



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:31 AM UTC

PDB ID : 2ANL / pdb_00002anl
Title : X-ray crystal structure of the aspartic protease plasmepsin 4 from the malarial parasite plasmodium malariae bound to an allophenylnorstatine based inhibitor
Authors : Clemente, J.C.; Govindasamy, L.; Madabushi, A.; Fisher, S.Z.; Moose, R.E.; Yowell, C.A.; Hidaka, K.; Kimura, T.; Hayashi, Y.; Kiso, Y.; Agbandje-McKenna, M.; Dame, J.B.; Dunn, B.M.; McKenna, R.
Deposited on : 2005-08-11
Resolution : 3.30 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
Ideal geometry (proteins)	:	Engh & Huber (2001)

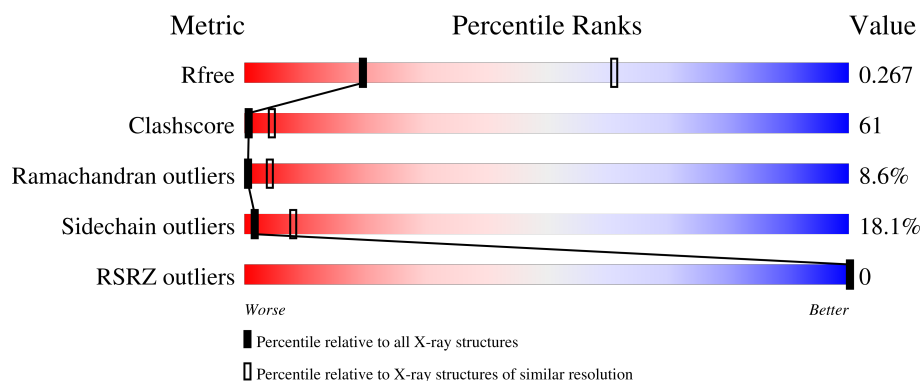
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	327	29% 48% 17% 6%
1	B	327	26% 51% 17% 6%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

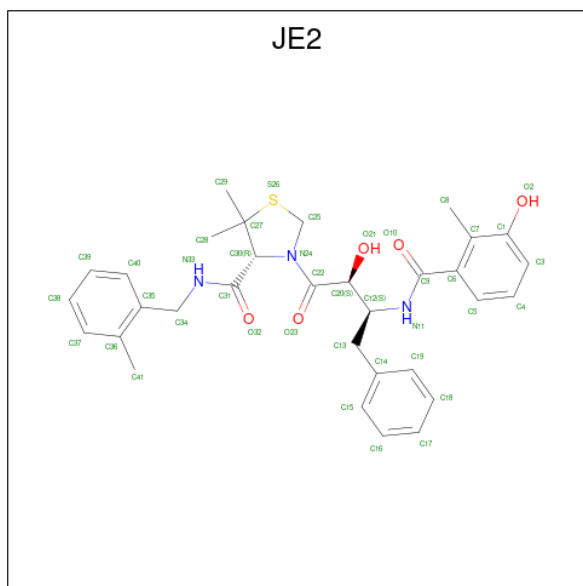
There are 3 unique types of molecules in this entry. The entry contains 5330 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 plasmepsin IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2617	1696	395	515	11			
1	B	327	Total	C	N	O	S	0	0	0
			2617	1696	395	515	11			

- Molecule 2 is (4R)-3-[(2S,3S)-2-hydroxy-3-[(3-hydroxy-2-methylbenzoyl)amino]-4-phenylbutanoyl]-5,5-dimethyl-N-(2-methylbenzyl)-1,3-thiazolidine-4-carboxamide (CCD ID: JE2) (formula: C₃₂H₃₇N₃O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			41	32	3	5	1		
2	B	1	Total	C	N	O	S	0	0
			41	32	3	5	1		

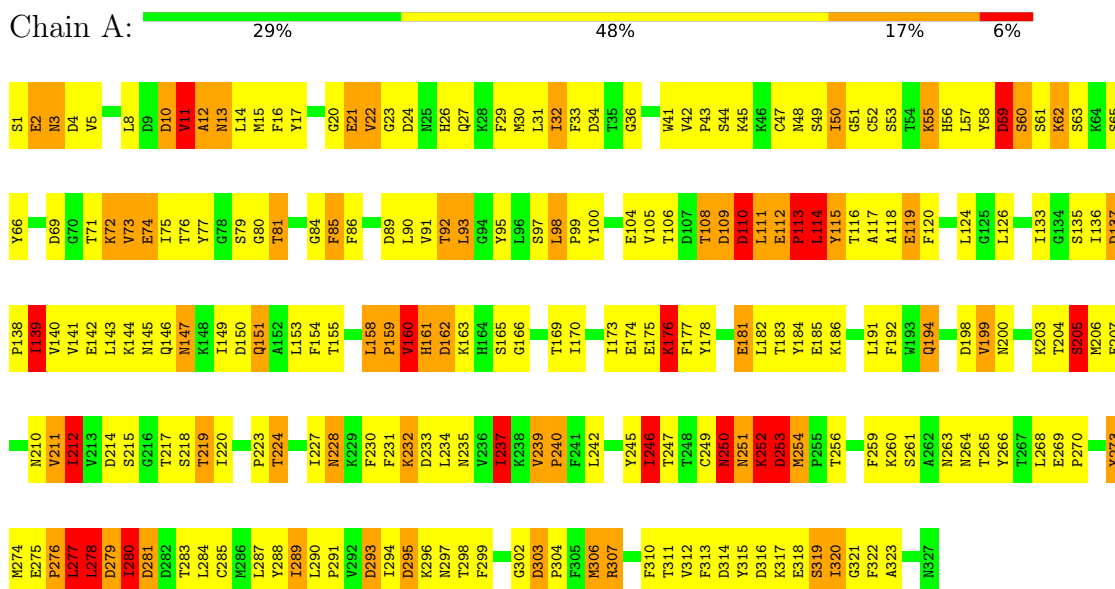
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total 7	O 7	0	0
3	B	7	Total 7	O 7	0	0

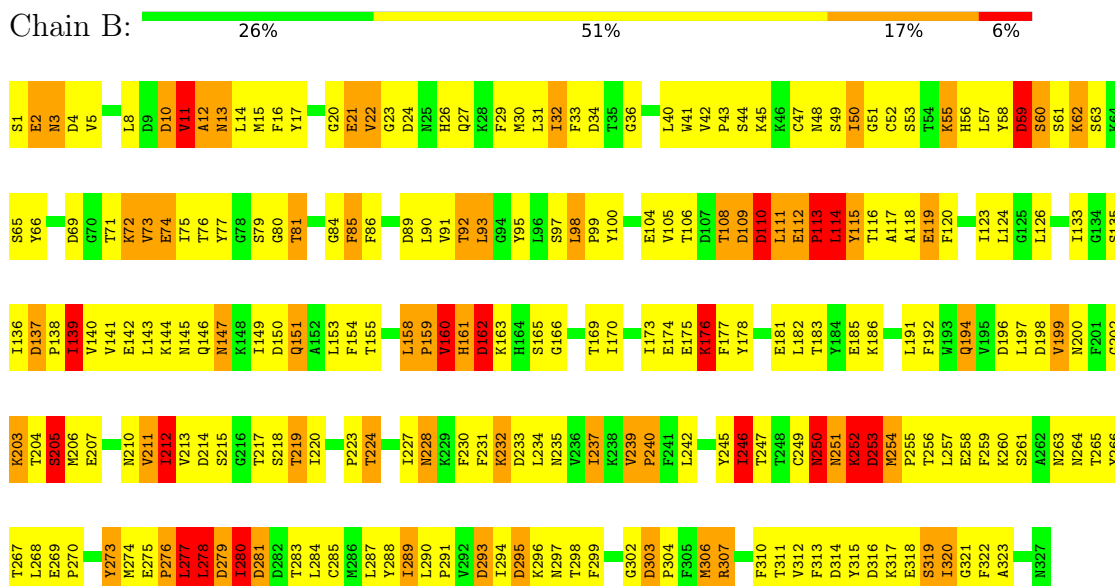
3 Residue-property plots

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: plasmepsin IV



• Molecule 1: plasmepsin IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.88Å 112.58Å 90.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.30 25.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-3.30) 79.4 (25.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 3.30Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.298 0.253 , 0.267	Depositor DCC
R_{free} test set	719 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 6.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5330	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: JE2

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	1.36	12/2681 (0.4%)	1.36	18/3636 (0.5%)
1	B	1.35	12/2681 (0.4%)	1.33	18/3636 (0.5%)
All	All	1.36	24/5362 (0.4%)	1.34	36/7272 (0.5%)

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	8
1	B	0	8
All	All	0	16

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	ASP	CA-CB	-7.96	1.40	1.53
1	A	295	ASP	N-CA	-7.10	1.37	1.46
1	B	295	ASP	N-CA	-7.08	1.37	1.46
1	B	289	ILE	CA-CB	-6.60	1.46	1.54
1	A	289	ILE	CA-CB	-6.59	1.46	1.54
1	B	2	GLU	CA-C	6.24	1.61	1.52
1	A	2	GLU	CA-C	6.24	1.61	1.52
1	B	181	GLU	CA-C	6.07	1.59	1.52
1	A	181	GLU	CA-C	6.01	1.59	1.52
1	A	5	VAL	CA-CB	-5.57	1.47	1.54
1	A	311	THR	CA-CB	-5.54	1.44	1.53
1	B	311	THR	CA-CB	-5.53	1.44	1.53
1	B	5	VAL	CA-CB	-5.53	1.47	1.54
1	B	211	VAL	N-CA	-5.46	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	ARG	NE-CZ	5.45	1.39	1.33
1	A	211	VAL	N-CA	-5.43	1.39	1.46
1	A	307	ARG	NE-CZ	5.38	1.39	1.33
1	A	170	ILE	CA-CB	-5.30	1.48	1.54
1	A	237	ILE	C-O	-5.29	1.18	1.24
1	B	237	ILE	C-O	-5.28	1.18	1.24
1	B	170	ILE	CA-CB	-5.27	1.48	1.54
1	B	136	ILE	CA-CB	-5.10	1.47	1.54
1	A	136	ILE	CA-CB	-5.05	1.47	1.54
1	B	213	VAL	N-CA	-5.03	1.39	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ASP	CB-CA-C	-19.00	80.26	111.23
1	B	253	ASP	N-CA-CB	17.20	139.56	110.49
1	A	253	ASP	N-CA-CB	17.20	139.56	110.49
1	B	111	LEU	N-CA-C	-16.70	94.01	113.21
1	A	111	LEU	N-CA-C	-16.69	94.02	113.21
1	B	279	ASP	CB-CA-C	-11.24	92.90	111.23
1	A	239	VAL	N-CA-C	-7.18	102.46	108.63
1	B	239	VAL	N-CA-C	-7.13	102.50	108.63
1	A	205	SER	N-CA-C	7.00	119.58	109.14
1	B	205	SER	N-CA-C	7.00	119.57	109.14
1	A	73	VAL	N-CA-C	6.86	116.07	107.70
1	B	73	VAL	N-CA-C	6.84	116.04	107.70
1	A	252	LYS	N-CA-C	-6.38	101.20	110.64
1	B	252	LYS	N-CA-C	-6.37	101.21	110.64
1	B	280	ILE	N-CA-CB	6.08	121.26	111.23
1	A	280	ILE	N-CA-CB	6.07	121.25	111.23
1	A	293	ASP	N-CA-C	5.74	117.27	109.11
1	A	158	LEU	N-CA-C	5.73	118.80	110.14
1	B	293	ASP	N-CA-C	5.72	117.23	109.11
1	B	158	LEU	N-CA-C	5.71	118.76	110.14
1	B	161	HIS	N-CA-C	5.68	117.16	108.12
1	B	246	ILE	CA-C-O	-5.68	116.27	121.72
1	A	161	HIS	N-CA-C	5.66	117.11	108.12
1	A	246	ILE	CA-C-O	-5.65	116.29	121.72
1	B	252	LYS	CB-CA-C	5.58	116.67	109.80
1	A	252	LYS	CB-CA-C	5.56	116.64	109.80
1	B	273	TYR	CB-CA-C	5.37	118.08	109.27
1	A	273	TYR	CB-CA-C	5.37	118.07	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	PHE	N-CA-C	-5.30	101.52	109.79
1	B	192	PHE	N-CA-C	-5.29	101.53	109.79
1	B	74	GLU	N-CA-C	5.20	117.09	109.24
1	B	110	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	74	GLU	N-CA-C	5.17	117.05	109.24
1	A	110	ASP	CA-CB-CG	5.16	117.75	112.60
1	B	85	PHE	N-CA-C	5.10	116.17	108.46
1	A	85	PHE	N-CA-C	5.09	116.15	108.46

