



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:21 AM UTC

PDB ID : 9GOW / pdb\_00009gow  
Title : Crystal structure of phosphorylated human IRE1a in complex with IA107  
Authors : Liu, Y.; Gasper, R.; Wu, P.  
Deposited on : 2024-09-06  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

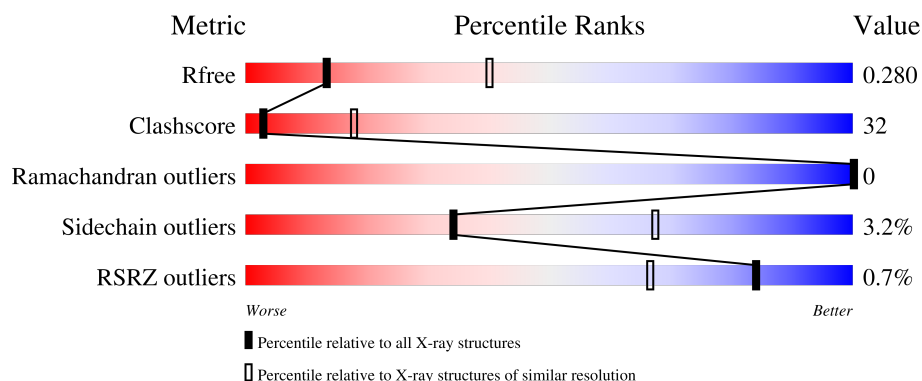
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	434	<div> <div>%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div>• 7%</div> </div> </div>
1	B	434	<div> <div></div> <div> <div>52%</div> <div>40%</div> <div>• 7%</div> </div> </div>
1	C	434	<div> <div></div> <div> <div>40%</div> <div>51%</div> <div>• 7%</div> </div> </div>
1	D	434	<div> <div>%</div> <div> <div></div> <div>26%</div> <div>41%</div> <div>•</div> <div>30%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12419 atoms, of which 60 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.

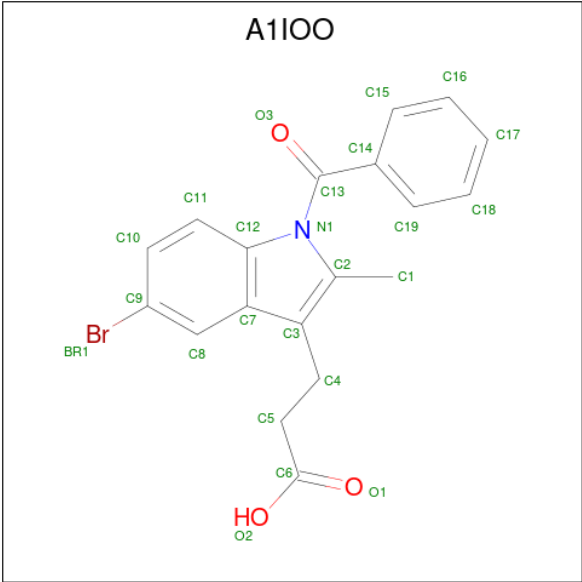
- Molecule 1 is a protein called Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	P	S	0	0	0
			3273	2076	580	594	3	20			
1	B	403	Total	C	N	O	P	S	0	0	0
			3273	2076	580	594	3	20			
1	C	403	Total	C	N	O	P	S	0	0	0
			3273	2076	580	594	3	20			
1	D	303	Total	C	N	O	P	S	0	0	0
			2444	1552	421	452	3	16			

There are 12 discrepancies between the modelled and reference sequences:

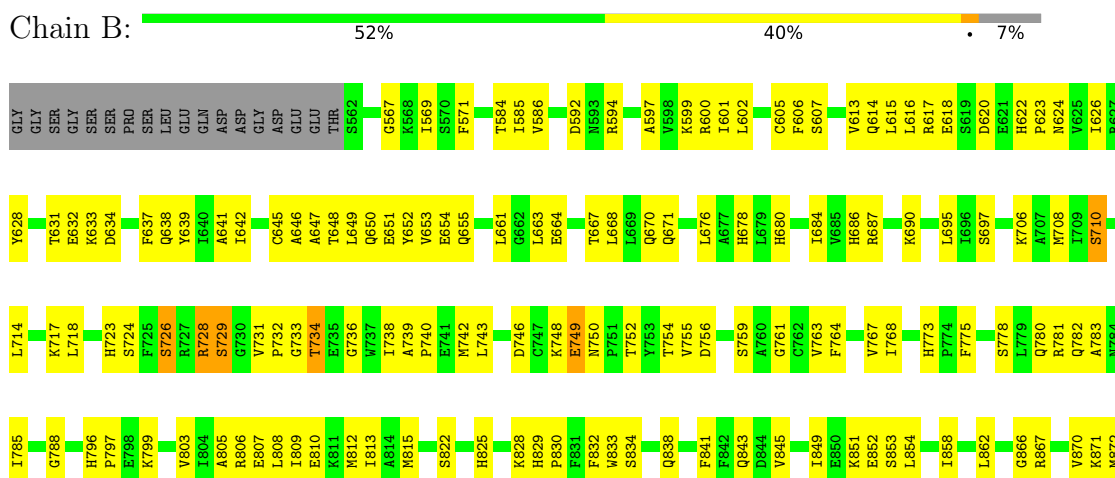
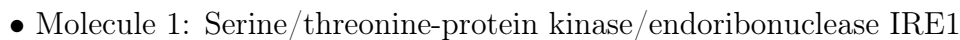
Chain	Residue	Modelled	Actual	Comment	Reference
A	544	GLY	-	expression tag	UNP O75460
A	545	GLY	-	expression tag	UNP O75460
A	546	SER	-	expression tag	UNP O75460
B	544	GLY	-	expression tag	UNP O75460
B	545	GLY	-	expression tag	UNP O75460
B	546	SER	-	expression tag	UNP O75460
C	544	GLY	-	expression tag	UNP O75460
C	545	GLY	-	expression tag	UNP O75460
C	546	SER	-	expression tag	UNP O75460
D	544	GLY	-	expression tag	UNP O75460
D	545	GLY	-	expression tag	UNP O75460
D	546	SER	-	expression tag	UNP O75460

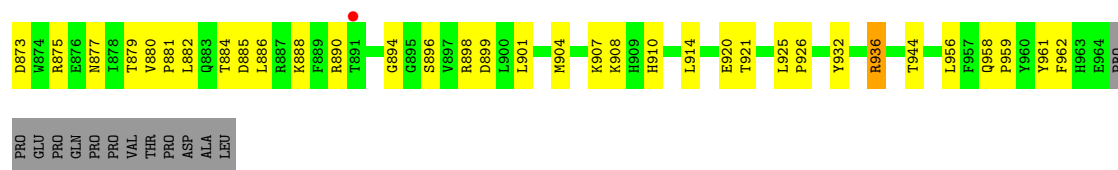
- Molecule 2 is 3-[5-bromanyl-2-methyl-1-(phenylcarbonyl)indol-3-yl]propanoic acid (CCD ID: A1IOO) (formula: C<sub>19</sub>H<sub>16</sub>BrNO<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	H	N	O	0	0
			39	1	19	15	1	3		
2	B	1	Total	Br	C	H	N	O	0	0
			39	1	19	15	1	3		
2	C	1	Total	Br	C	H	N	O	0	0
			39	1	19	15	1	3		
2	D	1	Total	Br	C	H	N	O	0	0
			39	1	19	15	1	3		

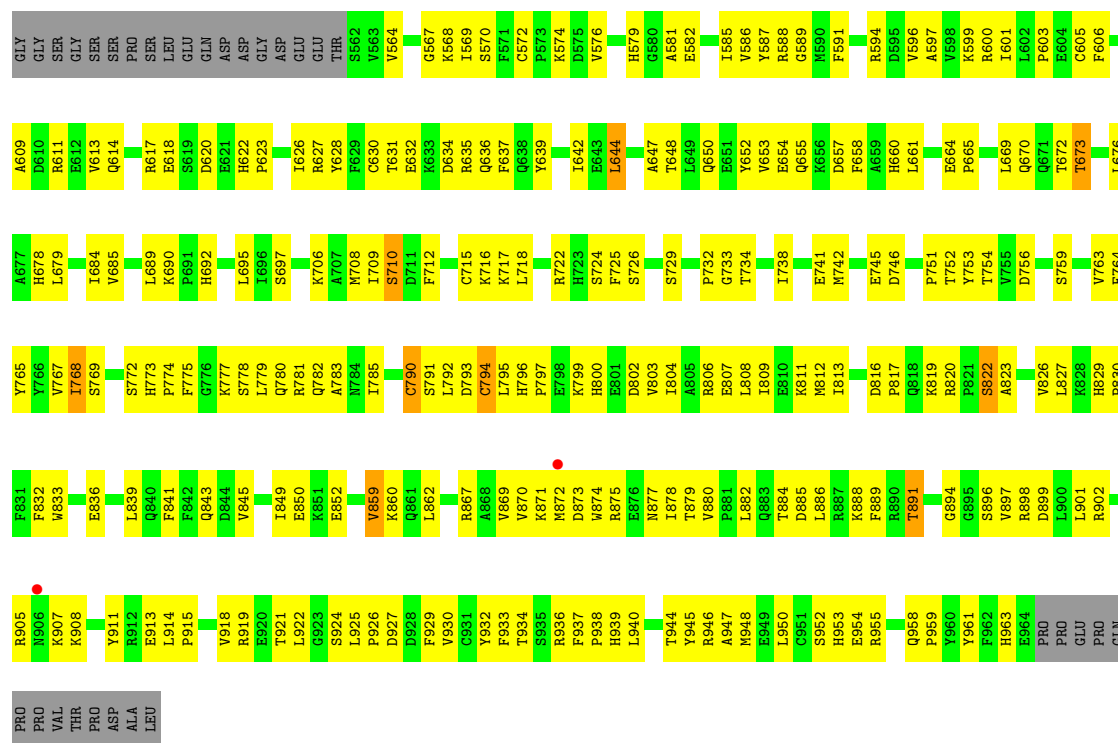
- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1





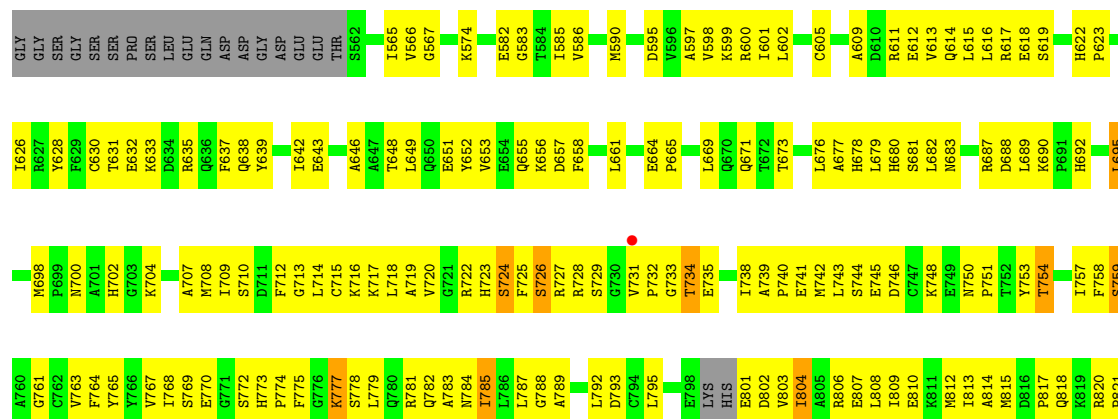
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain C: 40% 51% 7%



• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain D: 26% 41% 30%



THR	TYR	ASP	ARG	ALA	MET	E949	L950	C951		R955	L956	F957	Q958	P959	Y960	Y961	F962	H963	E964	PRO	PRO	GLU	GLU	PRO	PRO	GLN	THR	THR	ASP	ALA	ALA	LEU																														
THR	ASP	LEU	ARG	LYS	PHE	ARG	THR	TYR	LYS	GLY	GLY	SER	VAL	ARG	ASP	LEU	LEU	ASP	ARG	ALA	ALA	ALA	ASP	PRO	GLY	ILE	VAL	LYS	GLN	LEU	GLU	GLY	ARG	GLY	ARG	ALA	VAL	VAL	LYS	MET	ASP	TRP	ARG	ASN	GLU	ASN	THR	ILE	THR	VAL	PRO	PRO	LEU	GLN								
S822	K823	K824	H825	V826	L827	K828	H829	P830		W833	S834	L835	E836	K837	Q838	L839	Q840	F841	Q843	D844	V845		R848	T849	E850	LYS	GLU	SER	LEU	ASP	GLY	PRO	ILE	VAL	LYS	GLN	LEU	LEU	GLU	ARG	GLY	ARG	ALA	VAL	VAL	VAL	LYS	MET	ASP	TRP	ARG	ASN	GLU	ASN	THR	ILE	THR	VAL	PRO	PRO	LEU	GLN

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.18Å 77.50Å 141.06Å 74.61° 78.09° 65.63°	Depositor
Resolution (Å)	47.91 – 3.00 47.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (47.91-3.00) 91.9 (47.91-3.00)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487)	Depositor
R, $R_{free}$	0.231 , 0.281 0.231 , 0.280	Depositor DCC
$R_{free}$ test set	2287 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,h-k,h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12419	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, A1IOO

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	0.13	0/3320	0.30	0/4476
1	B	0.13	0/3320	0.30	0/4476
1	C	0.15	0/3320	0.34	0/4476
1	D	0.14	0/2469	0.31	0/3328
All	All	0.13	0/12429	0.31	0/16756

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	3273	0	3235	189	1
1	B	3273	0	3236	156	1
1	C	3273	0	3236	238	2
1	D	2444	0	2391	216	2
2	A	24	15	0	1	0
2	B	24	15	0	1	0
2	C	24	15	0	3	0
2	D	24	15	0	1	0
All	All	12359	60	12098	787	3

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 32.

