Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 12:05 AM EDT

PDB ID	:	1WOK
Title	:	Crystal structure of catalytic domain of human poly(ADP-ribose) polymerase complexed with a quinoxaline-type inhibitor
Authors	:	Iwashita, A.; Hattori, K.; Yamamoto, H.; Ishida, J.; Kido, Y.; Kamijo, K.; Murano, K.; Miyake, H.; Kinoshita, T.; Warizaya, M.; Ohkubo, M.; Matsuoka, N.; Mutoh, S.
Deposited on	:	2004-08-20
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

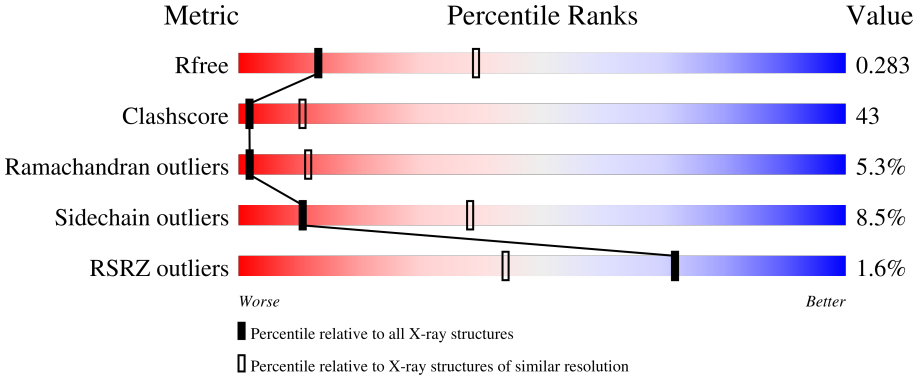
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 >=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 <=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	350	2% 49% 44% 7%
1	B	350	% 43% 49% 8%
1	C	350	% 40% 51% 9%
1	D	350	2% 28% 59% 11% •

2 Entry composition (i)

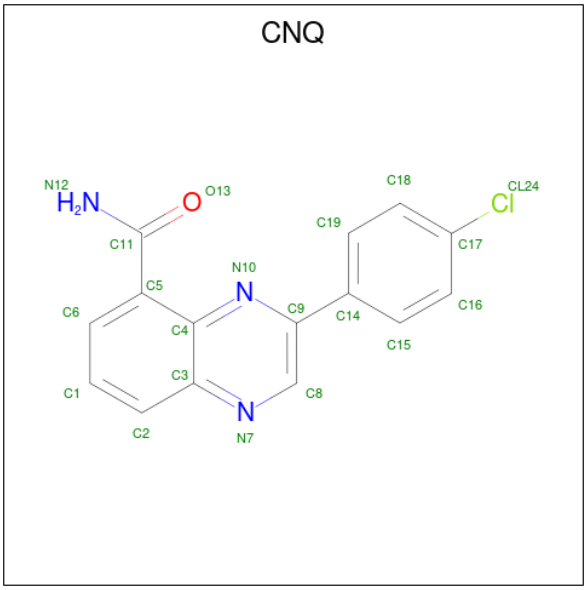
There are 2 unique types of molecules in this entry. The entry contains 11096 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Poly [ADP-ribose] polymerase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	2754	1752	465	526	11	0	0	0
1	B	350	2754	1752	465	526	11	0	0	0
1	C	350	2754	1752	465	526	11	0	0	0
1	D	350	2754	1752	465	526	11	0	0	0

- Molecule 2 is 3-(4-CHLOROPHENYL)QUINOXALINE-5-CARBOXAMIDE (three-letter code: CNQ) (formula: $C_{15}H_{10}ClN_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	20	15	1	3	1	0	0
2	B	1	20	15	1	3	1	0	0

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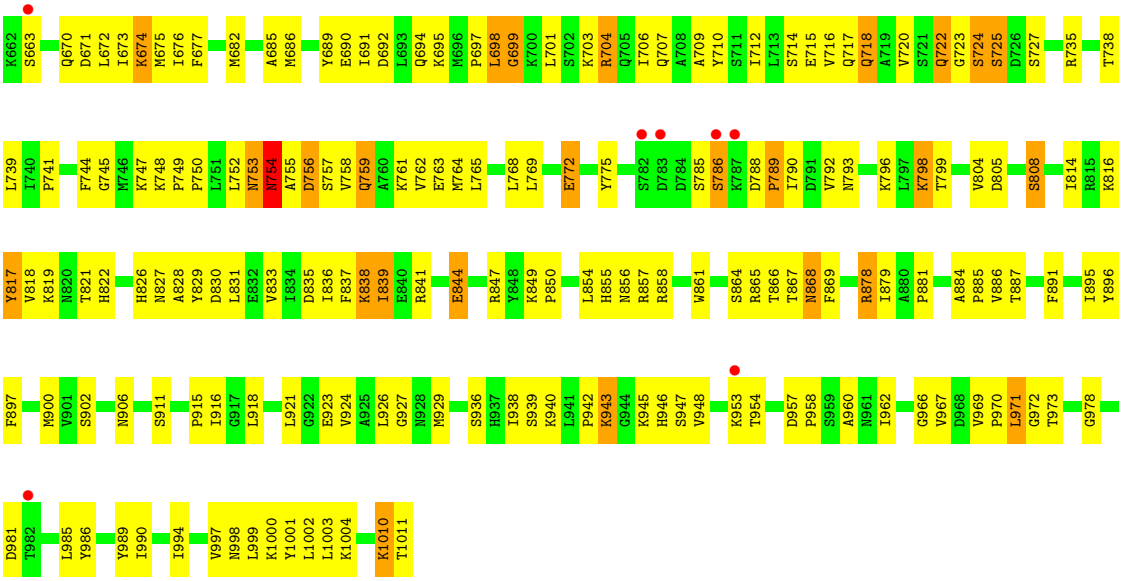
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	C	1	20	15	1	3	1	0	0
			Total	C	Cl	N	O		
2	D	1	20	15	1	3	1	0	0

3 Residue-property plots (i)

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.

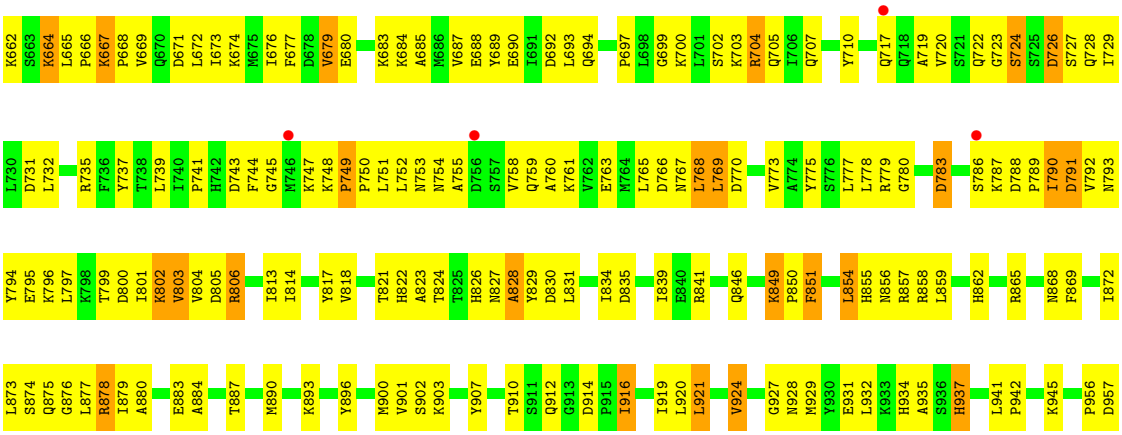
• Molecule 1: Poly [ADP-ribose] polymerase-1

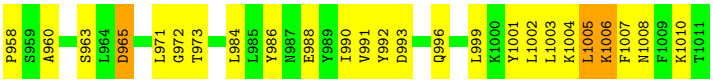
Chain A:



• Molecule 1: Poly [ADP-ribose] polymerase-1

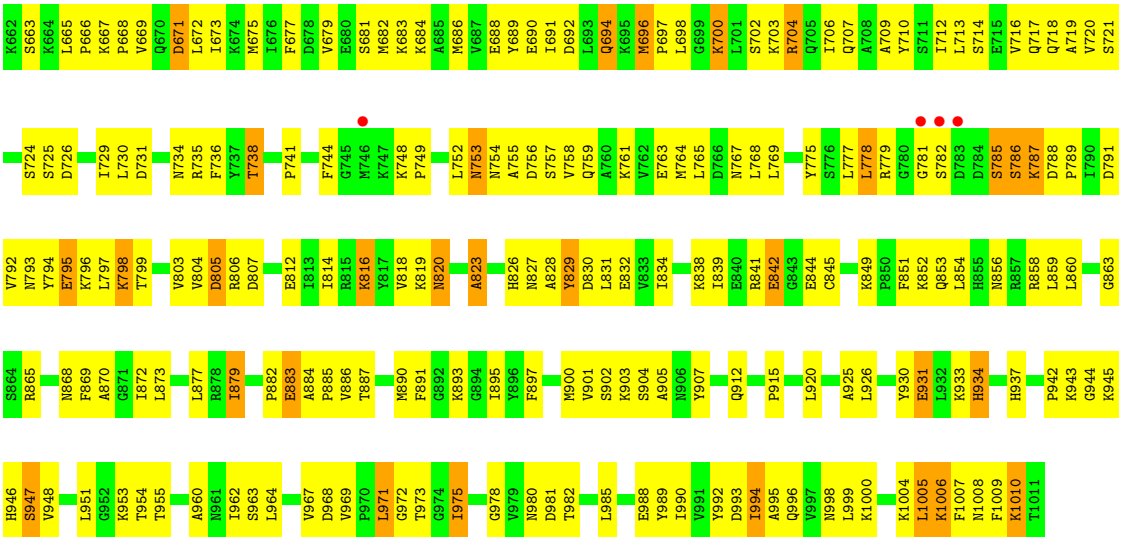
Chain B:





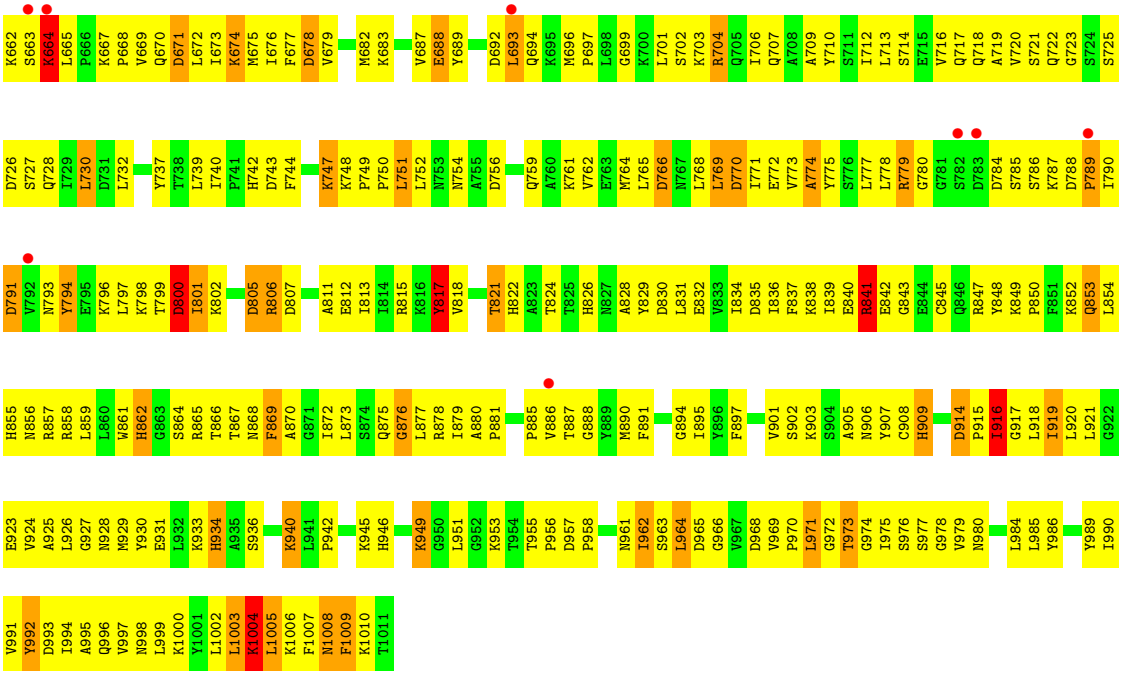
• Molecule 1: Poly [ADP-ribose] polymerase-1

Chain C:



• Molecule 1: Poly [ADP-ribose] polymerase-1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.05Å 77.08Å 113.72Å 90.00° 117.43° 90.00°	Depositor
Resolution (Å)	29.25 – 3.00 39.96 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.4 (29.25-3.00) 93.0 (39.96-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.12 (at 3.01Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.233 , 0.288 0.229 , 0.283	Depositor DCC
R_{free} test set	1271 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	50.8	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11096	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CNQ

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	0.37	0/2806	0.63	0/3786
1	B	0.36	0/2806	0.63	0/3786
1	C	0.40	0/2806	0.67	0/3786
1	D	0.30	0/2806	0.58	0/3786
All	All	0.36	0/11224	0.63	0/15144

