



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2020 – 10:09 AM EST

PDB ID : 6XK9
Title : Cereblon in complex with DDB1, CC-90009, and GSPT1
Authors : Clayton, T.L.; Tran, E.T.; Zhu, J.; Pagarigan, B.E.; Matyskiela, M.E.; Chamberlain, P.P.
Deposited on : 2020-06-25
Resolution : 3.64 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 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	:	2.14.6
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)	:	2.14.6

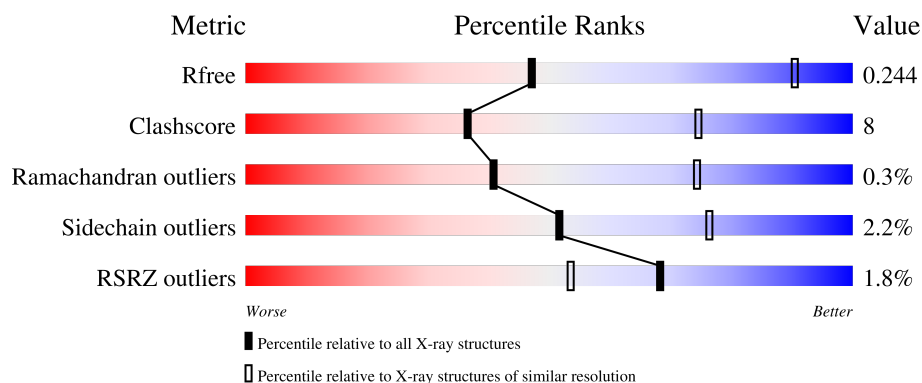
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 3.64 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	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	199	 71% 26% ..
1	X	199	 69% 28% ..
2	B	1140	 3% 77% 17% 5%
2	Y	1140	 % 76% 20% ..
3	C	406	 % 77% 17% 6%

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Mol	Chain	Length	Quality of chain
3	Z	406	<div><div><div>%</div><div><div></div></div><div>76%</div><div>18%</div><div>6%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25483 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	X	196	Total	C	N	O	S	0	0	0
			1454	925	253	264	12			
1	A	197	Total	C	N	O	S	0	0	0
			1459	927	254	267	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	435	GLY	-	expression tag	UNP P15170
X	436	SER	-	expression tag	UNP P15170
A	435	GLY	-	expression tag	UNP P15170
A	436	SER	-	expression tag	UNP P15170

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	1106	Total	C	N	O	S	0	0	0
			8402	5349	1411	1595	47			
2	B	1085	Total	C	N	O	S	0	0	0
			8186	5228	1365	1548	45			

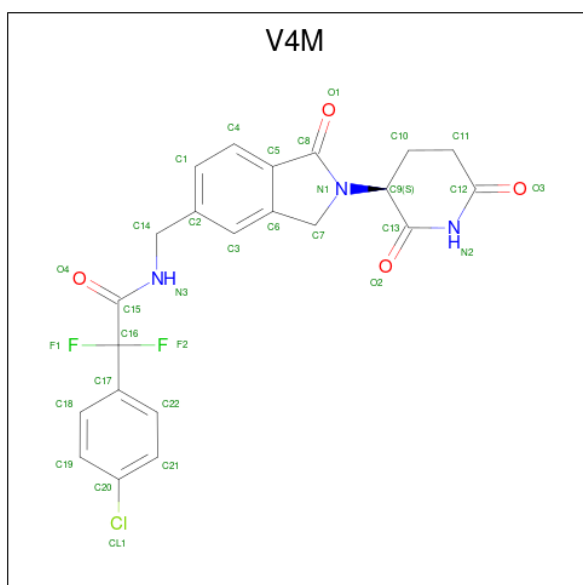
- Molecule 3 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	382	Total	C	N	O	S	0	0	0
			2981	1905	507	546	23			
3	C	381	Total	C	N	O	S	0	0	0
			2935	1876	498	538	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	37	GLY	-	expression tag	UNP Q96SW2
Z	38	SER	-	expression tag	UNP Q96SW2
Z	39	MET	-	expression tag	UNP Q96SW2
C	37	GLY	-	expression tag	UNP Q96SW2
C	38	SER	-	expression tag	UNP Q96SW2
C	39	MET	-	expression tag	UNP Q96SW2

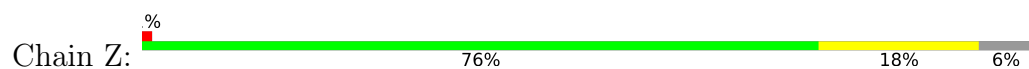
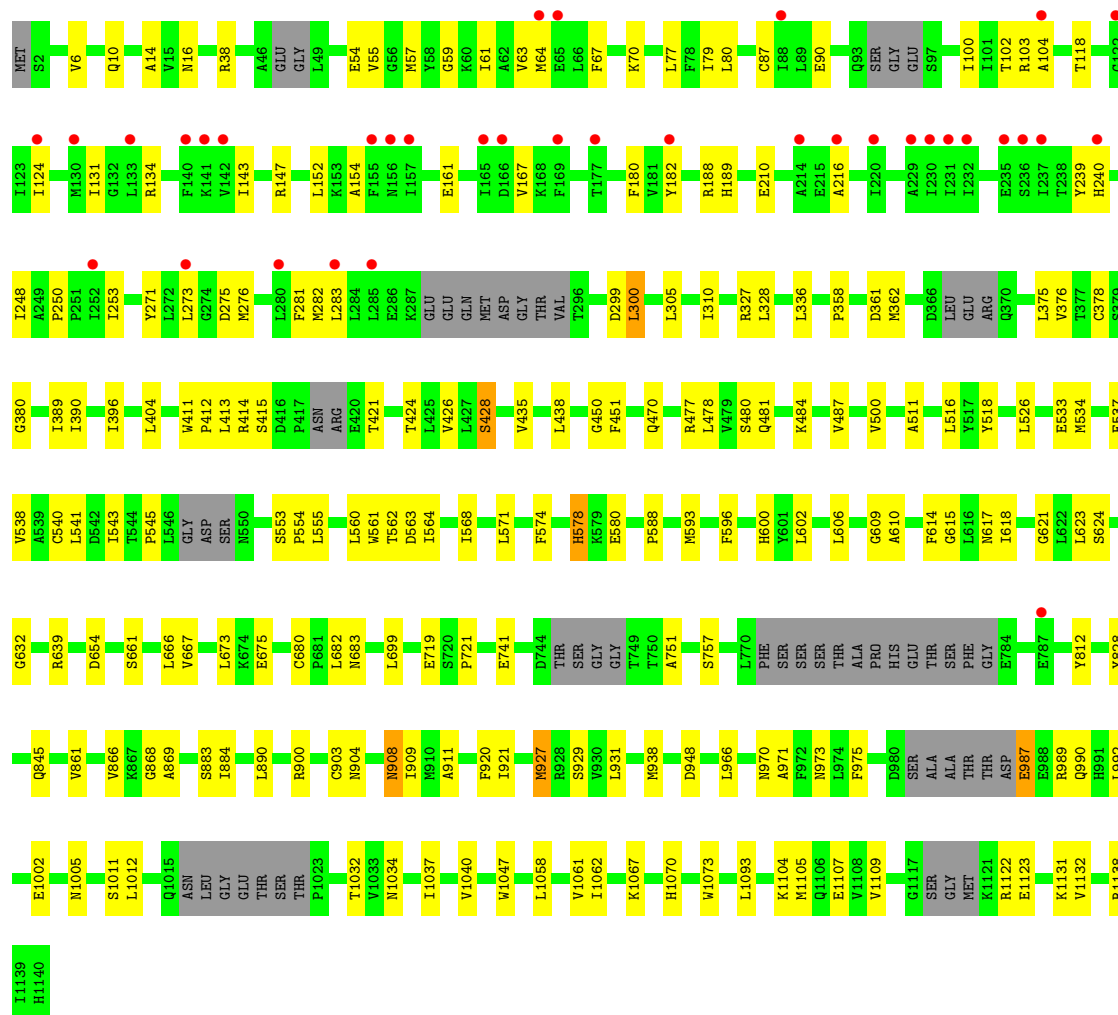
- Molecule 4 is 2-(4-chlorophenyl)-N-({2-[(3S)-2,6-dioxopiperidin-3-yl]-1-oxo-2,3-dihydro-1H-isoindol-5-yl}methyl)-2,2-difluoroacetamide (three-letter code: V4M) (formula: C₂₂H₁₈ClF₂N₃O₄) (labeled as "Ligand of Interest" by author).

