Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2023 – 08:15 PM EST

PDB ID	:	8G66
Title	:	Structure with SJ3149
Authors	:	Miller, D.J.; Young, S.M.; Fischer, M.
Deposited on	:	2023-02-14
Resolution	:	3.45 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
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:

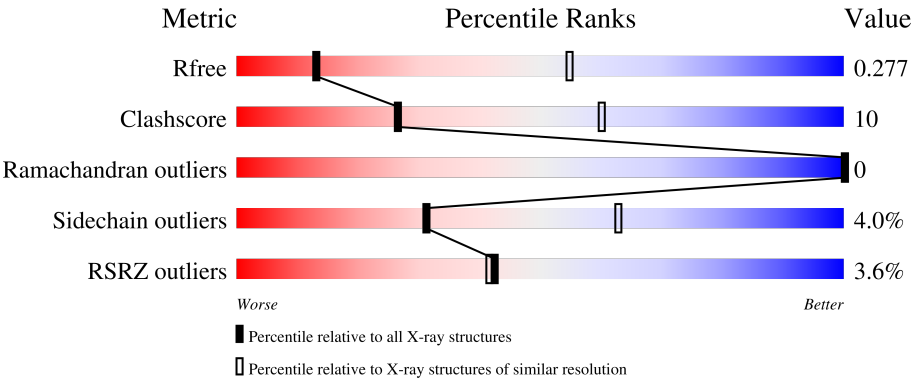
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.45 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}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	860	4% 72% 18% 10%
1	D	860	2% 66% 23% • 9%
2	B	426	2% 62% 24% • 13%
2	E	426	8% 53% 17% 29%
3	C	341	% 65% 19% • 15%

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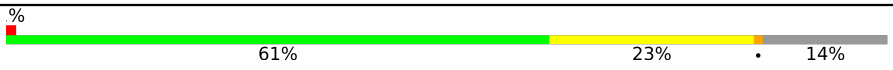
Mol	Chain	Length	Quality of chain
3	F	341	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21297 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	778	Total	C	N	O	S	0	0	0
			5713	3630	954	1099	30			
1	D	779	Total	C	N	O	S	0	0	0
			5835	3714	971	1116	34			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP Q16531
A	-22	GLY	-	expression tag	UNP Q16531
A	-21	SER	-	expression tag	UNP Q16531
A	-20	SER	-	expression tag	UNP Q16531
A	-19	HIS	-	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	SER	-	expression tag	UNP Q16531
A	-12	ALA	-	expression tag	UNP Q16531
A	-11	VAL	-	expression tag	UNP Q16531
A	-10	ASP	-	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	700	GLY	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531
D	-23	MET	-	initiating methionine	UNP Q16531
D	-22	GLY	-	expression tag	UNP Q16531
D	-21	SER	-	expression tag	UNP Q16531
D	-20	SER	-	expression tag	UNP Q16531
D	-19	HIS	-	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	SER	-	expression tag	UNP Q16531
D	-12	ALA	-	expression tag	UNP Q16531
D	-11	VAL	-	expression tag	UNP Q16531
D	-10	ASP	-	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	700	GLY	-	linker	UNP Q16531
D	701	ASN	-	linker	UNP Q16531
D	702	GLY	-	linker	UNP Q16531
D	703	ASN	-	linker	UNP Q16531
D	704	SER	-	linker	UNP Q16531
D	705	GLY	-	linker	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	372	Total	C	N	O	S	0	0	0
			2841	1818	478	523	22			
2	E	303	Total	C	N	O	S	0	0	0
			2186	1399	371	398	18			

There are 48 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
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	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	35	PHE	-	expression tag	UNP Q96SW2
E	36	GLN	-	expression tag	UNP Q96SW2
E	37	GLY	-	expression tag	UNP Q96SW2
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	289	Total	C	N	O	S	0	0	0
			2311	1487	397	412	15			
3	F	294	Total	C	N	O	S	0	0	0
			2381	1534	412	421	14			

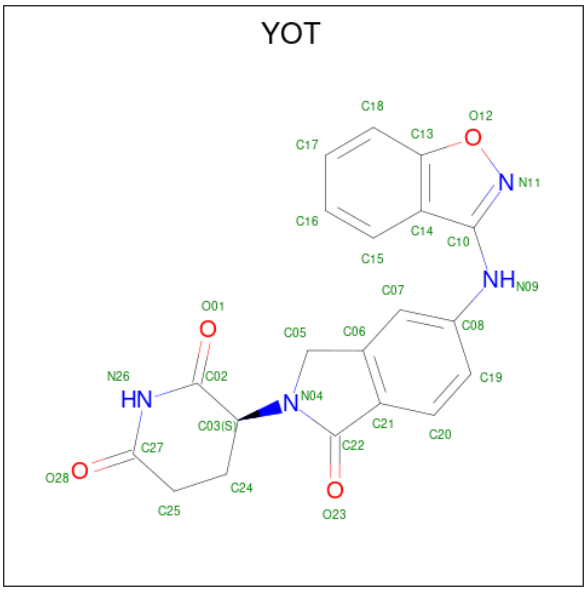
There are 8 discrepancies between the modelled and reference sequences:

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 (3S)-3-{5-[(1,2-benzoxazol-3-yl)amino]-1-oxo-1,3-dihydro-2H-isoindol-2-yl}piperidine-2,6-dione (three-letter code: YOT) (formula: $C_{20}H_{16}N_4O_4$) (labeled as "Ligand of Interest" by depositor).



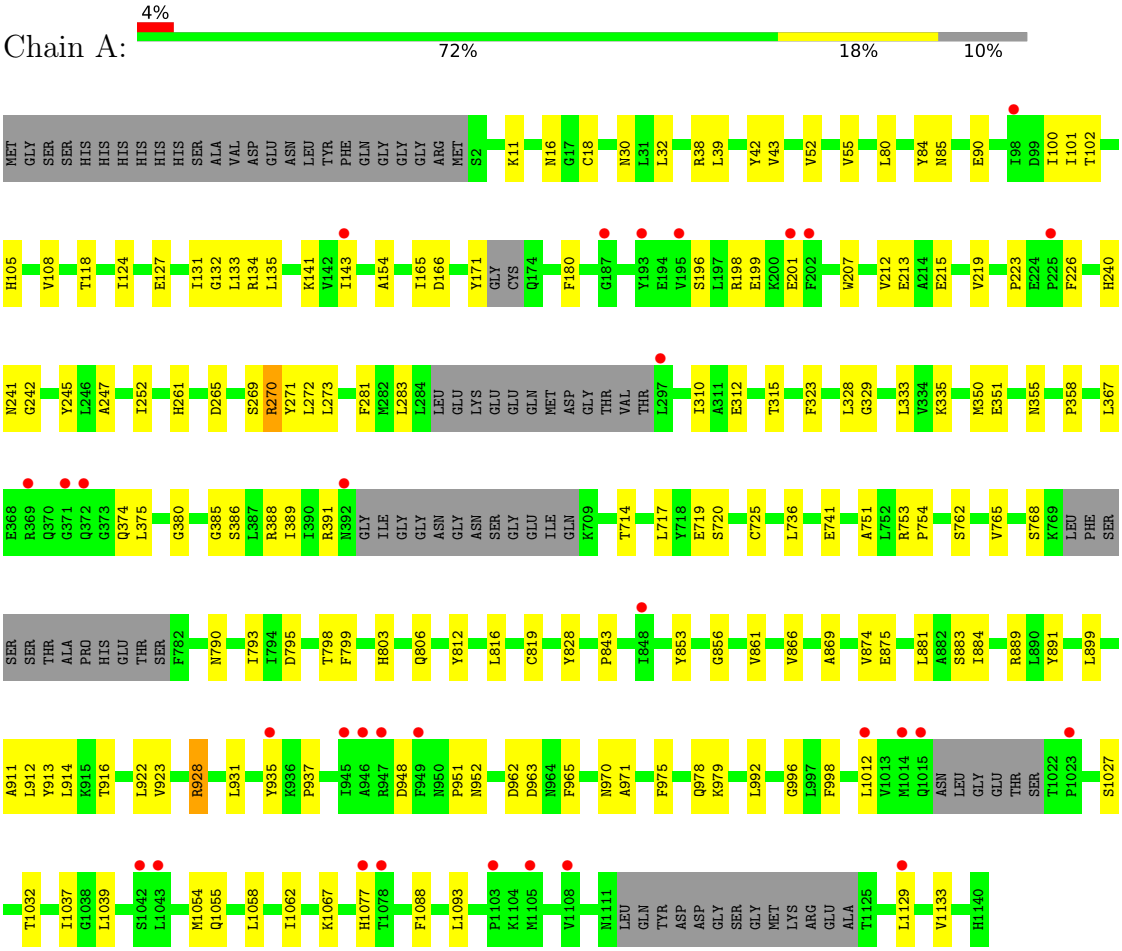
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			28	20	4	4		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