All (787) 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:849:ILE:HD12	1:C:898:ARG:HG3	1.26	1.15
1:B:788:GLY:HA2	1:B:815:MET:HE3	1.25	1.10
1:C:733:GLY:HA3	1:C:738:ILE:HD11	1.27	1.08
1:B:738:ILE:HG21	1:B:743:LEU:HD23	1.35	1.07
1:C:839:LEU:HD21	1:C:908:LYS:HE2	1.37	1.06
1:A:808:LEU:HG	1:A:812:MET:HE2	1.41	1.00
1:D:784:ASN:H	1:D:787:LEU:HD23	1.32	0.94
1:D:761:GLY:HA2	1:D:812:MET:HE3	1.50	0.93
1:D:757:ILE:HG22	1:D:812:MET:HB3	1.51	0.92
1:A:748:LYS:HE3	1:A:749:GLU:HB3	1.49	0.92
1:D:609:ALA:O	1:D:613:VAL:HG23	1.70	0.91
1:D:844:ASP:HB3	1:D:957:PHE:HE1	1.36	0.91
1:D:761:GLY:HA2	1:D:812:MET:CE	2.01	0.90
1:D:810:GLU:HA	1:D:813:ILE:HD11	1.52	0.90
1:D:795:LEU:HD23	1:D:806:ARG:HG3	1.52	0.89
1:C:706:LYS:HE2	1:C:708:MET:HE2	1.54	0.89
1:A:749:GLU:OE2	1:A:749:GLU:N	2.06	0.87
1:D:731:VAL:HG11	1:D:743:LEU:HD23	1.55	0.87
1:A:736:GLY:N	1:A:782:GLN:OE1	2.09	0.86
1:C:732:PRO:HD2	1:C:742:MET:HE1	1.58	0.86
1:D:688:ASP:HB2	1:D:714:LEU:HD11	1.57	0.85
1:A:801:GLU:OE1	1:A:801:GLU:N	2.08	0.85
1:D:733:GLY:HA3	1:D:738:ILE:HD11	1.57	0.84
1:C:634:ASP:HB2	1:C:639:TYR:HE1	1.43	0.84
1:A:888:LYS:HE2	1:A:889:PHE:HE2	1.42	0.84
1:C:600:ARG:HG3	1:C:637:PHE:HD1	1.42	0.83
1:A:907:LYS:NZ	1:A:914:LEU:HD21	1.93	0.83
1:C:940:LEU:O	1:C:944:THR:HG23	1.79	0.83
1:B:597:ALA:HB3	1:B:642:ILE:CD1	2.09	0.82
1:B:726:SEP:HA	1:B:750:ASN:OD1	1.78	0.82
1:A:799:LYS:O	1:A:803:VAL:HG23	1.79	0.82
1:B:569:ILE:HD13	1:B:641:ALA:HB2	1.61	0.82
1:C:932:TYR:O	1:C:936:ARG:HD2	1.79	0.82
1:A:890:ARG:HG2	1:A:890:ARG:HH11	1.45	0.81
1:D:565:ILE:HD12	1:D:565:ILE:O	1.80	0.81
1:C:878:ILE:HD12	1:C:882:LEU:HB3	1.63	0.81
1:C:623:PRO:O	1:C:706:LYS:HE3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:780:GLN:OE1	1:B:783:ALA:HB3	1.79	0.81
1:A:585:ILE:HG13	1:A:600:ARG:HH21	1.44	0.80
1:C:869:VAL:HG12	1:C:939:HIS:HB3	1.64	0.80
1:A:884:THR:HG22	1:A:887:ARG:HH21	1.46	0.80
1:D:828:LYS:HE3	1:D:962:PHE:HB2	1.63	0.79
1:A:650:GLN:O	1:A:654:GLU:HG3	1.81	0.79
1:A:888:LYS:HE2	1:A:889:PHE:CE2	2.18	0.79
1:C:779:LEU:HD12	1:C:780:GLN:N	1.98	0.79
1:B:732:PRO:HG2	1:B:742:MET:HE1	1.63	0.78
1:C:839:LEU:HD21	1:C:908:LYS:CE	2.12	0.78
1:C:763:VAL:O	1:C:767:VAL:HG23	1.83	0.78
1:C:945:TYR:O	1:C:961:TYR:OH	2.02	0.78
1:A:709:ILE:HG22	1:A:712:PHE:HE1	1.48	0.77
1:A:633:LYS:HD3	1:A:638:GLN:HE21	1.49	0.77
1:A:873:ASP:OD1	1:A:894:GLY:HA3	1.84	0.77
1:D:822:SER:HB3	1:D:825:HIS:CE1	2.20	0.77
1:D:652:TYR:OH	1:D:664:GLU:OE1	2.02	0.77
1:D:748:LYS:H	1:D:748:LYS:HD2	1.50	0.77
1:D:812:MET:O	1:D:820:ARG:HG2	1.85	0.77
1:A:666:ILE:HD12	1:A:666:ILE:H	1.50	0.76
1:A:915:PRO:HG2	1:A:918:VAL:HG23	1.66	0.76
1:C:733:GLY:HA3	1:C:738:ILE:CD1	2.14	0.76
1:A:714:LEU:HD23	1:A:732:PRO:HB3	1.69	0.75
1:B:888:LYS:HE2	1:D:617:ARG:HH22	1.49	0.75
1:A:907:LYS:HZ2	1:A:914:LEU:HD21	1.51	0.75
1:D:824:LYS:H	1:D:824:LYS:HD2	1.50	0.75
1:B:597:ALA:HB3	1:B:642:ILE:HD11	1.66	0.75
1:C:915:PRO:HD2	1:C:918:VAL:HG11	1.68	0.75
1:C:586:VAL:HG22	1:C:599:LYS:HG2	1.68	0.75
1:C:845:VAL:HG13	1:C:948:MET:CE	2.16	0.75
1:A:867:ARG:HH21	1:A:872:MET:HG3	1.51	0.74
1:C:745:GLU:OE1	1:C:745:GLU:N	2.20	0.74
1:C:915:PRO:HD2	1:C:918:VAL:CG1	2.17	0.74
1:D:757:ILE:HD12	1:D:757:ILE:H	1.50	0.74
1:D:643:GLU:CD	1:D:708:MET:HE1	2.12	0.74
1:D:616:LEU:HD13	1:D:628:TYR:HB2	1.67	0.74
1:D:764:PHE:O	1:D:768:ILE:HG12	1.86	0.74
1:B:843:GLN:OE1	1:B:908:LYS:NZ	2.20	0.74
1:D:784:ASN:O	1:D:788:GLY:N	2.18	0.74
1:C:839:LEU:CD2	1:C:908:LYS:HE2	2.17	0.74
1:C:780:GLN:OE1	1:C:783:ALA:HB3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:LEU:HA	1:B:904:MET:CE	2.17	0.74
1:D:754:THR:HA	1:D:757:ILE:HD13	1.70	0.73
1:A:586:VAL:HG22	1:A:599:LYS:HG2	1.70	0.73
1:D:809:ILE:O	1:D:813:ILE:HG13	1.89	0.73
1:D:848:ARG:HG2	1:D:957:PHE:HE2	1.53	0.73
1:A:572:CYS:HB3	1:A:575:ASP:OD2	1.88	0.73
1:C:609:ALA:O	1:C:613:VAL:HG12	1.87	0.73
1:A:866:GLY:O	1:A:870:VAL:HG22	1.89	0.73
1:C:841:PHE:O	1:C:845:VAL:HG23	1.88	0.73
1:C:795:LEU:O	1:C:806:ARG:NH1	2.21	0.73
1:D:566:VAL:HG21	1:D:639:TYR:CE2	2.23	0.73
1:B:925:LEU:HD23	1:B:926:PRO:HA	1.71	0.72
1:A:917:GLU:OE1	1:A:917:GLU:N	2.22	0.72
1:C:778:SER:HA	1:C:781:ARG:HG3	1.70	0.72
1:B:788:GLY:HA2	1:B:815:MET:CE	2.14	0.72
1:A:925:LEU:HD23	1:A:926:PRO:HA	1.72	0.72
1:D:754:THR:HA	1:D:757:ILE:CD1	2.19	0.72
1:C:768:ILE:HD11	1:C:809:ILE:HD11	1.72	0.72
1:C:800:HIS:CE1	1:C:804:ILE:HD11	2.25	0.72
1:D:795:LEU:CD2	1:D:806:ARG:HG3	2.20	0.71
1:C:733:GLY:CA	1:C:738:ILE:HD11	2.14	0.71
1:C:799:LYS:O	1:C:803:VAL:HG23	1.89	0.71
1:A:898:ARG:O	1:A:902:ARG:HG3	1.90	0.71
1:A:609:ALA:O	1:A:613:VAL:HG12	1.89	0.71
1:B:862:LEU:HD11	1:B:944:THR:HG22	1.73	0.71
1:C:822:SER:O	1:C:826:VAL:HG23	1.90	0.70
1:A:698:MET:HE3	1:A:699:PRO:HD2	1.74	0.70
1:C:925:LEU:HB2	1:C:926:PRO:HA	1.72	0.70
1:D:844:ASP:HB3	1:D:957:PHE:CE1	2.22	0.70
1:C:914:LEU:HB3	1:C:918:VAL:CG1	2.20	0.70
1:B:626:ILE:HD12	1:B:708:MET:HE2	1.74	0.70
1:B:714:LEU:HD22	1:B:732:PRO:HB3	1.72	0.70
1:D:845:VAL:O	1:D:849:ILE:HG12	1.92	0.70
1:B:649:LEU:O	1:B:653:VAL:HG23	1.92	0.69
1:B:858:ILE:HD12	1:B:858:ILE:H	1.56	0.69
1:C:614:GLN:NE2	1:C:618:GLU:OE2	2.26	0.69
1:C:879:THR:OG1	1:C:921:THR:HG21	1.91	0.69
1:C:765:TYR:OH	1:C:794:CYS:HB3	1.92	0.69
1:A:704:LYS:HA	1:A:704:LYS:HE2	1.73	0.69
1:B:633:LYS:HG3	1:B:638:GLN:HG3	1.75	0.69
1:B:569:ILE:CD1	1:B:641:ALA:HB2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:ILE:HG13	1:C:632:GLU:HG3	1.75	0.69
1:D:761:GLY:CA	1:D:812:MET:HE3	2.20	0.69
1:A:725:PHE:CZ	1:A:751:PRO:HB2	2.28	0.69
1:B:695:LEU:HD13	1:B:710:SER:OG	1.93	0.69
1:C:775:PHE:CE2	1:C:785:ILE:HA	2.27	0.69
1:D:740:PRO:HD2	1:D:820:ARG:HH22	1.58	0.69
1:A:808:LEU:CG	1:A:812:MET:HE2	2.20	0.68
1:C:642:ILE:C	1:C:642:ILE:HD12	2.18	0.68
1:D:585:ILE:HD13	1:D:600:ARG:NH2	2.07	0.68
1:D:777:LYS:O	1:D:781:ARG:HG3	1.93	0.68
1:B:763:VAL:O	1:B:767:VAL:HG23	1.93	0.68
1:D:835:LEU:HD12	1:D:835:LEU:H	1.57	0.68
1:D:689:LEU:HB2	1:D:759:SER:HB2	1.75	0.68
1:C:845:VAL:HG13	1:C:948:MET:HE2	1.75	0.68
1:D:793:ASP:N	1:D:793:ASP:OD1	2.26	0.68
1:B:633:LYS:HE3	1:B:638:GLN:HE21	1.59	0.68
1:C:836:GLU:HG2	1:C:926:PRO:HG3	1.76	0.68
1:A:633:LYS:HD3	1:A:638:GLN:NE2	2.08	0.67
1:A:867:ARG:NH2	1:A:872:MET:HA	2.09	0.67
1:C:741:GLU:OE2	1:C:820:ARG:NH1	2.27	0.67
1:C:796:HIS:ND1	1:C:797:PRO:HD2	2.10	0.67
1:D:769:SER:HB3	1:D:772:SER:HB3	1.75	0.67
1:A:724:SEP:O2P	1:C:635:ARG:NH2	2.25	0.67
1:A:879:THR:HG22	1:A:932:TYR:OH	1.94	0.67
1:B:851:LYS:O	1:B:851:LYS:HD3	1.94	0.67
1:A:882:LEU:HG	1:A:886:LEU:HD12	1.74	0.67
1:D:823:ALA:O	1:D:827:LEU:HD22	1.95	0.67
1:A:600:ARG:HH11	1:A:637:PHE:HE2	1.43	0.66
1:C:921:THR:HG22	1:C:932:TYR:HE2	1.59	0.66
1:C:914:LEU:HB3	1:C:918:VAL:HG13	1.76	0.66
1:A:628:TYR:HA	1:A:642:ILE:HG22	1.77	0.66
1:B:788:GLY:CA	1:B:815:MET:HE3	2.14	0.66
1:A:585:ILE:HG13	1:A:600:ARG:NH2	2.11	0.66
1:A:751:PRO:HB3	1:A:755:VAL:HG11	1.78	0.66
1:C:725:PHE:O	1:C:751:PRO:HD2	1.95	0.66
1:C:764:PHE:CD2	1:C:812:MET:HE1	2.32	0.66
1:C:879:THR:HG23	1:C:932:TYR:OH	1.94	0.66
1:A:634:ASP:HB2	1:A:639:TYR:HE1	1.61	0.65
1:C:947:ALA:O	1:C:950:LEU:HD23	1.96	0.65
1:D:643:GLU:OE1	1:D:708:MET:HE1	1.96	0.65
1:D:834:SER:O	1:D:838:GLN:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:764:PHE:CD2	1:D:812:MET:HE1	2.31	0.65
1:A:722:ARG:HG3	1:A:722:ARG:HH11	1.61	0.65
1:B:901:LEU:HA	1:B:904:MET:HE2	1.77	0.65
1:C:919:ARG:HB3	1:C:919:ARG:NH1	2.12	0.65
1:C:572:CYS:SG	1:C:574:LYS:HE2	2.36	0.65
1:B:731:VAL:HG23	1:B:731:VAL:O	1.96	0.65
1:C:888:LYS:HG3	1:C:889:PHE:CE1	2.32	0.65
1:B:714:LEU:HD22	1:B:732:PRO:CB	2.26	0.65
1:C:567:GLY:HA3	1:C:632:GLU:OE2	1.96	0.65
1:C:738:ILE:HB	1:C:782:GLN:HE22	1.61	0.65
1:D:848:ARG:O	1:D:848:ARG:NH1	2.27	0.65
1:A:591:PHE:O	1:A:594:ARG:HB2	1.96	0.65
1:B:615:LEU:HD12	1:B:684:ILE:HD13	1.79	0.64
1:A:725:PHE:O	1:A:751:PRO:HD2	1.97	0.64
1:D:741:GLU:HG2	1:D:817:PRO:HG3	1.78	0.64
1:D:792:LEU:HB2	1:D:806:ARG:NH1	2.12	0.64
1:D:964:GLU:OE1	1:D:964:GLU:N	2.31	0.64
1:C:613:VAL:HG23	1:C:628:TYR:CZ	2.33	0.64
1:A:853:SER:HA	1:D:728:ARG:HA	1.80	0.64
1:A:603:PRO:HA	1:A:606:PHE:CD1	2.33	0.64
1:B:664:GLU:O	1:B:668:LEU:HD13	1.98	0.64
1:B:746:ASP:OD2	1:B:748:LYS:HG3	1.97	0.64
1:C:634:ASP:HB2	1:C:639:TYR:CE1	2.31	0.64
1:D:649:LEU:O	1:D:653:VAL:HG23	1.97	0.64
1:A:616:LEU:HD13	1:A:628:TYR:HB2	1.78	0.64
1:C:572:CYS:SG	1:C:574:LYS:HG2	2.38	0.64
1:D:955:ARG:HA	1:D:958:GLN:HB2	1.80	0.64
1:D:590:MET:HE1	1:D:595:ASP:OD1	1.98	0.63
1:C:800:HIS:CD2	1:C:934:THR:HB	2.34	0.63
1:B:845:VAL:O	1:B:849:ILE:HG12	1.98	0.63
1:D:669:LEU:HD21	1:D:767:VAL:HG21	1.80	0.63
1:C:759:SER:O	1:C:763:VAL:HG23	1.99	0.63
1:C:816:ASP:HB3	1:C:819:LYS:HG3	1.79	0.63
1:C:880:VAL:O	1:C:884:THR:HG23	1.99	0.63
1:C:926:PRO:O	1:C:930:VAL:HG12	1.97	0.63
1:A:688:ASP:O	1:A:693:ASN:ND2	2.32	0.63
1:B:890:ARG:NH2	1:D:567:GLY:HA3	2.14	0.63
1:C:845:VAL:O	1:C:849:ILE:HG12	1.98	0.63
1:B:622:HIS:CG	1:B:623:PRO:HD2	2.34	0.63
1:B:759:SER:O	1:B:763:VAL:HG23	1.99	0.63
1:D:735:GLU:HG2	1:D:782:GLN:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:746:ASP:OD2	1:D:748:LYS:HE3	1.99	0.63
1:A:567:GLY:HA3	1:A:632:GLU:OE2	1.99	0.62
1:B:623:PRO:O	1:B:706:LYS:NZ	2.32	0.62
1:B:650:GLN:O	1:B:654:GLU:HG3	1.98	0.62
1:C:764:PHE:O	1:C:768:ILE:HG12	1.99	0.62
1:A:882:LEU:HG	1:A:886:LEU:CD1	2.29	0.62
1:C:669:LEU:HD11	1:C:767:VAL:HG21	1.81	0.62
1:A:613:VAL:HG23	1:A:628:TYR:CZ	2.35	0.62
1:D:808:LEU:HB2	1:D:829:HIS:NE2	2.14	0.62
1:B:761:GLY:HA2	1:B:812:MET:HE2	1.82	0.62
1:D:618:GLU:OE1	1:D:717:LYS:NZ	2.30	0.62
1:C:618:GLU:OE1	1:C:717:LYS:NZ	2.33	0.62
1:B:642:ILE:HD13	2:B:1001:A1IOO:C1	2.30	0.62
1:B:752:THR:HG23	1:B:754:THR:H	1.65	0.62
1:B:871:LYS:O	1:B:872:MET:HB2	1.99	0.62
1:D:848:ARG:HG2	1:D:957:PHE:CE2	2.34	0.61
1:A:915:PRO:HG2	1:A:918:VAL:CG2	2.29	0.61
1:A:807:GLU:HG2	1:A:829:HIS:HE2	1.65	0.61
1:C:780:GLN:OE1	1:C:780:GLN:HA	1.99	0.61
1:D:656:LYS:HB3	1:D:661:LEU:HD21	1.82	0.61
1:D:687:ARG:CZ	1:D:716:LYS:HB2	2.30	0.61
1:D:657:ASP:O	1:D:661:LEU:HD13	2.00	0.61
1:D:725:PHE:O	1:D:751:PRO:HD2	2.01	0.61
1:A:569:ILE:CD1	1:A:632:GLU:HG3	2.31	0.61
1:D:614:GLN:O	1:D:618:GLU:HG3	2.00	0.61
1:C:807:GLU:HG3	1:C:946:ARG:HH21	1.66	0.61
1:D:784:ASN:HA	1:D:787:LEU:HB2	1.83	0.61
1:D:759:SER:O	1:D:763:VAL:HG23	2.01	0.61
1:D:676:LEU:HD22	1:D:680:HIS:NE2	2.16	0.60
1:B:910:HIS:O	1:B:914:LEU:HD13	2.01	0.60
1:C:597:ALA:HB2	1:C:644:LEU:HD23	1.83	0.60
1:A:657:ASP:O	1:A:658:PHE:HB2	2.01	0.60
1:C:952:SER:OG	1:C:963:HIS:ND1	2.33	0.60
1:D:583:GLY:C	1:D:602:LEU:HD21	2.27	0.60
1:C:620:ASP:HB2	1:C:627:ARG:HA	1.84	0.60
1:A:808:LEU:HG	1:A:812:MET:CE	2.26	0.60
1:A:900:LEU:O	1:A:904:MET:HG3	2.01	0.60
1:B:584:THR:C	1:B:585:ILE:HD13	2.27	0.60
1:C:845:VAL:CG1	1:C:948:MET:HE2	2.32	0.60
1:B:888:LYS:HE2	1:D:617:ARG:NH2	2.16	0.60
1:C:852:GLU:HG3	1:C:859:VAL:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:800:HIS:O	1:C:804:ILE:HD12	2.01	0.59
1:D:566:VAL:HG12	1:D:632:GLU:HB3	1.82	0.59
1:D:583:GLY:O	1:D:602:LEU:HD21	2.02	0.59
1:A:748:LYS:HE3	1:A:749:GLU:CB	2.28	0.59
1:C:765:TYR:HD2	1:C:774:PRO:HD3	1.68	0.59
1:A:738:ILE:HB	1:A:782:GLN:NE2	2.17	0.59
1:B:799:LYS:O	1:B:803:VAL:HG23	2.03	0.59
1:C:600:ARG:HG3	1:C:637:PHE:CD1	2.32	0.59
1:D:949:GLU:N	1:D:961:TYR:HH	2.01	0.59
1:D:690:LYS:HE2	1:D:734:THR:HG21	1.84	0.59
1:A:890:ARG:HG2	1:A:890:ARG:NH1	2.15	0.58
1:D:758:PHE:HB2	1:D:820:ARG:NH1	2.18	0.58
1:C:601:ILE:HG23	1:C:605:CYS:HB2	1.84	0.58
1:C:634:ASP:OD1	1:C:635:ARG:N	2.34	0.58
1:D:841:PHE:O	1:D:845:VAL:HG22	2.03	0.58
1:A:687:ARG:NH1	1:A:729:SEP:O2P	2.31	0.58
1:A:896:SER:HB3	1:A:899:ASP:HB2	1.84	0.58
1:A:905:ARG:O	1:A:905:ARG:NH1	2.36	0.58
1:B:645:CYS:HB2	1:B:695:LEU:HD23	1.84	0.58
