



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2016 – 06:39 PM EDT

PDB ID : 5FQD
Title : Structural basis of Lenalidomide induced CK1a degradation by the crl4crbn ubiquitin ligase
Authors : Petzold, G.; Fischer, E.S.; Thoma, N.H.
Deposited on : 2015-12-09
Resolution : 2.45 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

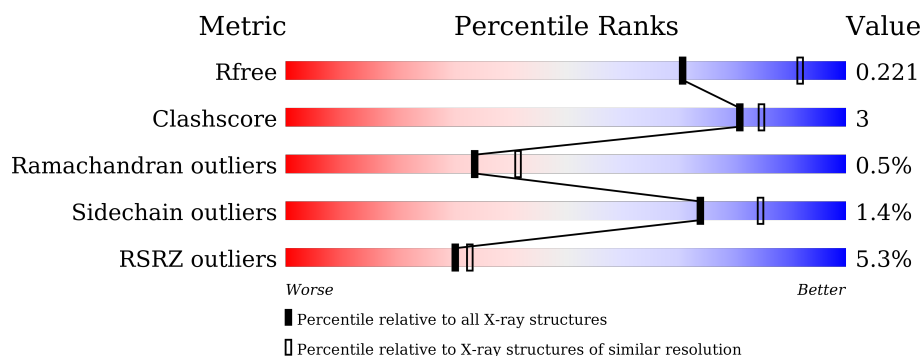
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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. 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	856	<div> <div>7%</div> <div>83% 9% 8%</div> </div>
1	D	856	<div> <div>2%</div> <div>82% 10% 8%</div> </div>
2	B	426	<div> <div>3%</div> <div>79% 9% 11%</div> </div>
2	E	426	<div> <div>14%</div> <div>77% 8% 14%</div> </div>
3	C	341	<div> <div>3%</div> <div>79% 7% 14%</div> </div>
3	F	341	<div> <div></div> <div>81% 5% 14%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23544 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA DAMAGE-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	789	Total	C	N	O	S	0	0	0
			6128	3892	1024	1178	34			
1	D	790	Total	C	N	O	S	0	0	0
			6196	3935	1042	1184	35			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q16531
A	-18	HIS	-	EXPRESSION TAG	UNP Q16531
A	-17	HIS	-	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	VAL	-	EXPRESSION TAG	UNP Q16531
A	-11	ASP	-	EXPRESSION TAG	UNP Q16531
A	-10	GLU	-	EXPRESSION TAG	UNP Q16531
A	-9	GLU	-	EXPRESSION TAG	UNP Q16531
A	-8	ASN	-	EXPRESSION TAG	UNP Q16531
A	-7	LEU	-	EXPRESSION TAG	UNP Q16531
A	-6	TYR	-	EXPRESSION TAG	UNP Q16531
A	-5	PHE	-	EXPRESSION TAG	UNP Q16531
A	-4	GLN	-	EXPRESSION TAG	UNP Q16531
A	-3	GLY	-	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
A	396	GLY	-	LINKER	UNP Q16531
A	397	ASN	-	LINKER	UNP Q16531
A	398	GLY	-	LINKER	UNP Q16531
A	399	ASN	-	LINKER	UNP Q16531
A	400	SER	-	LINKER	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	401	GLY	-	LINKER	UNP Q16531
D	-19	MET	-	EXPRESSION TAG	UNP Q16531
D	-18	HIS	-	EXPRESSION TAG	UNP Q16531
D	-17	HIS	-	EXPRESSION TAG	UNP Q16531
D	-16	HIS	-	EXPRESSION TAG	UNP Q16531
D	-15	HIS	-	EXPRESSION TAG	UNP Q16531
D	-14	HIS	-	EXPRESSION TAG	UNP Q16531
D	-13	HIS	-	EXPRESSION TAG	UNP Q16531
D	-12	VAL	-	EXPRESSION TAG	UNP Q16531
D	-11	ASP	-	EXPRESSION TAG	UNP Q16531
D	-10	GLU	-	EXPRESSION TAG	UNP Q16531
D	-9	GLU	-	EXPRESSION TAG	UNP Q16531
D	-8	ASN	-	EXPRESSION TAG	UNP Q16531
D	-7	LEU	-	EXPRESSION TAG	UNP Q16531
D	-6	TYR	-	EXPRESSION TAG	UNP Q16531
D	-5	PHE	-	EXPRESSION TAG	UNP Q16531
D	-4	GLN	-	EXPRESSION TAG	UNP Q16531
D	-3	GLY	-	EXPRESSION TAG	UNP Q16531
D	-2	GLY	-	EXPRESSION TAG	UNP Q16531
D	-1	GLY	-	EXPRESSION TAG	UNP Q16531
D	0	ARG	-	EXPRESSION TAG	UNP Q16531
D	396	GLY	-	LINKER	UNP Q16531
D	397	ASN	-	LINKER	UNP Q16531
D	398	GLY	-	LINKER	UNP Q16531
D	399	ASN	-	LINKER	UNP Q16531
D	400	SER	-	LINKER	UNP Q16531
D	401	GLY	-	LINKER	UNP Q16531