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	986	TYR	Sidechain

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	2754	0	2795	181	0
1	B	2754	0	2795	231	0
1	C	2754	0	2795	212	0
1	D	2754	0	2795	361	0
2	A	20	0	10	1	0
2	B	20	0	10	2	0
2	C	20	0	10	2	0
2	D	20	0	10	2	0
All	All	11096	0	11220	960	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (960) 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:879:ILE:HD13	1:C:879:ILE:H	1.19	1.03
1:B:717:GLN:HE22	1:B:887:THR:HB	1.23	1.00
1:B:697:PRO:HG2	1:B:700:LYS:HB2	1.40	1.00
1:B:920:LEU:HD21	1:B:999:LEU:HD13	1.43	0.99
1:D:998:ASN:HD22	1:D:1000:LYS:NZ	1.59	0.99
1:D:841:ARG:HB3	1:D:841:ARG:HH11	1.28	0.98
1:D:962:ILE:HG12	1:D:971:LEU:HD11	1.46	0.96
1:D:855:HIS:HA	1:D:857:ARG:HH12	1.29	0.94
1:C:697:PRO:HG2	1:C:700:LYS:HB2	1.50	0.93
1:D:839:ILE:HD13	1:D:1002:LEU:HB2	1.49	0.92
1:D:964:LEU:HD22	1:D:965:ASP:H	1.32	0.92
1:D:849:LYS:HA	1:D:852:LYS:HE2	1.52	0.90
1:C:782:SER:HA	1:C:792:VAL:HG11	1.51	0.90
1:C:703:LYS:HB3	1:C:704:ARG:NH1	1.87	0.89
1:B:717:GLN:NE2	1:B:887:THR:HB	1.86	0.89
1:C:754:ASN:HD22	1:C:757:SER:HB3	1.38	0.88
1:D:798:LYS:HB3	1:D:842:GLU:HB2	1.56	0.88
1:B:800:ASP:HB3	1:B:802:LYS:HE3	1.55	0.87
1:D:841:ARG:HB3	1:D:841:ARG:NH1	1.90	0.87
1:B:830:ASP:HB3	1:B:1008:ASN:HB2	1.57	0.87
1:C:962:ILE:HG22	1:C:963:SER:H	1.39	0.87
1:C:879:ILE:H	1:C:879:ILE:CD1	1.87	0.87
1:B:878:ARG:HH11	1:B:878:ARG:HB3	1.38	0.86
1:D:919:ILE:HD13	1:D:920:LEU:H	1.37	0.86
1:C:962:ILE:HG22	1:C:963:SER:N	1.91	0.86
1:D:706:ILE:HG23	1:D:765:LEU:HD22	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:SER:HB2	1:C:791:ASP:OD1	1.77	0.84
1:B:667:LYS:HB3	1:B:668:PRO:HD3	1.61	0.83
1:D:998:ASN:HD22	1:D:1000:LYS:HZ2	1.27	0.83
1:D:930:TYR:HB2	1:D:945:LYS:HE2	1.60	0.83
1:B:823:ALA:HB3	1:B:826:HIS:HD2	1.44	0.82
1:B:679:VAL:HG23	1:B:680:GLU:H	1.44	0.82
1:D:918:LEU:H	1:D:918:LEU:HD23	1.45	0.81
1:D:665:LEU:H	1:D:665:LEU:HD22	1.43	0.81
1:B:703:LYS:H	1:B:704:ARG:HH21	1.29	0.80
1:A:865:ARG:HB2	1:A:868:ASN:HB2	1.64	0.80
1:D:751:LEU:HD12	1:D:751:LEU:H	1.44	0.80
1:A:839:ILE:HD13	1:A:839:ILE:H	1.48	0.79
1:D:962:ILE:HG22	1:D:963:SER:H	1.47	0.79
1:C:720:VAL:HG13	1:C:721:SER:H	1.47	0.79
1:C:933:LYS:HB2	1:C:982:THR:HB	1.64	0.79
1:D:770:ASP:OD1	1:D:868:ASN:HA	1.83	0.78
1:B:920:LEU:HD13	1:B:1002:LEU:HD23	1.66	0.78
1:C:962:ILE:CG2	1:C:963:SER:H	1.96	0.78
1:D:919:ILE:CD1	1:D:920:LEU:H	1.97	0.78
1:C:720:VAL:HG13	1:C:721:SER:N	2.00	0.77
1:D:739:LEU:HD12	1:D:740:ILE:HG12	1.67	0.77
1:C:696:MET:HG3	1:C:741:PRO:HD2	1.66	0.77
1:C:683:LYS:HA	1:C:686:MET:HE3	1.65	0.77
1:C:831:LEU:HD12	1:C:1005:LEU:HD22	1.66	0.77
1:D:664:LYS:HD2	1:D:665:LEU:HD22	1.67	0.76
1:D:920:LEU:HD23	1:D:921:LEU:N	2.00	0.76
1:A:754:ASN:HD22	1:A:754:ASN:N	1.83	0.76
1:D:975:ILE:HG13	1:D:976:SER:H	1.51	0.76
1:C:704:ARG:HA	1:C:707:GLN:HE21	1.50	0.76
1:A:858:ARG:HD3	1:A:926:LEU:HD12	1.69	0.75
1:D:865:ARG:HB2	1:D:868:ASN:OD1	1.86	0.75
1:A:703:LYS:H	1:A:704:ARG:NH2	1.84	0.75
1:D:841:ARG:NH2	1:D:875:GLN:HA	2.01	0.75
1:A:717:GLN:O	1:A:720:VAL:HG12	1.88	0.74
1:D:1004:LYS:HB3	1:D:1004:LYS:HZ2	1.52	0.74
1:B:865:ARG:HB2	1:B:868:ASN:ND2	2.03	0.74
1:C:689:TYR:CD1	1:C:764:MET:HG2	2.23	0.73
1:D:799:THR:HG22	1:D:841:ARG:HA	1.68	0.73
1:D:895:ILE:HD11	1:D:994:ILE:HD13	1.71	0.73
1:B:777:LEU:HD11	1:B:796:LYS:HB3	1.71	0.72
1:A:923:GLU:O	1:A:923:GLU:HG3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:ARG:HD2	1:A:994:ILE:HG21	1.71	0.72
1:B:901:VAL:HG13	1:B:902:SER:N	2.05	0.72
1:B:991:VAL:HG11	1:B:996:GLN:HB2	1.72	0.71
1:C:734:ASN:O	1:C:738:THR:HG22	1.90	0.71
1:A:763:GLU:HA	2:A:1:CNQ:CL24	2.27	0.71
1:C:931:GLU:HG3	1:C:951:LEU:HD21	1.72	0.71
1:B:827:ASN:OD1	1:D:725:SER:HB3	1.91	0.71
1:B:849:LYS:HB3	1:B:850:PRO:HD3	1.73	0.70
1:C:704:ARG:HA	1:C:707:GLN:NE2	2.06	0.70
1:D:806:ARG:HG2	1:D:807:ASP:OD1	1.90	0.70
1:A:895:ILE:HD11	1:A:994:ILE:HG22	1.71	0.70
1:A:943:LYS:N	1:A:943:LYS:HE2	2.05	0.70
1:D:683:LYS:O	1:D:687:VAL:HG23	1.90	0.70
1:D:676:ILE:HG23	1:D:870:ALA:HA	1.74	0.70
1:C:788:ASP:HB2	1:C:789:PRO:HD2	1.75	0.69
1:A:748:LYS:HG2	1:C:688:GLU:HB3	1.72	0.69
1:C:706:ILE:HG23	1:C:765:LEU:HD22	1.72	0.69
1:D:821:THR:O	1:D:901:VAL:HG12	1.91	0.69
1:A:805:ASP:O	1:A:808:SER:HB3	1.93	0.69
1:C:696:MET:CE	1:C:700:LYS:HB3	2.23	0.69
1:C:895:ILE:O	1:C:990:ILE:HA	1.93	0.69
1:C:788:ASP:HB2	1:C:789:PRO:CD	2.23	0.69
1:D:841:ARG:HE	1:D:876:GLY:H	1.41	0.68
1:B:765:LEU:HA	1:B:768:LEU:HD12	1.75	0.68
1:D:744:PHE:HB3	1:D:747:LYS:HG3	1.75	0.68
1:C:903:LYS:NZ	1:C:988:GLU:HG3	2.09	0.68
1:B:717:GLN:O	1:B:720:VAL:HG12	1.93	0.68
1:C:943:LYS:HD3	1:C:944:GLY:H	1.59	0.68
1:D:704:ARG:HA	1:D:707:GLN:NE2	2.08	0.68
1:D:921:LEU:HD12	1:D:1003:LEU:HD11	1.74	0.68
1:D:998:ASN:HD22	1:D:1000:LYS:HZ1	1.40	0.68
1:D:963:SER:O	1:D:964:LEU:HB2	1.91	0.67
1:D:901:VAL:HG13	1:D:902:SER:N	2.09	0.67
1:A:926:LEU:O	1:A:946:HIS:HB2	1.94	0.67
1:C:826:HIS:HD2	1:C:902:SER:OG	1.76	0.67
1:A:849:LYS:HB3	1:A:850:PRO:HD3	1.75	0.67
1:C:989:TYR:C	1:C:990:ILE:HD12	2.15	0.67
1:D:662:LYS:O	1:D:787:LYS:HB3	1.95	0.67
1:D:826:HIS:ND1	1:D:902:SER:HB2	2.09	0.67
1:A:822:HIS:HA	1:A:902:SER:OG	1.95	0.67
1:B:748:LYS:HB2	1:D:688:GLU:HG3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1002:LEU:HD13	1:B:1003:LEU:N	2.10	0.67
1:C:860:LEU:HB3	1:C:897:PHE:HB3	1.77	0.67
1:D:664:LYS:HZ2	1:D:665:LEU:HD21	1.59	0.67
1:D:864:SER:O	1:D:908:CYS:HA	1.95	0.67
1:C:890:MET:HG2	1:C:891:PHE:CD2	2.30	0.66
1:D:748:LYS:HD2	1:D:749:PRO:HD2	1.78	0.66
1:D:1006:LYS:HZ2	1:D:1008:ASN:H	1.41	0.66
1:C:667:LYS:HB3	1:C:668:PRO:HD3	1.76	0.66
1:B:854:LEU:HD21	1:B:927:GLY:HA3	1.76	0.66
1:B:856:ASN:HB3	1:B:927:GLY:H	1.61	0.66
1:D:919:ILE:HG23	1:D:920:LEU:N	2.11	0.66
1:B:822:HIS:NE2	1:B:831:LEU:HD13	2.11	0.65
1:B:956:PRO:HB3	1:B:972:GLY:O	1.96	0.65
1:D:861:TRP:O	1:D:862:HIS:HB2	1.96	0.65
1:A:891:PHE:HB2	1:A:990:ILE:CD1	2.26	0.65
1:B:799:THR:HG23	1:B:801:ILE:HD11	1.76	0.65
1:C:704:ARG:H	1:C:704:ARG:NE	1.94	0.65
1:C:797:LEU:HB3	1:C:799:THR:HG22	1.79	0.65
1:D:859:LEU:HD23	1:D:923:GLU:HB3	1.78	0.65
1:D:933:LYS:HD2	1:D:979:VAL:CG1	2.26	0.65
1:A:826:HIS:HA	1:C:726:ASP:OD2	1.97	0.65
1:B:854:LEU:CD2	1:B:927:GLY:HA3	2.25	0.65
1:B:878:ARG:HB3	1:B:878:ARG:NH1	2.10	0.65
1:D:811:ALA:O	1:D:815:ARG:HG3	1.95	0.65
1:D:702:SER:HA	1:D:772:GLU:HG3	1.79	0.65
1:A:927:GLY:HA3	1:A:946:HIS:ND1	2.12	0.65
1:C:729:ILE:HG21	1:C:753:ASN:HD22	1.61	0.65
1:D:868:ASN:O	1:D:870:ALA:N	2.30	0.65
1:D:964:LEU:HD22	1:D:965:ASP:N	2.08	0.65
1:D:855:HIS:HA	1:D:857:ARG:NH1	2.08	0.65
1:D:875:GLN:O	1:D:876:GLY:O	2.16	0.65
1:D:770:ASP:CG	1:D:868:ASN:HA	2.17	0.64
1:A:830:ASP:O	1:A:831:LEU:HD23	1.96	0.64
1:D:835:ASP:HB3	1:D:837:PHE:CZ	2.33	0.64
1:B:690:GLU:HG2	1:B:744:PHE:CE1	2.32	0.64
1:C:729:ILE:HD12	1:C:729:ILE:H	1.61	0.64
1:D:845:CYS:O	1:D:849:LYS:HG3	1.98	0.64
1:C:890:MET:HG2	1:C:891:PHE:CE2	2.33	0.64
1:A:916:ILE:H	1:A:916:ILE:HD12	1.63	0.64
1:D:858:ARG:HA	1:D:968:ASP:H	1.63	0.64
1:A:798:LYS:NZ	1:A:798:LYS:HB3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:LYS:HE2	1:B:761:LYS:HA	1.80	0.64
1:B:823:ALA:HB3	1:B:826:HIS:CD2	2.30	0.64
1:C:816:LYS:HE2	1:C:820:ASN:CG	2.19	0.64
1:A:698:LEU:HD23	1:A:701:LEU:HD12	1.80	0.63
1:B:702:SER:HB3	1:B:705:GLN:HB3	1.79	0.63
1:B:813:ILE:HG22	1:B:814:ILE:N	2.12	0.63
1:A:692:ASP:OD2	1:A:695:LYS:HD3	1.98	0.63
1:C:665:LEU:HD23	1:C:791:ASP:OD1	1.98	0.63
1:A:703:LYS:NZ	1:A:769:LEU:HD22	2.13	0.63
1:A:839:ILE:HD12	1:A:1002:LEU:HB2	1.81	0.63
1:B:916:ILE:HG22	1:B:1006:LYS:HA	1.80	0.63
1:D:793:ASN:O	1:D:796:LYS:HG2	1.97	0.63
1:A:858:ARG:HD3	1:A:926:LEU:CD1	2.28	0.63
1:B:887:THR:HG22	1:B:887:THR:O	1.96	0.63
1:C:828:ALA:O	1:C:1010:LYS:HG2	1.98	0.63
1:B:931:GLU:O	1:B:932:LEU:HD23	1.98	0.63
1:C:841:ARG:HG2	1:C:841:ARG:HH11	1.63	0.63
1:A:672:LEU:HD12	1:A:673:ILE:N	2.14	0.63
1:C:702:SER:HB2	1:C:704:ARG:NH2	2.14	0.63
1:B:703:LYS:N	1:B:704:ARG:HH21	1.96	0.63
1:B:941:LEU:HD12	1:B:941:LEU:N	2.14	0.63
1:B:829:TYR:CE1	1:B:831:LEU:HD11	2.34	0.62
1:B:1006:LYS:HB2	1:B:1006:LYS:NZ	2.14	0.62
1:C:828:ALA:C	1:C:1010:LYS:HG2	2.20	0.62
1:D:674:LYS:HD2	1:D:675:MET:N	2.13	0.62
1:D:847:ARG:HD3	1:D:995:ALA:HA	1.80	0.62
1:A:804:VAL:HB	1:A:836:ILE:HG22	1.80	0.62
1:A:878:ARG:NH1	1:A:879:ILE:HG12	2.14	0.62
1:D:918:LEU:HD23	1:D:918:LEU:N	2.14	0.62
1:B:865:ARG:HH11	1:B:865:ARG:HG2	1.64	0.62
1:D:926:LEU:HD13	1:D:929:MET:HE1	1.82	0.62
1:B:993:ASP:HB3	1:B:996:GLN:HE21	1.64	0.62
1:D:693:LEU:HD12	1:D:697:PRO:HA	1.82	0.62
1:A:754:ASN:N	1:A:754:ASN:ND2	2.45	0.62
1:D:925:ALA:HB3	1:D:996:GLN:HG3	1.81	0.62
1:B:907:TYR:CD1	2:B:2:CNQ:H15	2.35	0.62
1:D:829:TYR:HA	1:D:1010:LYS:HE2	1.80	0.62
1:C:920:LEU:HD13	1:C:999:LEU:HD22	1.81	0.62
1:D:940:LYS:H	1:D:940:LYS:HD2	1.64	0.62
1:D:1004:LYS:HD2	1:D:1005:LEU:N	2.15	0.62
1:B:697:PRO:HG2	1:B:700:LYS:CB	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:ALA:HB3	1:A:972:GLY:HA3	1.83	0.61
1:B:770:ASP:HB3	1:B:868:ASN:HA	1.81	0.61
1:C:752:LEU:HB3	1:C:758:VAL:HG12	1.82	0.61
1:D:802:LYS:HB3	1:D:838:LYS:HB3	1.82	0.61
1:D:720:VAL:HG13	1:D:721:SER:N	2.15	0.61
1:D:671:ASP:O	1:D:674:LYS:HE2	1.99	0.61
1:B:841:ARG:HH12	1:B:874:SER:C	2.04	0.61
1:C:834:ILE:HD11	1:C:1006:LYS:CG	2.30	0.61
1:D:751:LEU:HD12	1:D:751:LEU:N	2.15	0.61
1:D:872:ILE:O	1:D:876:GLY:HA2	1.99	0.61
1:C:834:ILE:HB	1:C:1004:LYS:O	2.01	0.61
1:D:693:LEU:CD1	1:D:697:PRO:HA	2.31	0.61
1:A:703:LYS:N	1:A:704:ARG:NH2	2.49	0.61
1:B:862:HIS:NE2	1:B:877:LEU:HD21	2.15	0.61
1:B:865:ARG:HB2	1:B:868:ASN:HD21	1.66	0.61
1:D:692:ASP:C	1:D:694:GLN:H	2.04	0.61
1:B:788:ASP:OD1	1:B:789:PRO:HD2	2.00	0.61
1:A:694:GLN:HB3	1:A:695:LYS:HD2	1.83	0.60
1:A:739:LEU:O	1:A:741:PRO:HD3	2.01	0.60
1:A:891:PHE:HA	1:A:936:SER:O	2.01	0.60
1:D:821:THR:O	1:D:901:VAL:N	2.33	0.60
1:A:866:THR:HG23	1:A:867:THR:N	2.15	0.60
1:A:916:ILE:HD12	1:A:916:ILE:N	2.16	0.60
1:A:929:MET:HG2	1:A:947:SER:OG	2.01	0.60
1:B:729:ILE:HD13	1:B:753:ASN:HA	1.83	0.60
1:B:868:ASN:O	1:B:872:ILE:HG13	2.00	0.60
1:C:720:VAL:CG1	1:C:721:SER:H	2.14	0.60
1:D:663:SER:HB2	1:D:790:ILE:HD11	1.83	0.60
1:D:992:TYR:CD1	1:D:992:TYR:N	2.68	0.60
1:C:865:ARG:O	1:C:868:ASN:HB2	2.02	0.60
1:D:694:GLN:NE2	1:D:694:GLN:HA	2.15	0.60
1:A:754:ASN:ND2	1:A:754:ASN:H	1.99	0.60
1:D:806:ARG:H	1:D:806:ARG:HD2	1.64	0.60
1:D:994:ILE:O	1:D:997:VAL:HG12	2.02	0.60
1:D:722:GLN:O	1:D:722:GLN:HG2	2.00	0.60
1:A:670:GLN:O	1:A:674:LYS:HG2	2.02	0.60
1:A:672:LEU:HD23	1:A:837:PHE:CE2	2.37	0.60
1:B:692:ASP:HB2	1:B:743:ASP:HB2	1.84	0.60
1:C:767:ASN:HD22	1:C:865:ARG:HE	1.50	0.60
1:D:866:THR:HA	1:D:918:LEU:HD21	1.83	0.60
1:C:849:LYS:O	1:C:849:LYS:HD3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:858:ARG:HG3	1:C:860:LEU:HD21	1.84	0.60
