



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:13 PM UTC

PDB ID : 9HNE / pdb\_00009hne  
Title : Cereblon in complex with DDB1, GSPT1 and Compound-1  
Authors : Klejnot, M.; Walczak, M.J.  
Deposited on : 2024-12-10  
Resolution : 3.90 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

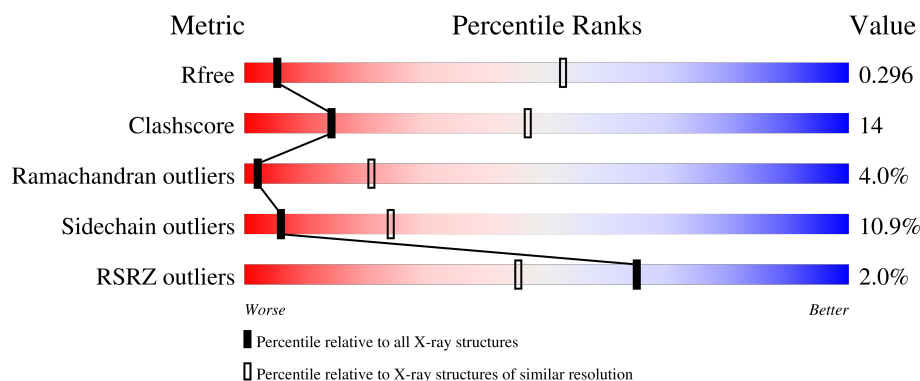
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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))
$R_{free}$	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	197	<div> <div>2%</div> <div>53% 31% 13% ..</div> </div>
1	D	197	<div> <div>4%</div> <div>47% 37% 15% ..</div> </div>
2	B	1140	<div> <div>2%</div> <div>62% 28% . 5%</div> </div>
2	E	1140	<div> <div>2%</div> <div>61% 30% . . 5%</div> </div>
3	C	404	<div> <div>2%</div> <div>59% 26% 6% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	404	<div><div></div><div>2%</div><div>57%</div><div>28%</div><div>6%</div><div>9%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26021 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 Eukaryotic peptide chain release factor GTP-binding subunit ERF3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1513	960	261	280	12			
1	D	196	Total	C	N	O	S	0	0	0
			1520	965	262	281	12			

- Molecule 2 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1081	Total	C	N	O	S	0	0	0
			8491	5397	1431	1617	46			
2	E	1082	Total	C	N	O	S	0	0	0
			8501	5402	1432	1621	46			

- Molecule 3 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	371	Total	C	N	O	S	0	0	0
			2996	1910	511	552	23			
3	F	367	Total	C	N	O	S	0	0	0
			2954	1892	502	536	24			

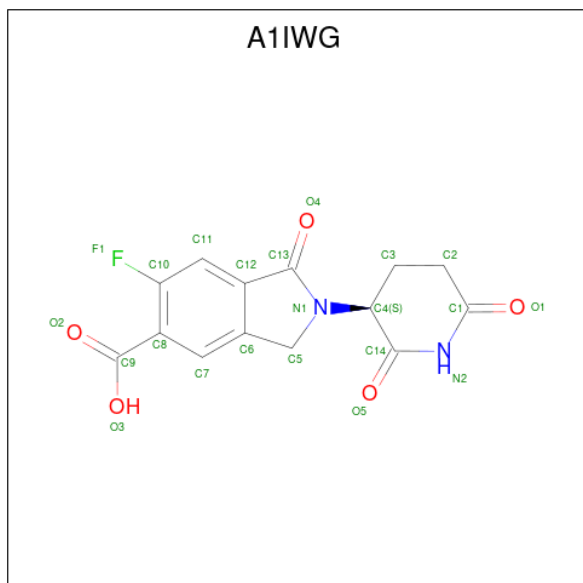
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	39	SER	-	expression tag	UNP Q96SW2
F	39	SER	-	expression tag	UNP Q96SW2

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

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

- Molecule 5 is 2-[(3 {S})-2,6-bis(oxidanylidene)piperidin-3-yl]-6-fluoranyl-1-oxidanylidene-3 {H}-isoindole-5-carboxylic acid (CCD ID: A1IWG) (formula: C<sub>14</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).

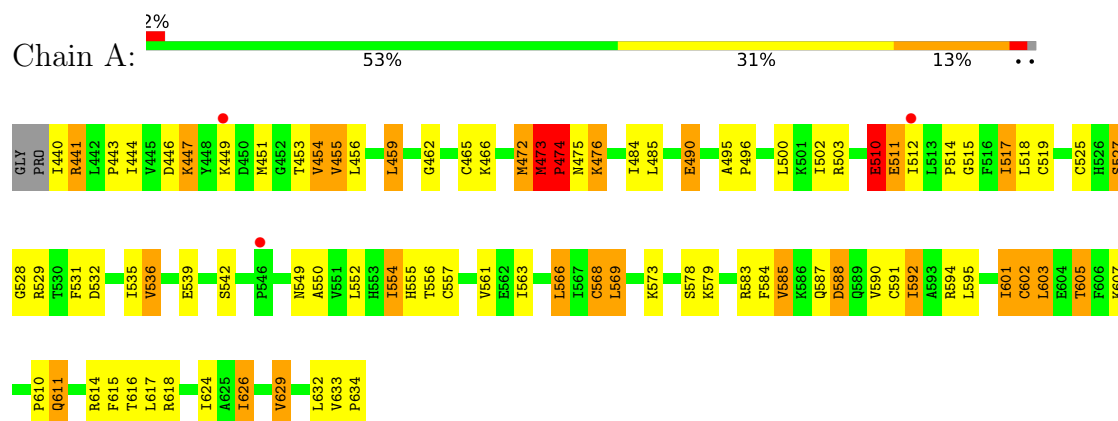


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	F	N	O	0	0
			22	14	1	2	5		
5	F	1	Total	C	F	N	O	0	0
			22	14	1	2	5		

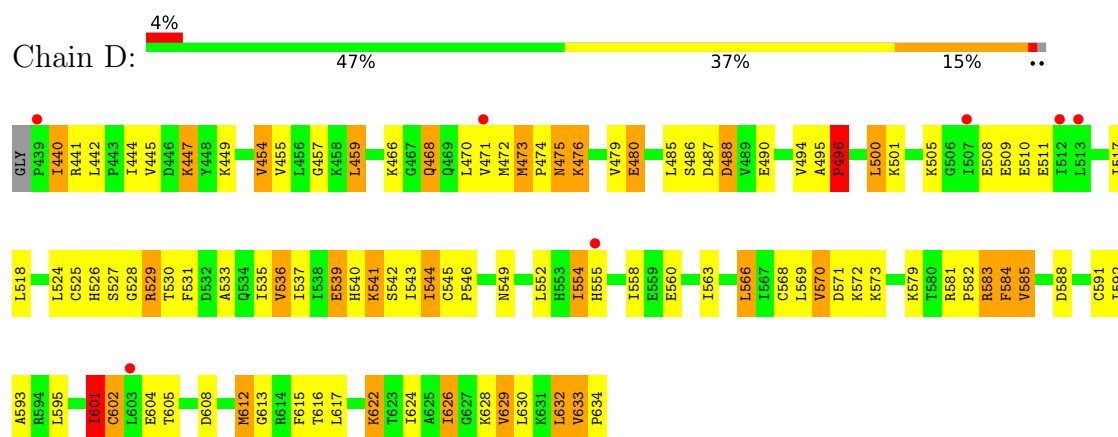
### 3 Residue-property plots [i](#)

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.

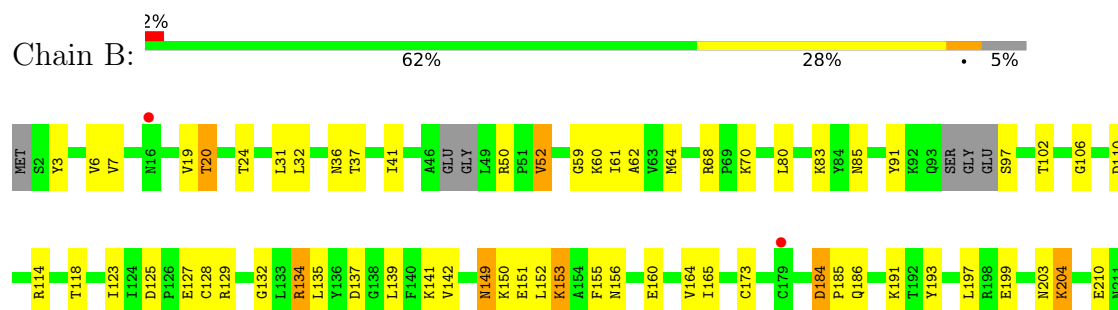
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A

