



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:27 PM UTC

PDB ID : 6MQ3 / pdb_00006mq3
Title : Structure of Cysteine-free Human Insulin-Degrading Enzyme in complex with Substrate-selective Macrocyclic Inhibitor 63
Authors : Tan, G.A.; Seeliger, M.A.; Welsh, A.J.; Maianti, J.P.; Liu, D.R.
Deposited on : 2018-10-09
Resolution : 3.57 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

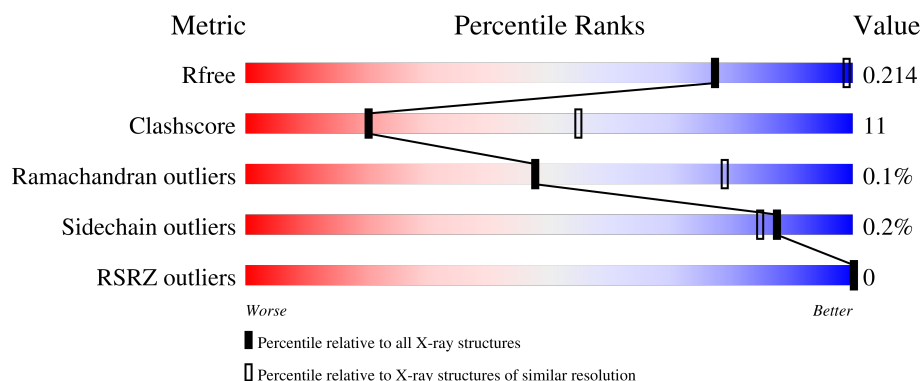
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	978	 75% 23% .
1	B	978	 72% 26% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15798 atoms, of which 102 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	959	Total	C	N	O	S	0	0	0
			7798	5021	1310	1445	22			
1	B	959	Total	C	N	O	S	0	0	0
			7798	5021	1310	1445	22			

There are 28 discrepancies between the modelled and reference sequences:

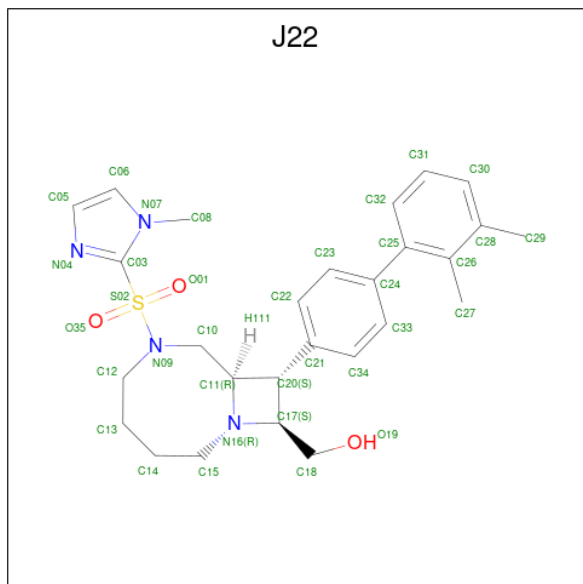
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is {(8R,9S,10S)-9-(2',3'-dimethyl[1,1'-biphenyl]-4-yl)-6-[(1-methyl-1H-imidazol-2-yl)sulfonyl]-1,6-diazabicyclo[6.2.0]decan-10-yl}methanol (CCD ID: J22) (formula: C₂₇H₃₄N₄O₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			69	27	34	4	3	1		
2	B	1	Total	C	H	N	O	S	0	0
			69	27	34	4	3	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



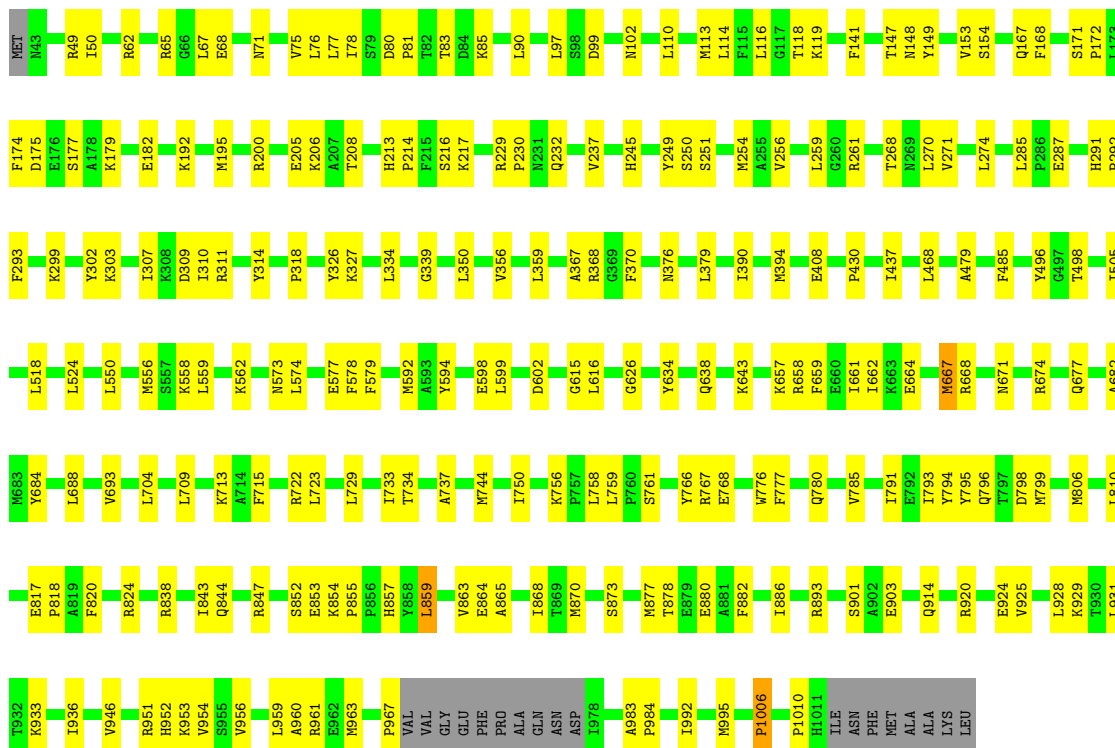
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
3	A	1	32	8	17	2	4	1	0	0
3	B	1	32	8	17	2	4	1	0	0

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.

