



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:05 AM UTC

PDB ID : 1FVV / pdb_00001fvv
Title : THE STRUCTURE OF CDK2/CYCLIN A IN COMPLEX WITH AN OXINDOLE INHIBITOR
Authors : Davis, S.T.; Benson, B.G.; Bramson, H.N.; Chapman, D.E.; Dickerson, S.H.; Dold, K.M.; Eberwein, D.J.; Edelstein, M.; Frye, S.V.; Gampe Jr., R.T.; Griffin, R.J.; Harris, P.A.; Hassell, A.M.; Holmes, W.D.; Hunter, R.N.; Knick, V.B.; Lackey, K.; Lovejoy, B.; Luzzio, M.J.; Murray, D.; Parker, P.; Rocque, W.J.; Shewchuk, L.; Veal, J.M.; Walker, D.H.; Kuyper, L.K.
Deposited on : 2000-09-20
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 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

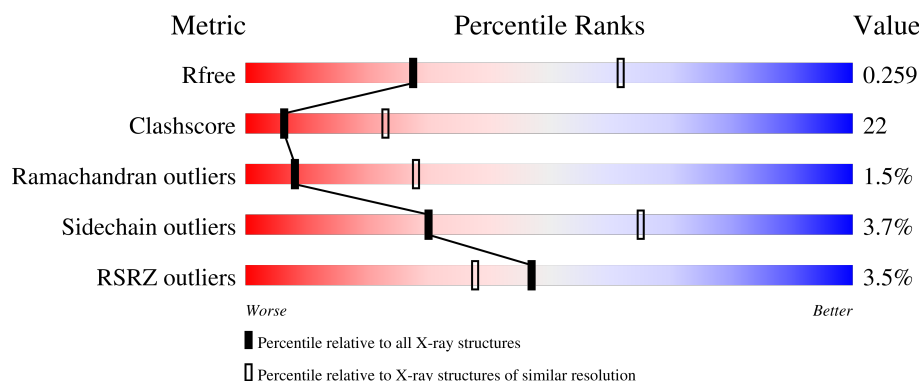
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	298	4% 62% 34% .
1	C	298	5% 54% 41% 5%
2	B	260	2% 53% 42% 5%

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	D	260	3% 63% 33%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9151 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.

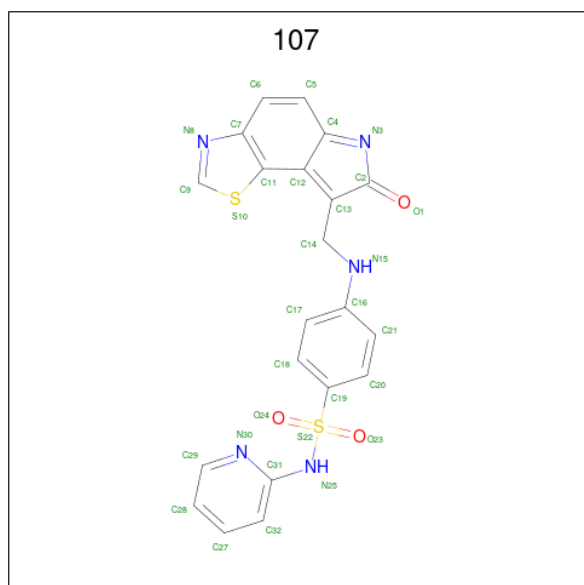
- Molecule 1 is a protein called CYCLIN-DEPENDENT KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2377	1546	405	418	8			
1	C	298	Total	C	N	O	S	0	0	0
			2381	1548	405	420	8			

- Molecule 2 is a protein called CYCLIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	0	0
			2101	1359	342	389	11			
2	D	260	Total	C	N	O	S	0	0	0
			2101	1359	342	389	11			

- Molecule 3 is 4-[(7-OXO-7H-THIAZOLO[5,4-E]INDOL-8-YLMETHYL)-AMINO]-N-PYRIDIN-2-YL-BENZENESULFONAMIDE (CCD ID: 107) (formula: C₂₁H₁₅N₅O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			31	21	5	3	2		
3	C	1	Total	C	N	O	S	0	0
			31	21	5	3	2		

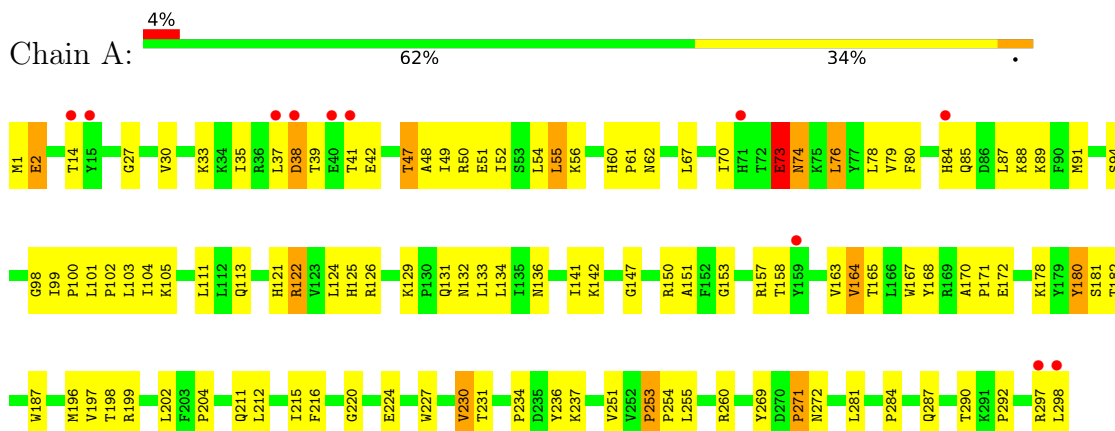
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	14	Total	O	0	0
			14	14		
4	C	18	Total	O	0	0
			18	18		
4	D	39	Total	O	0	0
			39	39		

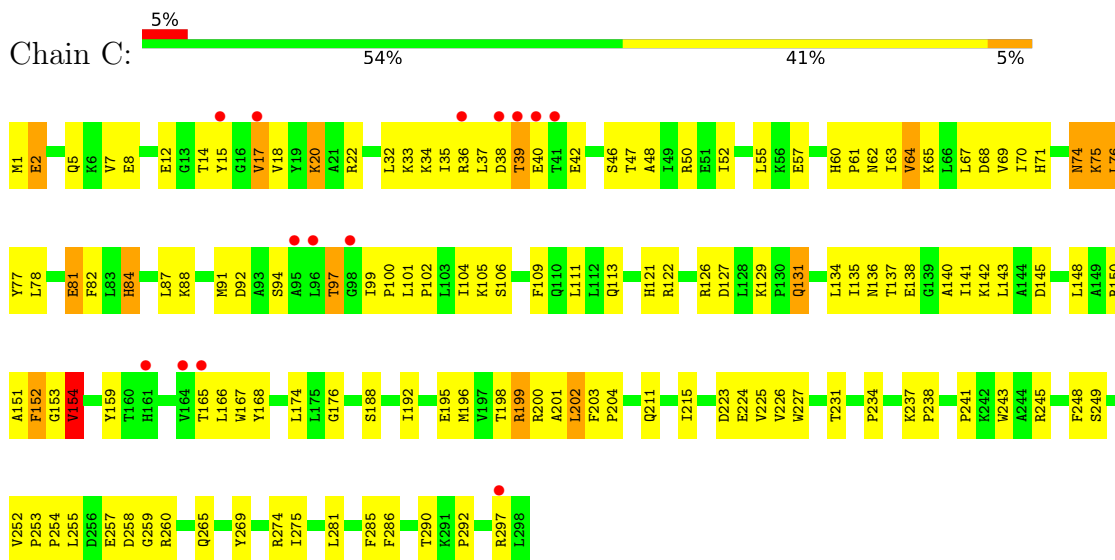
3 Residue-property plots

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.