- Molecule 2 is a protein called PROTEIN CEREBLON.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	381	Total	C	N	O	S	0	0	0
			3068	1954	521	569	24			
2	E	367	Total	C	N	O	S	0	0	0
			2949	1881	499	545	24			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	-	EXPRESSION TAG	UNP Q96SW2
B	18	ASP	-	EXPRESSION TAG	UNP Q96SW2
B	19	TRP	-	EXPRESSION TAG	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	36	GLN	-	EXPRESSION TAG	UNP Q96SW2
B	37	GLY	-	EXPRESSION TAG	UNP Q96SW2
B	38	GLY	-	EXPRESSION TAG	UNP Q96SW2
B	39	GLY	-	EXPRESSION TAG	UNP Q96SW2
B	40	ARG	-	EXPRESSION TAG	UNP Q96SW2
E	17	MET	-	EXPRESSION TAG	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	36	GLN	-	EXPRESSION TAG	UNP Q96SW2
E	37	GLY	-	EXPRESSION TAG	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	38	GLY	-	EXPRESSION TAG	UNP Q96SW2
E	39	GLY	-	EXPRESSION TAG	UNP Q96SW2
E	40	ARG	-	EXPRESSION TAG	UNP Q96SW2

- Molecule 3 is a protein called CASEIN KINASE I ISOFORM ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	294	Total	C	N	O	S	0	0	0
			2423	1561	423	424	15			
3	F	294	Total	C	N	O	S	0	0	0
			2435	1568	424	428	15			

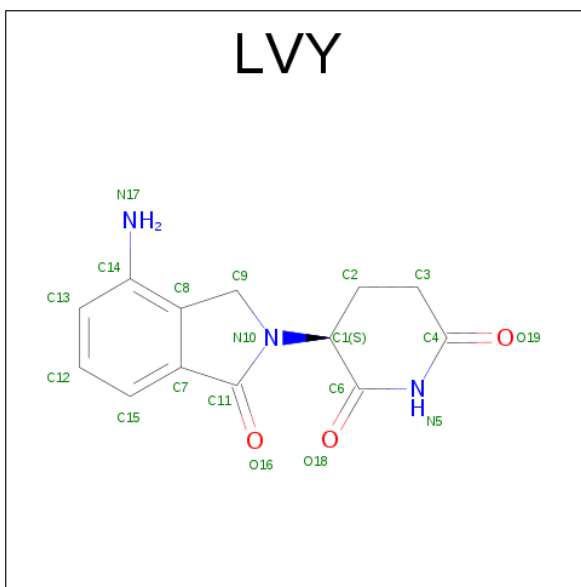
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	EXPRESSION TAG	UNP P48729
C	-2	GLY	-	EXPRESSION TAG	UNP P48729
C	-1	GLY	-	EXPRESSION TAG	UNP P48729
C	0	ARG	-	EXPRESSION TAG	UNP P48729
F	-3	GLY	-	EXPRESSION TAG	UNP P48729
F	-2	GLY	-	EXPRESSION TAG	UNP P48729
F	-1	GLY	-	EXPRESSION TAG	UNP P48729
F	0	ARG	-	EXPRESSION TAG	UNP P48729

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is S-LENALIDOMIDE (three-letter code: LVY) (formula: C₁₃H₁₃N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			19	13	3	3		
5	E	1	Total	C	N	O	0	0
			19	13	3	3		

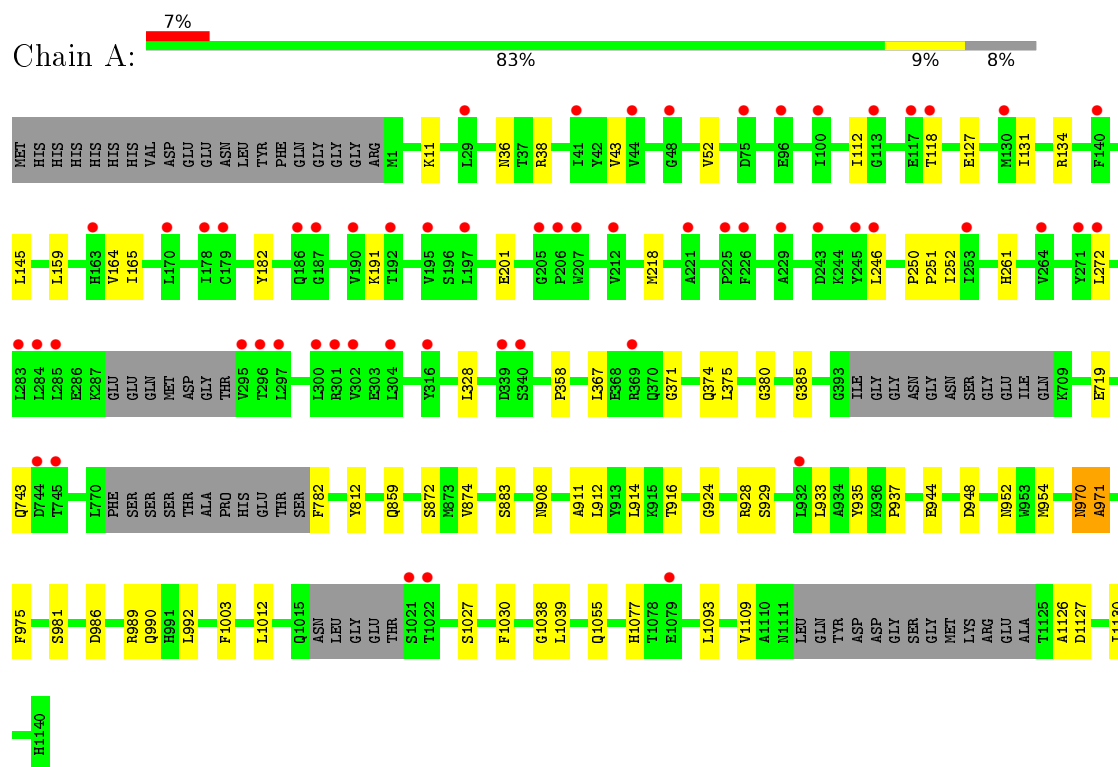
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total	O	0	0
			54	54		
6	B	52	Total	O	0	0
			52	52		
6	C	48	Total	O	0	0
			48	48		
6	D	93	Total	O	0	0
			93	93		
6	E	10	Total	O	0	0
			10	10		
6	F	48	Total	O	0	0
			48	48		