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	VAL	Peptide
1	A	112	GLU	Peptide
1	A	113	PRO	Peptide
1	A	114	LEU	Peptide
1	A	212	ILE	Peptide
1	A	277	LEU	Peptide
1	A	278	LEU	Peptide
1	A	59	ASP	Peptide
1	B	11	VAL	Peptide
1	B	112	GLU	Peptide
1	B	113	PRO	Peptide
1	B	114	LEU	Peptide
1	B	212	ILE	Peptide
1	B	277	LEU	Peptide
1	B	278	LEU	Peptide
1	B	59	ASP	Peptide

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	2617	0	2539	328	1
1	B	2617	0	2539	330	1
2	A	41	0	37	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	41	0	37	8	0
3	A	7	0	0	2	0
3	B	7	0	0	2	0
All	All	5330	0	5152	641	1

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 61.

All (641) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ILE:CD1	1:A:281:ASP:HB3	1.57	1.34
1:B:280:ILE:CD1	1:B:281:ASP:HB3	1.57	1.33
1:B:92:THR:C	1:B:93:LEU:HD23	1.63	1.24
1:A:92:THR:C	1:A:93:LEU:HD23	1.63	1.22
1:A:181:GLU:HG2	1:B:202:GLY:O	1.43	1.18
1:A:159:PRO:O	1:A:160:VAL:HG22	1.44	1.16
1:B:159:PRO:O	1:B:160:VAL:HG22	1.45	1.16
1:B:280:ILE:HD13	1:B:281:ASP:N	1.62	1.15
1:A:280:ILE:HD13	1:A:281:ASP:N	1.62	1.14
1:A:160:VAL:HB	1:A:163:LYS:HG3	1.28	1.13
1:B:280:ILE:HD13	1:B:280:ILE:C	1.76	1.10
1:A:280:ILE:HD13	1:A:280:ILE:C	1.76	1.09
1:A:110:ASP:C	1:A:112:GLU:H	1.51	1.09
1:B:280:ILE:HD13	1:B:281:ASP:HB3	1.35	1.09
1:B:160:VAL:HB	1:B:163:LYS:HG3	1.28	1.07
1:A:109:ASP:O	1:A:110:ASP:HB2	1.57	1.04
1:B:110:ASP:C	1:B:112:GLU:H	1.51	1.04
1:A:280:ILE:HD13	1:A:281:ASP:HB3	1.35	1.03
1:A:80:GLY:HA3	1:A:111:LEU:HD12	1.41	1.02
1:A:252:LYS:HD2	1:A:252:LYS:O	1.59	1.01
1:B:252:LYS:HD2	1:B:252:LYS:O	1.59	1.01
1:A:159:PRO:C	1:A:160:VAL:HG22	1.85	1.01
1:B:109:ASP:O	1:B:110:ASP:HB2	1.57	1.00
1:B:159:PRO:C	1:B:160:VAL:HG22	1.85	1.00
1:A:280:ILE:HD11	1:A:281:ASP:HB3	1.42	0.99
1:A:181:GLU:OE1	1:B:258:GLU:HG3	1.60	0.99
1:A:279:ASP:CG	1:A:279:ASP:O	1.98	0.99
1:B:280:ILE:HD11	1:B:281:ASP:HB3	1.42	0.99
1:B:80:GLY:HA3	1:B:111:LEU:HD12	1.41	0.98
1:A:280:ILE:HD13	1:A:281:ASP:CB	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:C	1:A:112:GLU:N	2.18	0.97
1:B:280:ILE:HD13	1:B:281:ASP:CB	1.94	0.97
1:A:314:ASP:OD2	1:A:317:LYS:HD2	1.64	0.96
1:A:112:GLU:OE2	1:A:116:THR:HG23	1.66	0.96
1:A:175:GLU:HB3	1:B:203:LYS:NZ	1.80	0.96
1:B:280:ILE:CD1	1:B:281:ASP:CB	2.44	0.96
1:B:45:LYS:HD2	1:B:59:ASP:HB2	1.48	0.95
1:A:280:ILE:CD1	1:A:281:ASP:CB	2.44	0.95
1:A:45:LYS:HD2	1:A:59:ASP:HB2	1.48	0.95
1:A:281:ASP:OD2	1:A:283:THR:HG22	1.67	0.94
1:B:112:GLU:OE2	1:B:116:THR:HG23	1.66	0.94
1:A:110:ASP:H	1:A:112:GLU:HB2	1.33	0.93
1:A:109:ASP:O	1:A:110:ASP:CB	2.15	0.93
1:B:281:ASP:OD2	1:B:283:THR:HG22	1.67	0.93
1:B:110:ASP:H	1:B:112:GLU:HB2	1.33	0.93
1:B:159:PRO:C	1:B:160:VAL:CG2	2.39	0.93
1:A:92:THR:O	1:A:93:LEU:HD23	1.68	0.92
1:B:275:GLU:O	1:B:276:PRO:O	1.87	0.92
1:B:92:THR:O	1:B:93:LEU:HD23	1.68	0.92
1:A:275:GLU:O	1:A:276:PRO:O	1.87	0.91
1:A:159:PRO:C	1:A:160:VAL:CG2	2.40	0.91
1:A:44:SER:HB2	1:A:104:GLU:HG2	1.53	0.90
1:B:114:LEU:HD23	1:B:114:LEU:H	1.37	0.90
1:B:109:ASP:O	1:B:110:ASP:CB	2.15	0.90
1:B:44:SER:HB2	1:B:104:GLU:HG2	1.53	0.89
1:A:160:VAL:CB	1:A:163:LYS:HG3	2.03	0.88
1:B:160:VAL:CB	1:B:163:LYS:HG3	2.03	0.88
1:A:114:LEU:HD23	1:A:114:LEU:H	1.37	0.88
1:B:110:ASP:C	1:B:112:GLU:N	2.18	0.87
1:A:181:GLU:OE1	1:B:200:ASN:HB2	1.75	0.87
1:B:232:LYS:HE2	1:B:233:ASP:N	1.92	0.85
1:B:275:GLU:C	1:B:276:PRO:O	2.19	0.84
1:A:232:LYS:HE2	1:A:233:ASP:N	1.92	0.84
1:A:181:GLU:CG	1:B:202:GLY:O	2.26	0.84
1:A:280:ILE:HD13	1:A:281:ASP:CA	2.11	0.81
1:B:280:ILE:HD13	1:B:281:ASP:CA	2.11	0.81
1:A:275:GLU:C	1:A:276:PRO:O	2.19	0.80
1:A:110:ASP:H	1:A:112:GLU:CB	1.94	0.80
1:A:93:LEU:HD23	1:A:93:LEU:N	1.87	0.80
1:B:110:ASP:H	1:B:112:GLU:CB	1.94	0.79
1:B:270:PRO:HA	1:B:273:TYR:CE2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:HB3	1:B:203:LYS:HZ3	1.47	0.77
1:B:93:LEU:HD23	1:B:93:LEU:N	1.87	0.77
1:A:254:MET:HE2	1:A:270:PRO:HB3	1.66	0.77
1:A:251:ASN:O	1:A:254:MET:HG2	1.85	0.77
1:A:270:PRO:HA	1:A:273:TYR:CE2	2.19	0.77
1:B:279:ASP:OD1	1:B:279:ASP:O	2.03	0.77
1:B:251:ASN:O	1:B:254:MET:HG2	1.85	0.77
1:A:111:LEU:O	1:A:114:LEU:HB2	1.84	0.77
1:B:111:LEU:O	1:B:114:LEU:HB2	1.84	0.77
1:B:254:MET:HE2	1:B:270:PRO:HB3	1.66	0.76
1:A:181:GLU:HB3	1:B:200:ASN:ND2	1.99	0.76
1:A:199:VAL:HG11	1:A:299:PHE:CE1	2.21	0.76
1:B:36:GLY:HA3	2:B:3152:JE2:O21	1.85	0.76
1:A:10:ASP:C	1:A:10:ASP:OD1	2.30	0.75
1:B:199:VAL:HG11	1:B:299:PHE:CE1	2.21	0.75
1:A:36:GLY:HA3	2:A:3151:JE2:O21	1.86	0.75
1:B:113:PRO:HD2	1:B:114:LEU:HD23	1.69	0.75
1:A:113:PRO:HD2	1:A:114:LEU:HD23	1.69	0.74
1:B:10:ASP:OD1	1:B:10:ASP:C	2.30	0.74
1:B:114:LEU:HD23	1:B:114:LEU:N	2.03	0.73
1:B:13:ASN:O	1:B:14:LEU:HD13	1.89	0.72
1:A:144:LYS:HD3	1:A:151:GLN:HA	1.72	0.72
1:A:234:LEU:H	1:A:234:LEU:HD23	1.53	0.72
1:B:22:VAL:CG2	1:B:22:VAL:O	2.38	0.72
1:B:234:LEU:HD23	1:B:234:LEU:H	1.53	0.72
1:A:13:ASN:O	1:A:14:LEU:HD13	1.89	0.71
1:A:108:THR:O	1:A:109:ASP:C	2.32	0.71
1:B:144:LYS:HD3	1:B:151:GLN:HA	1.72	0.71
1:B:275:GLU:O	1:B:276:PRO:C	2.32	0.71
1:A:22:VAL:O	1:A:22:VAL:CG2	2.38	0.71
1:A:114:LEU:H	1:A:114:LEU:CD2	2.03	0.71
1:B:108:THR:O	1:B:109:ASP:C	2.32	0.71
1:B:114:LEU:H	1:B:114:LEU:CD2	2.03	0.71
1:B:175:GLU:HA	1:B:178:TYR:CE2	2.26	0.70
1:A:114:LEU:HD23	1:A:114:LEU:N	2.03	0.70
1:A:175:GLU:HA	1:A:178:TYR:CE2	2.26	0.70
1:B:22:VAL:O	1:B:22:VAL:HG23	1.91	0.70
1:A:22:VAL:O	1:A:22:VAL:HG23	1.91	0.70
1:A:41:TRP:CE3	1:A:105:VAL:HG21	2.27	0.70
1:B:41:TRP:CE3	1:B:105:VAL:HG21	2.27	0.70
1:A:108:THR:O	1:A:109:ASP:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:THR:O	1:B:109:ASP:O	2.10	0.69
1:B:279:ASP:O	1:B:279:ASP:CG	2.34	0.69
1:A:159:PRO:O	1:A:160:VAL:CG2	2.33	0.69
1:A:278:LEU:HG	1:A:278:LEU:O	1.91	0.69
1:A:275:GLU:O	1:A:276:PRO:C	2.32	0.69
1:B:278:LEU:O	1:B:278:LEU:HG	1.91	0.69
1:A:175:GLU:HB3	1:B:203:LYS:HZ1	1.57	0.68
1:A:294:ILE:H	1:A:294:ILE:HD12	1.58	0.68
1:A:181:GLU:OE1	1:B:258:GLU:CG	2.38	0.68
1:A:114:LEU:CD2	1:A:114:LEU:N	2.57	0.68
1:A:59:ASP:OD2	1:A:59:ASP:C	2.36	0.68
1:B:150:ASP:HB3	1:B:151:GLN:NE2	2.09	0.68
1:B:59:ASP:C	1:B:59:ASP:OD2	2.36	0.68
1:A:150:ASP:HB3	1:A:151:GLN:NE2	2.09	0.68
1:B:294:ILE:HD12	1:B:294:ILE:H	1.58	0.68
1:A:97:SER:O	1:A:98:LEU:HB2	1.94	0.67
2:A:3151:JE2:HC83	2:A:3151:JE2:O10	1.93	0.67
1:B:114:LEU:N	1:B:114:LEU:CD2	2.57	0.67
1:A:1:SER:HB2	1:A:3:ASN:OD1	1.93	0.67
1:B:280:ILE:CD1	1:B:280:ILE:C	2.49	0.67
1:A:21:GLU:OE2	1:A:26:HIS:HB3	1.95	0.67
1:B:1:SER:HB2	1:B:3:ASN:OD1	1.93	0.67
1:B:11:VAL:HG23	1:B:15:MET:O	1.95	0.67
2:B:3152:JE2:HC83	2:B:3152:JE2:O10	1.93	0.67
1:B:278:LEU:O	1:B:278:LEU:CG	2.43	0.67
1:B:21:GLU:OE2	1:B:26:HIS:HB3	1.95	0.67
1:B:1:SER:HB3	3:B:410:HOH:O	1.95	0.66
1:A:280:ILE:CD1	1:A:280:ILE:C	2.49	0.66
1:A:278:LEU:O	1:A:278:LEU:CG	2.43	0.66
1:B:89:ASP:CG	1:B:90:LEU:H	2.04	0.66
1:A:138:PRO:HG2	1:A:141:VAL:CG2	2.26	0.66
1:A:224:THR:HG22	1:A:293:ASP:OD1	1.96	0.66
1:A:144:LYS:H	1:A:149:ILE:HD11	1.61	0.66
1:A:11:VAL:HG23	1:A:15:MET:O	1.95	0.66
1:A:1:SER:HB3	3:A:403:HOH:O	1.95	0.66