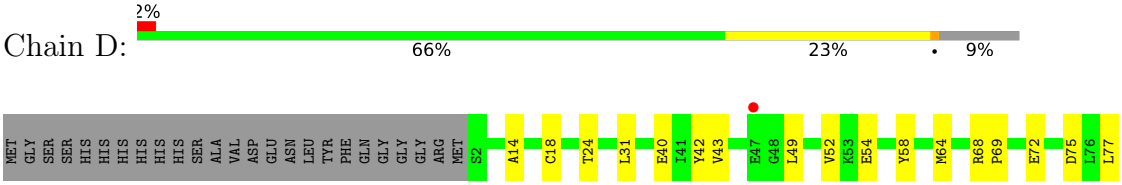
• Molecule 1: DNA damage-binding protein 1

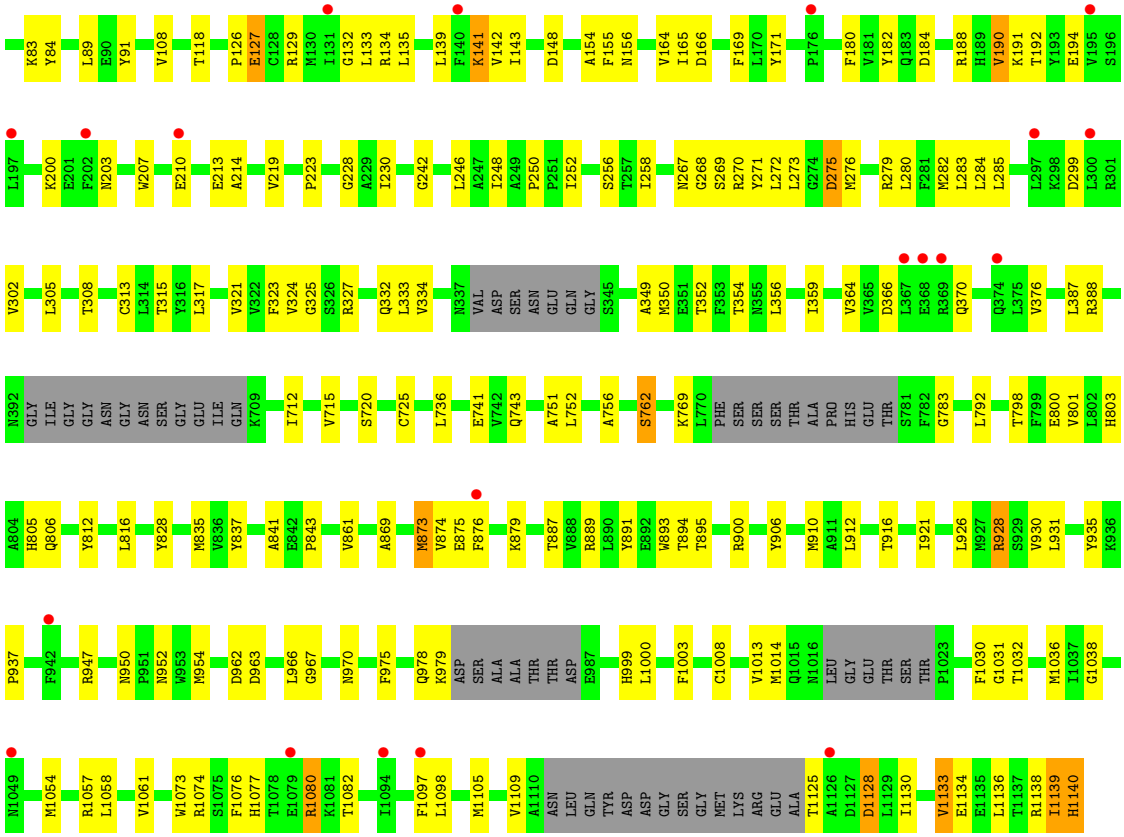
Chain A:



• Molecule 1: DNA damage-binding protein 1

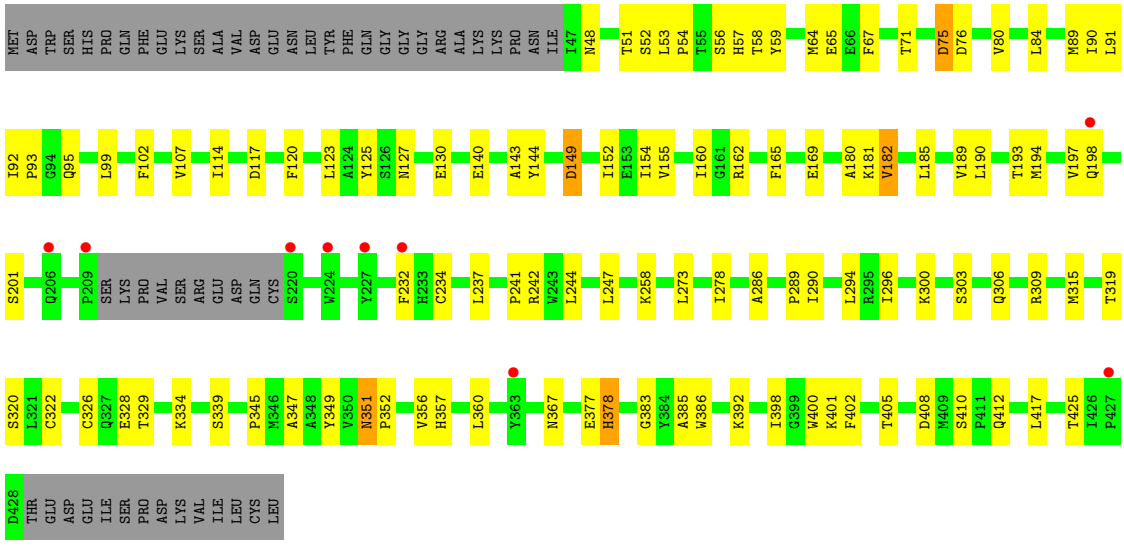
Chain D:





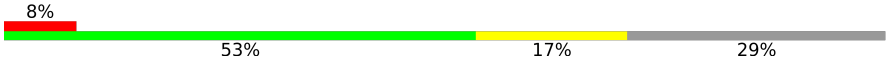
• Molecule 2: Protein cereblon

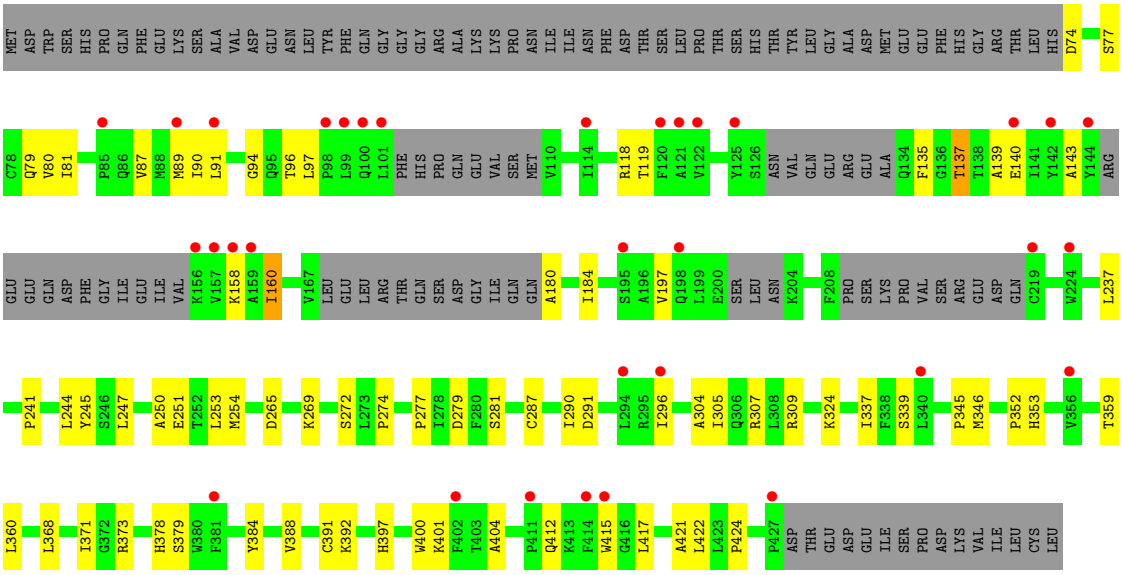
Chain B:

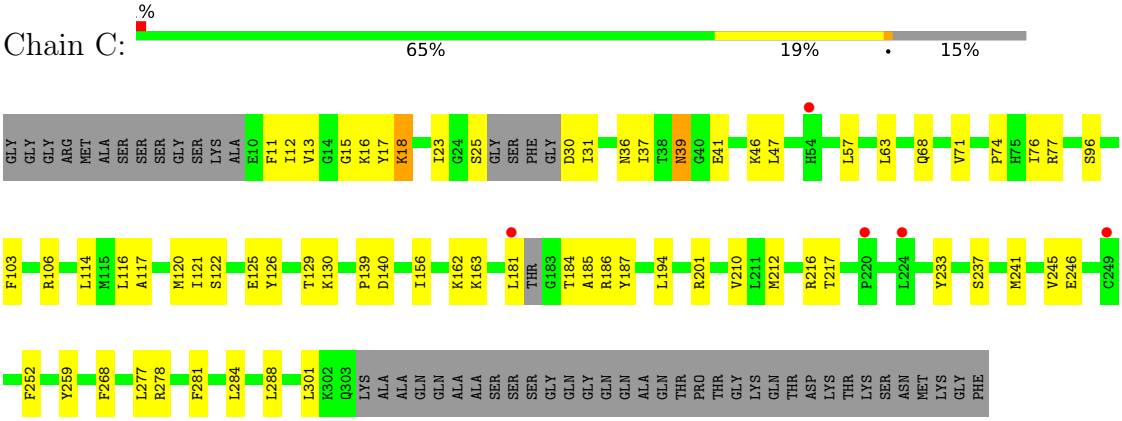


• Molecule 2: Protein cereblon

Chain E:







• Molecule 3: Casein kinase I isoform alpha

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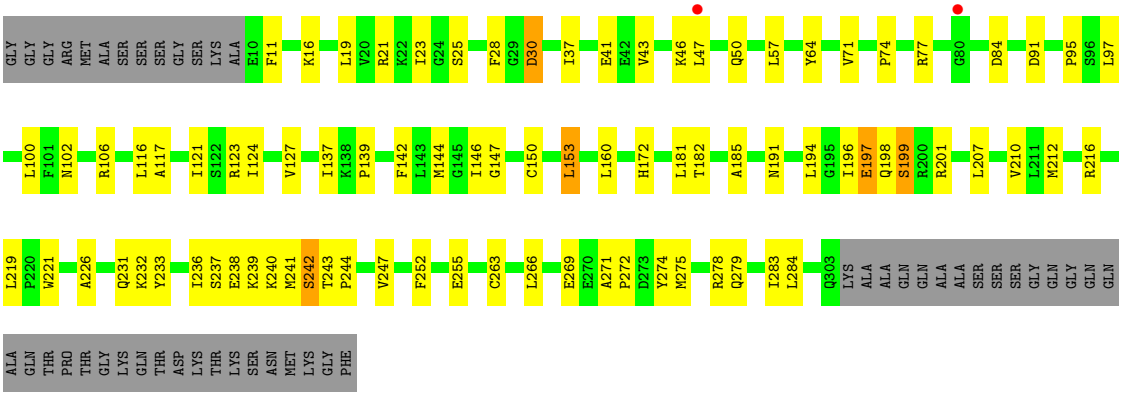

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	86.66Å 109.71Å 112.34Å 105.49° 94.41° 100.03°	Depositor
Resolution (Å)	48.25 – 3.45 48.78 – 3.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.25-3.45) 97.2 (48.78-3.45)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.213 , 0.272 0.216 , 0.277	Depositor DCC
R_{free} test set	1999 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å^2)	106.9	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 81.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21297	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: YOT, 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	0.44	0/5814	0.62	0/7920
1	D	0.46	0/5941	0.63	0/8076
2	B	0.46	0/2912	0.62	0/3979
2	E	0.41	0/2238	0.58	0/3070
3	C	0.47	0/2364	0.66	0/3195
3	F	0.53	0/2438	0.68	0/3290
All	All	0.46	0/21707	0.63	0/29530

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5713	0	5335	99	0
1	D	5835	0	5541	132	0
2	B	2841	0	2669	69	0
2	E	2186	0	1932	52	0
3	C	2311	0	2206	38	0
3	F	2381	0	2324	59	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
5	B	28	0	0	1	0
All	All	21297	0	20007	427	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 10.