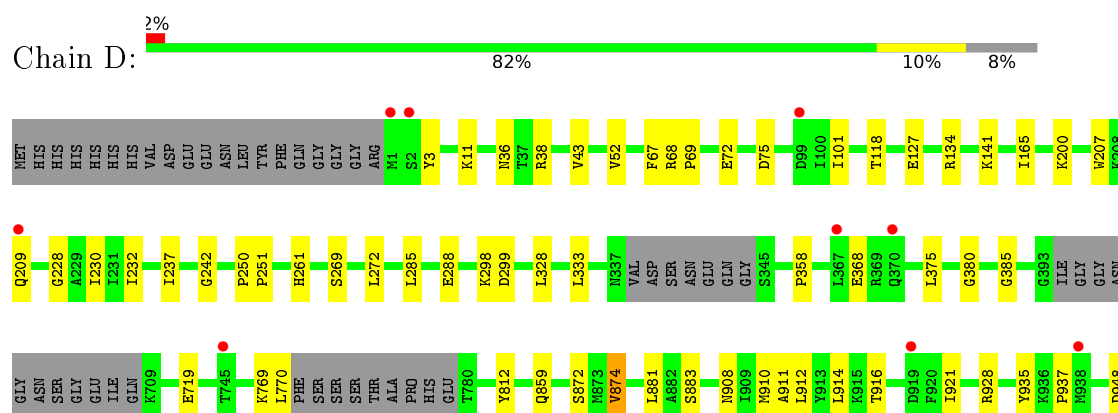
3 Residue-property plots [i](#)

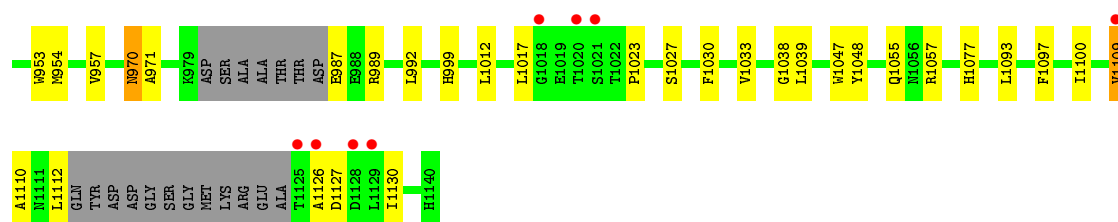
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

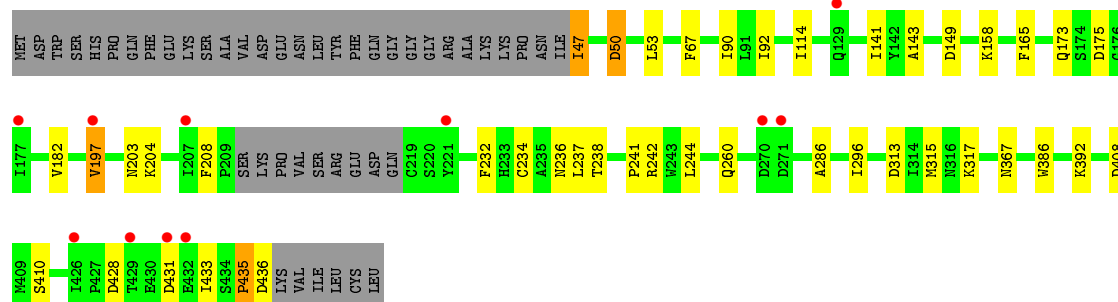
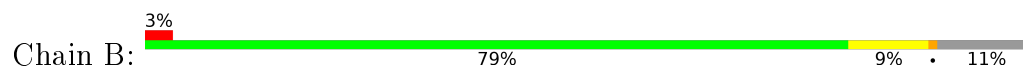


• Molecule 1: DNA DAMAGE-BINDING PROTEIN 1

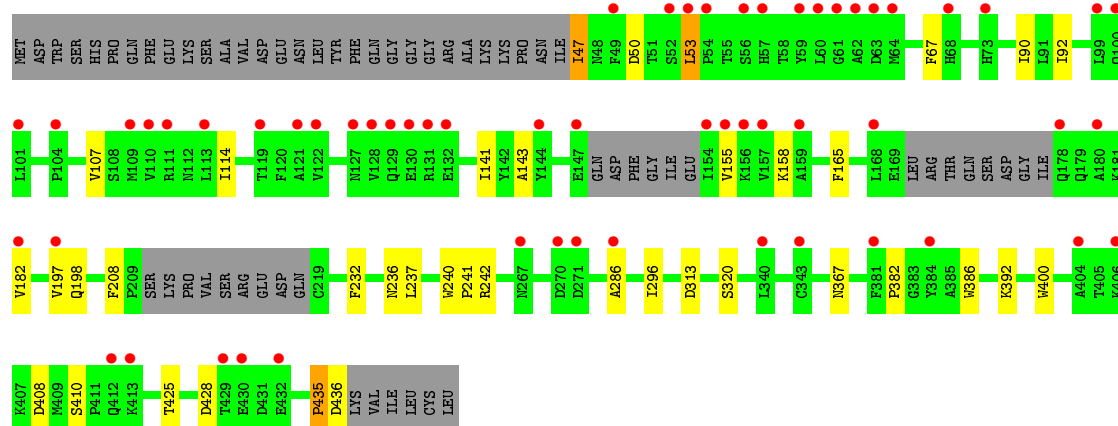
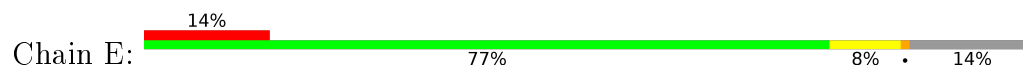