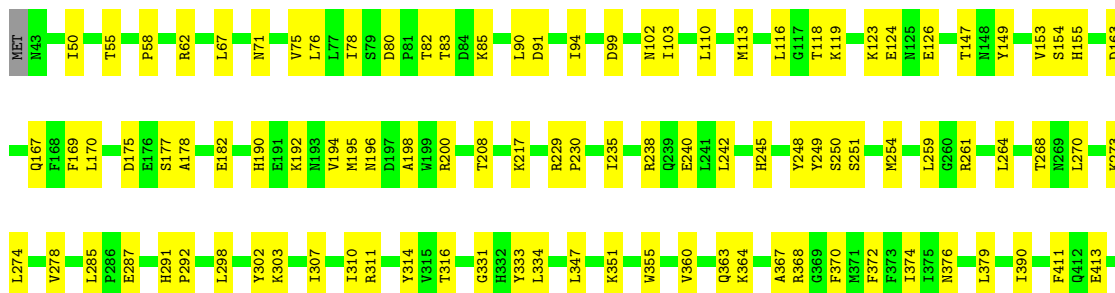
- Molecule 1: Insulin-degrading enzyme

Chain A: 



- Molecule 1: Insulin-degrading enzyme

Chain B: 



R950	R951	R952	K953	V954	L959	A960	R961	P967	VAL	VAL	GLY	GLU	PHE	PRO	ALA	GLN	ASN	ASP	1978	P984	1992	M995	P1006	P1010	H1011	ILE	ASN	PHE	MET	ALA	ALA	LYS	LEU										
I846	R847	S852	E853	K854		P855	F856	H857	Y858	L859	V863	E864	I868	T869	M870	S873	I874	M877	E880	A881	F882	R892	R893	L894	S901	A902	E903	Q914	Q915	Y916	R920	E924	V925	A926	Y927	L928	L931	T932	K933	I936	E942	M943	V946
L719		R722	L723	L729	I733	A737	M744	I750	L758	Y766	W776	F777	Q780	V785	H786	N787	E792	I793	Y794	Y795	Q796	D798	T799	M799	N805	L810	Q813	I814	E817	P818	A819	F820	L823	R824	I832	V833	R838	I843	Q844	G845			
P587	L588	Y594	E598	L599	L600	L616	Q638	K643	K648	F652	K657	R658	F659	E660	I661	I662	K663	E664	M667	R668	N671	R674	A675	E676	Q677	P678	H679	M683	L688	V693	E699	L700	L704	V707	T708	L709	K713	A714	F715				
D416	L417	V420	R423	F424	K425	E428	Y433	I437	E457	E458	F459	I464	L468	N475	F485	T498	L518	I531	L540	P548	A549	L550	I551	K552	M556	S557	K558	L559	K562	Q563	D564	D565	K566	N573	L574	E577	F578	F579	S580	P581			

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	263.25Å 263.25Å 91.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.81 – 3.57 65.81 – 3.57	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.81-3.57) 93.3 (65.81-3.57)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.162 , 0.211 0.165 , 0.214	Depositor DCC
R_{free} test set	2066 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15798	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, J22

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	0.09	0/7994	0.28	0/10824
1	B	0.09	0/7994	0.27	0/10824
All	All	0.09	0/15988	0.28	0/21648

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7798	0	7684	171	2
1	B	7798	0	7684	187	1
2	A	35	34	0	1	0
2	B	35	34	0	0	0
3	A	15	17	17	0	0
3	B	15	17	17	0	0
All	All	15696	102	15402	352	2

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 11.

