L	301	-	-	2/32/61/61	0/5/5/5
4	A1I58	I	301	-	-	0/32/61/61	0/5/5/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301	A1I58	CAK-CAI	13.91	1.67	1.47
4	L	301	A1I58	CAK-CAI	13.56	1.67	1.47
4	I	301	A1I58	CAK-CAI	13.18	1.66	1.47
4	F	301	A1I58	CAK-CAI	11.85	1.65	1.47
4	L	301	A1I58	CAG-N	5.74	1.44	1.34
4	C	301	A1I58	CAG-N	5.56	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	301	A1I58	CAG-N	5.09	1.43	1.34
4	F	301	A1I58	CAG-N	4.74	1.43	1.34
4	F	301	A1I58	CAS-CAR	4.49	1.59	1.52
4	I	301	A1I58	CAU-NAW	4.08	1.43	1.34
4	C	301	A1I58	CAU-NAW	3.93	1.42	1.34
4	F	301	A1I58	C-NAO	3.67	1.43	1.34
4	C	301	A1I58	CAC-N	3.57	1.53	1.47
4	F	301	A1I58	CAU-NAW	3.54	1.41	1.34
4	L	301	A1I58	CAU-NAW	3.35	1.41	1.34
4	I	301	A1I58	CA-N	3.34	1.51	1.47
4	I	301	A1I58	CAJ-CAI	3.30	1.52	1.47
4	F	301	A1I58	CAJ-CAI	3.28	1.52	1.47
4	L	301	A1I58	CAC-N	3.27	1.52	1.47
4	L	301	A1I58	CA-N	3.16	1.50	1.47
4	C	301	A1I58	C-NAO	3.02	1.41	1.34
4	C	301	A1I58	CAS-CAR	2.95	1.56	1.52
4	L	301	A1I58	C-NAO	2.93	1.41	1.34
4	I	301	A1I58	CAS-CAR	2.92	1.56	1.52
4	C	301	A1I58	CBK-CBG	2.76	1.55	1.50
4	C	301	A1I58	CAJ-CAI	2.73	1.51	1.47
4	F	301	A1I58	CAS-NAO	2.68	1.51	1.47
4	I	301	A1I58	C-NAO	2.65	1.40	1.34
4	L	301	A1I58	CAS-CAR	2.61	1.56	1.52
4	I	301	A1I58	CBA-CAY	2.53	1.43	1.39
4	I	301	A1I58	CAY-CAX	2.51	1.58	1.52
4	L	301	A1I58	CAJ-CAI	2.44	1.51	1.47
4	F	301	A1I58	CBA-CAY	2.43	1.43	1.39
4	C	301	A1I58	CBA-CAY	2.40	1.42	1.39
4	I	301	A1I58	CAS-NAO	2.36	1.51	1.47
4	I	301	A1I58	CAC-N	2.35	1.51	1.47
4	I	301	A1I58	CAP-CAU	2.34	1.58	1.52
4	L	301	A1I58	CBK-CBG	2.25	1.54	1.50
4	L	301	A1I58	CBB-CBA	2.24	1.42	1.38
4	L	301	A1I58	CBA-CAY	2.20	1.42	1.39
4	C	301	A1I58	CA-N	2.19	1.49	1.47
4	C	301	A1I58	CBE-CBD	2.19	1.42	1.38
4	I	301	A1I58	CAZ-CAX	2.16	1.57	1.52
4	C	301	A1I58	CAS-NAO	2.15	1.50	1.47
4	C	301	A1I58	CBB-CBA	2.14	1.42	1.38
4	I	301	A1I58	CBC-CBF	2.13	1.50	1.48
4	F	301	A1I58	CBK-CBG	2.05	1.53	1.50

