Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 06:33 PM EST

PDB ID	:	1UDU
Title	:	Crystal structure of Human Phosphodiesterase 5 complexed with tadalafil(Cialis)
Authors	:	Sung, B.-J.; Lee, J.I.; Heo, Y.-S.; Kim, J.H.; Moon, J.; Yoon, J.M.; Hyun, Y.-L.; Kim, E.; Eum, S.J.; Lee, T.G.; Cho, J.M.; Park, S.-Y.; Lee, J.-O.; Jeon, Y.H.; Hwang, K.Y.; Ro, S.
Deposited on	:	2003-05-06
Resolution	:	2.83 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

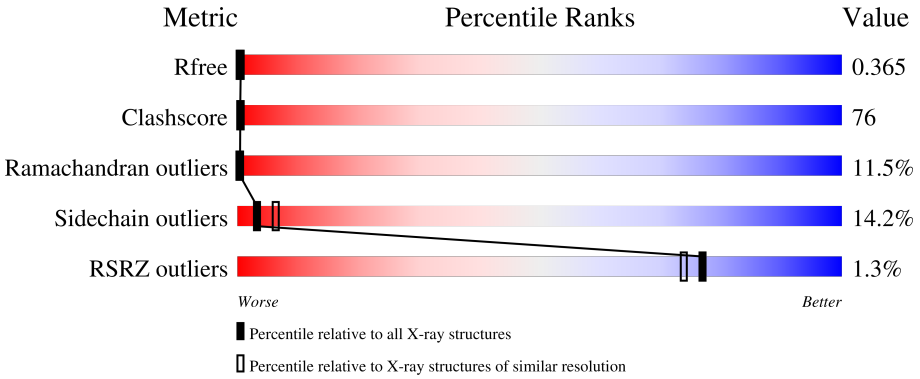
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	324	17% 60% 18%
1	B	324	18% 61% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5146 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 cGMP-specific 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2542	1617	442	465	18			
1	B	313	Total	C	N	O	S	0	0	0
			2542	1617	442	465	18			

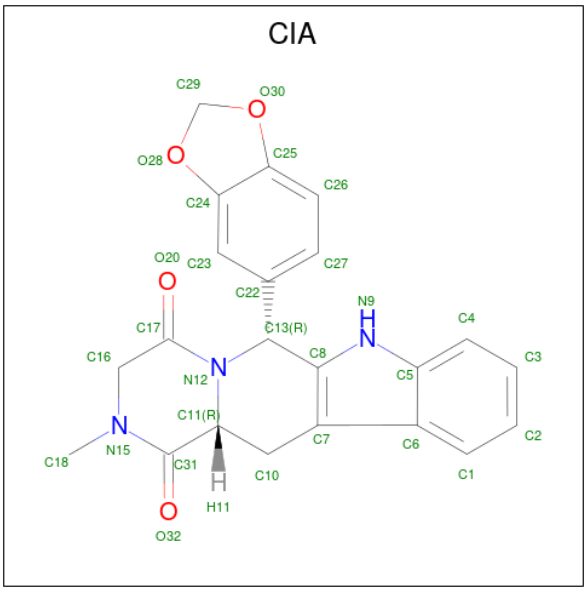
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 6-BENZO[1,3]DIOXOL-5-YL-2-METHYL-2,3,6,7,12,12A-HEXAHYDRO-PYRAZINO[1',2':1,6]PYRIDO[3,4-B]INDOLE-1,4-DIONE (three-letter code: CIA) (formula: $C_{22}H_{19}N_3O_4$).



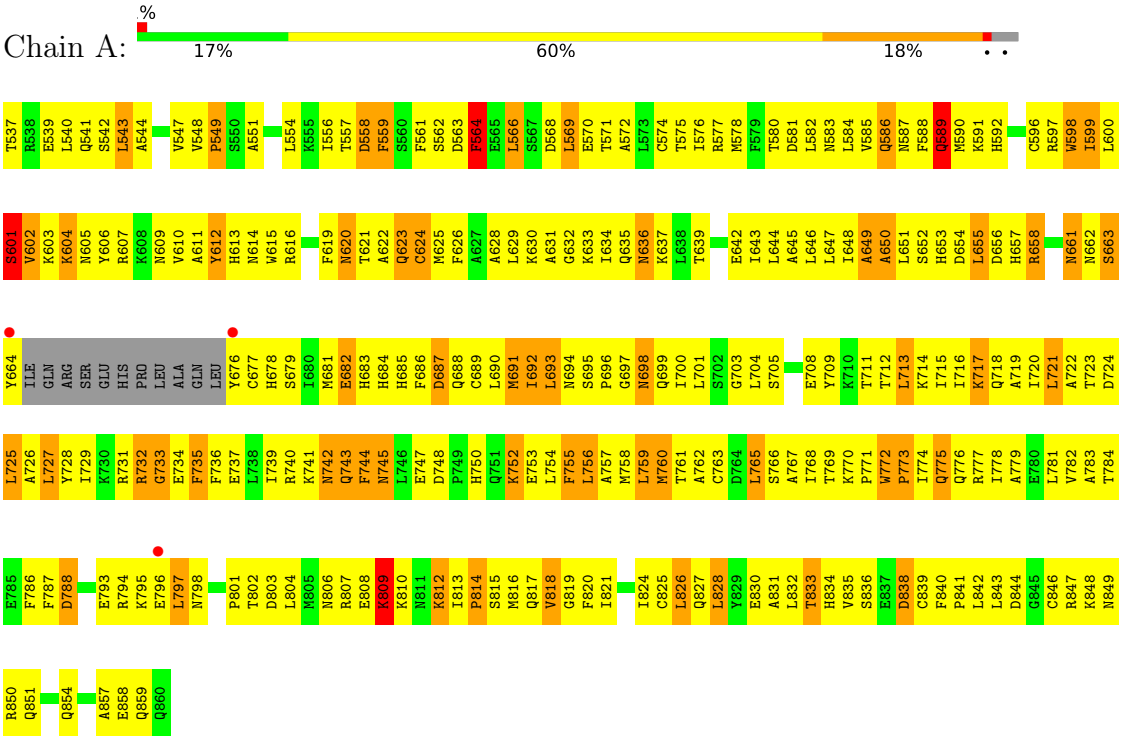
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 29 22 3 4	0	0
4	B	1	Total C N O 29 22 3 4	0	0

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.