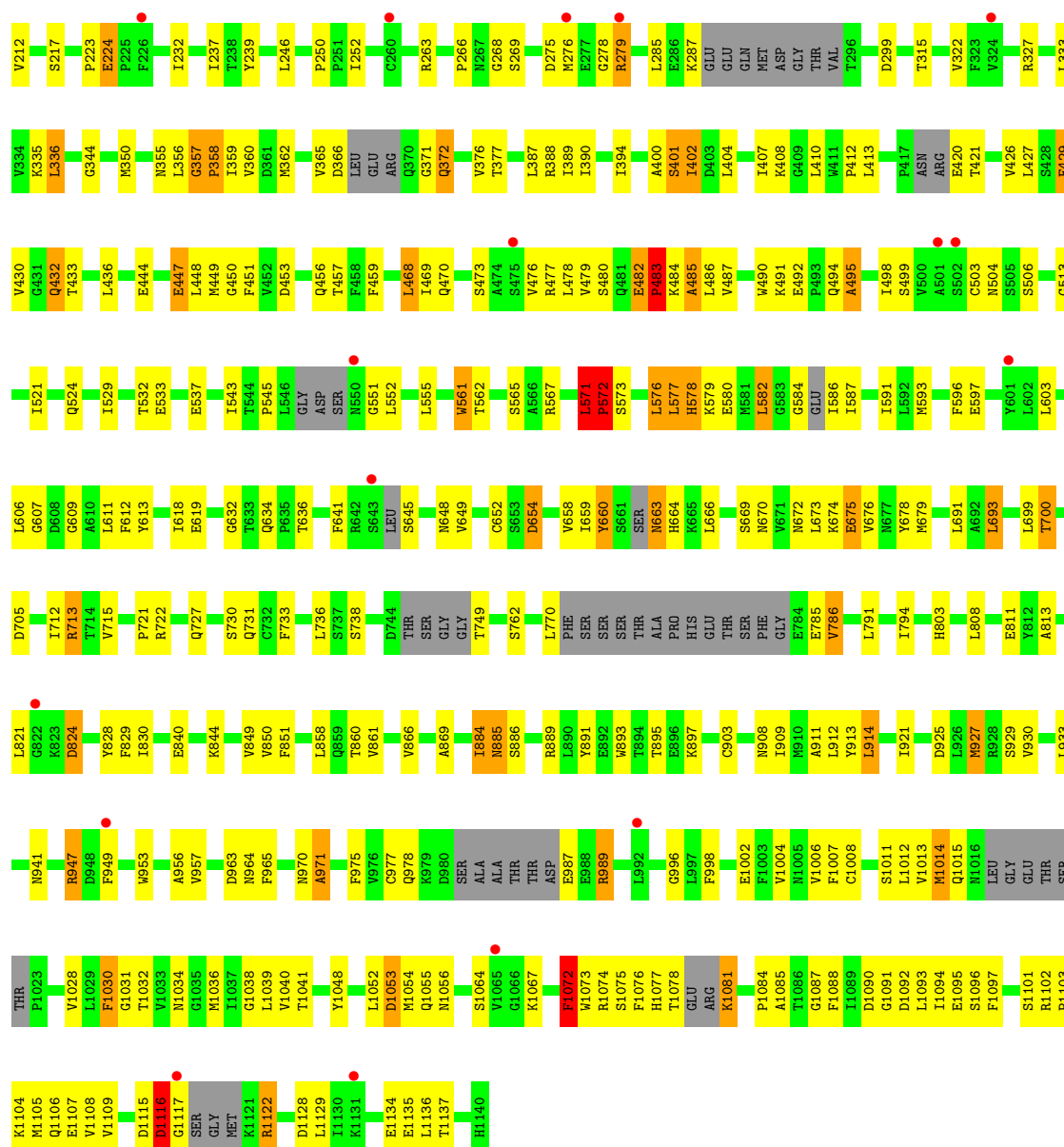


- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A

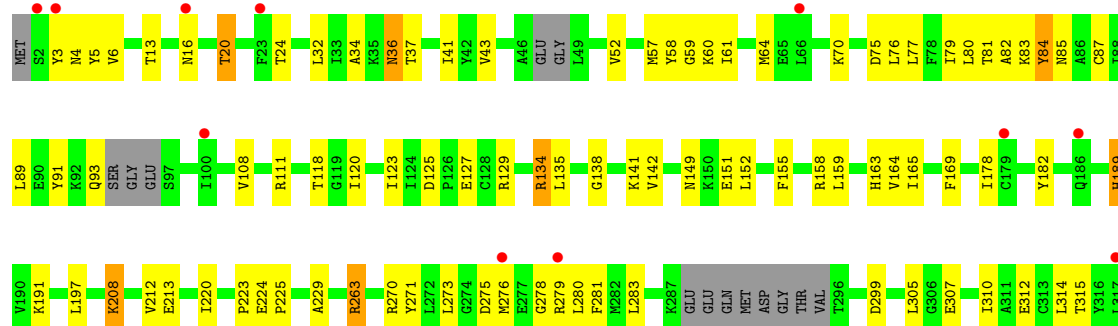


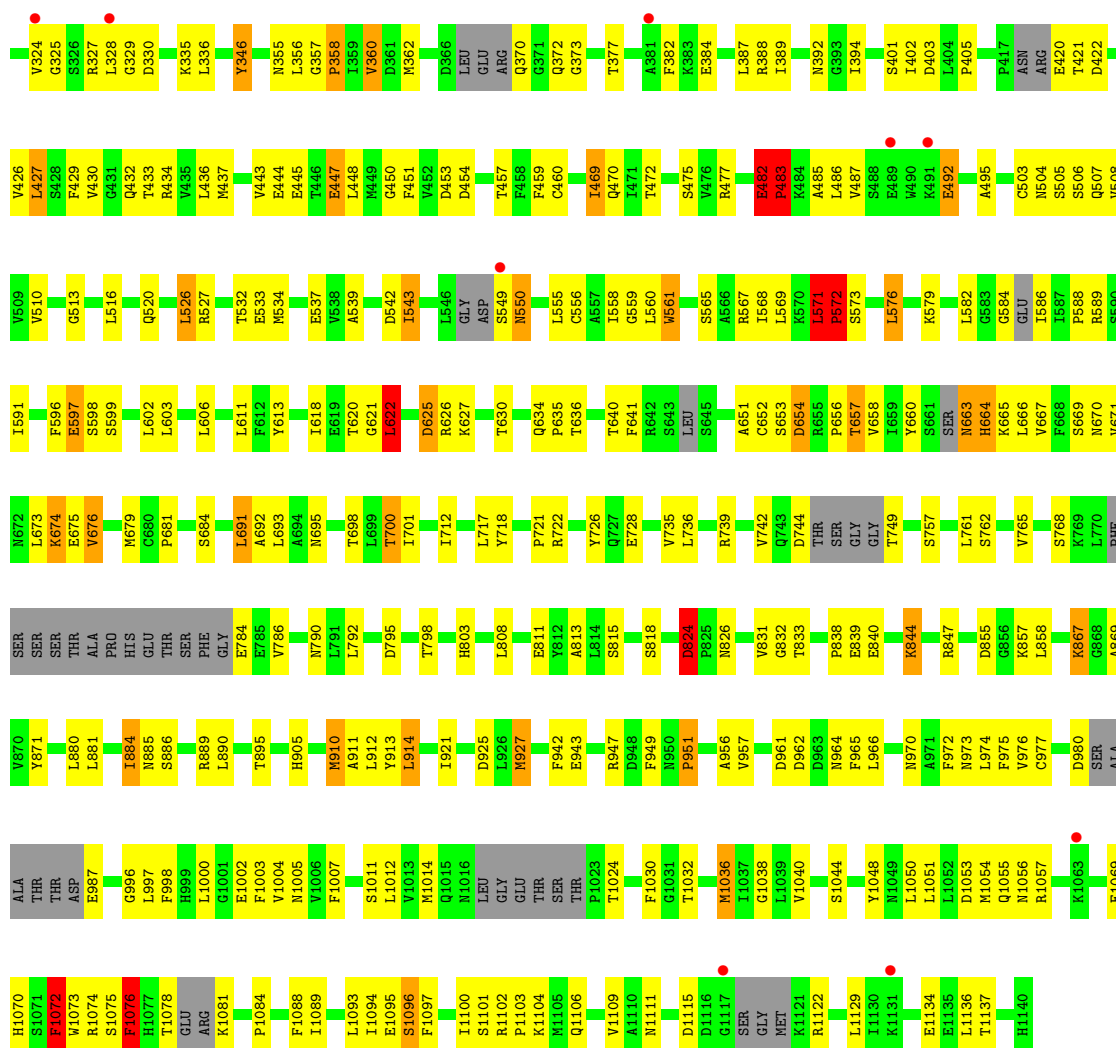
- Molecule 2: DNA damage-binding protein 1



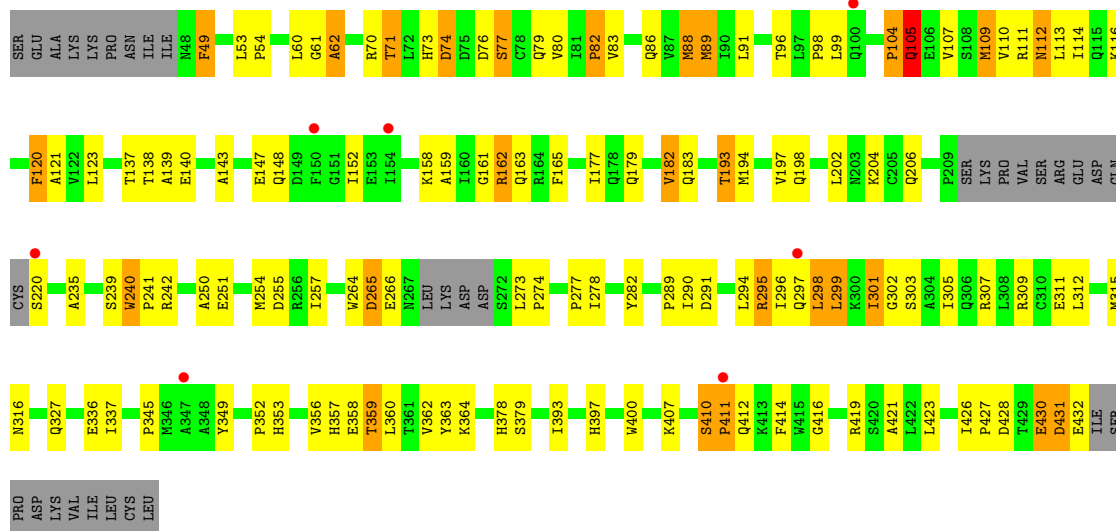


### • Molecule 2: DNA damage-binding protein 1



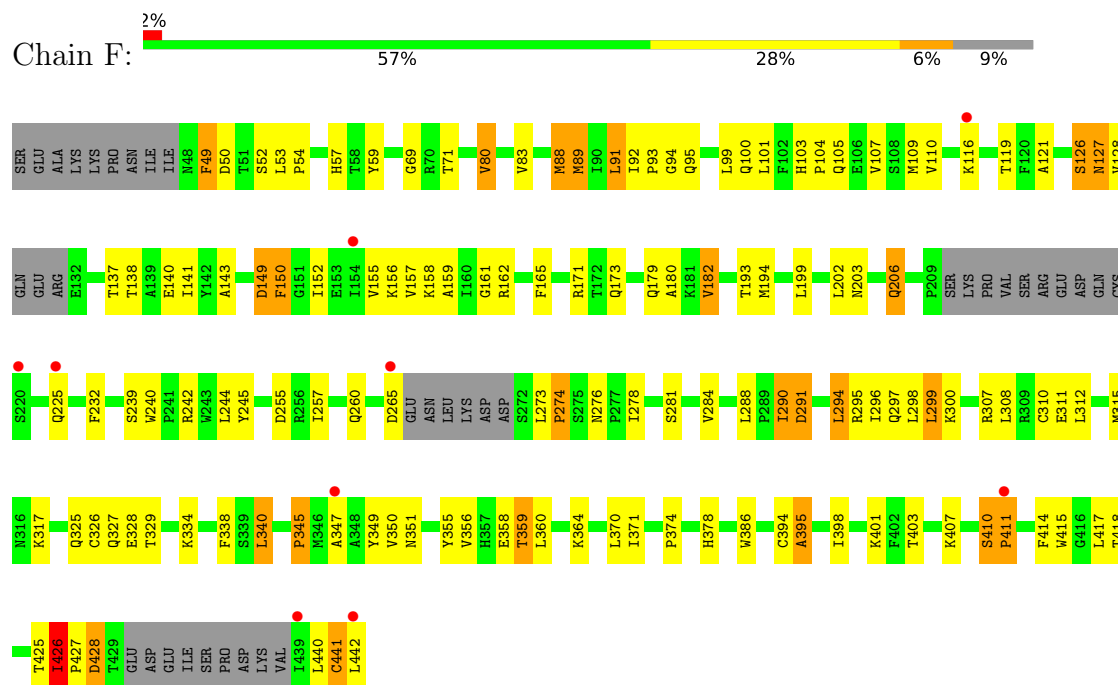


### • Molecule 3: Protein cereblon





● Molecule 3: Protein cereblon



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.34Å 112.38Å 177.94Å 90.00° 95.25° 90.00°	Depositor
Resolution (Å)	49.49 – 3.90 49.49 – 3.90	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.49-3.90) 96.5 (49.49-3.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.259 , 0.336 (Not available) , 0.296	Depositor DCC
$R_{free}$ test set	2100 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	107.4	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 183.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	26021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1IWG, 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	0.49	0/1534	1.11	1/2068 (0.0%)
1	D	0.49	0/1542	1.11	2/2079 (0.1%)
2	B	0.49	0/8637	1.01	17/11683 (0.1%)
2	E	0.49	0/8647	1.00	14/11696 (0.1%)
3	C	0.48	0/3067	1.06	10/4160 (0.2%)
3	F	0.48	0/3023	1.04	7/4099 (0.2%)
All	All	0.49	0/26450	1.03	51/35785 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	D	0	2
2	B	0	4
2	E	0	3
3	C	0	3
All	All	0	18

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	572	PRO	N-CA-CB	-8.46	94.36	103.25
2	B	572	PRO	N-CA-CB	-7.99	94.86	103.25
2	B	360	VAL	N-CA-CB	-7.69	105.33	111.64
2	B	1072	PHE	CA-CB-CG	7.39	121.19	113.80
2	B	1076	PHE	N-CA-CB	-7.30	99.30	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	291	ASP	CA-CB-CG	6.83	119.43	112.60
2	E	1072	PHE	CA-CB-CG	6.75	120.55	113.80
2	E	1076	PHE	N-CA-CB	-6.71	99.14	110.49
3	C	49	PHE	CA-CB-CG	6.57	120.36	113.80
2	B	483	PRO	N-CA-CB	-6.55	96.37	103.25
3	C	240	TRP	N-CA-C	6.18	113.78	108.22
2	B	1115	ASP	CA-CB-CG	6.17	118.77	112.60
3	C	291	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	474	PRO	N-CA-C	6.05	124.93	112.47
2	B	114	ARG	CB-CA-C	6.02	116.57	109.47
3	C	96	THR	CA-CB-OG1	-5.84	100.85	109.60
3	C	82	PRO	N-CA-CB	-5.74	97.22	103.25
3	F	359	THR	CA-CB-OG1	-5.67	101.09	109.60
3	F	49	PHE	CA-CB-CG	5.62	119.42	113.80
1	D	622	LYS	N-CA-CB	5.59	118.19	109.97
2	B	447	GLU	CB-CG-CD	5.57	122.06	112.60
2	B	365	VAL	N-CA-CB	-5.53	104.11	112.35
2	E	824	ASP	CA-CB-CG	5.51	118.11	112.60
3	C	431	ASP	CA-CB-CG	5.48	118.08	112.60
2	E	454	ASP	CA-CB-CG	5.48	118.08	112.60
2	B	1053	ASP	CA-CB-CG	5.40	118.00	112.60
2	B	705	ASP	CA-CB-CG	5.39	117.99	112.60
2	E	824	ASP	CB-CA-C	5.39	116.14	108.76
3	F	119	THR	CA-CB-OG1	-5.35	101.58	109.60
3	F	265	ASP	CA-CB-CG	5.29	117.89	112.60
3	C	359	THR	CA-CB-OG1	-5.27	101.69	109.60
3	C	414	PHE	CA-CB-CG	5.25	119.05	113.80
2	E	1115	ASP	CA-CB-CG	5.25	117.85	112.60
3	F	414	PHE	CA-CB-CG	5.22	119.03	113.80
2	B	453	ASP	CB-CA-C	-5.21	101.79	110.81
2	E	453	ASP	CA-CB-CG	5.21	117.81	112.60
2	E	572	PRO	N-CA-C	5.21	123.19	112.47
3	F	274	PRO	N-CA-C	5.18	119.62	111.38
2	B	1116	ASP	CA-CB-CG	5.15	117.75	112.60
3	C	336	GLU	CB-CG-CD	5.15	121.35	112.60
2	E	833	THR	CA-CB-OG1	-5.12	101.92	109.60
2	E	483	PRO	N-CA-CB	-5.12	97.88	103.25
2	B	366	ASP	CA-CB-CG	5.11	117.71	112.60
3	C	76	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	539	GLU	CB-CA-C	-5.11	102.28	110.14
2	B	453	ASP	CA-CB-CG	5.07	117.67	112.60
2	E	1003	PHE	CA-CB-CG	5.07	118.87	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	545	PRO	N-CA-CB	-5.06	97.94	103.25
2	E	447	GLU	CB-CG-CD	5.06	121.19	112.60
2	E	630	THR	CA-CB-OG1	-5.05	102.02	109.60
2	B	1030	PHE	CA-CB-CG	5.05	118.85	113.80

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	472	MET	Peptide
1	A	473	MET	Peptide
1	A	510	GLU	Peptide
1	A	588	ASP	Peptide
1	A	601	ILE	Peptide
1	A	603	LEU	Peptide
2	B	224	GLU	Peptide
2	B	327	ARG	Sidechain
2	B	571	LEU	Peptide
2	B	989	ARG	Sidechain
3	C	264	TRP	Peptide
3	C	265	ASP	Peptide
3	C	295	ARG	Sidechain
1	D	509	GLU	Peptide
1	D	601	ILE	Peptide
2	E	360	VAL	Peptide
2	E	482	GLU	Peptide
2	E	571	LEU	Peptide

## 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	1513	0	1584	64	0
1	D	1520	0	1592	81	0
2	B	8491	0	8487	202	0
2	E	8501	0	8496	232	0
3	C	2996	0	2971	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2954	0	2952	89	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
5	C	22	0	0	2	0
5	F	22	0	0	1	0
All	All	26021	0	26082	734	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 14.