1:B:867:ARG:NH1	1:B:872:MET:HE1	2.18	0.58
1:A:956:LEU:HD12	1:A:956:LEU:O	2.03	0.58
1:D:784:ASN:HB3	1:D:789:ALA:HB3	1.86	0.58
1:A:666:ILE:HD12	1:A:666:ILE:N	2.17	0.58
1:A:698:MET:HE3	1:A:699:PRO:CD	2.33	0.58
1:A:932:TYR:O	1:A:936:ARG:HD2	2.02	0.58
1:B:738:ILE:CG2	1:B:743:LEU:HD23	2.24	0.58
1:A:731:VAL:HG12	1:A:731:VAL:O	2.03	0.58
1:B:749:GLU:OE2	1:B:750:ASN:N	2.33	0.58
1:B:890:ARG:HH22	1:D:567:GLY:HA3	1.68	0.58
1:C:690:LYS:HE2	1:C:734:THR:OG1	2.04	0.58
1:B:571:PHE:HE1	1:B:639:TYR:HE2	1.50	0.58
1:A:569:ILE:HD11	1:A:632:GLU:HG3	1.85	0.58
1:D:718:LEU:HD21	1:D:725:PHE:HB3	1.84	0.58
1:A:649:LEU:O	1:A:653:VAL:HG23	2.04	0.58
1:B:663:LEU:O	1:B:667:THR:HG23	2.04	0.58
1:C:796:HIS:N	1:C:802:ASP:OD2	2.36	0.58
1:A:585:ILE:CG1	1:A:600:ARG:HH21	2.15	0.57
1:C:839:LEU:HD23	1:C:839:LEU:O	2.04	0.57
1:B:648:THR:OG1	1:B:651:GLU:HG3	2.04	0.57
1:C:779:LEU:HD12	1:C:780:GLN:CB	2.34	0.57
1:B:616:LEU:HD13	1:B:628:TYR:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:886:LEU:CD2	1:B:907:LYS:HE2	2.34	0.57
1:A:661:LEU:HD12	1:A:664:GLU:HB3	1.86	0.57
1:C:845:VAL:HG13	1:C:948:MET:HE3	1.83	0.57
1:A:697:SER:HB3	1:A:706:LYS:HG3	1.85	0.57
1:C:878:ILE:HD12	1:C:882:LEU:CB	2.32	0.57
1:D:669:LEU:HD22	1:D:764:PHE:CD1	2.39	0.57
1:C:885:ASP:C	1:C:886:LEU:HD23	2.28	0.57
1:B:752:THR:O	1:B:755:VAL:HG22	2.05	0.57
1:A:600:ARG:C	1:A:601:ILE:HD13	2.30	0.57
1:B:852:GLU:CD	1:B:858:ILE:HD13	2.29	0.57
1:C:869:VAL:HG12	1:C:939:HIS:CB	2.34	0.57
1:D:600:ARG:HD2	1:D:637:PHE:CD1	2.39	0.57
1:A:635:ARG:HB2	1:A:636:GLN:OE1	2.05	0.57
1:A:828:LYS:HD3	1:A:961:TYR:O	2.05	0.57
1:B:808:LEU:HB2	1:B:829:HIS:CE1	2.39	0.57
1:C:642:ILE:HD11	2:C:1001:A1IOO:C1	2.35	0.57
1:D:695:LEU:HD11	1:D:710:SER:OG	2.05	0.57
1:A:612:GLU:HB2	1:A:713:GLY:HA2	1.87	0.56
1:A:613:VAL:HG22	1:A:617:ARG:HH21	1.69	0.56
1:B:584:THR:O	1:B:585:ILE:HD13	2.04	0.56
1:A:695:LEU:HD12	1:A:695:LEU:N	2.20	0.56
1:D:712:PHE:HA	1:D:715:CYS:SG	2.45	0.56
1:A:812:MET:O	1:A:820:ARG:HD3	2.05	0.56
1:B:637:PHE:HB2	1:B:639:TYR:CE1	2.40	0.56
1:B:888:LYS:CE	1:D:617:ARG:HH22	2.17	0.56
1:B:932:TYR:O	1:B:936:ARG:HD2	2.04	0.56
1:C:582:GLU:N	1:C:582:GLU:OE1	2.38	0.56
1:C:843:GLN:OE1	1:C:908:LYS:NZ	2.35	0.56
1:D:758:PHE:HZ	1:D:785:ILE:HD13	1.69	0.56
1:B:654:GLU:O	1:B:655:GLN:NE2	2.39	0.56
1:B:586:VAL:HG22	1:B:599:LYS:HG2	1.87	0.56
1:C:870:VAL:HB	1:C:874:TRP:HB3	1.87	0.56
1:D:739:ALA:HA	1:D:758:PHE:CD2	2.40	0.56
1:D:809:ILE:HA	1:D:812:MET:HE2	1.88	0.56
1:A:879:THR:HG21	1:A:921:THR:OG1	2.06	0.56
1:C:925:LEU:HB3	1:C:929:PHE:CB	2.36	0.56
1:D:582:GLU:O	1:D:602:LEU:HD23	2.05	0.56
1:D:613:VAL:HG13	1:D:628:TYR:CZ	2.41	0.56
1:B:862:LEU:CD1	1:B:944:THR:HG22	2.35	0.56
1:D:837:LYS:NZ	1:D:837:LYS:HB3	2.20	0.56
1:A:634:ASP:HB2	1:A:639:TYR:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:MET:CA	1:A:815:MET:HE2	2.37	0.55
1:D:695:LEU:HD11	1:D:710:SER:CB	2.36	0.55
1:D:714:LEU:HD12	1:D:732:PRO:HB2	1.87	0.55
1:A:698:MET:CE	1:A:699:PRO:HD2	2.36	0.55
1:D:664:GLU:HB3	1:D:665:PRO:HD3	1.87	0.55
1:D:774:PRO:HG2	1:D:775:PHE:CD1	2.42	0.55
1:C:672:THR:HG23	1:C:709:ILE:HD11	1.88	0.55
1:C:782:GLN:OE1	1:C:782:GLN:HA	2.06	0.55
1:D:763:VAL:O	1:D:767:VAL:HG22	2.05	0.55
1:B:622:HIS:HB2	1:B:678:HIS:CE1	2.42	0.55
1:C:738:ILE:HB	1:C:782:GLN:NE2	2.22	0.55
1:C:898:ARG:HA	1:C:901:LEU:HD12	1.87	0.55
1:B:652:TYR:OH	1:B:661:LEU:HD12	2.06	0.55
1:C:809:ILE:O	1:C:813:ILE:HG12	2.06	0.55
1:D:600:ARG:HG2	1:D:600:ARG:HH11	1.71	0.55
1:D:731:VAL:HG11	1:D:743:LEU:CD2	2.32	0.55
1:A:774:PRO:HB3	1:A:792:LEU:HD21	1.88	0.55
1:C:845:VAL:CG1	1:C:948:MET:CE	2.85	0.55
1:B:622:HIS:ND1	1:B:623:PRO:HD2	2.22	0.55
1:B:718:LEU:HD23	1:B:723:HIS:HA	1.88	0.55
1:C:706:LYS:HE2	1:C:708:MET:CE	2.33	0.55
1:C:591:PHE:O	1:C:594:ARG:HB2	2.07	0.55
1:A:603:PRO:HA	1:A:606:PHE:CE1	2.42	0.54
1:C:888:LYS:HG3	1:C:889:PHE:CD1	2.41	0.54
1:D:741:GLU:OE2	1:D:820:ARG:NH1	2.40	0.54
1:D:801:GLU:O	1:D:804:ILE:N	2.40	0.54
1:C:870:VAL:HA	1:C:937:PHE:CD2	2.41	0.54
1:C:871:LYS:HD3	1:C:871:LYS:N	2.21	0.54
1:A:722:ARG:HG3	1:A:722:ARG:NH1	2.22	0.54
1:A:800:HIS:CG	1:A:934:THR:HB	2.43	0.54
1:A:867:ARG:NH2	1:A:872:MET:HG3	2.21	0.54
1:D:741:GLU:CG	1:D:817:PRO:HG3	2.37	0.54
1:D:773:HIS:CG	1:D:781:ARG:HD2	2.42	0.54
1:B:690:LYS:HD3	1:B:734:THR:HG21	1.89	0.54
1:C:860:LYS:O	1:C:860:LYS:HD3	2.08	0.54
1:C:922:LEU:HD13	1:C:929:PHE:CD2	2.43	0.54
1:A:731:VAL:CG1	1:A:738:ILE:HD13	2.38	0.54
1:A:903:ALA:O	1:A:907:LYS:HG2	2.08	0.54
1:B:624:ASN:ND2	1:B:671:GLN:HB3	2.22	0.54
1:B:729:SEP:O	1:B:732:PRO:HD3	2.08	0.54
1:B:879:THR:HG21	1:B:921:THR:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:678:HIS:NE2	1:D:682:LEU:HD11	2.23	0.54
1:D:733:GLY:CA	1:D:738:ILE:HD11	2.34	0.54
1:D:824:LYS:HA	1:D:827:LEU:HD23	1.89	0.53
1:C:647:ALA:HA	2:C:1001:A1IOO:C17	2.38	0.53
1:B:879:THR:HG22	1:B:932:TYR:OH	2.09	0.53
1:D:565:ILE:O	1:D:565:ILE:CD1	2.56	0.53
1:D:690:LYS:HG3	1:D:692:HIS:H	1.72	0.53
1:D:700:ASN:HD21	1:D:702:HIS:HB2	1.73	0.53
1:A:577:LEU:HB2	1:A:586:VAL:HG12	1.91	0.53
1:A:630:CYS:HA	1:B:592:ASP:OD2	2.08	0.53
1:A:746:ASP:OD2	1:A:746:ASP:C	2.51	0.53
1:D:783:ALA:O	1:D:785:ILE:N	2.37	0.53
1:A:658:PHE:HA	1:A:661:LEU:HB2	1.91	0.53
1:D:823:ALA:HB3	1:D:824:LYS:HE3	1.91	0.53
1:A:738:ILE:HG22	1:A:743:LEU:HD11	1.91	0.53
1:C:603:PRO:HA	1:C:606:PHE:CD1	2.44	0.53
1:C:919:ARG:HB3	1:C:919:ARG:HH11	1.73	0.53
1:D:781:ARG:O	1:D:785:ILE:HG13	2.07	0.53
1:C:873:ASP:OD1	1:C:875:ARG:HB2	2.09	0.53
1:C:907:LYS:CD	1:C:914:LEU:HD11	2.38	0.53
1:A:769:SER:HB2	1:A:772:SER:HB2	1.90	0.53
1:C:862:LEU:O	1:C:897:VAL:HG21	2.09	0.53
1:D:824:LYS:H	1:D:824:LYS:CD	2.19	0.53
1:C:773:HIS:CG	1:C:781:ARG:HD3	2.43	0.52
1:C:792:LEU:N	1:C:792:LEU:HD12	2.25	0.52
1:C:849:ILE:CD1	1:C:898:ARG:HG3	2.18	0.52
1:C:958:GLN:HG2	1:C:959:PRO:HD3	1.91	0.52
1:B:697:SER:OG	1:B:706:LYS:HG2	2.10	0.52
1:C:779:LEU:HD12	1:C:780:GLN:HB2	1.90	0.52
1:A:888:LYS:HG3	1:A:889:PHE:CD2	2.44	0.52
1:B:796:HIS:CG	1:B:797:PRO:HD2	2.45	0.52
1:B:854:LEU:HD22	1:B:854:LEU:N	2.25	0.52
1:C:684:ILE:HG13	1:C:717:LYS:HD2	1.92	0.52
1:C:839:LEU:HD23	1:C:839:LEU:C	2.34	0.52
1:A:668:LEU:O	1:A:672:THR:HG23	2.08	0.52
1:A:774:PRO:HB3	1:A:792:LEU:CD2	2.39	0.52
1:B:901:LEU:HA	1:B:904:MET:HE3	1.91	0.52
1:C:823:ALA:O	1:C:827:LEU:HD13	2.10	0.52
1:B:873:ASP:HA	1:B:894:GLY:O	2.10	0.52
1:D:626:ILE:HA	1:D:708:MET:HE2	1.92	0.52
1:B:633:LYS:CE	1:B:638:GLN:HE21	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:774:PRO:O	1:C:790:CYS:HA	2.10	0.51
1:C:808:LEU:HG	1:C:812:MET:HE2	1.91	0.51
1:A:574:LYS:HD2	1:A:574:LYS:N	2.24	0.51
1:A:636:GLN:OE1	1:A:636:GLN:N	2.43	0.51
1:B:601:ILE:HD12	1:B:601:ILE:N	2.24	0.51
1:D:614:GLN:OE1	1:D:614:GLN:HA	2.11	0.51
1:D:615:LEU:HD12	1:D:715:CYS:HB2	1.92	0.51
1:D:700:ASN:ND2	1:D:702:HIS:H	2.08	0.51
1:A:830:PRO:HD3	1:A:945:TYR:CZ	2.46	0.51
1:C:867:ARG:HH21	1:C:872:MET:HG3	1.75	0.51
1:A:907:LYS:NZ	1:A:914:LEU:CD2	2.72	0.51
1:C:600:ARG:O	1:C:600:ARG:HG2	2.10	0.51
1:C:692:HIS:C	1:C:692:HIS:CD2	2.88	0.51
1:A:622:HIS:HB2	1:A:678:HIS:CE1	2.45	0.51
1:B:670:GLN:HB2	1:B:832:PHE:CE1	2.45	0.51
1:B:866:GLY:O	1:B:870:VAL:HG22	2.10	0.51
1:D:614:GLN:OE1	1:D:617:ARG:NH2	2.36	0.51
1:D:792:LEU:HB2	1:D:806:ARG:HH11	1.76	0.51
1:A:754:THR:HB	1:A:820:ARG:HH11	1.76	0.51
1:A:815:MET:HE2	1:A:815:MET:HA	1.92	0.51
1:C:922:LEU:HD13	1:C:929:PHE:CE2	2.46	0.51
1:C:953:HIS:HD2	1:C:954:GLU:N	2.09	0.51
1:A:763:VAL:O	1:A:767:VAL:HG23	2.11	0.50
1:C:709:ILE:HG22	1:C:712:PHE:CE1	2.46	0.50
1:D:774:PRO:HG2	1:D:775:PHE:HD1	1.74	0.50
1:D:775:PHE:CD2	1:D:785:ILE:HD13	2.45	0.50
1:C:582:GLU:HB3	1:C:605:CYS:SG	2.51	0.50
1:D:669:LEU:HD22	1:D:764:PHE:HD1	1.76	0.50
1:A:748:LYS:HG3	1:A:749:GLU:OE2	2.11	0.50
1:D:818:GLN:OE1	1:D:818:GLN:N	2.44	0.50
1:A:652:TYR:O	1:A:656:LYS:HB2	2.11	0.50
1:B:613:VAL:HG13	1:B:628:TYR:CE2	2.46	0.50
1:B:901:LEU:HD23	1:B:904:MET:HE1	1.92	0.50
1:C:874:TRP:HB2	1:C:937:PHE:CZ	2.47	0.50
1:D:630:CYS:SG	1:D:631:THR:N	2.83	0.50
1:D:718:LEU:CD2	1:D:725:PHE:HB3	2.42	0.50
1:A:652:TYR:OH	1:A:661:LEU:HD12	2.11	0.50
1:A:695:LEU:HD11	1:A:710:SER:OG	2.12	0.50
1:A:829:HIS:CG	1:A:830:PRO:HD2	2.45	0.50
1:B:896:SER:HB3	1:B:899:ASP:HB2	1.92	0.50
1:B:841:PHE:O	1:B:845:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:956:LEU:HD12	1:B:956:LEU:O	2.11	0.50
1:C:631:THR:O	1:C:631:THR:HG23	2.12	0.50
1:C:672:THR:CG2	1:C:709:ILE:HD11	2.42	0.50
1:B:614:GLN:O	1:B:618:GLU:HG3	2.12	0.49
1:C:800:HIS:CE1	1:C:804:ILE:CD1	2.95	0.49
1:D:726:SEP:HA	1:D:750:ASN:ND2	2.26	0.49
1:A:612:GLU:HG3	1:A:712:PHE:HB2	1.95	0.49
1:B:886:LEU:HD21	1:B:907:LYS:HE2	1.94	0.49
1:A:907:LYS:HZ1	1:A:914:LEU:HD21	1.72	0.49
1:B:600:ARG:C	1:B:601:ILE:HD12	2.38	0.49
1:B:601:ILE:HG23	1:B:605:CYS:HB2	1.93	0.49
1:B:773:HIS:CD2	1:B:781:ARG:HD3	2.46	0.49
1:B:890:ARG:O	1:B:890:ARG:HG3	2.12	0.49
1:D:601:ILE:N	1:D:601:ILE:HD12	2.27	0.49
1:D:949:GLU:HA	1:D:961:TYR:CE2	2.47	0.49
1:C:905:ARG:HD2	1:C:905:ARG:O	2.13	0.49
1:B:879:THR:HG23	1:B:882:LEU:H	1.78	0.49
1:C:752:THR:HG23	1:C:753:TYR:N	2.27	0.49
1:C:915:PRO:HD2	1:C:918:VAL:HG12	1.95	0.49
1:D:837:LYS:HB3	1:D:837:LYS:HZ2	1.76	0.49
1:B:726:SEP:OG	1:B:728:ARG:NH1	2.45	0.49
1:B:761:GLY:CA	1:B:812:MET:HE2	2.42	0.49
1:C:812:MET:O	1:C:820:ARG:HD3	2.13	0.49
1:C:913:GLU:N	1:C:913:GLU:OE1	2.46	0.49
1:C:921:THR:HG22	1:C:932:TYR:CE2	2.45	0.49
1:D:814:ALA:O	1:D:820:ARG:NE	2.36	0.49
1:B:602:LEU:HD23	1:B:602:LEU:N	2.26	0.49
1:B:634:ASP:HB3	1:B:637:PHE:H	1.77	0.49
1:B:796:HIS:ND1	1:B:797:PRO:HD2	2.28	0.49
1:D:845:VAL:O	1:D:849:ILE:HG23	2.13	0.49
1:D:709:ILE:HG22	1:D:712:PHE:HE1	1.78	0.49
1:B:854:LEU:HD22	1:B:854:LEU:H	1.77	0.49
1:D:801:GLU:N	1:D:803:VAL:HG22	2.28	0.49
1:D:622:HIS:ND1	1:D:623:PRO:HD2	2.27	0.48
1:D:735:GLU:CG	1:D:782:GLN:HB2	2.43	0.48
1:C:657:ASP:O	1:C:661:LEU:HD23	2.13	0.48
1:D:648:THR:HG23	1:D:651:GLU:H	1.78	0.48
1:C:779:LEU:HD12	1:C:780:GLN:H	1.77	0.48
1:D:732:PRO:HD2	1:D:742:MET:HE1	1.95	0.48
1:C:685:VAL:CG2	1:C:716:LYS:HB3	2.43	0.48
1:D:631:THR:HG23	1:D:631:THR:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:LEU:HD21	1:B:756:ASP:HB3	1.95	0.48
1:C:564:VAL:O	1:C:570:SER:HA	2.14	0.48
1:D:695:LEU:CD1	1:D:710:SER:HB3	2.43	0.48
1:D:828:LYS:HZ1	1:D:962:PHE:HD1	1.59	0.48
1:A:807:GLU:OE1	1:A:811:LYS:HE3	2.13	0.48
1:D:731:VAL:HG13	1:D:742:MET:HB3	1.95	0.48
1:D:740:PRO:HG2	1:D:815:MET:SD	2.53	0.48
1:D:768:ILE:HD11	1:D:809:ILE:HD11	1.95	0.48
1:A:690:LYS:HE2	1:A:734:THR:OG1	2.13	0.48
1:A:809:ILE:O	1:A:813:ILE:HG12	2.13	0.48
1:C:769:SER:HB2	1:C:772:SER:HB2	1.96	0.48
1:C:873:ASP:OD1	1:C:894:GLY:HA3	2.14	0.48
1:C:882:LEU:O	1:C:886:LEU:HG	2.14	0.48
1:B:825:HIS:CD2	1:B:962:PHE:HB3	2.49	0.48
1:C:958:GLN:N	1:C:959:PRO:CD	2.77	0.48
1:D:817:PRO:HA	1:D:820:ARG:HD2	1.96	0.48
1:B:809:ILE:O	1:B:813:ILE:HG12	2.14	0.47
1:D:586:VAL:HG22	1:D:599:LYS:HG2	1.96	0.47
1:D:622:HIS:HB2	1:D:678:HIS:ND1	2.29	0.47
1:D:801:GLU:HG2	1:D:802:ASP:H	1.78	0.47
1:B:637:PHE:HB2	1:B:639:TYR:HE1	1.79	0.47
1:C:581:ALA:HB1	1:C:582:GLU:OE1	2.14	0.47
1:C:879:THR:HG21	1:C:921:THR:CG2	2.44	0.47
1:D:765:TYR:O	1:D:769:SER:HB2	2.14	0.47
1:A:807:GLU:OE2	1:A:946:ARG:HD2	2.14	0.47
1:A:882:LEU:O	1:A:886:LEU:HD12	2.14	0.47
1:A:888:LYS:HG3	1:A:889:PHE:CE2	2.49	0.47
1:C:807:GLU:O	1:C:811:LYS:HG3	2.13	0.47
1:C:896:SER:HB3	1:C:899:ASP:HB2	1.96	0.47
1:D:585:ILE:HD12	1:D:585:ILE:N	2.30	0.47
1:D:622:HIS:CG	1:D:623:PRO:HD2	2.50	0.47
1:D:733:GLY:HA3	1:D:738:ILE:CD1	2.35	0.47
1:A:622:HIS:CG	1:A:623:PRO:HD2	2.48	0.47
1:B:809:ILE:HD12	1:B:809:ILE:N	2.29	0.47
1:C:569:ILE:HD12	1:C:632:GLU:HB2	1.96	0.47
1:C:829:HIS:CG	1:C:830:PRO:HD2	2.50	0.47