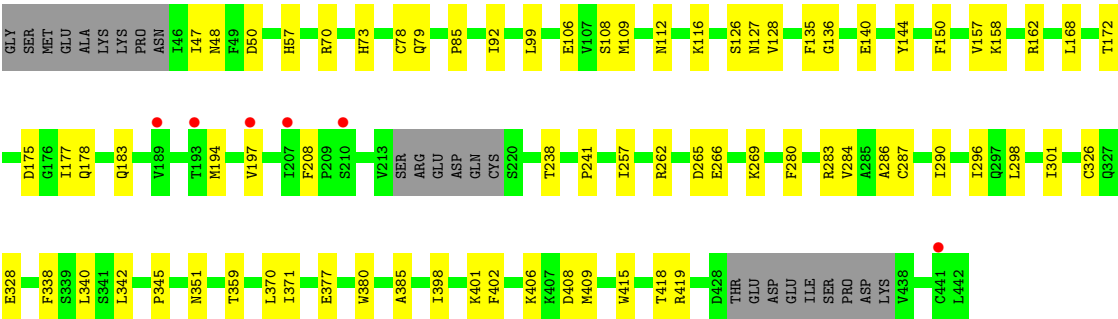


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	Z	1	Total	C	Cl	F	N	O	
			32	22	1	2	3	4	0
4	C	1	Total	C	Cl	F	N	O	
			32	22	1	2	3	4	0

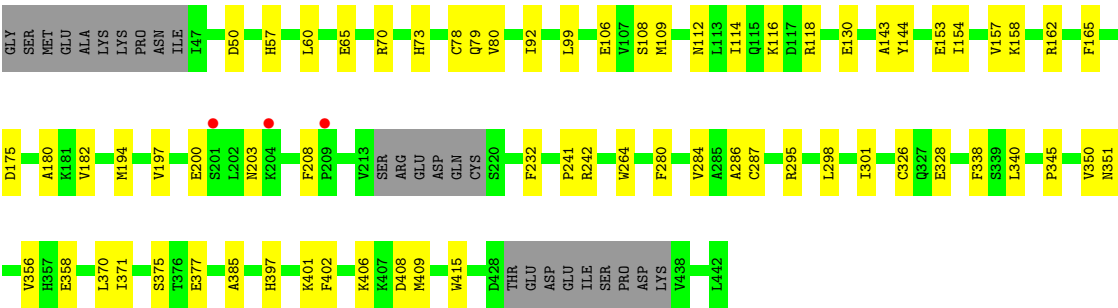
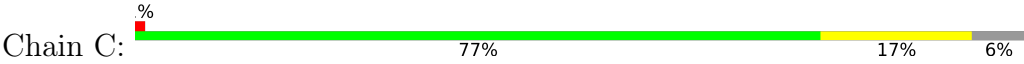
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Z	1	Total	Zn		
			1	1	0	0
5	C	1	Total	Zn		
			1	1	0	0





● Molecule 3: Protein cereblon



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.62Å 112.04Å 176.58Å 90.00° 95.79° 90.00°	Depositor
Resolution (Å)	74.45 – 3.64 112.04 – 3.64	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.45-3.64) 99.7 (112.04-3.64)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.208 , 0.245 0.208 , 0.244	Depositor DCC
R_{free} test set	3359 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25483	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, V4M

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	0.25	0/1481	0.54	0/2009
1	X	0.26	0/1475	0.55	0/1997
2	B	0.24	0/8335	0.46	0/11332
2	Y	0.25	0/8555	0.47	0/11623
3	C	0.26	0/3007	0.53	0/4102
3	Z	0.27	0/3052	0.52	0/4156
All	All	0.25	0/25905	0.49	0/35219

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 [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	1459	0	1467	32	0
1	X	1454	0	1471	33	0
2	B	8186	0	7918	116	0
2	Y	8402	0	8174	145	0
3	C	2935	0	2785	39	0
3	Z	2981	0	2880	45	0
4	C	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Z	32	0	0	0	0
5	C	1	0	0	0	0
5	Z	1	0	0	0	0
All	All	25483	0	24695	398	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 8.