All (734) 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:C:74:ASP:O	3:C:77:SER:OG	1.89	0.90
2:B:451:PHE:CE2	2:B:470:GLN:HB2	2.13	0.81
3:F:257:ILE:HG23	3:F:315:MET:HE1	1.62	0.81
2:B:433:THR:OG1	2:B:457:THR:OG1	1.99	0.80
2:E:1078:THR:HG1	2:E:1081:LYS:N	1.81	0.79
2:E:824:ASP:OD1	2:E:826:ASN:N	2.16	0.77
3:C:273:LEU:HB2	3:C:274:PRO:HD2	1.66	0.77
2:E:451:PHE:CE2	2:E:470:GLN:HB2	2.20	0.76
3:F:290:ILE:HD12	3:F:295:ARG:HA	1.69	0.75
2:B:571:LEU:HB3	2:B:572:PRO:CD	2.18	0.74
1:D:601:ILE:HG22	1:D:602:CYS:H	1.53	0.73
1:D:447:LYS:O	1:D:447:LYS:HG2	1.88	0.73
2:B:537:GLU:O	2:B:561:TRP:HB2	1.88	0.72
2:E:869:ALA:O	2:E:884:ILE:HA	1.89	0.72
3:C:83:VAL:HG22	3:C:121:ALA:HB3	1.73	0.71
2:E:795:ASP:HB3	2:E:798:THR:OG1	1.91	0.71
2:B:869:ALA:O	2:B:884:ILE:HA	1.90	0.71
2:B:674:LYS:O	2:B:675:GLU:O	2.10	0.70
2:E:913:TYR:CE1	2:E:956:ALA:HA	2.25	0.70
3:F:349:TYR:CD2	3:F:359:THR:HG22	2.27	0.70
3:F:273:LEU:HB2	3:F:274:PRO:HD2	1.74	0.69
1:A:633:VAL:HG12	1:A:634:PRO:HD2	1.74	0.69
1:A:601:ILE:HG22	1:A:602:CYS:N	2.07	0.69
3:C:112:ASN:C	3:C:114:ILE:H	2.00	0.69
2:B:359:ILE:HB	2:B:1032:THR:H	1.57	0.69
1:D:605:THR:HG22	1:D:630:LEU:O	1.93	0.69
2:E:472:THR:HG1	2:E:475:SER:H	1.40	0.68
2:E:13:THR:HB	2:E:355:ASN:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ILE:O	2:B:132:GLY:N	2.24	0.68
2:B:83:LYS:NZ	2:B:1075:SER:O	2.27	0.67
1:D:473:MET:SD	1:D:475:ASN:N	2.65	0.67
3:F:410:SER:HB3	3:F:411:PRO:HD2	1.76	0.67
2:B:565:SER:OG	2:B:567:ARG:NH1	2.28	0.67
2:E:1000:LEU:O	2:E:1074:ARG:NH1	2.28	0.67
2:E:537:GLU:O	2:E:561:TRP:HB2	1.95	0.67
2:E:584:GLY:O	2:E:586:ILE:N	2.28	0.67
3:F:359:THR:HA	3:F:417:LEU:O	1.95	0.67
3:F:83:VAL:HG22	3:F:121:ALA:HB3	1.76	0.67
3:F:273:LEU:HB2	3:F:274:PRO:CD	2.25	0.67
2:B:118:THR:HG21	2:B:165:ILE:O	1.96	0.66
3:C:112:ASN:O	3:C:114:ILE:N	2.29	0.66
2:E:355:ASN:O	2:E:357:GLY:N	2.29	0.66
2:B:1078:THR:HG1	2:B:1081:LYS:N	1.94	0.65
1:A:454:VAL:O	1:A:455:VAL:HG23	1.96	0.65
2:B:571:LEU:O	2:B:573:SER:N	2.30	0.65
2:E:663:ASN:C	2:E:663:ASN:HD22	2.05	0.65
2:E:913:TYR:CZ	3:F:240:TRP:HZ3	2.13	0.65
1:A:527:SER:OG	1:A:528:GLY:N	2.30	0.65
3:F:410:SER:HB3	3:F:411:PRO:CD	2.27	0.65
2:B:1102:ARG:N	2:B:1103:PRO:HD2	2.12	0.65
2:B:609:GLY:HA3	2:B:632:GLY:O	1.97	0.64
3:C:109:MET:HB2	3:C:177:ILE:CD1	2.27	0.64
3:F:378:HIS:O	5:F:502:A1IWG:N2	2.31	0.64
1:A:473:MET:HB3	1:A:474:PRO:CD	2.28	0.64
1:D:568:CYS:HB2	1:D:592:ILE:HD11	1.79	0.64
2:E:394:ILE:HD11	2:E:669:SER:OG	1.97	0.64
3:F:310:CYS:SG	3:F:442:LEU:HB3	2.38	0.64
2:B:149:ASN:ND2	2:B:153:LYS:O	2.31	0.63
2:B:59:GLY:HA2	2:B:1073:TRP:CZ3	2.33	0.63
1:A:633:VAL:CG1	1:A:634:PRO:HD2	2.29	0.63
1:D:536:VAL:HG13	1:D:626:ILE:HD12	1.81	0.63
2:B:634:GLN:HB2	2:B:654:ASP:OD1	1.98	0.63
2:E:651:ALA:HB3	2:E:657:THR:HB	1.80	0.63
2:E:1102:ARG:N	2:E:1103:PRO:HD2	2.14	0.62
1:A:451:MET:SD	1:A:503:ARG:HD3	2.40	0.62
1:D:486:SER:O	1:D:488:ASP:N	2.32	0.61
1:D:540:HIS:CD2	1:D:544:ILE:HG22	2.35	0.61
2:E:663:ASN:HB2	2:E:1134:GLU:OE1	2.00	0.61
2:B:450:GLY:O	2:B:477:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:442:LEU:HD23	1:D:518:LEU:HD12	1.83	0.61
2:B:355:ASN:C	2:B:357:GLY:H	2.09	0.61
2:E:426:VAL:C	2:E:427:LEU:HD12	2.25	0.61
2:E:597:GLU:OE2	2:E:663:ASN:N	2.33	0.61
2:E:913:TYR:CZ	3:F:240:TRP:CZ3	2.89	0.61
2:B:1109:VAL:HG12	2:B:1129:LEU:HD22	1.82	0.61
2:E:1095:GLU:C	2:E:1097:PHE:H	2.08	0.61
2:E:427:LEU:HD12	2:E:427:LEU:N	2.15	0.61
1:A:550:ALA:O	1:A:561:VAL:HG12	2.01	0.61
2:B:506:SER:OG	2:B:552:LEU:HD22	2.01	0.61
3:C:410:SER:HB3	3:C:411:PRO:CD	2.30	0.61
2:B:1054:MET:CE	2:B:1129:LEU:HD23	2.31	0.61
2:B:451:PHE:CD2	2:B:470:GLN:HB2	2.35	0.60
2:B:24:THR:HA	2:B:91:TYR:CD1	2.36	0.60
1:D:485:LEU:HB2	1:D:501:LYS:HB2	1.82	0.60
2:B:1054:MET:HE1	2:B:1129:LEU:HD23	1.81	0.60
3:C:165:PHE:CD1	3:C:182:VAL:CG2	2.84	0.60
2:B:582:LEU:HD23	2:B:612:PHE:CD2	2.37	0.60
3:C:337:ILE:HA	3:C:362:VAL:HG12	1.84	0.60
1:D:581:ARG:O	1:D:583:ARG:NH1	2.34	0.60
2:E:571:LEU:C	2:E:573:SER:H	2.09	0.60
2:E:134:ARG:NH2	2:E:164:VAL:O	2.35	0.60
1:A:601:ILE:HG22	1:A:602:CYS:H	1.65	0.59
2:B:571:LEU:HB3	2:B:572:PRO:HD2	1.85	0.59
1:A:473:MET:HB3	1:A:474:PRO:HD3	1.84	0.59
2:B:118:THR:HB	2:B:134:ARG:HH22	1.67	0.59
1:A:568:CYS:SG	1:A:578:SER:O	2.60	0.58
2:B:432:GLN:O	2:B:456:GLN:HA	2.02	0.58
2:B:964:ASN:HA	2:B:977:CYS:O	2.03	0.58
2:E:762:SER:O	2:E:803:HIS:HA	2.03	0.58
1:D:495:ALA:HB1	1:D:496:PRO:HD2	1.85	0.58
2:E:485:ALA:O	2:E:487:VAL:HG13	2.03	0.58
3:F:232:PHE:O	3:F:242:ARG:HG2	2.03	0.58
3:F:410:SER:O	3:F:411:PRO:C	2.45	0.58
2:B:1055:GLN:O	2:B:1056:ASN:C	2.45	0.58
2:B:913:TYR:CE1	2:B:956:ALA:HA	2.39	0.58
2:E:81:THR:HG22	2:E:85:ASN:HB2	1.86	0.58
2:B:636:THR:HA	2:B:652:CYS:O	2.02	0.58
1:D:572:LYS:NZ	1:D:588:ASP:OD2	2.27	0.58
3:F:149:ASP:O	3:F:150:PHE:C	2.46	0.58
2:B:1116:ASP:O	2:B:1117:GLY:C	2.47	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:SER:C	2:B:402:ILE:HG13	2.28	0.58
2:E:451:PHE:CD2	2:E:470:GLN:HB2	2.38	0.58
2:E:815:SER:O	2:E:831:VAL:HA	2.04	0.58
2:E:43:VAL:HG23	2:E:52:VAL:HG21	1.85	0.57
2:B:1032:THR:HB	2:B:1036:MET:O	2.04	0.57
2:B:1064:SER:OG	2:B:1067:LYS:HA	2.05	0.57
3:C:410:SER:CB	3:C:411:PRO:CD	2.82	0.57
2:E:450:GLY:O	2:E:477:ARG:NH2	2.37	0.57
3:C:296:ILE:O	3:C:297:GLN:C	2.47	0.57
2:E:636:THR:HA	2:E:652:CYS:O	2.04	0.57
2:E:79:ILE:HB	2:E:87:CYS:SG	2.43	0.57
2:E:613:TYR:CD2	2:E:666:LEU:HD12	2.40	0.57
1:D:605:THR:HG23	1:D:632:LEU:HD11	1.87	0.57
2:E:1078:THR:OG1	2:E:1081:LYS:N	2.38	0.57
2:E:1095:GLU:O	2:E:1097:PHE:N	2.37	0.57
2:E:571:LEU:HB3	2:E:572:PRO:CD	2.34	0.57
3:C:140:GLU:O	3:C:159:ALA:HA	2.05	0.57
2:E:1055:GLN:O	2:E:1056:ASN:C	2.48	0.57
3:F:410:SER:CB	3:F:411:PRO:CD	2.83	0.57
2:B:127:GLU:HB2	2:B:129:ARG:HG2	1.87	0.56
2:B:1013:VAL:O	2:B:1014:MET:O	2.23	0.56
2:B:106:GLY:HA3	2:B:152:LEU:HB2	1.86	0.56
3:C:109:MET:HB2	3:C:177:ILE:HD13	1.85	0.56
3:F:138:THR:OG1	3:F:162:ARG:HB2	2.05	0.56
3:F:296:ILE:O	3:F:299:LEU:N	2.37	0.56
3:C:257:ILE:HG23	3:C:315:MET:HE1	1.87	0.56
1:D:440:ILE:HD11	1:D:470:LEU:HD22	1.86	0.56
1:D:472:MET:HB2	1:D:518:LEU:HD23	1.87	0.56
2:E:472:THR:HG1	2:E:475:SER:N	2.03	0.56
3:C:410:SER:O	3:C:412:GLN:N	2.39	0.56
2:E:138:GLY:HA2	2:E:159:LEU:HB2	1.87	0.56
2:E:620:THR:OG1	2:E:621:GLY:N	2.39	0.56
2:E:914:LEU:HD21	2:E:921:ILE:HG23	1.87	0.56
3:F:143:ALA:HB3	3:F:158:LYS:HB2	1.88	0.56
2:E:1097:PHE:O	2:E:1100:ILE:HG12	2.05	0.56
2:E:358:PRO:O	2:E:360:VAL:HG23	2.05	0.55
2:B:1134:GLU:C	2:B:1136:LEU:H	2.14	0.55
2:B:1104:LYS:O	2:B:1108:VAL:HG23	2.06	0.55
2:E:695:ASN:OD1	2:E:698:THR:N	2.35	0.55
3:F:328:GLU:O	3:F:329:THR:OG1	2.22	0.55
1:A:459:LEU:HB2	1:A:500:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:558:ILE:HG12	2:E:569:LEU:HD23	1.89	0.55
2:B:663:ASN:HD22	2:B:663:ASN:C	2.14	0.55
2:B:1004:VAL:HG11	2:B:1007:PHE:CZ	2.42	0.55
1:D:536:VAL:HG13	1:D:626:ILE:CD1	2.37	0.55
2:B:884:ILE:HD12	2:B:884:ILE:N	2.22	0.55
2:E:57:MET:HE2	2:E:79:ILE:HG21	1.89	0.55
2:E:76:LEU:HD22	2:E:89:LEU:O	2.07	0.55
1:A:459:LEU:HD13	1:A:496:PRO:HA	1.89	0.54
2:E:656:PRO:O	2:E:671:VAL:HG23	2.07	0.54
1:A:568:CYS:HB2	1:A:592:ILE:HD11	1.88	0.54
1:D:633:VAL:HG12	1:D:634:PRO:HD2	1.90	0.54
3:F:100:GLN:HA	3:F:155:VAL:O	2.07	0.54
1:A:535:ILE:HG22	1:A:535:ILE:O	2.05	0.54
1:A:587:GLN:O	1:A:588:ASP:HB2	2.06	0.54
2:B:591:ILE:HG13	2:B:603:LEU:O	2.07	0.54
2:B:1032:THR:HG21	2:B:1036:MET:HB3	1.90	0.54
1:D:541:LYS:HE2	1:D:541:LYS:H	1.73	0.54
1:D:604:GLU:CG	1:D:612:MET:HE2	2.37	0.54
3:C:294:LEU:O	3:C:295:ARG:C	2.51	0.54
1:D:535:ILE:N	1:D:591:CYS:O	2.38	0.54
2:E:392:ASN:ND2	2:E:1012:LEU:O	2.40	0.54
2:E:871:TYR:CE1	3:F:244:LEU:HD13	2.42	0.54
2:E:556:CYS:HB2	2:E:571:LEU:HD11	1.89	0.54
2:E:1030:PHE:CZ	2:E:1038:GLY:HA3	2.43	0.54
2:B:357:GLY:O	2:B:358:PRO:C	2.51	0.54
2:B:648:ASN:OD1	2:B:660:TYR:HB3	2.08	0.54
2:E:61:ILE:HG23	2:E:79:ILE:HG23	1.90	0.54
2:E:275:ASP:OD1	2:E:276:MET:N	2.41	0.54
2:E:558:ILE:HG22	2:E:560:LEU:HD23	1.89	0.54
1:A:473:MET:O	1:A:475:ASN:N	2.38	0.54
2:B:275:ASP:HB2	2:B:279:ARG:O	2.08	0.54
2:B:914:LEU:HD21	2:B:921:ILE:HG23	1.89	0.54
1:D:566:LEU:CD2	1:D:585:VAL:HG12	2.38	0.54
1:D:633:VAL:O	1:D:634:PRO:C	2.51	0.54
2:B:824:ASP:C	2:B:824:ASP:OD1	2.50	0.53
3:C:88:MET:O	3:C:89:MET:CB	2.56	0.53
1:D:539:GLU:O	1:D:624:ILE:HG13	2.08	0.53
2:B:912:LEU:HB3	3:C:240:TRP:CH2	2.43	0.53
2:E:273:LEU:HB2	2:E:281:PHE:HB2	1.90	0.53
2:E:276:MET:HE2	3:F:202:LEU:HD22	1.89	0.53
2:B:250:PRO:HB2	2:B:252:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:721:PRO:O	2:B:722:ARG:HG2	2.08	0.53
1:A:441:ARG:HA	1:A:518:LEU:O	2.08	0.53
1:A:484:ILE:O	1:A:490:GLU:OE1	2.26	0.53
3:C:104:PRO:O	3:C:107:VAL:N	2.41	0.53
2:B:448:LEU:HD23	2:B:451:PHE:CD1	2.44	0.53
2:E:726:TYR:CZ	2:E:728:GLU:HA	2.44	0.53
2:B:486:LEU:HD12	2:B:487:VAL:N	2.23	0.53
3:C:410:SER:O	3:C:411:PRO:C	2.51	0.53
2:E:691:LEU:O	2:E:701:ILE:HA	2.09	0.53
3:F:394:CYS:O	3:F:395:ALA:HB3	2.09	0.53
2:B:278:GLY:O	2:B:279:ARG:C	2.51	0.53
2:B:555:LEU:HD13	2:B:593:MET:SD	2.49	0.53
3:C:250:ALA:HB2	3:C:305:ILE:HD11	1.90	0.53
2:E:589:ARG:HG3	2:E:635:PRO:HB3	1.90	0.53
3:F:349:TYR:CE2	3:F:359:THR:HG22	2.44	0.53
2:B:263:ARG:HH11	2:B:266:PRO:HA	1.74	0.52
2:B:371:GLY:O	2:B:372:GLN:C	2.51	0.52
2:B:394:ILE:CD1	2:B:658:VAL:HB	2.39	0.52
1:D:613:GLY:O	1:D:629:VAL:HG12	2.10	0.52
2:B:239:TYR:HB3	2:B:246:LEU:HB2	1.90	0.52
2:B:736:LEU:HD13	2:B:813:ALA:HB1	1.91	0.52
2:E:640:THR:O	2:E:641:PHE:HB3	2.10	0.52
2:B:649:VAL:HB	2:B:659:ILE:HB	1.92	0.52
3:C:352:PRO:O	3:C:353:HIS:CG	2.62	0.52
1:D:633:VAL:HG12	1:D:634:PRO:CD	2.39	0.52
2:E:998:PHE:HB2	2:E:1088:PHE:CD2	2.44	0.52
1:D:540:HIS:CD2	1:D:544:ILE:CG2	2.93	0.52
2:E:961:ASP:O	2:E:962:ASP:C	2.53	0.52
1:D:441:ARG:HG2	1:D:612:MET:HE1	1.91	0.52
2:B:410:LEU:CD1	2:B:427:LEU:HG	2.40	0.52
2:B:477:ARG:NH1	2:B:486:LEU:HD22	2.24	0.52
2:B:652:CYS:HB3	2:B:676:VAL:O	2.09	0.52
1:D:563:ILE:HG22	1:D:595:LEU:HD11	1.92	0.52
2:B:359:ILE:HG21	2:B:1031:GLY:HA3	1.93	0.51
1:D:584:PHE:O	1:D:584:PHE:CD1	2.63	0.51
2:E:64:MET:HG3	2:E:77:LEU:HD11	1.91	0.51
2:B:20:THR:HG23	2:B:315:THR:HG23	1.92	0.51
2:B:31:LEU:HD13	2:B:315:THR:HG21	1.90	0.51
1:A:447:LYS:H	1:A:447:LYS:HD3	1.75	0.51
1:D:441:ARG:HG3	1:D:525:CYS:SG	2.50	0.51
1:D:533:ALA:HA	1:D:628:LYS:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:LEU:HD11	2:E:41:ILE:HG23	1.93	0.51
2:E:224:GLU:N	2:E:225:PRO:CD	2.74	0.51
1:D:615:PHE:HE1	1:D:617:LEU:HD13	1.75	0.51
2:B:762:SER:O	2:B:803:HIS:HA	2.11	0.51
2:E:394:ILE:HD12	2:E:671:VAL:HG22	1.93	0.51
3:F:351:ASN:OD1	3:F:355:TYR:HB2	2.10	0.51
1:A:605:THR:HG22	1:A:632:LEU:HD11	1.92	0.51
2:B:165:ILE:HG21	2:B:217:SER:HA	1.92	0.51
1:D:454:VAL:HG12	1:D:455:VAL:H	1.76	0.51
2:E:824:ASP:OD1	2:E:824:ASP:C	2.54	0.51
2:E:881:LEU:HD12	2:E:889:ARG:O	2.09	0.51
3:F:203:ASN:O	3:F:206:GLN:HB2	2.11	0.51
2:E:60:LYS:N	2:E:81:THR:OG1	2.44	0.51