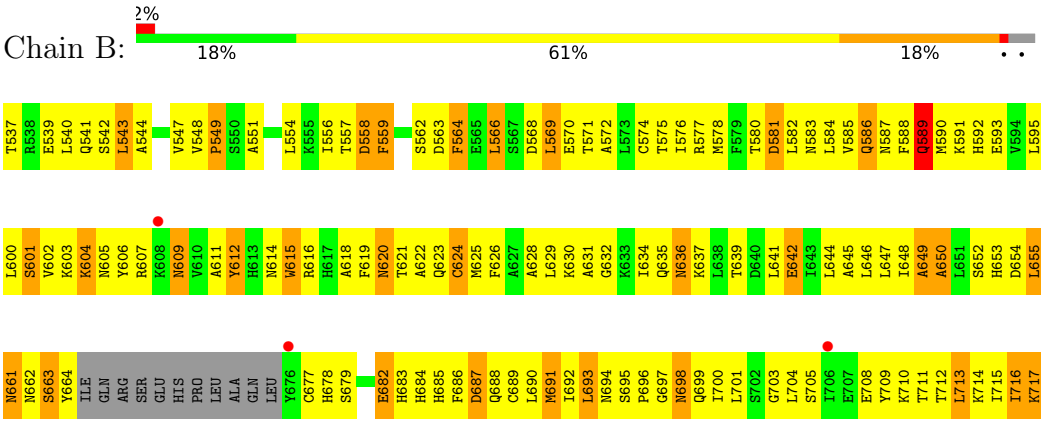
• Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase

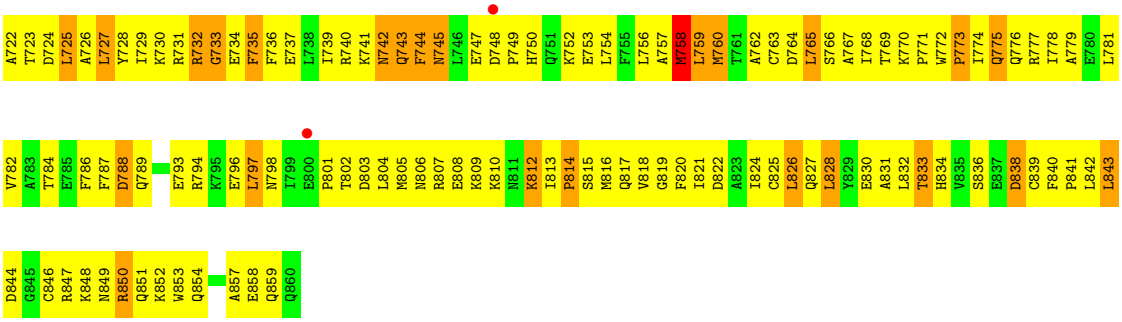
Chain A:



• Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase

Chain B:




A722 T723 D724 L725 A726 L727 Y728 I729 K730 R731 R732 G733 E734 F735 F736 E737 L738 I739 R740 K741 N742 Q743 F744 N745 L746 E747 D748 P749 H750 Q751 K752 E753 L754 F755 L756 A757 M758 L759 M760 T761 A762 C763 D764 L765 S766 A767 I768 T769 K770 P771 W772 P773 I774 Q775 Q776 R777 I778 A779 E780 L781
V782 A783 T784 E785 F786 F787 D788 Q789 E793 R794 K795 E796 L797 N798 I799 E800 P801 T802 D803 L804 M805 N806 R807 E808 K809 K810 N811 K812 I813 P814 S815 M816 Q817 V818 G819 F820 I821 D822 A823 I824 C825 L826 Q827 L828 Y829 E830 A831 L832 T833 H834 V835 S836 E837 D838 C839 F840 P841 L842 L843
D844 G845 C846 R847 K848 N849 R850 Q851 K852 W853 Q854 A857 E858 Q859 Q860

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.35Å 48.56Å 123.86Å 90.00° 117.28° 90.00°	Depositor
Resolution (Å)	19.59 – 2.83 20.13 – 2.83	Depositor EDS
% Data completeness (in resolution range)	71.5 (19.59-2.83) 71.6 (20.13-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 2.83Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.374 0.257 , 0.365	Depositor DCC
R_{free} test set	627 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	1.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5146	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CIA, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.46	0/2590	0.74	0/3493
1	B	0.49	0/2590	0.74	0/3493
All	All	0.47	0/5180	0.74	0/6986

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

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	2542	0	2552	395	0
1	B	2542	0	2552	397	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	29	0	19	8	0
4	B	29	0	19	1	0
All	All	5146	0	5142	778	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 76.

All (778) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:HIS:HA	1:A:720:ILE:HG23	1.26	1.14
1:B:653:HIS:HA	1:B:720:ILE:HG23	1.26	1.11
1:A:801:PRO:HB2	1:A:806:ASN:HB3	1.34	1.07
1:B:725:LEU:O	1:B:729:ILE:HG13	1.58	1.04
1:B:658:ARG:HG2	1:B:658:ARG:HH11	1.23	1.02
1:B:679:SER:HB3	1:B:682:GLU:HG3	1.39	1.02
1:B:801:PRO:HB2	1:B:806:ASN:HB3	1.35	1.02
1:B:797:LEU:H	1:B:797:LEU:HD22	1.22	1.02
1:A:808:GLU:HG3	1:A:809:LYS:H	1.20	1.01
1:B:543:LEU:HD11	1:B:572:ALA:HB1	1.43	0.99
1:B:808:GLU:HG3	1:B:809:LYS:H	1.26	0.98
1:B:572:ALA:O	1:B:576:ILE:HG13	1.67	0.95
1:A:821:ILE:HA	1:A:825:CYS:HB2	1.49	0.94
1:A:725:LEU:O	1:A:729:ILE:HG13	1.66	0.94
1:A:735:PHE:HB2	1:A:754:LEU:HD23	1.48	0.93
1:B:559:PHE:HD1	1:B:559:PHE:H	1.13	0.93
1:A:718:GLN:HE22	1:B:796:GLU:HB3	1.34	0.93
1:B:793:GLU:HA	1:B:797:LEU:HD23	1.52	0.92
1:B:652:SER:HB3	1:B:655:LEU:HD12	1.52	0.92
1:A:797:LEU:HD22	1:A:797:LEU:H	1.34	0.91
1:A:652:SER:HB3	1:A:655:LEU:HD12	1.50	0.90
1:B:607:ARG:NH2	1:B:658:ARG:HH21	1.68	0.90
1:B:735:PHE:HB2	1:B:754:LEU:HD23	1.52	0.89
1:B:765:LEU:O	1:B:768:ILE:HG22	1.73	0.89
1:A:830:GLU:HA	1:A:843:LEU:HD22	1.56	0.88
1:A:559:PHE:HD1	1:A:559:PHE:H	1.21	0.87
1:B:821:ILE:HA	1:B:825:CYS:HB2	1.58	0.86
1:A:677:CYS:HA	1:B:677:CYS:SG	2.16	0.85
1:B:727:LEU:HD23	1:B:728:TYR:N	1.89	0.85
1:B:632:GLY:HA2	1:B:838:ASP:HB3	1.56	0.85
1:B:828:LEU:O	1:B:828:LEU:HD22	1.77	0.85
1:A:679:SER:HB3	1:A:682:GLU:HG3	1.57	0.85
1:A:636:ASN:ND2	1:A:637:LYS:HG3	1.91	0.85
1:B:543:LEU:HD11	1:B:572:ALA:CB	2.08	0.84
1:B:653:HIS:HB2	1:B:723:THR:HG21	1.56	0.84
1:B:770:LYS:NZ	1:B:774:ILE:HG21	1.93	0.84