All (398) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:213:GLU:OE2	2:Y:214:ALA:N	2.04	0.90
2:Y:213:GLU:CD	2:Y:215:GLU:H	1.80	0.85
3:Z:287:CYS:HB2	3:Z:345:PRO:HD2	1.60	0.83
2:B:124:ILE:HG12	2:B:131:ILE:HG22	1.63	0.79
1:A:565:LEU:HD13	1:A:581:PRO:HG2	1.64	0.78
3:C:92:ILE:HD11	3:C:295:ARG:HD2	1.65	0.77
3:Z:172:THR:HG22	3:Z:178:GLN:HG2	1.67	0.76
2:Y:213:GLU:OE2	2:Y:215:GLU:N	2.20	0.74
2:Y:285:LEU:HD22	2:Y:300:LEU:HD22	1.68	0.74
2:B:578:HIS:HD2	2:B:623:LEU:H	1.32	0.74
1:X:499:LEU:HD23	1:X:501:ILE:HD11	1.70	0.73
2:Y:546:LEU:HD12	2:Y:547:GLY:H	1.52	0.72
1:A:578:LYS:HG2	1:A:579:THR:HG23	1.71	0.72
1:X:565:LEU:HD13	1:X:581:PRO:HG2	1.73	0.71
2:Y:545:PRO:HA	2:Y:553:SER:HB2	1.74	0.70
2:B:189:HIS:HB3	2:B:210:GLU:HA	1.73	0.70
3:Z:99:LEU:HB2	3:Z:157:VAL:HG22	1.73	0.70
2:B:415:SER:O	2:B:484:LYS:NZ	2.25	0.69
2:B:578:HIS:CD2	2:B:623:LEU:H	2.10	0.69
1:X:444:VAL:HG23	1:X:456:GLY:HA2	1.75	0.69
3:C:165:PHE:HB2	3:C:182:VAL:HG13	1.75	0.69
2:Y:762:SER:O	2:Y:803:HIS:ND1	2.26	0.68
2:B:654:ASP:HA	2:B:675:GLU:HG3	1.76	0.68
3:C:406:LYS:HE2	3:C:409:MET:HE3	1.76	0.67
1:A:499:LEU:HD23	1:A:501:ILE:HD11	1.76	0.67
3:Z:78:CYS:O	3:Z:79:GLN:NE2	2.24	0.67
2:Y:167:VAL:HG23	2:Y:180:PHE:HB3	1.76	0.66
2:Y:273:LEU:HB2	2:Y:281:PHE:HB2	1.78	0.66
2:B:6:VAL:HG22	2:B:1040:VAL:HG22	1.78	0.66
3:Z:283:ARG:HH12	3:Z:342:LEU:HD23	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1032:THR:HG22	2:B:1034:ASN:H	1.60	0.66
2:Y:6:VAL:HG22	2:Y:1040:VAL:HG22	1.77	0.65
2:Y:866:VAL:HG11	2:Y:884:ILE:HG12	1.76	0.65
3:Z:127:ASN:OD1	3:Z:128:VAL:N	2.28	0.65
2:Y:282:MET:HB2	2:Y:305:LEU:HD11	1.79	0.65
2:B:14:ALA:HB1	2:B:327:ARG:HG2	1.79	0.65
2:Y:297:LEU:HD21	2:Y:300:LEU:HD21	1.79	0.64
2:Y:1032:THR:HG22	2:Y:1034:ASN:H	1.62	0.64
2:B:426:VAL:HG22	2:B:435:VAL:HG22	1.80	0.64
2:Y:561:TRP:O	2:Y:563:ASP:N	2.31	0.64
2:B:903:CYS:SG	2:B:904:ASN:N	2.71	0.63
3:C:99:LEU:HB2	3:C:157:VAL:HG22	1.81	0.63
2:Y:948:ASP:HB2	2:Y:992:LEU:HB2	1.80	0.63
2:B:167:VAL:HG23	2:B:180:PHE:HB3	1.81	0.63
2:Y:14:ALA:HB1	2:Y:327:ARG:HG2	1.81	0.63
2:Y:909:ILE:HG23	2:Y:925:ASP:HB3	1.81	0.63
2:B:866:VAL:HG11	2:B:884:ILE:HG12	1.81	0.63
2:B:282:MET:HB2	2:B:305:LEU:HD11	1.81	0.62
2:B:411:TRP:HZ3	2:B:428:SER:HB3	1.64	0.62
2:Y:1122:ARG:NH2	2:Y:1123:GLU:O	2.32	0.62
2:Y:426:VAL:HG22	2:Y:435:VAL:HG22	1.80	0.62
3:Z:47:ILE:HG22	3:Z:48:ASN:H	1.63	0.62
2:B:273:LEU:HB2	2:B:281:PHE:HB2	1.82	0.62
2:B:970:ASN:O	2:B:973:ASN:ND2	2.33	0.61
2:Y:903:CYS:SG	2:Y:904:ASN:N	2.73	0.61
2:Y:1117:GLY:HA2	2:B:987:GLU:HG2	1.82	0.61
1:A:441:LEU:HD23	1:A:517:LEU:HD12	1.83	0.61
1:A:618:ASP:HB3	1:A:623:ILE:HD12	1.83	0.60
2:Y:90:GLU:OE1	2:Y:103:ARG:NH1	2.34	0.60
2:B:438:LEU:HD21	2:B:682:LEU:HD21	1.84	0.60
3:Z:370:LEU:HD21	3:Z:401:LYS:HD2	1.84	0.60
1:X:441:LEU:HD23	1:X:517:LEU:HD12	1.84	0.60
2:B:948:ASP:HB2	2:B:992:LEU:HB2	1.83	0.60
2:B:90:GLU:OE1	2:B:103:ARG:NH1	2.35	0.59
2:B:478:LEU:HB2	2:B:526:LEU:HD11	1.83	0.59
2:B:554:PRO:HD2	2:B:555:LEU:HD12	1.84	0.59
2:B:414:ARG:O	2:B:481:GLN:NE2	2.34	0.59
1:X:571:LYS:O	3:Z:351:ASN:ND2	2.35	0.59
2:B:375:LEU:HD23	2:B:390:ILE:HD12	1.85	0.59
3:Z:73:HIS:ND1	3:Z:79:GLN:OE1	2.36	0.59
1:A:444:VAL:HG23	1:A:456:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:603:GLU:HG2	1:X:608:PHE:HD2	1.68	0.58
2:B:561:TRP:O	2:B:563:ASP:N	2.37	0.58
1:A:604:THR:HA	1:A:628:VAL:HG13	1.84	0.58
2:B:545:PRO:HA	2:B:553:SER:HB2	1.86	0.58
2:Y:909:ILE:HD12	2:Y:931:LEU:HD13	1.86	0.57
3:Z:47:ILE:HG22	3:Z:48:ASN:N	2.19	0.57
2:Y:413:LEU:HB3	2:Y:424:THR:HB	1.87	0.57
2:Y:189:HIS:HB3	2:Y:210:GLU:HA	1.86	0.57
2:Y:478:LEU:HB2	2:Y:526:LEU:HD11	1.85	0.57
2:B:1047:TRP:HZ3	2:B:1132:VAL:HG13	1.68	0.57
2:Y:188:ARG:NH1	2:Y:216:ALA:O	2.37	0.57
2:B:450:GLY:O	2:B:477:ARG:NH2	2.34	0.57
2:Y:411:TRP:HZ3	2:Y:428:SER:HB3	1.69	0.57
2:Y:432:GLN:OE1	2:Y:434:ARG:NH1	2.36	0.57
3:Z:168:LEU:HD11	3:Z:183:GLN:HB2	1.86	0.57
3:Z:92:ILE:HD11	3:Z:286:ALA:HB2	1.88	0.56
2:B:188:ARG:NH1	2:B:216:ALA:O	2.38	0.56
1:A:605:PHE:HD2	1:A:627:LYS:HD2	1.70	0.56
1:A:573:SER:HB3	3:C:397:HIS:CD2	2.41	0.56
2:B:518:TYR:HB2	2:B:574:PHE:HZ	1.70	0.55
3:Z:126:SER:HA	3:Z:296:ILE:HD13	1.88	0.55
1:X:567:CYS:SG	1:X:577:SER:N	2.79	0.55
3:Z:112:ASN:HB3	3:Z:116:LYS:HE3	1.89	0.55
2:B:1061:VAL:HG13	2:B:1104:LYS:HE3	1.89	0.55
2:B:1070:HIS:CE1	2:B:1093:LEU:HD22	2.42	0.55
3:Z:338:PHE:CE2	3:Z:340:LEU:HG	2.41	0.55
2:B:654:ASP:OD1	2:B:654:ASP:N	2.39	0.55
1:X:509:GLU:OE2	1:X:509:GLU:N	2.41	0.54
2:B:310:ILE:HG21	2:B:328:LEU:HD12	1.89	0.54
3:C:338:PHE:CE2	3:C:340:LEU:HG	2.43	0.54
3:C:92:ILE:HD13	3:C:286:ALA:HA	1.89	0.54
3:Z:108:SER:O	3:Z:112:ASN:ND2	2.38	0.54
1:A:571:LYS:O	3:C:351:ASN:ND2	2.40	0.54
1:A:535:VAL:HG23	1:A:589:VAL:HG22	1.88	0.54
2:Y:183:GLN:NE2	2:Y:188:ARG:HE	2.05	0.54
3:Z:298:LEU:HA	3:Z:301:ILE:HD12	1.89	0.54
1:X:618:ASP:HB3	1:X:623:ILE:HD12	1.90	0.54
1:A:442:PRO:HA	1:A:516:ILE:HG22	1.90	0.54
3:C:73:HIS:CG	3:C:79:GLN:HE21	2.27	0.53
1:X:603:GLU:HG2	1:X:608:PHE:CD2	2.43	0.53
2:Y:546:LEU:CD1	2:Y:547:GLY:H	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:406:LYS:HE2	3:Z:409:MET:HE3	1.90	0.53
3:C:108:SER:O	3:C:112:ASN:ND2	2.40	0.53
2:Y:267:ASN:OD1	2:Y:268:GLY:N	2.42	0.53
3:C:287:CYS:HB2	3:C:345:PRO:HD2	1.91	0.53
2:Y:617:ASN:O	2:Y:621:GLY:N	2.39	0.53
2:Y:654:ASP:N	2:Y:654:ASP:OD2	2.34	0.53
3:C:295:ARG:NH2	3:C:358:GLU:OE1	2.32	0.53
2:B:593:MET:HG2	2:B:602:LEU:HD12	1.91	0.53
2:Y:10:GLN:HB3	2:Y:1037:ILE:HB	1.91	0.53
2:B:555:LEU:HD11	2:B:618:ILE:HG23	1.90	0.52
2:B:812:TYR:CZ	3:C:241:PRO:HB3	2.44	0.52
2:B:361:ASP:OD1	2:B:362:MET:N	2.43	0.52
3:C:57:HIS:HB2	3:C:158:LYS:HE2	1.91	0.52
2:B:538:VAL:HG21	2:B:541:LEU:HD21	1.92	0.52
2:Y:609:GLY:HA3	2:Y:632:GLY:O	2.10	0.52
2:Y:828:TYR:HE2	2:Y:861:VAL:HG21	1.74	0.52
2:B:600:HIS:CG	2:B:618:ILE:HD11	2.45	0.51
3:C:370:LEU:HD21	3:C:401:LYS:HD2	1.92	0.51
2:Y:1070:HIS:CE1	2:Y:1093:LEU:HD22	2.44	0.51
2:B:869:ALA:O	2:B:884:ILE:HA	2.11	0.51
2:Y:606:LEU:HD12	2:Y:610:ALA:HB3	1.93	0.51
2:Y:511:ALA:HA	2:Y:516:LEU:HA	1.91	0.51