1:D:803:VAL:HG23	1:D:804:ILE:N	2.29	0.47
1:D:829:HIS:CG	1:D:830:PRO:HD2	2.49	0.47
1:A:628:TYR:OH	1:A:631:THR:HG22	2.14	0.47
1:C:642:ILE:C	1:C:642:ILE:CD1	2.87	0.47
1:D:748:LYS:HD2	1:D:748:LYS:N	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:GLU:OE1	1:B:717:LYS:NZ	2.48	0.47
1:B:873:ASP:O	1:B:877:ASN:ND2	2.48	0.47
1:D:795:LEU:HD23	1:D:806:ARG:CG	2.37	0.47
1:D:739:ALA:HB1	1:D:741:GLU:OE1	2.14	0.47
1:D:773:HIS:CG	1:D:774:PRO:HD2	2.50	0.47
1:D:812:MET:HA	1:D:821:PRO:HD2	1.97	0.47
1:A:676:LEU:HD21	1:A:680:HIS:NE2	2.30	0.47
1:A:863:GLU:CD	1:A:897:VAL:HG22	2.40	0.47
1:D:677:ALA:HB2	1:D:823:ALA:HB1	1.97	0.47
1:A:564:VAL:HG23	1:A:573:PRO:HD3	1.97	0.46
1:A:594:ARG:NH2	1:B:620:ASP:OD2	2.48	0.46
1:B:601:ILE:CG2	1:B:605:CYS:HB2	2.45	0.46
1:D:761:GLY:HA2	1:D:812:MET:HE1	1.92	0.46
1:B:807:GLU:HG2	1:B:829:HIS:HE2	1.80	0.46
1:C:579:HIS:CE1	1:C:585:ILE:HG12	2.50	0.46
1:C:599:LYS:HE3	1:C:601:ILE:HD11	1.96	0.46
1:C:676:LEU:HD21	1:C:756:ASP:HB3	1.97	0.46
1:A:584:THR:HG22	1:A:601:ILE:HD12	1.97	0.46
1:A:738:ILE:HB	1:A:782:GLN:HE22	1.79	0.46
1:A:807:GLU:CD	1:A:946:ARG:HD2	2.40	0.46
1:C:670:GLN:HB2	1:C:832:PHE:CE1	2.50	0.46
1:D:602:LEU:N	1:D:602:LEU:HD22	2.31	0.46
1:D:633:LYS:HE2	1:D:638:GLN:OE1	2.15	0.46
1:C:650:GLN:O	1:C:654:GLU:HG3	2.16	0.46
1:C:925:LEU:HB3	1:C:929:PHE:HB2	1.97	0.46
1:B:606:PHE:CE1	1:B:638:GLN:HB2	2.50	0.46
1:B:785:ILE:O	1:B:815:MET:HE1	2.16	0.46
1:D:765:TYR:CE2	1:D:792:LEU:HD23	2.51	0.46
1:D:828:LYS:CE	1:D:962:PHE:HB2	2.39	0.46
1:A:667:THR:HG22	1:A:671:GLN:NE2	2.31	0.46
1:A:841:PHE:CE2	1:A:845:VAL:HG21	2.51	0.46
1:B:881:PRO:HG2	1:B:921:THR:HG21	1.98	0.46
1:D:958:GLN:HB3	1:D:959:PRO:HD3	1.97	0.46
1:A:579:HIS:HE1	1:A:583:GLY:HA2	1.80	0.46
1:B:829:HIS:CD2	1:B:830:PRO:HD2	2.51	0.46
1:C:732:PRO:HD2	1:C:742:MET:CE	2.39	0.46
1:D:773:HIS:CG	1:D:781:ARG:CD	2.99	0.46
1:A:862:LEU:O	1:A:897:VAL:HG21	2.16	0.45
1:B:645:CYS:CB	1:B:695:LEU:HD23	2.45	0.45
1:A:853:SER:CA	1:D:728:ARG:HG2	2.46	0.45
1:B:616:LEU:HD23	1:B:616:LEU:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:611:ARG:HH21	1:C:715:CYS:N	2.14	0.45
1:D:848:ARG:NE	1:D:951:CYS:SG	2.89	0.45
1:A:914:LEU:O	1:A:919:ARG:NH1	2.48	0.45
1:C:914:LEU:HB3	1:C:918:VAL:HG11	1.99	0.45
1:A:594:ARG:HG3	1:B:617:ARG:HD2	1.97	0.45
1:A:600:ARG:HG2	1:A:637:PHE:HD2	1.81	0.45
1:B:764:PHE:O	1:B:768:ILE:HG23	2.16	0.45
1:C:746:ASP:C	1:C:746:ASP:OD1	2.59	0.45
1:D:673:THR:HB	1:D:827:LEU:HD11	1.97	0.45
1:C:768:ILE:HD11	1:C:809:ILE:CD1	2.45	0.45
1:D:727:ARG:NH1	1:D:744:SER:O	2.49	0.45
1:A:743:LEU:HD12	1:A:743:LEU:H	1.82	0.45
1:B:851:LYS:HD3	1:B:851:LYS:C	2.42	0.45
1:B:920:GLU:HA	1:B:920:GLU:OE1	2.16	0.45
1:C:586:VAL:CG2	1:C:599:LYS:HG2	2.44	0.45
1:D:727:ARG:HH12	1:D:745:GLU:HA	1.81	0.45
1:D:744:SER:OG	1:D:748:LYS:NZ	2.50	0.45
1:D:775:PHE:CZ	1:D:813:ILE:HB	2.51	0.45
1:C:679:LEU:HD21	1:C:712:PHE:HE2	1.82	0.45
1:D:619:SER:HB3	1:D:682:LEU:HD13	1.98	0.45
1:A:741:GLU:OE2	1:A:755:VAL:HG12	2.17	0.45
1:C:635:ARG:C	1:C:636:GLN:HG2	2.41	0.45
1:C:765:TYR:CD2	1:C:774:PRO:HD3	2.51	0.45
1:C:802:ASP:O	1:C:806:ARG:HB2	2.17	0.45
1:D:722:ARG:HH21	1:D:724:SEP:P	2.39	0.45
1:A:688:ASP:OD1	1:A:690:LYS:HE2	2.16	0.44
1:A:796:HIS:CG	1:A:797:PRO:HD2	2.52	0.44
1:C:603:PRO:HA	1:C:606:PHE:CE1	2.53	0.44
1:B:834:SER:O	1:B:838:GLN:HG3	2.16	0.44
1:C:568:LYS:HB3	1:C:568:LYS:HE3	1.47	0.44
1:C:922:LEU:HD23	1:C:922:LEU:HA	1.83	0.44
1:D:622:HIS:HB2	1:D:678:HIS:CE1	2.52	0.44
1:A:845:VAL:HG11	1:A:944:THR:CG2	2.46	0.44
1:B:597:ALA:HB3	1:B:642:ILE:HD12	1.97	0.44
1:B:828:LYS:HE3	1:B:961:TYR:O	2.17	0.44
1:C:599:LYS:HB3	1:C:601:ILE:HD11	1.99	0.44
1:A:698:MET:HG3	1:A:699:PRO:HD2	2.00	0.44
1:A:907:LYS:HE3	1:A:914:LEU:HD11	1.99	0.44
1:B:748:LYS:H	1:B:748:LYS:NZ	2.15	0.44
1:B:879:THR:HG21	1:B:921:THR:CB	2.48	0.44
1:D:611:ARG:NH2	1:D:716:LYS:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:775:PHE:HZ	1:D:813:ILE:HB	1.81	0.44
1:C:626:ILE:HD12	1:C:708:MET:SD	2.57	0.44
1:C:841:PHE:CZ	1:C:945:TYR:HD1	2.36	0.44
1:D:646:ALA:HB2	1:D:698:MET:HA	1.99	0.44
1:D:658:PHE:HA	1:D:661:LEU:HD22	1.99	0.44
1:B:631:THR:HG23	1:B:639:TYR:O	2.17	0.44
1:D:601:ILE:HG23	1:D:605:CYS:HB2	2.00	0.44
1:D:635:ARG:HH11	1:D:635:ARG:HB2	1.83	0.44
1:B:676:LEU:HG	1:B:680:HIS:CE1	2.52	0.44
1:C:596:VAL:HB	1:C:642:ILE:O	2.17	0.44
1:D:678:HIS:O	1:D:681:SER:HB3	2.18	0.44
1:D:757:ILE:CG2	1:D:812:MET:HB3	2.34	0.44
1:A:829:HIS:CD2	1:A:830:PRO:HD2	2.53	0.44
1:B:852:GLU:O	1:B:898:ARG:NH1	2.50	0.44
1:C:830:PRO:HA	1:C:833:TRP:CD2	2.53	0.44
1:C:878:ILE:HD12	1:C:882:LEU:CG	2.47	0.44
1:D:671:GLN:OE1	1:D:707:ALA:N	2.46	0.44
1:A:626:ILE:HD12	1:A:626:ILE:HA	1.77	0.43
1:B:749:GLU:CD	1:B:750:ASN:N	2.76	0.43
1:C:808:LEU:HB2	1:C:829:HIS:CE1	2.53	0.43
1:D:719:ALA:O	1:D:722:ARG:HB2	2.18	0.43
1:A:666:ILE:H	1:A:666:ILE:CD1	2.25	0.43
1:C:614:GLN:HA	1:C:614:GLN:OE1	2.18	0.43
1:D:574:LYS:CD	1:D:574:LYS:H	2.31	0.43
1:D:695:LEU:CD1	1:D:710:SER:CB	2.96	0.43
1:A:613:VAL:CG2	1:A:617:ARG:HH21	2.31	0.43
1:A:622:HIS:HB2	1:A:678:HIS:ND1	2.33	0.43
1:B:667:THR:O	1:B:671:GLN:HG3	2.18	0.43
1:C:664:GLU:HB3	1:C:665:PRO:HD3	2.01	0.43
1:C:870:VAL:HA	1:C:937:PHE:HD2	1.82	0.43
1:D:679:LEU:HD21	1:D:712:PHE:CZ	2.53	0.43
1:D:784:ASN:H	1:D:787:LEU:CD2	2.15	0.43
1:A:602:LEU:HB3	1:A:603:PRO:CD	2.49	0.43
1:B:830:PRO:HA	1:B:833:TRP:CD2	2.53	0.43
1:C:601:ILE:O	1:C:606:PHE:HE1	2.01	0.43
1:C:722:ARG:HE	1:C:722:ARG:HB3	1.49	0.43
1:A:765:TYR:CD2	1:A:774:PRO:HG3	2.53	0.43
1:A:845:VAL:HG11	1:A:944:THR:HG21	2.01	0.43
1:B:601:ILE:C	1:B:602:LEU:HD23	2.44	0.43
1:B:958:GLN:N	1:B:959:PRO:CD	2.82	0.43
1:C:576:VAL:HG22	1:C:587:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:LYS:HE3	1:C:599:LYS:HB3	1.76	0.43
1:C:652:TYR:OH	1:C:664:GLU:OE2	2.35	0.43
1:C:829:HIS:ND1	1:C:830:PRO:HD2	2.33	0.43
1:A:613:VAL:HG23	1:A:628:TYR:CE2	2.53	0.43
1:C:870:VAL:HG13	1:C:897:VAL:HG12	1.99	0.43
1:D:669:LEU:HD11	1:D:767:VAL:CG2	2.47	0.43
1:D:619:SER:O	1:D:678:HIS:HE1	2.01	0.43
1:A:808:LEU:CD1	1:A:812:MET:HE2	2.48	0.43
1:C:613:VAL:HG23	1:C:628:TYR:CE2	2.54	0.43
1:C:613:VAL:HG22	1:C:617:ARG:CZ	2.48	0.43
1:C:622:HIS:HB2	1:C:678:HIS:CD2	2.54	0.43
1:C:642:ILE:CD1	2:C:1001:A1IOO:C1	2.97	0.43
1:C:679:LEU:HD21	1:C:712:PHE:CE2	2.54	0.43
1:C:690:LYS:C	1:C:692:HIS:H	2.26	0.43
1:C:830:PRO:HD3	1:C:945:TYR:CE2	2.54	0.43
1:D:635:ARG:CB	1:D:635:ARG:NH1	2.82	0.43
1:D:803:VAL:O	1:D:807:GLU:HG2	2.17	0.43
1:D:830:PRO:HG3	1:D:833:TRP:CZ3	2.54	0.43
1:C:628:TYR:HA	1:C:642:ILE:HG22	2.00	0.43
1:C:836:GLU:HG2	1:C:926:PRO:CG	2.45	0.43
1:C:877:ASN:HD22	1:C:877:ASN:HA	1.67	0.43
1:A:611:ARG:HG2	1:A:612:GLU:N	2.33	0.43
1:C:808:LEU:CG	1:C:812:MET:HE2	2.49	0.43
1:C:889:PHE:C	1:C:891:THR:H	2.26	0.43
1:D:635:ARG:HB3	1:D:635:ARG:CZ	2.49	0.43
1:D:655:GLN:O	1:D:656:LYS:HG2	2.18	0.43
1:C:752:THR:HG23	1:C:754:THR:H	1.84	0.42
1:D:773:HIS:CD2	1:D:781:ARG:HD2	2.52	0.42
1:A:775:PHE:CD2	1:A:785:ILE:HA	2.54	0.42
1:A:867:ARG:HE	1:A:867:ARG:HB3	1.59	0.42
1:A:890:ARG:NH1	1:A:890:ARG:CG	2.82	0.42
1:B:733:GLY:C	1:B:738:ILE:HD11	2.43	0.42
1:C:697:SER:HB2	1:C:708:MET:CE	2.48	0.42
1:A:765:TYR:O	1:A:769:SER:OG	2.29	0.42
1:C:658:PHE:HA	1:C:661:LEU:HB2	2.02	0.42
1:C:800:HIS:N	1:C:938:PRO:HB3	2.35	0.42
1:B:736:GLY:H	1:B:782:GLN:HG2	1.85	0.42
1:C:588:ARG:HG3	1:C:589:GLY:N	2.34	0.42
1:D:710:SER:HB2	2:D:1001:A1IOO:O1	2.19	0.42
1:A:631:THR:HG23	1:A:631:THR:O	2.20	0.42
1:A:642:ILE:HD11	2:A:1001:A1IOO:C4	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:VAL:O	1:B:731:VAL:CG2	2.65	0.42
1:C:650:GLN:O	1:C:653:VAL:HG22	2.18	0.42
1:C:673:THR:HB	1:C:827:LEU:HD11	2.00	0.42
1:C:911:TYR:HA	1:C:914:LEU:HD23	2.02	0.42
1:A:827:LEU:HD23	1:A:827:LEU:HA	1.92	0.42
1:B:809:ILE:HD12	1:B:809:ILE:H	1.83	0.42
1:C:955:ARG:HG3	1:C:955:ARG:HH11	1.85	0.42
1:D:725:PHE:CD1	1:D:726:SEP:O	2.73	0.42
1:A:620:ASP:OD2	1:B:594:ARG:NH2	2.41	0.42
1:A:834:SER:OG	1:A:835:LEU:N	2.52	0.42
1:B:764:PHE:CD1	1:B:812:MET:HE1	2.54	0.42
1:B:806:ARG:O	1:B:810:GLU:HB2	2.20	0.42
1:C:775:PHE:CD2	1:C:785:ILE:HG13	2.55	0.42
1:A:953:HIS:CD2	1:A:953:HIS:H	2.37	0.42
1:C:732:PRO:CD	1:C:742:MET:HE1	2.38	0.42
1:A:669:LEU:HD23	1:A:669:LEU:HA	1.85	0.42
1:A:884:THR:HG22	1:A:887:ARG:NH2	2.25	0.42
1:B:739:ALA:HB1	1:B:740:PRO:HD2	2.02	0.42
1:B:805:ALA:O	1:B:809:ILE:HD13	2.20	0.42
1:C:741:GLU:CD	1:C:820:ARG:HH22	2.28	0.42
1:C:873:ASP:HA	1:C:894:GLY:O	2.18	0.42
1:D:704:LYS:HA	1:D:704:LYS:HD2	1.83	0.42
1:A:918:VAL:O	1:A:922:LEU:HD12	2.19	0.42
1:A:945:TYR:O	1:A:961:TYR:OH	2.22	0.42
1:B:875:ARG:HE	1:B:875:ARG:HB2	1.48	0.42
1:A:679:LEU:HD21	1:A:712:PHE:CZ	2.55	0.41
1:A:693:ASN:O	1:A:695:LEU:HD12	2.20	0.41
1:C:775:PHE:CD2	1:C:785:ILE:HA	2.54	0.41
1:C:850:GLU:CD	1:C:902:ARG:HH11	2.27	0.41
1:D:716:LYS:HD2	1:D:716:LYS:HA	1.87	0.41
1:D:781:ARG:O	1:D:785:ILE:CG1	2.68	0.41
1:A:583:GLY:O	1:A:602:LEU:HD11	2.20	0.41
1:A:870:VAL:HG13	1:A:897:VAL:HG12	2.02	0.41
1:B:646:ALA:O	1:B:647:ALA:HB2	2.21	0.41
1:C:652:TYR:OH	1:C:661:LEU:CD1	2.68	0.41
1:C:741:GLU:OE2	1:C:817:PRO:HB3	2.20	0.41
1:C:953:HIS:CD2	1:C:954:GLU:N	2.88	0.41
1:D:612:GLU:HB2	1:D:713:GLY:HA2	2.01	0.41
1:A:616:LEU:HD23	1:A:616:LEU:HA	1.92	0.41
1:A:690:LYS:HE3	1:A:693:ASN:HD21	1.85	0.41
1:D:739:ALA:HA	1:D:758:PHE:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:ARG:O	1:A:601:ILE:HD13	2.20	0.41
1:B:567:GLY:HA3	1:B:632:GLU:OE2	2.20	0.41
1:B:885:ASP:OD2	1:B:907:LYS:HE3	2.21	0.41
1:C:775:PHE:HE2	1:C:785:ILE:HA	1.81	0.41
1:D:830:PRO:HA	1:D:833:TRP:CD2	2.54	0.41
1:B:686:HIS:O	1:B:687:ARG:HB2	2.19	0.41
1:B:775:PHE:CD2	1:B:785:ILE:HA	2.55	0.41
1:C:599:LYS:O	1:C:639:TYR:HA	2.20	0.41
1:D:808:LEU:HD21	1:D:826:VAL:HG13	2.02	0.41
1:D:834:SER:H	1:D:837:LYS:HB2	1.86	0.41
1:A:577:LEU:HD12	1:A:587:TYR:C	2.46	0.41
1:C:905:ARG:HD2	1:C:905:ARG:C	2.45	0.41
1:C:927:ASP:O	1:C:930:VAL:HG12	2.21	0.41
1:C:652:TYR:OH	1:C:661:LEU:HD12	2.21	0.41
1:D:795:LEU:CB	1:D:806:ARG:HG3	2.51	0.41
1:B:599:LYS:O	1:B:639:TYR:HA	2.21	0.41
1:C:648:THR:HG22	1:C:695:LEU:CD2	2.51	0.41
1:C:919:ARG:CB	1:C:919:ARG:CZ	2.98	0.41
1:B:849:ILE:HD12	1:B:898:ARG:CD	2.50	0.41
1:B:851:LYS:O	1:B:851:LYS:CD	2.66	0.41
1:C:718:LEU:HD12	1:C:753:TYR:OH	2.21	0.41
1:D:601:ILE:N	1:D:601:ILE:CD1	2.84	0.41
1:D:679:LEU:HD21	1:D:712:PHE:CE2	2.56	0.41
1:D:725:PHE:CD1	1:D:725:PHE:C	2.99	0.41
1:D:825:HIS:ND1	1:D:825:HIS:N	2.68	0.41
1:A:759:SER:O	1:A:763:VAL:HG23	2.21	0.41
1:A:907:LYS:HZ1	1:A:914:LEU:CD2	2.32	0.41
1:A:956:LEU:HD12	1:A:956:LEU:C	2.46	0.41
1:C:588:ARG:HG2	1:C:588:ARG:HH11	1.86	0.41
1:A:807:GLU:OE1	1:A:946:ARG:HD2	2.20	0.40
1:A:828:LYS:HD3	1:A:961:TYR:C	2.46	0.40
1:A:870:VAL:HG13	1:A:897:VAL:CG1	2.49	0.40
1:B:663:LEU:HA	1:B:663:LEU:HD23	1.79	0.40
1:B:853:SER:OG	1:B:854:LEU:N	2.55	0.40
1:B:852:GLU:OE1	1:B:858:ILE:HD13	2.22	0.40
1:C:679:LEU:HD22	1:C:684:ILE:CG2	2.51	0.40
1:C:695:LEU:HG	1:C:710:SER:OG	2.21	0.40
1:D:683:ASN:OD1	1:D:753:TYR:OH	2.39	0.40
1:A:599:LYS:O	1:A:639:TYR:HA	2.21	0.40
1:A:807:GLU:CG	1:A:829:HIS:HE2	2.31	0.40
1:A:922:LEU:HD22	1:A:929:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:PHE:CZ	1:C:630:CYS:HB2	2.57	0.40
1:C:807:GLU:OE1	1:C:811:LYS:HE2	2.21	0.40
1:C:860:LYS:HD3	1:C:860:LYS:C	2.46	0.40
1:D:669:LEU:HD11	1:D:767:VAL:HG21	2.03	0.40
1:D:835:LEU:HA	1:D:838:GLN:OE1	2.22	0.40
1:C:672:THR:HG23	1:C:709:ILE:CD1	2.51	0.40
1:D:597:ALA:O	1:D:642:ILE:HG22	2.21	0.40
1:A:600:ARG:HD2	1:A:637:PHE:CE2	2.57	0.40
1:C:669:LEU:HD11	1:C:767:VAL:CG2	2.51	0.40
1:C:922:LEU:HD21	1:C:933:PHE:CZ	2.57	0.40
1:D:599:LYS:HB3	1:D:599:LYS:HE3	1.95	0.40
1:D:635:ARG:HB2	1:D:635:ARG:NH1	2.36	0.40