1:D:678:ASP:O	1:D:682:MET:HG3	2.02	0.60
1:A:677:PHE:CE2	1:A:793:ASN:HB3	2.37	0.59
1:B:900:MET:CE	1:B:956:PRO:HG3	2.32	0.59
1:D:831:LEU:HB3	1:D:1005:LEU:HD22	1.84	0.59
1:D:862:HIS:HE2	1:D:877:LEU:HD22	1.65	0.59
1:B:699:GLY:HA2	1:B:775:TYR:CE2	2.37	0.59
1:C:816:LYS:HE3	1:C:816:LYS:HA	1.83	0.59
1:B:748:LYS:HD3	1:B:749:PRO:N	2.17	0.59
1:B:735:ARG:HH11	1:B:735:ARG:HG2	1.65	0.59
1:B:830:ASP:HB2	1:B:1010:LYS:NZ	2.17	0.59
1:D:836:ILE:HD12	1:D:836:ILE:N	2.17	0.59
1:B:690:GLU:OE2	1:B:744:PHE:HA	2.03	0.59
1:C:729:ILE:HD12	1:C:729:ILE:N	2.18	0.59
1:D:671:ASP:HA	1:D:674:LYS:HZ3	1.68	0.59
1:C:834:ILE:HD11	1:C:1006:LYS:HG2	1.84	0.59
1:D:739:LEU:CD1	1:D:740:ILE:HG12	2.31	0.59
1:D:747:LYS:HB2	1:D:747:LYS:NZ	2.18	0.59
1:A:759:GLN:HA	1:A:762:VAL:HG23	1.85	0.59
1:D:670:GLN:C	1:D:672:LEU:H	2.05	0.59
1:B:880:ALA:HB3	1:B:893:LYS:HG2	1.85	0.59
1:C:686:MET:HE2	1:C:698:LEU:HG	1.83	0.59
1:D:989:TYR:C	1:D:990:ILE:HD12	2.23	0.59
1:B:829:TYR:CD1	1:B:831:LEU:HD11	2.37	0.59
1:C:863:GLY:HA3	1:C:904:SER:O	2.03	0.59
1:D:855:HIS:CA	1:D:857:ARG:HH12	2.11	0.59
1:D:890:MET:SD	1:D:984:LEU:HD21	2.43	0.59
1:A:735:ARG:O	1:A:738:THR:HG22	2.02	0.58
1:C:689:TYR:O	1:C:690:GLU:HB2	2.03	0.58
1:D:831:LEU:N	1:D:831:LEU:HD22	2.17	0.58
1:B:859:LEU:HD13	1:B:921:LEU:HD21	1.85	0.58
1:B:878:ARG:HH12	1:B:879:ILE:HG12	1.67	0.58
1:D:1004:LYS:HD2	1:D:1004:LYS:C	2.23	0.58
1:B:855:HIS:O	1:B:927:GLY:HA2	2.03	0.58
1:B:991:VAL:HG13	1:B:996:GLN:NE2	2.18	0.58
1:B:739:LEU:HD13	1:B:739:LEU:O	2.02	0.58
1:B:859:LEU:HD22	1:B:921:LEU:HD23	1.86	0.58
1:D:694:GLN:HA	1:D:694:GLN:HE21	1.68	0.58
1:A:1003:LEU:HD12	1:A:1003:LEU:N	2.18	0.58
1:D:849:LYS:NZ	1:D:849:LYS:HB3	2.18	0.58
1:C:706:ILE:CG2	1:C:765:LEU:HD22	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:GLN:HE21	1:A:722:GLN:N	2.01	0.58
1:D:667:LYS:HB3	1:D:668:PRO:HD3	1.84	0.58
1:C:990:ILE:HD12	1:C:990:ILE:N	2.19	0.58
1:A:735:ARG:HA	1:A:738:THR:HG22	1.85	0.57
1:A:835:ASP:HB2	1:A:1004:LYS:HB3	1.85	0.57
1:C:778:LEU:HD23	1:C:778:LEU:O	2.03	0.57
1:C:943:LYS:HD3	1:C:944:GLY:N	2.18	0.57
1:D:664:LYS:HZ2	1:D:665:LEU:HD11	1.68	0.57
1:D:664:LYS:HZ2	1:D:665:LEU:CD2	2.16	0.57
1:D:788:ASP:CG	1:D:789:PRO:HD2	2.23	0.57
1:D:709:ALA:HB1	1:D:765:LEU:HD11	1.86	0.57
1:C:814:ILE:O	1:C:818:VAL:HG23	2.04	0.57
1:D:799:THR:HG21	1:D:873:LEU:HB3	1.87	0.57
1:D:868:ASN:C	1:D:870:ALA:H	2.08	0.57
1:B:878:ARG:NH1	1:B:879:ILE:N	2.52	0.57
1:C:759:GLN:HA	1:C:759:GLN:HE21	1.67	0.57
1:B:702:SER:HB3	1:B:705:GLN:CB	2.35	0.57
1:B:704:ARG:H	1:B:704:ARG:NE	2.02	0.57
1:B:747:LYS:HG2	1:B:748:LYS:N	2.18	0.57
1:B:830:ASP:HB3	1:B:1008:ASN:HD22	1.68	0.57
1:C:879:ILE:HD13	1:C:879:ILE:N	2.03	0.57
1:B:901:VAL:CG1	1:B:902:SER:N	2.67	0.57
1:C:669:VAL:O	1:C:673:ILE:HG12	2.05	0.57
1:C:946:HIS:O	1:C:947:SER:HB3	2.03	0.57
1:A:707:GLN:O	1:A:710:TYR:HB2	2.04	0.57
1:C:962:ILE:CG2	1:C:963:SER:N	2.55	0.57
1:D:849:LYS:HB2	1:D:850:PRO:HD3	1.87	0.57
1:A:938:ILE:HD12	1:A:948:VAL:HG21	1.87	0.57
1:B:669:VAL:O	1:B:673:ILE:HG12	2.04	0.57
1:B:878:ARG:NH1	1:B:879:ILE:H	2.03	0.57
1:D:931:GLU:HA	1:D:949:LYS:O	2.05	0.56
1:A:940:LYS:NZ	1:A:943:LYS:HE3	2.20	0.56
1:C:679:VAL:O	1:C:682:MET:HB2	2.06	0.56
1:C:754:ASN:HD22	1:C:757:SER:CB	2.13	0.56
1:D:1004:LYS:HB3	1:D:1004:LYS:NZ	2.18	0.56
1:A:709:ALA:HB2	1:A:739:LEU:HD23	1.88	0.56
1:C:744:PHE:HD2	1:C:749:PRO:HG3	1.70	0.56
1:D:778:LEU:C	1:D:780:GLY:H	2.07	0.56
1:D:917:GLY:H	1:D:1007:PHE:HE1	1.54	0.56
1:B:720:VAL:HG21	1:B:755:ALA:HB2	1.88	0.56
1:B:775:TYR:O	1:B:779:ARG:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:ILE:O	1:D:716:VAL:HG23	2.04	0.56
1:D:852:LYS:C	1:D:854:LEU:H	2.08	0.56
1:D:878:ARG:NH1	1:D:879:ILE:HG12	2.20	0.56
1:D:854:LEU:HD23	1:D:946:HIS:ND1	2.20	0.56
1:B:667:LYS:CB	1:B:668:PRO:HD3	2.35	0.56
1:B:1002:LEU:C	1:B:1003:LEU:HD12	2.25	0.56
1:C:754:ASN:O	1:C:756:ASP:N	2.36	0.56
1:D:861:TRP:CZ2	1:D:901:VAL:HB	2.41	0.56
1:A:706:ILE:HG23	1:A:765:LEU:HG	1.88	0.56
1:B:680:GLU:HA	1:B:683:LYS:HE2	1.88	0.56
1:D:663:SER:CB	1:D:790:ILE:HD11	2.35	0.56
1:D:689:TYR:CG	1:D:764:MET:HG3	2.41	0.56
1:D:975:ILE:HG13	1:D:976:SER:N	2.21	0.56
1:A:878:ARG:CZ	1:A:879:ILE:HG12	2.36	0.56
1:B:799:THR:CG2	1:B:801:ILE:HD11	2.35	0.56
1:C:988:GLU:HG2	2:C:3:CNQ:H2	1.87	0.56
1:D:930:TYR:CB	1:D:945:LYS:HE2	2.35	0.56
1:A:855:HIS:O	1:A:856:ASN:HB2	2.04	0.55
1:C:720:VAL:CG1	1:C:721:SER:N	2.69	0.55
1:C:930:TYR:HB3	1:C:948:VAL:HG22	1.88	0.55
1:D:1007:PHE:O	1:D:1008:ASN:C	2.43	0.55
1:B:920:LEU:CD1	1:B:1002:LEU:HD23	2.34	0.55
1:D:703:LYS:HE2	1:D:707:GLN:OE1	2.07	0.55
1:C:707:GLN:O	1:C:710:TYR:HB2	2.07	0.55
1:B:673:ILE:HD11	1:B:794:TYR:HD1	1.71	0.55
1:D:864:SER:HB3	1:D:869:PHE:CE1	2.41	0.55
1:C:663:SER:CB	1:C:791:ASP:OD1	2.54	0.55
1:C:731:ASP:OD2	1:C:735:ARG:HD2	2.06	0.55
1:D:963:SER:O	1:D:964:LEU:CB	2.54	0.55
1:A:838:LYS:HD2	1:A:1001:TYR:CE1	2.42	0.55
1:B:896:TYR:CE2	1:B:990:ILE:HG12	2.42	0.55
1:B:942:PRO:O	1:B:945:LYS:HB2	2.07	0.55
1:C:703:LYS:HB3	1:C:704:ARG:HH11	1.71	0.55
1:C:805:ASP:C	1:C:807:ASP:H	2.08	0.55
1:D:689:TYR:CD1	1:D:764:MET:HG3	2.41	0.55
1:D:887:THR:O	1:D:887:THR:HG22	2.07	0.55
1:D:1003:LEU:HD12	1:D:1003:LEU:H	1.73	0.55
1:A:748:LYS:HA	1:A:748:LYS:HE2	1.88	0.54
1:B:869:PHE:CE2	1:B:1002:LEU:HD21	2.42	0.54
1:D:709:ALA:CB	1:D:765:LEU:HD11	2.37	0.54
1:A:718:GLN:O	1:A:722:GLN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:LEU:HD12	1:B:1005:LEU:N	2.23	0.54
1:B:790:ILE:HG22	1:B:791:ASP:N	2.23	0.54
1:D:706:ILE:O	1:D:709:ALA:HB3	2.08	0.54
1:D:714:SER:O	1:D:717:GLN:HG2	2.08	0.54
1:A:752:LEU:HD11	1:A:761:LYS:NZ	2.22	0.54
1:A:792:VAL:O	1:A:796:LYS:HG3	2.07	0.54
1:B:907:TYR:CE1	2:B:2:CNQ:H15	2.42	0.54
1:B:859:LEU:HD13	1:B:921:LEU:CD2	2.37	0.54
1:C:849:LYS:O	1:C:852:LYS:HB3	2.07	0.54
1:D:891:PHE:HA	1:D:936:SER:O	2.07	0.54
1:D:712:ILE:HG13	1:D:739:LEU:HD21	1.90	0.54
1:B:818:VAL:O	1:B:901:VAL:HG11	2.07	0.54
1:C:777:LEU:HD11	1:C:796:LYS:HB3	1.89	0.54
1:C:798:LYS:HD2	1:C:842:GLU:CD	2.28	0.54
1:A:735:ARG:HA	1:A:738:THR:CG2	2.38	0.54
1:A:788:ASP:C	1:A:790:ILE:H	2.11	0.54
1:B:727:SER:OG	1:D:828:ALA:HA	2.07	0.54
1:D:662:LYS:HA	1:D:788:ASP:H	1.72	0.54
1:D:812:GLU:HA	1:D:815:ARG:HD2	1.89	0.54
1:D:964:LEU:HD13	1:D:965:ASP:N	2.23	0.54
1:D:770:ASP:OD2	1:D:868:ASN:O	2.26	0.54
1:D:779:ARG:HA	1:D:779:ARG:NE	2.22	0.54
1:A:962:ILE:HG12	1:A:971:LEU:HD11	1.89	0.53
1:B:792:VAL:O	1:B:795:GLU:HG3	2.08	0.53
1:D:710:TYR:OH	1:D:766:ASP:CG	2.46	0.53
1:D:839:ILE:CD1	1:D:1002:LEU:HB2	2.30	0.53
1:D:933:LYS:HD2	1:D:979:VAL:HG11	1.91	0.53
1:A:754:ASN:CG	1:A:757:SER:HB3	2.28	0.53
1:B:865:ARG:HG2	1:B:865:ARG:NH1	2.23	0.53
1:D:713:LEU:HD11	1:D:765:LEU:HD12	1.90	0.53
1:D:856:ASN:HB3	1:D:926:LEU:HB2	1.90	0.53
1:A:897:PHE:HB2	1:A:989:TYR:HB2	1.90	0.53
1:D:992:TYR:N	1:D:992:TYR:HD1	2.06	0.53
1:D:1003:LEU:HD12	1:D:1003:LEU:N	2.23	0.53
1:A:724:SER:O	1:A:725:SER:HB3	2.08	0.53
1:D:852:LYS:O	1:D:854:LEU:N	2.41	0.53
1:B:739:LEU:O	1:B:741:PRO:HD3	2.09	0.53
1:C:702:SER:HB2	1:C:704:ARG:HH21	1.71	0.53
1:D:720:VAL:HG13	1:D:721:SER:H	1.73	0.53
1:A:994:ILE:O	1:A:997:VAL:HG12	2.08	0.53
1:C:716:VAL:O	1:C:720:VAL:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:903:LYS:HZ3	1:C:988:GLU:HG3	1.73	0.53
1:D:664:LYS:HD2	1:D:665:LEU:H	1.73	0.53
1:D:692:ASP:O	1:D:694:GLN:N	2.42	0.53
1:D:794:TYR:HD2	1:D:794:TYR:O	1.92	0.53
1:D:879:ILE:CG2	1:D:894:GLY:HA2	2.39	0.53
1:B:739:LEU:HD13	1:B:739:LEU:C	2.29	0.52
1:C:960:ALA:HB3	1:C:972:GLY:HA3	1.90	0.52
1:D:832:GLU:O	1:D:834:ILE:HG12	2.09	0.52
1:B:667:LYS:HE3	1:B:671:ASP:OD2	2.10	0.52
1:A:735:ARG:C	1:A:738:THR:HG22	2.29	0.52
1:A:938:ILE:CD1	1:A:948:VAL:HG21	2.39	0.52
1:B:765:LEU:HD23	1:B:768:LEU:HD12	1.90	0.52
1:B:862:HIS:CD2	1:B:877:LEU:HD21	2.44	0.52
1:D:933:LYS:HD2	1:D:979:VAL:HG13	1.92	0.52
1:A:698:LEU:HD23	1:A:701:LEU:CD1	2.39	0.52
1:D:662:LYS:N	1:D:787:LYS:HG3	2.24	0.52
1:A:709:ALA:HB3	1:A:765:LEU:HD21	1.91	0.52
1:C:677:PHE:CE2	1:C:793:ASN:HB3	2.44	0.52
1:C:829:TYR:HD1	1:C:829:TYR:O	1.92	0.52
1:D:843:GLY:C	1:D:845:CYS:H	2.12	0.52
1:D:878:ARG:CZ	1:D:879:ILE:HG12	2.40	0.52
1:B:849:LYS:HZ2	1:B:849:LYS:HA	1.74	0.52
1:D:797:LEU:HB3	1:D:799:THR:OG1	2.10	0.52
1:A:710:TYR:CE2	1:A:881:PRO:HG3	2.45	0.52
1:C:729:ILE:H	1:C:729:ILE:CD1	2.23	0.52
1:A:703:LYS:HZ2	1:A:769:LEU:HD22	1.75	0.52
1:C:953:LYS:HE3	1:C:980:ASN:HB2	1.92	0.52
1:B:679:VAL:HG23	1:B:680:GLU:N	2.21	0.52
1:C:717:GLN:C	1:C:719:ALA:H	2.13	0.52
1:D:671:ASP:HA	1:D:674:LYS:NZ	2.25	0.52
1:D:805:ASP:OD2	1:D:805:ASP:N	2.43	0.52
1:A:788:ASP:OD1	1:A:790:ILE:HG12	2.10	0.51
1:A:911:SER:CB	1:C:748:LYS:HE3	2.40	0.51
1:A:962:ILE:CG1	1:A:971:LEU:HD11	2.40	0.51
1:B:671:ASP:HA	1:B:674:LYS:HD3	1.91	0.51
1:A:703:LYS:HG3	1:A:707:GLN:NE2	2.25	0.51
1:D:854:LEU:N	1:D:854:LEU:HD12	2.25	0.51
1:A:857:ARG:HA	1:A:924:VAL:O	2.10	0.51
1:D:861:TRP:O	1:D:862:HIS:CB	2.58	0.51
1:A:686:MET:O	1:A:691:ILE:HB	2.10	0.51
1:D:679:VAL:HA	1:D:682:MET:SD	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:919:ILE:HG22	1:D:1003:LEU:HB2	1.93	0.51
1:A:682:MET:O	1:A:685:ALA:HB3	2.09	0.51
1:D:670:GLN:C	1:D:672:LEU:N	2.64	0.51
1:D:674:LYS:HE2	1:D:675:MET:HG3	1.92	0.51
1:D:815:ARG:HB3	1:D:815:ARG:NH1	2.24	0.51
1:B:901:VAL:CG1	1:B:902:SER:H	2.24	0.51
1:A:896:TYR:CE2	1:A:990:ILE:HD11	2.46	0.51
1:D:858:ARG:HB3	1:D:968:ASP:HB3	1.92	0.51
1:D:924:VAL:HG23	1:D:926:LEU:HG	1.91	0.51
1:A:788:ASP:O	1:A:790:ILE:N	2.44	0.51
1:B:777:LEU:HD13	1:B:777:LEU:C	2.31	0.51
1:B:826:HIS:HA	1:D:726:ASP:OD2	2.10	0.51
1:C:767:ASN:ND2	1:C:865:ARG:HE	2.08	0.51
1:D:829:TYR:CA	1:D:1010:LYS:HE2	2.40	0.51
1:D:990:ILE:HG22	1:D:992:TYR:CE1	2.45	0.51
1:A:789:PRO:HA	1:A:792:VAL:CG2	2.41	0.51
1:B:821:THR:O	1:B:901:VAL:HG12	2.10	0.51
1:C:816:LYS:HE2	1:C:820:ASN:ND2	2.26	0.51
1:C:823:ALA:HB3	1:C:826:HIS:CD2	2.46	0.51
1:D:862:HIS:HA	2:D:4:CNQ:O13	2.10	0.51
1:D:901:VAL:CG1	1:D:902:SER:N	2.74	0.51
1:D:1003:LEU:O	1:D:1004:LYS:HB2	2.11	0.51
1:A:796:LYS:O	1:A:798:LYS:HG2	2.11	0.51
1:B:737:TYR:OH	1:B:750:PRO:HG2	2.11	0.51
1:C:933:LYS:HG2	1:C:934:HIS:ND1	2.25	0.51
1:D:853:GLN:C	1:D:854:LEU:HD12	2.32	0.51
1:A:788:ASP:OD1	1:A:789:PRO:HD2	2.12	0.50
1:B:702:SER:OG	1:B:704:ARG:NH2	2.45	0.50
1:B:890:MET:CE	1:B:935:ALA:HB2	2.41	0.50
1:C:1007:PHE:HB2	1:C:1009:PHE:CE1	2.46	0.50
1:D:665:LEU:H	1:D:665:LEU:CD2	2.20	0.50
1:D:775:TYR:O	1:D:778:LEU:N	2.42	0.50
1:D:842:GLU:O	1:D:842:GLU:HG3	2.11	0.50
1:A:714:SER:CB	1:A:885:PRO:HB3	2.42	0.50
1:B:685:ALA:O	1:B:688:GLU:HG2	2.11	0.50
1:C:731:ASP:OD2	1:C:731:ASP:C	2.49	0.50
1:D:662:LYS:HB3	1:D:788:ASP:HB2	1.94	0.50
1:A:838:LYS:HD2	1:A:1001:TYR:HE1	1.76	0.50
1:A:998:ASN:HD22	1:A:1000:LYS:HE2	1.76	0.50
1:D:862:HIS:ND1	2:D:4:CNQ:N12	2.59	0.50