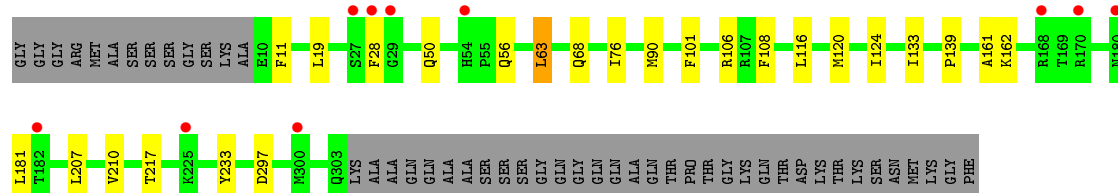
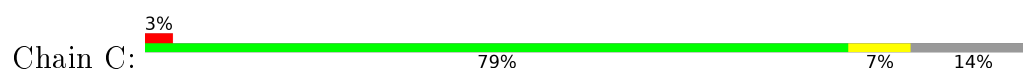
• Molecule 2: PROTEIN CEREBLON



• Molecule 2: PROTEIN CEREBLON



• Molecule 3: CASEIN KINASE I ISOFORM ALPHA



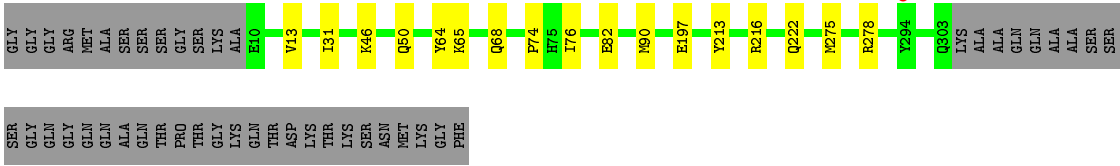
• Molecule 3: CASEIN KINASE I ISOFORM ALPHA

Chain F:

81%

5%

14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.97Å 109.93Å 112.40Å 106.02° 93.19° 101.63°	Depositor
Resolution (Å)	65.30 – 2.45 65.30 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.3 (65.30-2.45) 87.6 (65.30-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.181 , 0.210 0.193 , 0.221	Depositor DCC
R_{free} test set	6991 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 140746 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23544	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, LVY

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	0.47	0/6237	0.72	1/8449 (0.0%)
1	D	0.51	0/6305	0.73	1/8526 (0.0%)
2	B	0.52	0/3141	0.69	1/4264 (0.0%)
2	E	0.48	0/3018	0.68	1/4097 (0.0%)
3	C	0.55	0/2480	0.74	1/3336 (0.0%)
3	F	0.56	0/2492	0.73	1/3350 (0.0%)
All	All	0.51	0/23673	0.72	6/32022 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	970	ASN	C-N-CA	7.53	140.51	121.70
1	A	970	ASN	C-N-CA	6.06	136.84	121.70
2	B	435	PRO	C-N-CA	5.83	136.28	121.70
3	F	50	GLN	N-CA-C	-5.62	95.82	111.00
2	E	435	PRO	C-N-CA	5.56	135.59	121.70
3	C	50	GLN	N-CA-C	-5.54	96.05	111.00