All (427) 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:16:LYS:HA	3:F:37:ILE:HG12	1.62	0.82
1:A:118:THR:HG21	1:A:165:ILE:HA	1.61	0.81
1:D:248:ILE:HG13	1:D:250:PRO:HD3	1.63	0.79
2:E:352:PRO:HG3	2:E:378:HIS:CD2	2.17	0.79
1:D:118:THR:HB	1:D:134:ARG:HH22	1.49	0.76
2:B:398:ILE:HG22	2:B:417:LEU:HD22	1.68	0.75
3:F:43:VAL:HG12	3:F:77:ARG:HH11	1.51	0.75
1:D:743:GLN:HB3	1:D:783:GLY:H	1.54	0.72
2:B:92:ILE:HD13	2:B:286:ALA:HA	1.70	0.71
3:F:19:LEU:HD21	3:F:47:LEU:HD11	1.72	0.71
1:A:252:ILE:HG22	1:A:281:PHE:HE2	1.55	0.71
1:D:916:THR:HG22	1:D:921:ILE:HG13	1.73	0.71
1:D:272:LEU:HD22	1:D:280:LEU:HD11	1.74	0.70
1:D:250:PRO:HG3	1:D:302:VAL:HG21	1.74	0.69
2:B:189:VAL:HG22	2:B:278:ILE:HD11	1.74	0.68
3:C:13:VAL:HG23	3:C:17:TYR:HB2	1.76	0.68
2:E:269:LYS:HA	2:E:272:SER:HB2	1.75	0.68
1:D:69:PRO:HD2	1:D:72:GLU:HG3	1.76	0.67
1:D:912:LEU:HD21	2:E:244:LEU:HD21	1.77	0.66
3:F:64:TYR:HE1	3:F:74:PRO:HD2	1.61	0.66
2:B:385:ALA:O	2:B:402:PHE:HA	1.96	0.65
1:D:1058:LEU:HD21	1:D:1097:PHE:HD1	1.62	0.65
3:F:16:LYS:O	3:F:37:ILE:N	2.29	0.65
3:C:116:LEU:HB3	3:C:120:MET:HE2	1.79	0.65
2:E:290:ILE:HA	2:E:424:PRO:HG3	1.79	0.64
1:D:230:ILE:HD11	1:D:285:LEU:HD21	1.79	0.64
3:F:185:ALA:HB2	3:F:233:TYR:CE1	2.33	0.64
1:A:883:SER:HB2	1:A:911:ALA:HB3	1.80	0.63
2:E:417:LEU:HB2	2:E:422:LEU:HD11	1.78	0.63
3:F:219:LEU:HD13	3:F:221:TRP:HE1	1.62	0.63
3:C:117:ALA:O	3:C:121:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.82	0.62
1:D:43:VAL:HG23	1:D:52:VAL:HG21	1.82	0.62
2:B:351:ASN:ND2	3:C:37:ILE:O	2.29	0.62
1:A:207:TRP:CB	1:A:242:GLY:HA2	2.30	0.62
2:B:320:SER:HB3	2:B:425:THR:HB	1.83	0.61
2:E:90:ILE:HD13	2:E:296:ILE:HG13	1.83	0.61
1:D:58:TYR:HB3	1:D:1073:TRP:HB2	1.83	0.61
3:F:221:TRP:HB2	3:F:236:ILE:HG23	1.84	0.60
1:D:207:TRP:CB	1:D:242:GLY:HA2	2.31	0.60
2:E:143:ALA:HB3	2:E:158:LYS:H	1.66	0.60
1:D:356:LEU:HD21	1:D:712:ILE:HD13	1.82	0.59
2:B:194:MET:SD	2:B:232:PHE:HA	2.41	0.59
3:F:237:SER:O	3:F:241:MET:HG3	2.02	0.59
2:E:197:VAL:HG12	2:E:237:LEU:HD12	1.83	0.59
1:D:213:GLU:HG2	1:D:214:ALA:N	2.18	0.59
2:B:67:PHE:HZ	2:B:114:ILE:HG23	1.66	0.59
1:D:1013:VAL:HG11	1:D:1138:ARG:O	2.02	0.59
1:A:329:GLY:O	1:A:355:ASN:ND2	2.29	0.59
2:B:56:SER:HB2	2:B:58:THR:HG23	1.85	0.58
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.85	0.58
1:D:843:PRO:HG2	1:D:869:ALA:HB2	1.86	0.58
1:D:118:THR:HG21	1:D:165:ILE:O	2.03	0.58
3:C:114:LEU:HD22	3:C:281:PHE:HB3	1.86	0.58
1:A:912:LEU:HD21	2:B:244:LEU:HD11	1.86	0.58
3:F:244:PRO:HD2	3:F:247:VAL:HG21	1.86	0.57
1:A:196:SER:CB	1:A:199:GLU:HB2	2.35	0.57
2:B:80:VAL:HA	2:B:180:ALA:O	2.04	0.57
2:B:386:TRP:HA	2:B:401:LYS:O	2.04	0.57
1:D:928:ARG:HD2	1:D:950:ASN:O	2.04	0.57
2:B:289:PRO:HB3	2:B:360:LEU:HD22	1.84	0.57
1:D:1098:LEU:HD11	1:D:1133:VAL:HB	1.87	0.57
3:F:139:PRO:HG3	3:F:210:VAL:HG13	1.87	0.57
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.86	0.56
3:C:139:PRO:HG3	3:C:210:VAL:HG13	1.87	0.56
2:E:404:ALA:HB2	2:E:412:GLN:HA	1.87	0.56
3:F:194:LEU:HD21	3:F:241:MET:SD	2.44	0.56
1:D:954:MET:HE3	1:D:975:PHE:HZ	1.71	0.56
3:C:12:ILE:HG13	3:C:18:LYS:HG2	1.86	0.56
1:D:223:PRO:HD2	1:D:268:GLY:HA3	1.86	0.56
3:F:226:ALA:HB3	3:F:231:GLN:HB3	1.86	0.56
1:A:261:HIS:HA	1:A:272:LEU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:ASN:HB3	3:C:39:ASN:OD1	2.06	0.55
1:D:828:TYR:CE1	1:D:861:VAL:HG21	2.40	0.55
1:D:1130:ILE:O	1:D:1134:GLU:HG2	2.06	0.55
1:D:910:MET:O	1:D:912:LEU:N	2.38	0.55
3:F:239:LYS:O	3:F:243:THR:OG1	2.25	0.55
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.87	0.55
1:A:891:TYR:HB3	1:A:899:LEU:HD22	1.89	0.55
3:F:28:PHE:CZ	3:F:46:LYS:HG2	2.42	0.55
3:C:186:ARG:HD2	3:C:187:TYR:CZ	2.42	0.54
2:E:359:THR:HA	2:E:417:LEU:O	2.07	0.54
1:A:853:TYR:OH	1:A:856:GLY:HA2	2.07	0.54
2:B:140:GLU:OE1	2:B:162:ARG:NH1	2.38	0.54
2:B:90:ILE:HD13	2:B:296:ILE:HG13	1.88	0.54
1:D:967:GLY:HA3	1:D:975:PHE:CE2	2.43	0.54
1:A:874:VAL:HG11	1:A:916:THR:HG22	1.90	0.54
1:D:127:GLU:HB3	1:D:129:ARG:HG3	1.89	0.53
1:D:954:MET:HE3	1:D:975:PHE:CZ	2.43	0.53
1:D:14:ALA:HB1	1:D:327:ARG:HD2	1.91	0.53
1:A:196:SER:HB2	1:A:199:GLU:HB2	1.91	0.53
1:A:385:GLY:HA3	1:A:719:GLU:O	2.08	0.53
3:C:46:LYS:HE2	3:C:57:LEU:HD11	1.90	0.53
1:D:952:ASN:ND2	1:D:970:ASN:HB3	2.23	0.53
3:F:97:LEU:HD11	3:F:153:LEU:HD21	1.91	0.53
1:A:201:GLU:HG3	1:D:200:LYS:HE2	1.89	0.53
2:B:383:GLY:O	2:B:405:THR:HG23	2.09	0.53
1:D:963:ASP:OD1	1:D:979:LYS:HE3	2.09	0.53
1:A:265:ASP:OD2	1:A:269:SER:HB2	2.09	0.53
1:A:912:LEU:HD11	2:B:244:LEU:HD21	1.91	0.53
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.91	0.53
1:A:725:CYS:SG	1:A:816:LEU:HG	2.49	0.53
1:A:374:GLN:HG2	1:A:391:ARG:HB3	1.91	0.52
2:B:67:PHE:CZ	2:B:114:ILE:HG23	2.44	0.52
2:B:258:LYS:HG2	2:B:273:LEU:HD13	1.89	0.52
1:A:1055:GLN:HG2	1:A:1093:LEU:HD23	1.91	0.52
1:D:18:CYS:HG	1:D:313:CYS:HG	1.56	0.52
3:F:238:GLU:O	3:F:242:SER:HB3	2.10	0.52
2:B:57:HIS:HD1	2:B:59:TYR:HE1	1.58	0.52
1:D:118:THR:HG22	1:D:118:THR:O	2.10	0.52
1:D:271:TYR:HB2	1:D:283:LEU:HB3	1.91	0.52
2:E:324:LYS:N	2:E:421:ALA:O	2.33	0.52
2:B:107:VAL:HG22	2:B:155:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:ASP:HB3	1:D:370:GLN:HA	1.91	0.52
3:F:43:VAL:HG12	3:F:77:ARG:NH1	2.23	0.52
3:C:106:ARG:O	3:C:217:THR:HG22	2.10	0.52
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.92	0.52
1:D:334:VAL:HA	1:D:349:ALA:HA	1.92	0.52
1:A:84:TYR:CD1	1:A:135:LEU:HD13	2.45	0.51
1:A:108:VAL:O	1:A:141:LYS:HE2	2.10	0.51
1:A:367:LEU:HD12	1:A:374:GLN:NE2	2.26	0.51
2:B:319:THR:HG22	2:B:334:LYS:HE2	1.92	0.51
2:B:400:TRP:HZ2	3:C:39:ASN:HA	1.75	0.51
3:F:77:ARG:NH2	3:F:91:ASP:OD1	2.42	0.51
1:D:879:LYS:HB3	1:D:891:TYR:O	2.10	0.51
2:E:353:HIS:CG	3:F:37:ILE:HB	2.45	0.51
1:A:118:THR:OG1	1:A:134:ARG:NH2	2.37	0.51
1:A:765:VAL:HG12	1:A:806:GLN:HB3	1.92	0.51
1:D:324:VAL:HB	1:D:332:GLN:HB2	1.92	0.51
2:B:64:MET:HB3	2:B:144:TYR:O	2.10	0.51
3:F:219:LEU:HD13	3:F:221:TRP:NE1	2.25	0.51
2:B:352:PRO:HG3	2:B:378:HIS:CD2	2.45	0.51
1:D:270:ARG:HG2	1:D:284:LEU:HD23	1.91	0.51
1:D:275:ASP:OD1	1:D:279:ARG:N	2.44	0.51
1:D:364:VAL:HG23	1:D:1008:CYS:SG	2.51	0.51
1:A:335:LYS:HB2	1:A:350:MET:SD	2.50	0.51
1:D:31:LEU:HB3	1:D:42:TYR:HB2	1.93	0.51
1:D:841:ALA:O	2:E:247:LEU:HD21	2.11	0.51
1:D:108:VAL:HB	1:D:141:LYS:HE2	1.93	0.51
2:B:95:GLN:O	2:B:160:ILE:HA	2.11	0.51
1:D:315:THR:HG22	1:D:323:PHE:HB3	1.92	0.51
1:D:963:ASP:O	1:D:978:GLN:HA	2.10	0.51
2:E:80:VAL:HA	2:E:180:ALA:O	2.10	0.51
3:F:64:TYR:CE1	3:F:74:PRO:HD2	2.45	0.51
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.46	0.50
2:B:51:THR:O	2:B:54:PRO:HD2	2.11	0.50