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	301	A1I58	CAK-CAJ-CAI	8.61	67.90	60.48
4	L	301	A1I58	CAK-CAJ-CAI	8.42	67.74	60.48
4	I	301	A1I58	CAK-CAJ-CAI	7.58	67.02	60.48
4	F	301	A1I58	CA-C-NAO	7.10	135.21	117.72
4	F	301	A1I58	CAK-CAJ-CAI	7.02	66.53	60.48
4	L	301	A1I58	CA-C-NAO	6.13	132.81	117.72
4	I	301	A1I58	CA-C-NAO	5.70	131.76	117.72
4	F	301	A1I58	CAI-CAG-N	5.62	129.51	121.00
4	C	301	A1I58	CA-C-NAO	5.32	130.81	117.72
4	I	301	A1I58	O-C-NAO	-5.31	111.92	121.38
4	L	301	A1I58	O-C-NAO	-5.08	112.33	121.38
4	F	301	A1I58	O-C-NAO	-5.00	112.47	121.38
4	C	301	A1I58	CAB-CAC-N	4.89	118.33	110.67
4	C	301	A1I58	CAI-CAG-N	4.66	128.06	121.00
4	I	301	A1I58	CAA-CB-CA	4.64	119.89	111.23
4	L	301	A1I58	CAI-CAG-N	4.63	128.02	121.00
4	I	301	A1I58	CAI-CAG-N	4.54	127.88	121.00
4	C	301	A1I58	O-C-NAO	-4.37	113.59	121.38
4	L	301	A1I58	CAJ-CAK-CAI	-4.24	56.82	60.48
4	C	301	A1I58	CAJ-CAK-CAI	-4.14	56.90	60.48
4	C	301	A1I58	CAJ-CAI-CAK	-4.13	55.19	59.51
4	L	301	A1I58	CB-CA-N	3.96	116.03	110.53
4	F	301	A1I58	CAJ-CAI-CAK	-3.92	55.41	59.51
4	L	301	A1I58	CAJ-CAI-CAK	-3.89	55.44	59.51
4	I	301	A1I58	CB-CA-N	3.82	115.84	110.53
4	F	301	A1I58	O-C-CA	-3.79	112.31	120.22
4	I	301	A1I58	CAJ-CAI-CAK	-3.72	55.62	59.51
4	F	301	A1I58	CAQ-CAP-NAO	3.64	107.91	103.10
4	I	301	A1I58	CAJ-CAK-CAI	-3.61	57.37	60.48
4	L	301	A1I58	CAB-CAC-N	3.51	116.16	110.67
4	L	301	A1I58	CAA-CB-CA	3.38	117.52	111.23
4	F	301	A1I58	CAJ-CAK-CAI	-2.80	58.06	60.48
4	I	301	A1I58	CAQ-CAP-NAO	2.77	106.75	103.10
4	F	301	A1I58	CB-CA-N	2.69	114.27	110.53
4	L	301	A1I58	O-C-CA	-2.57	114.85	120.22
4	C	301	A1I58	CAP-CAU-NAW	2.55	122.27	116.58
4	F	301	A1I58	CAA-CB-CA	2.55	115.98	111.23
4	C	301	A1I58	CAQ-CAR-CAS	-2.50	100.22	103.31
4	F	301	A1I58	CAZ-CAX-CAY	-2.45	106.65	112.25
4	L	301	A1I58	CAQ-CAP-CAU	-2.39	106.55	111.32
4	L	301	A1I58	CAQ-CAP-NAO	2.34	106.19	103.10
4	L	301	A1I58	CAP-CAU-NAW	2.30	121.71	116.58
4	F	301	A1I58	CAP-CAU-NAW	2.27	121.64	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	301	A1I58	C-CA-N	-2.24	105.69	111.31
4	C	301	A1I58	O-C-CA	-2.21	115.60	120.22
4	I	301	A1I58	CBE-CAY-CBA	-2.21	115.54	118.29
4	C	301	A1I58	CB-CA-N	2.18	113.56	110.53
4	I	301	A1I58	CAX-NAW-CAU	2.10	125.89	122.93
4	L	301	A1I58	CBE-CAY-CBA	-2.05	115.73	118.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301	A1I58	N-CAG-CAI-CAJ
4	C	301	A1I58	N-CAG-CAI-CAK
4	C	301	A1I58	OAH-CAG-CAI-CAJ
4	L	301	A1I58	N-CAG-CAI-CAJ
4	F	301	A1I58	O-C-CA-N
4	L	301	A1I58	OAH-CAG-CAI-CAJ
4	F	301	A1I58	NAO-C-CA-N

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	301	A1I58	2	0
4	C	301	A1I58	1	0
4	L	301	A1I58	1	0
4	I	301	A1I58	2	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 then 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.