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	6128	0	6031	43	0
1	D	6196	0	6168	50	0
2	B	3068	0	3036	27	0
2	E	2949	0	2915	22	0
3	C	2423	0	2420	15	0
3	F	2435	0	2442	8	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	B	19	0	13	1	0
5	E	19	0	13	3	0
6	A	54	0	0	0	0
6	B	52	0	0	2	0
6	C	48	0	0	2	0
6	D	93	0	0	0	0
6	E	10	0	0	0	0
6	F	48	0	0	1	0
All	All	23544	0	23038	152	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 (152) 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:874:VAL:HG11	1:A:916:THR:HG22	1.38	1.02
2:E:313:ASP:OD2	2:E:435:PRO:HD2	1.72	0.88
3:C:11:PHE:HD2	3:C:19:LEU:HD22	1.39	0.87
2:B:313:ASP:OD2	2:B:435:PRO:HD2	1.74	0.86
1:D:971:ALA:HB3	1:D:1077:HIS:O	1.79	0.82
1:A:874:VAL:HG11	1:A:916:THR:CG2	2.14	0.76
3:C:106:ARG:HB2	6:C:2012:HOH:O	1.87	0.74
1:A:201:GLU:HG3	1:D:200:LYS:HE2	1.69	0.74
1:A:118:THR:HG21	1:A:165:ILE:O	1.90	0.72
1:D:118:THR:HG21	1:D:165:ILE:O	1.90	0.71
2:B:173:GLN:HB2	6:B:2020:HOH:O	1.90	0.69
1:A:954:MET:HE3	1:A:975:PHE:HZ	1.58	0.67
1:A:971:ALA:HB3	1:A:1077:HIS:O	1.95	0.66
1:D:11:LYS:HD3	1:D:38:ARG:HD2	1.77	0.66
2:B:53:LEU:HD23	6:B:2003:HOH:O	1.97	0.65
1:D:69:PRO:HD2	1:D:72:GLU:HG3	1.80	0.64
3:C:116:LEU:HB3	3:C:120:MET:HE2	1.79	0.63
1:D:954:MET:HE2	1:D:957:VAL:HB	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:LEU:HD21	3:C:161:ALA:HB3	1.82	0.62
2:E:47:ILE:N	2:E:410:SER:HG	1.98	0.61
1:A:812:TYR:CZ	2:B:241:PRO:HB3	2.35	0.61
3:C:124:ILE:HD12	3:C:207:LEU:HD22	1.81	0.60
2:E:165:PHE:HB2	2:E:182:VAL:HG13	1.83	0.59
2:B:197:VAL:HG11	2:B:238:THR:CG2	2.33	0.59
1:D:812:TYR:CZ	2:E:241:PRO:HB3	2.37	0.59
2:B:165:PHE:HB2	2:B:182:VAL:HG13	1.84	0.59
1:A:1109:VAL:HG11	1:A:1126:ALA:HA	1.85	0.58
2:B:317:LYS:NZ	2:B:433:ILE:HG23	2.17	0.58
1:D:1027:SER:OG	1:D:1039:LEU:HD11	2.04	0.57
1:A:908:ASN:O	2:B:435:PRO:HA	2.05	0.57
1:D:1109:VAL:HG11	1:D:1126:ALA:HA	1.87	0.56
1:D:43:VAL:HG23	1:D:52:VAL:HG21	1.88	0.56
1:A:367:LEU:HB2	1:A:374:GLN:HE21	1.71	0.56
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.88	0.55
1:A:1027:SER:OG	1:A:1039:LEU:HD11	2.06	0.55
2:B:47:ILE:N	2:B:410:SER:HG	2.03	0.55
1:D:948:ASP:HB2	1:D:992:LEU:HB2	1.88	0.55
1:A:948:ASP:HB2	1:A:992:LEU:HB2	1.88	0.55
3:F:90:MET:HE2	6:F:2011:HOH:O	2.06	0.55
1:D:328:LEU:HD21	2:E:237:LEU:HD21	1.89	0.55
1:A:118:THR:O	2:B:203:ASN:HB3	2.07	0.54
2:B:367:ASN:HA	2:B:392:LYS:HD2	1.90	0.54
2:E:367:ASN:HA	2:E:392:LYS:HD2	1.91	0.53
1:D:207:TRP:CH2	1:D:228:GLY:HA2	2.44	0.53
1:A:954:MET:HE3	1:A:975:PHE:CZ	2.43	0.52
1:D:908:ASN:O	2:E:435:PRO:HA	2.10	0.52
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.92	0.52
1:D:874:VAL:HG23	1:D:881:LEU:HB3	1.92	0.51
1:D:916:THR:HG22	1:D:921:ILE:HG13	1.91	0.51
3:C:181:LEU:HD23	3:C:233:TYR:CE2	2.44	0.51
1:D:954:MET:CE	1:D:957:VAL:HB	2.40	0.51
1:A:118:THR:HB	1:A:134:ARG:HH22	1.75	0.51
3:F:213:TYR:O	3:F:216:ARG:O	2.29	0.51
3:F:76:ILE:HD13	3:F:90:MET:HB3	1.92	0.50
3:C:76:ILE:HD13	3:C:90:MET:HB3	1.93	0.50
2:B:50:ASP:HB3	2:B:53:LEU:HD12	1.93	0.50
1:A:986:ASP:HA	1:A:989:ARG:HG2	1.94	0.50
2:E:320:SER:HB3	2:E:425:THR:HB	1.94	0.50
1:D:1127:ASP:HA	1:D:1130:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:THR:HB	1:D:134:ARG:HH22	1.76	0.49
2:E:90:ILE:HD13	2:E:296:ILE:HG13	1.93	0.49
1:A:218:MET:HE2	2:B:204:LYS:HE3	1.94	0.49
3:C:139:PRO:HG3	3:C:210:VAL:HG13	1.95	0.49
2:B:386:TRP:CZ2	5:B:1438:LVY:H92	2.48	0.49
3:F:13:VAL:HA	3:F:82:GLU:HG3	1.94	0.49
1:D:769:LYS:HB3	1:D:770:LEU:HD23	1.94	0.49
1:A:385:GLY:HA3	1:A:719:GLU:O	2.13	0.48
1:D:883:SER:HB2	1:D:911:ALA:HB3	1.95	0.48
2:B:114:ILE:HD11	2:B:141:ILE:HG21	1.95	0.48
1:A:1127:ASP:HA	1:A:1130:ILE:HD12	1.95	0.48
2:B:197:VAL:O	2:B:234:CYS:HB3	2.14	0.48
2:B:90:ILE:HD13	2:B:296:ILE:HG13	1.96	0.48
1:D:872:SER:HB3	1:D:914:LEU:HB2	1.96	0.48
2:E:386:TRP:CZ2	5:E:1438:LVY:H92	2.49	0.48
3:F:65:LYS:O	3:F:68:GLN:HG2	2.14	0.48
1:D:358:PRO:HD2	1:D:380:GLY:HA2	1.96	0.47