All (352) 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:B:118:THR:HG21	1:B:167:GLN:HB3	1.21	1.19
1:B:777:PHE:HB3	1:B:992:ILE:HD11	1.34	1.08
1:A:118:THR:HG21	1:A:167:GLN:HB3	1.22	1.08
1:A:880:GLU:HG3	1:B:457:GLU:HG3	1.10	1.06
1:A:777:PHE:HB3	1:A:992:ILE:HD11	1.33	1.03
1:A:880:GLU:HG3	1:B:457:GLU:CG	1.99	0.91
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.53	0.90
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.55	0.87
1:A:114:LEU:HD12	1:A:168:PHE:HB3	1.57	0.85
1:A:67:LEU:HD11	1:A:268:THR:HG23	1.59	0.84
1:A:777:PHE:HB3	1:A:992:ILE:CD1	2.06	0.84
1:B:67:LEU:HD11	1:B:268:THR:HG23	1.58	0.83
1:A:118:THR:HG21	1:A:167:GLN:CB	2.10	0.81
1:A:880:GLU:CG	1:B:457:GLU:HG3	2.02	0.81
1:B:118:THR:HG21	1:B:167:GLN:CB	2.06	0.81
1:A:311:ARG:NH1	1:A:379:LEU:O	2.12	0.80
1:B:76:LEU:HD23	1:B:437:ILE:HG21	1.65	0.79
1:B:777:PHE:HB3	1:B:992:ILE:CD1	2.11	0.79
1:B:311:ARG:NH1	1:B:379:LEU:O	2.16	0.78
1:B:562:LYS:NZ	1:B:903:GLU:OE2	2.17	0.77
1:A:195:MET:HG3	1:A:307:ILE:HD13	1.66	0.76
1:A:78:ILE:HB	1:A:259:LEU:HD23	1.68	0.76
1:B:78:ILE:HB	1:B:259:LEU:HD23	1.68	0.74
1:A:870:MET:HE2	1:A:870:MET:HA	1.68	0.74
1:B:99:ASP:O	1:B:217:LYS:NZ	2.18	0.73
1:B:880:GLU:N	1:B:880:GLU:OE1	2.21	0.73
1:A:113:MET:HE2	1:A:116:LEU:HD12	1.69	0.72
1:B:870:MET:HA	1:B:870:MET:HE2	1.71	0.72
1:A:817:GLU:HB3	1:A:818:PRO:HD3	1.72	0.71
1:B:810:LEU:HD23	1:B:936:ILE:HD11	1.71	0.71
1:B:688:LEU:HB3	1:B:995:MET:HE1	1.71	0.71
1:B:817:GLU:HB3	1:B:818:PRO:HD3	1.73	0.69
1:A:574:LEU:HD22	1:A:729:LEU:HD22	1.73	0.69
1:B:238:ARG:O	1:B:242:LEU:HD13	1.93	0.69
1:B:80:ASP:O	1:B:83:THR:HG22	1.94	0.67
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.76	0.67
1:B:195:MET:HG3	1:B:307:ILE:HD13	1.77	0.67
1:A:859:LEU:O	1:A:863:VAL:HG12	1.95	0.67
1:A:78:ILE:CG2	1:A:259:LEU:HD23	2.24	0.66
1:A:110:LEU:O	1:A:114:LEU:HD23	1.95	0.66
1:A:80:ASP:O	1:A:83:THR:HG22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:CG2	1:B:259:LEU:HD23	2.26	0.65
1:A:75:VAL:HG11	1:A:271:VAL:HG11	1.78	0.65
1:A:688:LEU:HB3	1:A:995:MET:HE1	1.79	0.65
1:A:119:LYS:HB2	1:A:171:SER:HB2	1.79	0.65
1:B:857:HIS:CD2	1:B:967:PRO:HD2	2.32	0.65
1:B:364:LYS:HE2	1:B:372:PHE:HB2	1.77	0.65
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.79	0.64
1:A:709:LEU:HD21	1:A:713:LYS:HE3	1.78	0.64
1:A:865:ALA:HB2	1:A:983:ALA:HA	1.80	0.63
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.80	0.63
1:B:540:LEU:HD12	1:B:563:GLN:CD	2.24	0.63
1:B:643:LYS:HA	1:B:744:MET:HE3	1.78	0.63
1:A:334:LEU:HD22	1:A:468:LEU:HD13	1.81	0.63
1:A:795:TYR:OH	1:A:864:GLU:OE2	2.16	0.62
1:A:192:LYS:HG3	1:A:677:GLN:OE1	2.00	0.62
1:A:78:ILE:CB	1:A:259:LEU:HD23	2.29	0.62
1:B:793:ILE:O	1:B:847:ARG:HA	2.00	0.62
1:B:793:ILE:HD12	1:B:863:VAL:HG11	1.82	0.61
1:B:813:GLN:OE1	1:B:892:ARG:NH1	2.33	0.61
1:B:113:MET:HE2	1:B:116:LEU:HD12	1.82	0.61
1:A:793:ILE:HD12	1:A:863:VAL:HG11	1.82	0.61
1:A:599:LEU:CD2	1:A:662:ILE:HD12	2.29	0.61
1:B:355:TRP:HB3	1:B:390:ILE:HD11	1.83	0.61
1:B:78:ILE:CB	1:B:259:LEU:HD23	2.30	0.60
1:A:878:THR:OG1	1:A:880:GLU:HG2	2.01	0.60
1:B:798:ASP:OD1	1:B:799:MET:N	2.32	0.60
1:A:71:ASN:HB2	1:A:251:SER:OG	2.01	0.60
1:B:118:THR:CG2	1:B:167:GLN:HB3	2.14	0.59
1:B:113:MET:HE3	1:B:182:GLU:HB3	1.84	0.59
1:B:857:HIS:NE2	1:B:967:PRO:HD2	2.18	0.59
1:A:77:LEU:HD21	1:A:271:VAL:HG21	1.84	0.58
1:B:797:THR:HG23	1:B:845:GLY:HA2	1.85	0.58
1:A:113:MET:CE	1:A:116:LEU:HD12	2.34	0.58
1:B:364:LYS:HD3	1:B:374:ILE:HG13	1.85	0.58
1:B:914:GLN:O	1:B:1010:PRO:HB3	2.03	0.58
1:B:733:ILE:HG13	1:B:737:ALA:HB3	1.85	0.58
1:B:287:GLU:HG2	1:B:368:ARG:HD2	1.84	0.57
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.36	0.57
1:B:683:MET:HA	1:B:792:GLU:OE1	2.04	0.57
1:B:83:THR:OG1	1:B:85:LYS:O	2.23	0.57
1:A:49:ARG:NE	1:A:68:GLU:OE1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LYS:HG3	1:B:677:GLN:OE1	2.04	0.57
1:B:946:VAL:HA	1:B:951:ARG:CZ	2.35	0.57
1:A:933:LYS:NZ	1:B:55:THR:HG22	2.20	0.56
1:A:270:LEU:HD12	1:A:274:LEU:HD13	1.86	0.56
1:B:577:GLU:HG2	1:B:579:PHE:CZ	2.40	0.56
1:A:682:ALA:HA	1:A:956:VAL:HG11	1.87	0.56
1:A:722:ARG:HA	1:A:756:LYS:O	2.05	0.56
1:A:857:HIS:CD2	1:A:967:PRO:HD2	2.41	0.56
1:B:270:LEU:HD12	1:B:274:LEU:HD13	1.88	0.56
1:A:175:ASP:OD2	1:A:177:SER:HB3	2.05	0.56
1:B:843:ILE:HG22	1:B:844:GLN:H	1.70	0.56
1:A:643:LYS:HA	1:A:744:MET:HE3	1.88	0.56
1:B:170:LEU:HD21	1:B:278:VAL:HG22	1.87	0.56
1:B:588:LEU:HD12	1:B:707:VAL:HG22	1.88	0.56
1:B:814:ILE:HG21	1:B:874:ILE:HD11	1.88	0.56
1:A:118:THR:HG22	1:A:119:LYS:N	2.21	0.56
1:A:172:PRO:HG2	1:A:174:PHE:CE2	2.41	0.56
1:A:914:GLN:O	1:A:1010:PRO:HB3	2.06	0.56
1:B:58:PRO:HG2	1:B:423:ARG:HG3	1.88	0.55
1:B:250:SER:O	1:B:254:MET:HG3	2.06	0.55
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.41	0.55
1:A:50:ILE:HG12	1:A:67:LEU:HD23	1.88	0.55
1:B:928:LEU:HA	1:B:931:LEU:HD13	1.87	0.55
1:A:843:ILE:HG22	1:A:844:GLN:H	1.71	0.55
1:A:793:ILE:O	1:A:847:ARG:HA	2.07	0.55
1:B:643:LYS:CA	1:B:744:MET:HE3	2.35	0.55
1:A:550:LEU:HD11	1:A:558:LYS:HG2	1.87	0.55
1:B:208:THR:HG21	1:B:302:TYR:CZ	2.41	0.54
1:A:820:PHE:CZ	1:A:824:ARG:HD3	2.41	0.54
1:A:81:PRO:HA	1:A:261:ARG:HG2	1.89	0.54
1:B:331:GLY:HA3	1:B:363:GLN:OE1	2.08	0.54
1:A:868:ILE:HD11	1:A:984:PRO:HG3	1.90	0.54
1:B:594:TYR:CZ	1:B:598:GLU:HG3	2.43	0.54
1:B:599:LEU:CD2	1:B:662:ILE:HD12	2.34	0.54