2:E:433:THR:OG1	2:E:457:THR:OG1	2.11	0.51
2:B:204:LYS:HE2	2:B:204:LYS:HA	1.92	0.51
1:A:552:LEU:HB2	1:A:561:VAL:HG11	1.92	0.50
2:B:80:LEU:HD12	2:B:85:ASN:O	2.11	0.50
3:C:349:TYR:CD2	3:C:359:THR:HG22	2.46	0.50
2:E:565:SER:OG	2:E:567:ARG:NH1	2.44	0.50
3:F:288:LEU:O	3:F:290:ILE:HG12	2.11	0.50
1:A:563:ILE:HG22	1:A:595:LEU:CD1	2.41	0.50
2:B:362:MET:HE3	2:B:1008:CYS:SG	2.51	0.50
3:C:360:LEU:O	3:C:416:GLY:HA2	2.11	0.50
1:D:474:PRO:C	1:D:476:LYS:H	2.18	0.50
1:D:601:ILE:HG22	1:D:602:CYS:N	2.23	0.50
2:B:503:CYS:SG	2:B:504:ASN:N	2.84	0.50
1:D:445:VAL:HG23	1:D:457:GLY:HA2	1.94	0.50
2:E:263:ARG:HA	2:E:271:TYR:CE1	2.46	0.50
1:D:563:ILE:HG22	1:D:595:LEU:CD1	2.42	0.50
2:E:625:ASP:O	2:E:626:ARG:HG3	2.12	0.50
1:D:568:CYS:HA	1:D:582:PRO:HD3	1.92	0.50
2:E:280:LEU:O	2:E:305:LEU:HB2	2.12	0.50
2:E:665:LYS:O	2:E:667:VAL:HG23	2.10	0.50
1:A:443:PRO:HA	1:A:517:ILE:HG22	1.93	0.50
2:E:970:ASN:O	2:E:973:ASN:ND2	2.45	0.50
3:F:398:ILE:O	3:F:418:THR:HG22	2.11	0.50
1:A:566:LEU:HD22	1:A:585:VAL:HG12	1.93	0.50
2:E:5:TYR:O	2:E:1040:VAL:HA	2.12	0.50
2:E:60:LYS:HE2	2:E:972:PHE:CE2	2.47	0.50
2:E:108:VAL:O	2:E:141:LYS:NZ	2.44	0.50
2:E:482:GLU:HG3	2:E:483:PRO:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:925:ASP:C	2:E:927:MET:H	2.20	0.50
1:D:542:SER:OG	1:D:543:ILE:N	2.44	0.49
2:B:1093:LEU:O	2:B:1094:ILE:C	2.55	0.49
1:D:480:GLU:HG3	1:D:505:LYS:HE2	1.94	0.49
2:E:736:LEU:HD13	2:E:813:ALA:HB1	1.94	0.49
1:A:552:LEU:CD1	1:A:615:PHE:CD1	2.95	0.49
1:A:603:LEU:HD22	1:A:629:VAL:HG21	1.93	0.49
3:C:378:HIS:O	5:C:502:A1IWG:N2	2.45	0.49
2:E:4:ASN:HD21	2:E:976:VAL:HG21	1.77	0.49
3:F:138:THR:O	3:F:161:GLY:HA2	2.12	0.49
2:E:182:TYR:CE1	2:E:189:HIS:HB2	2.48	0.49
2:E:549:SER:O	2:E:550:ASN:HB2	2.11	0.49
2:E:735:VAL:O	2:E:792:LEU:N	2.41	0.49
2:E:964:ASN:HA	2:E:977:CYS:O	2.12	0.49
2:E:1095:GLU:C	2:E:1097:PHE:N	2.67	0.49
1:A:563:ILE:HG22	1:A:595:LEU:HD11	1.94	0.49
2:B:459:PHE:CD1	2:B:459:PHE:C	2.90	0.49
2:B:1074:ARG:O	2:B:1085:ALA:HB2	2.12	0.49
2:E:975:PHE:HA	2:E:996:GLY:O	2.12	0.49
2:E:905:HIS:HB2	2:E:942:PHE:HD2	1.78	0.49
2:E:964:ASN:O	2:E:965:PHE:CD1	2.65	0.49
1:A:536:VAL:HG13	1:A:626:ILE:HD12	1.95	0.49
2:B:889:ARG:HD2	2:B:891:TYR:OH	2.13	0.49
1:D:442:LEU:HB3	1:D:518:LEU:HB2	1.95	0.49
1:D:447:LYS:HD3	1:D:447:LYS:H	1.78	0.49
3:F:317:LYS:O	3:F:426:ILE:HG22	2.13	0.49
3:F:370:LEU:O	3:F:371:ILE:HG23	2.13	0.49
3:C:309:ARG:C	3:C:311:GLU:H	2.21	0.49
3:C:379:SER:HA	5:C:502:A1IWG:O1	2.12	0.49
1:D:554:ILE:O	1:D:555:HIS:C	2.56	0.49
2:E:1036:MET:C	2:E:1036:MET:SD	2.96	0.49
1:A:601:ILE:CG2	1:A:602:CYS:N	2.75	0.49
2:B:149:ASN:O	2:B:150:LYS:C	2.55	0.49
2:E:571:LEU:O	2:E:573:SER:N	2.45	0.49
2:E:691:LEU:HD23	2:E:693:LEU:HD11	1.95	0.49
2:B:19:VAL:HG12	2:B:64:MET:HE3	1.95	0.49
2:B:355:ASN:C	2:B:357:GLY:N	2.70	0.49
2:B:377:THR:O	2:B:387:LEU:HA	2.13	0.49
2:B:504:ASN:HD22	2:B:543:ILE:HG23	1.77	0.49
2:B:929:SER:HB3	2:B:949:PHE:CD2	2.48	0.49
2:E:142:VAL:HB	2:E:155:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:808:LEU:HD13	2:E:847:ARG:NH2	2.28	0.49
1:A:473:MET:CB	1:A:474:PRO:CD	2.90	0.48
1:A:500:LEU:HD23	1:A:502:ILE:HD11	1.95	0.48
2:E:1102:ARG:N	2:E:1103:PRO:CD	2.75	0.48
3:F:93:PRO:C	3:F:95:GLN:H	2.20	0.48
3:F:99:LEU:HB2	3:F:157:VAL:HG23	1.95	0.48
2:E:372:GLN:HG3	2:E:373:GLY:H	1.79	0.48
3:F:165:PHE:CD1	3:F:182:VAL:CG2	2.96	0.48
3:C:194:MET:HE1	3:C:235:ALA:HA	1.95	0.48
2:B:486:LEU:HD12	2:B:487:VAL:H	1.78	0.48
2:B:1030:PHE:CE1	2:B:1036:MET:HE1	2.48	0.48
3:C:53:LEU:N	3:C:54:PRO:CD	2.77	0.48
2:E:1134:GLU:C	2:E:1136:LEU:H	2.21	0.48
1:A:440:ILE:C	1:A:440:ILE:HD12	2.38	0.48
2:B:389:ILE:HB	2:B:713:ARG:HB3	1.96	0.48
3:F:296:ILE:O	3:F:297:GLN:C	2.56	0.48
2:B:276:MET:HE2	3:C:202:LEU:HD22	1.94	0.48
3:C:165:PHE:CD1	3:C:182:VAL:HG22	2.48	0.48
2:E:803:HIS:CE1	2:E:858:LEU:HB3	2.47	0.48
2:B:543:ILE:HD11	2:B:571:LEU:HD21	1.95	0.48
2:B:404:LEU:HD22	2:B:407:ILE:HD11	1.95	0.48
2:B:613:TYR:CE2	2:B:666:LEU:HD12	2.48	0.48
3:C:397:HIS:HE1	3:C:400:TRP:CZ2	2.32	0.48
3:F:345:PRO:HB2	3:F:360:LEU:CD2	2.44	0.48
1:A:472:MET:HG3	1:A:518:LEU:HD23	1.95	0.48
3:C:73:HIS:CD2	3:C:79:GLN:HG3	2.49	0.48
1:D:472:MET:HG2	1:D:517:ILE:O	2.13	0.48
2:E:278:GLY:O	2:E:279:ARG:C	2.57	0.48
2:E:1051:LEU:HB3	2:E:1089:ILE:HD13	1.95	0.48
3:F:441:CYS:SG	3:F:442:LEU:HD23	2.54	0.48
2:B:355:ASN:O	2:B:357:GLY:N	2.42	0.48
2:E:59:GLY:HA2	2:E:1073:TRP:CE3	2.49	0.48
2:E:118:THR:HG21	2:E:165:ILE:O	2.13	0.48
2:E:663:ASN:HD22	2:E:664:HIS:N	2.12	0.48
3:F:104:PRO:HA	3:F:107:VAL:HB	1.96	0.48
2:E:1032:THR:HB	2:E:1036:MET:O	2.13	0.47
2:B:1102:ARG:N	2:B:1103:PRO:CD	2.77	0.47
2:E:998:PHE:CE1	2:E:1074:ARG:HD2	2.49	0.47
1:A:519:CYS:HG	1:A:525:CYS:HG	1.42	0.47
2:B:31:LEU:CD1	2:B:315:THR:HG21	2.44	0.47
2:B:715:VAL:HG12	2:B:715:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:749:THR:HG23	2:B:749:THR:O	2.14	0.47
2:B:1039:LEU:HD23	2:B:1040:VAL:N	2.28	0.47
3:C:410:SER:CB	3:C:411:PRO:HD3	2.42	0.47
2:E:36:ASN:HD22	2:E:37:THR:HG23	1.79	0.47
2:E:1093:LEU:O	2:E:1094:ILE:C	2.56	0.47
3:F:296:ILE:CG2	3:F:300:LYS:HE2	2.44	0.47
2:E:401:SER:C	2:E:402:ILE:HG13	2.39	0.47
2:E:588:PRO:HA	2:E:606:LEU:HD23	1.96	0.47
2:E:621:GLY:O	2:E:622:LEU:C	2.57	0.47
2:E:1002:GLU:HB3	2:E:1032:THR:HG23	1.96	0.47
2:B:576:LEU:O	2:B:577:LEU:HB2	2.14	0.47
3:C:112:ASN:C	3:C:114:ILE:N	2.65	0.47
1:D:444:ILE:HG23	1:D:455:VAL:HG13	1.96	0.47
2:E:83:LYS:O	2:E:84:TYR:HB2	2.15	0.47
2:E:571:LEU:C	2:E:573:SER:N	2.73	0.47
2:E:653:SER:O	2:E:654:ASP:C	2.56	0.47
3:F:427:PRO:O	3:F:428:ASP:HB2	2.14	0.47
1:A:473:MET:CB	1:A:474:PRO:HD3	2.45	0.47
2:B:596:PHE:CD1	2:B:666:LEU:HD21	2.49	0.47
2:B:613:TYR:CD2	2:B:666:LEU:HD12	2.50	0.47
1:D:545:CYS:HB2	1:D:546:PRO:HD2	1.97	0.47
3:C:165:PHE:HB2	3:C:183:GLN:O	2.14	0.47
2:E:34:ALA:HB2	2:E:64:MET:SD	2.54	0.47
2:E:1134:GLU:C	2:E:1136:LEU:N	2.73	0.47
3:C:250:ALA:HB2	3:C:305:ILE:CD1	2.45	0.47
3:C:428:ASP:HB3	3:C:430:GLU:HG2	1.96	0.47
2:E:273:LEU:N	2:E:281:PHE:O	2.48	0.47
2:E:964:ASN:C	2:E:965:PHE:CG	2.93	0.47
3:F:317:LYS:NZ	3:F:441:CYS:O	2.48	0.47
1:A:569:LEU:HD12	1:A:591:CYS:HB3	1.97	0.46
2:B:429:PHE:CD1	2:B:429:PHE:N	2.83	0.46
2:E:966:LEU:HD11	2:E:974:LEU:HD22	1.98	0.46
3:F:349:TYR:HD2	3:F:359:THR:HG22	1.77	0.46
2:B:469:ILE:O	2:B:469:ILE:HG23	2.15	0.46
2:B:903:CYS:SG	2:B:941:ASN:HA	2.56	0.46
3:F:57:HIS:ND1	3:F:59:TYR:HE1	2.14	0.46
3:F:295:ARG:O	3:F:298:LEU:HB2	2.15	0.46
3:C:88:MET:O	3:C:89:MET:HB2	2.15	0.46
3:C:120:PHE:CD1	3:C:139:ALA:O	2.68	0.46
2:E:20:THR:HG23	2:E:315:THR:CG2	2.44	0.46
2:E:24:THR:HA	2:E:91:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:329:GLY:HA3	2:E:384:GLU:HB3	1.98	0.46
2:B:884:ILE:O	2:B:885:ASN:C	2.58	0.46
2:B:1093:LEU:O	2:B:1096:SER:N	2.47	0.46
2:E:692:ALA:HA	2:E:700:THR:O	2.15	0.46
2:E:912:LEU:HB3	3:F:240:TRP:CH2	2.50	0.46
2:E:1097:PHE:CE2	2:E:1129:LEU:HB3	2.51	0.46
2:B:912:LEU:HB3	3:C:240:TRP:CZ2	2.51	0.46
2:E:20:THR:HG23	2:E:315:THR:HG21	1.98	0.46
2:E:808:LEU:CD1	2:E:847:ARG:NH2	2.79	0.46
1:A:550:ALA:O	1:A:561:VAL:CG1	2.64	0.46
2:B:733:PHE:N	2:B:794:ILE:O	2.41	0.46
2:B:1048:TYR:OH	2:B:1087:GLY:N	2.39	0.46
2:E:808:LEU:HD13	2:E:847:ARG:HH21	1.80	0.46
3:F:290:ILE:CD1	3:F:298:LEU:HD12	2.46	0.46
1:A:531:PHE:CE1	1:A:595:LEU:HB2	2.51	0.46
1:A:536:VAL:HB	1:A:590:VAL:HG22	1.96	0.46
2:B:506:SER:O	2:B:521:ILE:N	2.44	0.46
2:B:975:PHE:HA	2:B:996:GLY:O	2.16	0.46
3:C:273:LEU:C	3:C:273:LEU:HD12	2.41	0.46
1:D:511:GLU:HG3	1:D:511:GLU:O	2.16	0.46
1:D:524:LEU:C	1:D:524:LEU:HD12	2.41	0.46
1:D:552:LEU:HG	1:D:554:ILE:HG13	1.98	0.46
3:F:53:LEU:HB2	3:F:54:PRO:HD3	1.98	0.46
2:B:785:GLU:O	2:B:786:VAL:HG23	2.16	0.46
3:C:98:PRO:O	3:C:99:LEU:HG	2.15	0.46
2:E:507:GLN:NE2	2:E:571:LEU:CD2	2.79	0.46
2:E:910:MET:O	2:E:912:LEU:N	2.49	0.46
3:F:349:TYR:CE2	3:F:359:THR:CG2	2.99	0.46
2:B:494:GLN:O	2:B:495:ALA:HB3	2.16	0.45
3:C:250:ALA:O	3:C:251:GLU:C	2.59	0.45
2:E:83:LYS:NZ	2:E:1075:SER:O	2.49	0.45
3:F:80:VAL:HA	3:F:180:ALA:O	2.16	0.45
2:B:1030:PHE:CZ	2:B:1038:GLY:HA3	2.51	0.45
2:E:127:GLU:HB2	2:E:129:ARG:HG2	1.98	0.45
3:F:127:ASN:HD22	3:F:128:VAL:HG12	1.81	0.45
2:B:32:LEU:HD11	2:B:41:ILE:HG23	1.98	0.45
2:B:110:ASP:OD1	2:B:141:LYS:NZ	2.47	0.45
3:C:410:SER:OG	3:C:411:PRO:HD3	2.16	0.45
1:D:552:LEU:CD1	1:D:615:PHE:CD1	2.99	0.45
2:E:459:PHE:CG	2:E:460:CYS:N	2.85	0.45
2:E:913:TYR:OH	3:F:240:TRP:HZ3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:88:MET:O	3:F:89:MET:HB2	2.17	0.45
3:F:350:VAL:HA	3:F:355:TYR:O	2.16	0.45
1:A:495:ALA:HB1	1:A:496:PRO:CD	2.46	0.45
2:B:139:LEU:HD22	2:B:156:ASN:HB3	1.98	0.45
2:B:913:TYR:CZ	3:C:240:TRP:CZ3	3.05	0.45
3:C:426:ILE:HD12	3:C:427:PRO:HD2	1.98	0.45
1:D:539:GLU:O	1:D:540:HIS:HB2	2.15	0.45
2:E:362:MET:HE1	2:E:1030:PHE:C	2.42	0.45
2:E:1005:ASN:OD1	3:F:239:SER:N	2.50	0.45
2:B:927:MET:HE3	2:B:953:TRP:CZ3	2.52	0.45
1:D:472:MET:O	1:D:473:MET:HB3	2.16	0.45
1:D:531:PHE:CZ	1:D:595:LEU:HB2	2.52	0.45
1:D:604:GLU:O	1:D:629:VAL:CG1	2.65	0.45
2:E:437:MET:N	2:E:444:GLU:O	2.39	0.45
2:E:674:LYS:O	2:E:675:GLU:C	2.60	0.45
3:F:284:VAL:HG23	3:F:311:GLU:CD	2.42	0.45
3:C:302:GLY:O	3:C:307:ARG:NH2	2.50	0.45
1:D:459:LEU:HD13	1:D:459:LEU:O	2.16	0.45
1:D:604:GLU:HG3	1:D:612:MET:HE2	1.98	0.45
2:E:613:TYR:CE1	2:E:627:LYS:HB3	2.52	0.45
3:C:61:GLY:O	3:C:62:ALA:C	2.59	0.45
3:C:138:THR:OG1	3:C:163:GLN:N	2.44	0.45
2:E:492:GLU:O	2:E:495:ALA:N	2.47	0.45
1:A:473:MET:C	1:A:475:ASN:H	2.25	0.45
2:B:68:ARG:C	2:B:128:CYS:SG	3.00	0.45
2:B:376:VAL:HA	2:B:388:ARG:O	2.17	0.45
2:B:1072:PHE:CD1	2:B:1072:PHE:C	2.95	0.45
3:C:138:THR:O	3:C:161:GLY:HA2	2.16	0.45
2:E:357:GLY:O	2:E:358:PRO:C	2.59	0.45
2:E:1004:VAL:HG11	2:E:1007:PHE:CE1	2.51	0.45
2:E:1101:SER:OG	2:E:1104:LYS:HG2	2.17	0.45
2:B:427:LEU:N	2:B:427:LEU:HD12	2.32	0.45
2:B:485:ALA:O	2:B:487:VAL:HG13	2.17	0.45
2:B:1122:ARG:NH1	2:B:1128:ASP:OD2	2.50	0.45
3:C:419:ARG:C	3:C:421:ALA:H	2.23	0.45
2:E:472:THR:OG1	2:E:475:SER:N	2.31	0.45
2:E:1011:SER:O	2:E:1012:LEU:HD23	2.16	0.45
3:C:242:ARG:NH1	3:C:242:ARG:HB2	2.32	0.44
2:E:1053:ASP:O	2:E:1054:MET:C	2.59	0.44
3:F:401:LYS:HG3	3:F:415:TRP:CE2	2.51	0.44
1:A:554:ILE:O	1:A:556:THR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:GLY:O	2:B:285:LEU:HD12	2.17	0.44
2:B:849:VAL:HG12	2:B:851:PHE:CE1	2.52	0.44
2:B:1052:LEU:O	2:B:1053:ASP:C	2.60	0.44
2:B:62:ALA:N	2:B:80:LEU:O	2.37	0.44
2:B:80:LEU:HA	2:B:85:ASN:O	2.17	0.44
2:B:232:ILE:HD13	2:B:237:ILE:HG23	1.97	0.44
1:D:537:ILE:O	1:D:588:ASP:HA	2.18	0.44
2:E:450:GLY:C	2:E:477:ARG:HH21	2.25	0.44
2:E:469:ILE:HA	2:E:477:ARG:O	2.18	0.44
1:A:633:VAL:O	1:A:634:PRO:C	2.59	0.44
2:B:674:LYS:O	2:B:675:GLU:C	2.61	0.44
3:C:431:ASP:O	3:C:432:GLU:C	2.60	0.44
2:E:448:LEU:HD23	2:E:451:PHE:CD1	2.52	0.44
1:A:532:ASP:OD1	1:A:594:ARG:HG3	2.17	0.44
2:B:142:VAL:HB	2:B:155:PHE:CZ	2.52	0.44