1:B:47:CYS:SG	1:B:106:THR:O	2.55	0.66
1:B:224:THR:HG22	1:B:293:ASP:OD1	1.96	0.66
1:A:199:VAL:HG11	1:A:299:PHE:HE1	1.61	0.65
1:B:11:VAL:O	1:B:13:ASN:N	2.30	0.65
1:B:138:PRO:HG2	1:B:141:VAL:CG2	2.25	0.65
1:A:22:VAL:HG21	1:A:58:TYR:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:VAL:O	1:B:320:ILE:HG13	1.97	0.65
1:B:97:SER:O	1:B:98:LEU:HB2	1.94	0.65
1:A:89:ASP:CG	1:A:90:LEU:H	2.04	0.65
1:A:13:ASN:C	1:A:14:LEU:HD22	2.22	0.64
1:B:22:VAL:HG21	1:B:58:TYR:CD2	2.31	0.64
1:A:47:CYS:SG	1:A:106:THR:O	2.55	0.64
1:A:11:VAL:O	1:A:13:ASN:N	2.30	0.64
1:A:114:LEU:O	1:A:116:THR:N	2.31	0.64
1:B:158:LEU:HD23	1:B:159:PRO:HD2	1.79	0.64
1:A:112:GLU:OE2	1:A:116:THR:CG2	2.44	0.64
1:A:312:VAL:O	1:A:320:ILE:HG13	1.97	0.64
1:B:144:LYS:H	1:B:149:ILE:HD11	1.61	0.64
1:A:158:LEU:HD23	1:A:159:PRO:HD2	1.79	0.64
1:B:13:ASN:C	1:B:14:LEU:HD22	2.22	0.64
1:A:90:LEU:HD12	1:A:98:LEU:O	1.98	0.64
1:B:21:GLU:HA	1:B:27:GLN:O	1.98	0.63
1:A:140:VAL:HB	1:A:315:TYR:HE1	1.63	0.63
1:A:211:VAL:C	1:A:212:ILE:CG2	2.72	0.63
1:B:114:LEU:O	1:B:116:THR:N	2.31	0.63
1:B:280:ILE:HD11	1:B:281:ASP:CB	2.23	0.63
1:B:283:THR:HG23	1:B:284:LEU:N	2.14	0.63
1:A:21:GLU:HA	1:A:27:GLN:O	1.98	0.63
1:B:90:LEU:HD12	1:B:98:LEU:O	1.98	0.63
1:B:278:LEU:O	1:B:278:LEU:HD12	1.99	0.62
1:A:153:LEU:HB2	1:A:313:PHE:O	2.00	0.62
1:A:98:LEU:C	1:A:98:LEU:HD23	2.25	0.62
1:B:140:VAL:HB	1:B:315:TYR:HE1	1.63	0.62
1:A:278:LEU:O	1:A:278:LEU:HD12	1.99	0.62
1:A:283:THR:HG23	1:A:284:LEU:N	2.14	0.62
1:B:211:VAL:C	1:B:212:ILE:CG2	2.72	0.62
1:A:23:GLY:N	1:A:90:LEU:O	2.33	0.61
1:B:254:MET:HE2	1:B:270:PRO:CB	2.30	0.61
1:B:153:LEU:HB2	1:B:313:PHE:O	2.00	0.61
1:B:295:ASP:HB2	1:B:298:THR:OG1	2.00	0.61
1:A:186:LYS:HA	1:A:319:SER:HB2	1.83	0.60
1:B:98:LEU:HD23	1:B:98:LEU:C	2.25	0.60
1:A:295:ASP:HB2	1:A:298:THR:OG1	2.00	0.60
1:B:98:LEU:HD23	1:B:99:PRO:C	2.26	0.60
1:A:98:LEU:HD23	1:A:99:PRO:N	2.17	0.60
1:A:302:GLY:C	1:A:304:PRO:HD2	2.27	0.60
1:A:175:GLU:C	1:A:177:PHE:H	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:VAL:HG11	1:B:299:PHE:HE1	1.61	0.60
1:B:175:GLU:C	1:B:177:PHE:H	2.10	0.60
1:B:23:GLY:N	1:B:90:LEU:O	2.33	0.60
1:B:98:LEU:HD23	1:B:99:PRO:N	2.17	0.60
1:B:112:GLU:OE2	1:B:116:THR:CG2	2.44	0.60
1:B:186:LYS:HA	1:B:319:SER:HB2	1.83	0.60
1:B:302:GLY:C	1:B:304:PRO:HD2	2.27	0.60
1:A:80:GLY:CA	1:A:111:LEU:HD12	2.26	0.60
1:A:254:MET:HE2	1:A:270:PRO:CB	2.30	0.60
1:A:22:VAL:HG21	1:A:58:TYR:CE2	2.36	0.60
1:B:22:VAL:HG21	1:B:58:TYR:CE2	2.36	0.60
1:A:92:THR:O	1:A:93:LEU:CD2	2.46	0.59
1:A:314:ASP:OD2	1:A:317:LYS:CD	2.45	0.59
1:B:92:THR:O	1:B:93:LEU:CD2	2.46	0.59
1:A:314:ASP:HB3	1:A:317:LYS:HB2	1.83	0.59
1:B:278:LEU:O	1:B:280:ILE:HG23	2.02	0.59
1:A:280:ILE:HD11	1:A:281:ASP:CB	2.23	0.59
1:B:77:TYR:HA	2:B:3152:JE2:HC83	1.85	0.59
1:B:227:ILE:O	1:B:230:PHE:N	2.36	0.59
1:A:77:TYR:HA	2:A:3151:JE2:HC83	1.85	0.59
1:A:98:LEU:HD23	1:A:99:PRO:C	2.26	0.58
1:A:278:LEU:O	1:A:280:ILE:HG23	2.02	0.58
1:A:160:VAL:HB	1:A:163:LYS:CG	2.19	0.58
1:A:278:LEU:HD23	3:A:401:HOH:O	2.03	0.58
1:B:304:PRO:HA	1:B:307:ARG:HD2	1.86	0.58
1:A:227:ILE:O	1:A:228:ASN:C	2.46	0.58
1:B:227:ILE:O	1:B:228:ASN:C	2.46	0.58
1:B:275:GLU:HG3	1:B:288:TYR:OH	2.04	0.58
1:A:181:GLU:HB3	1:B:200:ASN:HD22	1.68	0.58
1:A:184:TYR:CB	1:B:207:GLU:OE2	2.52	0.58
1:B:278:LEU:HD23	3:B:408:HOH:O	2.03	0.58
1:B:50:ILE:O	1:B:51:GLY:C	2.47	0.58
1:A:22:VAL:CG2	1:A:58:TYR:CE2	2.87	0.58
1:A:198:ASP:OD1	1:A:207:GLU:HG3	2.04	0.58
1:A:227:ILE:O	1:A:230:PHE:N	2.36	0.58
1:A:275:GLU:HG3	1:A:288:TYR:OH	2.04	0.58
1:B:22:VAL:CG2	1:B:58:TYR:CE2	2.87	0.58
1:B:199:VAL:O	1:B:205:SER:OG	2.22	0.58
1:A:211:VAL:C	1:A:212:ILE:HG22	2.29	0.57
1:A:59:ASP:OD2	1:A:60:SER:N	2.37	0.57
1:A:217:THR:HG22	1:A:219:THR:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LYS:HD3	1:B:120:PHE:O	2.05	0.57
1:B:59:ASP:OD2	1:B:60:SER:N	2.37	0.57
1:A:199:VAL:O	1:A:205:SER:OG	2.22	0.57
1:A:50:ILE:O	1:A:51:GLY:C	2.47	0.57
1:A:304:PRO:HA	1:A:307:ARG:HD2	1.86	0.57
1:A:69:ASP:HB3	1:A:86:PHE:O	2.05	0.57
1:A:91:VAL:N	1:A:98:LEU:O	2.31	0.56
1:A:111:LEU:O	1:A:114:LEU:CB	2.54	0.56
1:B:69:ASP:HB3	1:B:86:PHE:O	2.05	0.56
1:B:89:ASP:OD2	1:B:90:LEU:N	2.38	0.56
1:B:217:THR:HG22	1:B:219:THR:HG23	1.86	0.56
1:B:278:LEU:O	1:B:278:LEU:CD1	2.53	0.56
1:A:55:LYS:HD3	1:A:120:PHE:O	2.04	0.56
1:A:278:LEU:O	1:A:278:LEU:CD1	2.53	0.56
1:B:198:ASP:OD1	1:B:207:GLU:HG3	2.04	0.56
1:A:80:GLY:HA3	1:A:111:LEU:CD1	2.28	0.56
1:B:91:VAL:N	1:B:98:LEU:O	2.31	0.56
1:B:211:VAL:C	1:B:212:ILE:HG22	2.29	0.56
1:B:110:ASP:N	1:B:112:GLU:HB2	2.13	0.56
1:B:92:THR:HB	1:B:97:SER:HA	1.88	0.56
1:B:138:PRO:HG2	1:B:141:VAL:HG21	1.88	0.56
1:B:277:LEU:HB3	1:B:278:LEU:HB3	1.88	0.55
1:B:10:ASP:OD1	1:B:11:VAL:N	2.39	0.55
1:A:138:PRO:HG2	1:A:141:VAL:HG21	1.88	0.55
1:B:161:HIS:CG	1:B:162:ASP:N	2.73	0.55
1:B:281:ASP:OD2	1:B:281:ASP:C	2.49	0.55
1:A:277:LEU:HB3	1:A:278:LEU:HB3	1.88	0.55
1:A:314:ASP:CG	1:A:317:LYS:HB2	2.32	0.55
1:A:85:PHE:CD1	1:A:85:PHE:N	2.74	0.55
1:B:75:ILE:HG12	1:B:133:ILE:HD12	1.89	0.55
1:B:85:PHE:CD1	1:B:85:PHE:N	2.74	0.55
1:A:10:ASP:OD1	1:A:11:VAL:N	2.39	0.55
1:A:281:ASP:OD2	1:A:281:ASP:C	2.49	0.55
1:B:259:PHE:HB2	1:B:266:TYR:HB2	1.89	0.55
1:A:92:THR:HB	1:A:97:SER:HA	1.88	0.54
1:A:259:PHE:HB2	1:A:266:TYR:HB2	1.89	0.54
1:A:251:ASN:O	1:A:252:LYS:C	2.50	0.54
1:B:10:ASP:CG	1:B:11:VAL:N	2.66	0.54
1:B:60:SER:O	1:B:61:SER:C	2.51	0.54
1:B:138:PRO:O	1:B:139:ILE:C	2.51	0.54
1:A:161:HIS:CG	1:A:162:ASP:N	2.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:PHE:CD1	1:A:322:PHE:N	2.76	0.54
1:A:75:ILE:HG12	1:A:133:ILE:HD12	1.89	0.54
1:A:89:ASP:OD2	1:A:90:LEU:N	2.38	0.54
1:B:1:SER:C	1:B:3:ASN:H	2.15	0.54
1:A:110:ASP:N	1:A:112:GLU:HB2	2.14	0.54
1:A:161:HIS:CG	1:A:162:ASP:H	2.26	0.54
1:A:173:ILE:HD12	1:A:173:ILE:N	2.23	0.54
1:B:173:ILE:N	1:B:173:ILE:HD12	2.23	0.54
1:B:239:VAL:HB	1:B:242:LEU:CD1	2.38	0.54
1:A:1:SER:C	1:A:3:ASN:H	2.15	0.53
1:A:198:ASP:OD1	1:A:207:GLU:CG	2.56	0.53
1:A:275:GLU:CG	1:A:288:TYR:OH	2.56	0.53
1:B:234:LEU:H	1:B:234:LEU:CD2	2.21	0.53
1:A:60:SER:O	1:A:61:SER:C	2.51	0.53
1:B:80:GLY:HA3	1:B:111:LEU:CD1	2.28	0.53
1:B:198:ASP:OD1	1:B:207:GLU:CG	2.56	0.53
1:B:322:PHE:CD1	1:B:322:PHE:N	2.76	0.53
1:A:138:PRO:O	1:A:139:ILE:C	2.51	0.53
1:A:247:THR:O	1:A:285:CYS:N	2.39	0.53
1:B:320:ILE:HG12	1:B:322:PHE:CE1	2.44	0.53
1:B:100:TYR:OH	1:B:137:ASP:O	2.25	0.53
1:A:31:LEU:O	1:A:32:ILE:HG13	2.09	0.53
1:A:263:ASN:ND2	1:B:263:ASN:HA	2.24	0.53
1:B:247:THR:O	1:B:285:CYS:N	2.39	0.53
1:B:275:GLU:CG	1:B:288:TYR:OH	2.56	0.53
1:A:239:VAL:HB	1:A:242:LEU:CD1	2.38	0.53
1:A:320:ILE:HG12	1:A:322:PHE:CE1	2.44	0.53
1:A:10:ASP:CG	1:A:11:VAL:N	2.65	0.53
1:B:160:VAL:HB	1:B:163:LYS:CG	2.19	0.52
1:A:62:LYS:N	1:A:62:LYS:HD2	2.23	0.52
1:A:194:GLN:HB2	1:A:210:ASN:HD21	1.75	0.52
1:B:251:ASN:O	1:B:252:LYS:C	2.50	0.52
1:A:154:PHE:CE2	1:A:313:PHE:CD2	2.98	0.52
1:A:155:THR:OG1	1:A:169:THR:HB	2.10	0.52
1:A:217:THR:HG22	1:A:218:SER:N	2.25	0.52
1:A:223:PRO:HD2	1:A:299:PHE:CE2	2.45	0.52
1:B:161:HIS:CG	1:B:162:ASP:H	2.26	0.52