1:A:310:ILE:HA	1:A:668:ARG:NH1	2.23	0.54
1:A:556:MET:HE1	1:A:750:ILE:HD11	1.89	0.53
1:B:556:MET:HE1	1:B:750:ILE:HD11	1.90	0.53
1:A:796:GLN:HB3	1:A:952:HIS:HB2	1.91	0.53
1:A:113:MET:HE3	1:A:182:GLU:HB3	1.90	0.53
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.42	0.53
1:B:118:THR:HG22	1:B:119:LYS:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:HG2	1:A:496:TYR:HB3	1.91	0.53
1:A:810:LEU:HD23	1:A:936:ILE:HD11	1.91	0.53
1:B:675:ALA:HA	1:B:785:VAL:HG21	1.90	0.52
1:A:693:VAL:HB	1:A:766:TYR:CE1	2.44	0.52
1:B:175:ASP:OD2	1:B:177:SER:HB3	2.09	0.52
1:B:794:TYR:HB3	1:B:954:VAL:HG13	1.92	0.52
1:A:785:VAL:O	1:A:961:ARG:NH1	2.42	0.52
1:B:873:SER:O	1:B:877:MET:HB2	2.10	0.52
1:A:367:ALA:HB3	1:A:370:PHE:CE1	2.45	0.52
1:B:190:HIS:O	1:B:194:VAL:HG23	2.09	0.52
1:B:693:VAL:HB	1:B:766:TYR:CE1	2.45	0.52
1:A:76:LEU:HD23	1:A:437:ILE:HG21	1.92	0.52
1:B:573:ASN:HD21	1:B:901:SER:HA	1.75	0.52
1:A:578:PHE:O	1:A:626:GLY:HA3	2.10	0.51
1:A:77:LEU:CD2	1:A:271:VAL:HG21	2.41	0.51
1:B:820:PHE:CE1	1:B:824:ARG:HD3	2.45	0.51
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.46	0.51
1:A:287:GLU:HG2	1:A:368:ARG:HD2	1.93	0.51
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.91	0.51
1:A:65:ARG:O	1:A:76:LEU:HD12	2.11	0.51
1:A:855:PRO:O	1:A:859:LEU:HD13	2.09	0.51
1:B:270:LEU:O	1:B:274:LEU:HD13	2.10	0.51
1:A:798:ASP:OD1	1:A:799:MET:N	2.40	0.50
1:A:62:ARG:HG2	1:A:80:ASP:HB2	1.93	0.50
1:B:843:ILE:HG22	1:B:844:GLN:N	2.25	0.50
1:B:868:ILE:HD11	1:B:984:PRO:HG3	1.93	0.50
1:B:50:ILE:HG12	1:B:67:LEU:HD23	1.94	0.50
1:A:310:ILE:HA	1:A:668:ARG:HH12	1.76	0.50
1:B:942:GLU:HA	1:B:949:PRO:HD2	1.93	0.50
1:A:615:GLY:HA3	1:A:634:TYR:HE2	1.77	0.50
1:B:303:LYS:HB3	1:B:485:PHE:CD2	2.47	0.50
1:B:588:LEU:CD1	1:B:707:VAL:HG22	2.42	0.50
1:B:71:ASN:HB2	1:B:251:SER:OG	2.12	0.49
1:B:616:LEU:HD11	1:B:638:GLN:HG3	1.93	0.49
1:B:62:ARG:HG2	1:B:80:ASP:HB2	1.95	0.49
1:B:709:LEU:HD21	1:B:713:LYS:HE3	1.94	0.49
1:B:657:LYS:O	1:B:661:ILE:HG13	2.12	0.49
1:B:920:ARG:O	1:B:924:GLU:HG3	2.13	0.49
1:A:200:ARG:NH2	1:A:498:THR:HA	2.28	0.49
1:A:780:GLN:NE2	1:A:959:LEU:HD11	2.27	0.49
1:A:864:GLU:OE2	1:A:953:LYS:HE3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ILE:HA	1:B:668:ARG:NH1	2.27	0.49
1:A:179:LYS:HD2	1:A:237:VAL:HB	1.94	0.49
1:B:417:LEU:HD21	1:B:531:ILE:HG12	1.95	0.49
1:A:67:LEU:CD1	1:A:268:THR:HG23	2.37	0.49
1:A:250:SER:O	1:A:254:MET:HG3	2.13	0.49
1:A:709:LEU:HD21	1:A:713:LYS:CE	2.42	0.49
1:B:245:HIS:O	1:B:249:TYR:HB2	2.13	0.49
1:B:67:LEU:HB2	1:B:75:VAL:HB	1.93	0.49
1:B:943:MET:HE1	1:B:950:ARG:NH1	2.28	0.49
1:B:102:ASN:HD22	1:B:235:ILE:CD1	2.25	0.48
1:B:838:ARG:O	1:B:844:GLN:HA	2.13	0.48
1:A:723:LEU:C	1:A:758:LEU:HD13	2.38	0.48
1:B:316:THR:OG1	1:B:374:ILE:HD13	2.13	0.48
1:A:208:THR:HG21	1:A:302:TYR:CZ	2.48	0.48
1:A:303:LYS:HB3	1:A:485:PHE:CD2	2.48	0.48
1:A:562:LYS:NZ	1:A:903:GLU:OE2	2.44	0.48
1:A:820:PHE:CE1	1:A:824:ARG:HD3	2.49	0.48
1:A:960:ALA:HB3	1:A:963:MET:HE3	1.95	0.48
1:B:785:VAL:O	1:B:961:ARG:NH1	2.47	0.48
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.49	0.48
1:A:229:ARG:O	1:A:232:GLN:HB3	2.13	0.48
1:B:291:HIS:ND1	1:B:292:PRO:HD2	2.29	0.48
1:A:854:LYS:HB2	1:A:859:LEU:HD11	1.96	0.47
1:B:163:ASP:HA	1:B:274:LEU:HD23	1.97	0.47
1:B:580:SER:HB2	1:B:723:LEU:HD23	1.96	0.47
1:B:715:PHE:CZ	1:B:719:LEU:HD22	2.50	0.47
1:B:868:ILE:HD11	1:B:984:PRO:HB3	1.96	0.47
1:A:350:LEU:HB3	1:A:356:VAL:HG22	1.95	0.47
1:A:946:VAL:HA	1:A:951:ARG:CZ	2.44	0.47
1:B:787:ASN:C	1:B:960:ALA:HB1	2.39	0.47
1:A:97:LEU:CD1	1:A:367:ALA:HB2	2.45	0.47
1:A:886:ILE:HG23	1:A:928:LEU:HG	1.96	0.47
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.97	0.47
1:A:602:ASP:OD2	1:A:658:ARG:NH2	2.34	0.47
1:A:843:ILE:HG22	1:A:844:GLN:N	2.28	0.47
1:B:298:LEU:HD13	1:B:475:ASN:HA	1.96	0.47
1:B:411:PHE:CD1	1:B:459:PHE:HB2	2.50	0.47
1:B:805:ASN:HA	1:B:844:GLN:HE22	1.78	0.47
1:A:90:LEU:HD12	1:A:256:VAL:HG22	1.97	0.47
1:B:777:PHE:CB	1:B:992:ILE:HD11	2.24	0.47
1:A:592:MET:HE3	1:A:715:PHE:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:LEU:HA	1:A:931:LEU:HD13	1.96	0.47
1:B:723:LEU:C	1:B:758:LEU:HD13	2.40	0.47
1:B:820:PHE:CZ	1:B:824:ARG:HD3	2.50	0.47
1:A:599:LEU:HD21	1:A:659:PHE:HA	1.96	0.46
1:B:347:LEU:O	1:B:351:LYS:HB2	2.15	0.46
1:A:110:LEU:HD23	1:A:114:LEU:HD23	1.97	0.46
1:A:643:LYS:CA	1:A:744:MET:HE3	2.45	0.46
1:A:767:ARG:NH1	1:A:1006:PRO:HA	2.31	0.46
1:A:671:ASN:O	1:A:674:ARG:HG2	2.15	0.46
1:A:859:LEU:H	1:A:859:LEU:CD1	2.29	0.46
1:B:600:LEU:HD11	1:B:648:LYS:HB3	1.97	0.46
1:B:882:PHE:CE2	1:B:933:LYS:HA	2.50	0.46
1:B:102:ASN:HD22	1:B:235:ILE:HD11	1.80	0.46
1:B:550:LEU:HD11	1:B:558:LYS:HG2	1.97	0.46
1:A:83:THR:OG1	1:A:85:LYS:O	2.32	0.46
1:A:838:ARG:O	1:A:844:GLN:HA	2.16	0.45
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.52	0.45
1:B:163:ASP:O	1:B:167:GLN:HG2	2.16	0.45
1:B:413:GLU:O	1:B:417:LEU:HD23	2.16	0.45
1:A:213:HIS:ND1	1:A:214:PRO:HD2	2.32	0.45
1:A:270:LEU:O	1:A:274:LEU:HD13	2.16	0.45
1:B:285:LEU:HD21	1:B:368:ARG:NE	2.32	0.45
1:B:797:THR:OG1	1:B:798:ASP:N	2.43	0.45
1:A:791:ILE:HA	1:A:956:VAL:O	2.16	0.45
1:B:333:TYR:CD1	1:B:464:ILE:HD13	2.51	0.45
1:B:722:ARG:C	1:B:758:LEU:HD11	2.41	0.45
1:A:118:THR:HG22	1:A:119:LYS:H	1.81	0.45
1:B:110:LEU:HD23	1:B:110:LEU:O	2.17	0.45