1:D:385:GLY:HA3	1:D:719:GLU:O	2.14	0.47
2:E:400:TRP:NE1	5:E:1438:LVY:H22C	2.30	0.47
1:A:883:SER:HB2	1:A:911:ALA:HB3	1.95	0.47
1:A:11:LYS:HD3	1:A:38:ARG:HD2	1.96	0.47
1:D:1023:PRO:HB3	1:D:1047:TRP:CZ2	2.50	0.47
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.97	0.46
3:C:108:PHE:HA	3:C:297:ASP:OD2	2.15	0.46
1:D:288:GLU:HB2	1:D:298:LYS:HB2	1.97	0.46
1:A:874:VAL:CG1	1:A:916:THR:CG2	2.90	0.46
2:E:143:ALA:HB3	2:E:158:LYS:HB2	1.97	0.46
1:A:924:GLY:HA2	1:A:929:SER:O	2.16	0.46
1:D:207:TRP:HH2	1:D:228:GLY:HA2	1.79	0.46
1:D:987:GLU:HG3	1:D:989:ARG:HG3	1.98	0.46
1:A:328:LEU:HD21	2:B:237:LEU:HD21	1.97	0.46
2:B:92:ILE:HD13	2:B:286:ALA:HA	1.97	0.45
1:D:3:TYR:HB3	1:D:1048:TYR:HB2	1.98	0.45
1:D:1057:ARG:HH12	1:D:1110:ALA:HB3	1.82	0.45
1:D:910:MET:CE	1:D:912:LEU:HD13	2.47	0.45
1:D:1097:PHE:O	1:D:1100:ILE:HG12	2.17	0.45
1:D:971:ALA:O	1:D:999:HIS:CE1	2.70	0.45
1:A:872:SER:HB3	1:A:914:LEU:HB2	1.99	0.44
2:B:143:ALA:HB3	2:B:158:LYS:HB2	1.99	0.44
2:B:232:PHE:O	2:B:242:ARG:HG2	2.18	0.44
1:A:367:LEU:HB2	1:A:374:GLN:NE2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:232:PHE:O	2:E:242:ARG:HG2	2.18	0.44
3:F:275:MET:CE	3:F:278:ARG:HH21	2.30	0.44
3:C:101:PHE:CE2	3:C:106:ARG:HG3	2.52	0.44
2:E:114:ILE:HD11	2:E:141:ILE:HG21	2.00	0.44
2:E:386:TRP:CG	5:E:1438:LVY:H31C	2.52	0.44
2:B:317:LYS:HZ3	2:B:433:ILE:HG23	1.80	0.43
1:D:1030:PHE:CZ	1:D:1038:GLY:HA3	2.53	0.43
1:A:935:TYR:O	1:A:937:PRO:HD3	2.18	0.43
1:D:935:TYR:O	1:D:937:PRO:HD3	2.19	0.43
1:D:953:TRP:HB2	1:D:970:ASN:HB2	2.01	0.43
1:D:1055:GLN:HG2	1:D:1093:LEU:HD23	2.01	0.43
1:A:1003:PHE:CE2	2:B:197:VAL:HG22	2.54	0.43
3:C:133:ILE:HD11	3:C:162:LYS:HE2	2.00	0.43
1:D:250:PRO:HA	1:D:251:PRO:HD3	1.95	0.43
2:E:92:ILE:HD13	2:E:286:ALA:HA	2.00	0.43
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.54	0.43
2:E:53:LEU:HD22	2:E:382:PRO:HG2	2.01	0.43
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	2.00	0.43
1:A:159:LEU:HD21	1:A:164:VAL:HG21	2.00	0.42
1:D:68:ARG:HB2	1:D:75:ASP:OD1	2.19	0.42
3:F:64:TYR:HE1	3:F:74:PRO:HD2	1.85	0.42
3:C:63:LEU:CD2	3:C:161:ALA:HB3	2.48	0.42
1:A:912:LEU:HD11	2:B:244:LEU:HD21	2.02	0.42
1:D:67:PHE:CE2	1:D:69:PRO:HG3	2.54	0.42
2:E:165:PHE:CB	2:E:182:VAL:HG13	2.48	0.42
3:C:217:THR:HA	6:C:2013:HOH:O	2.19	0.42
3:C:28:PHE:HB3	3:C:56:GLN:HG2	2.02	0.42
1:D:912:LEU:HG	2:E:240:TRP:CZ2	2.55	0.42
1:A:131:ILE:HD11	1:A:145:LEU:HD21	2.02	0.41
1:D:261:HIS:HA	1:D:272:LEU:O	2.19	0.41
1:D:912:LEU:HD12	1:D:912:LEU:HA	1.82	0.41
1:A:986:ASP:O	1:A:990:GLN:HG2	2.20	0.41
2:E:107:VAL:HG22	2:E:155:VAL:HG12	2.02	0.41
1:A:182:TYR:HE1	1:A:191:LYS:HB2	1.85	0.41
1:D:333:LEU:HD23	1:D:333:LEU:HA	1.95	0.41
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.95	0.41
2:B:165:PHE:CB	2:B:182:VAL:HG13	2.48	0.41
2:E:67:PHE:HZ	2:E:114:ILE:HG23	1.86	0.41
1:D:358:PRO:HA	1:D:1033:VAL:O	2.21	0.41
1:D:375:LEU:HB2	1:D:1012:LEU:HD21	2.02	0.41
1:A:261:HIS:HA	1:A:272:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:ASN:OD1	1:A:970:ASN:HB3	2.20	0.41
3:C:63:LEU:HD21	3:C:161:ALA:CB	2.49	0.41
3:F:31:ILE:HG12	3:F:46:LYS:HG2	2.02	0.41
1:D:812:TYR:OH	2:E:241:PRO:HB3	2.21	0.41
1:D:232:ILE:HG12	1:D:237:ILE:HG12	2.01	0.41
1:A:1055:GLN:HG2	1:A:1093:LEU:HD23	2.02	0.40
1:A:933:LEU:HD23	1:A:944:GLU:HA	2.03	0.40
2:B:260:GLN:HG2	2:B:315:MET:SD	2.61	0.40
1:D:230:ILE:HD11	1:D:285:LEU:HD21	2.03	0.40
2:B:67:PHE:HZ	2:B:114:ILE:HG23	1.87	0.40
1:A:743:GLN:HB3	1:A:782:PHE:HB3	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	777/856 (91%)	744 (96%)	29 (4%)	4 (0%)	34	41
1	D	778/856 (91%)	744 (96%)	30 (4%)	4 (0%)	34	41
2	B	377/426 (88%)	364 (97%)	10 (3%)	3 (1%)	24	28
2	E	359/426 (84%)	347 (97%)	9 (2%)	3 (1%)	24	28
3	C	292/341 (86%)	282 (97%)	10 (3%)	0	100	100
3	F	292/341 (86%)	279 (96%)	13 (4%)	0	100	100
All	All	2875/3246 (89%)	2760 (96%)	101 (4%)	14 (0%)	34	41