1:B:194:GLN:HB2	1:B:210:ASN:HD21	1.75	0.52
1:A:33:PHE:CD1	1:A:33:PHE:N	2.77	0.52
1:A:161:HIS:C	1:A:163:LYS:N	2.68	0.52
1:A:251:ASN:O	1:A:254:MET:CG	2.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:O	1:B:32:ILE:HG13	2.09	0.52
1:B:220:ILE:HD11	1:B:304:PRO:HB2	1.92	0.52
1:A:43:PRO:O	1:A:57:LEU:HA	2.10	0.52
1:A:140:VAL:HB	1:A:315:TYR:CE1	2.45	0.52
1:B:111:LEU:O	1:B:114:LEU:CB	2.54	0.52
1:B:223:PRO:HD2	1:B:299:PHE:CE2	2.45	0.52
1:A:178:TYR:CE1	1:A:182:LEU:HD11	2.45	0.51
1:A:227:ILE:HD12	1:A:291:PRO:HB3	1.91	0.51
1:B:161:HIS:C	1:B:163:LYS:N	2.68	0.51
1:A:277:LEU:CB	1:A:278:LEU:HB3	2.40	0.51
1:A:280:ILE:CD1	1:A:281:ASP:N	2.54	0.51
1:B:217:THR:HG22	1:B:218:SER:N	2.25	0.51
1:B:303:ASP:HB2	1:B:304:PRO:HD3	1.93	0.51
1:A:220:ILE:HD11	1:A:304:PRO:HB2	1.92	0.51
1:B:33:PHE:N	1:B:33:PHE:CD1	2.77	0.51
1:B:154:PHE:CE2	1:B:313:PHE:CD2	2.98	0.51
1:A:234:LEU:H	1:A:234:LEU:CD2	2.21	0.51
1:B:17:TYR:CE1	1:B:30:MET:HG2	2.46	0.51
1:B:43:PRO:O	1:B:57:LEU:HA	2.10	0.51
1:B:155:THR:OG1	1:B:169:THR:HB	2.10	0.51
1:B:175:GLU:C	1:B:177:PHE:N	2.67	0.51
1:A:175:GLU:C	1:A:177:PHE:N	2.67	0.51
1:B:227:ILE:HD12	1:B:291:PRO:HB3	1.91	0.51
1:B:277:LEU:CB	1:B:278:LEU:HB3	2.40	0.51
1:B:36:GLY:HA3	2:B:3152:JE2:H21	1.72	0.51
1:B:251:ASN:O	1:B:254:MET:CG	2.56	0.51
1:A:100:TYR:OH	1:A:137:ASP:O	2.25	0.51
1:B:80:GLY:CA	1:B:111:LEU:HD12	2.26	0.51
1:B:153:LEU:C	1:B:153:LEU:HD12	2.36	0.51
1:B:182:LEU:N	1:B:182:LEU:HD12	2.26	0.51
1:B:252:LYS:HD2	1:B:252:LYS:C	2.35	0.51
1:A:211:VAL:CG1	1:A:212:ILE:N	2.73	0.51
1:A:252:LYS:HD2	1:A:252:LYS:C	2.35	0.51
1:B:140:VAL:HB	1:B:315:TYR:CE1	2.45	0.51
1:B:314:ASP:HB3	1:B:317:LYS:HB3	1.92	0.51
1:A:17:TYR:CE1	1:A:30:MET:HG2	2.46	0.51
1:B:283:THR:HG23	1:B:284:LEU:H	1.76	0.51
1:B:62:LYS:HD2	1:B:62:LYS:N	2.22	0.50
1:A:182:LEU:N	1:A:182:LEU:HD12	2.26	0.50
1:A:230:PHE:O	1:A:233:ASP:HB2	2.11	0.50
1:B:178:TYR:CE1	1:B:182:LEU:HD11	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:VAL:HB	1:B:242:LEU:HG	1.94	0.50
1:A:278:LEU:O	1:A:280:ILE:N	2.44	0.50
1:B:108:THR:O	1:B:110:ASP:HB3	2.11	0.50
1:A:108:THR:O	1:A:110:ASP:HB3	2.11	0.50
1:A:153:LEU:C	1:A:153:LEU:HD12	2.36	0.50
1:B:11:VAL:O	1:B:12:ALA:C	2.54	0.50
1:A:113:PRO:O	1:A:114:LEU:O	2.30	0.50
1:A:279:ASP:O	1:A:279:ASP:OD2	2.26	0.50
1:B:230:PHE:O	1:B:233:ASP:HB2	2.11	0.50
1:A:303:ASP:HB2	1:A:304:PRO:HD3	1.93	0.50
1:B:12:ALA:O	1:B:13:ASN:O	2.30	0.50
1:B:50:ILE:O	1:B:53:SER:N	2.45	0.50
1:B:278:LEU:O	1:B:280:ILE:N	2.44	0.50
1:A:4:ASP:CG	1:A:95:TYR:HB3	2.37	0.50
1:B:72:LYS:H	1:B:72:LYS:HD2	1.77	0.50
1:B:113:PRO:O	1:B:114:LEU:O	2.30	0.50
1:A:11:VAL:O	1:A:12:ALA:C	2.54	0.49
1:B:1:SER:C	1:B:3:ASN:N	2.71	0.49
1:B:4:ASP:CG	1:B:95:TYR:HB3	2.37	0.49
1:A:50:ILE:O	1:A:53:SER:N	2.45	0.49
1:A:98:LEU:HG	1:A:99:PRO:HD2	1.94	0.49
1:B:155:THR:HB	1:B:310:PHE:CE2	2.47	0.49
1:A:55:LYS:HD2	1:A:115:TYR:CZ	2.48	0.49
1:A:72:LYS:H	1:A:72:LYS:HD2	1.77	0.49
1:A:155:THR:HB	1:A:310:PHE:CE2	2.47	0.49
1:A:239:VAL:HB	1:A:242:LEU:HG	1.94	0.49
1:A:261:SER:HB3	1:A:264:ASN:HB2	1.95	0.49
1:B:211:VAL:CG1	1:B:212:ILE:N	2.73	0.49
1:A:1:SER:C	1:A:3:ASN:N	2.71	0.49
1:B:98:LEU:HG	1:B:99:PRO:HD2	1.94	0.49
1:A:184:TYR:CZ	1:B:207:GLU:HB2	2.48	0.49
1:A:254:MET:HE2	1:A:254:MET:HB3	1.62	0.49
1:A:283:THR:HG23	1:A:284:LEU:H	1.76	0.49
1:B:217:THR:HG22	1:B:219:THR:H	1.77	0.49
1:B:261:SER:HB3	1:B:264:ASN:HB2	1.95	0.49
1:A:139:ILE:O	1:A:142:GLU:N	2.41	0.48
1:A:273:TYR:HA	1:A:288:TYR:HD1	1.78	0.48
1:A:12:ALA:O	1:A:13:ASN:O	2.30	0.48
1:A:161:HIS:C	1:A:161:HIS:CD2	2.90	0.48
1:A:296:LYS:H	1:A:296:LYS:HD3	1.78	0.48
1:A:110:ASP:N	1:A:112:GLU:CB	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:THR:HG22	1:A:219:THR:H	1.77	0.48
1:B:50:ILE:O	1:B:53:SER:OG	2.31	0.48
1:B:55:LYS:HD2	1:B:115:TYR:CZ	2.48	0.48
1:B:297:ASN:OD1	1:B:297:ASN:N	2.45	0.48
1:A:113:PRO:O	1:A:114:LEU:C	2.56	0.48
1:A:184:TYR:CG	1:B:207:GLU:OE2	2.67	0.48
1:B:227:ILE:HD12	1:B:291:PRO:CA	2.44	0.48
1:A:45:LYS:C	1:A:47:CYS:H	2.22	0.48
1:A:200:ASN:OD1	1:A:205:SER:OG	2.29	0.48
1:B:159:PRO:C	1:B:160:VAL:HG23	2.35	0.48
1:A:160:VAL:CG2	1:A:163:LYS:HG3	2.44	0.48
1:A:227:ILE:HD12	1:A:291:PRO:CA	2.44	0.48
1:A:297:ASN:N	1:A:297:ASN:OD1	2.45	0.48
1:B:296:LYS:H	1:B:296:LYS:HD3	1.78	0.48
1:A:246:ILE:HG13	1:A:247:THR:N	2.29	0.48
1:A:302:GLY:O	1:A:303:ASP:C	2.57	0.48
1:B:113:PRO:O	1:B:114:LEU:C	2.56	0.48
1:B:159:PRO:O	1:B:160:VAL:CG2	2.33	0.48
1:B:273:TYR:HA	1:B:288:TYR:HD1	1.78	0.48
1:A:17:TYR:CZ	1:A:30:MET:HE3	2.49	0.47
1:A:239:VAL:HB	1:A:242:LEU:HD11	1.96	0.47
1:B:239:VAL:HB	1:B:242:LEU:HD11	1.96	0.47
1:A:314:ASP:CB	1:A:317:LYS:HB2	2.42	0.47
1:B:17:TYR:CZ	1:B:30:MET:HE3	2.49	0.47
1:B:161:HIS:C	1:B:163:LYS:H	2.22	0.47
1:B:45:LYS:C	1:B:47:CYS:H	2.22	0.47
1:B:50:ILE:HA	1:B:53:SER:OG	2.14	0.47
1:B:302:GLY:O	1:B:303:ASP:C	2.57	0.47
1:B:280:ILE:CD1	1:B:281:ASP:N	2.54	0.47
1:A:77:TYR:CD2	2:A:3151:JE2:C8	2.97	0.47
1:B:214:ASP:OD1	2:B:3152:JE2:O23	2.33	0.47
1:A:161:HIS:C	1:A:163:LYS:H	2.21	0.47
1:A:211:VAL:HG22	1:A:299:PHE:HB2	1.97	0.47
1:B:161:HIS:C	1:B:161:HIS:CD2	2.90	0.47
1:B:304:PRO:HG3	1:B:307:ARG:NH1	2.30	0.47
1:A:22:VAL:CG2	1:A:58:TYR:CD2	2.97	0.47
1:A:200:ASN:HA	1:A:205:SER:OG	2.15	0.47
1:B:211:VAL:HG22	1:B:299:PHE:HB2	1.96	0.47
1:A:45:LYS:HA	1:A:57:LEU:HB3	1.97	0.47
1:A:52:CYS:HB3	1:A:57:LEU:HD21	1.97	0.47
1:B:160:VAL:CG2	1:B:163:LYS:HG3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ILE:HG13	1:B:247:THR:N	2.29	0.47
1:A:214:ASP:OD1	2:A:3151:JE2:O23	2.33	0.47
1:A:215:SER:HA	1:A:306:MET:HE1	1.96	0.47
1:A:283:THR:CG2	1:A:284:LEU:N	2.78	0.47
1:A:304:PRO:HG3	1:A:307:ARG:NH1	2.30	0.47
1:B:52:CYS:HB3	1:B:57:LEU:HD21	1.97	0.47
1:B:215:SER:HB3	1:B:306:MET:HE1	1.97	0.47
1:A:50:ILE:HA	1:A:53:SER:OG	2.14	0.46
1:A:245:TYR:CD1	1:A:245:TYR:N	2.83	0.46
1:A:50:ILE:O	1:A:53:SER:OG	2.31	0.46
1:B:45:LYS:HA	1:B:57:LEU:HB3	1.97	0.46
1:B:77:TYR:CD2	2:B:3152:JE2:C8	2.97	0.46
1:B:100:TYR:CZ	1:B:139:ILE:HG23	2.50	0.46
1:A:100:TYR:CZ	1:A:139:ILE:HG23	2.50	0.46
1:B:22:VAL:CG2	1:B:58:TYR:CD2	2.97	0.46
1:B:89:ASP:CG	1:B:90:LEU:N	2.73	0.46
1:B:200:ASN:HA	1:B:205:SER:OG	2.15	0.46
1:A:150:ASP:HB3	1:A:151:GLN:HE22	1.80	0.46
1:B:215:SER:HA	1:B:306:MET:HE1	1.96	0.46
1:B:251:ASN:OD1	1:B:252:LYS:O	2.34	0.46
1:A:314:ASP:CG	1:A:317:LYS:HD2	2.39	0.46
1:A:118:ALA:O	1:A:120:PHE:N	2.46	0.46
1:B:110:ASP:N	1:B:112:GLU:CB	2.71	0.46
1:A:174:GLU:HB3	1:A:176:LYS:HG3	1.98	0.46
1:A:254:MET:CE	1:A:270:PRO:HB3	2.42	0.46
1:B:245:TYR:CD1	1:B:245:TYR:N	2.83	0.46
1:B:254:MET:CE	1:B:270:PRO:HB3	2.42	0.46
1:B:283:THR:CG2	1:B:284:LEU:N	2.78	0.46
1:B:34:ASP:O	1:B:126:LEU:N	2.46	0.46
1:B:76:THR:HG23	1:B:81:THR:OG1	2.16	0.46
1:A:114:LEU:O	1:A:117:ALA:N	2.49	0.46
1:B:182:LEU:HD12	1:B:182:LEU:H	1.81	0.46
1:B:182:LEU:HA	1:B:323:ALA:HB2	1.98	0.46
1:A:76:THR:HG23	1:A:81:THR:OG1	2.16	0.45
1:B:150:ASP:HB3	1:B:151:GLN:HE22	1.80	0.45
1:A:251:ASN:OD1	1:A:252:LYS:O	2.34	0.45
1:B:313:PHE:CE1	1:B:320:ILE:HD12	2.52	0.45
1:B:118:ALA:O	1:B:120:PHE:N	2.46	0.45