3:C:114:ILE:HA	3:C:118:ARG:HG2	1.92	0.51
2:Y:38:ARG:NH2	2:Y:54:GLU:OE2	2.38	0.51
2:Y:869:ALA:O	2:Y:884:ILE:HA	2.10	0.51
2:B:909:ILE:HD13	2:B:931:LEU:HD13	1.93	0.51
2:B:118:THR:HB	2:B:134:ARG:HH22	1.76	0.51
2:B:568:ILE:HD11	2:B:602:LEU:HD13	1.92	0.51
1:X:604:THR:HA	1:X:628:VAL:HG13	1.93	0.51
3:Z:408:ASP:N	3:Z:408:ASP:OD2	2.42	0.51
2:B:57:MET:HG3	2:B:61:ILE:HD11	1.92	0.50
2:Y:92:LYS:HD2	2:Y:101:ILE:HD13	1.92	0.50
2:B:271:TYR:HB2	2:B:283:LEU:HB3	1.92	0.50
1:X:552:HIS:HB2	1:X:615:THR:HG23	1.92	0.50
2:B:543:ILE:HD11	2:B:571:LEU:HD11	1.92	0.50
2:B:358:PRO:HD2	2:B:380:GLY:HA2	1.92	0.50
2:Y:450:GLY:O	2:Y:477:ARG:NH2	2.43	0.50
2:Y:408:LYS:HA	2:Y:678:TYR:CE2	2.46	0.50
2:B:248:ILE:HG13	2:B:250:PRO:HD3	1.94	0.50
2:B:421:THR:OG1	2:B:683:ASN:O	2.29	0.50
2:B:609:GLY:HA3	2:B:632:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:605:PHE:HD2	1:X:627:LYS:HB3	1.76	0.50
1:A:466:GLY:HA2	1:A:480:VAL:O	2.12	0.49
2:B:299:ASP:OD1	2:B:300:LEU:N	2.44	0.49
1:A:578:LYS:HD3	1:A:578:LYS:H	1.77	0.49
2:B:1032:THR:HG22	2:B:1034:ASN:N	2.28	0.49
2:B:511:ALA:HA	2:B:516:LEU:HA	1.94	0.49
3:Z:70:ARG:HD3	3:Z:162:ARG:HH12	1.77	0.49
2:B:396:ILE:HD12	2:B:673:LEU:HD13	1.93	0.49
2:B:596:PHE:HB3	2:B:661:SER:HB3	1.94	0.49
2:Y:507:GLN:HB3	2:Y:518:TYR:HE2	1.78	0.49
3:C:60:LEU:HD12	3:C:158:LYS:HE3	1.94	0.49
2:Y:605:ALA:HB1	2:Y:636:THR:HB	1.94	0.49
2:B:1105:MET:O	2:B:1109:VAL:HG12	2.12	0.49
1:X:529:THR:HB	1:X:632:VAL:HB	1.93	0.49
2:Y:1004:VAL:HG11	2:Y:1007:PHE:CZ	2.48	0.49
2:B:239:TYR:O	2:B:240:HIS:ND1	2.46	0.48
2:Y:331:SER:HB2	2:Y:353:PHE:HB2	1.95	0.48
2:B:143:ILE:HG12	2:B:154:ALA:HB2	1.95	0.48
3:C:114:ILE:HG21	3:C:144:TYR:CE1	2.47	0.48
2:Y:361:ASP:OD1	2:Y:362:MET:N	2.45	0.48
2:Y:618:ILE:H	2:Y:618:ILE:HD12	1.79	0.48
2:B:970:ASN:OD1	2:B:971:ALA:N	2.45	0.48
1:X:560:VAL:HG21	1:X:594:LEU:HD23	1.96	0.48
2:Y:812:TYR:CZ	3:Z:241:PRO:HB3	2.48	0.48
1:A:473:PRO:HG2	1:A:515:PHE:CG	2.48	0.48
1:X:473:PRO:HG2	1:X:515:PHE:CD1	2.49	0.48
3:Z:283:ARG:NH1	3:Z:342:LEU:O	2.46	0.48
3:C:73:HIS:CD2	3:C:79:GLN:HG3	2.48	0.48
1:A:485:SER:HA	1:A:499:LEU:HA	1.96	0.47
2:B:534:MET:HG2	2:B:560:LEU:HD21	1.95	0.47
1:X:442:PRO:HA	1:X:516:ILE:HG22	1.95	0.47
2:Y:507:GLN:NE2	2:Y:518:TYR:OH	2.39	0.47
2:B:413:LEU:HB3	2:B:424:THR:HB	1.95	0.47
3:C:375:SER:OG	3:C:377:GLU:HG3	2.15	0.47
3:Z:265:ASP:OD1	3:Z:266:GLU:N	2.47	0.47
2:B:16:ASN:OD1	2:B:327:ARG:NH1	2.48	0.47
2:B:828:TYR:HE2	2:B:861:VAL:HG21	1.79	0.47
3:Z:106:GLU:O	3:Z:109:MET:HG3	2.14	0.47
2:B:518:TYR:HB2	2:B:574:PHE:CZ	2.49	0.47
1:A:552:HIS:HB2	1:A:615:THR:HG23	1.96	0.47
3:C:406:LYS:HE2	3:C:409:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:197:VAL:HG21	3:Z:238:THR:HG22	1.97	0.47
1:A:578:LYS:CD	1:A:578:LYS:H	2.28	0.47
1:A:478:VAL:HG23	1:A:505:GLY:HA3	1.95	0.47
3:C:298:LEU:HA	3:C:301:ILE:HD12	1.97	0.47
2:Y:532:THR:HG1	2:Y:574:PHE:HD1	1.61	0.47
3:Z:406:LYS:HE2	3:Z:409:MET:CE	2.43	0.47
1:X:473:PRO:HG3	1:X:601:CYS:SG	2.54	0.46
2:Y:275:ASP:OD1	2:Y:276:MET:N	2.46	0.46
1:A:440:ARG:NH2	1:A:603:GLU:OE2	2.44	0.46
3:C:70:ARG:HD2	3:C:162:ARG:HH12	1.79	0.46
3:Z:194:MET:HA	3:Z:197:VAL:HG12	1.97	0.46
2:Y:358:PRO:HD2	2:Y:380:GLY:HA2	1.97	0.46
2:Y:891:TYR:HB3	2:Y:899:LEU:HD22	1.97	0.46
2:Y:717:LEU:HD12	2:Y:721:PRO:HG3	1.98	0.46
2:Y:118:THR:HB	2:Y:134:ARG:NH2	2.31	0.46
2:Y:17:GLY:HA2	2:Y:313:CYS:SG	2.56	0.46
3:Z:398:ILE:O	3:Z:418:THR:HG22	2.16	0.46
1:X:593:ARG:HD3	1:X:632:VAL:HG21	1.98	0.46
2:B:64:MET:HG3	2:B:77:LEU:HD11	1.97	0.45
1:X:544:CYS:HB2	1:X:545:PRO:HD2	1.97	0.45
1:X:567:CYS:HB3	1:X:591:ILE:HD11	1.98	0.45
2:Y:206:PRO:HB2	2:Y:207:TRP:CD1	2.51	0.45
2:Y:600:HIS:CG	2:Y:618:ILE:HD11	2.51	0.45
1:A:449:ASP:OD1	1:A:450:MET:HG2	2.15	0.45
2:B:719:GLU:OE2	2:B:757:SER:N	2.48	0.45
2:Y:661:SER:HB2	2:Y:663:ASN:N	2.32	0.45
3:Z:257:ILE:HG21	3:Z:284:VAL:HG11	1.97	0.45
1:A:552:HIS:CE1	1:A:617:ARG:HD3	2.52	0.45
1:X:439:ILE:HD11	1:X:463:ILE:HB	1.98	0.45
1:X:482:GLY:H	1:X:502:ARG:HB3	1.82	0.45
2:Y:316:TYR:HA	2:Y:322:VAL:HG22	1.98	0.45
1:X:627:LYS:NZ	3:Z:377:GLU:OE1	2.43	0.45
2:B:1011:SER:OG	2:B:1012:LEU:N	2.50	0.45
2:B:617:ASN:O	2:B:621:GLY:N	2.42	0.45
2:Y:420:GLU:HB2	2:Y:421:THR:H	1.48	0.45
2:Y:23:PHE:N	2:Y:30:ASN:OD1	2.42	0.45
2:B:182:TYR:CZ	2:B:189:HIS:HB2	2.52	0.45
2:B:275:ASP:OD1	2:B:276:MET:N	2.47	0.45
3:C:350:VAL:HG12	3:C:356:VAL:HG22	1.99	0.45
2:B:883:SER:HB2	2:B:911:ALA:HB3	1.98	0.45
2:B:336:LEU:HD23	2:B:336:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:TRP:CZ3	3:C:345:PRO:HG3	2.51	0.45
2:Y:231:ILE:HA	2:Y:231:ILE:HD13	1.84	0.45
2:Y:845:GLN:HA	2:Y:868:GLY:H	1.82	0.45
2:Y:18:CYS:SG	2:Y:31:LEU:HD11	2.57	0.44
2:Y:642:ARG:NH2	2:Y:645:SER:HA	2.32	0.44
2:Y:72:GLU:OE1	2:Y:103:ARG:NH2	2.46	0.44
2:B:537:GLU:HG3	2:B:561:TRP:CG	2.52	0.44
1:X:613:ARG:HD3	3:Z:150:PHE:CE1	2.52	0.44
2:Y:1047:TRP:HZ3	2:Y:1132:VAL:HG13	1.83	0.44
2:Y:542:ASP:OD1	2:Y:544:THR:OG1	2.35	0.44
2:Y:134:ARG:NH1	2:Y:134:ARG:O	2.51	0.44
2:Y:541:LEU:HA	2:Y:557:ALA:O	2.18	0.44
1:A:464:CYS:HA	1:A:492:THR:HG22	1.99	0.44
2:Y:652:CYS:HB3	2:Y:676:VAL:HG12	2.00	0.44
2:Y:987:GLU:OE2	2:Y:988:GLU:N	2.36	0.44
2:Y:183:GLN:HE21	2:Y:188:ARG:HE	1.65	0.44
2:Y:376:VAL:HG22	2:Y:389:ILE:HG13	1.99	0.44
2:Y:411:TRP:CZ3	2:Y:428:SER:HB3	2.51	0.44
3:C:385:ALA:O	3:C:402:PHE:HA	2.18	0.44
2:Y:59:GLY:HA2	2:Y:1073:TRP:CZ3	2.53	0.44
2:Y:803:HIS:HD2	2:Y:858:LEU:HB2	1.82	0.44
1:A:529:THR:HG23	1:A:595:ARG:HG2	2.00	0.44
2:Y:16:ASN:ND2	2:Y:36:ASN:HA	2.32	0.44
2:B:63:VAL:HB	2:B:80:LEU:HB3	1.99	0.44
3:Z:57:HIS:HB2	3:Z:158:LYS:HE2	2.00	0.44
3:C:106:GLU:O	3:C:109:MET:HG3	2.17	0.44
3:C:194:MET:HA	3:C:197:VAL:HG12	2.00	0.44
1:X:485:SER:HA	1:X:499:LEU:HA	2.00	0.44
2:Y:1032:THR:HG22	2:Y:1034:ASN:N	2.31	0.44
3:C:112:ASN:HB3	3:C:116:LYS:NZ	2.33	0.43
3:C:232:PHE:O	3:C:242:ARG:HG2	2.17	0.43
3:C:326:CYS:C	3:C:328:GLU:H	2.22	0.43
2:B:451:PHE:CE2	2:B:470:GLN:HB2	2.53	0.43
2:B:618:ILE:HD12	2:B:618:ILE:H	1.82	0.43
1:X:568:LEU:HD23	1:X:590:CYS:HB3	1.99	0.43
2:B:661:SER:HB2	2:B:666:LEU:HD23	2.00	0.43