1:D:901:VAL:HG13	1:D:902:SER:H	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:ASP:OD1	1:A:981:ASP:N	2.43	0.50
1:B:793:ASN:HA	1:B:796:LYS:HD2	1.94	0.50
1:C:759:GLN:HA	1:C:759:GLN:NE2	2.26	0.50
1:C:985:LEU:HD22	1:C:985:LEU:N	2.27	0.50
1:B:841:ARG:NH1	1:B:873:LEU:O	2.45	0.50
1:D:726:ASP:O	1:D:730:LEU:HB2	2.12	0.50
1:D:701:LEU:O	1:D:702:SER:HB3	2.12	0.50
1:D:713:LEU:CD1	1:D:765:LEU:HD12	2.42	0.50
1:D:955:THR:CG2	1:D:977:SER:HB3	2.42	0.50
1:C:1007:PHE:HD1	1:C:1007:PHE:H	1.60	0.50
1:D:664:LYS:HZ2	1:D:665:LEU:CD1	2.25	0.50
1:D:664:LYS:NZ	1:D:665:LEU:HD11	2.26	0.50
1:A:861:TRP:CZ3	1:A:921:LEU:HG	2.47	0.49
1:B:830:ASP:HB2	1:B:1010:LYS:HZ1	1.76	0.49
1:D:790:ILE:HG13	1:D:791:ASP:N	2.26	0.49
1:D:865:ARG:HH21	1:D:909:HIS:CE1	2.30	0.49
1:B:702:SER:OG	1:B:704:ARG:CZ	2.60	0.49
1:B:703:LYS:H	1:B:704:ARG:NH2	2.05	0.49
1:D:919:ILE:HD13	1:D:920:LEU:N	2.16	0.49
1:D:759:GLN:HE21	1:D:759:GLN:HA	1.78	0.49
1:A:844:GLU:OE1	1:A:999:LEU:N	2.45	0.49
1:D:669:VAL:O	1:D:673:ILE:HG12	2.11	0.49
1:D:797:LEU:O	1:D:799:THR:HG23	2.13	0.49
1:A:924:VAL:HG23	1:A:926:LEU:HG	1.94	0.49
1:B:901:VAL:HG13	1:B:902:SER:H	1.73	0.49
1:A:844:GLU:HA	1:A:847:ARG:HG2	1.93	0.49
1:B:683:LYS:O	1:B:687:VAL:HG23	2.12	0.49
1:B:775:TYR:O	1:B:778:LEU:HB3	2.12	0.49
1:C:782:SER:CA	1:C:792:VAL:HG11	2.34	0.49
1:D:754:ASN:O	1:D:756:ASP:N	2.39	0.49
1:D:835:ASP:HB3	1:D:837:PHE:CE2	2.47	0.49
1:A:866:THR:CG2	1:A:867:THR:N	2.76	0.49
1:B:786:SER:O	1:B:787:LYS:HD2	2.12	0.49
1:C:782:SER:HA	1:C:792:VAL:CG1	2.34	0.49
1:C:882:PRO:O	1:C:884:ALA:N	2.46	0.49
1:D:854:LEU:HD23	1:D:927:GLY:HA3	1.95	0.49
1:D:854:LEU:HB3	1:D:927:GLY:HA2	1.94	0.49
1:D:933:LYS:HG2	1:D:951:LEU:HB2	1.94	0.49
1:A:723:GLY:O	1:A:724:SER:HB3	2.13	0.49
1:D:682:MET:CE	1:D:774:ALA:HB3	2.43	0.49
1:D:737:TYR:OH	1:D:750:PRO:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:841:ARG:HH11	1:D:841:ARG:CB	2.11	0.49
1:D:879:ILE:O	1:D:880:ALA:C	2.51	0.49
1:B:717:GLN:C	1:B:720:VAL:HG12	2.33	0.49
1:D:841:ARG:HE	1:D:876:GLY:N	2.08	0.49
1:B:752:LEU:HB3	1:B:758:VAL:HG12	1.95	0.49
1:B:839:ILE:HD11	1:B:920:LEU:HD11	1.94	0.49
1:A:715:GLU:OE2	1:A:735:ARG:NH2	2.46	0.48
1:B:822:HIS:CD2	1:B:831:LEU:HD22	2.48	0.48
1:C:905:ALA:C	1:C:907:TYR:H	2.15	0.48
1:C:901:VAL:HG13	1:C:902:SER:N	2.28	0.48
1:D:778:LEU:O	1:D:780:GLY:N	2.46	0.48
1:D:838:LYS:HE2	1:D:840:GLU:OE2	2.13	0.48
1:B:823:ALA:O	1:B:826:HIS:HB2	2.13	0.48
1:B:827:ASN:O	1:B:828:ALA:HB2	2.14	0.48
1:C:778:LEU:HD23	1:C:778:LEU:C	2.33	0.48
1:A:827:ASN:HD21	1:C:725:SER:HB2	1.77	0.48
1:B:717:GLN:HA	1:B:720:VAL:HG12	1.95	0.48
1:B:890:MET:HG3	1:B:935:ALA:CB	2.44	0.48
1:C:681:SER:HA	1:C:684:LYS:HG3	1.94	0.48
1:D:964:LEU:C	1:D:966:GLY:H	2.15	0.48
1:A:826:HIS:ND1	1:A:902:SER:CB	2.76	0.48
1:B:687:VAL:HG22	1:B:693:LEU:HD23	1.96	0.48
1:B:719:ALA:HB1	1:B:724:SER:OG	2.13	0.48
1:C:872:ILE:HG23	1:C:877:LEU:HD23	1.94	0.48
1:B:722:GLN:HA	1:B:722:GLN:OE1	2.14	0.48
1:A:718:GLN:C	1:A:718:GLN:NE2	2.67	0.48
1:C:697:PRO:CG	1:C:700:LYS:HB2	2.34	0.48
1:D:765:LEU:HD23	1:D:768:LEU:HD12	1.95	0.48
1:D:855:HIS:O	1:D:856:ASN:HB2	2.14	0.48
1:B:707:GLN:HB3	1:B:883:GLU:HG2	1.95	0.48
1:C:744:PHE:CD2	1:C:749:PRO:HG3	2.49	0.48
1:C:856:ASN:HD21	1:C:858:ARG:HH11	1.61	0.48
1:A:706:ILE:CD1	1:A:768:LEU:HB3	2.44	0.48
1:A:753:ASN:C	1:A:755:ALA:H	2.17	0.48
1:B:887:THR:HG23	1:B:937:HIS:CD2	2.48	0.48
1:C:679:VAL:HA	1:C:682:MET:HE3	1.96	0.48
1:D:662:LYS:CA	1:D:788:ASP:H	2.26	0.48
1:D:813:ILE:HD12	1:D:813:ILE:N	2.28	0.48
1:A:744:PHE:O	1:A:747:LYS:HG2	2.13	0.48
1:A:798:LYS:HB3	1:A:798:LYS:HZ2	1.79	0.48
1:B:858:ARG:NH2	1:B:929:MET:HE1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:TYR:HB3	1:A:764:MET:HE2	1.96	0.47
1:A:942:PRO:O	1:A:945:LYS:HG2	2.14	0.47
1:B:869:PHE:HE2	1:B:1002:LEU:HD21	1.79	0.47
1:C:832:GLU:O	1:C:834:ILE:HD12	2.13	0.47
1:D:841:ARG:HH21	1:D:875:GLN:HA	1.77	0.47
1:D:903:LYS:O	1:D:906:ASN:HB2	2.14	0.47
1:B:801:ILE:N	1:B:801:ILE:HD13	2.29	0.47
1:B:839:ILE:HD13	1:B:1002:LEU:HB2	1.95	0.47
1:C:763:GLU:HA	2:C:3:CNQ:CL24	2.51	0.47
1:D:670:GLN:O	1:D:672:LEU:N	2.46	0.47
1:D:964:LEU:HD13	1:D:965:ASP:CB	2.44	0.47
1:A:735:ARG:CA	1:A:738:THR:HG22	2.45	0.47
1:B:827:ASN:HD21	1:D:725:SER:CB	2.27	0.47
1:B:827:ASN:HD21	1:D:725:SER:HB3	1.79	0.47
1:B:857:ARG:HA	1:B:924:VAL:O	2.14	0.47
1:C:900:MET:O	1:C:901:VAL:C	2.53	0.47
1:D:702:SER:CA	1:D:772:GLU:HG3	2.43	0.47
1:D:703:LYS:HG2	1:D:707:GLN:OE1	2.14	0.47
1:D:759:GLN:HA	1:D:759:GLN:NE2	2.29	0.47
1:A:826:HIS:ND1	1:A:902:SER:HB2	2.29	0.47
1:B:827:ASN:ND2	1:D:725:SER:HB3	2.29	0.47
1:D:975:ILE:CG1	1:D:976:SER:H	2.26	0.47
1:A:759:GLN:HA	1:A:759:GLN:HE21	1.79	0.47
1:A:772:GLU:OE1	1:A:772:GLU:C	2.53	0.47
1:B:672:LEU:O	1:B:676:ILE:HG12	2.14	0.47
1:C:777:LEU:HD13	1:C:796:LYS:HD3	1.96	0.47
1:A:703:LYS:HB3	1:A:704:ARG:NH1	2.30	0.47
1:A:718:GLN:C	1:A:718:GLN:HE21	2.18	0.47
1:B:689:TYR:O	1:B:690:GLU:HB3	2.15	0.47
1:B:872:ILE:O	1:B:876:GLY:N	2.45	0.47
1:B:941:LEU:N	1:B:941:LEU:CD1	2.77	0.47
1:C:714:SER:HA	1:C:885:PRO:HB3	1.95	0.47
1:C:879:ILE:CD1	1:C:879:ILE:N	2.65	0.47
1:D:831:LEU:N	1:D:831:LEU:CD2	2.77	0.47
1:D:862:HIS:NE2	1:D:877:LEU:HD22	2.29	0.47
1:A:706:ILE:HD12	1:A:769:LEU:HD23	1.97	0.47
1:B:688:GLU:HA	1:D:747:LYS:HA	1.96	0.47
1:B:777:LEU:HD11	1:B:796:LYS:CB	2.44	0.47
1:B:830:ASP:C	1:B:831:LEU:HD12	2.35	0.47
1:C:869:PHE:HA	1:C:872:ILE:HD12	1.97	0.47
1:D:915:PRO:HB3	1:D:1009:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:931:GLU:HB3	1:D:949:LYS:HB3	1.97	0.47
1:D:1009:PHE:O	1:D:1010:LYS:HD3	2.14	0.47
1:B:834:ILE:HB	1:B:1004:LYS:HG2	1.97	0.47
1:B:856:ASN:HB3	1:B:927:GLY:N	2.27	0.47
1:C:942:PRO:O	1:C:945:LYS:HB2	2.14	0.47
1:D:794:TYR:O	1:D:797:LEU:HB2	2.14	0.47
1:D:831:LEU:HD12	1:D:1005:LEU:CD1	2.45	0.47
1:B:763:GLU:O	1:B:766:ASP:HB2	2.15	0.47
1:B:797:LEU:CB	1:B:799:THR:HG22	2.45	0.47
1:B:803:VAL:HG12	1:B:804:VAL:N	2.29	0.47
1:D:849:LYS:O	1:D:852:LYS:HG3	2.15	0.47
1:A:826:HIS:CE1	1:A:906:ASN:HD21	2.33	0.47
1:A:841:ARG:HG2	1:A:841:ARG:HH11	1.80	0.47
1:B:690:GLU:OE1	1:D:747:LYS:HE2	2.15	0.47
1:B:759:GLN:O	1:B:763:GLU:HG2	2.15	0.47
1:B:846:GLN:NE2	1:B:846:GLN:HA	2.30	0.47
1:D:768:LEU:O	1:D:771:ILE:N	2.47	0.47
1:D:762:VAL:O	1:D:766:ASP:OD1	2.33	0.46
1:D:777:LEU:HD13	1:D:777:LEU:C	2.34	0.46
1:A:758:VAL:O	1:A:762:VAL:HG23	2.15	0.46
1:A:911:SER:HB3	1:C:748:LYS:HE3	1.97	0.46
1:C:797:LEU:HB3	1:C:799:THR:CG2	2.45	0.46
1:D:798:LYS:HB3	1:D:842:GLU:CB	2.38	0.46
1:D:915:PRO:O	1:D:916:ILE:HG23	2.15	0.46
1:D:985:LEU:HD23	1:D:986:TYR:CE2	2.49	0.46
1:A:671:ASP:O	1:A:674:LYS:HG3	2.15	0.46
1:A:697:PRO:O	1:A:698:LEU:C	2.53	0.46
1:C:912:GLN:O	1:C:915:PRO:HD3	2.15	0.46
1:C:955:THR:O	1:C:975:ILE:N	2.46	0.46
1:D:702:SER:O	1:D:706:ILE:HG13	2.15	0.46
1:D:822:HIS:CD2	1:D:831:LEU:HD23	2.50	0.46
1:D:1007:PHE:O	1:D:1009:PHE:N	2.48	0.46
1:D:664:LYS:HD2	1:D:665:LEU:N	2.30	0.46
1:B:851:PHE:CD1	1:B:996:GLN:HG2	2.51	0.46
1:B:934:HIS:ND1	1:B:934:HIS:N	2.64	0.46
1:A:701:LEU:HD21	1:A:768:LEU:HD22	1.98	0.46
1:A:839:ILE:HD13	1:A:839:ILE:N	2.24	0.46
1:A:869:PHE:CE1	1:A:918:LEU:HB2	2.51	0.46
1:B:720:VAL:HG11	1:B:755:ALA:HB2	1.98	0.46
1:C:859:LEU:HB2	1:C:969:VAL:HG22	1.97	0.46
1:C:873:LEU:HD23	1:C:873:LEU:HA	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1007:PHE:CD1	1:C:1007:PHE:N	2.84	0.46
1:D:861:TRP:CE3	1:D:921:LEU:HD21	2.50	0.46
1:D:964:LEU:C	1:D:966:GLY:N	2.69	0.46
1:A:953:LYS:HD2	1:A:985:LEU:HD12	1.98	0.46
1:B:887:THR:HG23	1:B:937:HIS:NE2	2.30	0.46
1:D:677:PHE:CE2	1:D:793:ASN:HB3	2.51	0.46
1:A:858:ARG:HA	1:A:967:VAL:HG13	1.98	0.46
1:C:830:ASP:O	1:C:1008:ASN:ND2	2.42	0.46
1:C:953:LYS:HD3	1:C:980:ASN:HB3	1.98	0.46
1:D:662:LYS:O	1:D:788:ASP:N	2.47	0.46
1:D:692:ASP:C	1:D:694:GLN:N	2.69	0.46
1:D:920:LEU:HD21	1:D:999:LEU:HD22	1.97	0.46
1:B:748:LYS:CB	1:D:688:GLU:HG3	2.42	0.46
1:B:827:ASN:CG	1:D:725:SER:HB3	2.36	0.46
1:D:670:GLN:OE1	1:D:790:ILE:HD12	2.16	0.46
1:A:788:ASP:C	1:A:790:ILE:N	2.69	0.45
1:A:821:THR:HB	1:A:900:MET:HA	1.99	0.45
1:C:744:PHE:CE2	1:C:749:PRO:HB3	2.51	0.45
1:C:975:ILE:HD12	1:C:975:ILE:HA	1.74	0.45
1:D:730:LEU:HD23	1:D:730:LEU:HA	1.78	0.45
1:B:677:PHE:CD2	1:B:793:ASN:HB3	2.50	0.45
1:B:806:ARG:NH1	1:B:806:ARG:HB2	2.32	0.45
1:B:859:LEU:HD22	1:B:921:LEU:CD2	2.46	0.45
1:B:880:ALA:HB3	1:B:893:LYS:CG	2.46	0.45
1:C:779:ARG:O	1:C:779:ARG:HG3	2.16	0.45
1:C:829:TYR:HA	1:C:1010:LYS:HD3	1.97	0.45
1:C:851:PHE:C	1:C:853:GLN:N	2.69	0.45
1:D:699:GLY:HA2	1:D:775:TYR:CE2	2.50	0.45
1:D:801:ILE:O	1:D:801:ILE:HG22	2.16	0.45
1:D:822:HIS:HD2	1:D:831:LEU:HD23	1.81	0.45
1:D:832:GLU:HB3	1:D:1006:LYS:HG2	1.98	0.45
1:D:861:TRP:HA	1:D:921:LEU:HD23	1.98	0.45
1:D:964:LEU:HD13	1:D:965:ASP:HB2	1.97	0.45
1:A:878:ARG:NH2	1:A:879:ILE:O	2.49	0.45
1:C:691:ILE:HG22	1:C:692:ASP:N	2.31	0.45
1:C:712:ILE:HG21	1:C:736:PHE:HB2	1.98	0.45
1:C:962:ILE:HB	1:C:971:LEU:HD11	1.99	0.45
1:D:662:LYS:O	1:D:788:ASP:HB3	2.16	0.45
1:D:728:GLN:OE1	1:D:728:GLN:N	2.49	0.45
1:D:853:GLN:O	1:D:853:GLN:HG3	2.17	0.45
1:D:879:ILE:HG21	1:D:894:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:VAL:HG12	1:A:819:LYS:N	2.31	0.45
1:C:887:THR:HG22	1:C:937:HIS:CD2	2.52	0.45
1:D:670:GLN:HE22	1:D:790:ILE:CD1	2.29	0.45
1:D:762:VAL:CG2	1:D:885:PRO:HG3	2.46	0.45
1:D:817:TYR:CE1	1:D:821:THR:HG21	2.51	0.45
1:D:886:VAL:C	1:D:888:GLY:H	2.20	0.45
1:A:1011:THR:HB	1:C:730:LEU:HD11	1.99	0.45
1:C:826:HIS:HD2	1:C:902:SER:CB	2.30	0.45
1:C:844:GLU:OE1	1:C:998:ASN:HA	2.17	0.45
1:A:816:LYS:HE3	1:A:816:LYS:HB2	1.77	0.45
1:B:677:PHE:CE2	1:B:793:ASN:HB3	2.52	0.45
1:B:731:ASP:O	1:B:735:ARG:HG3	2.17	0.45
1:B:749:PRO:HA	1:B:750:PRO:HD2	1.81	0.45
1:B:1004:LYS:C	1:B:1005:LEU:HD12	2.37	0.45
1:D:663:SER:OG	1:D:790:ILE:HD11	2.16	0.45
1:D:794:TYR:C	1:D:794:TYR:CD2	2.90	0.45
1:C:709:ALA:O	1:C:713:LEU:HD23	2.17	0.45
1:C:854:LEU:HD23	1:C:925:ALA:HB1	1.98	0.45
1:D:677:PHE:CD1	1:D:778:LEU:HD22	2.52	0.45
1:D:790:ILE:HG13	1:D:791:ASP:OD1	2.17	0.45
1:B:748:LYS:HD3	1:B:748:LYS:C	2.36	0.45
1:B:777:LEU:HD13	1:B:777:LEU:O	2.17	0.45
1:C:704:ARG:N	1:C:704:ARG:CD	2.79	0.45
1:D:717:GLN:CG	1:D:718:GLN:N	2.80	0.45
1:D:806:ARG:HD2	1:D:806:ARG:N	2.29	0.45
1:D:858:ARG:HH21	1:D:970:PRO:CG	2.29	0.45
1:A:942:PRO:HB2	1:A:945:LYS:HG3	1.98	0.45
1:A:943:LYS:HE2	1:A:943:LYS:CA	2.46	0.45
1:B:854:LEU:HD22	1:B:855:HIS:O	2.16	0.45
1:C:686:MET:O	1:C:689:TYR:HB2	2.17	0.45
1:C:761:LYS:HA	1:C:761:LYS:HD3	1.73	0.45
1:A:704:ARG:CZ	1:A:704:ARG:H	2.30	0.44
1:B:903:LYS:NZ	1:B:988:GLU:HG2	2.32	0.44
1:C:785:SER:O	1:C:786:SER:C	2.54	0.44
1:D:777:LEU:HD22	1:D:777:LEU:O	2.18	0.44
1:D:848:TYR:CG	1:D:848:TYR:O	2.69	0.44
1:D:914:ASP:N	1:D:915:PRO:CD	2.80	0.44
1:A:695:LYS:HD2	1:A:695:LYS:N	2.33	0.44
1:A:828:ALA:O	1:A:829:TYR:HB3	2.16	0.44