All (3) 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:655:GLN:OE1	1:B:778:SER:OG[1_455]	1.98	0.22
1:C:777:LYS:NZ	1:D:770:GLU:OE1[1_565]	2.05	0.15
1:C:655:GLN:NE2	1:D:778:SER:OG[1_565]	2.13	0.07

## 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	398/434 (92%)	375 (94%)	23 (6%)	0	100	100
1	B	398/434 (92%)	372 (94%)	26 (6%)	0	100	100
1	C	398/434 (92%)	372 (94%)	26 (6%)	0	100	100
1	D	294/434 (68%)	276 (94%)	18 (6%)	0	100	100
All	All	1488/1736 (86%)	1395 (94%)	93 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	354/380 (93%)	348 (98%)	6 (2%)	53	78
1	B	354/380 (93%)	345 (98%)	9 (2%)	42	72
1	C	354/380 (93%)	340 (96%)	14 (4%)	28	62
1	D	265/380 (70%)	252 (95%)	13 (5%)	22	56
All	All	1327/1520 (87%)	1285 (97%)	42 (3%)	34	67

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	564	VAL
1	A	574	LYS
1	A	576	VAL
1	A	626	ILE
1	A	627	ARG
1	A	921	THR
1	B	607	SER
1	B	710	SER
1	B	728	ARG
1	B	734	THR
1	B	749	GLU
1	B	822	SER
1	B	880	VAL
1	B	884	THR
1	B	936	ARG
1	C	644	LEU
1	C	660	HIS
1	C	673	THR
1	C	689	LEU
1	C	710	SER
1	C	768	ILE
1	C	790	CYS