2:Y:1011:SER:OG	2:Y:1012:LEU:N	2.52	0.43
2:Y:63:VAL:HB	2:Y:80:LEU:HB3	1.99	0.43
2:B:1058:LEU:HB3	2:B:1062:ILE:HD12	2.00	0.43
2:B:927:MET:C	2:B:929:SER:H	2.20	0.43
2:Y:842:GLU:HG3	2:Y:843:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:PRO:HG2	2:B:253:ILE:HG12	2.01	0.43
2:B:376:VAL:HG22	2:B:389:ILE:HG13	2.01	0.43
2:B:741:GLU:HG2	2:B:751:ALA:HA	2.00	0.43
2:Y:503:CYS:SG	2:Y:504:ASN:N	2.91	0.43
2:Y:845:GLN:HA	2:Y:868:GLY:N	2.32	0.43
2:Y:80:LEU:HA	2:Y:85:ASN:O	2.19	0.43
2:B:10:GLN:HB3	2:B:1037:ILE:HB	2.00	0.43
3:Z:135:PHE:CG	3:Z:136:GLY:N	2.87	0.43
2:Y:535:GLU:OE2	2:Y:567:ARG:NH2	2.50	0.43
2:Y:70:LYS:HE2	2:Y:70:LYS:HB2	1.79	0.43
2:B:908:ASN:N	2:B:908:ASN:OD1	2.51	0.43
2:B:987:GLU:HG3	2:B:989:ARG:HH21	1.84	0.43
1:X:449:ASP:OD1	1:X:450:MET:N	2.51	0.43
2:Y:64:MET:HG3	2:Y:77:LEU:HD11	2.01	0.43
2:B:59:GLY:HA2	2:B:1073:TRP:CZ3	2.53	0.43
2:B:606:LEU:HD12	2:B:610:ALA:HB3	2.00	0.43
1:X:542:ILE:HG22	1:X:585:LYS:HG2	2.01	0.43
2:Y:238:THR:HG23	2:Y:247:ALA:HB2	2.00	0.43
2:Y:336:LEU:HD23	2:Y:336:LEU:H	1.84	0.43
2:Y:60:LYS:HB3	2:Y:60:LYS:HE3	1.82	0.43
2:Y:673:LEU:HD23	2:Y:673:LEU:HA	1.86	0.43
2:Y:821:LEU:HB3	2:Y:893:TRP:HB2	2.01	0.43
2:B:1104:LYS:HA	2:B:1107:GLU:HB3	2.00	0.42
2:B:639:ARG:HE	2:B:639:ARG:HB3	1.56	0.42
2:B:70:LYS:HE2	2:B:70:LYS:HB2	1.80	0.42
2:Y:1002:GLU:HB3	2:Y:1032:THR:HG21	2.01	0.42
3:Z:340:LEU:HD23	3:Z:340:LEU:HA	1.89	0.42
2:B:411:TRP:CZ3	2:B:428:SER:HB3	2.50	0.42
2:B:564:ILE:HG23	2:B:588:PRO:HD3	2.01	0.42
2:Y:161:GLU:N	2:Y:161:GLU:OE1	2.47	0.42
2:Y:908:ASN:OD1	2:Y:908:ASN:N	2.52	0.42
2:Y:883:SER:HB2	2:Y:911:ALA:HB3	1.99	0.42
1:X:575:GLU:HA	3:Z:371:ILE:HD11	2.00	0.42
1:A:556:CYS:SG	1:A:600:ILE:HG12	2.59	0.42
2:B:412:PRO:HD3	2:B:680:CYS:HB2	2.02	0.42
2:Y:191:LYS:HG3	2:Y:208:LYS:HE2	2.01	0.42
2:Y:480:SER:HB3	2:Y:487:VAL:HG11	2.01	0.42
2:Y:481:GLN:OE1	2:Y:484:LYS:NZ	2.52	0.42
3:Z:385:ALA:O	3:Z:402:PHE:HA	2.20	0.42
1:A:567:CYS:HB2	1:A:591:ILE:HD11	2.01	0.42
2:Y:213:GLU:OE2	2:Y:214:ALA:CA	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:586:ILE:HG13	2:Y:608:ASP:HB3	2.01	0.42
2:Y:987:GLU:OE1	2:Y:989:ARG:NH2	2.52	0.42
2:B:537:GLU:HG3	2:B:561:TRP:CD1	2.55	0.42
2:Y:124:ILE:HG12	2:Y:131:ILE:HG12	2.00	0.42
2:Y:719:GLU:OE2	2:Y:757:SER:N	2.46	0.42
2:Y:123:ILE:HD13	2:Y:167:VAL:HG13	2.01	0.42
2:Y:438:LEU:HD21	2:Y:682:LEU:HD21	2.01	0.42
3:Z:85:PRO:HD3	3:Z:177:ILE:HD13	2.00	0.42
2:B:920:PHE:O	2:B:921:ILE:HG13	2.19	0.42
3:C:78:CYS:HA	3:C:182:VAL:O	2.20	0.42
3:C:280:PHE:O	3:C:284:VAL:HG22	2.20	0.42
2:Y:378:CYS:HB3	2:Y:721:PRO:HB2	2.01	0.42
3:Z:280:PHE:O	3:Z:284:VAL:HG22	2.19	0.42
3:Z:326:CYS:C	3:Z:328:GLU:H	2.23	0.42
2:B:102:THR:HG21	2:B:1067:LYS:HG3	2.02	0.42
2:B:161:GLU:OE1	2:B:161:GLU:N	2.46	0.42
2:B:378:CYS:HB3	2:B:721:PRO:HB2	2.01	0.42
2:B:890:LEU:HB3	2:B:903:CYS:HB3	2.02	0.42
2:B:404:LEU:HD13	2:B:699:LEU:HD12	2.02	0.42
2:B:500:VAL:HG11	2:B:540:CYS:HA	2.01	0.42
3:Z:359:THR:HG21	3:Z:380:TRP:CZ3	2.55	0.42
2:Y:931:LEU:HD11	2:Y:947:ARG:NH2	2.35	0.42
3:Z:262:ARG:HH22	3:Z:269:LYS:HD3	1.85	0.42
1:X:464:CYS:HA	1:X:492:THR:HG22	2.02	0.41
1:A:482:GLY:H	1:A:502:ARG:HB3	1.85	0.41
1:X:473:PRO:HG2	1:X:515:PHE:CG	2.55	0.41
2:Y:264:VAL:HG13	2:Y:316:TYR:CG	2.55	0.41
2:Y:476:VAL:HB	2:Y:490:TRP:HB3	2.02	0.41
2:Y:764:SER:N	2:Y:803:HIS:HE1	2.19	0.41
2:Y:909:ILE:HD11	2:Y:949:PHE:CZ	2.55	0.41
2:B:667:VAL:HG22	2:B:1138:ARG:HD3	2.02	0.41
2:B:38:ARG:NH2	2:B:54:GLU:OE2	2.38	0.41
2:Y:414:ARG:O	2:Y:481:GLN:NE2	2.52	0.41
2:Y:522:HIS:CE1	2:Y:527:ARG:HH12	2.37	0.41
2:Y:921:ILE:HB	2:Y:933:LEU:HB2	2.01	0.41
2:Y:471:ILE:HG12	2:Y:476:VAL:HG13	2.03	0.41
2:B:1122:ARG:NH2	2:B:1123:GLU:O	2.52	0.41
2:Y:176:PRO:HG2	2:Y:195:VAL:O	2.20	0.41
2:Y:310:ILE:HG21	2:Y:328:LEU:HD12	2.02	0.41
2:Y:909:ILE:CG2	2:Y:925:ASP:HB3	2.49	0.41
1:A:455:LEU:HG	1:A:500:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:938:MET:HE2	2:Y:938:MET:H	1.85	0.41
2:Y:966:LEU:HD12	2:Y:975:PHE:O	2.21	0.41
3:Z:140:GLU:HB2	3:Z:162:ARG:HG3	2.03	0.41
1:A:575:GLU:HG3	3:C:371:ILE:HD13	2.01	0.41
3:C:200:GLU:HA	3:C:203:ASN:ND2	2.35	0.41
1:X:580:ARG:HB3	1:X:582:ARG:HH12	1.86	0.41
2:Y:413:LEU:HA	2:Y:413:LEU:HD12	1.90	0.41
2:Y:466:GLN:O	2:Y:481:GLN:HB2	2.21	0.41
2:B:79:ILE:HB	2:B:87:CYS:SG	2.60	0.41
2:Y:498:ILE:HA	2:Y:512:VAL:HG22	2.03	0.41
2:Y:421:THR:OG1	2:Y:683:ASN:O	2.37	0.41
2:Y:807:PHE:CZ	2:Y:831:VAL:HG11	2.55	0.41
1:A:575:GLU:HA	3:C:371:ILE:HD11	2.03	0.41
2:B:413:LEU:HD12	2:B:413:LEU:HA	1.83	0.41
3:C:153:GLU:O	3:C:154:ILE:HD13	2.20	0.41
2:Y:55:VAL:HG11	2:Y:100:ILE:HD12	2.02	0.41
2:Y:812:TYR:OH	3:Z:241:PRO:HB3	2.20	0.41
2:B:104:ALA:HB1	2:B:152:LEU:HG	2.03	0.41
2:Y:333:LEU:HA	2:Y:333:LEU:HD23	1.97	0.41
2:Y:928:ARG:O	2:Y:930:VAL:HG23	2.21	0.41
2:B:615:GLY:N	2:B:624:SER:O	2.47	0.40
3:C:80:VAL:HA	3:C:180:ALA:O	2.21	0.40
2:Y:329:GLY:O	2:Y:355:ASN:ND2	2.33	0.40
2:B:480:SER:HB3	2:B:487:VAL:HG11	2.03	0.40
2:Y:639:ARG:HE	2:Y:639:ARG:HB3	1.54	0.40
2:B:55:VAL:HG11	2:B:100:ILE:HD12	2.03	0.40
2:B:966:LEU:HD12	2:B:975:PHE:O	2.21	0.40
2:Y:422:ASP:O	2:Y:684:SER:HA	2.21	0.40
2:Y:927:MET:C	2:Y:929:SER:H	2.24	0.40
1:A:440:ARG:HB2	1:A:460:SER:HB3	2.03	0.40
1:A:446:LYS:H	1:A:446:LYS:HD3	1.87	0.40
2:Y:1093:LEU:O	2:Y:1096:SER:OG	2.39	0.40
2:Y:183:GLN:HB2	2:Y:188:ARG:HG2	2.02	0.40
2:Y:451:PHE:CE2	2:Y:470:GLN:HB2	2.56	0.40
2:Y:480:SER:O	2:Y:484:LYS:HA	2.22	0.40
2:B:1002:GLU:HB3	2:B:1032:THR:CG2	2.52	0.40
2:B:580:GLU:HG2	2:B:614:PHE:CE2	2.56	0.40
2:B:845:GLN:HA	2:B:868:GLY:N	2.37	0.40
3:C:65:GLU:O	3:C:143:ALA:HA	2.20	0.40
3:Z:290:ILE:O	3:Z:419:ARG:HD2	2.22	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	195/199 (98%)	175 (90%)	18 (9%)	2 (1%)	15	54
1	X	194/199 (98%)	170 (88%)	21 (11%)	3 (2%)	10	46
2	B	1061/1140 (93%)	985 (93%)	75 (7%)	1 (0%)	51	83
2	Y	1090/1140 (96%)	1005 (92%)	83 (8%)	2 (0%)	47	79
3	C	375/406 (92%)	358 (96%)	15 (4%)	2 (0%)	29	67
3	Z	376/406 (93%)	358 (95%)	17 (4%)	1 (0%)	41	74
All	All	3291/3490 (94%)	3051 (93%)	229 (7%)	11 (0%)	41	74