2:B:484:LYS:O	2:B:485:ALA:HB2	2.17	0.44
2:B:584:GLY:O	2:B:586:ILE:N	2.50	0.44
3:C:70:ARG:O	3:C:71:THR:HB	2.18	0.44
2:E:314:LEU:HD23	2:E:324:VAL:HA	1.99	0.44
2:E:394:ILE:CD1	2:E:658:VAL:HB	2.47	0.44
2:E:832:GLY:HA2	2:E:847:ARG:O	2.17	0.44
3:F:307:ARG:O	3:F:311:GLU:N	2.50	0.44
2:B:1105:MET:O	2:B:1106:GLN:C	2.60	0.44
1:D:555:HIS:NE2	1:D:612:MET:HB3	2.33	0.44
3:F:338:PHE:CE2	3:F:340:LEU:HG	2.52	0.44
1:A:585:VAL:HG11	1:A:591:CYS:SG	2.57	0.44
1:D:568:CYS:H	1:D:592:ILE:HG13	1.82	0.44
2:E:433:THR:HG22	2:E:434:ARG:N	2.32	0.44
2:E:844:LYS:O	2:E:867:LYS:C	2.61	0.44
2:B:555:LEU:N	2:B:571:LEU:HD23	2.33	0.44
2:B:679:MET:HA	2:B:693:LEU:HA	1.99	0.44
3:C:83:VAL:CG2	3:C:121:ALA:HB3	2.46	0.44
2:E:613:TYR:CZ	2:E:627:LYS:HB3	2.53	0.44
2:E:1075:SER:OG	2:E:1084:PRO:HA	2.18	0.44
3:F:110:VAL:HG11	3:F:155:VAL:HG11	2.00	0.44
1:A:447:LYS:CG	1:A:447:LYS:O	2.66	0.44
2:B:476:VAL:HB	2:B:490:TRP:HB3	1.98	0.44
2:B:964:ASN:C	2:B:965:PHE:CG	2.95	0.44
2:B:1002:GLU:OE1	2:B:1034:ASN:CG	2.61	0.44
2:B:1095:GLU:C	2:B:1097:PHE:H	2.26	0.44
3:C:296:ILE:O	3:C:298:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:503:CYS:SG	2:E:504:ASN:N	2.91	0.44
2:E:1093:LEU:O	2:E:1096:SER:OG	2.32	0.44
3:F:242:ARG:HH11	3:F:242:ARG:HB2	1.83	0.44
2:B:68:ARG:C	2:B:128:CYS:HG	2.25	0.43
2:B:803:HIS:CE1	2:B:858:LEU:HB3	2.52	0.43
2:B:913:TYR:CE1	3:C:240:TRP:CH2	3.06	0.43
3:C:257:ILE:HG12	3:C:312:LEU:HG	2.00	0.43
1:A:552:LEU:HG	1:A:554:ILE:CG1	2.48	0.43
2:B:908:ASN:OD1	2:B:908:ASN:N	2.52	0.43
2:E:123:ILE:O	2:E:169:PHE:HE2	2.01	0.43
2:E:142:VAL:HB	2:E:155:PHE:CE1	2.53	0.43
2:B:389:ILE:O	2:B:712:ILE:HA	2.18	0.43
2:B:925:ASP:C	2:B:927:MET:H	2.24	0.43
1:D:454:VAL:O	1:D:455:VAL:HG23	2.18	0.43
1:D:527:SER:OG	1:D:528:GLY:N	2.52	0.43
2:E:539:ALA:HB2	2:E:561:TRP:CD1	2.53	0.43
3:F:59:TYR:CE2	3:F:350:VAL:O	2.72	0.43
3:F:103:HIS:O	3:F:107:VAL:HG23	2.18	0.43
3:C:295:ARG:HG2	3:C:295:ARG:HH11	1.84	0.43
3:C:298:LEU:HD21	3:C:311:GLU:HG3	1.99	0.43
1:D:584:PHE:CD1	1:D:584:PHE:C	2.97	0.43
2:E:312:GLU:HG2	2:E:327:ARG:HG3	1.99	0.43
2:E:520:GLN:O	2:E:526:LEU:HA	2.19	0.43
3:F:93:PRO:O	3:F:95:GLN:N	2.52	0.43
1:A:510:GLU:O	1:A:511:GLU:CB	2.65	0.43
2:B:372:GLN:OE1	2:B:670:ASN:ND2	2.51	0.43
3:C:138:THR:O	3:C:162:ARG:N	2.51	0.43
3:C:345:PRO:HB2	3:C:360:LEU:HD12	2.00	0.43
1:D:605:THR:OG1	1:D:608:ASP:HB2	2.19	0.43
2:E:59:GLY:HA2	2:E:1073:TRP:CZ3	2.54	0.43
2:E:558:ILE:HG22	2:E:559:GLY:N	2.34	0.43
3:F:290:ILE:HD12	3:F:295:ARG:CA	2.42	0.43
3:C:182:VAL:O	3:C:182:VAL:CG1	2.66	0.43
1:D:533:ALA:HB1	1:D:628:LYS:O	2.19	0.43
1:D:537:ILE:CG1	1:D:585:VAL:HG22	2.49	0.43
3:C:397:HIS:CE1	3:C:400:TRP:CZ2	3.06	0.43
2:E:328:LEU:HA	2:E:358:PRO:HD2	2.01	0.43
2:E:427:LEU:N	2:E:427:LEU:CD1	2.80	0.43
2:E:744:ASP:O	2:E:749:THR:N	2.51	0.43
1:A:446:ASP:O	1:A:455:VAL:HA	2.18	0.43
2:B:217:SER:HB2	3:C:204:LYS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:645:SER:O	2:B:645:SER:OG	2.35	0.43
2:B:921:ILE:N	2:B:933:LEU:O	2.45	0.43
2:E:925:ASP:C	2:E:927:MET:N	2.75	0.43
2:E:1057:ARG:NH2	2:E:1111:ASN:O	2.52	0.43
1:A:472:MET:HE1	1:A:512:ILE:HG22	2.01	0.43
1:D:552:LEU:HD21	1:D:554:ILE:HD11	2.00	0.43
2:E:16:ASN:HD21	2:E:36:ASN:HA	1.83	0.43
2:E:58:TYR:CE1	2:E:1070:HIS:HB2	2.54	0.43
2:B:60:LYS:O	2:B:61:ILE:C	2.61	0.42
2:B:184:ASP:O	2:B:186:GLN:N	2.52	0.42
2:B:468:LEU:O	2:B:478:LEU:HD12	2.18	0.42
2:E:880:LEU:O	2:E:890:LEU:HD12	2.19	0.42
3:F:91:LEU:HD22	3:F:92:ILE:N	2.34	0.42
2:B:603:LEU:HB3	2:B:611:LEU:HD11	2.01	0.42
2:B:963:ASP:O	2:B:978:GLN:HA	2.20	0.42
3:C:104:PRO:O	3:C:105:GLN:C	2.62	0.42
3:C:295:ARG:O	3:C:298:LEU:HB2	2.19	0.42
2:E:224:GLU:N	2:E:225:PRO:HD2	2.34	0.42
2:E:997:LEU:HB3	2:E:1076:PHE:CD2	2.54	0.42
2:E:1032:THR:CB	2:E:1036:MET:O	2.67	0.42
3:F:307:ARG:O	3:F:308:LEU:C	2.62	0.42
3:F:427:PRO:O	3:F:428:ASP:CB	2.67	0.42
2:B:429:PHE:O	2:B:430:VAL:C	2.62	0.42
3:C:194:MET:O	3:C:198:GLN:HB2	2.20	0.42
3:C:296:ILE:O	3:C:299:LEU:N	2.52	0.42
1:D:459:LEU:HB2	1:D:500:LEU:HD22	2.01	0.42
2:E:16:ASN:ND2	2:E:36:ASN:HA	2.34	0.42
2:E:429:PHE:CD1	2:E:429:PHE:N	2.87	0.42
2:E:591:ILE:HG13	2:E:603:LEU:O	2.18	0.42
2:E:721:PRO:C	2:E:722:ARG:HG2	2.45	0.42
3:F:101:LEU:CD1	3:F:110:VAL:HG21	2.49	0.42
3:F:374:PRO:HA	3:F:386:TRP:O	2.19	0.42
1:A:611:GLN:HA	1:A:614:ARG:HD2	2.00	0.42
1:A:615:PHE:CD1	1:A:615:PHE:C	2.97	0.42
2:B:850:VAL:HG21	2:B:893:TRP:CZ3	2.55	0.42
2:B:1091:GLY:C	2:B:1093:LEU:N	2.76	0.42
2:B:1105:MET:O	2:B:1108:VAL:N	2.52	0.42
3:C:254:MET:SD	3:C:277:PRO:HB3	2.59	0.42
1:D:540:HIS:ND1	1:D:542:SER:O	2.53	0.42
2:E:81:THR:OG1	2:E:82:ALA:N	2.49	0.42
2:E:191:LYS:HG2	2:E:208:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:640:THR:HG22	2:E:641:PHE:N	2.35	0.42
3:F:257:ILE:CG1	3:F:312:LEU:HG	2.49	0.42
2:B:83:LYS:HE3	2:B:1077:HIS:HB2	2.01	0.42
2:B:730:SER:O	2:B:731:GLN:C	2.62	0.42
2:B:1028:VAL:O	2:B:1039:LEU:HA	2.19	0.42
2:E:312:GLU:HB3	2:E:325:GLY:O	2.19	0.42
2:E:389:ILE:O	2:E:712:ILE:HA	2.20	0.42
2:E:516:LEU:C	2:E:516:LEU:HD12	2.44	0.42
2:E:681:PRO:HA	2:E:691:LEU:HD12	2.01	0.42
2:E:808:LEU:HD13	2:E:811:GLU:OE1	2.20	0.42
2:E:1072:PHE:O	2:E:1075:SER:HB2	2.19	0.42
3:F:126:SER:O	3:F:127:ASN:C	2.63	0.42
1:A:539:GLU:O	1:A:624:ILE:HG13	2.19	0.42
2:E:151:GLU:O	2:E:152:LEU:C	2.62	0.42
2:E:178:ILE:O	2:E:178:ILE:HG13	2.19	0.42
2:E:220:ILE:O	2:E:229:ALA:HA	2.19	0.42
3:F:165:PHE:CD1	3:F:165:PHE:C	2.98	0.42
1:A:527:SER:HA	1:A:602:CYS:HA	2.02	0.42
2:B:727:GLN:HB2	2:B:829:PHE:CZ	2.54	0.42
2:B:770:LEU:C	2:E:445:GLU:OE2	2.63	0.42
2:E:263:ARG:HA	2:E:271:TYR:HE1	1.83	0.42
2:E:568:ILE:C	2:E:569:LEU:HD22	2.44	0.42
1:A:531:PHE:CZ	1:A:595:LEU:HB2	2.55	0.42
1:A:554:ILE:O	1:A:557:CYS:N	2.53	0.42
2:B:426:VAL:C	2:B:427:LEU:HD12	2.44	0.42
2:B:909:ILE:HB	2:B:925:ASP:HB3	2.01	0.42
2:E:838:PRO:HB2	3:F:225:GLN:NE2	2.35	0.42
2:B:1054:MET:SD	2:B:1129:LEU:HD23	2.60	0.42
3:C:83:VAL:HG11	3:C:123:LEU:HG	2.02	0.42
3:C:110:VAL:O	3:C:111:ARG:C	2.63	0.42
2:E:84:TYR:O	2:E:108:VAL:HG22	2.20	0.42
3:F:394:CYS:O	3:F:395:ALA:CB	2.67	0.42
2:B:1134:GLU:C	2:B:1136:LEU:N	2.73	0.42
1:D:605:THR:HA	1:D:629:VAL:O	2.19	0.42
3:F:100:GLN:OE1	3:F:156:LYS:NZ	2.43	0.42
2:B:333:LEU:O	2:B:350:MET:HB2	2.19	0.41
2:B:808:LEU:HB2	2:B:811:GLU:HB2	2.02	0.41
2:E:549:SER:O	2:E:550:ASN:CB	2.68	0.41
3:F:69:GLY:HA3	3:F:140:GLU:OE2	2.19	0.41
3:F:296:ILE:HG22	3:F:300:LYS:HE2	2.01	0.41
2:E:327:ARG:HD3	3:F:199:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:387:LEU:O	2:E:388:ARG:HD3	2.20	0.41
1:A:569:LEU:H	1:A:578:SER:HB3	1.85	0.41
2:B:953:TRP:CZ2	3:C:193:THR:HG23	2.55	0.41
1:D:494:VAL:HG11	1:D:500:LEU:HD11	2.02	0.41
1:D:533:ALA:O	1:D:593:ALA:N	2.40	0.41
2:E:127:GLU:HB2	2:E:129:ARG:CG	2.50	0.41
2:E:273:LEU:HD11	2:E:283:LEU:HB2	2.01	0.41
2:E:558:ILE:HG22	2:E:560:LEU:CD2	2.50	0.41
3:F:281:SER:O	3:F:311:GLU:OE1	2.38	0.41
2:B:269:SER:OG	2:B:287:LYS:NZ	2.46	0.41
2:B:828:TYR:HB3	2:B:851:PHE:O	2.20	0.41
2:B:482:GLU:O	2:B:483:PRO:C	2.64	0.41
2:E:32:LEU:CD1	2:E:41:ILE:HG23	2.51	0.41
3:F:50:ASP:OD2	3:F:52:SER:OG	2.34	0.41
2:B:1075:SER:OG	2:B:1084:PRO:HA	2.21	0.41
3:C:278:ILE:O	3:C:282:TYR:CD2	2.73	0.41
2:E:3:TYR:HB3	2:E:1048:TYR:CG	2.56	0.41
2:E:739:ARG:NH1	2:E:757:SER:OG	2.54	0.41
3:F:294:LEU:O	3:F:295:ARG:C	2.63	0.41
2:B:390:ILE:HG12	2:B:712:ILE:HG12	2.02	0.41
2:B:450:GLY:C	2:B:477:ARG:NH2	2.79	0.41
3:C:165:PHE:CD1	3:C:165:PHE:C	2.99	0.41
3:C:410:SER:HB3	3:C:411:PRO:HD3	2.02	0.41
1:D:485:LEU:HG	1:D:490:GLU:HB3	2.03	0.41
3:F:194:MET:HE2	3:F:245:TYR:CG	2.55	0.41
1:A:484:ILE:C	1:A:485:LEU:HD12	2.45	0.41
2:B:3:TYR:HB3	2:B:1048:TYR:CG	2.55	0.41
2:B:436:LEU:HA	2:B:444:GLU:O	2.20	0.41
2:B:998:PHE:HB2	2:B:1088:PHE:CD2	2.55	0.41
1:D:563:ILE:O	1:D:563:ILE:HG13	2.21	0.41
1:D:572:LYS:O	1:D:573:LYS:C	2.64	0.41
2:E:118:THR:HB	2:E:134:ARG:NH2	2.35	0.41
2:E:508:VAL:HG12	2:E:510:VAL:HG13	2.02	0.41
2:E:571:LEU:HB3	2:E:572:PRO:HD3	2.03	0.41
3:F:59:TYR:HE2	3:F:350:VAL:O	2.04	0.41
3:F:141:ILE:HA	3:F:159:ALA:HA	2.01	0.41
1:A:444:ILE:O	1:A:514:PRO:HA	2.21	0.41
1:A:515:GLY:HA2	1:A:557:CYS:HB2	2.03	0.41
2:B:322:VAL:HG23	2:B:336:LEU:HD21	2.03	0.41
2:B:1101:SER:C	2:B:1103:PRO:HD2	2.45	0.41
3:C:410:SER:HB3	3:C:411:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:LEU:HA	1:D:490:GLU:HA	2.03	0.41
1:D:505:LYS:HG2	1:D:505:LYS:O	2.21	0.41
1:D:529:ARG:HD3	1:D:530:THR:OG1	2.21	0.41
2:E:477:ARG:NH1	2:E:486:LEU:HD22	2.36	0.41
2:E:613:TYR:CE2	2:E:627:LYS:HD3	2.56	0.41
2:E:679:MET:C	2:E:679:MET:SD	3.04	0.41
2:B:473:SER:O	2:B:498:ILE:N	2.37	0.41
1:D:466:LYS:C	1:D:468:GLN:H	2.28	0.41
2:E:80:LEU:HA	2:E:85:ASN:O	2.21	0.41
2:E:120:ILE:HG23	2:E:135:LEU:HD23	2.02	0.41
2:E:327:ARG:O	2:E:358:PRO:HD2	2.20	0.41
1:A:473:MET:CG	1:A:474:PRO:HD3	2.51	0.40
2:B:102:THR:HG23	2:B:102:THR:O	2.22	0.40
2:B:479:VAL:CG1	2:B:480:SER:N	2.84	0.40
2:B:970:ASN:O	2:B:971:ALA:HB3	2.21	0.40
2:B:1011:SER:O	2:B:1012:LEU:HD23	2.21	0.40
2:E:542:ASP:CG	2:E:543:ILE:H	2.29	0.40
2:E:652:CYS:HB3	2:E:676:VAL:O	2.21	0.40
2:B:400:ALA:O	2:B:700:THR:HA	2.21	0.40
2:B:408:LYS:HA	2:B:678:TYR:CE2	2.56	0.40
2:B:821:LEU:HD11	2:B:830:ILE:HD11	2.03	0.40
3:C:302:GLY:O	3:C:303:SER:C	2.64	0.40
3:C:357:HIS:O	3:C:359:THR:N	2.54	0.40
2:E:346:TYR:N	2:E:346:TYR:CD2	2.89	0.40
1:A:455:VAL:CG1	1:A:456:LEU:N	2.84	0.40
2:B:203:ASN:O	2:B:204:LYS:C	2.64	0.40
2:B:587:ILE:C	2:B:606:LEU:HD23	2.47	0.40
2:B:736:LEU:HD23	2:B:791:LEU:HD13	2.04	0.40
2:B:930:VAL:O	2:B:947:ARG:HA	2.21	0.40
1:D:540:HIS:NE2	1:D:544:ILE:HG22	2.34	0.40
2:E:559:GLY:HA2	2:E:565:SER:O	2.20	0.40
3:F:347:ALA:O	3:F:358:GLU:HA	2.21	0.40
1:A:615:PHE:HE1	1:A:617:LEU:CD1	2.34	0.40
3:C:104:PRO:HG2	3:C:105:GLN:OE1	2.21	0.40
3:C:298:LEU:HD23	3:C:307:ARG:HG3	2.02	0.40
2:E:436:LEU:HB3	2:E:443:VAL:HG13	2.03	0.40
2:E:602:LEU:HD23	2:E:602:LEU:O	2.21	0.40
2:E:658:VAL:HG23	2:E:671:VAL:CG2	2.51	0.40
2:E:757:SER:HB3	2:E:792:LEU:HD21	2.03	0.40
3:F:165:PHE:CD1	3:F:182:VAL:HG21	2.56	0.40
2:B:191:LYS:HE2	2:B:193:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:607:GLY:C	2:B:609:GLY:N	2.78	0.40
2:B:641:PHE:CZ	2:B:648:ASN:HB2	2.57	0.40
3:C:143:ALA:HB3	3:C:158:LYS:HB2	2.02	0.40
1:D:552:LEU:HG	1:D:554:ILE:CG1	2.52	0.40
2:E:433:THR:O	2:E:434:ARG:CD	2.70	0.40
2:E:596:PHE:CD2	2:E:666:LEU:HD21	2.57	0.40
2:E:717:LEU:O	2:E:718:TYR:HB2	2.22	0.40
2:E:1072:PHE:CD1	2:E:1072:PHE:C	3.00	0.40
3:F:276:ASN:HD21	3:F:278:ILE:HD12	1.84	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	193/197 (98%)	152 (79%)	30 (16%)	11 (6%)	1	16
1	D	194/197 (98%)	149 (77%)	36 (19%)	9 (5%)	2	19
2	B	1049/1140 (92%)	884 (84%)	126 (12%)	39 (4%)	2	22
2	E	1050/1140 (92%)	880 (84%)	135 (13%)	35 (3%)	3	24
3	C	365/404 (90%)	287 (79%)	61 (17%)	17 (5%)	2	19
3	F	357/404 (88%)	287 (80%)	53 (15%)	17 (5%)	2	18
All	All	3208/3482 (92%)	2639 (82%)	441 (14%)	128 (4%)	2	21