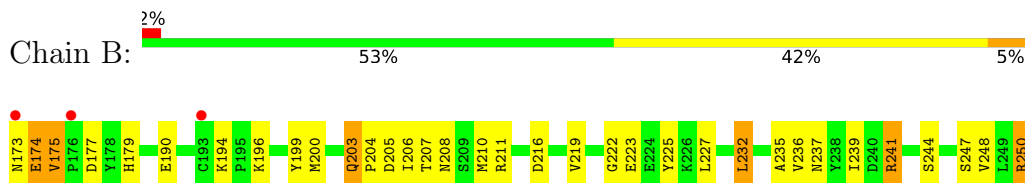
• Molecule 1: CYCLIN-DEPENDENT KINASE 2

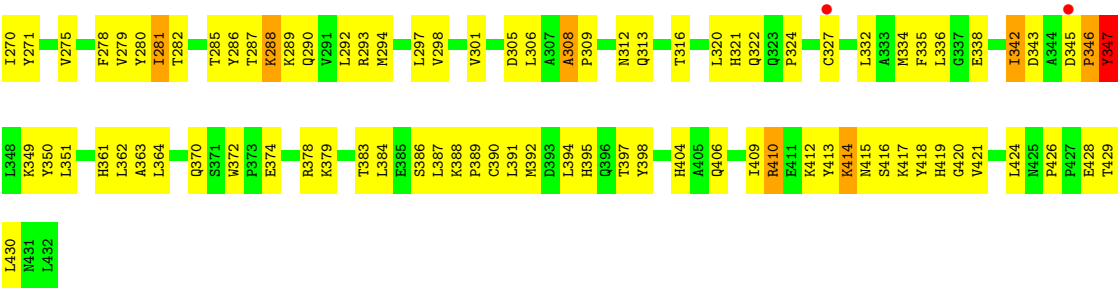


• Molecule 1: CYCLIN-DEPENDENT KINASE 2

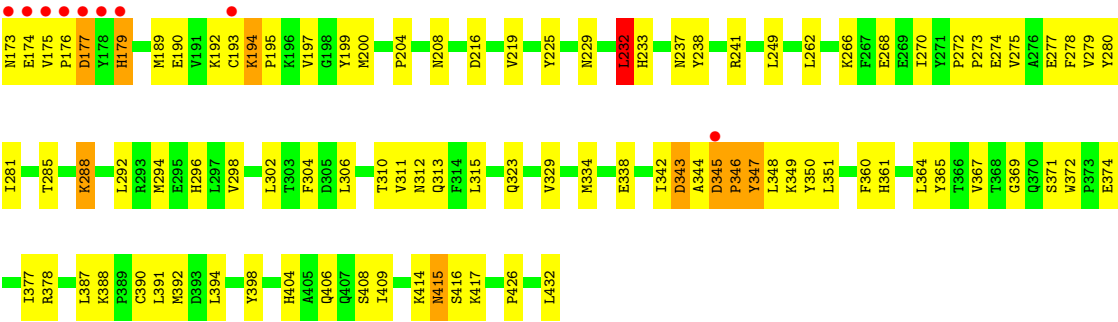


• Molecule 2: CYCLIN A





● Molecule 2: CYCLIN A



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.95Å 184.95Å 212.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.9 (20.00-2.80) 95.5 (20.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.260 , 0.260 0.216 , 0.259	Depositor DCC
R_{free} test set	5407 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9151	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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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	0.46	0/2438	0.97	9/3310 (0.3%)
1	C	0.43	0/2442	0.94	7/3315 (0.2%)
2	B	0.45	0/2151	0.98	14/2920 (0.5%)
2	D	0.48	0/2151	0.97	10/2920 (0.3%)
All	All	0.45	0/9182	0.96	40/12465 (0.3%)

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
2	B	0	1

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	347	TYR	N-CA-C	9.26	123.89	112.23
2	B	342	ILE	N-CA-C	8.62	118.63	110.53
2	D	344	ALA	N-CA-C	-8.47	101.99	111.82
1	C	84	HIS	N-CA-C	7.98	121.08	111.82
2	D	347	TYR	N-CA-C	7.68	121.92	112.54
2	D	285	THR	N-CA-C	-7.68	103.74	113.72
2	B	177	ASP	N-CA-C	7.12	119.70	111.02
2	B	414	LYS	N-CA-C	-7.08	104.67	113.38
1	A	269	TYR	N-CA-C	6.97	119.53	111.02
1	A	153	GLY	N-CA-C	-6.55	104.65	113.24
1	C	154	VAL	N-CA-C	-6.34	94.48	107.92
1	C	81	GLU	N-CA-C	-6.31	101.60	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	THR	N-CA-C	-6.03	105.75	113.23
2	D	343	ASP	N-CA-C	6.03	119.49	107.62
1	A	272	ASN	N-CA-C	-6.01	106.28	113.97
1	A	251	VAL	N-CA-C	-5.96	105.91	111.45
2	B	288	LYS	N-CA-C	-5.88	104.87	111.28
2	D	414	LYS	N-CA-C	-5.64	105.51	112.90
2	B	268	GLU	N-CA-C	5.62	120.14	113.12
1	C	249	SER	N-CA-C	-5.55	105.32	111.71
1	A	180	TYR	N-CA-C	-5.55	101.76	110.36
2	D	342	ILE	N-CA-C	5.51	115.71	110.42
1	A	253	PRO	N-CA-C	5.49	117.40	110.70
1	A	202	LEU	N-CA-C	5.45	116.91	111.07
1	C	65	LYS	N-CA-C	5.40	118.43	109.46
2	D	268	GLU	N-CA-C	5.39	119.94	112.45
2	D	197	VAL	N-CA-C	5.31	115.75	110.23
2	B	203	GLN	CA-C-N	5.27	124.72	119.24
2	B	203	GLN	C-N-CA	5.27	124.72	119.24
1	C	166	LEU	N-CA-C	5.19	119.94	111.37
2	D	232	LEU	N-CA-C	-5.19	105.31	110.97
2	B	270	ILE	N-CA-C	-5.18	105.66	110.53
2	B	205	ASP	N-CA-C	5.17	120.23	113.30
1	A	178	LYS	N-CA-C	5.14	116.69	111.14
2	B	175	VAL	CA-C-N	5.07	126.18	119.84
2	B	175	VAL	C-N-CA	5.07	126.18	119.84
2	B	308	ALA	N-CA-C	5.07	116.05	109.72
1	C	153	GLY	N-CA-C	-5.05	101.91	114.74
2	B	384	LEU	N-CA-C	-5.04	105.79	111.28
2	D	177	ASP	N-CA-C	5.00	118.80	111.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	347	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2377	0	2424	98	0
1	C	2381	0	2428	125	0
2	B	2101	0	2119	113	0
2	D	2101	0	2119	79	0
3	A	31	0	15	2	0
3	C	31	0	15	0	0
4	A	58	0	0	3	0
4	B	14	0	0	1	0
4	C	18	0	0	2	0
4	D	39	0	0	3	0
All	All	9151	0	9120	401	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 22.