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Z	50	ASP
3	C	50	ASP
3	C	130	GLU
1	X	599	THR
2	Y	551	GLY
1	X	609	PRO
2	Y	562	THR
1	A	609	PRO
2	B	562	THR
1	X	506	ILE
1	A	506	ILE

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	156/175 (89%)	148 (95%)	8 (5%)	24	58
1	X	155/175 (89%)	149 (96%)	6 (4%)	32	64
2	B	865/999 (87%)	851 (98%)	14 (2%)	62	82
2	Y	896/999 (90%)	873 (97%)	23 (3%)	46	73
3	C	307/368 (83%)	303 (99%)	4 (1%)	69	85
3	Z	319/368 (87%)	315 (99%)	4 (1%)	69	85
All	All	2698/3084 (88%)	2639 (98%)	59 (2%)	52	76

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	446	LYS
1	X	519	ASP
1	X	544	CYS
1	X	565	LEU
1	X	605	PHE
1	X	617	ARG
2	Y	18	CYS
2	Y	67	PHE
2	Y	147	ARG
2	Y	196	SER
2	Y	213	GLU
2	Y	299	ASP
2	Y	366	ASP
2	Y	428	SER
2	Y	492	GLU
2	Y	503	CYS
2	Y	533	GLU
2	Y	670	ASN
2	Y	803	HIS
2	Y	855	ASP
2	Y	900	ARG
2	Y	908	ASN
2	Y	927	MET
2	Y	938	MET
2	Y	987	GLU
2	Y	990	GLN
2	Y	1005	ASN
2	Y	1111	ASN
2	Y	1131	LYS
3	Z	144	TYR

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Mol	Chain	Res	Type
3	Z	175	ASP
3	Z	208	PHE
3	Z	415	TRP
1	A	446	LYS
1	A	519	ASP
1	A	528	ARG
1	A	565	LEU
1	A	578	LYS
1	A	601	CYS
1	A	605	PHE
1	A	615	THR
2	B	67	PHE
2	B	147	ARG
2	B	300	LEU
2	B	428	SER
2	B	533	GLU
2	B	578	HIS
2	B	900	ARG
2	B	908	ASN
2	B	927	MET
2	B	938	MET
2	B	987	GLU
2	B	990	GLN
2	B	1005	ASN
2	B	1131	LYS
3	C	175	ASP
3	C	208	PHE
3	C	408	ASP
3	C	415	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	Y	183	GLN
3	Z	397	HIS
2	B	578	HIS
2	B	907	ASN
3	C	73	HIS
3	C	79	GLN

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 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	$\# Z > 2$
4	V4M	C	501	-	35,35,35	2.75	13 (37%)	47,52,52	2.36	15 (31%)
4	V4M	Z	501	-	35,35,35	2.75	13 (37%)	47,52,52	2.34	12 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	V4M	C	501	-	-	8/21/46/46	0/4/4/4
4	V4M	Z	501	-	-	4/21/46/46	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	V4M	C8-N1	9.39	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	501	V4M	C8-N1	9.26	1.45	1.36
4	Z	501	V4M	C7-N1	6.23	1.51	1.46
4	C	501	V4M	C7-N1	6.16	1.51	1.46
4	Z	501	V4M	C15-N3	5.87	1.45	1.34
4	C	501	V4M	C15-N3	5.72	1.45	1.34
4	Z	501	V4M	C7-C6	4.69	1.56	1.50
4	C	501	V4M	C7-C6	4.62	1.56	1.50
4	Z	501	V4M	C12-N2	3.71	1.43	1.37
4	C	501	V4M	C12-N2	3.70	1.43	1.37
4	Z	501	V4M	C13-N2	3.55	1.43	1.37
4	C	501	V4M	C13-N2	3.51	1.43	1.37
4	C	501	V4M	C5-C6	-3.28	1.35	1.39
4	Z	501	V4M	C5-C6	-3.27	1.35	1.39
4	C	501	V4M	C16-C17	3.02	1.53	1.50
4	Z	501	V4M	C16-C17	2.86	1.53	1.50
4	Z	501	V4M	C16-C15	-2.51	1.53	1.55
4	C	501	V4M	C16-C15	-2.38	1.53	1.55
4	Z	501	V4M	O4-C15	-2.25	1.19	1.22
4	Z	501	V4M	O2-C13	-2.23	1.19	1.23
4	C	501	V4M	O2-C13	-2.23	1.19	1.23
4	C	501	V4M	O4-C15	-2.21	1.19	1.22
4	C	501	V4M	O3-C12	-2.17	1.18	1.23
4	Z	501	V4M	O3-C12	-2.15	1.18	1.23
4	Z	501	V4M	C20-CL1	2.05	1.79	1.74
4	C	501	V4M	C20-CL1	2.01	1.78	1.74