1:B:599:LEU:HD21	1:B:659:PHE:HA	1.99	0.45
1:A:767:ARG:HH12	1:A:1006:PRO:HA	1.82	0.45
1:A:794:TYR:HB3	1:A:954:VAL:HG13	1.98	0.45
1:B:852:SER:HB3	1:B:859:LEU:HD11	1.99	0.45
1:A:615:GLY:HA3	1:A:634:TYR:CE2	2.51	0.45
1:B:76:LEU:CD2	1:B:437:ILE:HG21	2.40	0.45
1:A:259:LEU:HD12	1:A:430:PRO:HB3	1.99	0.45
1:A:479:ALA:HB2	2:A:1101:J22:C30	2.47	0.45
1:B:259:LEU:C	1:B:259:LEU:HD13	2.42	0.45
1:B:776:TRP:HA	1:B:953:LYS:O	2.16	0.45
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.52	0.44
1:A:920:ARG:O	1:A:924:GLU:HG3	2.16	0.44
1:B:270:LEU:HD12	1:B:274:LEU:CD1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:MET:HE3	1:B:882:PHE:HD2	1.83	0.44
1:A:259:LEU:HD13	1:A:259:LEU:C	2.43	0.44
1:A:768:GLU:HB3	1:A:843:ILE:HG13	1.98	0.44
1:A:594:TYR:CZ	1:A:598:GLU:HG3	2.53	0.44
1:A:50:ILE:HG12	1:A:67:LEU:CD2	2.46	0.44
1:A:390:ILE:HG22	1:A:394:MET:HE3	1.99	0.44
1:B:192:LYS:HG3	1:B:677:GLN:CD	2.42	0.44
1:B:360:VAL:HB	1:B:376:ASN:HB3	1.98	0.44
1:B:915:GLN:OE1	1:B:920:ARG:NH2	2.51	0.44
1:B:334:LEU:HD22	1:B:468:LEU:HD13	2.00	0.44
1:B:868:ILE:HD11	1:B:984:PRO:CG	2.48	0.44
1:A:205:GLU:HG2	1:A:293:PHE:HZ	1.83	0.44
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.53	0.44
1:A:270:LEU:HD12	1:A:274:LEU:CD1	2.48	0.44
1:B:376:ASN:C	1:B:376:ASN:OD1	2.60	0.44
1:A:524:LEU:HD23	1:A:524:LEU:HA	1.84	0.43
1:B:616:LEU:CD1	1:B:638:GLN:HG3	2.48	0.43
1:B:364:LYS:NZ	1:B:374:ILE:HD11	2.33	0.43
1:B:416:ASP:O	1:B:420:VAL:HG23	2.18	0.43
1:B:548:PRO:HA	1:B:562:LYS:HB2	2.00	0.43
1:B:671:ASN:O	1:B:674:ARG:HG2	2.18	0.43
1:B:367:ALA:HB3	1:B:370:PHE:CE1	2.53	0.43
1:B:780:GLN:NE2	1:B:959:LEU:HD11	2.33	0.43
1:A:777:PHE:CB	1:A:992:ILE:HD11	2.24	0.43
1:B:110:LEU:HD11	1:B:245:HIS:HB2	2.00	0.43
1:B:679:HIS:CE1	1:B:832:ILE:HD13	2.53	0.43
1:A:616:LEU:HD11	1:A:638:GLN:HG3	1.98	0.43
1:A:559:LEU:HD11	1:A:729:LEU:HG	1.99	0.43
1:B:118:THR:HG22	1:B:119:LYS:H	1.83	0.43
1:B:433:TYR:CZ	1:B:437:ILE:HD11	2.54	0.43
1:B:518:LEU:HD23	1:B:518:LEU:HA	1.76	0.43
1:A:153:VAL:HG22	1:A:154:SER:N	2.33	0.43
1:A:657:LYS:O	1:A:661:ILE:HG13	2.19	0.43
1:A:878:THR:HG21	1:B:457:GLU:OE2	2.19	0.43
1:B:90:LEU:HD23	1:B:91:ASP:N	2.34	0.43
1:A:518:LEU:HA	1:A:518:LEU:HD23	1.68	0.43
1:B:264:LEU:HD23	1:B:264:LEU:HA	1.91	0.43
1:A:865:ALA:HB2	1:A:983:ALA:CA	2.46	0.42
1:B:153:VAL:HG22	1:B:154:SER:N	2.34	0.42
1:B:796:GLN:HB3	1:B:952:HIS:HB2	2.01	0.42
1:B:90:LEU:HD13	1:B:169:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:PRO:HD3	1:B:758:LEU:HD21	2.00	0.42
1:A:206:LYS:HB3	1:A:216:SER:HA	2.01	0.42
1:A:229:ARG:HB3	1:A:230:PRO:HD3	2.02	0.42
1:A:594:TYR:CE2	1:A:598:GLU:HG3	2.55	0.42
1:A:97:LEU:HD11	1:A:367:ALA:HB2	2.01	0.42
1:A:99:ASP:O	1:A:217:LYS:NZ	2.38	0.42
1:A:114:LEU:HD12	1:A:168:PHE:CB	2.38	0.42
1:A:285:LEU:HD21	1:A:368:ARG:NE	2.34	0.42
1:B:90:LEU:HD23	1:B:90:LEU:C	2.44	0.42
1:B:94:ILE:HG13	1:B:248:TYR:HB3	2.00	0.42
1:A:577:GLU:HG2	1:A:579:PHE:CZ	2.54	0.42
1:A:376:ASN:OD1	1:A:376:ASN:C	2.62	0.42
1:A:873:SER:O	1:A:877:MET:HB2	2.20	0.42
1:B:103:ILE:HD11	1:B:235:ILE:HG21	2.00	0.42
1:B:196:ASN:OD1	1:B:198:ALA:N	2.53	0.42
1:B:942:GLU:OE1	1:B:950:ARG:HD3	2.20	0.42
1:A:245:HIS:O	1:A:249:TYR:HB2	2.20	0.42
1:A:299:LYS:HA	1:A:505:ILE:HD12	2.01	0.42
1:B:50:ILE:HG12	1:B:67:LEU:CD2	2.49	0.42
1:B:102:ASN:OD1	1:B:102:ASN:N	2.45	0.42
1:B:648:LYS:O	1:B:652:PHE:HB2	2.19	0.42
1:A:796:GLN:HE21	1:A:843:ILE:HG21	1.84	0.42
1:A:925:VAL:O	1:A:929:LYS:HG3	2.19	0.42
1:B:823:LEU:HB2	1:B:833:VAL:HG11	2.01	0.42
1:A:339:GLY:HA2	1:A:359:LEU:CD2	2.50	0.42
1:A:776:TRP:HA	1:A:953:LYS:O	2.20	0.42
1:B:314:TYR:HE2	1:B:376:ASN:ND2	2.18	0.42
1:B:587:PRO:HB3	1:B:700:LEU:HD23	2.01	0.42
1:A:573:ASN:HD21	1:A:901:SER:HA	1.85	0.41
1:B:894:LEU:HD11	1:B:925:VAL:HG11	2.02	0.41
1:A:309:ASP:O	1:A:668:ARG:NH1	2.52	0.41
1:A:195:MET:CG	1:A:307:ILE:HD13	2.44	0.41
1:A:314:TYR:HE2	1:A:376:ASN:ND2	2.19	0.41
1:A:684:TYR:CZ	1:A:688:LEU:HD11	2.56	0.41
1:A:806:MET:HE1	1:A:893:ARG:HH12	1.85	0.41
1:B:124:GLU:OE2	1:B:178:ALA:HB2	2.21	0.41
1:B:273:LYS:HG2	1:B:274:LEU:HD12	2.01	0.41
1:A:859:LEU:CD1	1:A:859:LEU:N	2.84	0.41
1:B:200:ARG:NH2	1:B:498:THR:HA	2.36	0.41
1:B:552:LYS:HB3	1:B:559:LEU:HB3	2.02	0.41
1:B:914:GLN:HA	1:B:916:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:TYR:CE1	1:A:953:LYS:HD2	2.56	0.41
1:B:565:ASP:OD1	1:B:566:LYS:HG3	2.21	0.41
1:A:102:ASN:OD1	1:A:102:ASN:N	2.47	0.41
1:A:141:PHE:CE2	1:A:148:ASN:HB3	2.56	0.41
1:A:326:TYR:OH	1:A:327:LYS:NZ	2.54	0.41
1:B:103:ILE:CD1	1:B:240:GLU:HG3	2.51	0.41
1:B:110:LEU:HD23	1:B:110:LEU:C	2.46	0.41
1:B:314:TYR:CE2	1:B:376:ASN:ND2	2.89	0.41
1:B:425:LYS:HD2	1:B:428:GLU:OE1	2.20	0.41
1:B:667:MET:HG3	1:B:704:LEU:HD23	2.03	0.41
1:B:787:ASN:HB2	1:B:961:ARG:NH2	2.36	0.41
1:A:709:LEU:C	1:A:709:LEU:HD23	2.46	0.41
1:A:882:PHE:CE1	1:A:886:ILE:HD11	2.56	0.41
1:A:667:MET:HG3	1:A:704:LEU:HD23	2.03	0.40
1:B:113:MET:CE	1:B:116:LEU:HD12	2.48	0.40
1:A:852:SER:OG	1:A:853:GLU:N	2.54	0.40
1:A:192:LYS:HB3	1:A:192:LYS:HE3	1.87	0.40
1:A:733:ILE:HG13	1:A:737:ALA:HB3	2.02	0.40
1:A:933:LYS:HZ1	1:B:55:THR:HG22	1.86	0.40
1:B:78:ILE:HG22	1:B:259:LEU:HD23	2.00	0.40
1:B:155:HIS:ND1	1:B:261:ARG:HD2	2.36	0.40
1:B:854:LYS:HB3	1:B:855:PRO:HD2	2.03	0.40
1:A:291:HIS:ND1	1:A:292:PRO:HD2	2.37	0.40
1:B:864:GLU:CD	1:B:951:ARG:HH22	2.30	0.40