3:C:162:LYS:HG2	3:C:163:LYS:O	2.11	0.50
1:D:256:SER:HB3	1:D:275:ASP:OD2	2.10	0.50
2:B:296:ILE:O	2:B:300:LYS:HG3	2.11	0.50
3:F:144:MET:SD	3:F:153:LEU:HD12	2.52	0.50
1:A:736:LEU:HG	1:A:816:LEU:HD22	1.94	0.50
1:A:922:LEU:HD22	1:A:965:PHE:HD2	1.75	0.50
1:A:812:TYR:CE1	2:B:241:PRO:HG3	2.47	0.50
1:A:935:TYR:O	1:A:937:PRO:HD3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:PHE:HA	1:A:996:GLY:O	2.12	0.50
1:D:725:CYS:SG	1:D:816:LEU:HG	2.52	0.50
1:D:18:CYS:SG	1:D:313:CYS:SG	3.10	0.50
3:F:226:ALA:CB	3:F:231:GLN:HB3	2.41	0.50
1:A:367:LEU:HB2	1:A:374:GLN:HE21	1.76	0.50
2:E:244:LEU:O	2:E:244:LEU:HG	2.12	0.50
1:D:126:PRO:HD3	1:D:169:PHE:HB3	1.93	0.49
2:B:296:ILE:HG22	2:B:300:LYS:HE3	1.94	0.49
3:C:181:LEU:HD23	3:C:233:TYR:CE2	2.47	0.49
3:F:197:GLU:HG3	3:F:198:GLN:N	2.27	0.49
3:C:77:ARG:HH11	3:C:77:ARG:HG2	1.77	0.49
1:D:762:SER:O	1:D:803:HIS:HA	2.12	0.49
1:A:198:ARG:NH1	1:D:156:ASN:O	2.46	0.49
1:A:386:SER:HA	1:A:717:LEU:HG	1.95	0.49
1:D:68:ARG:HB2	1:D:75:ASP:OD1	2.13	0.49
2:E:274:PRO:HB2	2:E:279:ASP:HB2	1.94	0.49
3:C:103:PHE:HE2	3:C:301:LEU:HB2	1.77	0.49
3:F:172:HIS:CG	3:F:269:GLU:HG2	2.48	0.49
1:A:245:TYR:CZ	1:A:247:ALA:HB2	2.48	0.49
3:C:185:ALA:HB2	3:C:233:TYR:CE1	2.48	0.49
1:D:258:ILE:HD13	1:D:273:LEU:HD13	1.93	0.49
2:E:352:PRO:HG3	2:E:378:HIS:NE2	2.27	0.49
1:A:753:ARG:HG3	1:A:754:PRO:O	2.12	0.48
3:C:284:LEU:O	3:C:288:LEU:HG	2.13	0.48
1:D:1003:PHE:CE2	2:E:197:VAL:HG22	2.47	0.48
2:B:92:ILE:HG22	2:B:93:PRO:O	2.13	0.48
3:C:25:SER:HA	3:C:30:ASP:HA	1.95	0.48
1:D:49:LEU:HG	1:D:333:LEU:HD11	1.94	0.48
2:E:384:TYR:CD1	2:E:404:ALA:HA	2.49	0.48
3:F:232:LYS:O	3:F:236:ILE:HG13	2.14	0.48
2:B:357:HIS:CD2	2:B:400:TRP:HH2	2.31	0.48
1:D:83:LYS:HE2	1:D:1077:HIS:HB2	1.96	0.48
1:D:828:TYR:HE1	1:D:861:VAL:HG21	1.76	0.48
2:B:165:PHE:HB2	2:B:182:VAL:HG13	1.94	0.48
1:D:282:MET:HB2	1:D:305:LEU:HD21	1.96	0.48
2:E:250:ALA:O	2:E:254:MET:HG3	2.14	0.48
2:E:337:ILE:HG23	2:E:360:LEU:HD11	1.96	0.48
1:A:913:TYR:O	1:A:914:LEU:HD23	2.13	0.48
2:E:384:TYR:HD1	2:E:404:ALA:HA	1.78	0.48
1:D:935:TYR:O	1:D:937:PRO:HD3	2.14	0.47
2:B:48:ASN:OD1	2:B:410:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:VAL:HG12	1:A:240:HIS:HE1	1.79	0.47
1:A:881:LEU:HD12	1:A:889:ARG:O	2.14	0.47
2:B:408:ASP:OD1	2:B:408:ASP:N	2.45	0.47
1:D:207:TRP:CH2	1:D:228:GLY:HA2	2.49	0.47
1:D:966:LEU:HD12	1:D:975:PHE:O	2.15	0.47
3:F:121:ILE:HD12	3:F:278:ARG:HA	1.97	0.47
1:A:315:THR:CG2	1:A:323:PHE:HB3	2.44	0.47
1:A:741:GLU:HG2	1:A:751:ALA:HA	1.97	0.47
1:D:1098:LEU:HG	1:D:1133:VAL:HG11	1.96	0.47
1:A:312:GLU:OE2	2:B:201:SER:HB3	2.13	0.47
1:A:315:THR:HG23	1:A:323:PHE:HB3	1.97	0.47
2:B:367:ASN:HA	2:B:392:LYS:HD2	1.95	0.47
1:D:143:ILE:HG12	1:D:154:ALA:HB2	1.95	0.47
2:E:119:THR:HA	2:E:139:ALA:O	2.14	0.47
2:B:102:PHE:CD2	2:B:154:ILE:HD12	2.50	0.47
2:B:197:VAL:HG22	2:B:237:LEU:HD12	1.95	0.47
2:B:326:CYS:C	2:B:328:GLU:H	2.18	0.47
3:C:125:GLU:O	3:C:129:THR:HG23	2.15	0.47
1:D:1128:ASP:OD1	1:D:1128:ASP:N	2.48	0.47
1:D:58:TYR:HB3	1:D:1073:TRP:CB	2.43	0.47
3:C:194:LEU:HD21	3:C:241:MET:SD	2.55	0.47
2:E:94:GLY:HA2	2:E:160:ILE:HD11	1.97	0.47
1:D:246:LEU:HD11	1:D:299:ASP:HA	1.97	0.46
3:F:102:ASN:OD1	3:F:106:ARG:HD3	2.14	0.46
2:B:165:PHE:CD1	2:B:182:VAL:HG22	2.50	0.46
1:D:313:CYS:SG	1:D:325:GLY:HA3	2.54	0.46
1:A:84:TYR:CE1	1:A:135:LEU:HD13	2.50	0.46
3:C:74:PRO:HG3	3:C:156:ILE:HG22	1.96	0.46
2:E:251:GLU:HA	2:E:254:MET:HE3	1.97	0.46
3:F:255:GLU:OE2	3:F:284:LEU:HB2	2.16	0.46
1:A:952:ASN:OD1	1:A:970:ASN:HB3	2.15	0.46
2:E:253:LEU:HD13	2:E:309:ARG:HG3	1.98	0.46
3:F:124:ILE:HD12	3:F:207:LEU:HD22	1.98	0.46
3:C:16:LYS:HE2	3:C:36:ASN:HD21	1.79	0.46
1:A:389:ILE:HG12	1:A:799:PHE:CZ	2.50	0.46
1:D:952:ASN:CG	1:D:970:ASN:HB3	2.36	0.46
1:A:310:ILE:HG21	1:A:328:LEU:HD12	1.98	0.46
3:C:237:SER:O	3:C:241:MET:HG3	2.16	0.46
1:D:743:GLN:HB3	1:D:783:GLY:N	2.25	0.46
1:D:889:ARG:HD2	1:D:891:TYR:CZ	2.51	0.46
2:E:81:ILE:O	2:E:180:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:CG	1:A:223:PRO:HA	2.51	0.46
2:B:315:MET:O	2:B:334:LYS:NZ	2.40	0.46
1:D:1136:LEU:HA	1:D:1139:ILE:HD13	1.96	0.46
2:E:265:ASP:HB2	2:E:339:SER:HB2	1.98	0.46
1:A:166:ASP:HB3	1:A:219:VAL:HG23	1.98	0.46
1:A:793:ILE:HG21	1:A:853:TYR:CD1	2.51	0.46
2:B:149:ASP:O	2:B:152:ILE:HG12	2.15	0.46
1:D:887:THR:HG23	1:D:906:TYR:CD1	2.50	0.46
3:F:199:SER:OG	3:F:201:ARG:HG2	2.16	0.46
3:F:275:MET:HE2	3:F:278:ARG:HH21	1.81	0.46
1:A:843:PRO:HG2	1:A:869:ALA:HB2	1.96	0.45
2:B:339:SER:HA	2:B:345:PRO:HA	1.97	0.45
1:D:1076:PHE:O	1:D:1082:THR:HA	2.16	0.45
1:D:387:LEU:HB2	1:D:715:VAL:HB	1.98	0.45
1:D:1080:ARG:H	1:D:1080:ARG:HG2	1.59	0.45
3:F:275:MET:CE	3:F:278:ARG:HH21	2.29	0.45
1:A:55:VAL:HG11	1:A:100:ILE:HG13	1.97	0.45
1:A:90:GLU:HB3	1:A:101:ILE:HD11	1.98	0.45
2:E:401:LYS:HB2	2:E:415:TRP:CZ3	2.52	0.45
1:A:912:LEU:CD2	2:B:244:LEU:HD11	2.45	0.45
2:B:412:GLN:HE21	2:B:412:GLN:HB2	1.56	0.45
1:D:315:THR:CG2	1:D:323:PHE:HB3	2.47	0.45
1:D:1057:ARG:O	1:D:1061:VAL:HG13	2.17	0.45
3:F:263:CYS:HA	3:F:266:LEU:HD12	1.99	0.45
1:A:1027:SER:OG	1:A:1039:LEU:HD11	2.17	0.45
1:A:271:TYR:HB2	1:A:283:LEU:HB3	1.99	0.45
1:D:207:TRP:HB2	1:D:242:GLY:HA2	1.98	0.45
1:D:267:ASN:ND2	1:D:269:SER:OG	2.49	0.45
3:F:160:LEU:HD13	3:F:182:THR:HG22	1.99	0.45
2:E:388:VAL:HG21	3:F:41:GLU:HB2	1.98	0.44
3:F:25:SER:HA	3:F:30:ASP:HA	1.98	0.44
2:B:303:SER:HB3	2:B:306:GLN:HG3	1.99	0.44
3:C:39:ASN:OD1	3:C:41:GLU:HB3	2.17	0.44
2:E:135:PHE:N	2:E:135:PHE:CD1	2.85	0.44
1:D:952:ASN:OD1	1:D:970:ASN:HB3	2.17	0.44
2:E:250:ALA:HB2	2:E:305:ILE:HD11	1.99	0.44
3:F:21:ARG:HG3	3:F:23:ILE:HG23	2.00	0.44
3:F:117:ALA:O	3:F:121:ILE:HG13	2.17	0.44
1:A:367:LEU:HB2	1:A:374:GLN:NE2	2.33	0.44
2:B:294:LEU:HD23	2:B:294:LEU:HA	1.86	0.44
1:D:40:GLU:HB3	1:D:42:TYR:HE1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:89:MET:SD	2:E:97:LEU:HD13	2.57	0.44
3:F:50:GLN:HG3	3:F:84:ASP:O	2.17	0.44
3:F:137:ILE:HG22	3:F:210:VAL:HG21	1.99	0.44
3:F:191:ASN:HB3	3:F:196:ILE:HD12	1.99	0.44
1:D:180:PHE:CE1	1:D:191:LYS:HB3	2.52	0.44
1:A:388:ARG:NE	1:A:714:THR:HG23	2.33	0.44
3:C:46:LYS:HE3	3:C:46:LYS:HB3	1.82	0.44
3:C:122:SER:OG	3:C:278:ARG:NH1	2.51	0.44
1:D:190:VAL:HG12	1:D:210:GLU:H	1.83	0.44
1:A:80:LEU:HD12	1:A:85:ASN:O	2.17	0.44
1:A:869:ALA:O	1:A:884:ILE:HA	2.18	0.44
2:B:84:LEU:HD12	2:B:120:PHE:CE2	2.52	0.44
1:D:321:VAL:HG22	1:D:350:MET:SD	2.58	0.44
1:D:916:THR:CG2	1:D:921:ILE:HG13	2.44	0.44
2:E:339:SER:HA	2:E:345:PRO:HA	1.99	0.44
1:A:333:LEU:HB2	1:A:351:GLU:HB2	2.00	0.44
3:C:15:GLY:O	3:C:37:ILE:HD11	2.18	0.44