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	501	V4M	C7-N1-C8	-7.97	109.84	113.12
4	C	501	V4M	C7-N1-C8	-7.62	109.99	113.12
4	C	501	V4M	C9-N1-C8	5.23	130.14	121.81
4	Z	501	V4M	C9-N1-C8	5.20	130.09	121.81
4	C	501	V4M	C12-N2-C13	-4.75	120.00	126.61
4	Z	501	V4M	F2-C16-F1	4.74	108.90	105.23
4	Z	501	V4M	C12-N2-C13	-4.56	120.26	126.61
4	C	501	V4M	F2-C16-F1	4.49	108.70	105.23
4	Z	501	V4M	C10-C11-C12	-4.12	106.82	114.12
4	C	501	V4M	C10-C11-C12	-4.05	106.96	114.12
4	C	501	V4M	C7-N1-C9	-3.97	119.87	123.69
4	Z	501	V4M	C7-N1-C9	-3.77	120.07	123.69
4	Z	501	V4M	C10-C9-N1	-3.64	110.19	114.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	V4M	C11-C12-N2	3.57	120.66	116.65
4	Z	501	V4M	C11-C12-N2	3.46	120.54	116.65
4	Z	501	V4M	C6-C5-C8	3.44	110.78	108.94
4	C	501	V4M	C6-C5-C8	3.31	110.71	108.94
4	C	501	V4M	C6-C7-N1	-3.11	101.14	102.18
4	C	501	V4M	C10-C9-N1	-3.09	110.77	114.11
4	C	501	V4M	O4-C15-C16	2.60	121.50	118.44
4	Z	501	V4M	C9-C13-N2	2.50	119.61	116.25
4	C	501	V4M	C9-C13-N2	2.46	119.56	116.25
4	C	501	V4M	C2-C14-N3	-2.45	107.80	113.05
4	Z	501	V4M	C6-C7-N1	-2.43	101.37	102.18
4	C	501	V4M	C1-C2-C3	2.21	121.64	118.54
4	C	501	V4M	C4-C1-C2	-2.15	118.06	121.03
4	Z	501	V4M	O4-C15-C16	2.14	120.96	118.44

There are no chirality outliers.

All (12) torsion outliers are listed below:

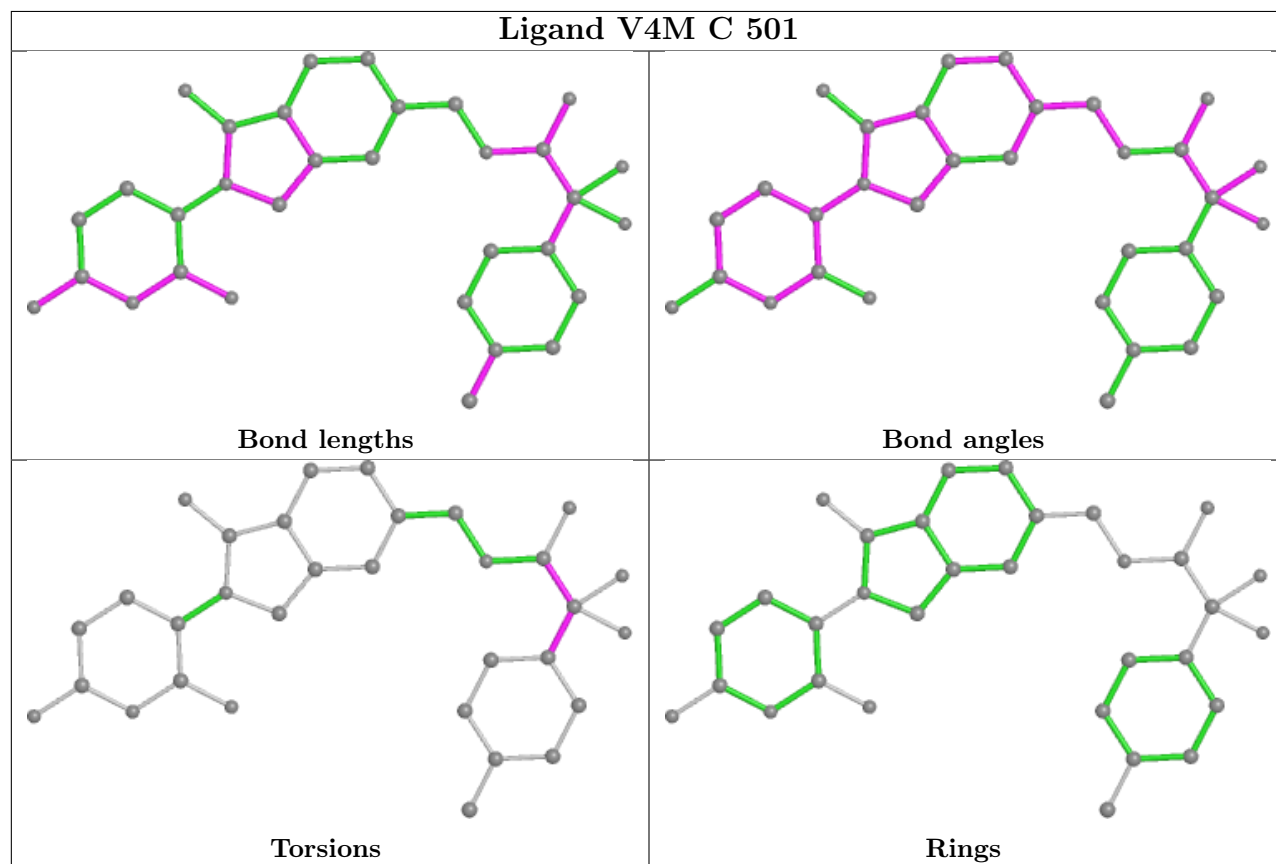
Mol	Chain	Res	Type	Atoms
4	C	501	V4M	N3-C15-C16-C17
4	C	501	V4M	N3-C15-C16-F1
4	C	501	V4M	O4-C15-C16-F1
4	C	501	V4M	C15-C16-C17-C18
4	C	501	V4M	F2-C16-C17-C18
4	C	501	V4M	F2-C16-C17-C22
4	Z	501	V4M	N3-C15-C16-C17
4	Z	501	V4M	N3-C15-C16-F2
4	Z	501	V4M	O4-C15-C16-F2
4	C	501	V4M	O4-C15-C16-C17
4	Z	501	V4M	O4-C15-C16-C17
4	C	501	V4M	F1-C16-C17-C22