1:B:277:LEU:HB3	1:B:278:LEU:CB	2.47	0.45
1:A:17:TYR:CD1	1:A:30:MET:HG2	2.52	0.45
1:A:185:GLU:OE1	1:A:261:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LYS:HE3	1:A:265:THR:HB	1.99	0.45
1:A:313:PHE:CE1	1:A:320:ILE:HD12	2.52	0.45
1:A:34:ASP:O	1:A:126:LEU:N	2.46	0.45
1:B:114:LEU:O	1:B:117:ALA:N	2.49	0.45
1:B:79:SER:HB2	2:B:3152:JE2:C29	2.47	0.45
1:B:8:LEU:HB2	1:B:166:GLY:HA3	1.99	0.45
1:B:17:TYR:CD1	1:B:30:MET:HG2	2.52	0.45
1:B:62:LYS:N	1:B:62:LYS:CD	2.80	0.45
1:B:230:PHE:O	1:B:231:PHE:C	2.59	0.45
1:A:79:SER:HB2	2:A:3151:JE2:C29	2.47	0.45
1:A:182:LEU:HD12	1:A:182:LEU:H	1.81	0.45
1:A:182:LEU:HA	1:A:323:ALA:HB2	1.98	0.45
1:B:174:GLU:HB3	1:B:176:LYS:HG3	1.98	0.45
1:A:114:LEU:O	1:A:115:TYR:C	2.60	0.45
1:B:254:MET:HA	1:B:255:PRO:HD2	1.84	0.45
1:B:16:PHE:HE2	1:B:158:LEU:HD11	1.83	0.44
1:B:200:ASN:OD1	1:B:205:SER:OG	2.29	0.44
1:B:260:LYS:HE3	1:B:265:THR:HB	1.99	0.44
1:A:8:LEU:HB2	1:A:166:GLY:HA3	1.99	0.44
1:A:61:SER:O	1:A:63:SER:O	2.36	0.44
1:A:215:SER:HB3	1:A:306:MET:HE1	1.97	0.44
1:B:44:SER:CB	1:B:104:GLU:HG2	2.37	0.44
1:B:199:VAL:HG22	1:B:259:PHE:CD1	2.53	0.44
1:B:232:LYS:HE2	1:B:232:LYS:C	2.42	0.44
1:A:89:ASP:CG	1:A:90:LEU:N	2.73	0.44
1:A:174:GLU:HB3	1:A:176:LYS:CG	2.47	0.44
1:A:184:TYR:HB3	1:B:207:GLU:OE2	2.18	0.44
1:A:268:LEU:HA	1:A:268:LEU:HD12	1.68	0.44
1:B:61:SER:O	1:B:63:SER:O	2.36	0.44
1:B:145:ASN:C	1:B:147:ASN:H	2.25	0.44
1:B:185:GLU:OE1	1:B:261:SER:HB2	2.17	0.44
1:A:175:GLU:O	1:A:177:PHE:N	2.51	0.44
1:B:4:ASP:OD1	1:B:93:LEU:O	2.36	0.44
1:A:144:LYS:HA	1:A:144:LYS:HD2	1.83	0.44
1:A:184:TYR:CD2	1:B:207:GLU:OE2	2.71	0.44
1:B:174:GLU:HB3	1:B:176:LYS:CG	2.47	0.44
1:A:16:PHE:CE2	1:A:158:LEU:HD11	2.53	0.44
1:A:97:SER:O	1:A:98:LEU:CB	2.64	0.44
1:A:181:GLU:OE1	1:B:200:ASN:CB	2.57	0.44
1:B:114:LEU:O	1:B:115:TYR:C	2.60	0.44
1:A:277:LEU:HB3	1:A:278:LEU:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HD2	1:A:115:TYR:CE1	2.53	0.43
1:A:4:ASP:OD1	1:A:93:LEU:O	2.36	0.43
1:A:154:PHE:CE2	1:A:313:PHE:CG	3.07	0.43
1:B:47:CYS:O	1:B:48:ASN:OD1	2.37	0.43
1:B:175:GLU:O	1:B:177:PHE:N	2.51	0.43
1:B:199:VAL:O	1:B:199:VAL:HG12	2.19	0.43
1:B:204:THR:HG21	1:B:230:PHE:HB2	2.00	0.43
1:A:142:GLU:O	1:A:146:GLN:HG3	2.19	0.43
1:B:239:VAL:O	1:B:240:PRO:C	2.62	0.43
1:A:16:PHE:HE2	1:A:158:LEU:HD11	1.83	0.43
1:A:43:PRO:HG2	1:A:56:HIS:O	2.18	0.43
1:A:155:THR:HG1	1:A:169:THR:HB	1.83	0.43
1:A:199:VAL:HG22	1:A:259:PHE:CD1	2.53	0.43
1:B:49:SER:O	1:B:50:ILE:C	2.61	0.43
1:B:178:TYR:CZ	1:B:182:LEU:HD11	2.54	0.43
1:B:55:LYS:HD2	1:B:115:TYR:CE1	2.53	0.43
1:B:256:THR:HG1	1:B:268:LEU:C	2.27	0.43
1:A:178:TYR:CZ	1:A:182:LEU:HD11	2.54	0.43
1:A:232:LYS:HE2	1:A:232:LYS:C	2.42	0.43
1:A:90:LEU:HD12	1:A:98:LEU:C	2.43	0.43
1:A:145:ASN:C	1:A:147:ASN:H	2.25	0.43
1:A:204:THR:HG21	1:A:230:PHE:HB2	2.01	0.43
1:B:161:HIS:CD2	1:B:162:ASP:N	2.87	0.43
1:B:242:LEU:HD12	1:B:242:LEU:O	2.19	0.43
1:A:49:SER:O	1:A:50:ILE:C	2.61	0.43
1:B:16:PHE:CE2	1:B:158:LEU:HD11	2.53	0.43
1:B:43:PRO:HG2	1:B:56:HIS:O	2.18	0.43
1:B:77:TYR:CD2	2:B:3152:JE2:HC83	2.54	0.43
1:A:62:LYS:N	1:A:62:LYS:CD	2.80	0.42
1:B:142:GLU:O	1:B:146:GLN:HG3	2.19	0.42
1:A:249:CYS:O	1:A:254:MET:SD	2.77	0.42
1:B:249:CYS:O	1:B:254:MET:SD	2.77	0.42
1:A:161:HIS:CD2	1:A:162:ASP:N	2.87	0.42
1:A:230:PHE:O	1:A:231:PHE:C	2.59	0.42
1:A:303:ASP:N	1:A:304:PRO:CD	2.83	0.42
1:B:154:PHE:CE2	1:B:313:PHE:CG	3.07	0.42
1:B:274:MET:HG2	1:B:287:LEU:HD23	2.01	0.42
1:B:316:ASP:C	1:B:318:GLU:H	2.27	0.42
1:A:50:ILE:O	1:A:53:SER:CB	2.68	0.42
1:A:84:GLY:C	1:A:85:PHE:HD1	2.27	0.42
1:A:159:PRO:C	1:A:160:VAL:HG23	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LEU:HD12	1:B:191:LEU:HA	1.80	0.42
1:A:242:LEU:HD12	1:A:242:LEU:O	2.19	0.42
1:B:84:GLY:C	1:B:85:PHE:HD1	2.28	0.42
1:A:47:CYS:O	1:A:48:ASN:OD1	2.37	0.42
1:A:77:TYR:CD2	2:A:3151:JE2:HC83	2.54	0.42
1:A:256:THR:HG1	1:A:268:LEU:C	2.27	0.42
1:A:99:PRO:O	1:A:99:PRO:HG2	2.20	0.42
1:A:184:TYR:CD2	1:B:207:GLU:CD	2.97	0.42
1:B:97:SER:O	1:B:98:LEU:CB	2.64	0.42
1:B:139:ILE:O	1:B:142:GLU:N	2.41	0.42
1:A:316:ASP:C	1:A:318:GLU:H	2.27	0.42
1:B:42:VAL:HG23	1:B:42:VAL:O	2.19	0.42
1:B:93:LEU:HD22	1:B:93:LEU:HA	1.77	0.42
1:B:99:PRO:O	1:B:99:PRO:HG2	2.20	0.42
1:A:153:LEU:HB3	1:A:314:ASP:HA	2.01	0.42
1:A:199:VAL:O	1:A:199:VAL:HG12	2.19	0.42
1:B:51:GLY:HA2	1:B:116:THR:HG22	2.02	0.42
1:B:138:PRO:HG2	1:B:141:VAL:HB	2.02	0.42
1:A:42:VAL:O	1:A:42:VAL:HG23	2.19	0.41
1:B:29:PHE:HE1	1:B:56:HIS:O	2.03	0.41
1:B:50:ILE:O	1:B:53:SER:CB	2.68	0.41
1:B:111:LEU:HD12	1:B:111:LEU:HA	1.90	0.41
1:B:153:LEU:HB3	1:B:314:ASP:HA	2.01	0.41
1:A:227:ILE:HD12	1:A:291:PRO:CB	2.50	0.41
1:A:239:VAL:O	1:A:240:PRO:C	2.61	0.41
1:B:239:VAL:HB	1:B:242:LEU:CG	2.50	0.41
1:B:303:ASP:N	1:B:304:PRO:CD	2.83	0.41
1:A:138:PRO:HG2	1:A:141:VAL:HB	2.02	0.41
1:A:191:LEU:HD12	1:A:191:LEU:HA	1.79	0.41
1:B:250:ASN:O	1:B:252:LYS:N	2.54	0.41
1:B:227:ILE:HD12	1:B:291:PRO:CB	2.50	0.41
1:A:210:ASN:O	1:A:298:THR:HA	2.20	0.41
1:B:90:LEU:HD12	1:B:98:LEU:C	2.43	0.41
1:B:254:MET:HE2	1:B:254:MET:HB3	1.62	0.41
1:A:29:PHE:HE1	1:A:56:HIS:O	2.04	0.41
1:A:43:PRO:HB2	1:A:57:LEU:HD23	2.03	0.41
1:A:51:GLY:HA2	1:A:116:THR:HG22	2.02	0.41
1:A:250:ASN:O	1:A:252:LYS:N	2.53	0.41
1:B:113:PRO:HD2	1:B:114:LEU:CD2	2.46	0.41
1:B:210:ASN:O	1:B:298:THR:HA	2.20	0.41
1:A:239:VAL:HB	1:A:242:LEU:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:MET:HG2	1:A:287:LEU:HD23	2.01	0.41
1:A:283:THR:CG2	1:A:284:LEU:H	2.34	0.41
1:A:289:ILE:O	1:A:290:LEU:HD23	2.20	0.41
1:A:321:GLY:C	1:A:322:PHE:CD1	2.99	0.41
1:A:98:LEU:HD12	1:A:143:LEU:CD2	2.51	0.41
1:A:217:THR:HG22	1:A:219:THR:N	2.36	0.41
1:B:20:GLY:O	1:B:29:PHE:N	2.54	0.41
1:B:45:LYS:HD2	1:B:59:ASP:CB	2.34	0.41
1:B:98:LEU:HD12	1:B:143:LEU:CD2	2.51	0.41
1:B:137:ASP:HA	1:B:138:PRO:HD2	1.90	0.41
1:B:144:LYS:HA	1:B:144:LYS:HD2	1.83	0.41
1:B:302:GLY:C	1:B:304:PRO:CD	2.93	0.41
1:B:316:ASP:C	1:B:318:GLU:N	2.78	0.41
1:B:321:GLY:C	1:B:322:PHE:CD1	2.99	0.41
1:A:237:ILE:HD12	1:A:246:ILE:HD11	2.03	0.41
1:A:303:ASP:N	1:A:303:ASP:OD1	2.47	0.41
1:B:268:LEU:HA	1:B:268:LEU:HD12	1.68	0.41
1:A:231:PHE:O	1:A:234:LEU:HD23	2.21	0.40
1:B:231:PHE:O	1:B:234:LEU:HD23	2.21	0.40
1:A:20:GLY:O	1:A:29:PHE:N	2.54	0.40
1:A:22:VAL:HG23	1:A:58:TYR:HE2	1.86	0.40
1:B:43:PRO:HB2	1:B:57:LEU:HD23	2.03	0.40
1:B:84:GLY:C	1:B:85:PHE:CD1	3.00	0.40
1:B:155:THR:HB	1:B:310:PHE:CZ	2.56	0.40
1:B:22:VAL:HG23	1:B:58:TYR:HE2	1.86	0.40
1:B:99:PRO:O	1:B:99:PRO:CG	2.69	0.40
1:A:153:LEU:CB	1:A:313:PHE:O	2.67	0.40
1:A:175:GLU:OE1	1:B:203:LYS:HB3	2.21	0.40
1:B:217:THR:CG2	1:B:219:THR:HG23	2.49	0.40
1:B:257:LEU:O	1:B:267:THR:HA	2.22	0.40
1:A:43:PRO:HA	1:A:105:VAL:HB	2.03	0.40
1:A:155:THR:HB	1:A:310:PHE:CZ	2.56	0.40
1:A:217:THR:CG2	1:A:219:THR:HG23	2.49	0.40
1:A:302:GLY:C	1:A:304:PRO:CD	2.93	0.40
1:B:40:LEU:HA	1:B:123:ILE:O	2.22	0.40
1:B:196:ASP:O	1:B:197:LEU:HD23	2.22	0.40
1:B:289:ILE:O	1:B:290:LEU:HD23	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:N	1:B:279:ASP:CB[3_645]	1.93	0.27