1:A:604:LYS:HB2	1:A:604:LYS:NZ	1.93	0.83
1:A:787:PHE:HB3	1:A:807:ARG:HD2	1.59	0.83
1:A:793:GLU:HA	1:A:797:LEU:HD23	1.61	0.83
1:A:658:ARG:HG2	1:A:658:ARG:HH11	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:LEU:H	1:B:566:LEU:HD23	1.44	0.82
1:A:543:LEU:HD11	1:A:572:ALA:HB1	1.60	0.82
1:B:693:LEU:HD22	1:B:701:LEU:HD12	1.61	0.82
1:B:712:THR:O	1:B:716:ILE:HG13	1.80	0.81
1:A:727:LEU:HD23	1:A:728:TYR:N	1.94	0.81
1:B:642:GLU:O	1:B:646:LEU:HD23	1.79	0.81
1:B:679:SER:HB3	1:B:682:GLU:CG	2.10	0.81
1:A:607:ARG:NH2	1:A:658:ARG:HH21	1.77	0.81
1:B:604:LYS:HB2	1:B:604:LYS:NZ	1.96	0.80
1:A:663:SER:HA	4:A:1003:CIA:H182	1.64	0.80
1:B:813:ILE:HA	1:B:816:MET:HE3	1.63	0.80
1:A:572:ALA:O	1:A:576:ILE:HG13	1.81	0.79
1:B:603:LYS:HG3	1:B:615:TRP:CD1	2.17	0.79
1:A:661:ASN:C	1:A:662:ASN:HD22	1.85	0.79
1:B:569:LEU:O	1:B:572:ALA:HB3	1.81	0.79
1:A:693:LEU:HD22	1:A:701:LEU:HD12	1.64	0.79
1:A:770:LYS:NZ	1:A:774:ILE:HG21	1.97	0.79
1:A:539:GLU:HG2	1:A:600:LEU:HD11	1.63	0.79
1:B:827:GLN:HA	1:B:830:GLU:HG2	1.63	0.78
1:A:632:GLY:HA2	1:A:838:ASP:HB3	1.64	0.78
1:A:653:HIS:HB2	1:A:723:THR:HG21	1.63	0.78
1:B:820:PHE:CE1	1:B:824:ILE:HD12	2.19	0.78
1:B:563:ASP:HB3	1:B:620:ASN:HD21	1.49	0.78
1:A:765:LEU:O	1:A:768:ILE:HG22	1.84	0.77
1:B:549:PRO:HG2	1:B:554:LEU:HD21	1.67	0.77
1:B:636:ASN:HD22	1:B:636:ASN:C	1.87	0.77
1:B:787:PHE:HB3	1:B:807:ARG:HD2	1.67	0.77
1:A:543:LEU:HD11	1:A:572:ALA:CB	2.14	0.77
1:A:566:LEU:HD23	1:A:566:LEU:H	1.48	0.77
1:A:582:LEU:HD21	1:A:629:LEU:HD23	1.66	0.77
1:B:734:GLU:C	1:B:736:PHE:H	1.86	0.76
1:B:770:LYS:HZ3	1:B:774:ILE:HG21	1.51	0.76
1:B:636:ASN:ND2	1:B:637:LYS:HG3	2.01	0.76
1:A:705:SER:HB2	1:A:708:GLU:HG2	1.68	0.76
1:A:712:THR:O	1:A:716:ILE:HG13	1.85	0.75
1:A:770:LYS:HZ3	1:A:774:ILE:HG21	1.50	0.75
1:A:630:LYS:O	1:A:632:GLY:N	2.18	0.75
1:B:806:ASN:HD21	1:B:809:LYS:HG2	1.50	0.74
1:A:759:LEU:O	1:A:759:LEU:HD12	1.87	0.74
1:B:639:THR:OG1	1:B:642:GLU:HG3	1.87	0.74
1:B:826:LEU:HD23	1:B:827:GLN:N	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:PHE:CD2	1:B:841:PRO:HB2	2.23	0.74
1:B:586:GLN:HA	1:B:586:GLN:HE21	1.52	0.74
1:A:586:GLN:HA	1:A:586:GLN:HE21	1.51	0.74
1:B:692:ILE:O	1:B:695:SER:N	2.21	0.73
1:B:630:LYS:O	1:B:632:GLY:N	2.21	0.73
1:A:642:GLU:O	1:A:646:LEU:HD23	1.89	0.73
1:A:808:GLU:HG3	1:A:809:LYS:N	2.00	0.73
1:A:558:ASP:N	1:A:558:ASP:OD2	2.20	0.73
1:A:636:ASN:C	1:A:636:ASN:HD22	1.91	0.72
1:A:696:PRO:HA	1:A:699:GLN:HE21	1.54	0.72
1:A:717:LYS:HG2	1:A:721:LEU:HD11	1.71	0.72
1:A:787:PHE:HB2	1:A:807:ARG:NH1	2.03	0.72
1:B:607:ARG:HH21	1:B:658:ARG:HH21	1.35	0.72
1:B:704:LEU:HB3	1:B:708:GLU:HB2	1.72	0.72
1:B:705:SER:HB2	1:B:708:GLU:HG2	1.71	0.72
1:B:658:ARG:HH11	1:B:658:ARG:CG	2.02	0.71
1:B:762:ALA:HA	1:B:828:LEU:HD11	1.70	0.71
1:B:575:THR:O	1:B:578:MET:HB2	1.90	0.71
1:B:658:ARG:HG2	1:B:658:ARG:NH1	2.00	0.71
1:A:663:SER:HA	4:A:1003:CIA:C18	2.21	0.71
1:A:826:LEU:HD23	1:A:827:GLN:N	2.06	0.70
1:A:711:THR:O	1:A:715:ILE:HG13	1.91	0.70
1:B:584:LEU:HD13	1:B:644:LEU:HD12	1.72	0.70
1:A:652:SER:HB3	1:A:655:LEU:CD1	2.21	0.70
1:B:759:LEU:HD12	1:B:759:LEU:O	1.91	0.70
1:A:767:ALA:HA	1:A:770:LYS:CG	2.22	0.70
1:B:833:THR:HG22	1:B:834:HIS:N	2.06	0.70
1:A:636:ASN:HD21	1:A:637:LYS:HG3	1.56	0.70
1:B:801:PRO:HB2	1:B:806:ASN:CB	2.19	0.69
1:A:742:ASN:C	1:A:744:PHE:H	1.94	0.69
1:A:828:LEU:HD22	1:A:828:LEU:O	1.92	0.69
1:A:718:GLN:NE2	1:B:796:GLU:HB3	2.07	0.69
1:B:571:THR:HA	1:B:619:PHE:CZ	2.28	0.69
1:A:716:ILE:O	1:A:719:ALA:HB3	1.93	0.69
1:A:563:ASP:HB2	1:A:616:ARG:HH11	1.58	0.69
1:A:597:ARG:HG2	1:A:698:ASN:OD1	1.93	0.69
1:A:695:SER:HB2	1:A:698:ASN:HD22	1.57	0.69