All (401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLN:H	1:C:131:GLN:NE2	1.55	1.03
2:B:203:GLN:HG2	2:B:206:ILE:HG12	1.43	0.99
2:D:404:HIS:HD2	2:D:406:GLN:H	1.10	0.98
2:B:250:ARG:HH11	2:B:250:ARG:HB3	1.25	0.97
2:D:415:ASN:ND2	2:D:417:LYS:H	1.69	0.91
1:A:227:TRP:O	1:A:230:VAL:HG23	1.69	0.90
2:B:287:THR:HG22	2:B:289:LYS:H	1.39	0.88
2:D:345:ASP:HB2	2:D:346:PRO:HD3	1.56	0.86
2:D:415:ASN:HD22	2:D:417:LYS:H	1.24	0.86
2:B:345:ASP:HB3	2:B:346:PRO:HD3	1.59	0.84
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.56	0.84
2:B:207:THR:HG22	2:B:210:MET:HG3	1.58	0.83
1:C:131:GLN:H	1:C:131:GLN:HE21	1.22	0.83
1:C:2:GLU:H	1:C:2:GLU:CD	1.87	0.82
2:B:289:LYS:O	2:B:293:ARG:HG3	1.81	0.81
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.60	0.80
2:D:200:MET:HG2	2:D:208:ASN:ND2	1.97	0.80
2:D:415:ASN:HD22	2:D:416:SER:N	1.80	0.80
1:A:61:PRO:O	1:A:142:LYS:HE2	1.82	0.79
1:A:172:GLU:HG2	1:A:271:PRO:HG3	1.65	0.79
2:D:404:HIS:CD2	2:D:406:GLN:H	1.98	0.78
1:A:163:VAL:HB	4:A:555:HOH:O	1.83	0.77
2:B:417:LYS:HE3	2:B:418:TYR:CE1	2.20	0.77
2:D:345:ASP:CB	2:D:346:PRO:HD3	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:174:GLU:HG3	2:D:176:PRO:HD2	1.66	0.77
2:B:404:HIS:HE1	2:B:406:GLN:HE21	1.32	0.77
1:C:60:HIS:HD2	1:C:62:ASN:H	1.30	0.77
2:B:237:ASN:HD21	2:B:241:ARG:HE	1.31	0.76
2:B:250:ARG:HH11	2:B:250:ARG:CB	1.98	0.76
2:B:237:ASN:ND2	2:B:241:ARG:HE	1.84	0.75
2:B:428:GLU:HG3	2:B:429:THR:HG23	1.69	0.75
2:B:210:MET:HE1	2:B:250:ARG:CB	2.17	0.75
1:C:5:GLN:HB3	1:C:22:ARG:HG2	1.68	0.74
2:B:336:LEU:HD13	2:B:362:LEU:HD23	1.67	0.74
2:B:250:ARG:HB3	2:B:250:ARG:NH1	2.03	0.73
1:C:61:PRO:O	1:C:142:LYS:HE2	1.89	0.72
1:C:201:ALA:HB3	1:C:204:PRO:HG3	1.70	0.71
2:D:391:LEU:HD23	2:D:432:LEU:HD11	1.71	0.71
1:A:33:LYS:HB3	1:A:78:LEU:HB2	1.72	0.71
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.72	0.71
1:C:91:MET:HE3	1:C:196:MET:HG2	1.71	0.71
1:C:165:THR:HG22	4:C:607:HOH:O	1.89	0.70
2:D:175:VAL:HA	2:D:179:HIS:CD2	2.26	0.70
2:B:361:HIS:HD2	2:B:372:TRP:H	1.37	0.70
1:A:47:THR:HG22	1:A:147:GLY:O	1.92	0.69
1:C:150:ARG:HD2	4:C:610:HOH:O	1.92	0.69
2:B:410:ARG:HB3	2:B:410:ARG:NH1	2.07	0.69
1:A:30:VAL:HG21	1:A:79:VAL:HG12	1.74	0.69
2:B:203:GLN:HG2	2:B:206:ILE:CG1	2.21	0.69
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.73	0.68
1:A:74:ASN:HD22	1:A:74:ASN:H	1.41	0.68
2:D:262:LEU:HD11	2:D:266:LYS:HE3	1.73	0.68
1:C:136:ASN:HD21	1:C:138:GLU:HB2	1.58	0.68
1:C:136:ASN:ND2	1:C:138:GLU:HB2	2.09	0.68
1:A:51:GLU:O	1:A:55:LEU:HB2	1.94	0.68
1:A:52:ILE:O	1:A:56:LYS:HG3	1.94	0.67
1:C:241:PRO:HB2	1:C:243:TRP:CZ3	2.29	0.67
2:D:345:ASP:HB2	2:D:346:PRO:CD	2.25	0.67
2:B:207:THR:CG2	2:B:210:MET:HG3	2.25	0.67
1:C:104:ILE:HG23	1:C:196:MET:HE3	1.77	0.67
2:B:287:THR:HB	2:B:290:GLN:HG3	1.76	0.66
1:C:38:ASP:HB3	1:C:42:GLU:HB3	1.77	0.66
1:A:182:THR:HG23	2:B:173:ASN:N	2.09	0.66
1:A:165:THR:HG21	1:A:168:TYR:HD1	1.59	0.66
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:CD2	1:A:62:ASN:H	2.14	0.66
1:C:1:MET:HG2	1:C:70:ILE:HG21	1.78	0.66
1:C:74:ASN:HD22	1:C:75:LYS:CD	2.09	0.66
1:C:60:HIS:CD2	1:C:62:ASN:H	2.14	0.64
2:D:415:ASN:HD22	2:D:415:ASN:C	2.03	0.64
1:C:252:VAL:HG21	1:C:255:LEU:HD12	1.79	0.64
2:B:404:HIS:CE1	2:B:406:GLN:HE21	2.16	0.63
1:C:200:ARG:HD2	1:C:201:ALA:H	1.63	0.63
1:C:40:GLU:O	2:D:288:LYS:HD3	1.98	0.63
2:D:204:PRO:HG2	4:D:49:HOH:O	1.98	0.63
2:D:312:ASN:OD1	2:D:334:MET:HE1	1.99	0.63
1:C:74:ASN:HD22	1:C:75:LYS:HD2	1.65	0.62
2:D:374:GLU:HG3	2:D:378:ARG:NH1	2.15	0.62
1:A:60:HIS:HD2	1:A:62:ASN:H	1.47	0.61
1:A:74:ASN:H	1:A:74:ASN:ND2	1.97	0.61
1:A:30:VAL:HG21	1:A:79:VAL:CG1	2.30	0.61
2:D:277:GLU:HA	2:D:280:TYR:CD1	2.36	0.61
1:A:231:THR:HA	1:A:236:TYR:CD2	2.35	0.61
1:C:131:GLN:HE21	1:C:131:GLN:N	1.95	0.61
1:C:126:ARG:HH12	1:C:159:TYR:HE1	1.48	0.61
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.35	0.60
1:C:34:LYS:HZ1	1:C:75:LYS:NZ	1.99	0.60
1:C:203:PHE:CE2	1:C:215:ILE:HA	2.35	0.60
1:A:38:ASP:OD1	1:A:39:THR:HG23	2.01	0.60
2:D:346:PRO:O	2:D:349:LYS:HG2	2.01	0.60
2:B:282:THR:O	2:B:285:THR:HG23	2.01	0.60
2:B:374:GLU:HG3	2:B:378:ARG:NH2	2.17	0.60
1:A:164:VAL:HG12	1:A:165:THR:N	2.17	0.59
2:B:223:GLU:OE2	2:B:412:LYS:HE3	2.02	0.59
1:C:34:LYS:HE2	1:C:77:TYR:OH	2.02	0.59
1:C:36:ARG:O	1:C:37:LEU:HB2	2.02	0.59
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.85	0.59
2:B:225:TYR:HE2	2:B:281:ILE:HG21	1.68	0.58
2:B:312:ASN:OD1	2:B:334:MET:HE1	2.03	0.58
1:A:85:GLN:NE2	1:A:89:LYS:HD3	2.19	0.58