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	325/327 (99%)	240 (74%)	57 (18%)	28 (9%)	0	4
1	B	325/327 (99%)	240 (74%)	57 (18%)	28 (9%)	0	4
All	All	650/654 (99%)	480 (74%)	114 (18%)	56 (9%)	0	4

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	113	PRO
1	A	114	LEU
1	A	159	PRO
1	A	160	VAL
1	A	240	PRO
1	A	276	PRO
1	A	278	LEU
1	B	13	ASN
1	B	113	PRO
1	B	114	LEU
1	B	159	PRO
1	B	160	VAL
1	B	240	PRO
1	B	276	PRO
1	B	278	LEU
1	A	50	ILE
1	A	109	ASP
1	A	110	ASP
1	A	115	TYR

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Mol	Chain	Res	Type
1	A	162	ASP
1	A	176	LYS
1	A	251	ASN
1	A	253	ASP
1	B	50	ILE
1	B	109	ASP
1	B	110	ASP
1	B	115	TYR
1	B	162	ASP
1	B	176	LYS
1	B	251	ASN
1	B	253	ASP
1	A	2	GLU
1	A	3	ASN
1	A	32	ILE
1	A	66	TYR
1	A	98	LEU
1	A	135	SER
1	A	250	ASN
1	B	2	GLU
1	B	3	ASN
1	B	32	ILE
1	B	66	TYR
1	B	98	LEU
1	B	135	SER
1	B	250	ASN
1	A	12	ALA
1	A	65	SER
1	B	12	ALA
1	B	65	SER
1	A	119	GLU
1	B	119	GLU
1	A	228	ASN
1	B	228	ASN
1	A	139	ILE
1	B	139	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	295/295 (100%)	242 (82%)	53 (18%)	2	8
1	B	295/295 (100%)	241 (82%)	54 (18%)	2	7
All	All	590/590 (100%)	483 (82%)	107 (18%)	2	8