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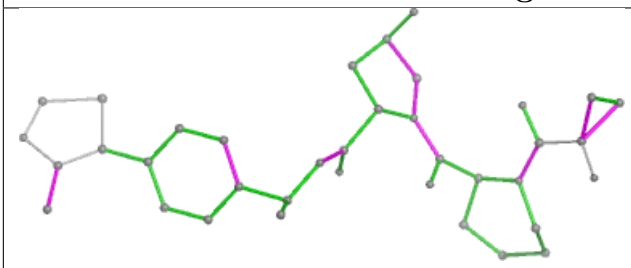
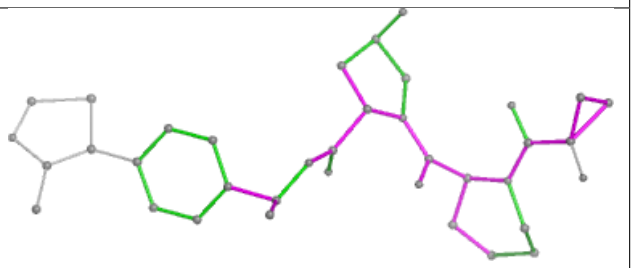
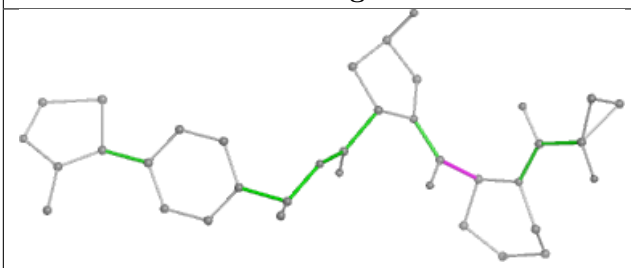