All (2) 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:408:GLU:OE2	1:A:734:THR:OG1[3_655]	2.12	0.08
1:A:761:SER:OG	1:B:699:GLU:OE2[5_555]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	955/978 (98%)	914 (96%)	40 (4%)	1 (0%)	48	79
1	B	955/978 (98%)	913 (96%)	41 (4%)	1 (0%)	48	79
All	All	1910/1956 (98%)	1827 (96%)	81 (4%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1006	PRO
1	B	1006	PRO

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	842/870 (97%)	839 (100%)	3 (0%)	84	80
1	B	842/870 (97%)	841 (100%)	1 (0%)	88	87
All	All	1684/1740 (97%)	1680 (100%)	4 (0%)	87	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	667	MET
1	A	759	LEU
1	A	859	LEU
1	B	82	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	167	GLN

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Mol	Chain	Res	Type
1	A	312	ASN
1	A	323	GLN
1	A	857	HIS
1	A	982	GLN
1	B	52	ASN
1	B	111	GLN
1	B	190	HIS
1	B	336	HIS
1	B	376	ASN
1	B	396	GLN
1	B	442	HIS
1	B	605	ASN
1	B	724	HIS
1	B	736	GLN
1	B	752	HIS

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](#)

4 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	EPE	A	1102	-	15,15,15	0.75	1 (6%)	19,20,20	1.71	3 (15%)
2	J22	A	1101	-	35,39,39	2.55	16 (45%)	38,58,58	2.16	7 (18%)
3	EPE	B	1102	-	15,15,15	0.77	1 (6%)	19,20,20	1.82	4 (21%)
2	J22	B	1101	-	35,39,39	2.87	15 (42%)	38,58,58	2.12	5 (13%)

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	EPE	A	1102	-	-	7/9/19/19	0/1/1/1
2	J22	A	1101	-	-	6/20/49/49	0/4/5/5
3	EPE	B	1102	-	-	5/9/19/19	0/1/1/1
2	J22	B	1101	-	-	10/20/49/49	0/4/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	J22	C11-N16	7.72	1.54	1.49
2	B	1101	J22	C03-S02	7.24	1.86	1.78
2	B	1101	J22	C03-N04	6.88	1.36	1.32
2	A	1101	J22	C03-N04	6.60	1.36	1.32
2	A	1101	J22	C11-N16	6.46	1.53	1.49
2	A	1101	J22	C03-S02	4.61	1.83	1.78
2	B	1101	J22	C10-N09	4.41	1.53	1.47
2	A	1101	J22	O01-S02	3.14	1.46	1.43
2	A	1101	J22	C06-C05	3.13	1.42	1.35
2	B	1101	J22	O01-S02	3.10	1.46	1.43
2	B	1101	J22	C06-C05	3.05	1.42	1.35
2	A	1101	J22	C13-C12	2.96	1.58	1.52
2	A	1101	J22	C12-N09	2.76	1.52	1.48
2	B	1101	J22	C12-N09	2.73	1.52	1.48
2	B	1101	J22	C18-C17	2.69	1.56	1.52
2	A	1101	J22	C14-C15	2.65	1.57	1.52
3	A	1102	EPE	C10-S	2.50	1.81	1.77
3	B	1102	EPE	C10-S	2.50	1.81	1.77
2	B	1101	J22	C25-C24	-2.49	1.45	1.49
2	A	1101	J22	C32-C25	2.46	1.43	1.40
2	A	1101	J22	C31-C30	2.44	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	J22	C17-N16	2.41	1.50	1.49
2	B	1101	J22	C31-C30	2.26	1.42	1.38
2	A	1101	J22	C34-C33	2.25	1.42	1.38
2	A	1101	J22	C25-C26	2.25	1.44	1.40
2	A	1101	J22	C25-C24	-2.23	1.45	1.49
2	A	1101	J22	C23-C22	2.17	1.42	1.38
2	B	1101	J22	C34-C33	2.13	1.42	1.38
2	A	1101	J22	C33-C24	2.12	1.43	1.39
2	B	1101	J22	C32-C25	2.12	1.43	1.40
2	B	1101	J22	C14-C15	2.11	1.56	1.52
2	B	1101	J22	C23-C22	2.06	1.42	1.38
2	A	1101	J22	C31-C32	2.04	1.42	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	J22	O35-S02-O01	-10.99	103.91	119.69
2	B	1101	J22	O35-S02-O01	-10.95	103.98	119.69
3	A	1102	EPE	C5-N4-C3	4.67	118.89	108.84
3	B	1102	EPE	C5-N4-C3	4.20	117.89	108.84
3	B	1102	EPE	C7-N4-C5	3.68	121.05	111.24
3	B	1102	EPE	C7-N4-C3	3.59	120.81	111.24
3	A	1102	EPE	C7-N4-C5	3.40	120.29	111.24
2	B	1101	J22	O35-S02-N09	3.24	112.91	107.26
2	A	1101	J22	O35-S02-N09	3.13	112.72	107.26
2	A	1101	J22	C12-N09-S02	2.84	122.32	116.64
2	A	1101	J22	C06-C05-N04	-2.77	107.11	110.74
2	B	1101	J22	C06-C05-N04	-2.63	107.30	110.74
2	A	1101	J22	O01-S02-N09	2.49	111.60	107.26
2	B	1101	J22	O01-S02-N09	2.47	111.56	107.26
2	A	1101	J22	O19-C18-C17	-2.35	106.36	111.55
3	A	1102	EPE	C7-N4-C3	2.20	117.09	111.24
2	A	1101	J22	C21-C20-C17	-2.15	113.23	118.21
2	B	1101	J22	C13-C14-C15	-2.12	111.38	115.69
3	B	1102	EPE	O2S-S-C10	2.02	109.78	106.73