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	MET
1	A	474	PRO
1	A	511	GLU

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Mol	Chain	Res	Type
1	A	555	HIS
1	A	584	PHE
2	B	210	GLU
2	B	372	GLN
2	B	483	PRO
2	B	495	ALA
2	B	572	PRO
2	B	675	GLU
2	B	897	LYS
2	B	1014	MET
3	C	62	ALA
3	C	89	MET
3	C	265	ASP
3	C	266	GLU
3	C	410	SER
3	C	411	PRO
2	E	223	PRO
2	E	358	PRO
2	E	483	PRO
2	E	550	ASN
2	E	572	PRO
2	E	911	ALA
2	E	1076	PHE
3	F	127	ASN
3	F	152	ILE
3	F	327	GLN
3	F	410	SER
3	F	428	ASP
3	F	441	CYS
1	A	476	LYS
1	A	527	SER
1	A	607	LYS
1	A	610	PRO
2	B	279	ARG
2	B	358	PRO
2	B	513	GLY
2	B	576	LEU
2	B	578	HIS
2	B	885	ASN
3	C	71	THR
3	C	86	GLN
3	C	113	LEU

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Mol	Chain	Res	Type
3	C	327	GLN
3	C	358	GLU
1	D	488	ASP
1	D	584	PHE
2	E	84	TYR
2	E	212	VAL
2	E	513	GLY
2	E	664	HIS
2	E	1096	SER
3	F	116	LYS
2	B	185	PRO
2	B	223	PRO
2	B	577	LEU
2	B	664	HIS
2	B	861	VAL
2	B	911	ALA
2	B	1090	ASP
1	D	475	ASN
1	D	487	ASP
1	D	496	PRO
1	D	570	VAL
2	E	36	ASN
2	E	356	LEU
2	E	622	LEU
2	E	761	LEU
2	E	885	ASN
3	F	89	MET
3	F	150	PHE
3	F	395	ALA
3	F	411	PRO
1	A	542	SER
2	B	356	LEU
2	B	485	ALA
2	B	1092	ASP
1	D	468	GLN
2	E	149	ASN
2	E	543	ILE
2	E	576	LEU
2	E	910	MET
2	E	1014	MET
3	F	94	GLY
2	B	52	VAL