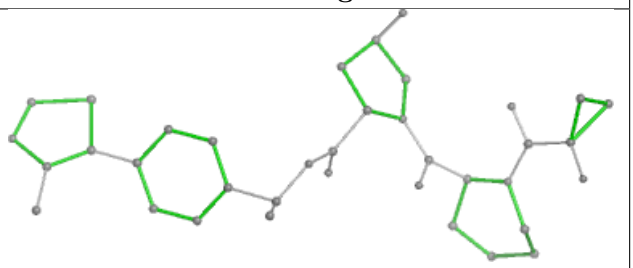
Bond lengths



Bond angles

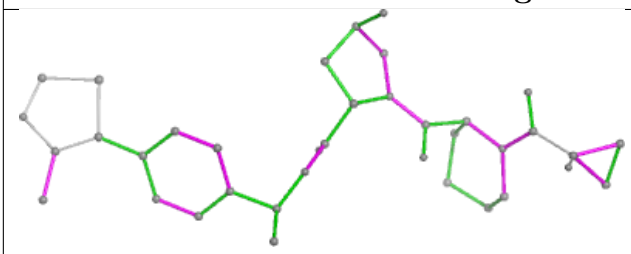


Torsions

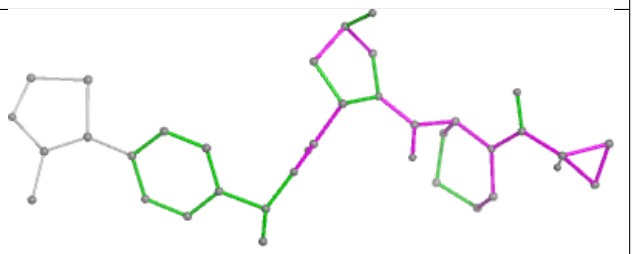


Rings

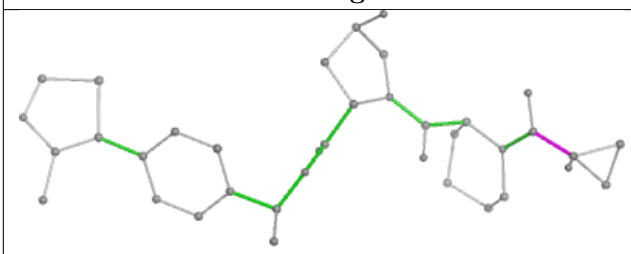
Ligand A1I58 C 301



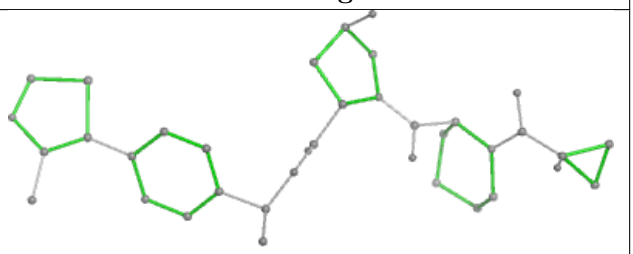
Bond lengths



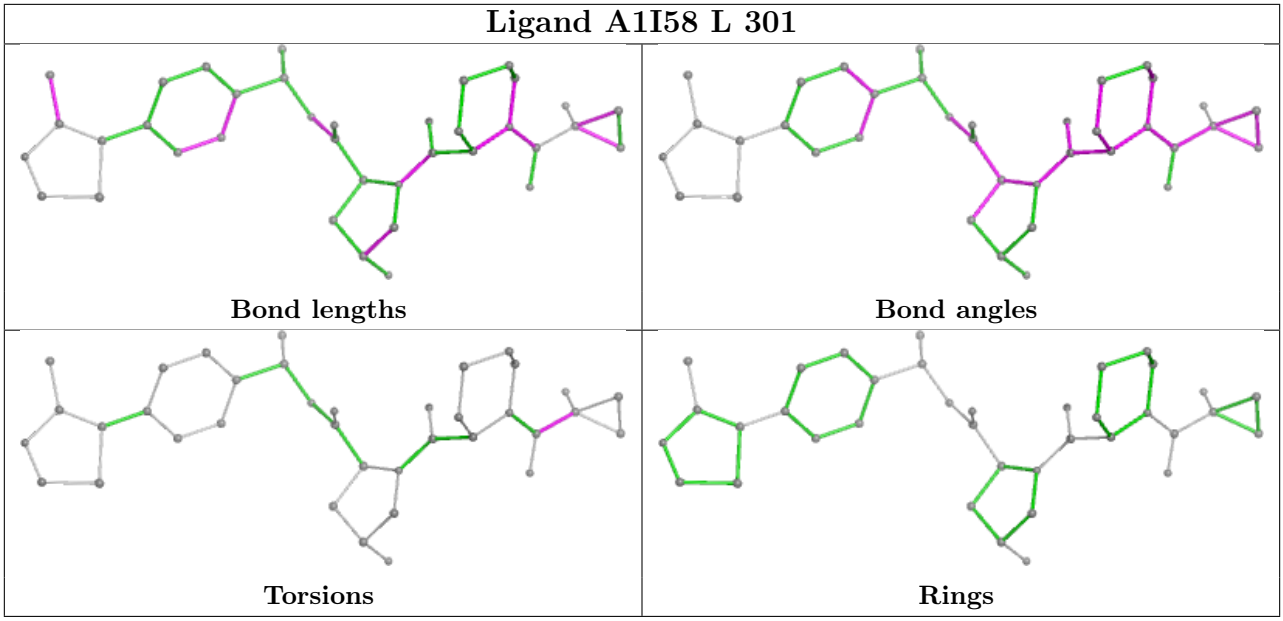
Bond angles

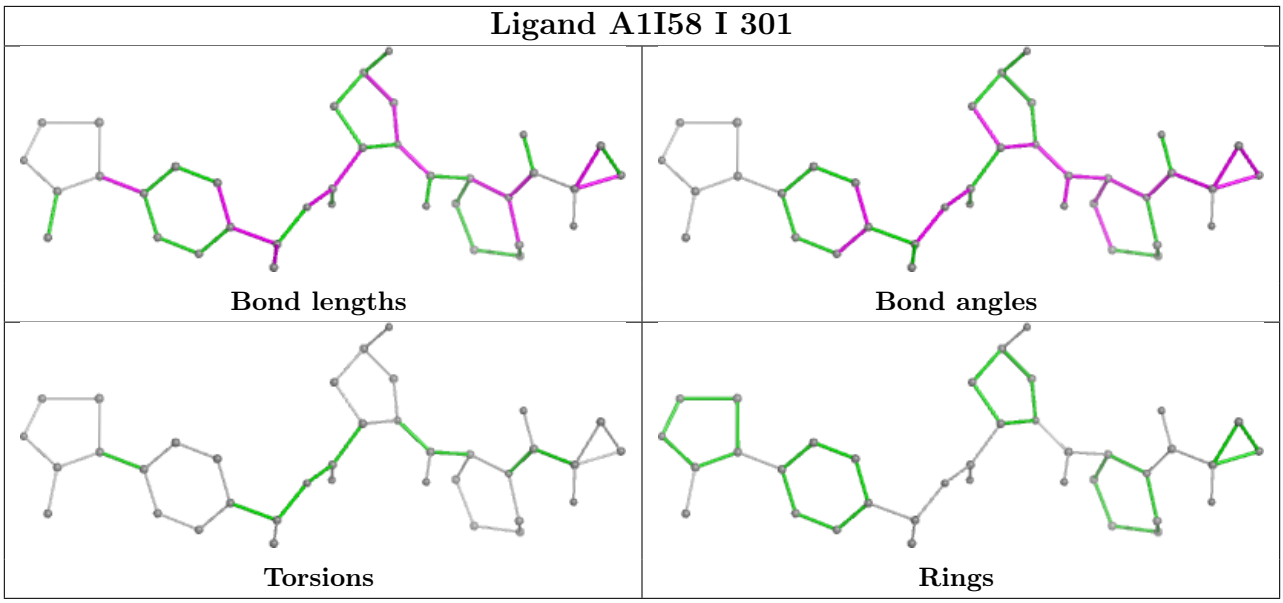


Torsions



Rings





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, 95^{th} 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	103/129 (79%)	0.20	4 (3%)	44	40	44, 61, 98, 111	0
1	D	100/129 (77%)	0.84	9 (9%)	17	15	58, 84, 106, 117	0
1	G	102/129 (79%)	0.58	4 (3%)	44	40	57, 76, 96, 107	0
1	J	103/129 (79%)	0.11	5 (4%)	36	33	46, 60, 95, 125	0
2	B	89/97 (91%)	0.33	3 (3%)	48	45	49, 63, 91, 101	0
2	E	87/97 (89%)	0.55	3 (3%)	48	45	56, 75, 95, 100	0
2	H	86/97 (88%)	1.21	14 (16%)	5	5	59, 82, 101, 115	0
2	K	88/97 (90%)	0.44	3 (3%)	48	45	48, 63, 88, 110	0
3	C	144/203 (70%)	0.72	9 (6%)	27	25	50, 68, 101, 114	0
3	F	142/203 (69%)	0.51	7 (4%)	36	33	51, 70, 98, 108	0
3	I	146/203 (71%)	0.75	9 (6%)	28	26	51, 69, 105, 115	0
3	L	145/203 (71%)	0.50	8 (5%)	32	29	43, 60, 96, 111	0
All	All	1335/1716 (77%)	0.56	78 (5%)	30	28	43, 69, 101, 125	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	207	ALA	5.6
3	L	207	ALA	4.7
3	C	205	ARG	4.4
1	D	83	ASP	4.1
2	H	107	ALA	4.1
2	K	112	CYS	3.7
3	I	206	ILE	3.6
3	F	185	TYR	3.6
2	K	109	PHE	3.4
2	H	99	ILE	3.4
2	H	46	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
3	L	62	VAL	3.4
3	L	182	ARG	3.3