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Mol	Chain	Res	Type
1	C	791	SER
1	C	793	ASP
1	C	794	CYS
1	C	822	SER
1	C	859	VAL
1	C	891	THR
1	C	924	SER
1	D	598	VAL
1	D	695	LEU
1	D	720	VAL
1	D	723	HIS
1	D	734	THR
1	D	754	THR
1	D	759	SER
1	D	777	LYS
1	D	779	LEU
1	D	785	ILE
1	D	804	ILE
1	D	824	LYS
1	D	950	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	624	ASN
1	A	638	GLN
1	A	655	GLN
1	A	683	ASN
1	A	693	ASN
1	A	700	ASN
1	A	840	GLN
1	A	883	GLN
1	A	909	HIS
1	A	939	HIS
1	A	953	HIS
1	B	638	GLN
1	B	655	GLN
1	B	825	HIS
1	B	861	GLN
1	B	910	HIS
1	C	579	HIS
1	C	678	HIS

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Mol	Chain	Res	Type
1	C	692	HIS
1	C	750	ASN
1	C	861	GLN
1	C	877	ASN
1	C	943	HIS
1	C	953	HIS
1	D	593	ASN
1	D	693	ASN
1	D	700	ASN
1	D	750	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	SEP	B	724	1	8,9,10	1.65	1 (12%)	7,12,14	1.48	1 (14%)
1	SEP	B	729	1	8,9,10	1.64	1 (12%)	7,12,14	1.27	1 (14%)
1	SEP	A	729	1	8,9,10	1.61	1 (12%)	7,12,14	0.98	0
1	SEP	C	729	1	8,9,10	1.64	1 (12%)	7,12,14	1.36	1 (14%)
1	SEP	C	724	1	8,9,10	1.64	1 (12%)	7,12,14	1.32	1 (14%)
1	SEP	D	726	1	8,9,10	1.61	1 (12%)	7,12,14	1.29	1 (14%)
1	SEP	B	726	1	8,9,10	1.64	1 (12%)	7,12,14	1.07	1 (14%)
1	SEP	A	726	1	8,9,10	1.64	1 (12%)	7,12,14	1.43	1 (14%)
1	SEP	A	724	1	8,9,10	1.63	1 (12%)	7,12,14	0.90	0
1	SEP	C	726	1	8,9,10	1.62	1 (12%)	7,12,14	1.40	1 (14%)
1	SEP	D	729	1	8,9,10	1.63	1 (12%)	7,12,14	1.44	1 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	D	724	1	8,9,10	1.61	1 (12%)	7,12,14	1.32	1 (14%)

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
1	SEP	B	724	1	-	3/6/8/10	-
1	SEP	B	729	1	-	5/6/8/10	-
1	SEP	A	729	1	-	0/6/8/10	-
1	SEP	C	729	1	-	0/6/8/10	-
1	SEP	C	724	1	-	6/6/8/10	-
1	SEP	D	726	1	-	4/6/8/10	-
1	SEP	B	726	1	-	2/6/8/10	-
1	SEP	A	726	1	-	1/6/8/10	-
1	SEP	A	724	1	-	3/6/8/10	-
1	SEP	C	726	1	-	2/6/8/10	-
1	SEP	D	729	1	-	0/6/8/10	-
1	SEP	D	724	1	-	3/6/8/10	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	724	SEP	P-O1P	3.62	1.61	1.50
1	B	729	SEP	P-O1P	3.59	1.61	1.50
1	B	726	SEP	P-O1P	3.58	1.61	1.50
1	D	729	SEP	P-O1P	3.58	1.61	1.50
1	C	724	SEP	P-O1P	3.58	1.61	1.50
1	A	724	SEP	P-O1P	3.57	1.61	1.50
1	D	726	SEP	P-O1P	3.56	1.61	1.50
1	C	729	SEP	P-O1P	3.55	1.61	1.50
1	A	726	SEP	P-O1P	3.55	1.61	1.50
1	C	726	SEP	P-O1P	3.54	1.61	1.50
1	D	724	SEP	P-O1P	3.54	1.61	1.50
1	A	729	SEP	P-O1P	3.53	1.61	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	724	SEP	OG-CB-CA	3.38	111.43	108.14
1	A	726	SEP	OG-CB-CA	3.27	111.33	108.14
1	C	726	SEP	OG-CB-CA	3.18	111.24	108.14
1	D	729	SEP	OG-CB-CA	3.14	111.20	108.14
1	C	729	SEP	OG-CB-CA	3.02	111.08	108.14
1	D	726	SEP	OG-CB-CA	2.83	110.90	108.14
1	D	724	SEP	OG-CB-CA	2.82	110.89	108.14
1	B	729	SEP	OG-CB-CA	2.81	110.88	108.14
1	C	724	SEP	OG-CB-CA	2.80	110.87	108.14
1	B	726	SEP	OG-CB-CA	2.07	110.16	108.14