2:E:74:ASP:O	2:E:77:SER:HB3	2.18	0.44
1:D:1030:PHE:CZ	1:D:1038:GLY:HA3	2.53	0.43
2:E:77:SER:OG	2:E:79:GLN:OE1	2.35	0.43
1:A:270:ARG:HE	1:A:270:ARG:HB2	1.73	0.43
1:A:18:CYS:HA	1:A:32:LEU:O	2.18	0.43
1:D:166:ASP:HB3	1:D:219:VAL:HG23	1.99	0.43
1:D:741:GLU:HG2	1:D:751:ALA:HA	2.00	0.43
1:A:213:GLU:HG2	1:A:215:GLU:H	1.84	0.43
1:A:866:VAL:HG21	1:A:884:ILE:HG12	2.00	0.43
2:B:71:THR:HG21	2:B:117:ASP:HB2	2.00	0.43
1:D:1058:LEU:HD21	1:D:1097:PHE:CD1	2.47	0.43
2:E:353:HIS:CD2	3:F:37:ILE:HB	2.53	0.43
1:D:250:PRO:HB2	1:D:252:ILE:HG22	2.01	0.43
1:D:928:ARG:HB2	1:D:952:ASN:O	2.18	0.43
2:E:371:ILE:HG21	3:F:41:GLU:HG3	1.99	0.43
3:F:212:MET:HE1	3:F:252:PHE:CD2	2.53	0.43
2:B:247:LEU:O	2:B:309:ARG:HD2	2.19	0.43
3:C:16:LYS:HA	3:C:37:ILE:HG12	1.99	0.43
3:F:279:GLN:O	3:F:283:ILE:HG13	2.19	0.43
1:D:893:TRP:HA	1:D:893:TRP:CE3	2.52	0.43
2:B:378:HIS:O	5:B:502:YOT:N26	2.52	0.43
1:D:84:TYR:CE1	1:D:135:LEU:HD13	2.53	0.43
1:D:812:TYR:CZ	2:E:241:PRO:HB3	2.54	0.43
2:E:373:ARG:NE	3:F:146:ILE:HG23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:ASP:O	2:B:76:ASP:HB2	2.19	0.43
2:B:349:TYR:O	2:B:356:VAL:HA	2.19	0.43
3:F:181:LEU:HB3	3:F:233:TYR:HE2	1.83	0.43
1:A:16:ASN:HA	1:A:312:GLU:HG2	2.00	0.43
2:B:89:MET:HE1	2:B:91:LEU:HD13	2.01	0.43
3:C:259:TYR:CE1	3:C:277:LEU:HD13	2.53	0.43
1:D:1139:ILE:HG12	1:D:1140:HIS:N	2.34	0.43
1:A:793:ILE:HG21	1:A:853:TYR:CE1	2.54	0.42
2:B:92:ILE:O	2:B:95:GLN:HB2	2.19	0.42
2:B:169:GLU:O	2:B:181:LYS:N	2.50	0.42
3:C:126:TYR:OH	3:C:130:LYS:HE3	2.18	0.42
1:D:308:THR:HB	1:D:332:GLN:OE1	2.18	0.42
1:D:805:HIS:CD2	1:D:806:GLN:O	2.72	0.42
1:D:835:MET:HB3	1:D:837:TYR:CE1	2.54	0.42
2:E:397:HIS:HE1	2:E:400:TRP:CZ2	2.37	0.42
3:C:16:LYS:HE2	3:C:36:ASN:ND2	2.34	0.42
1:D:1105:MET:O	1:D:1109:VAL:HG13	2.19	0.42
2:E:368:LEU:O	2:E:392:LYS:NZ	2.51	0.42
1:A:388:ARG:CZ	1:A:714:THR:HG23	2.49	0.42
1:A:1058:LEU:HD22	1:A:1062:ILE:HD11	2.01	0.42
1:D:876:PHE:CE2	1:D:921:ILE:HD11	2.55	0.42
1:A:819:CYS:HB2	1:A:875:GLU:HG3	2.00	0.42
1:A:828:TYR:CE1	1:A:861:VAL:HG21	2.53	0.42
1:D:194:GLU:HB2	1:D:203:ASN:HB2	2.01	0.42
1:D:928:ARG:O	1:D:930:VAL:HG23	2.19	0.42
1:A:39:LEU:HB3	1:A:55:VAL:HG23	2.02	0.42
1:D:132:GLY:O	1:D:133:LEU:HD23	2.19	0.42
1:D:999:HIS:HB3	1:D:1074:ARG:HA	2.02	0.42
3:F:57:LEU:HD23	3:F:57:LEU:HA	1.80	0.42
3:F:144:MET:HE3	3:F:150:CYS:O	2.20	0.42
2:B:123:LEU:HB2	2:B:125:TYR:CZ	2.54	0.42
3:C:114:LEU:HD23	3:C:114:LEU:HA	1.87	0.42
1:D:141:LYS:HB2	1:D:156:ASN:OD1	2.19	0.42
1:A:762:SER:O	1:A:803:HIS:HA	2.20	0.42
1:D:134:ARG:NH1	1:D:164:VAL:O	2.50	0.42
1:A:795:ASP:OD2	1:A:798:THR:HG23	2.20	0.42
2:B:198:GLN:HA	2:B:234:CYS:SG	2.60	0.42
2:B:290:ILE:HD12	2:B:294:LEU:HB3	2.01	0.42
3:C:201:ARG:CZ	3:C:268:PHE:HA	2.49	0.42
1:D:1054:MET:O	1:D:1058:LEU:HD12	2.20	0.42
3:F:123:ARG:O	3:F:127:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:TYR:CZ	2:B:241:PRO:HB3	2.55	0.42
1:A:978:GLN:O	1:A:992:LEU:HA	2.20	0.42
3:C:57:LEU:HD12	3:C:57:LEU:HA	1.78	0.42
2:E:135:PHE:HD1	2:E:135:PHE:H	1.66	0.42
3:C:246:GLU:OE1	3:C:246:GLU:N	2.50	0.42
1:D:126:PRO:HB3	1:D:171:TYR:CE1	2.54	0.42
1:D:873:MET:HE2	1:D:873:MET:HB2	1.96	0.42
3:F:241:MET:HE2	3:F:241:MET:HB3	1.85	0.42
3:C:212:MET:HE1	3:C:252:PHE:CD2	2.55	0.41
1:D:931:LEU:HD12	1:D:947:ARG:HB3	2.02	0.41
2:E:373:ARG:NH2	3:F:147:GLY:H	2.18	0.41
1:A:375:LEU:HD23	1:A:1037:ILE:HD13	2.02	0.41
1:A:963:ASP:O	1:A:978:GLN:HA	2.19	0.41
1:D:182:TYR:O	1:D:188:ARG:HA	2.20	0.41
1:D:843:PRO:CG	1:D:869:ALA:HB2	2.50	0.41
2:E:118:ARG:O	2:E:140:GLU:HA	2.20	0.41
1:A:951:PRO:O	2:B:190:LEU:HD21	2.19	0.41
1:D:926:LEU:HD21	2:E:245:TYR:CD1	2.56	0.41
1:A:30:ASN:HA	1:A:42:TYR:O	2.20	0.41
1:A:105:HIS:CD2	1:A:1067:LYS:HD2	2.55	0.41
1:A:998:PHE:HB2	1:A:1088:PHE:CD2	2.54	0.41
3:C:76:ILE:HD13	3:C:76:ILE:HA	1.88	0.41
1:D:166:ASP:OD2	1:D:219:VAL:N	2.47	0.41
1:A:1054:MET:SD	1:A:1129:LEU:HD21	2.60	0.41
1:D:143:ILE:CG1	1:D:154:ALA:HB2	2.50	0.41
1:D:376:VAL:HA	1:D:388:ARG:O	2.21	0.41
1:A:11:LYS:HD3	1:A:38:ARG:HD2	2.03	0.41
2:B:165:PHE:HA	2:B:185:LEU:HG	2.01	0.41
2:B:347:ALA:HB3	2:B:349:TYR:CZ	2.56	0.41
1:D:42:TYR:CD2	1:D:49:LEU:HB3	2.55	0.41
1:D:317:LEU:HD12	1:D:321:VAL:HG12	2.03	0.41
1:A:226:PHE:O	1:A:241:ASN:ND2	2.54	0.41
1:A:853:TYR:CZ	1:A:856:GLY:HA2	2.56	0.41
1:D:736:LEU:HG	1:D:816:LEU:HD22	2.03	0.41
2:E:277:PRO:O	2:E:304:ALA:HB1	2.21	0.41
2:E:281:SER:OG	2:E:307:ARG:HD2	2.21	0.41
1:A:923:VAL:HB	1:A:931:LEU:HB3	2.02	0.41
2:B:306:GLN:HG3	2:B:306:GLN:H	1.70	0.41
1:D:798:THR:OG1	1:D:800:GLU:HG2	2.21	0.41
2:E:291:ASP:OD1	2:E:291:ASP:N	2.54	0.41
3:F:116:LEU:HD23	3:F:116:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:THR:HB	1:A:1067:LYS:HE3	2.03	0.41
1:A:132:GLY:O	1:A:133:LEU:HD23	2.21	0.41
1:A:912:LEU:HA	1:A:912:LEU:HD23	1.69	0.41
2:B:99:LEU:HA	2:B:99:LEU:HD23	1.62	0.41
1:D:916:THR:HG22	1:D:921:ILE:HA	2.02	0.41
2:E:287:CYS:HA	2:E:346:MET:HE3	2.03	0.41
2:E:401:LYS:HB2	2:E:415:TRP:CE3	2.55	0.41
1:A:1129:LEU:O	1:A:1133:VAL:HG23	2.21	0.41
2:B:127:ASN:HB3	2:B:130:GLU:CB	2.51	0.41
1:D:64:MET:HG2	1:D:77:LEU:HD11	2.03	0.41
1:D:333:LEU:O	1:D:350:MET:N	2.54	0.41
3:F:95:PRO:HG2	3:F:100:LEU:HD21	2.03	0.41
3:F:142:PHE:HB3	3:F:153:LEU:HD21	2.03	0.40
1:A:928:ARG:NH2	1:A:948:ASP:OD2	2.55	0.40
1:D:24:THR:HA	1:D:91:TYR:CD2	2.57	0.40
1:D:142:VAL:HB	1:D:155:PHE:CZ	2.57	0.40
1:D:756:ALA:HB1	1:D:801:VAL:HG21	2.03	0.40
1:D:1000:LEU:HD21	1:D:1030:PHE:CE1	2.56	0.40
3:F:271:ALA:HA	3:F:272:PRO:HD3	1.97	0.40
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	2.04	0.40
2:E:91:LEU:HB3	2:E:137:THR:HG21	2.03	0.40
1:A:971:ALA:HB3	1:A:1077:HIS:O	2.21	0.40
2:B:65:GLU:O	2:B:143:ALA:HA	2.21	0.40
1:D:359:ILE:HG21	1:D:1031:GLY:HA3	2.04	0.40
3:F:244:PRO:HD2	3:F:247:VAL:CG2	2.52	0.40
2:B:322:CYS:HB3	2:B:329:THR:O	2.22	0.40
1:D:910:MET:HE3	1:D:910:MET:HB3	1.86	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	764/860 (89%)	730 (96%)	34 (4%)	0	100	100
1	D	765/860 (89%)	732 (96%)	33 (4%)	0	100	100
2	B	368/426 (86%)	362 (98%)	6 (2%)	0	100	100
2	E	289/426 (68%)	281 (97%)	8 (3%)	0	100	100
3	C	283/341 (83%)	264 (93%)	19 (7%)	0	100	100
3	F	292/341 (86%)	276 (94%)	16 (6%)	0	100	100
All	All	2761/3254 (85%)	2645 (96%)	116 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	575/746 (77%)	565 (98%)	10 (2%)	60	82
1	D	604/746 (81%)	569 (94%)	35 (6%)	20	52
2	B	293/385 (76%)	283 (97%)	10 (3%)	37	67
2	E	203/385 (53%)	196 (97%)	7 (3%)	37	67
3	C	233/293 (80%)	219 (94%)	14 (6%)	19	51
3	F	246/293 (84%)	236 (96%)	10 (4%)	30	62
All	All	2154/2848 (76%)	2068 (96%)	86 (4%)	31	63