1:B:558:ASP:OD2	1:B:558:ASP:N	2.24	0.69
1:B:745:ASN:ND2	1:B:748:ASP:HB2	2.08	0.69
1:A:639:THR:OG1	1:A:642:GLU:HG3	1.93	0.69
1:A:658:ARG:HG2	1:A:658:ARG:NH1	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:GLU:C	1:A:736:PHE:H	1.95	0.68
1:B:574:CYS:O	1:B:577:ARG:HB3	1.93	0.68
1:B:584:LEU:HD13	1:B:644:LEU:CD1	2.23	0.68
1:A:636:ASN:HD22	1:A:637:LYS:N	1.92	0.68
1:B:559:PHE:CD1	1:B:559:PHE:N	2.59	0.68
1:B:597:ARG:HG2	1:B:698:ASN:OD1	1.94	0.68
1:B:716:ILE:O	1:B:719:ALA:HB3	1.94	0.68
1:B:717:LYS:HG2	1:B:721:LEU:HD11	1.75	0.68
1:A:679:SER:HB3	1:A:682:GLU:CG	2.23	0.68
1:A:704:LEU:HB3	1:A:708:GLU:HB2	1.75	0.68
1:B:661:ASN:C	1:B:662:ASN:HD22	1.96	0.68
1:A:692:ILE:O	1:A:695:SER:N	2.26	0.68
1:A:818:VAL:HG12	1:A:819:GLY:N	2.07	0.68
1:B:583:ASN:HB3	1:B:587:ASN:HD21	1.57	0.68
1:B:844:ASP:O	1:B:848:LYS:HG3	1.93	0.68
1:A:549:PRO:HG2	1:A:554:LEU:HD21	1.77	0.67
1:A:725:LEU:HD12	1:A:725:LEU:H	1.60	0.67
1:B:582:LEU:HD21	1:B:629:LEU:HD23	1.76	0.67
1:B:604:LYS:HB2	1:B:604:LYS:HZ2	1.58	0.67
1:B:830:GLU:O	1:B:833:THR:HB	1.94	0.67
1:B:770:LYS:HZ3	1:B:774:ILE:CG2	2.08	0.67
1:B:578:MET:O	1:B:582:LEU:HD12	1.95	0.67
1:A:779:ALA:HB1	1:A:817:GLN:NE2	2.09	0.66
1:B:724:ASP:OD2	1:B:726:ALA:HB3	1.96	0.66
1:B:695:SER:HB2	1:B:698:ASN:HD22	1.61	0.66
1:B:742:ASN:C	1:B:744:PHE:H	1.99	0.66
1:B:636:ASN:HD22	1:B:637:LYS:N	1.93	0.66
1:B:549:PRO:HB2	1:B:554:LEU:HG	1.78	0.66
1:B:585:VAL:O	1:B:589:GLN:HA	1.96	0.66
1:A:568:ASP:O	1:A:571:THR:N	2.29	0.65
1:A:724:ASP:OD2	1:A:726:ALA:HB3	1.97	0.65
1:A:761:THR:O	1:A:765:LEU:HD13	1.96	0.65
1:B:727:LEU:O	1:B:731:ARG:HG3	1.95	0.65
1:B:731:ARG:O	1:B:733:GLY:N	2.29	0.65
1:A:709:TYR:CE2	1:A:713:LEU:HD11	2.32	0.65
1:A:821:ILE:HA	1:A:825:CYS:CB	2.26	0.65
1:A:563:ASP:HB2	1:A:616:ARG:NH1	2.12	0.65
1:B:797:LEU:HD22	1:B:797:LEU:N	2.05	0.65
1:B:583:ASN:O	1:B:587:ASN:ND2	2.29	0.65
1:B:717:LYS:HE2	1:B:721:LEU:HD11	1.79	0.65
1:B:632:GLY:CA	1:B:838:ASP:HB3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:ASN:ND2	1:B:809:LYS:HG2	2.13	0.64
1:B:806:ASN:ND2	1:B:808:GLU:HB3	2.12	0.64
1:B:808:GLU:HG3	1:B:809:LYS:N	2.06	0.64
1:B:779:ALA:HB1	1:B:817:GLN:NE2	2.12	0.64
1:A:654:ASP:HA	1:A:685:HIS:CE1	2.32	0.64
1:A:731:ARG:O	1:A:733:GLY:N	2.31	0.64
1:A:695:SER:O	1:A:699:GLN:HG3	1.98	0.64
1:A:745:ASN:ND2	1:A:748:ASP:HB2	2.13	0.64
1:B:598:TRP:HA	1:B:698:ASN:HB3	1.80	0.64
1:B:603:LYS:O	1:B:606:TYR:HB2	1.97	0.64
1:B:734:GLU:C	1:B:736:PHE:N	2.50	0.64
1:A:814:PRO:HB2	1:A:857:ALA:HB2	1.79	0.64
1:B:582:LEU:O	1:B:583:ASN:HB2	1.98	0.64
1:B:833:THR:HG22	1:B:834:HIS:HD2	1.62	0.63
1:A:578:MET:O	1:A:582:LEU:HD12	1.98	0.63
1:B:696:PRO:HA	1:B:699:GLN:HE21	1.63	0.63
1:A:767:ALA:HA	1:A:770:LYS:HG3	1.79	0.63
1:A:813:ILE:CG1	1:A:814:PRO:HD3	2.29	0.63
1:B:709:TYR:CE2	1:B:713:LEU:HD11	2.34	0.63
1:B:652:SER:HB3	1:B:655:LEU:CD1	2.27	0.63
1:B:821:ILE:HA	1:B:825:CYS:CB	2.28	0.63
1:B:711:THR:O	1:B:715:ILE:HG13	1.99	0.63
1:B:830:GLU:HA	1:B:843:LEU:HD22	1.81	0.63
1:B:779:ALA:HB1	1:B:817:GLN:HE22	1.63	0.63
1:A:806:ASN:ND2	1:A:808:GLU:HB3	2.14	0.63
1:B:598:TRP:O	1:B:602:VAL:HG23	1.98	0.63
1:B:725:LEU:HD12	1:B:725:LEU:H	1.64	0.63
1:B:839:CYS:C	1:B:841:PRO:HD2	2.20	0.63
1:B:683:HIS:O	1:B:687:ASP:OD1	2.17	0.62
1:B:787:PHE:HB2	1:B:807:ARG:NH1	2.14	0.62
1:A:778:ILE:HA	1:A:781:LEU:HD12	1.81	0.62
1:B:689:CYS:SG	1:B:720:ILE:HD11	2.40	0.62
1:B:767:ALA:HA	1:B:770:LYS:CG	2.30	0.62
1:A:621:THR:HG23	1:A:763:CYS:O	2.00	0.62
1:A:679:SER:O	1:A:683:HIS:ND1	2.30	0.62
1:A:779:ALA:HB1	1:A:817:GLN:HE22	1.62	0.62
1:A:735:PHE:CE2	1:A:758:MET:HG2	2.34	0.62
1:A:563:ASP:HB3	1:A:620:ASN:HD21	1.65	0.62