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	J22	N16-C17-C18-O19
2	B	1101	J22	N04-C03-S02-O35

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Mol	Chain	Res	Type	Atoms
2	B	1101	J22	C20-C17-C18-O19
2	B	1101	J22	N16-C17-C18-O19
2	B	1101	J22	C12-N09-S02-C03
3	A	1102	EPE	C10-C9-N1-C2
3	A	1102	EPE	C8-C7-N4-C5
3	A	1102	EPE	C9-C10-S-O2S
3	B	1102	EPE	C9-C10-S-O1S
3	B	1102	EPE	C9-C10-S-O3S
3	A	1102	EPE	C9-C10-S-O3S
2	A	1101	J22	C12-N09-S02-O01
2	B	1101	J22	C12-N09-S02-O35
2	A	1101	J22	C12-N09-S02-C03
2	B	1101	J22	C10-N09-S02-O35
3	A	1102	EPE	C9-C10-S-O1S
3	B	1102	EPE	C9-C10-S-O2S
3	B	1102	EPE	C8-C7-N4-C5
2	A	1101	J22	C12-N09-S02-O35
2	A	1101	J22	N04-C03-S02-O01
3	A	1102	EPE	C10-C9-N1-C6
3	B	1102	EPE	N4-C7-C8-O8
2	B	1101	J22	C23-C24-C25-C26
2	B	1101	J22	C33-C24-C25-C26
2	B	1101	J22	C23-C24-C25-C32
2	B	1101	J22	C33-C24-C25-C32
2	A	1101	J22	C20-C17-C18-O19
3	A	1102	EPE	C8-C7-N4-C3

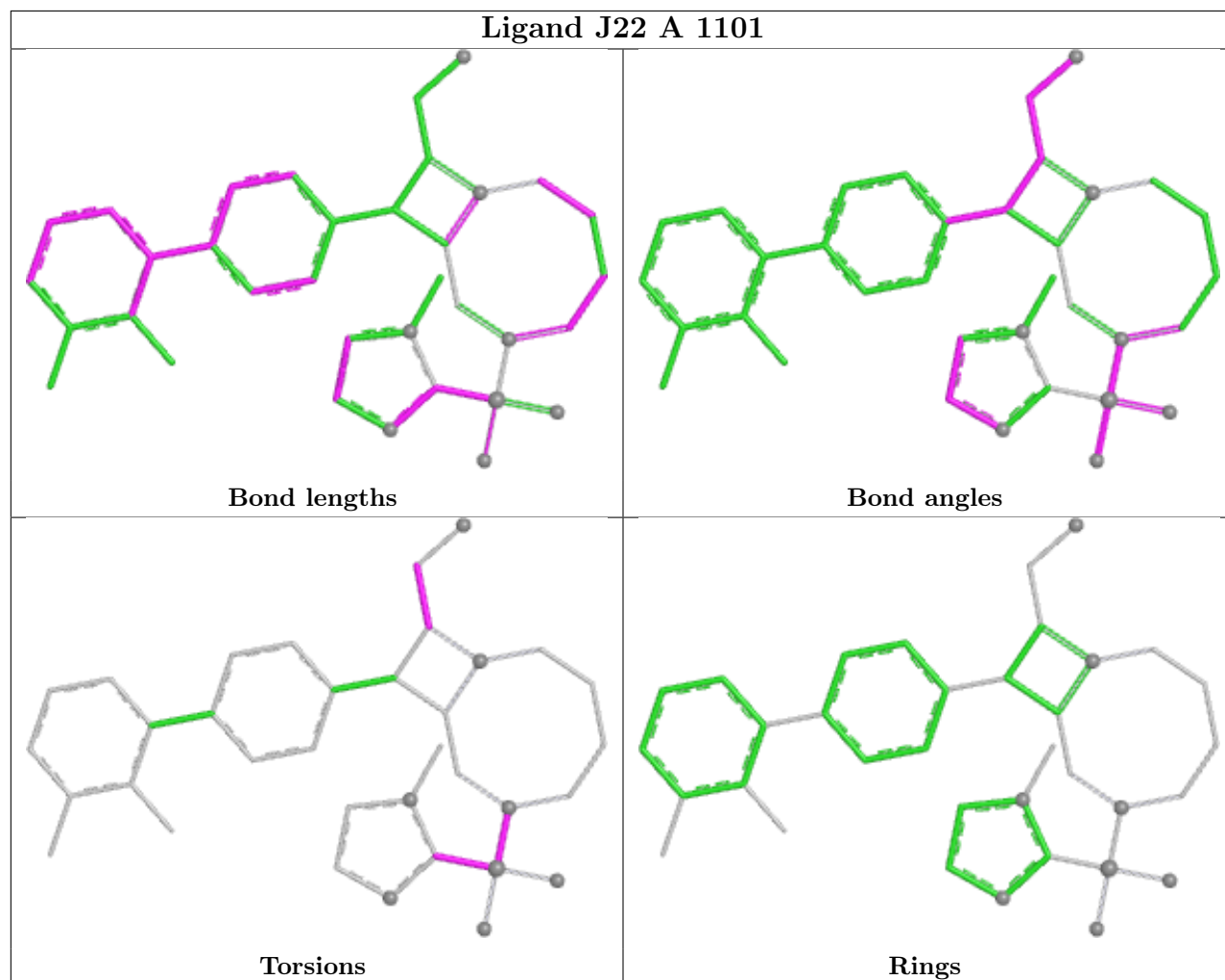
There are no ring outliers.