3	L	185	TYR	3.2
1	A	83	ASP	3.2
3	F	62	VAL	3.1
2	H	57	THR	3.1
3	F	106	GLY	3.1
3	I	184	LEU	3.1
3	I	62	VAL	3.0
3	I	181	VAL	3.0
3	C	106	GLY	2.9
3	I	205	ARG	2.9
3	L	143	ASP	2.9
2	H	110	LEU	2.9
3	L	206	ILE	2.9
3	C	204	GLU	2.9
3	F	109	ILE	2.8
2	K	47	SER	2.8
2	H	104	LEU	2.8
3	C	179	ASP	2.7
1	A	102	VAL	2.7
1	D	103	MET	2.7
2	H	108	ASN	2.7
3	C	152	THR	2.7
2	H	77	PHE	2.7
2	B	16	MET	2.6
2	E	62	PHE	2.6
3	F	148	PHE	2.5
1	D	102	VAL	2.5
1	D	65	GLN	2.5
2	H	105	MET	2.5
3	I	178	LEU	2.5
1	D	85	PHE	2.5
3	F	204	GLU	2.4
1	A	82	ASP	2.4
2	E	47	SER	2.4
1	G	57	LEU	2.4
2	H	103	LEU	2.4
2	B	48	GLY	2.4
1	D	12	THR	2.3
1	D	80	ARG	2.3
1	G	83	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	48	ASP	2.3
2	B	112	CYS	2.3
1	J	102	VAL	2.3
2	H	36	ALA	2.3
2	H	100	ALA	2.3
3	I	144	GLY	2.2
2	H	111	ASP	2.2
3	C	195	GLN	2.2
1	A	52	ASP	2.2
3	C	203	GLN	2.2
1	J	99	LEU	2.2
2	H	62	PHE	2.2
3	L	183	SER	2.2
1	J	101	ASP	2.2
3	C	142	VAL	2.2
1	D	52	ASP	2.1
1	G	103	MET	2.1
1	D	93	PHE	2.1
1	J	60	CYS	2.1
3	L	180	ILE	2.1
2	E	46	LEU	2.1
3	I	142	VAL	2.1
3	C	143	ASP	2.1
3	F	181	VAL	2.0
1	G	97	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, 95^{th} 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	CAS	D	89	9/10	0.71	0.16	94,97,124,152	0
1	CAS	A	89	9/10	0.86	0.13	66,69,99,132	0
1	CAS	G	89	9/10	0.87	0.12	61,74,97,130	0
3	CAS	F	77	9/10	0.89	0.13	61,71,94,110	0
1	CAS	J	89	9/10	0.91	0.11	49,63,86,118	0
3	CAS	C	77	9/10	0.92	0.14	62,68,92,101	0
3	CAS	I	77	9/10	0.95	0.09	48,60,75,96	0
3	CAS	L	77	9/10	0.97	0.11	49,54,64,79	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