1:A:858:ARG:O	1:A:923:GLU:HA	2.17	0.44
1:C:696:MET:CG	1:C:741:PRO:HD2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:852:LYS:O	1:C:852:LYS:HG3	2.16	0.44
1:C:868:ASN:O	1:C:872:ILE:HG13	2.18	0.44
1:D:717:GLN:HE22	1:D:886:VAL:HG23	1.82	0.44
1:D:920:LEU:HD23	1:D:920:LEU:C	2.36	0.44
1:A:674:LYS:HG3	1:A:675:MET:N	2.33	0.44
1:B:726:ASP:C	1:D:828:ALA:HB2	2.37	0.44
1:B:910:THR:HB	1:B:914:ASP:O	2.16	0.44
1:C:954:THR:HG22	1:C:955:THR:N	2.31	0.44
1:C:993:ASP:HB3	1:C:996:GLN:HE21	1.82	0.44
1:D:676:ILE:CG2	1:D:870:ALA:HA	2.43	0.44
1:D:895:ILE:HD11	1:D:994:ILE:CD1	2.45	0.44
1:A:1010:LYS:HD2	1:A:1010:LYS:N	2.33	0.44
1:B:920:LEU:HD21	1:B:999:LEU:CD1	2.28	0.44
1:B:958:PRO:C	1:B:960:ALA:H	2.21	0.44
1:C:841:ARG:HG2	1:C:841:ARG:NH1	2.32	0.44
1:C:994:ILE:HD13	1:C:994:ILE:N	2.32	0.44
1:D:775:TYR:CZ	1:D:779:ARG:HD2	2.52	0.44
1:D:779:ARG:HA	1:D:779:ARG:HE	1.81	0.44
1:B:662:LYS:HE2	1:B:788:ASP:OD2	2.18	0.44
1:C:793:ASN:O	1:C:796:LYS:HB2	2.18	0.44
1:C:826:HIS:CD2	1:C:902:SER:OG	2.65	0.44
1:D:768:LEU:O	1:D:769:LEU:C	2.56	0.44
1:A:759:GLN:O	1:A:763:GLU:HG3	2.18	0.44
1:B:1006:LYS:HB2	1:B:1006:LYS:HZ3	1.83	0.44
1:C:754:ASN:ND2	1:C:757:SER:HB3	2.20	0.44
1:D:682:MET:HE3	1:D:774:ALA:HB3	1.99	0.44
1:D:843:GLY:C	1:D:845:CYS:N	2.70	0.44
1:D:901:VAL:CG1	1:D:902:SER:H	2.29	0.44
1:A:828:ALA:CB	1:C:726:ASP:HB3	2.48	0.44
1:B:684:LYS:O	1:B:684:LYS:HD3	2.17	0.44
1:B:689:TYR:HE2	1:B:767:ASN:ND2	2.15	0.44
1:C:869:PHE:O	1:C:870:ALA:C	2.56	0.44
1:D:786:SER:C	1:D:787:LYS:HD2	2.37	0.44
1:A:699:GLY:HA2	1:A:775:TYR:CE2	2.53	0.44
1:A:828:ALA:HB2	1:C:726:ASP:HB3	2.00	0.44
1:A:938:ILE:HG22	1:A:939:SER:N	2.32	0.44
1:B:801:ILE:HD12	1:B:839:ILE:HG22	1.99	0.44
1:D:699:GLY:HA2	1:D:775:TYR:HE2	1.83	0.44
1:A:759:GLN:HA	1:A:762:VAL:CG2	2.46	0.43
1:A:915:PRO:HG2	1:A:916:ILE:HD12	2.00	0.43
1:B:666:PRO:O	1:B:667:LYS:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:PHE:CD1	1:B:1007:PHE:N	2.85	0.43
1:A:663:SER:HB3	1:A:670:GLN:CD	2.39	0.43
1:A:672:LEU:HD12	1:A:673:ILE:HD13	2.00	0.43
1:A:814:ILE:CG2	1:A:1003:LEU:HD21	2.48	0.43
1:A:864:SER:OG	1:A:865:ARG:N	2.51	0.43
1:B:665:LEU:HB3	1:B:669:VAL:HB	2.00	0.43
1:C:1006:LYS:HE2	1:C:1006:LYS:HB2	1.70	0.43
1:D:778:LEU:HD13	1:D:793:ASN:OD1	2.19	0.43
1:A:759:GLN:HE21	1:A:759:GLN:CA	2.31	0.43
1:B:890:MET:HG3	1:B:935:ALA:HB1	1.99	0.43
1:C:703:LYS:HG2	1:C:707:GLN:CD	2.38	0.43
1:D:716:VAL:HG22	1:D:732:LEU:HD13	1.99	0.43
1:D:905:ALA:C	1:D:907:TYR:H	2.21	0.43
1:C:694:GLN:HA	1:C:694:GLN:HE21	1.82	0.43
1:A:978:GLY:HA3	1:D:942:PRO:HA	2.00	0.43
1:B:834:ILE:HD13	1:B:834:ILE:HA	1.83	0.43
1:C:666:PRO:O	1:C:667:LYS:C	2.57	0.43
1:D:856:ASN:OD1	1:D:927:GLY:O	2.36	0.43
1:D:918:LEU:HB3	1:D:1004:LYS:HG2	1.99	0.43
1:D:928:ASN:O	1:D:945:LYS:HE3	2.18	0.43
1:A:881:PRO:HG2	1:A:884:ALA:HB2	1.99	0.43
1:B:872:ILE:O	1:B:876:GLY:HA2	2.19	0.43
1:C:754:ASN:O	1:C:755:ALA:HB3	2.19	0.43
1:D:717:GLN:HG3	1:D:718:GLN:N	2.33	0.43
1:D:849:LYS:CA	1:D:852:LYS:HE2	2.36	0.43
1:D:861:TRP:CE2	1:D:901:VAL:HB	2.54	0.43
1:D:878:ARG:NH2	1:D:879:ILE:O	2.52	0.43
1:A:785:SER:O	1:A:786:SER:HB2	2.18	0.43
1:B:664:LYS:HE3	1:B:791:ASP:OD1	2.19	0.43
1:C:794:TYR:O	1:C:797:LEU:N	2.49	0.43
1:D:674:LYS:CE	1:D:675:MET:HG3	2.48	0.43
1:A:833:VAL:O	1:A:833:VAL:HG12	2.18	0.43
1:B:673:ILE:O	1:B:677:PHE:HB2	2.18	0.43
1:A:804:VAL:O	1:A:804:VAL:HG12	2.18	0.43
1:B:689:TYR:HE2	1:B:767:ASN:HD22	1.65	0.43
1:D:839:ILE:HD13	1:D:1002:LEU:HD12	2.01	0.43
1:D:868:ASN:C	1:D:870:ALA:N	2.72	0.43
1:D:953:LYS:HE2	1:D:953:LYS:HB2	1.82	0.43
1:D:973:THR:HG23	1:D:973:THR:O	2.18	0.43
1:B:710:TYR:CD1	1:B:765:LEU:HD12	2.53	0.43
1:B:775:TYR:CE2	1:B:779:ARG:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:829:TYR:CD1	1:C:829:TYR:C	2.92	0.43
1:D:752:LEU:HD21	1:D:761:LYS:HE3	2.01	0.43
1:D:866:THR:HG23	1:D:918:LEU:HD21	2.01	0.43
1:A:857:ARG:HH21	1:A:966:GLY:HA3	1.84	0.42
1:B:878:ARG:HH22	1:B:879:ILE:HG12	1.84	0.42
1:B:879:ILE:HG13	1:B:880:ALA:O	2.19	0.42
1:B:963:SER:O	1:B:965:ASP:N	2.50	0.42
1:C:992:TYR:CD1	1:C:992:TYR:N	2.87	0.42
1:D:895:ILE:HG22	1:D:897:PHE:CE1	2.54	0.42
1:B:788:ASP:CG	1:B:789:PRO:HD2	2.40	0.42
1:B:849:LYS:HA	1:B:849:LYS:NZ	2.34	0.42
1:D:865:ARG:NE	1:D:909:HIS:HB2	2.34	0.42
1:D:1006:LYS:NZ	1:D:1006:LYS:HB2	2.32	0.42
1:B:704:ARG:H	1:B:704:ARG:HE	1.66	0.42
1:B:829:TYR:CD1	1:B:831:LEU:CD1	3.03	0.42
1:C:672:LEU:O	1:C:675:MET:HB3	2.19	0.42
1:C:926:LEU:HD23	1:C:947:SER:OG	2.19	0.42
1:C:971:LEU:HD12	1:C:971:LEU:H	1.85	0.42
1:A:866:THR:C	1:A:868:ASN:H	2.23	0.42
1:B:748:LYS:HD3	1:B:749:PRO:CD	2.50	0.42
1:B:824:THR:C	1:B:826:HIS:N	2.72	0.42
1:C:805:ASP:O	1:C:807:ASP:N	2.50	0.42
1:D:869:PHE:HA	1:D:872:ILE:HD12	2.02	0.42
1:D:991:VAL:C	1:D:992:TYR:CD1	2.92	0.42
1:A:886:VAL:HG23	1:A:887:THR:N	2.35	0.42
1:A:969:VAL:HA	1:A:970:PRO:HD3	1.69	0.42
1:B:729:ILE:HG22	1:B:751:LEU:HD11	2.00	0.42
1:B:942:PRO:HA	1:C:978:GLY:HA3	2.01	0.42
1:C:667:LYS:CB	1:C:668:PRO:HD3	2.46	0.42
1:C:792:VAL:O	1:C:795:GLU:HG3	2.20	0.42
1:C:860:LEU:CB	1:C:897:PHE:HB3	2.48	0.42
1:D:905:ALA:C	1:D:907:TYR:N	2.72	0.42
1:D:990:ILE:HD12	1:D:990:ILE:N	2.35	0.42
1:B:797:LEU:HB3	1:B:799:THR:HG22	2.02	0.42
1:D:728:GLN:O	1:D:732:LEU:HG	2.20	0.42
1:D:821:THR:C	1:D:901:VAL:HG12	2.39	0.42
1:D:998:ASN:ND2	1:D:1000:LYS:HZ1	2.13	0.42
1:B:775:TYR:HE2	1:B:779:ARG:HH11	1.68	0.42
1:B:1002:LEU:HD22	1:B:1002:LEU:HA	1.74	0.42
1:C:838:LYS:HB2	1:C:838:LYS:HE3	1.80	0.42
1:C:851:PHE:HE2	1:C:995:ALA:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:716:VAL:O	1:D:719:ALA:HB3	2.20	0.42
1:A:817:TYR:CE1	1:A:821:THR:HG21	2.54	0.42
1:B:830:ASP:CB	1:B:1008:ASN:HD22	2.33	0.42
1:D:786:SER:O	1:D:787:LYS:HD2	2.20	0.42
1:D:993:ASP:O	1:D:996:GLN:HB3	2.20	0.42
1:B:692:ASP:HB2	1:B:743:ASP:CB	2.49	0.42
1:C:816:LYS:C	1:C:816:LYS:HD3	2.40	0.42
1:A:706:ILE:HD13	1:A:768:LEU:HB3	2.02	0.42
1:A:712:ILE:O	1:A:715:GLU:HB2	2.20	0.42
1:B:744:PHE:CZ	1:B:750:PRO:HD2	2.55	0.42
1:C:671:ASP:O	1:C:675:MET:HB2	2.20	0.42
1:C:710:TYR:HB3	1:C:883:GLU:O	2.20	0.42
1:C:803:VAL:HG12	1:C:804:VAL:N	2.35	0.42
1:D:676:ILE:HG23	1:D:870:ALA:CA	2.45	0.42
1:D:696:MET:HE1	1:D:701:LEU:HA	2.01	0.42
1:D:710:TYR:OH	1:D:766:ASP:OD1	2.38	0.42
1:D:754:ASN:C	1:D:756:ASP:H	2.21	0.42
1:D:829:TYR:CD1	1:D:830:ASP:N	2.87	0.42
1:D:957:ASP:HA	1:D:958:PRO:HD2	1.88	0.42
1:D:972:GLY:O	1:D:973:THR:C	2.57	0.42
1:A:754:ASN:C	1:A:756:ASP:H	2.23	0.41
1:C:882:PRO:O	1:C:893:LYS:HE3	2.20	0.41
1:D:1002:LEU:HD23	1:D:1003:LEU:O	2.20	0.41
1:A:749:PRO:HA	1:A:750:PRO:HD2	1.87	0.41
1:A:752:LEU:HD11	1:A:761:LYS:HZ3	1.85	0.41
1:B:662:LYS:O	1:B:787:LYS:HG3	2.19	0.41
1:B:710:TYR:HB3	1:B:884:ALA:HA	2.02	0.41
1:C:734:ASN:O	1:C:735:ARG:C	2.59	0.41
1:C:839:ILE:HG12	1:C:1000:LYS:O	2.20	0.41
1:C:851:PHE:C	1:C:853:GLN:H	2.23	0.41
1:D:663:SER:OG	1:D:664:LYS:N	2.53	0.41
1:D:826:HIS:CD2	1:D:826:HIS:N	2.88	0.41
1:B:760:ALA:HA	1:B:763:GLU:HG3	2.01	0.41
1:C:933:LYS:HB2	1:C:982:THR:CB	2.43	0.41
1:D:677:PHE:HE1	1:D:777:LEU:HD12	1.85	0.41
1:D:841:ARG:NE	1:D:876:GLY:H	2.11	0.41
1:D:972:GLY:O	1:D:974:GLY:N	2.53	0.41
1:A:716:VAL:O	1:A:720:VAL:HB	2.21	0.41
1:A:957:ASP:HA	1:A:958:PRO:HD2	1.91	0.41
1:B:690:GLU:O	1:B:690:GLU:HG3	2.21	0.41
1:B:921:LEU:HB3	1:B:1001:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:717:GLN:O	1:C:719:ALA:N	2.46	0.41
1:C:887:THR:HA	1:C:937:HIS:CE1	2.56	0.41
1:D:664:LYS:NZ	1:D:665:LEU:HD21	2.33	0.41
1:D:720:VAL:CG1	1:D:721:SER:N	2.83	0.41
1:D:765:LEU:HA	1:D:768:LEU:HD12	2.02	0.41
1:B:991:VAL:CG1	1:B:992:TYR:N	2.84	0.41
1:C:698:LEU:HD22	1:C:775:TYR:CD1	2.56	0.41
1:A:753:ASN:O	1:A:755:ALA:N	2.54	0.41
1:A:798:LYS:HB3	1:A:798:LYS:HZ3	1.83	0.41
1:B:903:LYS:NZ	1:B:988:GLU:CG	2.83	0.41
1:D:876:GLY:O	1:D:877:LEU:C	2.57	0.41
1:B:827:ASN:OD1	1:B:827:ASN:O	2.39	0.41
1:C:724:SER:HB3	1:C:725:SER:H	1.66	0.41
1:C:768:LEU:HD23	1:C:768:LEU:HA	1.88	0.41
1:C:863:GLY:N	1:C:904:SER:HB2	2.35	0.41
1:D:677:PHE:O	1:D:679:VAL:N	2.54	0.41
1:D:800:ASP:O	1:D:802:LYS:N	2.45	0.41
1:D:918:LEU:N	1:D:918:LEU:CD2	2.84	0.41
1:A:804:VAL:HB	1:A:836:ILE:CG2	2.48	0.41
1:B:728:GLN:O	1:B:732:LEU:HB2	2.21	0.41
1:C:829:TYR:HD1	1:C:829:TYR:C	2.24	0.41
1:C:903:LYS:HZ1	1:C:988:GLU:HG3	1.81	0.41
1:D:778:LEU:C	1:D:780:GLY:N	2.73	0.41
1:D:920:LEU:HD11	1:D:999:LEU:HD13	2.02	0.41
1:A:727:SER:HB3	1:C:827:ASN:ND2	2.35	0.41
1:A:878:ARG:NH1	1:A:879:ILE:CG1	2.84	0.41
1:A:878:ARG:CD	1:A:994:ILE:HG21	2.47	0.41
1:A:938:ILE:CG2	1:A:939:SER:N	2.84	0.41
1:A:942:PRO:HA	1:D:978:GLY:HA3	2.03	0.41
1:B:722:GLN:O	1:B:723:GLY:C	2.58	0.41
1:B:957:ASP:OD2	1:B:957:ASP:C	2.59	0.41
1:C:755:ALA:O	1:C:759:GLN:HB2	2.19	0.41
1:C:787:LYS:HD2	1:C:787:LYS:N	2.36	0.41
1:C:882:PRO:C	1:C:884:ALA:H	2.24	0.41
1:D:662:LYS:C	1:D:787:LYS:HB3	2.42	0.41
1:D:727:SER:HB3	1:D:728:GLN:OE1	2.20	0.41
1:D:765:LEU:HD23	1:D:765:LEU:HA	1.84	0.41
1:A:689:TYR:O	1:A:690:GLU:HB2	2.21	0.41
1:A:714:SER:HB3	1:A:885:PRO:HB3	2.02	0.41
1:B:735:ARG:HG2	1:B:735:ARG:NH1	2.35	0.41
1:B:769:LEU:O	1:B:773:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:824:THR:C	1:B:826:HIS:H	2.24	0.41
1:B:839:ILE:CD1	1:B:920:LEU:HD11	2.50	0.41
1:B:872:ILE:O	1:B:876:GLY:CA	2.69	0.41
1:C:812:GLU:O	1:C:816:LYS:HB2	2.21	0.41
1:D:934:HIS:ND1	1:D:934:HIS:N	2.68	0.41
1:D:953:LYS:NZ	1:D:980:ASN:HA	2.37	0.41
1:D:956:PRO:HB3	1:D:970:PRO:O	2.21	0.41
1:C:704:ARG:H	1:C:704:ARG:CZ	2.33	0.40
1:D:692:ASP:HA	1:D:743:ASP:HB2	2.03	0.40
1:A:748:LYS:CG	1:C:688:GLU:HB3	2.46	0.40
1:B:802:LYS:N	1:B:802:LYS:HE2	2.37	0.40
1:D:748:LYS:HA	1:D:749:PRO:HD3	1.91	0.40
1:D:847:ARG:NH1	1:D:994:ILE:HG22	2.37	0.40
1:D:849:LYS:HG2	1:D:852:LYS:HE2	2.03	0.40
1:D:866:THR:HG23	1:D:918:LEU:CD2	2.52	0.40
1:D:953:LYS:O	1:D:953:LYS:HG3	2.22	0.40
1:A:985:LEU:HD23	1:A:986:TYR:HE2	1.86	0.40
1:B:677:PHE:CZ	1:B:777:LEU:HD12	2.56	0.40
1:B:792:VAL:HG12	1:B:796:LYS:HE3	2.03	0.40
1:C:754:ASN:ND2	1:C:757:SER:CB	2.83	0.40
1:C:805:ASP:C	1:C:807:ASP:N	2.74	0.40
1:D:665:LEU:HB3	1:D:669:VAL:HB	2.03	0.40
1:D:969:VAL:HG23	1:D:969:VAL:O	2.21	0.40
1:A:866:THR:C	1:A:868:ASN:N	2.74	0.40
1:B:958:PRO:C	1:B:960:ALA:N	2.73	0.40
1:C:697:PRO:O	1:C:698:LEU:C	2.59	0.40
1:C:803:VAL:CG1	1:C:804:VAL:N	2.85	0.40
1:A:857:ARG:O	1:A:967:VAL:HA	2.21	0.40
1:B:684:LYS:HD3	1:B:684:LYS:C	2.42	0.40
1:D:714:SER:C	1:D:716:VAL:H	2.23	0.40
1:D:815:ARG:CB	1:D:815:ARG:HH11	2.35	0.40
1:D:924:VAL:HG12	1:D:997:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	348/350 (99%)	294 (84%)	44 (13%)	10 (3%)	4 24
1	B	348/350 (99%)	275 (79%)	56 (16%)	17 (5%)	2 13
1	C	348/350 (99%)	279 (80%)	55 (16%)	14 (4%)	3 17
1	D	348/350 (99%)	254 (73%)	61 (18%)	33 (10%)	0 3
All	All	1392/1400 (99%)	1102 (79%)	216 (16%)	74 (5%)	2 11