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	50	ASP

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Mol	Chain	Res	Type
2	E	50	ASP
1	D	368	GLU
1	D	1017	LEU
1	A	371	GLY
2	E	198	GLN
2	B	428	ASP
2	B	431	ASP
1	D	36	ASN
1	D	1109	VAL
2	E	428	ASP
1	A	36	ASN
1	A	971	ALA
1	A	981	SER

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	671/744 (90%)	665 (99%)	6 (1%)	84	91
1	D	686/744 (92%)	676 (98%)	10 (2%)	72	84
2	B	344/385 (89%)	336 (98%)	8 (2%)	58	74
2	E	330/385 (86%)	323 (98%)	7 (2%)	61	77
3	C	256/293 (87%)	254 (99%)	2 (1%)	86	92
3	F	260/293 (89%)	258 (99%)	2 (1%)	86	92
All	All	2547/2844 (90%)	2512 (99%)	35 (1%)	74	85

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ILE
1	A	127	GLU
1	A	246	LEU
1	A	252	ILE
1	A	859	GLN

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Mol	Chain	Res	Type
1	A	928	ARG
2	B	47	ILE
2	B	149	ASP
2	B	175	ASP
2	B	197	VAL
2	B	208	PHE
2	B	236	ASN
2	B	408	ASP
2	B	436	ASP
3	C	63	LEU
3	C	68	GLN
1	D	101	ILE
1	D	127	GLU
1	D	141	LYS
1	D	209	GLN
1	D	269	SER
1	D	299	ASP
1	D	859	GLN
1	D	874	VAL
1	D	928	ARG
1	D	1112	LEU
2	E	47	ILE
2	E	53	LEU
2	E	197	VAL
2	E	208	PHE
2	E	236	ASN
2	E	408	ASP
2	E	436	ASP
3	F	197	GLU
3	F	222	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	727	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	LVY	B	1438	-	20,21,21	1.26	2 (10%)	25,31,31	2.84	10 (40%)
5	LVY	E	1438	-	20,21,21	1.15	1 (5%)	25,31,31	2.28	9 (36%)

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	LVY	B	1438	-	-	0/4/29/29	0/3/3/3
5	LVY	E	1438	-	-	0/4/29/29	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1438	LVY	C12-C13	2.09	1.43	1.38
5	E	1438	LVY	C9-C8	2.60	1.53	1.50
5	B	1438	LVY	C9-C8	2.73	1.54	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1438	LVY	C8-C7-C11	-5.97	104.76	108.77
5	B	1438	LVY	C9-N10-C11	-4.51	111.52	113.03
5	B	1438	LVY	O16-C11-C7	-3.96	120.91	128.70
5	E	1438	LVY	C9-N10-C11	-3.29	111.93	113.03
5	E	1438	LVY	C8-C7-C11	-3.22	106.61	108.77
5	E	1438	LVY	O16-C11-C7	-2.95	122.90	128.70
5	B	1438	LVY	C2-C3-C4	-2.56	109.54	114.34
5	B	1438	LVY	C8-C14-N17	-2.18	118.23	120.50
5	E	1438	LVY	C8-C14-N17	2.56	123.17	120.50
5	B	1438	LVY	C3-C2-C1	2.70	114.57	109.95
5	B	1438	LVY	C1-C6-N5	2.73	119.56	116.50
5	E	1438	LVY	C3-C4-N5	3.07	119.86	116.62
5	E	1438	LVY	C3-C2-C1	3.33	115.65	109.95
5	E	1438	LVY	O16-C11-N10	3.45	127.60	125.17
5	E	1438	LVY	C1-C6-N5	4.15	121.17	116.50
5	B	1438	LVY	C3-C4-N5	4.37	121.23	116.62
5	B	1438	LVY	O16-C11-N10	5.03	128.71	125.17
5	E	1438	LVY	C7-C11-N10	5.33	109.43	106.48
5	B	1438	LVY	C7-C11-N10	7.01	110.36	106.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1438	LVY	1	0
5	E	1438	LVY	3	0

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	789/856 (92%)	0.37	57 (7%)	18 19	53, 106, 181, 202	0
1	D	790/856 (92%)	0.01	17 (2%)	65 68	50, 82, 131, 172	0
2	B	381/426 (89%)	0.16	11 (2%)	55 58	54, 78, 134, 159	0
2	E	367/426 (86%)	0.83	58 (15%)	3 2	57, 114, 206, 218	0
3	C	294/341 (86%)	0.01	10 (3%)	49 52	56, 77, 126, 165	1 (0%)
3	F	294/341 (86%)	-0.12	1 (0%)	94 95	52, 76, 117, 162	2 (0%)
All	All	2915/3246 (89%)	0.22	154 (5%)	30 33	50, 88, 172, 218	3 (0%)