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Mol	Chain	Res	Type
2	B	135	LEU
2	B	529	ILE
2	B	551	GLY
2	B	580	GLU
2	B	597	GLU
2	B	971	ALA
3	C	60	LEU
3	C	105	GLN
3	C	363	TYR
1	D	476	LYS
1	D	601	ILE
2	E	382	PHE
2	E	403	ASP
2	E	422	ASP
2	E	506	SER
2	E	597	GLU
2	E	598	SER
2	E	765	VAL
2	E	855	ASP
2	E	1109	VAL
3	F	149	ASP
3	F	345	PRO
1	A	462	GLY
2	B	36	ASN
2	B	212	VAL
2	B	357	GLY
2	B	571	LEU
2	B	1015	GLN
2	B	1135	GLU
3	F	71	THR
3	F	325	GLN
2	B	344	GLY
3	C	104	PRO
2	E	571	LEU
3	C	301	ILE
2	E	430	VAL
2	B	224	GLU
3	C	152	ILE
2	E	310	ILE
2	E	951	PRO
3	F	426	ILE

### 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	173/174 (99%)	140 (81%)	33 (19%)	1	10
1	D	174/174 (100%)	137 (79%)	37 (21%)	1	6
2	B	951/999 (95%)	865 (91%)	86 (9%)	9	31
2	E	953/999 (95%)	857 (90%)	96 (10%)	7	27
3	C	335/367 (91%)	298 (89%)	37 (11%)	6	24
3	F	331/367 (90%)	301 (91%)	30 (9%)	9	31
All	All	2917/3080 (95%)	2598 (89%)	319 (11%)	6	24

All (319) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	ARG
1	A	447	LYS
1	A	449	LYS
1	A	453	THR
1	A	454	VAL
1	A	455	VAL
1	A	459	LEU
1	A	465	CYS
1	A	466	LYS
1	A	474	PRO
1	A	476	LYS
1	A	490	GLU
1	A	510	GLU
1	A	517	ILE
1	A	529	ARG
1	A	536	VAL
1	A	549	ASN
1	A	554	ILE
1	A	566	LEU
1	A	568	CYS
1	A	569	LEU
1	A	573	LYS

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Mol	Chain	Res	Type
1	A	579	LYS
1	A	583	ARG
1	A	585	VAL
1	A	592	ILE
1	A	602	CYS
1	A	605	THR
1	A	611	GLN
1	A	616	THR
1	A	618	ARG
1	A	626	ILE
1	A	629	VAL
2	B	6	VAL
2	B	7	VAL
2	B	20	THR
2	B	37	THR
2	B	50	ARG
2	B	52	VAL
2	B	70	LYS
2	B	97	SER
2	B	125	ASP
2	B	134	ARG
2	B	137	ASP
2	B	149	ASN
2	B	151	GLU
2	B	153	LYS
2	B	160	GLU
2	B	164	VAL
2	B	173	CYS
2	B	184	ASP
2	B	197	LEU
2	B	199	GLU
2	B	204	LYS
2	B	299	ASP
2	B	335	LYS
2	B	336	LEU
2	B	401	SER
2	B	402	ILE
2	B	412	PRO
2	B	413	LEU
2	B	420	GLU
2	B	421	THR
2	B	429	PHE

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Mol	Chain	Res	Type
2	B	432	GLN
2	B	447	GLU
2	B	449	MET
2	B	468	LEU
2	B	482	GLU
2	B	483	PRO
2	B	491	LYS
2	B	492	GLU
2	B	499	SER
2	B	524	GLN
2	B	532	THR
2	B	533	GLU
2	B	561	TRP
2	B	562	THR
2	B	572	PRO
2	B	578	HIS
2	B	579	LYS
2	B	582	LEU
2	B	618	ILE
2	B	619	GLU
2	B	654	ASP
2	B	660	TYR
2	B	663	ASN
2	B	669	SER
2	B	672	ASN
2	B	673	LEU
2	B	691	LEU
2	B	693	LEU
2	B	699	LEU
2	B	700	THR
2	B	713	ARG
2	B	738	SER
2	B	786	VAL
2	B	824	ASP
2	B	840	GLU
2	B	844	LYS
2	B	860	THR
2	B	866	VAL
2	B	884	ILE
2	B	886	SER
2	B	895	THR
2	B	914	LEU

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Mol	Chain	Res	Type
2	B	927	MET
2	B	947	ARG
2	B	957	VAL
2	B	987	GLU
2	B	989	ARG
2	B	1006	VAL
2	B	1041	THR
2	B	1072	PHE
2	B	1081	LYS
2	B	1107	GLU
2	B	1116	ASP
2	B	1122	ARG
2	B	1137	THR
3	C	49	PHE
3	C	74	ASP
3	C	77	SER
3	C	80	VAL
3	C	82	PRO
3	C	88	MET
3	C	91	LEU
3	C	105	GLN
3	C	109	MET
3	C	112	ASN
3	C	116	LYS
3	C	120	PHE
3	C	137	THR
3	C	147	GLU
3	C	148	GLN
3	C	162	ARG
3	C	179	GLN
3	C	182	VAL
3	C	193	THR
3	C	197	VAL
3	C	206	GLN
3	C	220	SER
3	C	239	SER
3	C	241	PRO
3	C	255	ASP
3	C	289	PRO
3	C	290	ILE
3	C	298	LEU
3	C	299	LEU

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Mol	Chain	Res	Type
3	C	301	ILE
3	C	316	ASN
3	C	356	VAL
3	C	364	LYS
3	C	393	ILE
3	C	407	LYS
3	C	423	LEU
3	C	430	GLU
1	D	440	ILE
1	D	447	LYS
1	D	449	LYS
1	D	454	VAL
1	D	459	LEU
1	D	471	VAL
1	D	473	MET
1	D	479	VAL
1	D	480	GLU
1	D	496	PRO
1	D	500	LEU
1	D	508	GLU
1	D	510	GLU
1	D	526	HIS
1	D	529	ARG
1	D	536	VAL
1	D	541	LYS
1	D	544	ILE
1	D	549	ASN
1	D	554	ILE
1	D	558	ILE
1	D	560	GLU
1	D	566	LEU
1	D	569	LEU
1	D	570	VAL
1	D	571	ASP
1	D	579	LYS
1	D	583	ARG
1	D	585	VAL
1	D	602	CYS
1	D	612	MET
1	D	616	THR
1	D	622	LYS
1	D	626	ILE

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Mol	Chain	Res	Type
1	D	629	VAL
1	D	632	LEU
1	D	633	VAL
2	E	6	VAL
2	E	20	THR
2	E	70	LYS
2	E	75	ASP
2	E	93	GLN
2	E	111	ARG
2	E	125	ASP
2	E	134	ARG
2	E	158	ARG
2	E	163	HIS
2	E	189	HIS
2	E	197	LEU
2	E	208	LYS
2	E	213	GLU
2	E	263	ARG
2	E	270	ARG
2	E	299	ASP
2	E	307	GLU
2	E	330	ASP
2	E	335	LYS
2	E	336	LEU
2	E	346	TYR
2	E	370	GLN
2	E	377	THR
2	E	405	PRO
2	E	420	GLU
2	E	421	THR
2	E	427	LEU
2	E	432	GLN
2	E	447	GLU
2	E	469	ILE
2	E	482	GLU
2	E	483	PRO
2	E	492	GLU
2	E	505	SER
2	E	526	LEU
2	E	527	ARG
2	E	532	THR
2	E	533	GLU

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Mol	Chain	Res	Type
2	E	534	MET
2	E	555	LEU
2	E	561	TRP
2	E	572	PRO
2	E	576	LEU
2	E	579	LYS
2	E	582	LEU
2	E	599	SER
2	E	611	LEU
2	E	618	ILE
2	E	622	LEU
2	E	625	ASP
2	E	634	GLN
2	E	654	ASP
2	E	657	THR
2	E	660	TYR
2	E	663	ASN
2	E	670	ASN
2	E	673	LEU
2	E	674	LYS
2	E	676	VAL
2	E	684	SER
2	E	691	LEU
2	E	700	THR
2	E	742	VAL
2	E	768	SER
2	E	784	GLU
2	E	786	VAL
2	E	790	ASN
2	E	818	SER
2	E	824	ASP
2	E	839	GLU
2	E	840	GLU
2	E	844	LYS
2	E	857	LYS
2	E	867	LYS
2	E	884	ILE
2	E	886	SER
2	E	895	THR
2	E	914	LEU
2	E	927	MET
2	E	943	GLU

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Mol	Chain	Res	Type
2	E	947	ARG
2	E	949	PHE
2	E	951	PRO
2	E	957	VAL
2	E	980	ASP
2	E	987	GLU
2	E	1024	THR
2	E	1036	MET
2	E	1044	SER
2	E	1050	LEU
2	E	1069	GLU
2	E	1072	PHE
2	E	1106	GLN
2	E	1122	ARG
2	E	1137	THR
3	F	49	PHE
3	F	80	VAL
3	F	88	MET
3	F	91	LEU
3	F	105	GLN
3	F	109	MET
3	F	126	SER
3	F	137	THR
3	F	171	ARG
3	F	173	GLN
3	F	179	GLN
3	F	182	VAL
3	F	193	THR
3	F	206	GLN
3	F	255	ASP
3	F	260	GLN
3	F	290	ILE
3	F	291	ASP
3	F	294	LEU
3	F	299	LEU
3	F	326	CYS
3	F	334	LYS
3	F	340	LEU
3	F	356	VAL
3	F	364	LYS
3	F	403	THR
3	F	407	LYS