1:A:604:LYS:HB2	1:A:604:LYS:HZ3	1.65	0.62
1:A:628:ALA:O	1:A:634:ILE:HB	1.99	0.62
1:A:578:MET:O	1:A:582:LEU:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:ILE:CG1	1:B:814:PRO:HD3	2.30	0.61
1:A:786:PHE:HD1	1:A:804:LEU:HG	1.64	0.61
1:B:562:SER:OG	1:B:777:ARG:NH2	2.30	0.61
1:B:827:GLN:HA	1:B:830:GLU:CG	2.30	0.61
1:A:571:THR:HA	1:A:619:PHE:CZ	2.35	0.61
1:A:683:HIS:O	1:A:687:ASP:OD1	2.18	0.61
1:B:583:ASN:HB3	1:B:587:ASN:ND2	2.15	0.61
1:B:820:PHE:HE1	1:B:824:ILE:HD12	1.63	0.61
1:A:769:THR:HG22	1:A:846:CYS:HB2	1.80	0.61
1:B:778:ILE:HA	1:B:781:LEU:HD12	1.81	0.61
1:A:559:PHE:CD2	1:A:841:PRO:HB2	2.34	0.61
1:B:563:ASP:HB2	1:B:616:ARG:HH11	1.66	0.61
1:A:539:GLU:HG2	1:A:600:LEU:CD1	2.31	0.61
1:A:583:ASN:O	1:A:587:ASN:ND2	2.33	0.61
1:A:844:ASP:O	1:A:848:LYS:HG3	2.01	0.61
1:B:630:LYS:C	1:B:632:GLY:H	2.04	0.61
1:B:679:SER:CB	1:B:682:GLU:HG3	2.24	0.61
1:B:814:PRO:HB2	1:B:857:ALA:HB2	1.83	0.61
1:A:582:LEU:HD11	1:A:626:PHE:HD1	1.64	0.61
1:B:763:CYS:O	1:B:766:SER:HB3	2.00	0.61
1:A:549:PRO:HB2	1:A:554:LEU:HG	1.84	0.60
1:B:597:ARG:HD2	1:B:697:GLY:O	2.01	0.60
1:B:762:ALA:CA	1:B:828:LEU:HD11	2.31	0.60
1:B:684:HIS:O	1:B:688:GLN:HB2	2.02	0.60
1:B:750:HIS:O	1:B:753:GLU:HB2	2.02	0.60
1:B:830:GLU:CG	1:B:831:ALA:H	2.14	0.60
1:A:692:ILE:O	1:A:694:ASN:N	2.34	0.60
1:A:585:VAL:O	1:A:589:GLN:HA	2.01	0.60
1:A:786:PHE:CD1	1:A:804:LEU:HG	2.37	0.60
1:B:712:THR:HA	1:B:715:ILE:HD12	1.83	0.60
1:A:693:LEU:HD22	1:A:701:LEU:CD1	2.32	0.59
1:A:630:LYS:C	1:A:632:GLY:H	2.05	0.59
1:B:658:ARG:CG	1:B:658:ARG:NH1	2.63	0.59
1:A:597:ARG:HD2	1:A:697:GLY:O	2.01	0.59
1:A:575:THR:O	1:A:578:MET:HB2	2.02	0.59
1:B:695:SER:O	1:B:699:GLN:HG3	2.02	0.59
1:A:604:LYS:HB2	1:A:604:LYS:HZ2	1.68	0.59
1:A:623:GLN:O	1:A:625:MET:N	2.36	0.59
1:A:762:ALA:HA	1:A:828:LEU:HD11	1.84	0.59
1:A:559:PHE:CD1	1:A:559:PHE:N	2.61	0.59
1:A:734:GLU:C	1:A:736:PHE:N	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:SER:HG	1:B:777:ARG:HH22	1.50	0.59
1:B:551:ALA:HB2	1:B:581:ASP:OD1	2.03	0.59
1:A:813:ILE:HG12	1:A:814:PRO:HD3	1.84	0.59
1:A:624:CYS:O	1:A:624:CYS:SG	2.61	0.58
1:A:684:HIS:O	1:A:688:GLN:HB2	2.02	0.58
1:A:796:GLU:HB2	1:B:717:LYS:HZ3	1.67	0.58
1:B:578:MET:O	1:B:582:LEU:HB2	2.03	0.58
1:A:559:PHE:HD2	1:A:842:LEU:HG	1.69	0.58
1:B:636:ASN:HD21	1:B:637:LYS:HG3	1.67	0.58
1:B:775:GLN:HG3	1:B:776:GLN:N	2.18	0.58
1:A:607:ARG:HH21	1:A:658:ARG:HH21	1.48	0.58
1:A:709:TYR:HE2	1:A:713:LEU:HD11	1.66	0.58
1:A:759:LEU:HD12	1:A:759:LEU:C	2.24	0.58
1:A:847:ARG:O	1:A:851:GLN:HG3	2.03	0.58
1:A:644:LEU:HG	1:A:648:ILE:HD12	1.86	0.58
1:B:615:TRP:O	1:B:615:TRP:CE3	2.57	0.58
1:B:540:LEU:CD2	1:B:597:ARG:HE	2.16	0.58
1:B:559:PHE:CD2	1:B:842:LEU:HG	2.39	0.58
1:B:622:ALA:O	1:B:625:MET:HB3	2.03	0.58
1:B:580:THR:C	1:B:582:LEU:H	2.08	0.58
1:B:630:LYS:HD3	1:B:635:GLN:NE2	2.19	0.57
1:B:770:LYS:HZ1	1:B:774:ILE:HG21	1.67	0.57
1:B:814:PRO:O	1:B:817:GLN:N	2.35	0.57
1:A:582:LEU:O	1:A:583:ASN:HB2	2.03	0.57
1:A:634:ILE:HD13	1:A:836:SER:HB2	1.86	0.57
1:B:767:ALA:HA	1:B:770:LYS:HG3	1.85	0.57
1:A:547:VAL:O	1:A:549:PRO:HD3	2.05	0.57
1:A:557:THR:HG22	1:A:557:THR:O	2.04	0.57
1:A:801:PRO:HB2	1:A:806:ASN:CB	2.22	0.57
1:A:813:ILE:HA	1:A:816:MET:HE3	1.87	0.57
1:B:654:ASP:HA	1:B:685:HIS:CE1	2.40	0.57
1:B:584:LEU:HD12	1:B:647:LEU:CD1	2.35	0.57
1:B:769:THR:HG22	1:B:846:CYS:HB2	1.86	0.57
1:A:750:HIS:O	1:A:753:GLU:HB2	2.05	0.57
1:A:843:LEU:HD12	1:A:843:LEU:O	2.03	0.57
1:B:705:SER:H	1:B:708:GLU:HB2	1.70	0.57
1:A:623:GLN:O	1:A:626:PHE:N	2.37	0.57
1:A:787:PHE:CB	1:A:807:ARG:HH11	2.17	0.57
1:A:830:GLU:O	1:A:833:THR:HB	2.05	0.57
1:A:559:PHE:CD2	1:A:842:LEU:HG	2.40	0.56