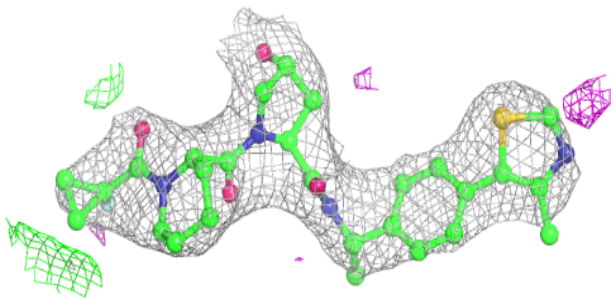
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

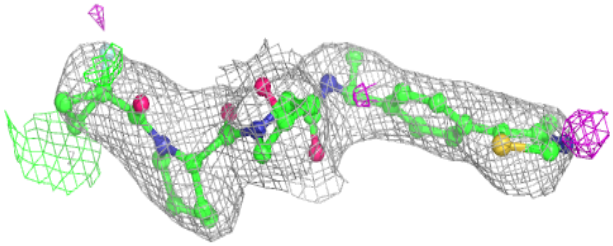
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	A1I58	C	301	37/37	0.89	0.12	50,61,74,85	0
4	A1I58	F	301	37/37	0.90	0.11	50,68,81,86	0
4	A1I58	I	301	37/37	0.90	0.11	54,66,82,86	0
4	A1I58	L	301	37/37	0.93	0.12	49,59,76,78	0

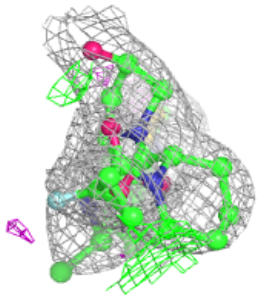
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1I58 C 301:

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

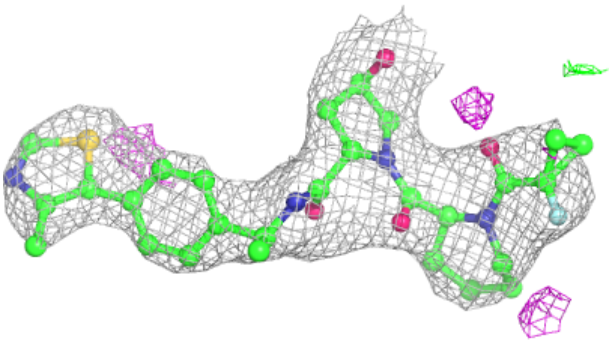


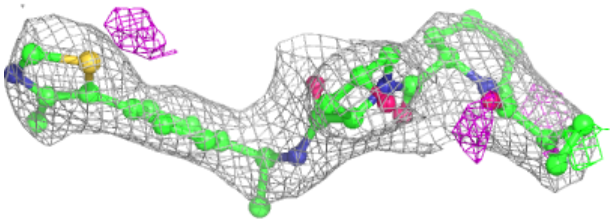


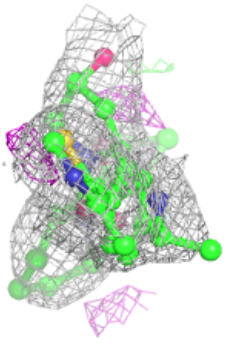


Electron density around A1I58 F 301:

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

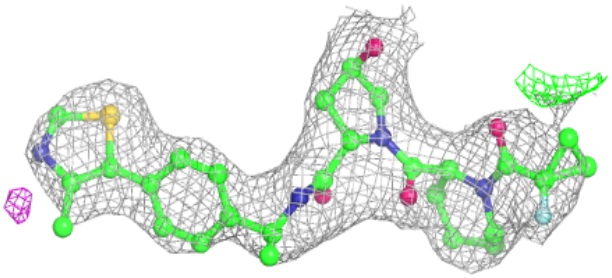


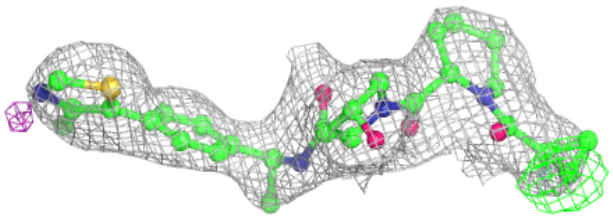


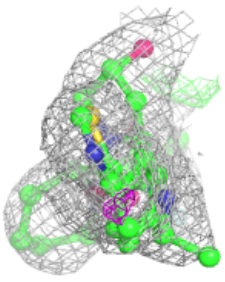


Electron density around A1I58 I 301:

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

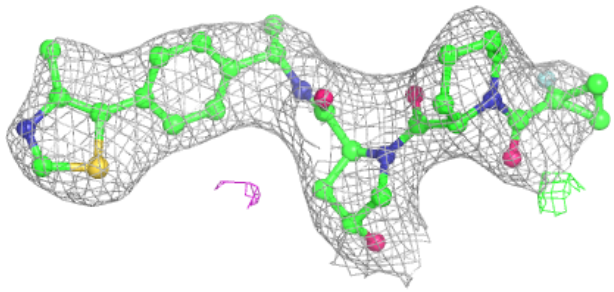


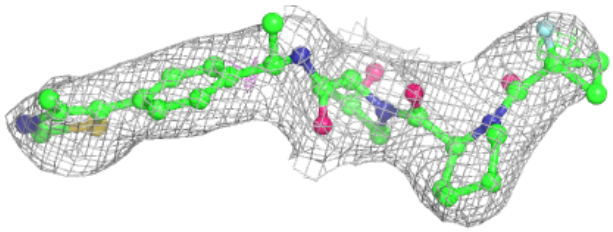


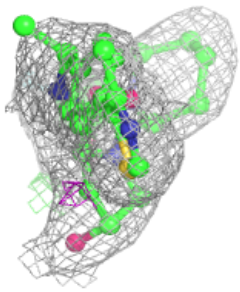


Electron density around A1I58 L 301:

$2mF_o$-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.