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLU
1	A	180	PHE
1	A	270	ARG
1	A	720	SER
1	A	768	SER
1	A	790	ASN
1	A	928	ARG

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Mol	Chain	Res	Type
1	A	962	ASP
1	A	979	LYS
1	A	1032	THR
2	B	52	SER
2	B	53	LEU
2	B	75	ASP
2	B	149	ASP
2	B	182	VAL
2	B	193	THR
2	B	242	ARG
2	B	351	ASN
2	B	377	GLU
2	B	378	HIS
3	C	11	PHE
3	C	18	LYS
3	C	23	ILE
3	C	31	ILE
3	C	39	ASN
3	C	47	LEU
3	C	63	LEU
3	C	68	GLN
3	C	71	VAL
3	C	96	SER
3	C	140	ASP
3	C	184	THR
3	C	216	ARG
3	C	245	VAL
1	D	54	GLU
1	D	89	LEU
1	D	127	GLU
1	D	139	LEU
1	D	141	LYS
1	D	148	ASP
1	D	184	ASP
1	D	190	VAL
1	D	192	THR
1	D	275	ASP
1	D	276	MET
1	D	352	THR
1	D	354	THR
1	D	720	SER
1	D	752	LEU

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Mol	Chain	Res	Type
1	D	762	SER
1	D	769	LYS
1	D	792	LEU
1	D	873	MET
1	D	874	VAL
1	D	875	GLU
1	D	894	THR
1	D	895	THR
1	D	900	ARG
1	D	928	ARG
1	D	962	ASP
1	D	1014	MET
1	D	1032	THR
1	D	1036	MET
1	D	1080	ARG
1	D	1125	THR
1	D	1128	ASP
1	D	1133	VAL
1	D	1139	ILE
1	D	1140	HIS
2	E	87	VAL
2	E	96	THR
2	E	137	THR
2	E	160	ILE
2	E	184	ILE
2	E	379	SER
2	E	391	CYS
3	F	11	PHE
3	F	30	ASP
3	F	71	VAL
3	F	153	LEU
3	F	197	GLU
3	F	199	SER
3	F	216	ARG
3	F	240	LYS
3	F	242	SER
3	F	274	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN

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Mol	Chain	Res	Type
1	A	189	HIS
2	B	79	GLN
3	C	151	ASN
3	C	198	GLN
3	C	290	HIS
1	D	85	ASN
1	D	107	ASN
1	D	337	ASN
1	D	790	ASN
2	E	306	GLN
2	E	316	ASN
2	E	369	ASN
3	F	50	GLN
3	F	141	ASN
3	F	149	HIS
3	F	215	ASN
3	F	290	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	YOT	B	502	-	28,32,32	0.69	1 (3%)	36,47,47	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	YOT	B	502	-	-	0/6/33/33	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	YOT	C14-C13	-2.23	1.38	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