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Mol	Chain	Res	Type
3	F	425	THR
3	F	426	ILE
3	F	440	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	ASN
1	A	549	ASN
1	A	589	GLN
2	B	85	ASN
2	B	156	ASN
2	B	189	HIS
2	B	319	ASN
2	B	355	ASN
2	B	455	GLN
2	B	462	ASN
2	B	497	ASN
2	B	578	HIS
2	B	663	ASN
2	B	670	ASN
2	B	677	ASN
2	B	696	ASN
2	B	796	GLN
2	B	990	GLN
2	B	1055	GLN
2	B	1059	ASN
3	C	73	HIS
3	C	95	GLN
3	C	198	GLN
3	C	367	ASN
3	C	397	HIS
2	E	4	ASN
2	E	85	ASN
2	E	183	GLN
2	E	262	ASN
2	E	319	ASN
2	E	397	HIS
2	E	455	GLN
2	E	466	GLN
2	E	481	GLN
2	E	497	ASN

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Mol	Chain	Res	Type
2	E	578	HIS
2	E	648	ASN
2	E	663	ASN
2	E	670	ASN
2	E	672	ASN
2	E	803	HIS
2	E	810	ASN
2	E	905	HIS
2	E	950	ASN
2	E	964	ASN
2	E	1056	ASN
2	E	1106	GLN
3	F	79	GLN
3	F	95	GLN
3	F	103	HIS
3	F	115	GLN
3	F	134	GLN
3	F	173	GLN
3	F	179	GLN
3	F	198	GLN
3	F	206	GLN
3	F	233	HIS
3	F	297	GLN
3	F	397	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 oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

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	A1IWG	F	502	-	24,24,24	0.73	0	36,36,36	0.96	3 (8%)
5	A1IWG	C	502	-	24,24,24	0.72	0	36,36,36	0.87	1 (2%)

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	A1IWG	F	502	-	-	4/8/33/33	0/3/3/3
5	A1IWG	C	502	-	-	0/8/33/33	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	502	A1IWG	C11-C10-C8	-2.36	120.87	123.48
5	F	502	A1IWG	C14-C4-N1	-2.32	108.18	110.32
5	F	502	A1IWG	C7-C8-C10	2.23	119.59	116.83
5	C	502	A1IWG	C7-C8-C10	2.00	119.31	116.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

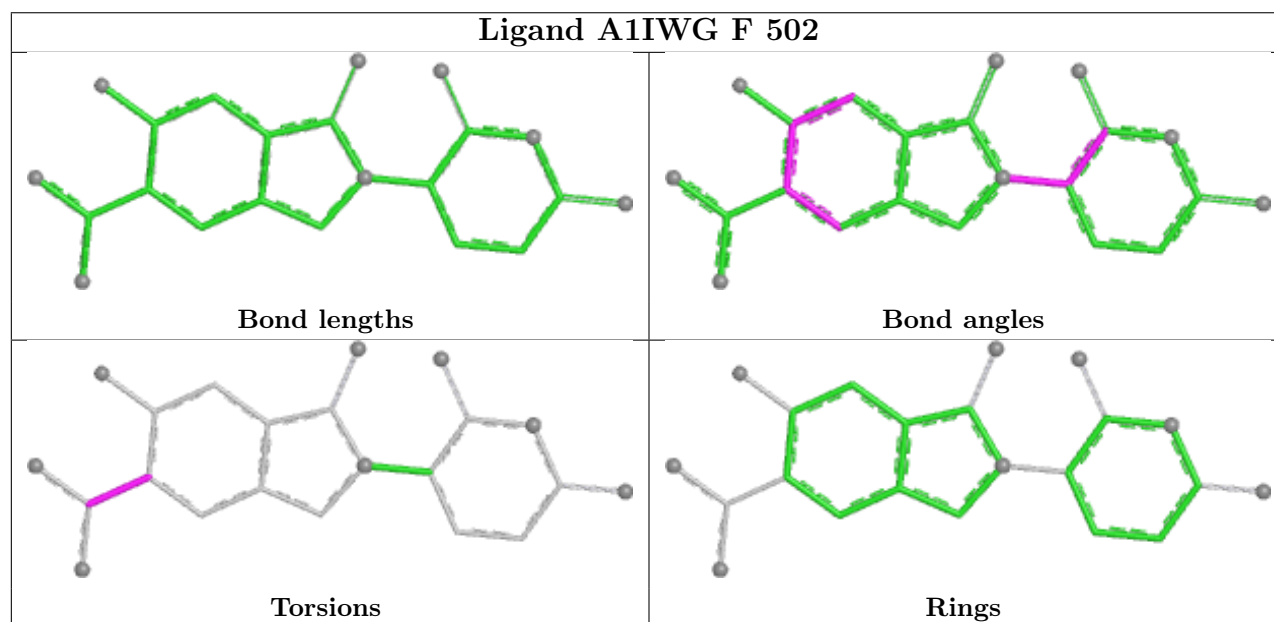
Mol	Chain	Res	Type	Atoms
5	F	502	A1IWG	C10-C8-C9-O2
5	F	502	A1IWG	C10-C8-C9-O3
5	F	502	A1IWG	C7-C8-C9-O2
5	F	502	A1IWG	C7-C8-C9-O3

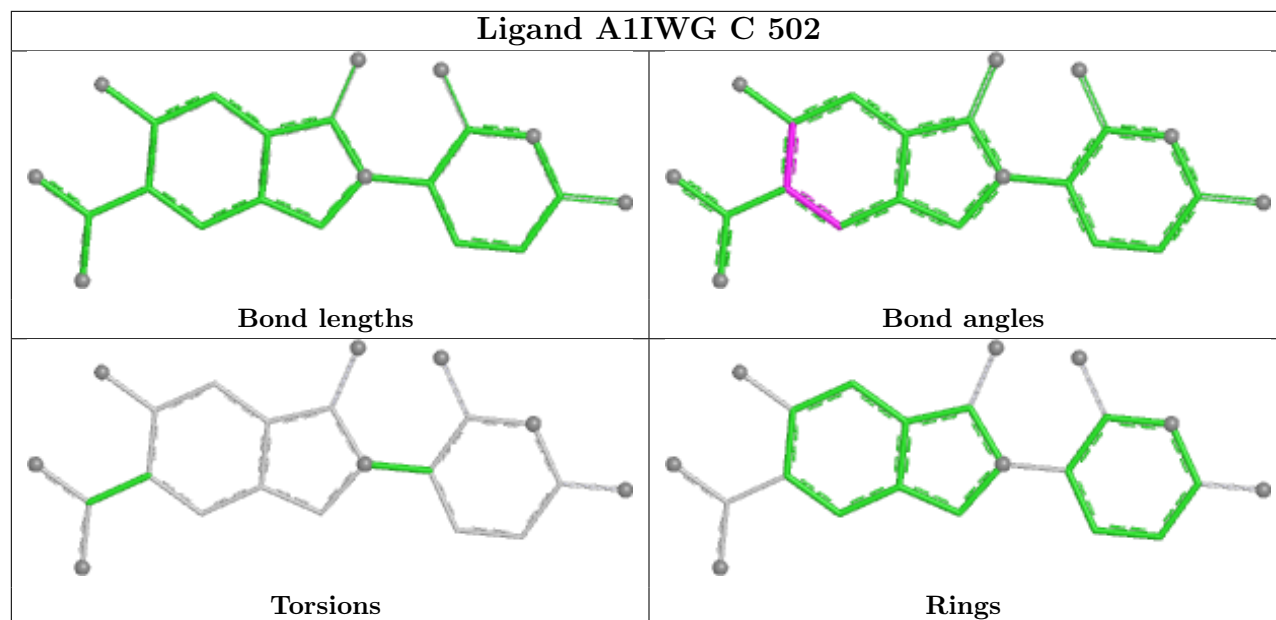
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	502	A1IWG	1	0
5	C	502	A1IWG	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	195/197 (98%)	0.19	3 (1%)	72 50	69, 145, 271, 323	0
1	D	196/197 (99%)	0.25	7 (3%)	46 33	60, 143, 239, 326	0
2	B	1081/1140 (94%)	0.01	19 (1%)	67 47	31, 125, 203, 284	5 (0%)
2	E	1082/1140 (94%)	0.08	20 (1%)	67 47	31, 130, 221, 308	5 (0%)
3	C	371/404 (91%)	0.05	7 (1%)	66 46	63, 122, 211, 291	0
3	F	367/404 (90%)	0.09	9 (2%)	58 41	59, 122, 198, 262	0
All	All	3292/3482 (94%)	0.07	65 (1%)	65 45	31, 128, 219, 326	10 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	226	PHE	4.4
2	B	260	CYS	4.0
2	E	179	CYS	4.0
1	D	555	HIS	3.9
2	E	276	MET	3.9
3	C	297	GLN	3.7
2	B	16	ASN	3.6
2	B	1131	LYS	3.4
2	E	1117	GLY	3.3
3	C	347	ALA	3.3
3	F	411	PRO	3.2
2	B	276	MET	3.2
2	B	501	ALA	3.2
2	B	324	VAL	3.1
2	B	279	ARG	3.1
2	E	1131	LYS	3.1
3	C	411	PRO	3.0
1	A	512	ILE	2.9
2	B	179	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	16	ASN	2.9
2	B	550	ASN	2.9
3	F	154	ILE	2.9
3	F	439	ILE	2.8
2	E	23	PHE	2.8
3	F	220	SER	2.7
1	D	507	ILE	2.7
2	B	1117	GLY	2.6
2	B	992	LEU	2.6
2	B	1065	VAL	2.5
2	E	381	ALA	2.5
3	C	154	ILE	2.5
3	F	116	LYS	2.5
1	A	546	PRO	2.5
2	E	66	LEU	2.5
2	E	2	SER	2.5
3	F	442	LEU	2.4
2	B	822	GLY	2.4
2	E	279	ARG	2.4
3	F	347	ALA	2.4
2	B	502	SER	2.3
1	D	513	LEU	2.3
1	A	449	LYS	2.3
2	E	317	LEU	2.3
3	C	220	SER	2.3
2	E	3	TYR	2.2
2	E	100	ILE	2.2
2	E	186	GLN	2.2
3	C	150	PHE	2.2
3	F	265	ASP	2.2
2	E	1063	LYS	2.2
2	B	601	TYR	2.2
3	F	225	GLN	2.1
2	E	549	SER	2.1
1	D	512	ILE	2.1
2	E	324	VAL	2.1
2	E	489	GLU	2.1
2	B	475	SER	2.1
2	E	491	LYS	2.1
1	D	439	PRO	2.1
3	C	100	GLN	2.1
1	D	603	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	643	SER	2.1
1	D	471	VAL	2.1
2	E	328	LEU	2.0
2	B	949	PHE	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

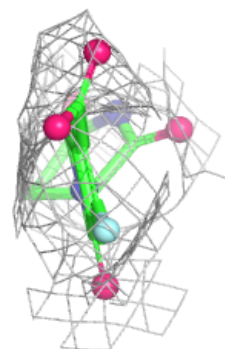
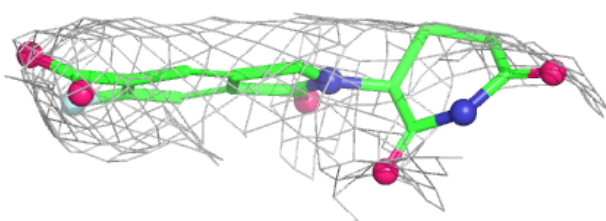
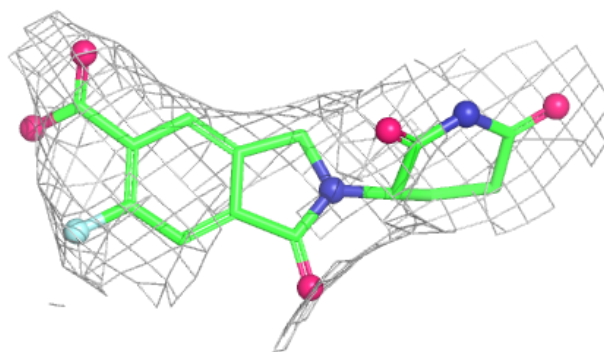
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	A1IWG	F	502	22/22	0.95	0.08	72,88,105,113	0
5	A1IWG	C	502	22/22	0.96	0.08	69,88,107,115	0
4	ZN	C	501	1/1	1.00	0.03	113,113,113,113	0
4	ZN	F	501	1/1	1.00	0.02	100,100,100,100	0

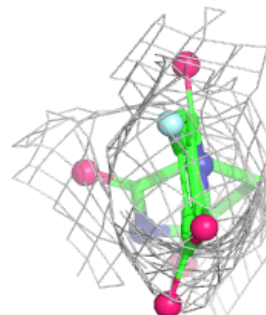
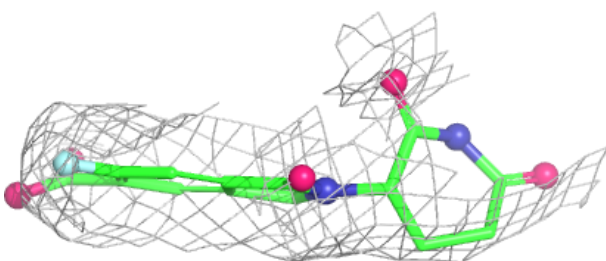
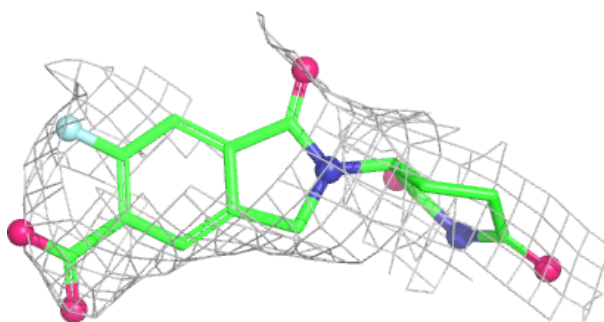
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1IWG F 502:**

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

**Electron density around A1IWG C 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.