1:A:121:HIS:O	1:A:122:ARG:HG3	2.03	0.58
1:C:224:GLU:OE2	1:C:231:THR:HB	2.03	0.58
2:D:229:ASN:HD22	2:D:334:MET:CE	2.16	0.58
1:C:74:ASN:ND2	1:C:75:LYS:HD2	2.19	0.57
2:D:189:MET:HE1	2:D:192:LYS:HD2	1.86	0.57
2:D:345:ASP:CB	2:D:346:PRO:CD	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:O	1:A:98:GLY:N	2.34	0.57
2:B:361:HIS:HD2	2:B:372:TRP:N	2.02	0.57
1:C:101:LEU:N	1:C:102:PRO:HD2	2.19	0.57
1:A:298:LEU:C	1:A:298:LEU:HD23	2.29	0.57
2:B:428:GLU:CG	2:B:429:THR:HG23	2.33	0.57
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.86	0.57
1:C:152:PHE:C	1:C:154:VAL:H	2.13	0.56
1:C:94:SER:HA	1:C:97:THR:HG23	1.85	0.56
2:D:388:LYS:O	2:D:392:MET:HG2	2.05	0.56
1:C:63:ILE:O	1:C:64:VAL:C	2.47	0.56
2:D:329:VAL:HG22	2:D:367:VAL:HB	1.88	0.56
1:C:55:LEU:C	1:C:57:GLU:H	2.14	0.56
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.86	0.56
2:B:271:TYR:CD1	2:B:271:TYR:O	2.59	0.56
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.41	0.55
2:B:410:ARG:HB3	2:B:410:ARG:HH11	1.70	0.55
2:D:189:MET:CE	2:D:192:LYS:HD2	2.36	0.55
2:B:398:TYR:CE2	2:B:426:PRO:HB3	2.41	0.55
1:C:84:HIS:CD2	1:C:137:THR:HG23	2.42	0.55
2:B:173:ASN:O	2:B:175:VAL:HG22	2.07	0.55
1:A:74:ASN:HD22	1:A:74:ASN:N	1.99	0.55
1:A:2:GLU:H	1:A:2:GLU:CD	2.14	0.55
1:C:34:LYS:HZ1	1:C:75:LYS:HZ3	1.55	0.55
1:C:202:LEU:HD13	1:C:203:PHE:CE1	2.42	0.55
2:D:278:PHE:O	2:D:281:ILE:HG12	2.07	0.55
1:A:121:HIS:C	1:A:122:ARG:HG3	2.31	0.54
1:C:33:LYS:HB3	1:C:78:LEU:HB2	1.88	0.54
2:D:225:TYR:HE1	2:D:277:GLU:HB3	1.72	0.54
2:B:410:ARG:HH11	2:B:410:ARG:CB	2.20	0.54
1:C:131:GLN:NE2	1:C:131:GLN:N	2.40	0.54
1:A:50:ARG:NE	1:A:150:ARG:NH1	2.55	0.54
1:A:129:LYS:HE2	1:A:132:ASN:ND2	2.23	0.54
2:B:222:GLY:HA2	2:B:227:LEU:HD12	1.90	0.54
1:C:34:LYS:HZ1	1:C:36:ARG:NH1	2.06	0.54
2:D:190:GLU:HG3	2:D:351:LEU:HD22	1.89	0.54
2:D:350:TYR:CE2	2:D:390:CYS:HB2	2.43	0.54
1:A:87:LEU:O	1:A:91:MET:HG3	2.07	0.54
1:C:2:GLU:OE2	1:C:2:GLU:N	2.41	0.54
1:C:111:LEU:HD21	1:C:141:ILE:HD13	1.89	0.54
1:C:135:ILE:HA	1:C:140:ALA:O	2.07	0.54
2:D:237:ASN:OD1	2:D:241:ARG:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:O	1:A:298:LEU:C	2.50	0.53
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.43	0.53
1:A:100:PRO:O	1:A:104:ILE:HG13	2.08	0.53
2:B:414:LYS:HA	2:B:420:GLY:HA2	1.89	0.53
1:C:245:ARG:NH2	1:C:248:PHE:CE1	2.76	0.53
2:B:343:ASP:O	2:B:346:PRO:HD2	2.09	0.53
1:C:94:SER:HA	1:C:97:THR:CG2	2.38	0.53
2:B:203:GLN:CG	2:B:206:ILE:HG12	2.27	0.53
1:C:167:TRP:CD1	1:C:204:PRO:HA	2.44	0.53
2:D:174:GLU:HG3	2:D:176:PRO:CD	2.36	0.53
2:D:194:LYS:HG2	2:D:195:PRO:N	2.24	0.53
1:A:157:ARG:HG3	4:A:556:HOH:O	2.08	0.52
2:B:235:ALA:O	2:B:239:ILE:HG13	2.10	0.52
2:D:338:GLU:HB3	2:D:409:ILE:HD13	1.92	0.52
2:B:313:GLN:O	2:B:316:THR:HB	2.10	0.52
1:C:91:MET:HE3	1:C:196:MET:CG	2.38	0.52
2:D:199:TYR:CE2	2:D:348:LEU:HD21	2.44	0.52
2:B:175:VAL:HG23	2:B:175:VAL:O	2.10	0.52
1:C:84:HIS:HD2	1:C:136:ASN:HA	1.73	0.52
2:D:387:LEU:O	2:D:391:LEU:HB2	2.10	0.52
2:D:398:TYR:CE1	2:D:426:PRO:HB3	2.45	0.52
2:B:196:LYS:HB2	2:B:199:TYR:HB3	1.91	0.52
2:B:216:ASP:HB2	2:B:406:GLN:HG2	1.92	0.52
2:B:374:GLU:HG3	2:B:378:ARG:HH22	1.74	0.52
2:D:371:SER:O	2:D:372:TRP:C	2.53	0.52
1:A:129:LYS:HE3	1:A:131:GLN:HG2	1.92	0.51
2:B:350:TYR:CZ	2:B:390:CYS:HA	2.45	0.51
1:C:223:ASP:H	1:C:226:VAL:CG1	2.23	0.51
1:C:223:ASP:OD1	1:C:226:VAL:HG12	2.10	0.51
1:C:34:LYS:NZ	1:C:75:LYS:HZ3	2.09	0.51
1:C:248:PHE:HB3	1:C:260:ARG:HD2	1.92	0.51
1:A:85:GLN:HA	3:A:501:107:C20	2.40	0.51
1:A:41:THR:HB	2:B:288:LYS:NZ	2.26	0.51
1:C:100:PRO:C	1:C:102:PRO:HD2	2.36	0.51
2:B:297:LEU:O	2:B:301:VAL:HG23	2.10	0.50
1:C:34:LYS:NZ	1:C:75:LYS:NZ	2.58	0.50
2:D:174:GLU:CG	2:D:176:PRO:HD2	2.38	0.50
1:A:27:GLY:HA3	2:D:249:LEU:HD12	1.94	0.50
1:C:127:ASP:HB2	1:C:148:LEU:HD12	1.92	0.50
1:C:57:GLU:OE1	1:C:122:ARG:NH2	2.38	0.50
2:D:346:PRO:HG2	2:D:347:TYR:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:HG22	1:C:39:THR:O	2.10	0.50
1:A:227:TRP:HB3	1:A:230:VAL:CG2	2.42	0.50
2:B:200:MET:HG2	2:B:208:ASN:ND2	2.26	0.50
1:C:201:ALA:CB	1:C:204:PRO:HG3	2.42	0.50
2:D:311:VAL:O	2:D:315:LEU:HB2	2.12	0.49
1:C:109:PHE:HB2	1:C:286:PHE:CE1	2.47	0.49
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.48	0.49
2:B:322:GLN:HB3	2:B:324:PRO:O	2.12	0.49
1:A:227:TRP:CD2	1:A:230:VAL:HG22	2.47	0.49
1:C:38:ASP:C	1:C:40:GLU:H	2.20	0.49
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.48	0.49
1:A:216:PHE:O	1:A:220:GLY:N	2.44	0.49
1:A:284:PRO:HA	1:A:287:GLN:HG3	1.94	0.49