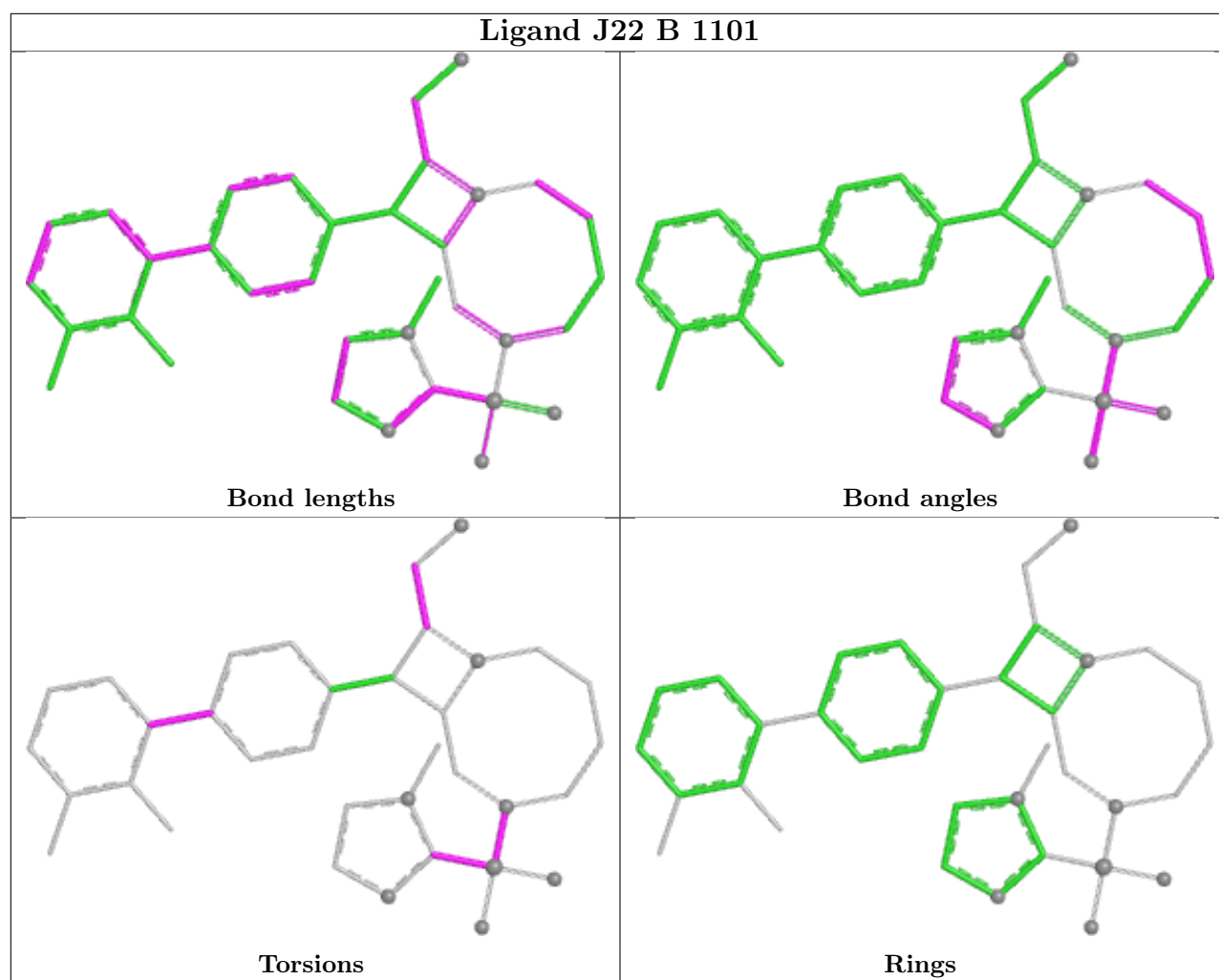
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	J22	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	959/978 (98%)	-0.54	0 100 100	42, 65, 88, 133	0
1	B	959/978 (98%)	-0.45	0 100 100	49, 73, 96, 135	0
All	All	1918/1956 (98%)	-0.49	0 100 100	42, 69, 92, 135	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.

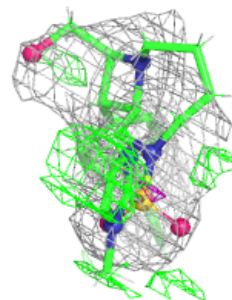
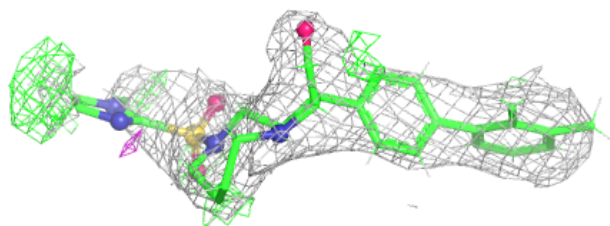
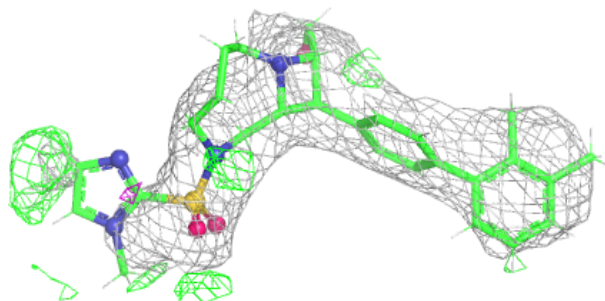
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	J22	B	1101	35/35	0.91	0.17	68,110,154,169	0
3	EPE	A	1102	15/15	0.91	0.14	60,81,101,106	32
3	EPE	B	1102	15/15	0.94	0.12	57,75,96,101	32
2	J22	A	1101	35/35	0.95	0.15	55,91,116,132	69

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.

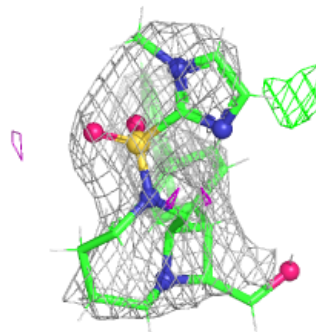
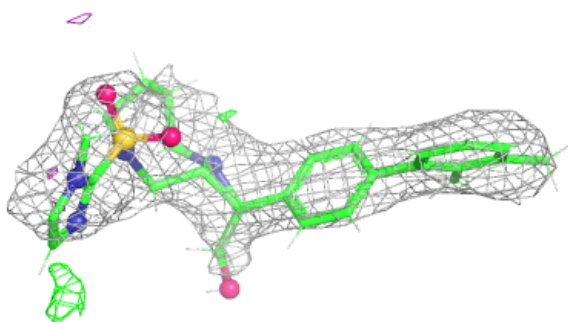
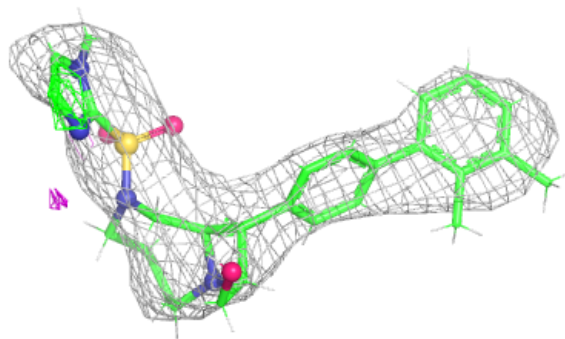
Electron density around J22 B 1101:

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



Electron density around J22 A 1101:

$2mF_o-DF_c$ (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.