1:A:632:GLY:CA	1:A:838:ASP:HB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:LEU:HD11	1:A:847:ARG:NE	2.20	0.56
1:B:656:ASP:H	1:B:685:HIS:HD2	1.53	0.56
1:B:720:ILE:O	1:B:723:THR:HG23	2.06	0.56
1:B:735:PHE:CE2	1:B:758:MET:HG2	2.40	0.56
1:B:847:ARG:O	1:B:851:GLN:HG3	2.05	0.56
1:A:725:LEU:O	1:A:729:ILE:CG1	2.49	0.56
1:A:833:THR:HG22	1:A:834:HIS:N	2.21	0.56
1:B:818:VAL:HG12	1:B:819:GLY:N	2.21	0.56
1:A:705:SER:H	1:A:708:GLU:CG	2.19	0.56
1:A:727:LEU:O	1:A:731:ARG:HG3	2.04	0.56
1:A:767:ALA:HA	1:A:770:LYS:HG2	1.85	0.56
1:B:559:PHE:CE2	1:B:841:PRO:HB2	2.41	0.56
1:B:570:GLU:C	1:B:572:ALA:H	2.08	0.56
1:A:562:SER:HG	1:A:777:ARG:HH22	1.51	0.56
1:A:677:CYS:C	1:A:678:HIS:CG	2.80	0.56
1:B:609:ASN:N	1:B:609:ASN:ND2	2.52	0.56
1:A:540:LEU:CD2	1:A:597:ARG:HE	2.19	0.56
1:A:787:PHE:CB	1:A:807:ARG:NH1	2.68	0.56
1:B:830:GLU:HG3	1:B:831:ALA:H	1.70	0.56
1:B:692:ILE:O	1:B:694:ASN:N	2.38	0.56
1:B:758:MET:HG3	1:B:828:LEU:HD23	1.88	0.56
1:B:810:LYS:HA	1:B:813:ILE:HG23	1.88	0.56
1:B:539:GLU:HG2	1:B:600:LEU:HD11	1.87	0.55
1:B:588:PHE:CD2	1:B:704:LEU:HD21	2.40	0.55
1:B:734:GLU:O	1:B:736:PHE:N	2.39	0.55
1:B:742:ASN:O	1:B:744:PHE:N	2.39	0.55
1:A:820:PHE:CE1	1:A:824:ILE:HD12	2.41	0.55
1:A:609:ASN:N	1:A:609:ASN:HD22	2.05	0.55
1:A:742:ASN:O	1:A:744:PHE:N	2.39	0.55
1:A:763:CYS:O	1:A:766:SER:HB3	2.06	0.55
1:A:771:PRO:O	1:A:773:PRO:N	2.38	0.55
1:B:628:ALA:O	1:B:634:ILE:HB	2.06	0.55
1:B:677:CYS:C	1:B:678:HIS:CG	2.80	0.55
1:A:712:THR:HA	1:A:715:ILE:HD12	1.87	0.55
1:A:717:LYS:HZ3	1:B:796:GLU:CB	2.20	0.55
1:A:802:THR:O	1:A:804:LEU:N	2.38	0.55
1:B:679:SER:O	1:B:683:HIS:ND1	2.37	0.55
1:B:559:PHE:HD2	1:B:842:LEU:HG	1.72	0.55
1:A:584:LEU:HD12	1:A:647:LEU:CD1	2.37	0.54
1:A:840:PHE:N	1:A:841:PRO:CD	2.70	0.54
1:B:609:ASN:N	1:B:609:ASN:HD22	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:THR:O	1:A:619:PHE:CE1	2.60	0.54
1:A:742:ASN:C	1:A:744:PHE:N	2.61	0.54
1:B:802:THR:O	1:B:804:LEU:N	2.40	0.54
1:A:801:PRO:CB	1:A:806:ASN:HB3	2.24	0.54
1:B:582:LEU:HD11	1:B:626:PHE:HD1	1.72	0.54
1:B:724:ASP:O	1:B:726:ALA:N	2.41	0.54
1:A:701:LEU:HD23	1:A:704:LEU:CD1	2.37	0.54
1:A:775:GLN:HG3	1:A:776:GLN:N	2.21	0.54
1:B:727:LEU:HG	1:B:731:ARG:HD2	1.90	0.54
1:A:695:SER:CB	1:A:698:ASN:HD22	2.21	0.54
1:A:735:PHE:CB	1:A:754:LEU:HD23	2.30	0.54
1:A:765:LEU:CD1	1:A:765:LEU:H	2.21	0.54
1:B:797:LEU:H	1:B:797:LEU:CD2	2.02	0.54
1:A:584:LEU:HD13	1:A:644:LEU:CD1	2.37	0.54
1:A:598:TRP:HA	1:A:698:ASN:HB3	1.89	0.54
1:A:609:ASN:N	1:A:609:ASN:ND2	2.52	0.54
1:B:636:ASN:C	1:B:636:ASN:ND2	2.59	0.54
1:A:759:LEU:O	1:A:762:ALA:HB3	2.08	0.54
1:B:762:ALA:HA	1:B:828:LEU:CD1	2.38	0.54
1:A:551:ALA:HB2	1:A:581:ASP:OD1	2.08	0.54
1:A:574:CYS:O	1:A:577:ARG:HB3	2.08	0.54
1:A:765:LEU:CD1	1:A:765:LEU:N	2.71	0.54
1:A:857:ALA:C	1:A:859:GLN:H	2.11	0.54
1:B:607:ARG:NE	1:B:658:ARG:HE	2.06	0.54
1:A:603:LYS:O	1:A:606:TYR:HB2	2.09	0.53
1:A:611:ALA:O	1:A:781:LEU:HB3	2.08	0.53
1:A:705:SER:H	1:A:708:GLU:HB2	1.73	0.53
1:B:810:LYS:O	1:B:813:ILE:HG12	2.08	0.53
1:A:709:TYR:O	1:A:713:LEU:HG	2.09	0.53
1:A:758:MET:HG3	1:A:828:LEU:HD23	1.90	0.53
1:A:827:GLN:HA	1:A:830:GLU:HG2	1.90	0.53
1:A:717:LYS:HE2	1:A:721:LEU:HD11	1.90	0.53
1:A:737:GLU:O	1:A:741:LYS:HB2	2.08	0.53
1:A:770:LYS:HZ3	1:A:774:ILE:CG2	2.19	0.53
1:B:686:PHE:HA	1:B:689:CYS:HB2	1.89	0.53
1:A:570:GLU:C	1:A:572:ALA:H	2.11	0.53
1:B:574:CYS:O	1:B:577:ARG:N	2.42	0.53
1:B:679:SER:C	1:B:682:GLU:HG2	2.29	0.53
1:B:812:LYS:O	1:B:816:MET:HG3	2.08	0.53
1:B:563:ASP:HB2	1:B:616:ARG:NH1	2.22	0.53
1:B:646:LEU:N	1:B:646:LEU:CD2	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:GLU:C	1:B:739:ILE:N	2.62	0.53