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	PHE	8.9
2	E	429	THR	8.7
2	B	429	THR	7.4
2	E	340	LEU	6.9
2	E	270	ASP	6.8
3	C	28	PHE	6.8
1	A	285	LEU	6.5
1	A	297	LEU	6.2
2	E	155	VAL	5.9
2	E	384	TYR	5.7
3	C	182	THR	5.5
1	A	246	LEU	5.5
1	A	302	VAL	5.1
1	A	300	LEU	5.1
2	E	62	ALA	5.1
1	D	1126	ALA	4.9
2	E	131	ARG	4.9
2	E	113	LEU	4.8
1	A	225	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	432	GLU	4.7
2	E	271	ASP	4.6
1	A	1021	SER	4.6
1	A	207	TRP	4.5
2	B	197	VAL	4.5
2	E	128	VAL	4.5
2	E	157	VAL	4.4
1	A	130	MET	4.4
2	E	154	ILE	4.3
1	A	243	ASP	4.3
1	A	96	GLU	4.2
1	A	301	ARG	4.1
1	A	186	GLN	4.0
1	A	295	VAL	4.0
2	E	61	GLY	3.9
3	C	27	SER	3.9
2	E	49	PHE	3.8
3	C	168	ARG	3.8
2	E	412	GLN	3.8
2	E	119	THR	3.8
2	E	144	TYR	3.8
2	E	430	GLU	3.7
1	A	1022	THR	3.6
1	A	271	TYR	3.6
1	A	140	PHE	3.6
3	C	29	GLY	3.5
2	E	68	HIS	3.5
2	E	127	ASN	3.5
3	C	225	LYS	3.5
2	E	404	ALA	3.5
1	D	209	GLN	3.4
2	E	52	SER	3.4
2	B	270	ASP	3.3
1	D	1018	GLY	3.3
1	A	744	ASP	3.3
1	D	1	MET	3.2
1	A	192	THR	3.2
1	D	1125	THR	3.2
2	E	168	LEU	3.2
2	E	109	MET	3.2
1	A	197	LEU	3.1
2	E	132	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	367	LEU	3.1
2	E	180	ALA	3.1
2	B	271	ASP	3.0
2	E	182	VAL	3.0
1	A	48	GLY	3.0
1	D	938	MET	2.9
2	E	406	LYS	2.9
1	A	195	VAL	2.9
1	A	187	GLY	2.8
2	B	221	TYR	2.8
2	E	56	SER	2.8
2	E	267	ASN	2.8
2	E	413	LYS	2.8
1	A	253	ILE	2.7
1	A	369	ARG	2.7
1	A	339	ASP	2.7
2	E	110	VAL	2.7
2	E	63	ASP	2.7
2	E	381	PHE	2.7
3	C	54	HIS	2.6
3	C	180	ASN	2.6
1	A	178	ILE	2.6
1	D	1129	LEU	2.6
1	A	163	HIS	2.6
2	E	129	GLN	2.6
1	D	99	ASP	2.6
2	E	54	PRO	2.5
2	E	122	VAL	2.5
2	E	59	TYR	2.5
2	E	121	ALA	2.5
1	A	29	LEU	2.5
1	A	1079	GLU	2.5
1	A	41	ILE	2.5
1	A	212	VAL	2.5
2	E	156	LYS	2.5
1	A	205	GLY	2.5
2	E	73	HIS	2.5
1	D	745	THR	2.5
1	A	264	VAL	2.5
2	E	53	LEU	2.5
2	B	207	ILE	2.4
2	E	101	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	57	HIS	2.4
1	A	316	TYR	2.4
1	A	272	LEU	2.4
1	A	117	GLU	2.4
2	E	130	GLU	2.4
2	E	286	ALA	2.4
1	A	118	THR	2.4
1	D	370	GLN	2.4
1	D	1021	SER	2.4
1	A	179	CYS	2.4
1	D	1128	ASP	2.3
2	B	431	ASP	2.3
1	A	100	ILE	2.3
2	E	64	MET	2.3
2	E	343	CYS	2.3
1	D	2	SER	2.3
2	E	100	GLN	2.3
1	A	75	ASP	2.3
2	B	177	ILE	2.3
2	E	99	LEU	2.3
2	E	147	GLU	2.3
2	E	178	GLN	2.2
2	E	432	GLU	2.2
1	A	113	GLY	2.2
1	A	190	VAL	2.2
1	A	170	LEU	2.2
1	A	304	LEU	2.2
2	E	104	PRO	2.2
3	C	170	ARG	2.2
1	A	284	LEU	2.2
1	A	245	TYR	2.1
1	A	44	VAL	2.1
1	A	932	LEU	2.1
3	C	300	MET	2.1
2	E	197	VAL	2.1
1	A	229	ALA	2.1
2	B	129	GLN	2.1
1	A	296	THR	2.1
1	A	745	THR	2.1
2	B	426	ILE	2.1
1	A	283	LEU	2.1
2	E	60	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	111	ARG	2.1
1	A	206	PRO	2.1
3	F	294	TYR	2.1
1	A	340	SER	2.0
1	A	221	ALA	2.0
1	D	1020	THR	2.0
2	E	159	ALA	2.0
1	D	1109	VAL	2.0
1	D	919	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	LVY	E	1438	19/19	0.93	0.25	1.46	81,92,113,114	0
5	LVY	B	1438	19/19	0.98	0.15	0.25	48,55,58,61	0
4	ZN	E	1437	1/1	0.99	0.10	-0.84	101,101,101,101	0
4	ZN	B	1437	1/1	0.99	0.10	-1.60	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.