2:B:190:GLU:O	2:B:194:LYS:HB3	2.12	0.49
2:B:203:GLN:OE1	2:B:248:VAL:N	2.43	0.49
2:B:294:MET:O	2:B:298:VAL:HG23	2.12	0.49
2:B:346:PRO:O	2:B:349:LYS:HG2	2.13	0.48
1:C:134:LEU:O	1:C:141:ILE:HA	2.12	0.48
1:A:231:THR:HA	1:A:236:TYR:CE2	2.48	0.48
2:B:278:PHE:O	2:B:282:THR:HG23	2.13	0.48
1:C:87:LEU:O	1:C:91:MET:HG3	2.13	0.48
2:D:238:TYR:OH	2:D:306:LEU:HB3	2.13	0.48
1:A:88:LYS:HD2	1:A:131:GLN:HB3	1.95	0.48
1:C:99:ILE:HG22	1:C:104:ILE:HG13	1.96	0.48
1:C:121:HIS:C	1:C:122:ARG:HG3	2.38	0.48
2:B:237:ASN:O	2:B:241:ARG:HB2	2.14	0.48
2:B:383:THR:N	2:B:386:SER:OG	2.46	0.48
2:B:388:LYS:O	2:B:392:MET:HG2	2.13	0.48
2:B:388:LYS:HG3	2:B:392:MET:HE3	1.94	0.48
1:C:152:PHE:CD1	1:C:152:PHE:N	2.82	0.48
1:C:165:THR:HG23	1:C:165:THR:O	2.13	0.48
1:C:188:SER:O	1:C:192:ILE:HG13	2.14	0.47
1:C:265:GLN:HB3	1:C:275:ILE:HB	1.95	0.47
2:D:200:MET:HE3	2:D:208:ASN:HD22	1.79	0.47
1:C:111:LEU:HD21	1:C:141:ILE:CD1	2.43	0.47
1:C:14:THR:HG23	1:C:15:TYR:N	2.29	0.47
1:A:181:SER:HB3	2:B:174:GLU:HG3	1.95	0.47
1:A:111:LEU:CD2	1:A:133:LEU:HD22	2.45	0.47
1:A:158:THR:HA	1:A:180:TYR:CE2	2.50	0.47
2:B:237:ASN:HD21	2:B:241:ARG:NE	2.07	0.47
1:C:105:LYS:HE2	1:C:285:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:334:MET:HE2	4:D:122:HOH:O	2.15	0.47
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.97	0.47
1:A:50:ARG:HD3	1:A:150:ARG:NH1	2.30	0.47
1:C:84:HIS:CD2	1:C:137:THR:H	2.32	0.47
1:C:122:ARG:HD2	1:C:122:ARG:O	2.15	0.47
2:D:374:GLU:HG3	2:D:378:ARG:HH12	1.78	0.47
1:C:34:LYS:NZ	1:C:36:ARG:NH1	2.62	0.46
2:D:275:VAL:O	2:D:279:VAL:HG23	2.15	0.46
2:B:179:HIS:HD2	2:B:320:LEU:HD13	1.80	0.46
1:A:197:VAL:HG11	1:A:255:LEU:HG	1.97	0.46
1:C:75:LYS:HD2	1:C:75:LYS:N	2.30	0.46
1:C:227:TRP:CE3	1:C:269:TYR:HB3	2.50	0.46
1:A:30:VAL:HG23	1:A:67:LEU:HD12	1.97	0.46
1:C:70:ILE:HG22	1:C:70:ILE:O	2.14	0.46
2:B:275:VAL:HG21	2:B:292:LEU:HD11	1.98	0.46
2:B:404:HIS:CE1	2:B:406:GLN:HB2	2.51	0.46
1:C:7:VAL:HB	1:C:20:LYS:O	2.16	0.46
1:A:35:ILE:HD12	1:A:76:LEU:HD13	1.98	0.46
1:A:54:LEU:HD21	1:A:151:ALA:HB2	1.98	0.46
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.50	0.46
1:A:84:HIS:CD2	1:A:136:ASN:HA	2.51	0.45
2:D:241:ARG:CZ	2:D:302:LEU:HD22	2.46	0.45
1:A:111:LEU:HD22	1:A:133:LEU:HD22	1.97	0.45
2:B:287:THR:HG22	2:B:289:LYS:N	2.19	0.45
2:D:233:HIS:HD2	4:D:123:HOH:O	1.99	0.45
1:A:181:SER:CB	2:B:174:GLU:HG3	2.47	0.45
2:B:241:ARG:NH2	2:B:305:ASP:O	2.45	0.45
1:C:174:LEU:C	1:C:176:GLY:H	2.24	0.45
1:C:200:ARG:HD2	1:C:201:ALA:N	2.30	0.45
1:A:1:MET:CE	1:A:70:ILE:HD12	2.47	0.45
2:B:203:GLN:HA	2:B:204:PRO:HD2	1.84	0.45
1:C:165:THR:HG23	1:C:168:TYR:HD1	1.81	0.45
1:A:37:LEU:HD22	1:A:76:LEU:HB2	1.99	0.45
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.23	0.45
2:B:216:ASP:O	2:B:219:VAL:HB	2.16	0.45
2:B:210:MET:HE1	2:B:250:ARG:HB3	1.96	0.45
2:B:388:LYS:HE3	2:B:392:MET:HE3	1.99	0.45
1:A:35:ILE:HD13	1:A:48:ALA:HB2	1.99	0.45
2:B:199:TYR:CD1	2:B:199:TYR:C	2.95	0.45
2:B:279:VAL:HG21	2:B:288:LYS:HA	1.99	0.45
1:C:113:GLN:HG3	1:C:281:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:HB2	1:A:74:ASN:H	1.56	0.44
2:B:211:ARG:HG2	2:B:211:ARG:HH11	1.83	0.44
2:B:232:LEU:O	2:B:236:VAL:HG23	2.17	0.44
2:B:345:ASP:HB3	2:B:346:PRO:CD	2.40	0.44
1:C:88:LYS:HD2	1:C:131:GLN:OE1	2.17	0.44
1:C:81:GLU:OE2	1:C:142:LYS:NZ	2.45	0.44
2:D:225:TYR:CE1	2:D:277:GLU:HB3	2.52	0.44
2:B:321:HIS:NE2	2:B:379:LYS:HD2	2.32	0.44
2:D:350:TYR:CD2	2:D:390:CYS:HB2	2.53	0.44
1:A:105:LYS:HE3	1:A:105:LYS:HB2	1.82	0.44
1:A:134:LEU:O	1:A:141:ILE:HA	2.17	0.44
2:D:360:PHE:O	2:D:364:LEU:HB2	2.18	0.44
1:A:101:LEU:N	1:A:102:PRO:CD	2.81	0.44
1:A:150:ARG:NH1	2:B:267:PHE:O	2.51	0.44
2:B:364:LEU:HG	2:B:370:GLN:HB2	1.99	0.44
1:C:50:ARG:HE	1:C:150:ARG:NH1	2.15	0.44
1:C:69:VAL:CG1	1:C:76:LEU:HD21	2.48	0.44
1:C:198:THR:O	1:C:200:ARG:N	2.51	0.44
1:A:212:LEU:HG	1:A:216:PHE:CZ	2.52	0.44
2:B:211:ARG:HG2	2:B:211:ARG:NH1	2.32	0.44
2:B:417:LYS:HE3	2:B:418:TYR:HE1	1.77	0.44
2:B:286:TYR:HA	2:B:290:GLN:OE1	2.17	0.44
1:A:164:VAL:CG1	1:A:165:THR:N	2.81	0.43
1:A:253:PRO:HD2	1:A:254:PRO:HD3	2.00	0.43
2:B:421:VAL:HA	2:B:424:LEU:HG	2.00	0.43
2:D:199:TYR:CD1	2:D:199:TYR:C	2.96	0.43
2:D:310:THR:OG1	2:D:313:GLN:HG3	2.17	0.43
2:D:174:GLU:C	2:D:176:PRO:HD2	2.43	0.43
1:A:198:THR:O	1:A:199:ARG:HB2	2.19	0.43
2:B:210:MET:CE	2:B:250:ARG:HB2	2.40	0.43
1:C:223:ASP:H	1:C:226:VAL:HG12	1.83	0.43
1:A:165:THR:HG21	1:A:168:TYR:CD1	2.46	0.43
2:D:225:TYR:CE2	2:D:281:ILE:CG2	3.01	0.43
1:A:1:MET:HE2	1:A:70:ILE:HG21	2.00	0.43