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	724	SEP	CB-OG-P-O1P
1	A	724	SEP	CB-OG-P-O2P
1	A	724	SEP	CB-OG-P-O3P
1	B	724	SEP	CB-OG-P-O1P
1	B	724	SEP	CB-OG-P-O3P
1	B	726	SEP	N-CA-CB-OG
1	B	726	SEP	C-CA-CB-OG
1	B	729	SEP	N-CA-CB-OG
1	B	729	SEP	C-CA-CB-OG
1	B	729	SEP	CB-OG-P-O2P
1	B	729	SEP	CB-OG-P-O3P
1	C	724	SEP	C-CA-CB-OG
1	C	724	SEP	CB-OG-P-O2P
1	C	724	SEP	CB-OG-P-O3P
1	C	726	SEP	C-CA-CB-OG
1	D	724	SEP	N-CA-CB-OG
1	D	724	SEP	C-CA-CB-OG
1	D	726	SEP	N-CA-CB-OG
1	D	726	SEP	CB-OG-P-O1P
1	D	726	SEP	CB-OG-P-O2P
1	D	726	SEP	CB-OG-P-O3P
1	C	724	SEP	CB-OG-P-O1P
1	A	726	SEP	CA-CB-OG-P
1	C	724	SEP	CA-CB-OG-P
1	C	726	SEP	CA-CB-OG-P
1	D	724	SEP	CA-CB-OG-P
1	C	724	SEP	N-CA-CB-OG
1	B	724	SEP	CB-OG-P-O2P

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Mol	Chain	Res	Type	Atoms
1	B	729	SEP	CB-OG-P-O1P

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	729	SEP	1	0
1	A	729	SEP	1	0
1	D	726	SEP	2	0
1	B	726	SEP	2	0
1	A	724	SEP	1	0
1	D	724	SEP	1	0

## 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	$\# Z  > 2$
2	A1IOO	B	1001	-	26,26,26	0.55	0	37,37,37	0.60	0
2	A1IOO	A	1001	-	26,26,26	0.56	0	37,37,37	0.57	0
2	A1IOO	D	1001	-	26,26,26	0.52	0	37,37,37	0.54	0
2	A1IOO	C	1001	-	26,26,26	0.55	0	37,37,37	0.76	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1IOO	B	1001	-	-	2/13/13/13	0/3/3/3
2	A1IOO	A	1001	-	-	2/13/13/13	0/3/3/3
2	A1IOO	D	1001	-	-	3/13/13/13	0/3/3/3
2	A1IOO	C	1001	-	-	2/13/13/13	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	A1IOO	C12-N1-C13	2.51	131.01	125.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1001	A1IOO	O3-C13-N1-C2
2	B	1001	A1IOO	C4-C5-C6-O1
2	C	1001	A1IOO	C4-C5-C6-O1
2	D	1001	A1IOO	C4-C5-C6-O2
2	D	1001	A1IOO	C4-C5-C6-O1
2	B	1001	A1IOO	C4-C5-C6-O2
2	A	1001	A1IOO	C4-C5-C6-O2
2	C	1001	A1IOO	C4-C5-C6-O2
2	A	1001	A1IOO	C4-C5-C6-O1

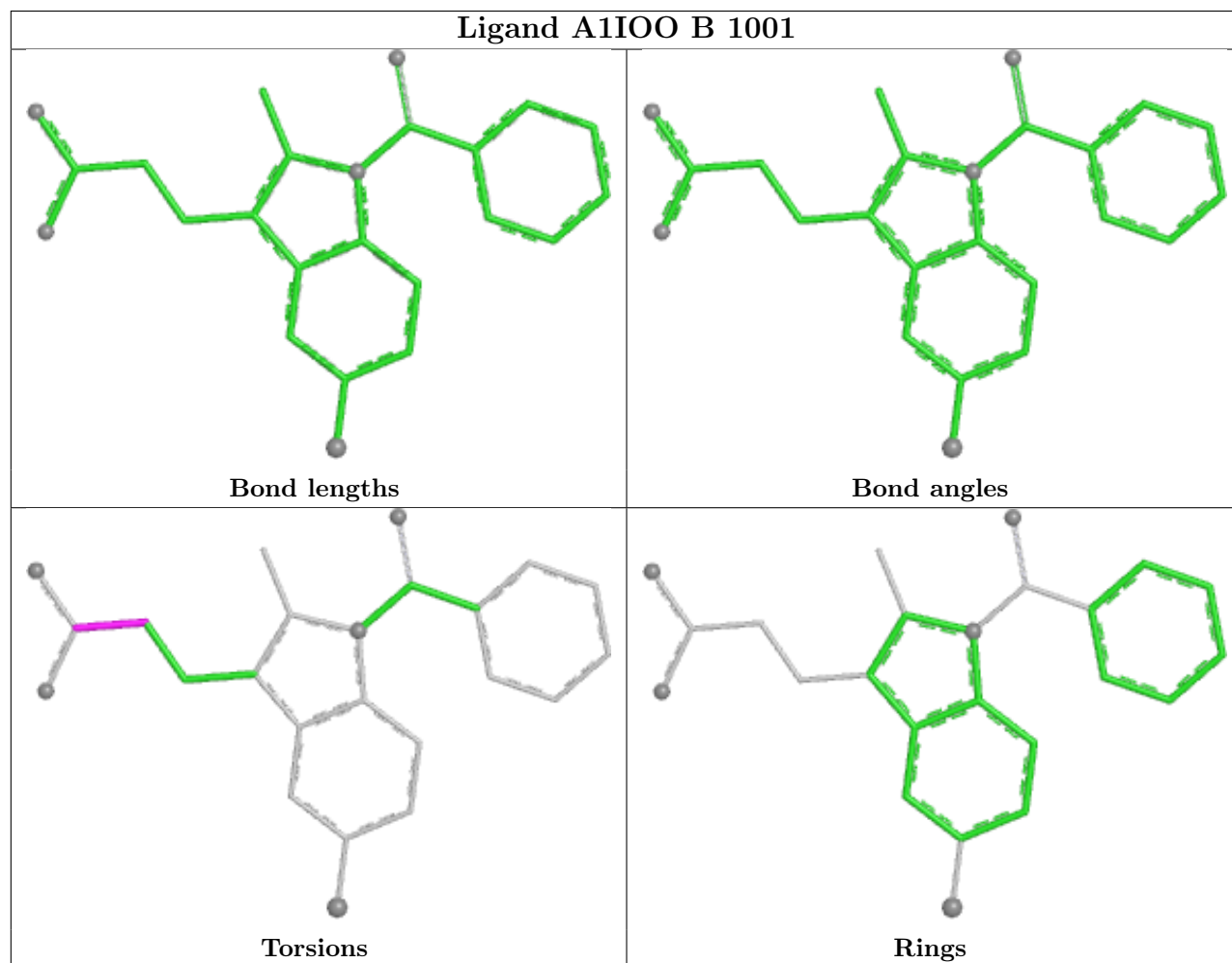
There are no ring outliers.

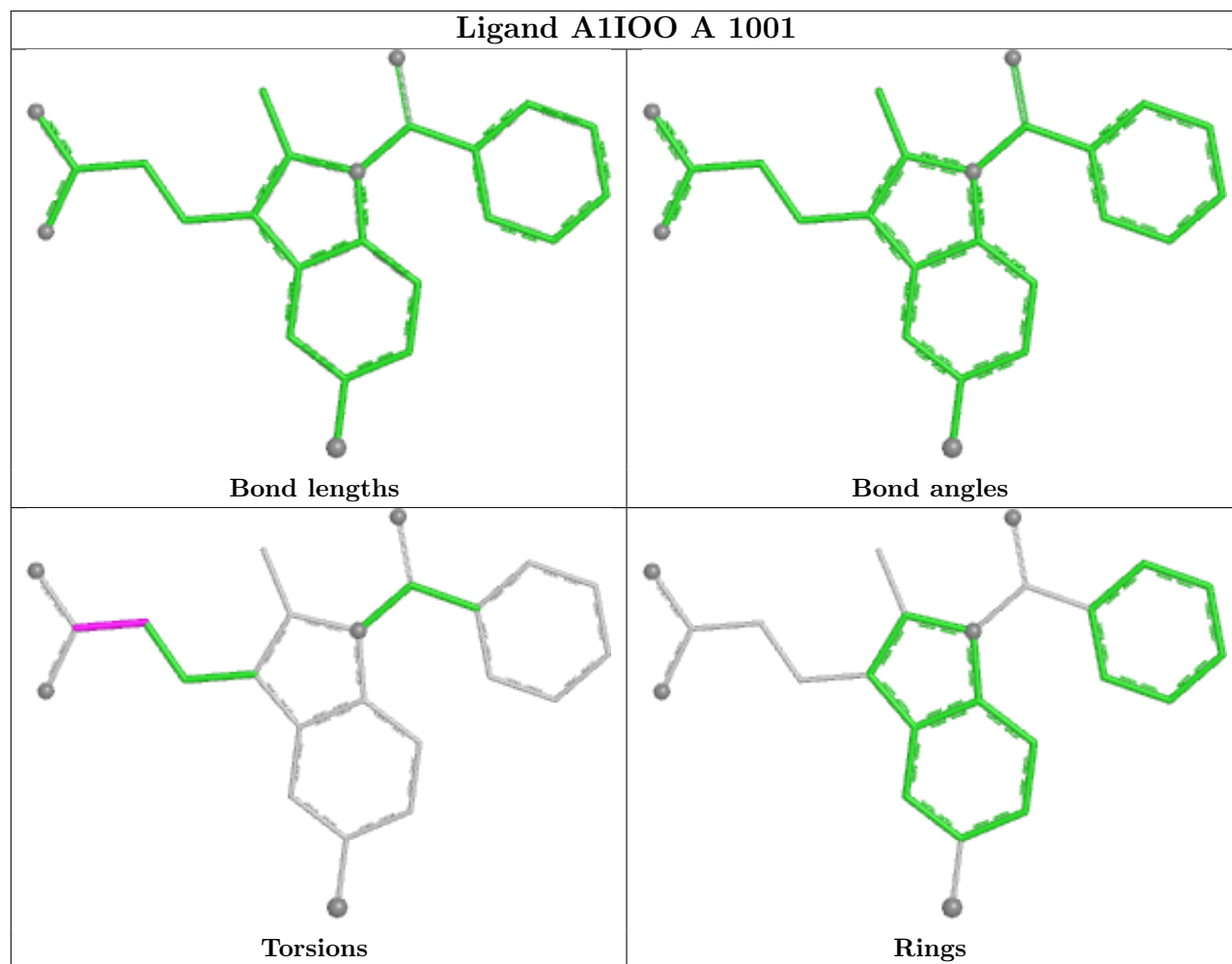
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	A1IOO	1	0
2	A	1001	A1IOO	1	0
2	D	1001	A1IOO	1	0
2	C	1001	A1IOO	3	0

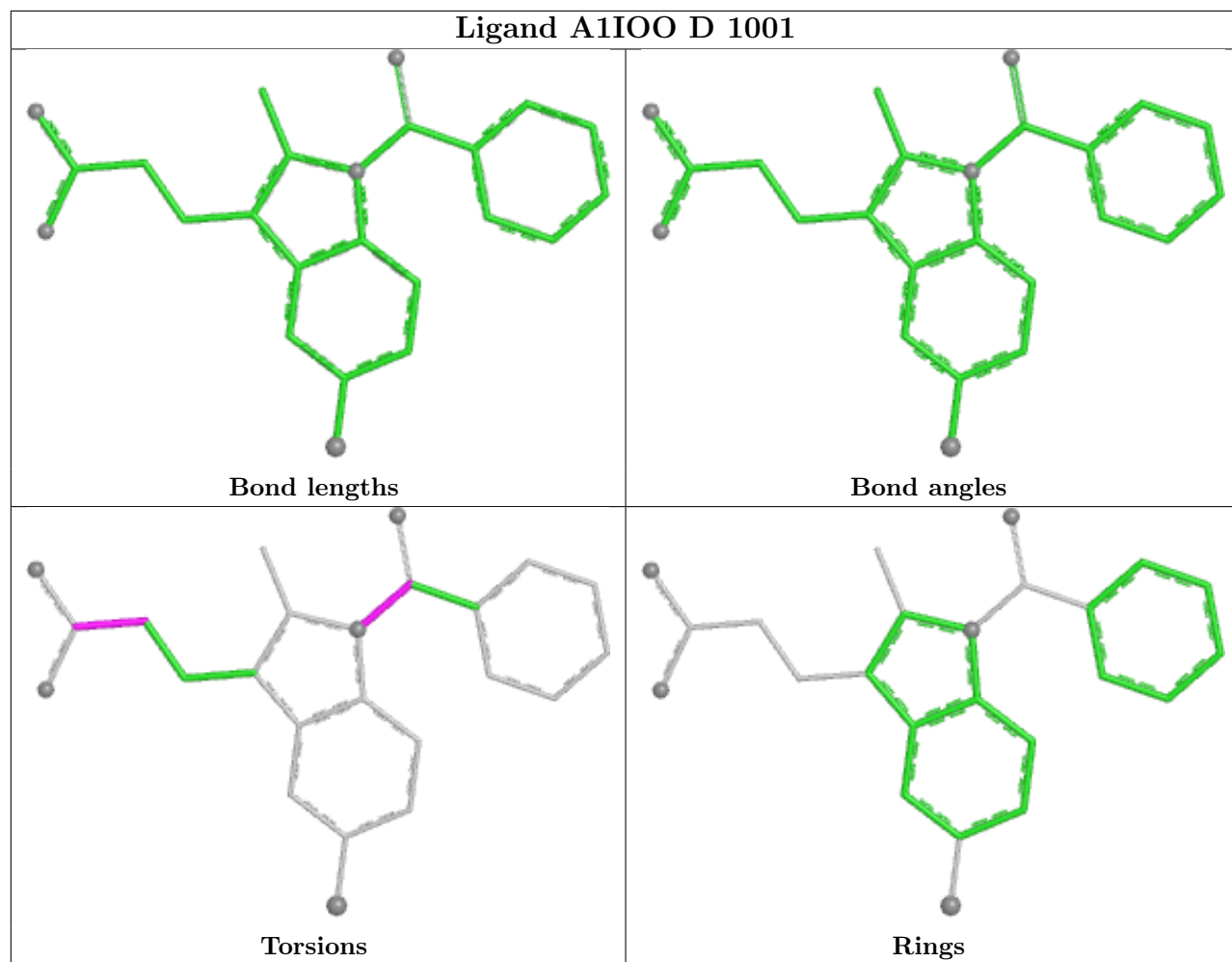
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