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	724	SER
1	A	786	SER
1	B	724	SER
1	B	828	ALA
1	B	965	ASP
1	C	753	ASN
1	C	785	SER
1	C	786	SER
1	C	883	GLU
1	D	693	LEU
1	D	841	ARG
1	D	862	HIS
1	D	869	PHE
1	D	876	GLY
1	D	964	LEU
1	D	1008	ASN
1	A	725	SER
1	A	753	ASN
1	B	783	ASP
1	B	790	ILE
1	C	781	GLY
1	C	806	ARG
1	C	947	SER
1	C	981	ASP
1	D	678	ASP
1	D	784	ASP
1	D	785	SER
1	D	800	ASP

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Mol	Chain	Res	Type
1	D	853	GLN
1	D	916	ILE
1	D	962	ILE
1	D	1004	LYS
1	A	745	GLY
1	A	754	ASN
1	B	667	LYS
1	B	768	LEU
1	B	806	ARG
1	C	718	GLN
1	C	823	ALA
1	C	842	GLU
1	D	671	ASP
1	D	779	ARG
1	D	801	ILE
1	D	817	TYR
1	D	909	HIS
1	D	973	THR
1	D	1003	LEU
1	D	1009	PHE
1	B	745	GLY
1	B	803	VAL
1	D	664	LYS
1	D	774	ALA
1	D	961	ASN
1	A	698	LEU
1	B	754	ASN
1	B	780	GLY
1	B	851	PHE
1	B	937	HIS
1	C	931	GLU
1	C	967	VAL
1	D	769	LEU
1	D	821	THR
1	A	789	PRO
1	B	679	VAL
1	B	749	PRO
1	B	805	ASP
1	C	778	LEU
1	D	914	ASP
1	D	881	PRO
1	A	699	GLY