1:A:125:HIS:O	1:A:126:ARG:HB2	2.18	0.43
2:B:210:MET:HE1	2:B:250:ARG:HH11	1.83	0.43
2:D:347:TYR:OH	2:D:394:LEU:HA	2.19	0.43
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.54	0.43
1:C:7:VAL:HG11	1:C:20:LYS:HE3	2.00	0.43
1:C:84:HIS:CD2	1:C:136:ASN:HA	2.53	0.43
2:D:274:GLU:O	2:D:275:VAL:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.78	0.43
2:B:190:GLU:HG3	2:B:351:LEU:HD22	2.00	0.43
1:C:106:SER:HB2	1:C:290:THR:O	2.19	0.43
2:B:203:GLN:OE1	2:B:247:SER:HA	2.19	0.43
2:B:415:ASN:OD1	2:B:416:SER:N	2.52	0.43
2:D:415:ASN:ND2	2:D:415:ASN:C	2.74	0.43
1:A:41:THR:HB	2:B:288:LYS:HZ3	1.83	0.42
1:C:122:ARG:O	1:C:151:ALA:HA	2.18	0.42
1:C:257:GLU:OE1	1:C:257:GLU:HA	2.19	0.42
2:D:272:PRO:HA	2:D:273:PRO:HD3	1.89	0.42
2:D:275:VAL:HG21	2:D:292:LEU:HD21	2.00	0.42
1:A:62:ASN:HA	1:A:142:LYS:HG2	2.00	0.42
2:B:395:HIS:ND1	2:B:430:LEU:HG	2.34	0.42
1:A:255:LEU:O	1:A:260:ARG:NH1	2.52	0.42
1:C:46:SER:O	1:C:50:ARG:HG3	2.19	0.42
1:C:64:VAL:HG12	1:C:143:LEU:O	2.19	0.42
2:D:343:ASP:OD1	2:D:404:HIS:HE1	2.01	0.42
1:A:37:LEU:HB3	1:A:74:ASN:O	2.20	0.42
1:A:171:PRO:HD3	1:A:187:TRP:CZ2	2.54	0.42
1:C:126:ARG:NH1	1:C:159:TYR:HE1	2.14	0.42
1:C:226:VAL:O	1:C:226:VAL:HG22	2.20	0.42
1:A:181:SER:HA	2:B:173:ASN:HB3	2.02	0.42
2:B:308:ALA:HA	2:B:309:PRO:HD3	1.97	0.42
2:B:387:LEU:O	2:B:391:LEU:HB2	2.20	0.42
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.02	0.42
1:C:258:ASP:O	1:C:259:GLY:C	2.60	0.42
2:D:194:LYS:HB3	2:D:194:LYS:HE2	1.76	0.42
2:D:216:ASP:OD2	2:D:408:SER:HB2	2.20	0.42
2:D:398:TYR:CD1	2:D:426:PRO:HB3	2.54	0.42
1:A:30:VAL:CG2	1:A:80:PHE:O	2.68	0.42
1:A:170:ALA:HB1	1:A:172:GLU:OE2	2.19	0.42
2:D:294:MET:O	2:D:298:VAL:HG23	2.20	0.42
2:B:173:ASN:HD22	2:B:173:ASN:HA	1.69	0.42
1:C:88:LYS:HD2	1:C:131:GLN:HG3	2.02	0.42
1:C:150:ARG:NH2	2:D:270:ILE:HA	2.35	0.42
1:A:42:GLU:OE1	2:B:275:VAL:HG23	2.20	0.41
1:A:165:THR:HG22	4:A:535:HOH:O	2.18	0.41
1:A:290:THR:C	1:A:292:PRO:HD3	2.45	0.41
1:C:35:ILE:O	1:C:75:LYS:HB2	2.19	0.41
1:C:60:HIS:HD2	1:C:62:ASN:N	2.08	0.41
2:D:374:GLU:CG	2:D:378:ARG:HH12	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:HIS:O	2:B:420:GLY:C	2.63	0.41
1:C:203:PHE:HB2	1:C:211:GLN:HE22	1.85	0.41
1:A:99:ILE:HG23	1:A:103:LEU:HD23	2.02	0.41
1:A:211:GLN:O	1:A:215:ILE:HG13	2.20	0.41
2:B:287:THR:N	2:B:290:GLN:OE1	2.44	0.41
1:C:18:VAL:HA	1:C:32:LEU:O	2.20	0.41
1:C:20:LYS:HG3	1:C:82:PHE:CZ	2.55	0.41
2:D:394:LEU:HA	2:D:394:LEU:HD12	1.90	0.41
1:A:39:THR:C	1:A:41:THR:H	2.28	0.41
1:A:89:LYS:HD2	3:A:501:107:S22	2.60	0.41
2:B:338:GLU:O	2:B:409:ILE:HD13	2.21	0.41
1:C:237:LYS:HA	1:C:238:PRO:HD3	1.94	0.41
1:C:290:THR:C	1:C:292:PRO:HD3	2.46	0.41
1:A:165:THR:HG23	1:A:168:TYR:H	1.86	0.41
1:C:227:TRP:CD1	1:C:227:TRP:C	2.98	0.41
1:A:124:LEU:CD2	1:A:182:THR:HA	2.50	0.41
2:B:196:LYS:HG2	2:B:244:SER:HB3	2.01	0.41
1:C:67:LEU:O	1:C:68:ASP:HB2	2.21	0.41
2:D:347:TYR:C	2:D:349:LYS:H	2.27	0.41
2:B:280:TYR:C	2:B:282:THR:H	2.28	0.41
2:B:287:THR:HG22	2:B:288:LYS:N	2.36	0.41
2:B:342:ILE:HG22	2:B:343:ASP:OD1	2.21	0.41
2:D:175:VAL:N	2:D:176:PRO:CD	2.84	0.41
1:A:73:GLU:H	1:A:73:GLU:HG3	1.43	0.41
1:A:91:MET:HE3	1:A:196:MET:HG2	2.03	0.41
1:A:113:GLN:HG3	1:A:281:LEU:HD21	2.02	0.41
1:C:17:VAL:CG2	1:C:18:VAL:N	2.83	0.41
1:C:71:HIS:NE2	2:D:296:HIS:CD2	2.89	0.41
1:C:91:MET:HE1	1:C:195:GLU:HB3	2.03	0.41
2:D:175:VAL:N	2:D:176:PRO:HD2	2.36	0.41
1:A:50:ARG:CD	1:A:150:ARG:NH1	2.84	0.41
2:B:293:ARG:HH22	1:C:2:GLU:HB2	1.85	0.41
2:B:397:THR:HG23	4:B:56:HOH:O	2.21	0.41
1:A:101:LEU:HD23	1:A:104:ILE:HD12	2.02	0.40
1:C:129:LYS:HA	1:C:192:ILE:HD11	2.03	0.40
2:D:229:ASN:HD22	2:D:334:MET:HE2	1.85	0.40
2:D:365:TYR:O	2:D:369:GLY:HA2	2.21	0.40
1:C:92:ASP:C	1:C:94:SER:H	2.29	0.40
1:A:56:LYS:HE2	1:A:56:LYS:HB3	1.86	0.40
1:A:236:TYR:CG	1:A:237:LYS:N	2.88	0.40
2:B:250:ARG:HG3	2:B:251:GLY:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LYS:HG3	1:C:77:TYR:CE2	2.57	0.40
1:C:48:ALA:O	1:C:52:ILE:HG13	2.21	0.40
1:C:12:GLU:HA	1:C:17:VAL:HA	2.04	0.40
1:C:165:THR:CG2	1:C:168:TYR:HD1	2.34	0.40
2:D:415:ASN:HD22	2:D:417:LYS:N	2.04	0.40
2:B:196:LYS:CG	2:B:244:SER:HB3	2.51	0.40
2:B:347:TYR:OH	2:B:394:LEU:HA	2.22	0.40
1:C:274:ARG:O	1:C:275:ILE:C	2.65	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	296/298 (99%)	274 (93%)	17 (6%)	5 (2%)	7	25
1	C	296/298 (99%)	255 (86%)	35 (12%)	6 (2%)	6	21
2	B	258/260 (99%)	240 (93%)	15 (6%)	3 (1%)	10	34
2	D	258/260 (99%)	242 (94%)	13 (5%)	3 (1%)	10	34
All	All	1108/1116 (99%)	1011 (91%)	80 (7%)	17 (2%)	8	28