1:B:759:LEU:HD12	1:B:759:LEU:C	2.28	0.53
1:A:642:GLU:OE1	1:A:752:LYS:NZ	2.41	0.53
1:A:725:LEU:H	1:A:725:LEU:CD1	2.22	0.53
1:A:741:LYS:C	1:A:743:GLN:H	2.12	0.53
1:A:704:LEU:HB3	1:A:708:GLU:CB	2.39	0.53
1:B:740:ARG:HG3	1:B:740:ARG:HH11	1.73	0.53
1:B:840:PHE:N	1:B:841:PRO:CD	2.71	0.53
1:A:657:HIS:O	1:A:658:ARG:HD3	2.09	0.52
1:B:813:ILE:HG13	1:B:814:PRO:HD3	1.90	0.52
1:B:854:GLN:HA	1:B:854:GLN:OE1	2.09	0.52
1:A:728:TYR:OH	1:A:828:LEU:HB2	2.09	0.52
1:B:646:LEU:N	1:B:646:LEU:HD22	2.23	0.52
1:B:732:ARG:HG3	1:B:733:GLY:N	2.24	0.52
1:A:752:LYS:O	1:A:756:LEU:HB2	2.10	0.52
1:A:797:LEU:HD22	1:A:797:LEU:N	2.16	0.52
1:B:704:LEU:HB3	1:B:708:GLU:CB	2.40	0.52
1:B:639:THR:HG23	1:B:642:GLU:OE1	2.09	0.52
1:B:815:SER:HA	1:B:818:VAL:HB	1.92	0.52
1:A:622:ALA:O	1:A:625:MET:HB3	2.10	0.52
1:A:810:LYS:HA	1:A:813:ILE:HG23	1.92	0.52
1:B:705:SER:H	1:B:708:GLU:CG	2.23	0.52
1:A:717:LYS:NZ	1:B:796:GLU:HG2	2.25	0.52
1:B:537:THR:C	1:B:539:GLU:H	2.13	0.52
1:B:557:THR:HG22	1:B:557:THR:O	2.10	0.52
1:B:793:GLU:HA	1:B:797:LEU:CD2	2.32	0.52
1:A:549:PRO:HB2	1:A:554:LEU:CG	2.39	0.52
1:A:639:THR:HG1	1:A:642:GLU:HG3	1.74	0.52
1:B:657:HIS:O	1:B:658:ARG:HD3	2.09	0.52
1:A:582:LEU:HG	1:A:626:PHE:CE1	2.45	0.52
1:A:679:SER:C	1:A:682:GLU:HG2	2.29	0.52
1:A:740:ARG:HG3	1:A:740:ARG:HH11	1.74	0.52
1:B:648:ILE:CD1	1:B:700:ILE:HD11	2.40	0.52
1:B:833:THR:CG2	1:B:834:HIS:N	2.73	0.51
1:B:548:VAL:HG23	1:B:548:VAL:O	2.09	0.51
1:A:717:LYS:HG2	1:A:721:LEU:CD1	2.38	0.51
1:A:757:ALA:O	1:A:760:MET:N	2.43	0.51
1:B:571:THR:HG22	1:B:619:PHE:CE2	2.46	0.51
1:B:623:GLN:O	1:B:626:PHE:N	2.43	0.51
1:A:564:PHE:CE1	1:A:777:ARG:HD3	2.46	0.51
1:B:715:ILE:O	1:B:719:ALA:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:ILE:N	1:B:814:PRO:CD	2.74	0.51
1:B:830:GLU:HG3	1:B:831:ALA:N	2.26	0.51
1:B:663:SER:HG	1:B:664:TYR:HD1	1.58	0.51
1:A:839:CYS:C	1:A:841:PRO:HD2	2.31	0.51
1:B:607:ARG:HG2	1:B:607:ARG:HH11	1.75	0.51
1:B:611:ALA:O	1:B:781:LEU:HB3	2.10	0.51
1:B:653:HIS:CA	1:B:720:ILE:HG23	2.19	0.51
1:B:737:GLU:O	1:B:741:LYS:HG3	2.11	0.51
1:A:636:ASN:ND2	1:A:636:ASN:C	2.62	0.51
1:A:806:ASN:OD1	1:A:809:LYS:HB2	2.10	0.51
1:B:547:VAL:O	1:B:549:PRO:HD3	2.11	0.51
1:B:649:ALA:O	1:B:652:SER:N	2.44	0.51
1:B:715:ILE:O	1:B:719:ALA:CB	2.59	0.51
1:A:569:LEU:O	1:A:572:ALA:HB3	2.11	0.50
1:B:578:MET:HA	1:B:626:PHE:CE1	2.45	0.50
1:B:830:GLU:CG	1:B:831:ALA:N	2.73	0.50
1:B:639:THR:HG1	1:B:642:GLU:HG3	1.77	0.50
1:A:583:ASN:HB3	1:A:587:ASN:ND2	2.27	0.50
1:A:585:VAL:HG13	1:A:590:MET:HB2	1.93	0.50
1:A:588:PHE:O	1:A:589:GLN:C	2.49	0.50
1:A:814:PRO:O	1:A:817:GLN:N	2.42	0.50
1:B:696:PRO:HA	1:B:699:GLN:NE2	2.25	0.50
1:A:574:CYS:O	1:A:577:ARG:N	2.44	0.50
1:B:695:SER:CB	1:B:698:ASN:HD22	2.23	0.50
1:B:720:ILE:O	1:B:722:ALA:N	2.45	0.50
1:A:714:LYS:O	1:A:718:GLN:HB2	2.12	0.50
1:B:818:VAL:HG23	1:B:853:TRP:HB3	1.93	0.50
1:A:582:LEU:CD1	1:A:626:PHE:HD1	2.25	0.50
1:B:770:LYS:O	1:B:775:GLN:HB3	2.12	0.50
1:A:601:SER:O	1:A:602:VAL:C	2.50	0.50
1:A:717:LYS:O	1:A:721:LEU:HG	2.12	0.50
1:A:808:GLU:C	1:A:810:LYS:H	2.15	0.50
1:B:563:ASP:HB3	1:B:620:ASN:ND2	2.23	0.50
1:B:621:THR:HG23	1:B:763:CYS:O	2.10	0.50
1:A:548:VAL:HG23	1:A:548:VAL:O	2.11	0.50
1:A:770:LYS:HZ1	1:A:774:ILE:HG21	1.75	0.50
1:B:709:TYR:HE2	1:B:713:LEU:HD11	1.76	0.50
1:B:820:PHE:CZ	4:B:2003:CIA:H11	2.47	0.50
1:A:813:ILE:N	1:A:814:PRO:CD	2.76	0.49
1:A:832:LEU:O	1:A:833:THR:C	2.50	0.49
1:B:559:PHE:HD2	1:B:842:LEU:CD2	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:SER:HA	1:A:818:VAL:HB	1.94	0.49
1:B:735:PHE:CB	1:B:754:LEU:HD23	2.34	0.49