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Mol	Chain	Res	Type
1	D	818	VAL
1	D	773	VAL
1	A	676	ILE
1	D	723	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/308 (100%)	285 (92%)	23 (8%)	13	43
1	B	308/308 (100%)	283 (92%)	25 (8%)	11	40
1	C	308/308 (100%)	280 (91%)	28 (9%)	9	34
1	D	308/308 (100%)	279 (91%)	29 (9%)	8	32
All	All	1232/1232 (100%)	1127 (92%)	105 (8%)	10	38

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	674	LYS
1	A	704	ARG
1	A	718	GLN
1	A	722	GLN
1	A	754	ASN
1	A	756	ASP
1	A	759	GLN
1	A	772	GLU
1	A	798	LYS
1	A	799	THR
1	A	808	SER
1	A	817	TYR
1	A	838	LYS
1	A	839	ILE
1	A	844	GLU
1	A	854	LEU
1	A	868	ASN

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Mol	Chain	Res	Type
1	A	878	ARG
1	A	943	LYS
1	A	954	THR
1	A	971	LEU
1	A	973	THR
1	A	1010	LYS
1	B	664	LYS
1	B	694	GLN
1	B	704	ARG
1	B	726	ASP
1	B	769	LEU
1	B	783	ASP
1	B	791	ASP
1	B	802	LYS
1	B	817	TYR
1	B	835	ASP
1	B	849	LYS
1	B	854	LEU
1	B	875	GLN
1	B	878	ARG
1	B	912	GLN
1	B	916	ILE
1	B	919	ILE
1	B	921	LEU
1	B	924	VAL
1	B	928	ASN
1	B	971	LEU
1	B	973	THR
1	B	984	LEU
1	B	1005	LEU
1	B	1006	LYS
1	C	671	ASP
1	C	694	GLN
1	C	696	MET
1	C	700	LYS
1	C	704	ARG
1	C	738	THR
1	C	769	LEU
1	C	787	LYS
1	C	795	GLU
1	C	798	LYS
1	C	805	ASP

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Mol	Chain	Res	Type
1	C	816	LYS
1	C	819	LYS
1	C	820	ASN
1	C	829	TYR
1	C	845	CYS
1	C	879	ILE
1	C	886	VAL
1	C	934	HIS
1	C	964	LEU
1	C	968	ASP
1	C	971	LEU
1	C	973	THR
1	C	975	ILE
1	C	994	ILE
1	C	1005	LEU
1	C	1006	LYS
1	C	1010	LYS
1	D	664	LYS
1	D	674	LYS
1	D	688	GLU
1	D	704	ARG
1	D	730	LEU
1	D	742	HIS
1	D	747	LYS
1	D	751	LEU
1	D	766	ASP
1	D	770	ASP
1	D	789	PRO
1	D	791	ASP
1	D	794	TYR
1	D	800	ASP
1	D	805	ASP
1	D	806	ARG
1	D	817	TYR
1	D	824	THR
1	D	841	ARG
1	D	867	THR
1	D	916	ILE
1	D	919	ILE
1	D	934	HIS
1	D	940	LYS
1	D	949	LYS

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Mol	Chain	Res	Type
1	D	971	LEU
1	D	992	TYR
1	D	1004	LYS
1	D	1005	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	694	GLN
1	A	707	GLN
1	A	718	GLN
1	A	722	GLN
1	A	754	ASN
1	A	759	GLN
1	A	906	ASN
1	A	912	GLN
1	A	961	ASN
1	A	980	ASN
1	A	996	GLN
1	A	1008	ASN
1	B	707	GLN
1	B	717	GLN
1	B	718	GLN
1	B	826	HIS
1	B	846	GLN
1	B	853	GLN
1	B	856	ASN
1	B	868	ASN
1	B	961	ASN
1	B	996	GLN
1	C	670	GLN
1	C	694	GLN
1	C	707	GLN
1	C	722	GLN
1	C	734	ASN
1	C	754	ASN
1	C	759	GLN
1	C	767	ASN
1	C	820	ASN
1	C	826	HIS
1	C	856	ASN
1	C	987	ASN

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Mol	Chain	Res	Type
1	C	996	GLN
1	D	694	GLN
1	D	717	GLN
1	D	759	GLN
1	D	767	ASN
1	D	928	ASN
1	D	961	ASN
1	D	998	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	CNQ	A	1	-	20,22,22	2.29	10 (50%)	24,31,31	2.25	8 (33%)
2	CNQ	C	3	-	20,22,22	2.36	11 (55%)	24,31,31	2.39	8 (33%)
2	CNQ	D	4	-	20,22,22	2.18	10 (50%)	24,31,31	2.23	7 (29%)
2	CNQ	B	2	-	20,22,22	2.29	9 (45%)	24,31,31	2.40	7 (29%)

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	CNQ	A	1	-	-	1/4/8/8	0/3/3/3
2	CNQ	C	3	-	-	2/4/8/8	0/3/3/3
2	CNQ	D	4	-	-	2/4/8/8	0/3/3/3
2	CNQ	B	2	-	-	0/4/8/8	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	CNQ	C8-N7	5.98	1.37	1.30
2	B	2	CNQ	C8-N7	5.48	1.37	1.30
2	A	1	CNQ	C8-N7	5.32	1.36	1.30
2	D	4	CNQ	C8-N7	5.32	1.36	1.30
2	A	1	CNQ	C6-C5	3.56	1.44	1.38
2	C	3	CNQ	C6-C5	3.36	1.44	1.38
2	B	2	CNQ	C19-C18	3.25	1.43	1.36
2	B	2	CNQ	C6-C5	3.20	1.43	1.38
2	C	3	CNQ	C4-C3	3.18	1.47	1.42
2	C	3	CNQ	C19-C18	3.05	1.43	1.36
2	B	2	CNQ	C4-C3	2.99	1.47	1.42
2	D	4	CNQ	C19-C18	2.92	1.42	1.36
2	A	1	CNQ	C4-C3	2.90	1.47	1.42
2	C	3	CNQ	C9-N10	2.90	1.40	1.35
2	A	1	CNQ	C9-N10	2.85	1.40	1.35
2	A	1	CNQ	C19-C18	2.80	1.42	1.36
2	D	4	CNQ	C6-C5	2.78	1.43	1.38
2	D	4	CNQ	C9-N10	2.78	1.39	1.35
2	A	1	CNQ	C4-N10	2.76	1.40	1.35
2	B	2	CNQ	C15-C16	2.74	1.42	1.36
2	D	4	CNQ	C4-C3	2.73	1.46	1.42
2	B	2	CNQ	C9-N10	2.73	1.39	1.35
2	A	1	CNQ	C15-C16	2.65	1.42	1.36
2	C	3	CNQ	C15-C16	2.59	1.42	1.36
2	B	2	CNQ	C4-N10	2.59	1.40	1.35
2	D	4	CNQ	C15-C16	2.52	1.41	1.36
2	C	3	CNQ	C18-C17	2.47	1.42	1.38
2	C	3	CNQ	C1-C6	2.47	1.44	1.38
2	A	1	CNQ	C1-C2	2.39	1.42	1.36
2	B	2	CNQ	C1-C2	2.30	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	CNQ	C18-C17	2.28	1.42	1.38
2	D	4	CNQ	C4-N10	2.28	1.39	1.35
2	C	3	CNQ	C1-C2	2.23	1.41	1.36
2	D	4	CNQ	C1-C2	2.20	1.41	1.36
2	D	4	CNQ	C18-C17	2.19	1.42	1.38
2	C	3	CNQ	C4-N10	2.15	1.39	1.35
2	A	1	CNQ	C1-C6	2.13	1.43	1.38
2	A	1	CNQ	C16-C17	2.07	1.41	1.38
2	C	3	CNQ	C16-C17	2.01	1.41	1.38
2	D	4	CNQ	C16-C17	2.01	1.41	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	CNQ	O13-C11-C5	6.58	127.98	120.22
2	B	2	CNQ	O13-C11-C5	5.90	127.18	120.22
2	A	1	CNQ	O13-C11-C5	5.59	126.81	120.22
2	B	2	CNQ	C3-C4-N10	-5.21	116.93	121.56
2	D	4	CNQ	O13-C11-C5	5.20	126.35	120.22
2	D	4	CNQ	C3-C4-N10	-5.02	117.10	121.56
2	C	3	CNQ	C4-N10-C9	4.90	122.60	117.02
2	B	2	CNQ	C4-N10-C9	4.87	122.56	117.02
2	C	3	CNQ	C3-C4-N10	-4.78	117.31	121.56
2	D	4	CNQ	C4-N10-C9	4.75	122.43	117.02
2	A	1	CNQ	C3-C4-N10	-4.73	117.35	121.56
2	A	1	CNQ	C4-N10-C9	4.57	122.23	117.02
2	B	2	CNQ	O13-C11-N12	-3.79	117.19	122.58
2	C	3	CNQ	O13-C11-N12	-3.25	117.97	122.58
2	B	2	CNQ	C8-C9-N10	-3.22	118.68	122.33
2	A	1	CNQ	C8-C9-N10	-3.16	118.75	122.33
2	A	1	CNQ	C8-N7-C3	3.15	122.03	117.69
2	D	4	CNQ	O13-C11-N12	-3.02	118.28	122.58
2	C	3	CNQ	C8-C9-N10	-3.00	118.93	122.33
2	D	4	CNQ	C8-N7-C3	2.97	121.77	117.69
2	A	1	CNQ	O13-C11-N12	-2.96	118.37	122.58
2	B	2	CNQ	C5-C4-N10	2.94	123.93	120.30
2	C	3	CNQ	C8-N7-C3	2.93	121.72	117.69
2	B	2	CNQ	C8-N7-C3	2.91	121.70	117.69
2	D	4	CNQ	C8-C9-N10	-2.90	119.04	122.33
2	D	4	CNQ	C5-C4-N10	2.81	123.76	120.30
2	C	3	CNQ	C5-C11-N12	-2.77	114.06	118.28
2	A	1	CNQ	C5-C4-N10	2.54	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	CNQ	C5-C11-N12	-2.28	114.81	118.28
2	C	3	CNQ	C5-C4-N10	2.22	123.04	120.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	CNQ	N12-C11-C5-C4
2	C	3	CNQ	N12-C11-C5-C4
2	C	3	CNQ	O13-C11-C5-C4
2	D	4	CNQ	N12-C11-C5-C4
2	D	4	CNQ	O13-C11-C5-C4

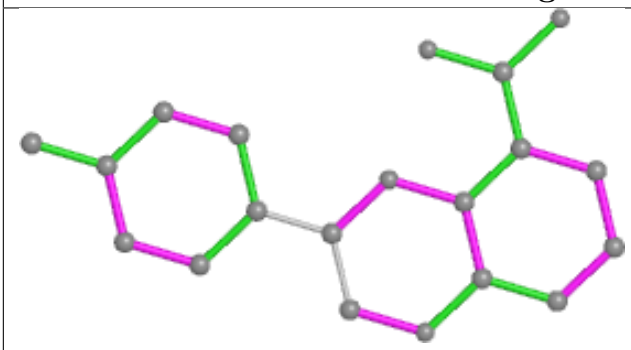
There are no ring outliers.

4 monomers are involved in 7 short contacts:

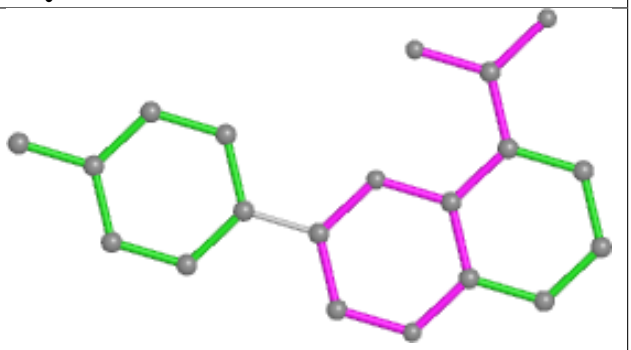
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	CNQ	1	0
2	C	3	CNQ	2	0
2	D	4	CNQ	2	0
2	B	2	CNQ	2	0