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	11	VAL
1	A	21	GLU
1	A	22	VAL
1	A	24	ASP
1	A	55	LYS
1	A	59	ASP
1	A	60	SER
1	A	62	LYS
1	A	71	THR
1	A	72	LYS
1	A	73	VAL
1	A	74	GLU
1	A	81	THR
1	A	92	THR
1	A	93	LEU
1	A	108	THR
1	A	114	LEU
1	A	119	GLU
1	A	124	LEU
1	A	137	ASP
1	A	139	ILE
1	A	147	ASN
1	A	151	GLN
1	A	160	VAL
1	A	165	SER
1	A	176	LYS
1	A	183	THR
1	A	194	GLN
1	A	199	VAL
1	A	203	LYS
1	A	205	SER
1	A	206	MET

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Mol	Chain	Res	Type
1	A	212	ILE
1	A	219	THR
1	A	224	THR
1	A	232	LYS
1	A	235	ASN
1	A	237	ILE
1	A	246	ILE
1	A	250	ASN
1	A	252	LYS
1	A	253	ASP
1	A	254	MET
1	A	269	GLU
1	A	277	LEU
1	A	278	LEU
1	A	280	ILE
1	A	281	ASP
1	A	303	ASP
1	A	306	MET
1	A	319	SER
1	A	320	ILE
1	B	10	ASP
1	B	11	VAL
1	B	21	GLU
1	B	22	VAL
1	B	24	ASP
1	B	55	LYS
1	B	59	ASP
1	B	60	SER
1	B	62	LYS
1	B	71	THR
1	B	72	LYS
1	B	73	VAL
1	B	74	GLU
1	B	81	THR
1	B	92	THR
1	B	93	LEU
1	B	108	THR
1	B	114	LEU
1	B	119	GLU
1	B	124	LEU
1	B	137	ASP
1	B	139	ILE

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Mol	Chain	Res	Type
1	B	147	ASN
1	B	151	GLN
1	B	160	VAL
1	B	162	ASP
1	B	165	SER
1	B	176	LYS
1	B	183	THR
1	B	194	GLN
1	B	199	VAL
1	B	203	LYS
1	B	205	SER
1	B	206	MET
1	B	212	ILE
1	B	219	THR
1	B	224	THR
1	B	232	LYS
1	B	235	ASN
1	B	237	ILE
1	B	246	ILE
1	B	250	ASN
1	B	252	LYS
1	B	253	ASP
1	B	254	MET
1	B	269	GLU
1	B	277	LEU
1	B	278	LEU
1	B	280	ILE
1	B	281	ASP
1	B	303	ASP
1	B	306	MET
1	B	319	SER
1	B	320	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	151	GLN
1	A	161	HIS
1	A	194	GLN
1	A	210	ASN
1	A	250	ASN

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Mol	Chain	Res	Type
1	B	13	ASN
1	B	151	GLN
1	B	164	HIS
1	B	194	GLN
1	B	200	ASN
1	B	210	ASN
1	B	250	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	JE2	A	3151	-	44,44,44	1.83	7 (15%)	55,63,63	2.01	13 (23%)
2	JE2	B	3152	-	44,44,44	1.83	7 (15%)	55,63,63	2.00	13 (23%)

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
2	JE2	A	3151	-	-	2/33/49/49	0/4/4/4
2	JE2	B	3152	-	-	2/33/49/49	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3151	JE2	C27-S26	-6.46	1.72	1.85
2	B	3152	JE2	C27-S26	-6.43	1.72	1.85
2	B	3152	JE2	C20-C22	-4.99	1.48	1.53
2	A	3151	JE2	C20-C22	-4.95	1.48	1.53
2	A	3151	JE2	O10-C9	4.25	1.33	1.23
2	B	3152	JE2	O10-C9	4.25	1.33	1.23
2	A	3151	JE2	C25-S26	-3.45	1.75	1.83
2	B	3152	JE2	C25-S26	-3.43	1.75	1.83
2	B	3152	JE2	C9-N11	-3.32	1.26	1.34
2	A	3151	JE2	C9-N11	-3.32	1.26	1.34
2	A	3151	JE2	C6-C7	-3.20	1.36	1.40
2	B	3152	JE2	C6-C7	-3.19	1.36	1.40
2	B	3152	JE2	C30-N24	2.06	1.48	1.46
2	A	3151	JE2	C30-N24	2.03	1.48	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3152	JE2	C29-C27-S26	-5.21	100.79	109.19
2	A	3151	JE2	C29-C27-S26	-5.20	100.81	109.19
2	A	3151	JE2	C13-C12-N11	-4.82	103.23	110.08
2	B	3152	JE2	C5-C6-C7	-4.80	117.31	120.74
2	B	3152	JE2	C13-C12-N11	-4.79	103.27	110.08
2	A	3151	JE2	C5-C6-C7	-4.76	117.34	120.74
2	B	3152	JE2	C6-C7-C1	4.26	121.23	116.88
2	A	3151	JE2	C6-C7-C1	4.26	121.22	116.88
2	B	3152	JE2	C29-C27-C30	3.97	120.17	111.61
2	A	3151	JE2	C29-C27-C30	3.96	120.15	111.61
2	B	3152	JE2	C27-C30-C31	-3.31	106.89	113.29
2	A	3151	JE2	C27-C30-C31	-3.30	106.91	113.29
2	B	3152	JE2	C8-C7-C6	-3.08	117.70	122.29
2	A	3151	JE2	C8-C7-C6	-3.07	117.70	122.29
2	A	3151	JE2	C14-C13-C12	-3.04	108.25	113.40
2	A	3151	JE2	O2-C1-C7	3.03	124.24	116.83
2	B	3152	JE2	C14-C13-C12	-3.03	108.26	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3152	JE2	O2-C1-C7	3.03	124.23	116.83
2	A	3151	JE2	C29-C27-C28	2.31	114.46	110.70
2	B	3152	JE2	C29-C27-C28	2.30	114.44	110.70
2	A	3151	JE2	C37-C36-C35	2.30	121.51	118.59
2	B	3152	JE2	C37-C36-C35	2.27	121.48	118.59
2	A	3151	JE2	C35-C34-N33	-2.26	108.59	113.15
2	B	3152	JE2	C35-C34-N33	-2.24	108.62	113.15
2	B	3152	JE2	O10-C9-N11	-2.24	118.21	122.47
2	A	3151	JE2	O10-C9-N11	-2.22	118.24	122.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