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
2	B	346	PRO
1	C	39	THR
2	D	346	PRO
1	C	199	ARG
1	C	297	ARG
1	C	145	ASP

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Mol	Chain	Res	Type
2	B	327	CYS
2	D	304	PHE
1	C	234	PRO
1	A	234	PRO
2	D	345	ASP
1	A	271	PRO
2	B	281	ILE
1	A	230	VAL
1	C	64	VAL
1	A	164	VAL

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	259/263 (98%)	251 (97%)	8 (3%)	35	70
1	C	260/263 (99%)	245 (94%)	15 (6%)	18	49
2	B	234/234 (100%)	229 (98%)	5 (2%)	47	79
2	D	234/234 (100%)	225 (96%)	9 (4%)	29	64
All	All	987/994 (99%)	950 (96%)	37 (4%)	30	65

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	38	ASP
1	A	47	THR
1	A	55	LEU
1	A	73	GLU
1	A	74	ASN
1	A	76	LEU
1	A	122	ARG
2	B	174	GLU
2	B	232	LEU
2	B	241	ARG

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Mol	Chain	Res	Type
2	B	250	ARG
2	B	410	ARG
1	C	2	GLU
1	C	8	GLU
1	C	17	VAL
1	C	20	LYS
1	C	47	THR
1	C	74	ASN
1	C	75	LYS
1	C	76	LEU
1	C	97	THR
1	C	131	GLN
1	C	152	PHE
1	C	154	VAL
1	C	199	ARG
1	C	202	LEU
1	C	225	VAL
2	D	173	ASN
2	D	177	ASP
2	D	179	HIS
2	D	193	CYS
2	D	194	LYS
2	D	232	LEU
2	D	288	LYS
2	D	323	GLN
2	D	415	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	60	HIS
1	A	62	ASN
1	A	74	ASN
1	A	84	HIS
1	A	85	GLN
1	A	113	GLN
1	A	246	GLN
1	A	272	ASN
1	A	287	GLN
2	B	173	ASN
2	B	179	HIS

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Mol	Chain	Res	Type
2	B	208	ASN
2	B	237	ASN
2	B	361	HIS
2	B	370	GLN
2	B	396	GLN
2	B	403	GLN
2	B	406	GLN
1	C	60	HIS
1	C	62	ASN
1	C	84	HIS
1	C	85	GLN
1	C	113	GLN
1	C	119	HIS
1	C	131	GLN
1	C	265	GLN
1	C	268	HIS
2	D	183	HIS
2	D	208	ASN
2	D	229	ASN
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS
2	D	313	GLN
2	D	322	GLN
2	D	396	GLN
2	D	404	HIS
2	D	406	GLN
2	D	415	ASN
2	D	431	ASN

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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	107	A	501	-	32,35,35	4.30	20 (62%)	38,51,51	2.10	11 (28%)
3	107	C	601	-	32,35,35	4.29	20 (62%)	38,51,51	2.80	13 (34%)

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
3	107	A	501	-	-	4/16/28/28	0/5/5/5
3	107	C	601	-	-	4/16/28/28	0/5/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	107	C7-C11	10.95	1.52	1.40
3	C	601	107	C7-C11	9.97	1.51	1.40
3	C	601	107	C20-C19	6.84	1.49	1.38
3	A	501	107	C17-C16	6.59	1.50	1.39
3	A	501	107	C5-C4	6.42	1.48	1.40
3	A	501	107	C18-C19	6.28	1.48	1.38
3	C	601	107	C6-C5	6.07	1.48	1.38
3	C	601	107	C5-C4	6.05	1.47	1.40
3	A	501	107	C20-C19	5.88	1.48	1.38
3	C	601	107	C18-C19	5.88	1.48	1.38
3	C	601	107	C17-C16	5.84	1.49	1.39
3	C	601	107	C31-N30	5.70	1.44	1.34
3	A	501	107	C21-C16	5.63	1.48	1.39
3	A	501	107	C21-C20	5.59	1.47	1.38
3	A	501	107	C31-N30	5.57	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	107	C27-C32	5.54	1.48	1.38
3	C	601	107	C21-C20	5.43	1.47	1.38
3	C	601	107	C21-C16	5.21	1.48	1.39
3	A	501	107	C6-C5	5.20	1.47	1.38
3	C	601	107	C18-C17	5.10	1.47	1.38
3	C	601	107	C9-N8	5.04	1.36	1.29
3	C	601	107	C29-N30	4.88	1.44	1.34
3	A	501	107	C9-N8	4.87	1.36	1.29
3	A	501	107	C32-C31	4.82	1.50	1.39
3	A	501	107	C27-C32	4.78	1.47	1.38
3	C	601	107	C28-C27	4.70	1.48	1.38
3	A	501	107	C28-C27	4.68	1.48	1.38
3	A	501	107	C18-C17	4.56	1.46	1.38
3	A	501	107	C29-N30	4.51	1.44	1.34
3	C	601	107	C32-C31	4.37	1.49	1.39
3	C	601	107	C6-C7	4.34	1.46	1.40
3	A	501	107	C28-C29	3.77	1.48	1.37
3	A	501	107	C6-C7	3.64	1.45	1.40
3	C	601	107	C28-C29	3.64	1.48	1.37
3	C	601	107	C11-S10	-3.13	1.67	1.76
3	A	501	107	C9-S10	-2.91	1.69	1.73
3	A	501	107	C11-S10	-2.76	1.68	1.76
3	C	601	107	C9-S10	-2.57	1.69	1.73
3	A	501	107	C14-N15	2.51	1.49	1.45
3	C	601	107	S22-N25	2.49	1.67	1.63

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	107	C7-N8-C9	9.26	114.50	109.83
3	C	601	107	C11-S10-C9	7.14	93.58	88.90
3	A	501	107	C7-N8-C9	6.77	113.24	109.83
3	C	601	107	S10-C9-N8	-6.60	112.87	117.01
3	A	501	107	C11-S10-C9	5.05	92.21	88.90
3	C	601	107	C2-C13-C12	-4.77	103.59	107.06
3	A	501	107	C2-C13-C12	-3.81	104.29	107.06
3	A	501	107	S10-C9-N8	-3.42	114.86	117.01
3	C	601	107	O23-S22-C19	-3.41	103.68	107.98
3	A	501	107	C12-C11-S10	3.37	131.38	127.20
3	C	601	107	C29-N30-C31	3.36	122.01	117.21
3	C	601	107	N25-C31-N30	3.18	117.67	114.13
3	A	501	107	C29-N30-C31	3.06	121.58	117.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	107	C14-N15-C16	2.69	127.63	122.42
3	A	501	107	C5-C6-C7	-2.53	119.63	122.03
3	C	601	107	C5-C6-C7	-2.53	119.64	122.03
3	C	601	107	C12-C11-S10	2.51	130.32	127.20
3	C	601	107	C14-N15-C16	2.43	127.12	122.42
3	C	601	107	O24-S22-C19	2.36	110.96	107.98
3	C	601	107	O24-S22-O23	-2.34	116.68	119.52
3	C	601	107	C31-N25-S22	2.28	130.06	124.83
3	A	501	107	C18-C19-S22	-2.14	117.40	119.76
3	A	501	107	C21-C16-N15	-2.14	116.12	120.96
3	A	501	107	N25-C31-N30	2.11	116.48	114.13

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	107	C2-C13-C14-N15
3	A	501	107	C12-C13-C14-N15
3	C	601	107	C2-C13-C14-N15
3	C	601	107	C12-C13-C14-N15
3	C	601	107	C17-C16-N15-C14
3	C	601	107	C21-C16-N15-C14
3	A	501	107	C21-C16-N15-C14
3	A	501	107	C17-C16-N15-C14