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

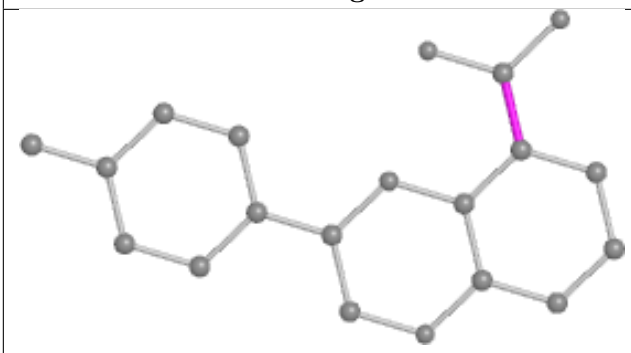
Ligand CNQ A 1



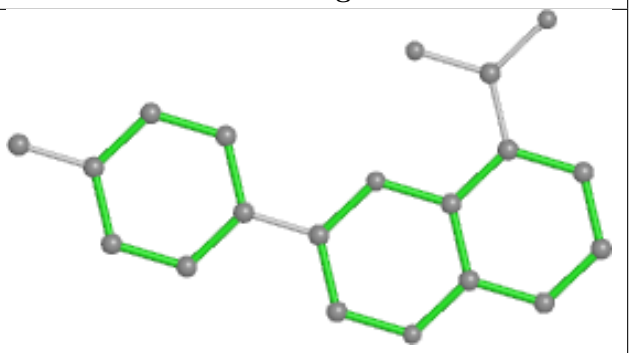
Bond lengths



Bond angles

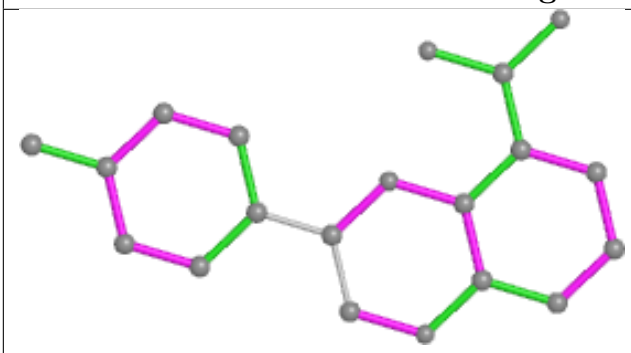


Torsions

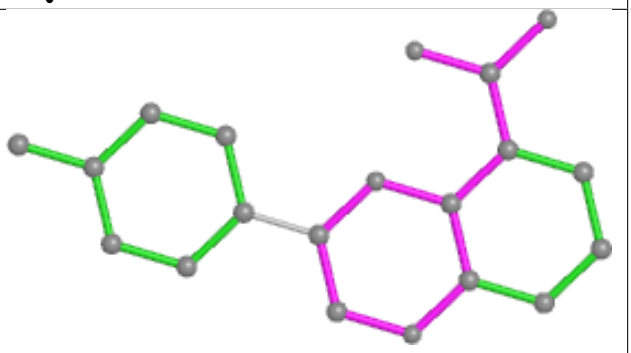


Rings

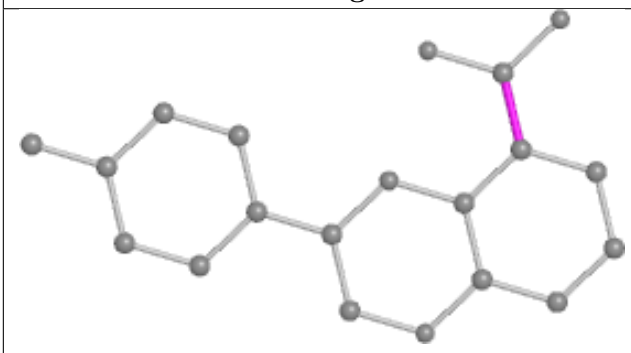
Ligand CNQ C 3



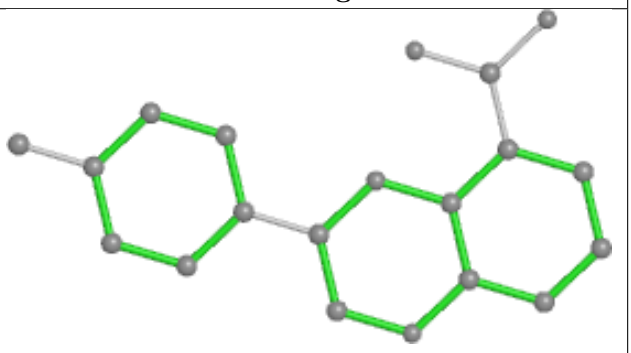
Bond lengths



Bond angles

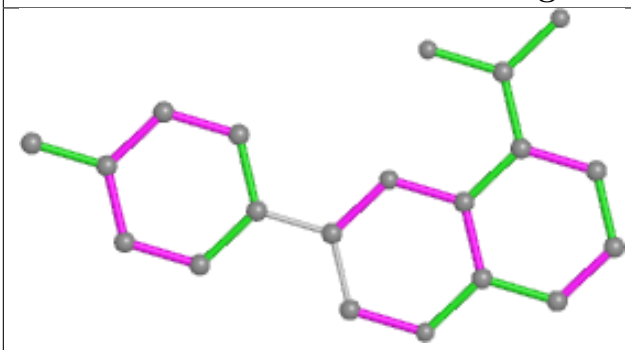


Torsions

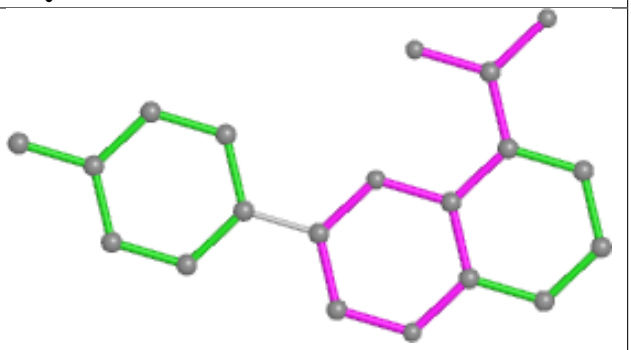


Rings

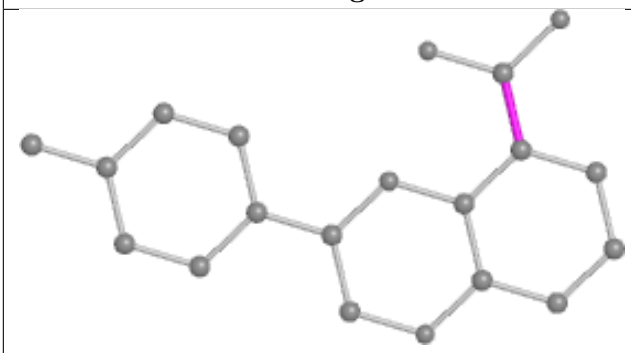
Ligand CNQ D 4



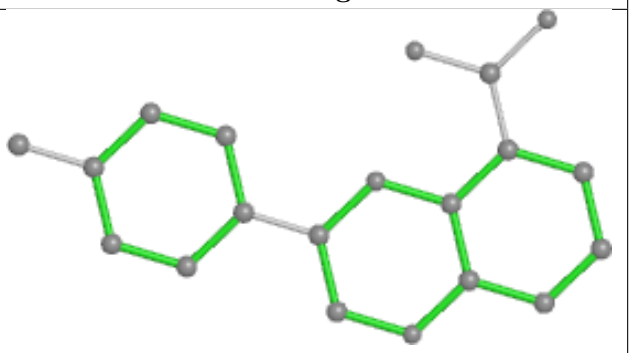
Bond lengths



Bond angles

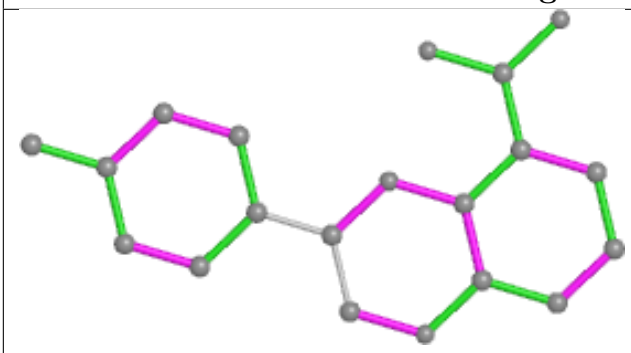


Torsions

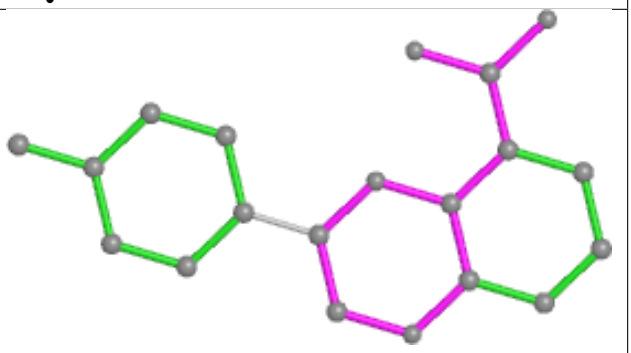


Rings

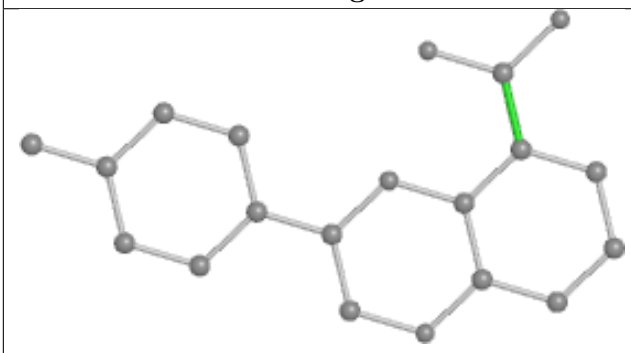
Ligand CNQ B 2



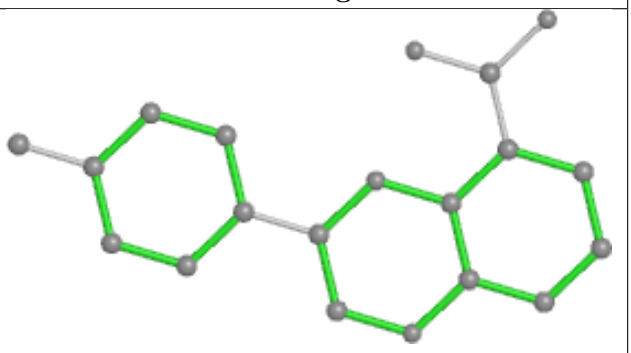
Bond lengths



Bond angles



Torsions



Rings

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	350/350 (100%)	-0.47	7 (2%)	65	36	10, 34, 85, 147	0
1	B	350/350 (100%)	-0.42	4 (1%)	80	56	9, 42, 102, 124	0
1	C	350/350 (100%)	-0.54	4 (1%)	80	56	9, 30, 77, 129	0
1	D	350/350 (100%)	-0.03	8 (2%)	60	31	15, 71, 126, 145	0
All	All	1400/1400 (100%)	-0.36	23 (1%)	72	44	9, 41, 111, 147	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	782	SER	8.8
1	A	783	ASP	5.0
1	A	786	SER	4.1
1	B	786	SER	4.1
1	A	787	LYS	3.5
1	D	789	PRO	3.4
1	C	782	SER	3.3
1	A	663	SER	3.2
1	D	663	SER	3.2
1	B	746	MET	3.1
1	C	783	ASP	3.0
1	D	782	SER	2.8
1	D	886	VAL	2.8
1	D	664	LYS	2.8
1	D	783	ASP	2.7
1	B	756	ASP	2.6
1	C	746	MET	2.6
1	A	982	THR	2.5
1	C	781	GLY	2.5
1	D	792	VAL	2.4
1	D	693	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	953	LYS	2.2
1	B	717	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

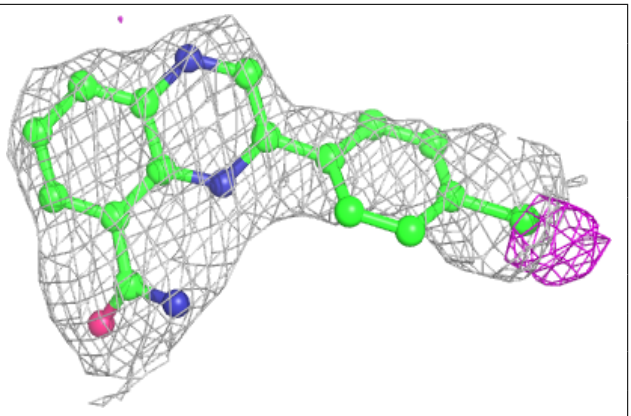
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

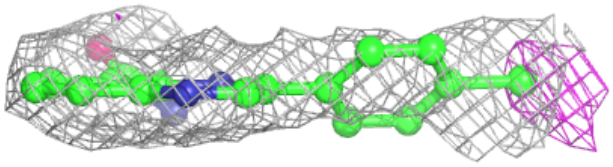
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CNQ	A	1	20/20	0.88	0.24	31,50,65,67	0
2	CNQ	D	4	20/20	0.90	0.27	52,84,101,101	0
2	CNQ	C	3	20/20	0.92	0.23	11,40,56,58	0
2	CNQ	B	2	20/20	0.92	0.19	34,45,49,50	0

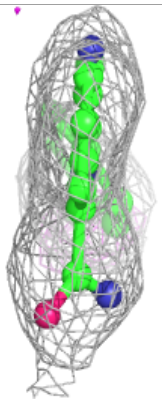
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CNQ A 1:

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

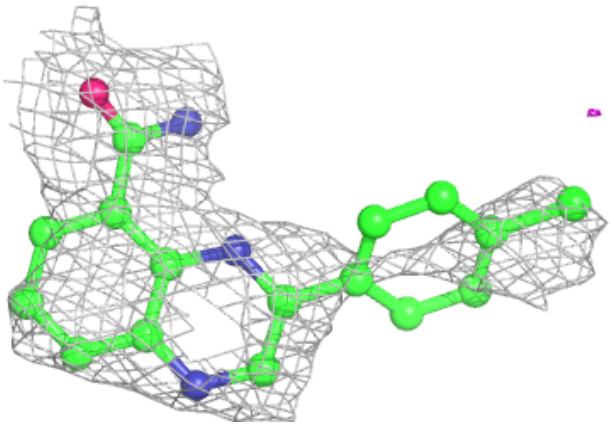


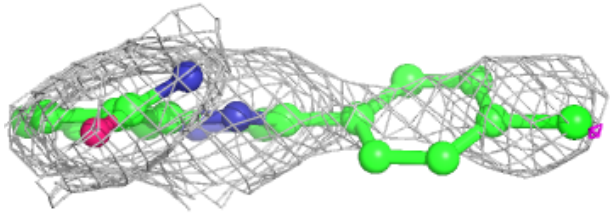


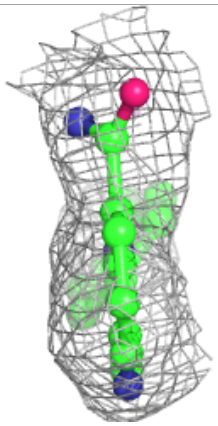


Electron density around CNQ D 4:

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

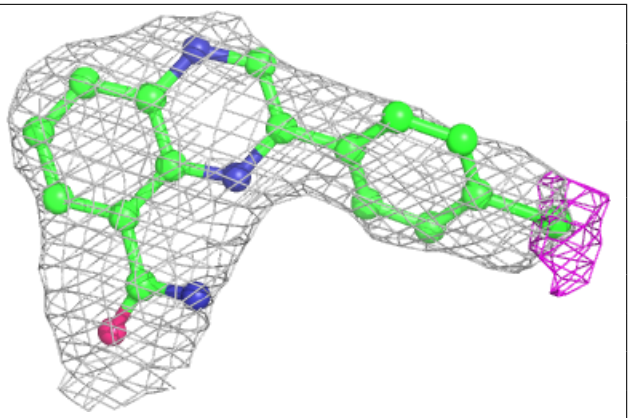


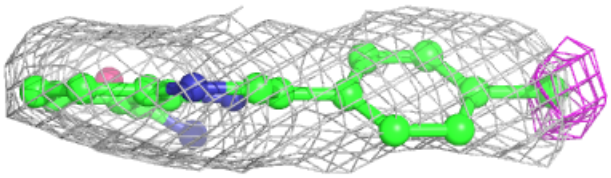


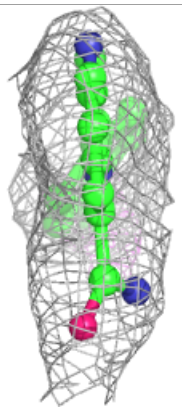


Electron density around CNQ C 3:

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

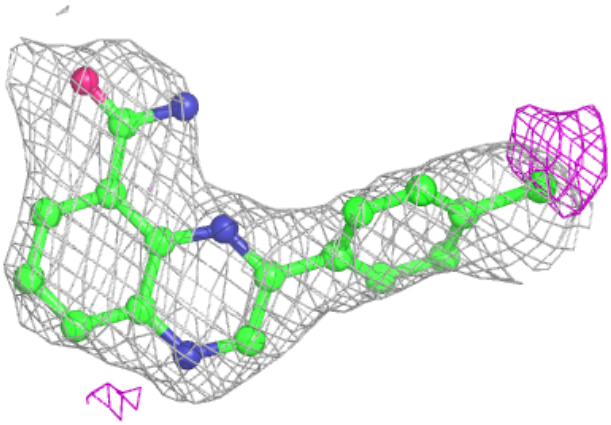


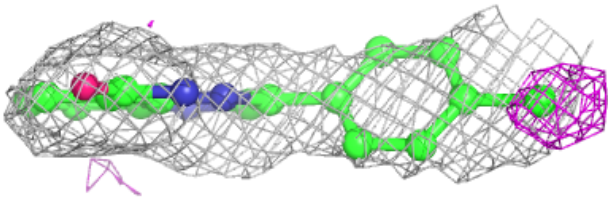


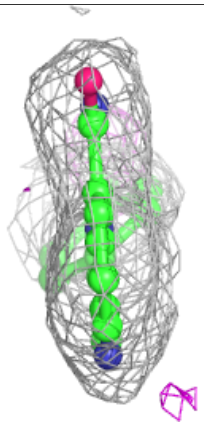


Electron density around CNQ B 2:

$2mF_o$-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.