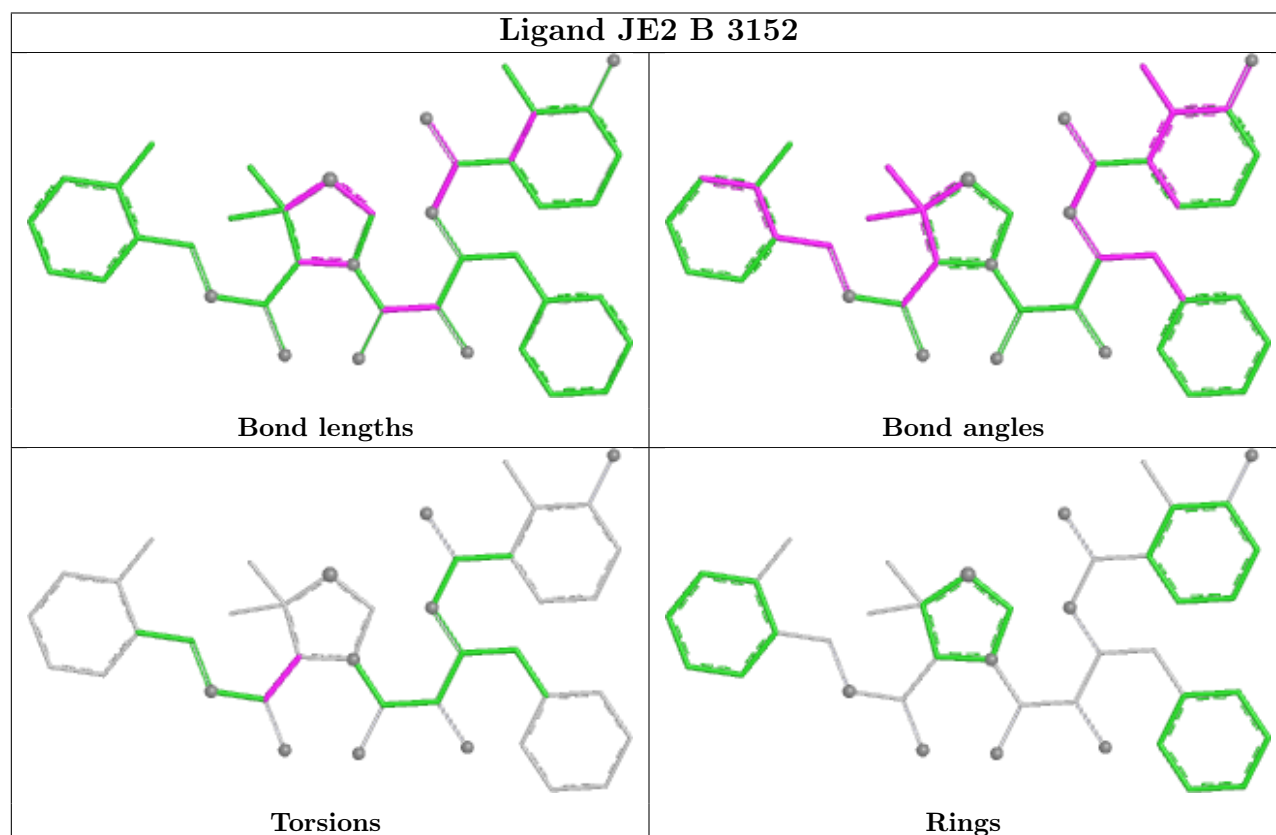
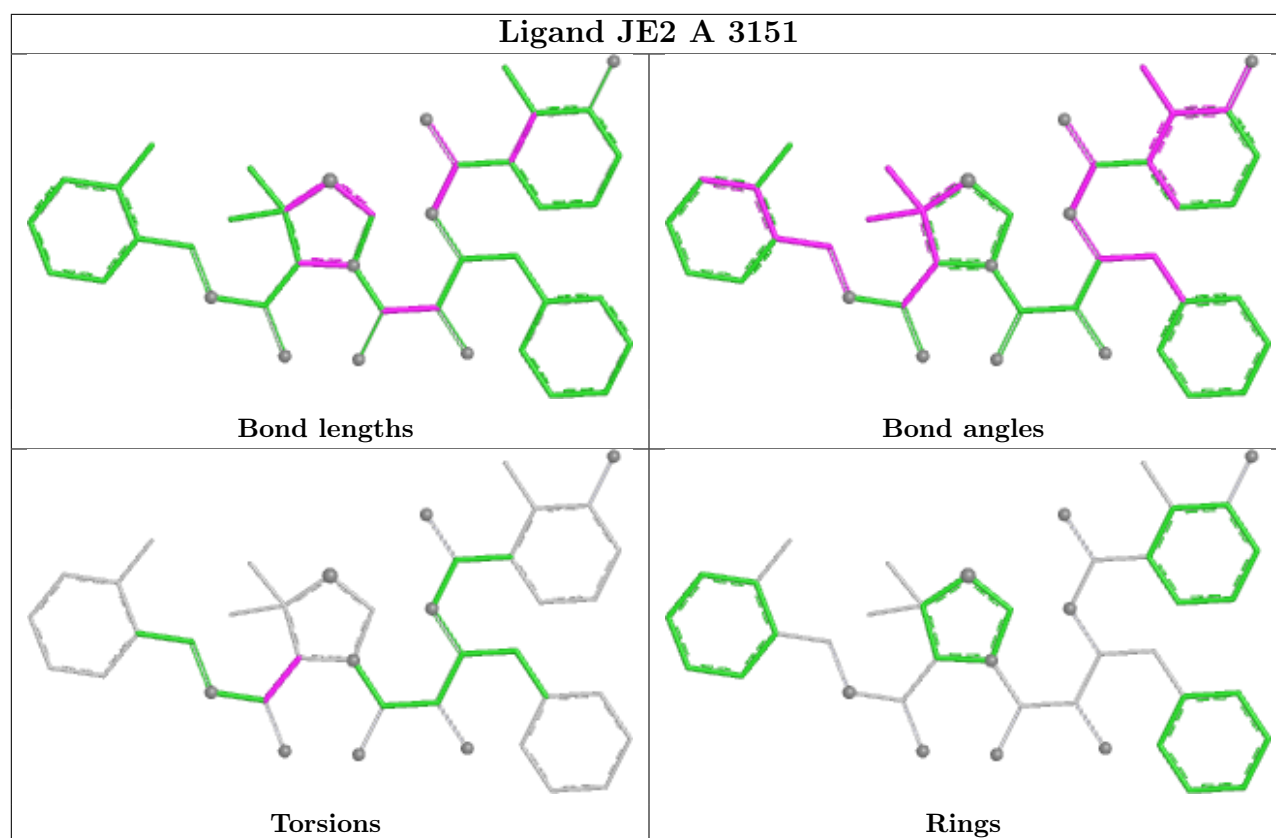
Mol	Chain	Res	Type	Atoms
2	A	3151	JE2	N24-C30-C31-N33
2	B	3152	JE2	N24-C30-C31-N33
2	A	3151	JE2	N24-C30-C31-O32
2	B	3152	JE2	N24-C30-C31-O32

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3151	JE2	7	0
2	B	3152	JE2	8	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	327/327 (100%)	-1.62	0 100 100	24, 55, 57, 58	0
1	B	327/327 (100%)	-1.60	0 100 100	24, 55, 57, 58	0
All	All	654/654 (100%)	-1.61	0 100 100	24, 55, 57, 58	0

There are no RSRZ outliers to report.

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](#)

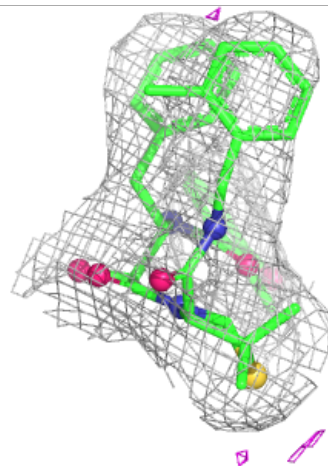
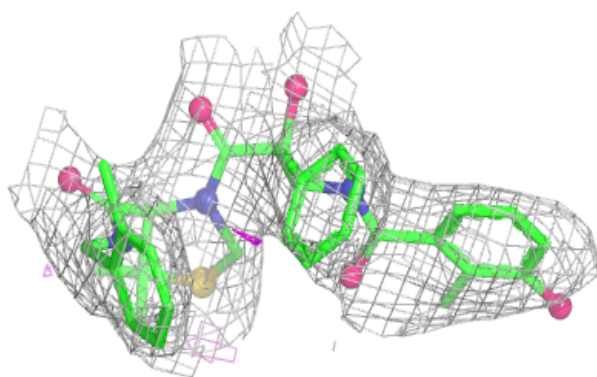
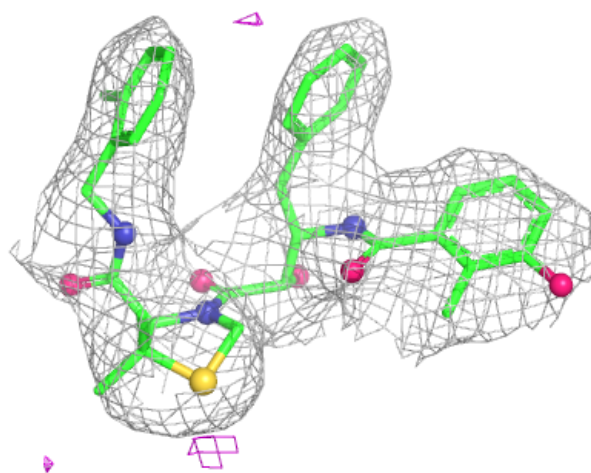
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	JE2	A	3151	41/41	0.99	0.04	44,52,56,57	0
2	JE2	B	3152	41/41	0.99	0.05	44,52,56,57	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.

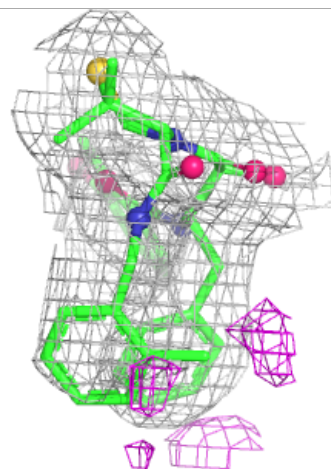
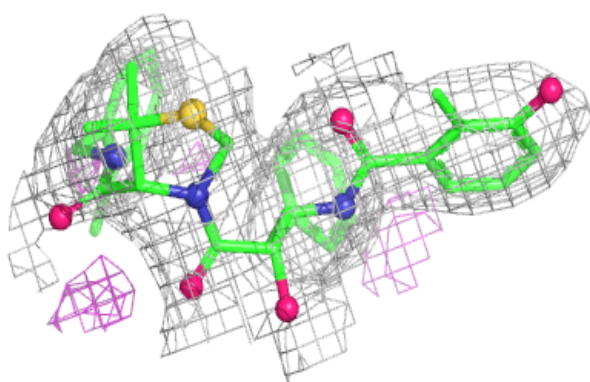
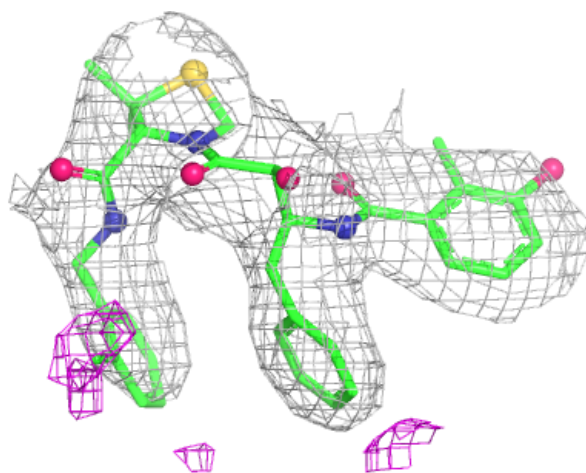
Electron density around JE2 A 3151:

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



Electron density around JE2 B 3152:

$2mF_o-DF_c$ (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.