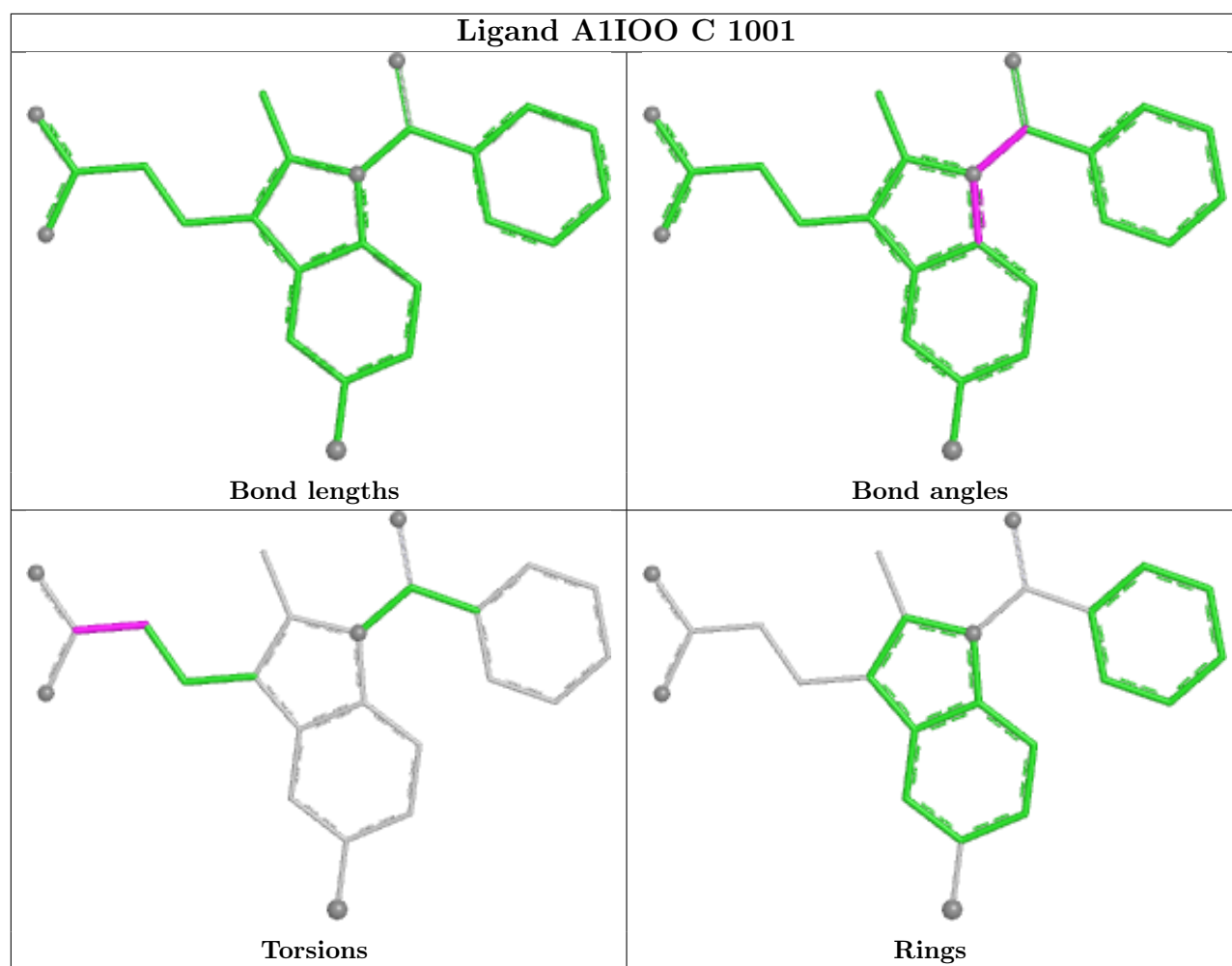
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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





## Ligand A1IOO D 1001





## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	400/434 (92%)	-0.05	3 (0%) 82 64	52, 77, 114, 139	0
1	B	400/434 (92%)	-0.14	1 (0%) 90 79	51, 72, 100, 122	0
1	C	400/434 (92%)	0.12	2 (0%) 87 72	58, 91, 122, 180	0
1	D	300/434 (69%)	0.25	4 (1%) 75 53	62, 93, 131, 154	0
All	All	1500/1736 (86%)	0.03	10 (0%) 84 66	51, 82, 121, 180	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	563	VAL	3.4
1	D	731	VAL	2.8
1	B	891	THR	2.6
1	D	841	PHE	2.5
1	A	645	CYS	2.5
1	D	842	PHE	2.5
1	C	906	ASN	2.2
1	C	872	MET	2.2
1	A	582	GLU	2.0
1	D	839	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	C	726	10/11	0.71	0.10	126,137,148,148	0
1	SEP	D	724	10/11	0.73	0.10	127,130,132,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SEP	C	729	10/11	0.77	0.10	124,140,147,147	0
1	SEP	D	726	10/11	0.78	0.10	120,127,129,130	0
1	SEP	B	726	10/11	0.80	0.13	97,108,120,124	0
1	SEP	D	729	10/11	0.83	0.09	112,118,123,127	0
1	SEP	C	724	10/11	0.86	0.08	113,122,129,133	0
1	SEP	B	729	10/11	0.88	0.10	93,103,110,111	0
1	SEP	A	726	10/11	0.89	0.09	83,92,104,108	0
1	SEP	B	724	10/11	0.91	0.07	83,88,104,106	0
1	SEP	A	724	10/11	0.92	0.07	85,90,106,109	0
1	SEP	A	729	10/11	0.94	0.07	75,80,87,95	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

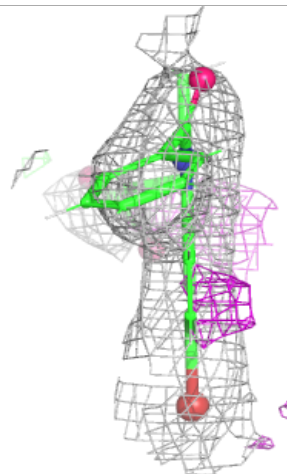
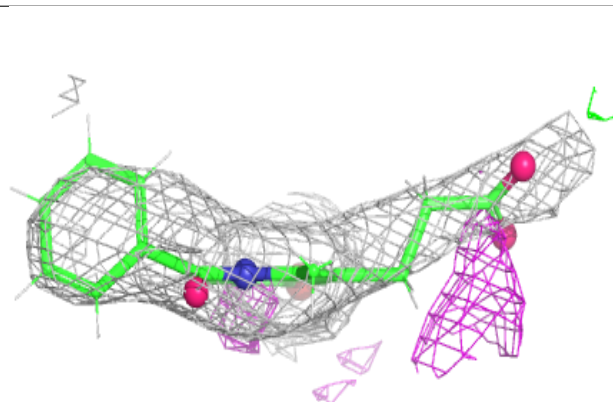
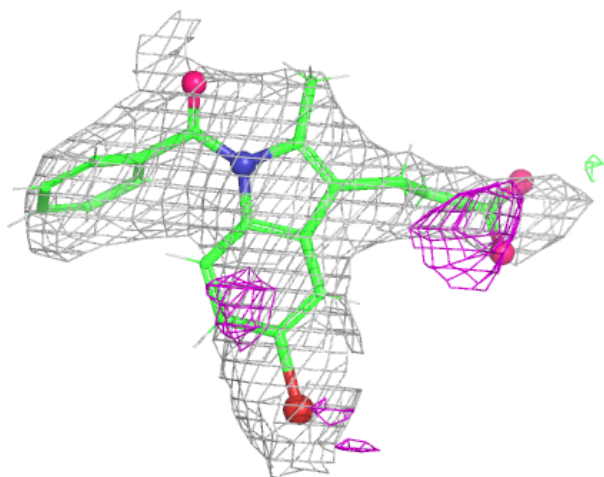
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1IOO	A	1001	24/24	0.84	0.12	79,96,128,165	0
2	A1IOO	C	1001	24/24	0.88	0.11	77,93,116,147	0
2	A1IOO	D	1001	24/24	0.94	0.09	73,80,97,113	0
2	A1IOO	B	1001	24/24	0.95	0.08	64,77,93,117	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.

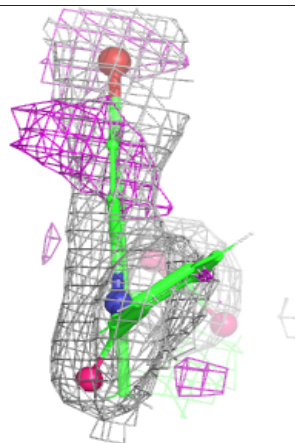
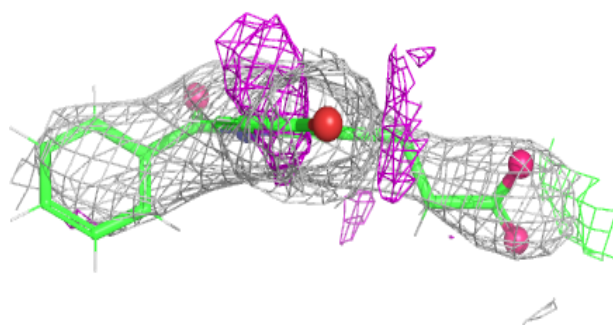
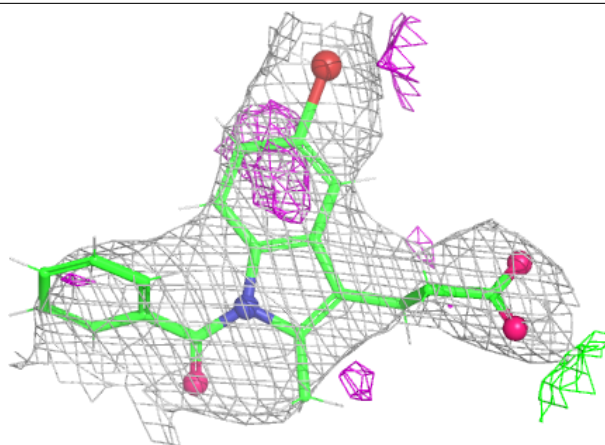
**Electron density around A1IOO A 1001:**

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



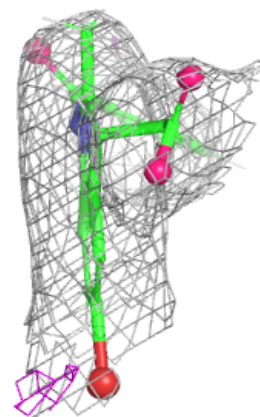
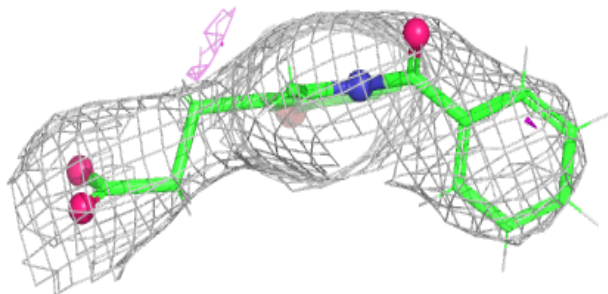
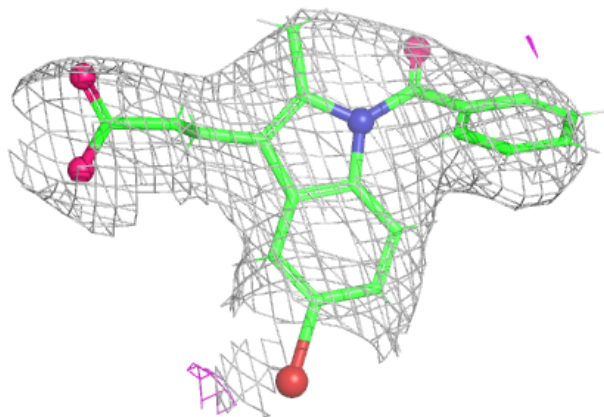
**Electron density around A1IOO C 1001:**

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



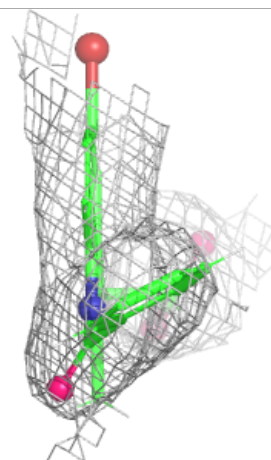
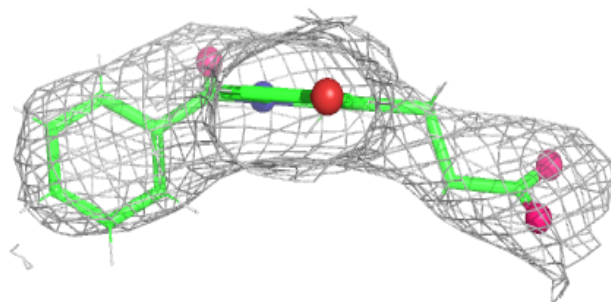
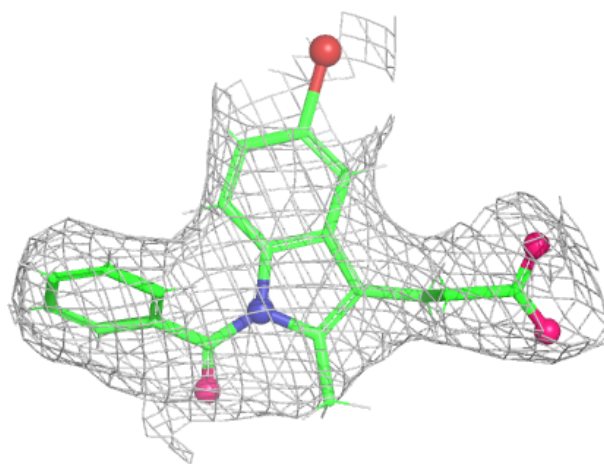
**Electron density around A1IOO D 1001:**

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



**Electron density around A1IOO B 1001:**

$2mF_o-DF_c$  (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.