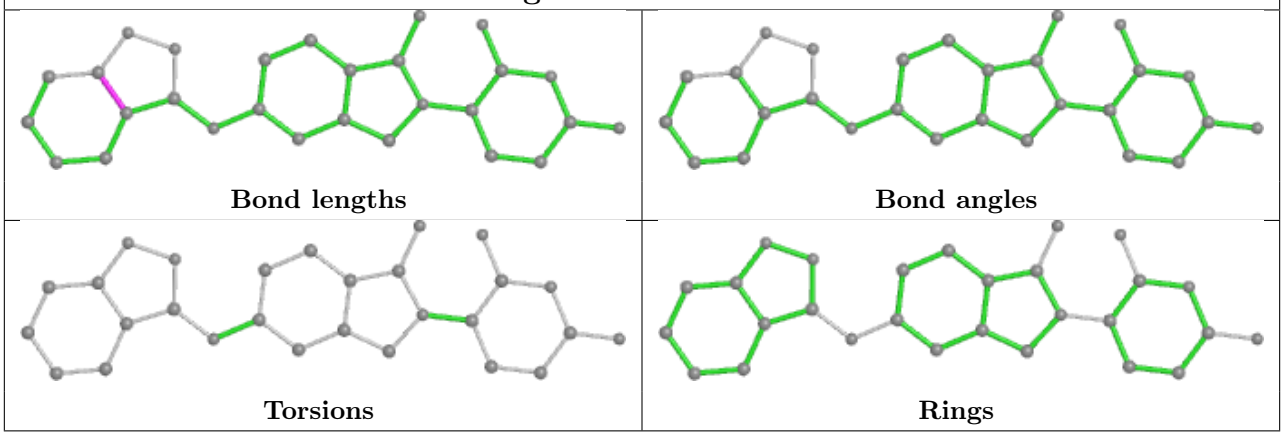
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	YOT	1	0

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

Ligand YOT B 502



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	778/860 (90%)	0.11	31 (3%) 38 36	74, 129, 191, 243	0
1	D	779/860 (90%)	0.11	21 (2%) 54 52	62, 117, 181, 256	0
2	B	372/426 (87%)	-0.02	9 (2%) 59 56	82, 114, 199, 304	0
2	E	303/426 (71%)	0.48	33 (10%) 5 8	87, 147, 196, 253	0
3	C	289/341 (84%)	0.03	5 (1%) 70 67	78, 109, 162, 202	0
3	F	294/341 (86%)	-0.13	2 (0%) 87 85	66, 98, 149, 195	0
All	All	2815/3254 (86%)	0.10	101 (3%) 42 41	62, 119, 188, 304	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	227	TYR	4.7
1	A	1108	VAL	4.5
1	D	368	GLU	4.2
2	B	198	GLN	4.1
2	E	411	PRO	4.1
2	E	121	ALA	3.9
2	B	206	GLN	3.9
2	E	198	GLN	3.6
2	E	402	PHE	3.6
1	D	1049	ASN	3.6
3	C	224	LEU	3.5
1	A	372	GLN	3.5
2	E	120	PHE	3.5
1	D	374	GLN	3.3
1	A	945	ILE	3.3
1	A	187	GLY	3.3
1	A	1023	PRO	3.3
2	E	340	LEU	3.3
2	E	158	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	98	PRO	3.2
2	B	224	TRP	3.2
1	A	1078	THR	3.1
2	E	157	VAL	3.1
1	A	1043	LEU	3.1
1	A	392	ASN	3.0
1	A	1077	HIS	3.0
2	E	414	PHE	3.0
2	E	100	GLN	3.0
1	D	369	ARG	2.9
1	A	1129	LEU	2.9
2	E	122	VAL	2.9
2	E	156	LYS	2.8
2	E	415	TRP	2.8
1	A	201	GLU	2.7
2	E	91	LEU	2.7
1	D	1097	PHE	2.7
2	E	219	CYS	2.7
2	B	427	PRO	2.7
2	E	159	ALA	2.7
3	C	181	LEU	2.6
1	A	371	GLY	2.6
1	A	297	LEU	2.6
2	E	296	ILE	2.6
2	E	85	PRO	2.6
2	E	99	LEU	2.6
3	C	54	HIS	2.6
1	D	942	PHE	2.5
2	E	224	TRP	2.5
1	A	1042	SER	2.5
3	F	47	LEU	2.5
2	B	220	SER	2.5
1	D	876	PHE	2.5
1	D	300	LEU	2.4
1	D	176	PRO	2.4
2	E	142	TYR	2.4
1	A	1014	MET	2.4
1	D	195	VAL	2.4
1	A	193	TYR	2.4
1	A	946	ALA	2.4
1	A	369	ARG	2.4
2	E	195	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1015	GLN	2.3
1	A	225	PRO	2.3
1	A	1012	LEU	2.3
1	D	197	LEU	2.3
1	D	297	LEU	2.3
1	A	202	PHE	2.3
2	B	209	PRO	2.3
1	A	195	VAL	2.3
3	F	80	GLY	2.3
1	D	367	LEU	2.3
1	A	1105	MET	2.3
3	C	220	PRO	2.3
1	A	935	TYR	2.3
1	A	98	ILE	2.2
2	E	114	ILE	2.2
2	B	232	PHE	2.2
2	E	140	GLU	2.2
1	A	143	ILE	2.2
2	E	356	VAL	2.2
1	A	1103	PRO	2.2
2	E	427	PRO	2.2
2	E	89	MET	2.1
2	E	101	LEU	2.1
1	D	47	GLU	2.1
1	D	1094	ILE	2.1
2	E	381	PHE	2.1
1	D	131	ILE	2.1
1	D	1126	ALA	2.1
3	C	249	CYS	2.1
2	E	294	LEU	2.1
1	A	949	PHE	2.1
1	A	848	ILE	2.1
1	D	140	PHE	2.0
1	D	210	GLU	2.0
1	D	1079	GLU	2.0
2	E	125	TYR	2.0
1	A	947	ARG	2.0
2	E	144	TYR	2.0
1	D	202	PHE	2.0
2	B	363	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

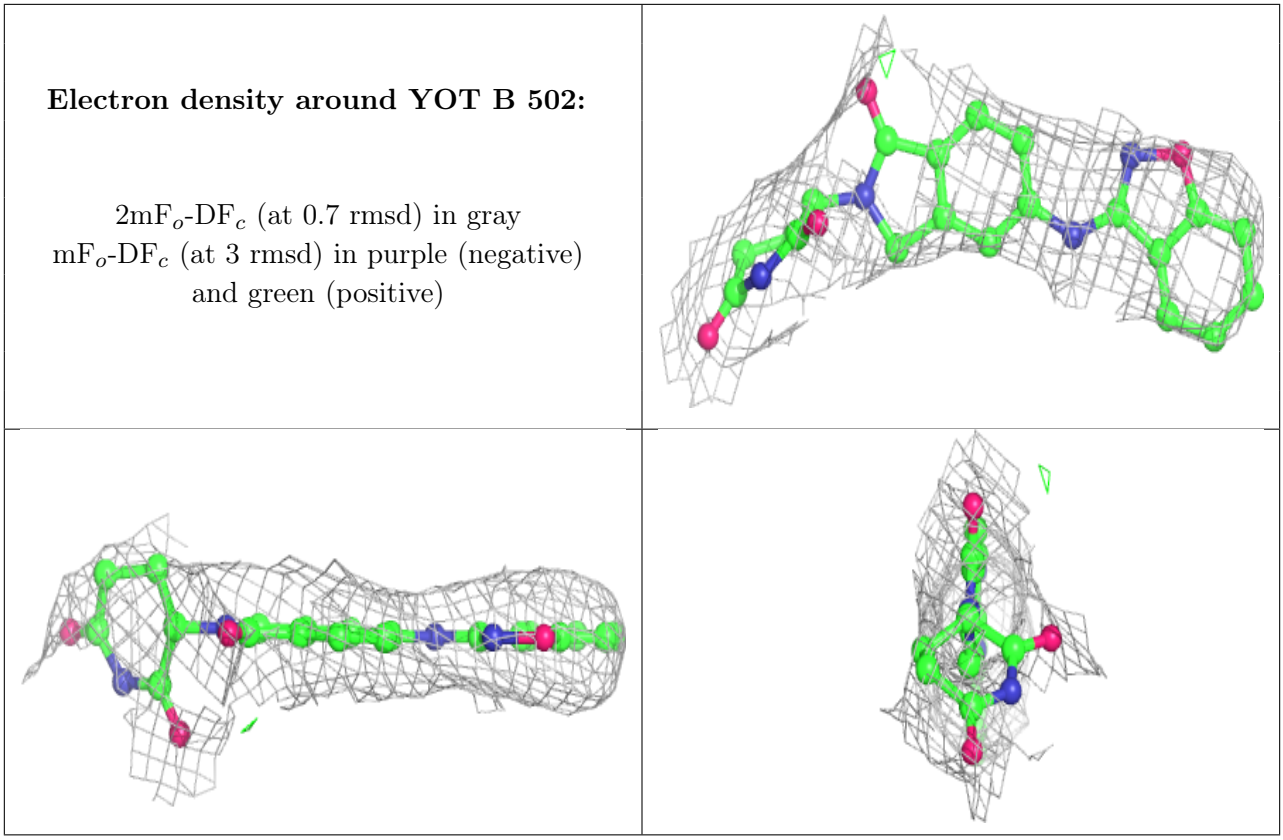
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	YOT	B	502	28/28	0.93	0.22	80,94,117,118	0
4	ZN	E	501	1/1	1.00	0.11	115,115,115,115	0
4	ZN	B	501	1/1	1.00	0.14	110,110,110,110	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 YOT B 502:

$2mF_o$-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.