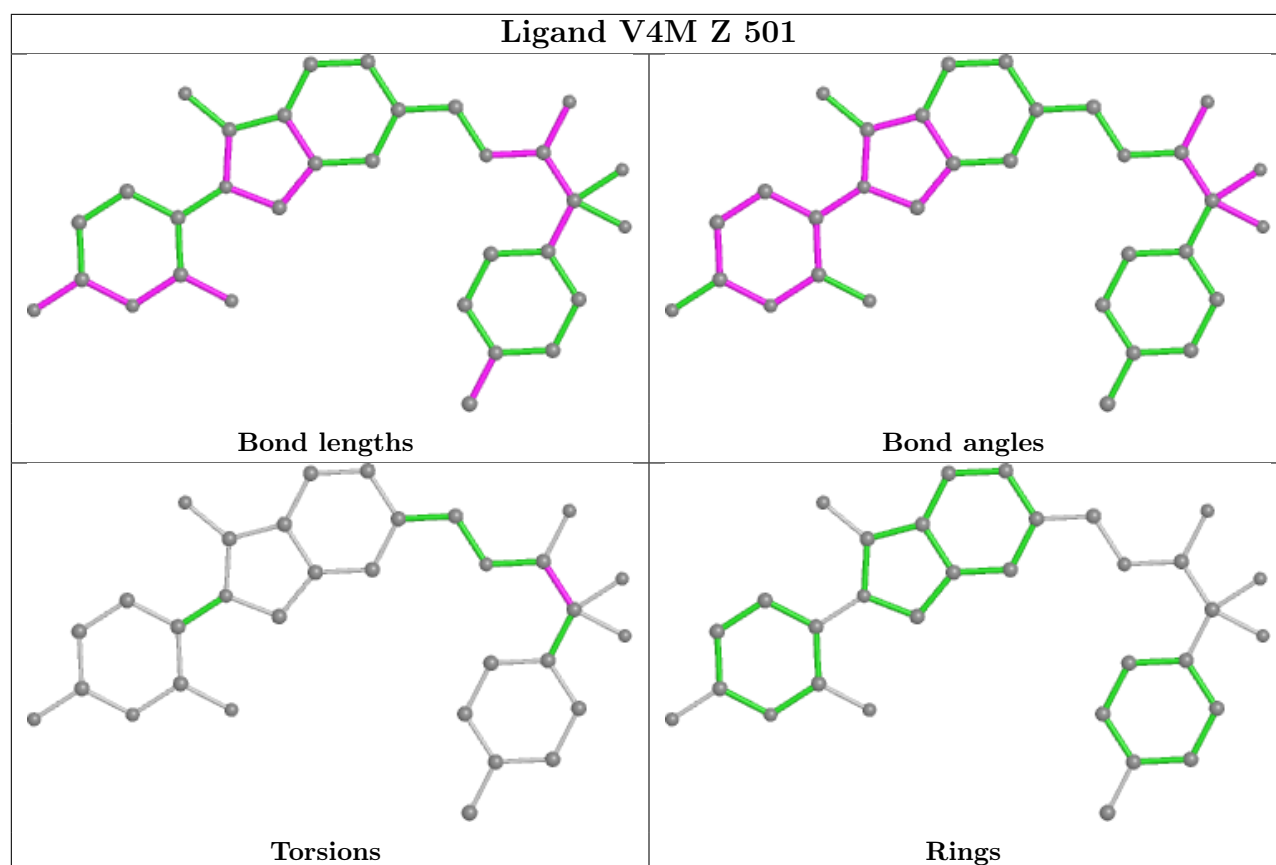
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	197/199 (98%)	-0.01	0	100	100	51, 87, 126, 133	0
1	X	196/199 (98%)	0.01	0	100	100	53, 90, 127, 138	0
2	B	1085/1140 (95%)	0.15	36 (3%)	46	31	52, 92, 141, 162	0
2	Y	1106/1140 (97%)	0.09	14 (1%)	77	64	51, 91, 129, 151	0
3	C	381/406 (93%)	0.05	3 (0%)	86	76	61, 89, 135, 161	0
3	Z	382/406 (94%)	0.12	6 (1%)	72	58	57, 89, 129, 154	0
All	All	3347/3490 (95%)	0.10	59 (1%)	68	53	51, 90, 134, 162	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	236	SER	4.4
3	C	209	PRO	4.4
2	B	140	PHE	4.0
2	Y	166	ASP	3.6
3	C	201	SER	3.6
2	Y	232	ILE	3.6
2	B	237	ILE	3.6
2	Y	179	CYS	3.5
2	B	141	LYS	3.4
2	B	166	ASP	3.4
2	B	232	ILE	3.4
3	Z	210	SER	3.1
2	B	65	GLU	3.1
2	B	230	ILE	3.1
2	B	220	ILE	3.1
2	B	130	MET	3.0
2	B	157	ILE	2.9
2	B	235	GLU	2.8
2	B	231	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	283	LEU	2.7
2	B	124	ILE	2.7
2	Y	180	PHE	2.7
2	B	156	ASN	2.6
2	B	88	ILE	2.6
2	B	273	LEU	2.6
2	B	142	VAL	2.6
2	B	155	PHE	2.5
2	B	64	MET	2.5
2	B	214	ALA	2.5
2	B	133	LEU	2.5
3	Z	441	CYS	2.5
2	Y	237	ILE	2.5
2	B	165	ILE	2.4
2	B	285	LEU	2.4
2	B	169	PHE	2.4
2	B	216	ALA	2.4
2	B	252	ILE	2.3
2	B	182	TYR	2.3
2	Y	231	ILE	2.3
3	Z	207	ILE	2.3
2	Y	315	THR	2.3
2	B	787	GLU	2.2
2	B	104	ALA	2.2
2	B	122	GLY	2.2
2	Y	140	PHE	2.2
3	Z	189	VAL	2.2
2	Y	195	VAL	2.2
2	B	177	THR	2.2
2	B	280	LEU	2.2
2	Y	273	LEU	2.1
2	Y	156	ASN	2.1
3	C	204	LYS	2.1
2	B	240	HIS	2.1
2	Y	120	ILE	2.1
2	Y	197	LEU	2.1
3	Z	197	VAL	2.0
2	B	229	ALA	2.0
3	Z	193	THR	2.0
2	Y	300	LEU	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](#)

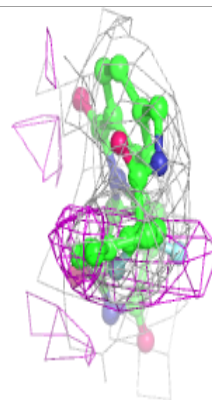
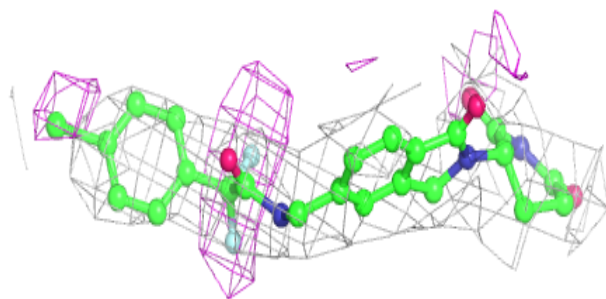
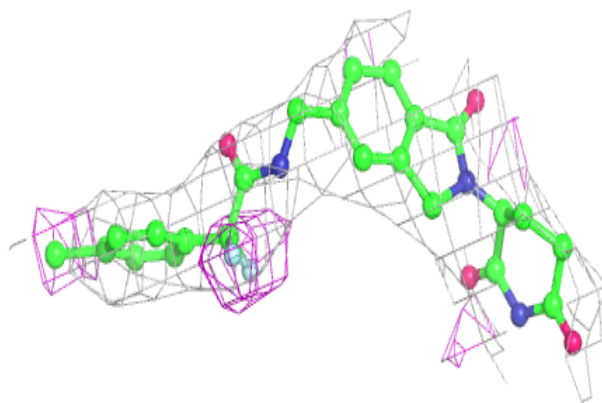
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ZN	C	502	1/1	0.92	0.22	99,99,99,99	0
4	V4M	Z	501	32/32	0.93	0.42	57,70,98,112	0
4	V4M	C	501	32/32	0.94	0.38	57,68,98,122	0
5	ZN	Z	502	1/1	0.97	0.25	133,133,133,133	0

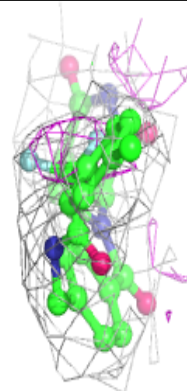
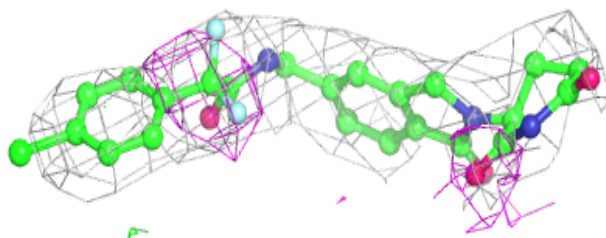
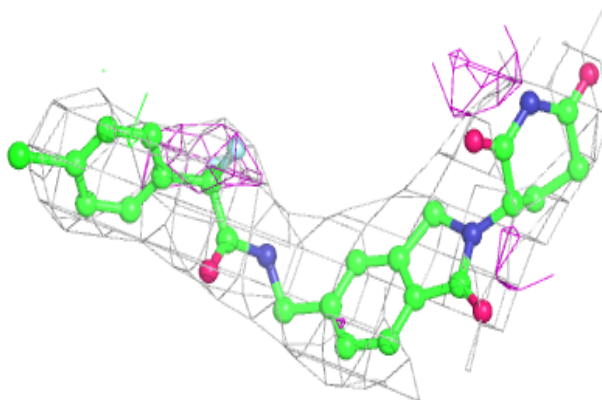
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V4M Z 501:

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

**Electron density around V4M C 501:**

$2mF_o-DF_c$ (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.