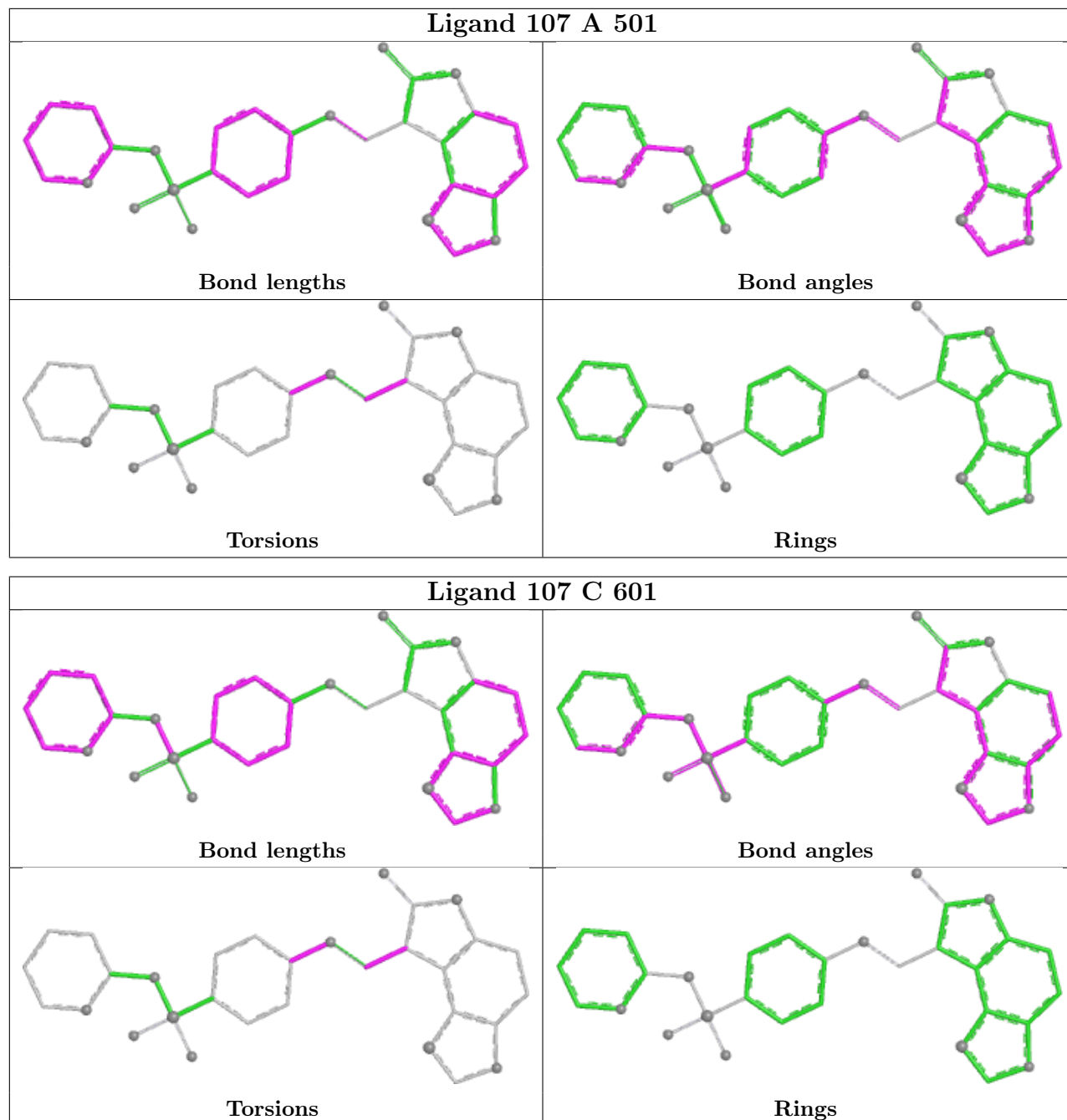
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	107	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, 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	298/298 (100%)	-0.23	11 (3%) 45 36	31, 46, 83, 99	0
1	C	298/298 (100%)	0.15	14 (4%) 36 29	38, 62, 87, 97	0
2	B	260/260 (100%)	-0.14	5 (1%) 66 57	34, 53, 75, 95	0
2	D	260/260 (100%)	-0.30	9 (3%) 47 38	29, 43, 73, 103	0
All	All	1116/1116 (100%)	-0.12	39 (3%) 47 38	29, 51, 84, 103	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	174	GLU	6.8
2	D	175	VAL	6.1
2	D	173	ASN	6.0
2	D	176	PRO	5.4
2	D	345	ASP	5.0
1	A	298	LEU	4.7
2	D	193	CYS	4.0
2	D	178	TYR	4.0
2	B	173	ASN	3.9
2	B	345	ASP	3.9
1	A	40	GLU	3.8
2	B	193	CYS	3.8
1	C	15	TYR	3.5
2	D	177	ASP	3.1
1	C	17	VAL	3.0
1	C	164	VAL	2.9
1	A	84	HIS	2.9
1	A	41	THR	2.9
1	A	159	TYR	2.8
1	C	297	ARG	2.8
1	A	71	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	165	THR	2.7
1	C	36	ARG	2.7
1	A	15	TYR	2.6
1	C	161	HIS	2.5
1	A	14	THR	2.5
1	A	297	ARG	2.4
1	C	40	GLU	2.3
2	D	179	HIS	2.3
1	A	38	ASP	2.2
1	A	37	LEU	2.2
1	C	41	THR	2.2
2	B	176	PRO	2.1
1	C	38	ASP	2.1
1	C	96	LEU	2.1
1	C	95	ALA	2.1
2	B	327	CYS	2.1
1	C	98	GLY	2.0
1	C	39	THR	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, 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.

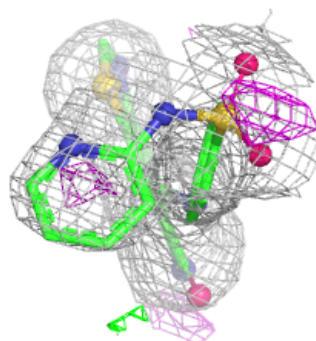
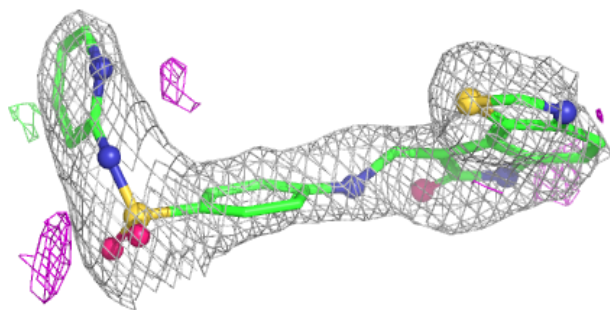
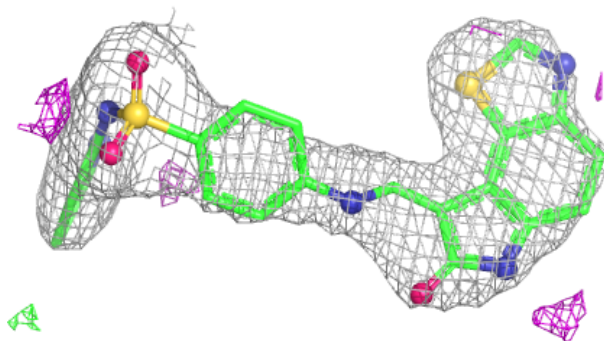
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	107	C	601	31/31	0.93	0.12	69,72,76,76	0
3	107	A	501	31/31	0.96	0.08	39,48,58,58	0

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.

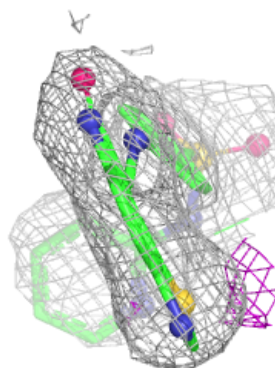
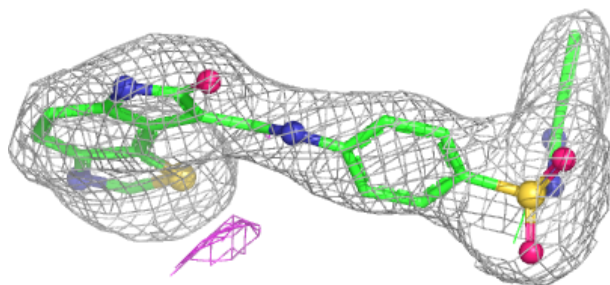
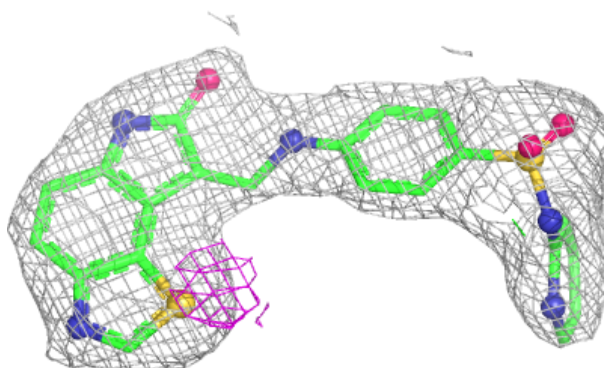
Electron density around 107 C 601:

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



Electron density around 107 A 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.