1:B:541:GLN:O	1:B:544:ALA:HB3	2.12	0.49
1:B:731:ARG:O	1:B:732:ARG:C	2.50	0.49
1:A:705:SER:HB2	1:A:708:GLU:CG	2.41	0.49
1:A:854:GLN:OE1	1:A:854:GLN:HA	2.12	0.49
1:B:607:ARG:HG2	1:B:607:ARG:NH1	2.27	0.49
1:B:623:GLN:O	1:B:625:MET:N	2.45	0.49
1:B:742:ASN:C	1:B:744:PHE:N	2.65	0.49
1:A:548:VAL:HG11	1:A:576:ILE:CG2	2.42	0.49
1:A:737:GLU:C	1:A:739:ILE:H	2.15	0.49
1:A:793:GLU:HA	1:A:797:LEU:CD2	2.37	0.49
1:B:757:ALA:O	1:B:760:MET:N	2.45	0.49
1:B:634:ILE:HD13	1:B:836:SER:HB2	1.93	0.49
1:A:584:LEU:HD13	1:A:644:LEU:HD12	1.94	0.49
1:A:737:GLU:C	1:A:739:ILE:N	2.64	0.49
1:A:765:LEU:HD13	1:A:765:LEU:H	1.77	0.49
1:B:750:HIS:CD2	1:B:754:LEU:HD13	2.48	0.49
1:A:644:LEU:HG	1:A:648:ILE:CD1	2.42	0.49
1:B:727:LEU:HD23	1:B:728:TYR:H	1.75	0.49
1:A:661:ASN:C	1:A:662:ASN:ND2	2.60	0.49
1:B:590:MET:HE1	1:B:644:LEU:CD1	2.42	0.49
1:B:687:ASP:O	1:B:691:MET:HB2	2.13	0.49
1:B:808:GLU:CG	1:B:809:LYS:H	2.10	0.49
1:A:583:ASN:HB3	1:A:587:ASN:HD21	1.77	0.49
1:A:732:ARG:HG3	1:A:733:GLY:N	2.28	0.49
1:A:808:GLU:C	1:A:810:LYS:N	2.66	0.49
1:B:653:HIS:HD2	1:B:764:ASP:OD2	1.96	0.49
1:A:765:LEU:N	1:A:765:LEU:HD12	2.28	0.48
1:B:679:SER:CA	1:B:682:GLU:HG2	2.42	0.48
1:B:720:ILE:C	1:B:722:ALA:H	2.16	0.48
1:B:745:ASN:HD22	1:B:748:ASP:HB2	1.75	0.48
1:B:767:ALA:HA	1:B:770:LYS:HG2	1.93	0.48
1:A:568:ASP:O	1:A:569:LEU:C	2.51	0.48
1:B:717:LYS:HG2	1:B:721:LEU:CD1	2.43	0.48
1:A:607:ARG:CZ	1:A:658:ARG:HE	2.25	0.48
1:A:656:ASP:H	1:A:685:HIS:HD2	1.59	0.48
1:A:808:GLU:O	1:A:810:LYS:N	2.46	0.48
1:B:736:PHE:O	1:B:737:GLU:OE1	2.31	0.48
1:A:705:SER:H	1:A:708:GLU:HG3	1.77	0.48
1:B:832:LEU:O	1:B:833:THR:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:VAL:HG11	1:A:613:HIS:HB2	1.95	0.48
1:B:586:GLN:HE21	1:B:586:GLN:CA	2.16	0.48
1:B:735:PHE:O	1:B:735:PHE:CD2	2.67	0.48
1:A:656:ASP:H	1:A:685:HIS:CD2	2.32	0.48
1:B:813:ILE:HG12	1:B:814:PRO:HD3	1.96	0.48
1:A:783:ALA:HA	4:A:1003:CIA:H291	1.95	0.48
1:B:549:PRO:HB2	1:B:554:LEU:CG	2.42	0.48
1:B:715:ILE:O	1:B:719:ALA:N	2.46	0.48
1:A:582:LEU:HD11	1:A:626:PHE:CD1	2.48	0.47
1:A:808:GLU:CG	1:A:809:LYS:H	2.03	0.47
1:B:539:GLU:HG2	1:B:600:LEU:CD1	2.43	0.47
1:B:705:SER:H	1:B:708:GLU:HG3	1.79	0.47
1:B:772:TRP:HB3	1:B:773:PRO:HD3	1.96	0.47
1:B:717:LYS:HE2	1:B:721:LEU:CD1	2.43	0.47
1:A:598:TRP:O	1:A:599:ILE:C	2.53	0.47
1:A:717:LYS:HZ3	1:B:796:GLU:CG	2.28	0.47
1:B:570:GLU:C	1:B:572:ALA:N	2.67	0.47
1:B:584:LEU:HD12	1:B:647:LEU:HD13	1.96	0.47
1:B:607:ARG:CZ	1:B:658:ARG:HE	2.26	0.47
1:A:705:SER:H	1:A:708:GLU:CB	2.27	0.47
1:A:731:ARG:O	1:A:732:ARG:C	2.52	0.47
1:B:820:PHE:CD1	1:B:824:ILE:HD12	2.49	0.47
1:A:621:THR:HG23	1:A:763:CYS:C	2.34	0.47
1:B:709:TYR:O	1:B:713:LEU:HG	2.14	0.47
1:B:749:PRO:O	1:B:752:LYS:N	2.47	0.47
1:B:756:LEU:HD23	1:B:759:LEU:HD23	1.97	0.47
1:A:580:THR:C	1:A:582:LEU:H	2.18	0.47
1:A:646:LEU:O	1:A:650:ALA:CB	2.62	0.47
1:A:816:MET:HB2	4:A:1003:CIA:H26	1.94	0.47
1:A:612:TYR:OH	4:A:1003:CIA:H2	2.14	0.47
1:A:719:ALA:HB1	1:A:760:MET:CE	2.45	0.47
1:A:736:PHE:O	1:A:737:GLU:OE1	2.33	0.47
1:A:797:LEU:HD13	1:B:718:GLN:NE2	2.30	0.47
1:B:543:LEU:HD22	1:B:576:ILE:HD11	1.96	0.47
1:B:645:ALA:O	1:B:649:ALA:CB	2.62	0.47
1:B:741:LYS:C	1:B:743:GLN:H	2.18	0.47
1:A:679:SER:CA	1:A:682:GLU:HG2	2.45	0.47
1:A:561:PHE:CD2	1:A:623:GLN:HG3	2.50	0.47
1:A:629:LEU:HG	1:A:635:GLN:HB2	1.96	0.47
1:A:813:ILE:HA	1:A:816:MET:CE	2.44	0.47
1:B:641:LEU:O	1:B:644:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:LEU:O	1:B:650:ALA:HB3	2.15	0.47
1:B:728:TYR:OH	1:B:828:LEU:HB2	2.15	0.47
1:A:720:ILE:C	1:A:722:ALA:H	2.19	0.47
1:A:797:LEU:HD11	1:B:717:LYS:NZ	2.30	0.47
1:B:656:ASP:HB3	1:B:684:HIS:NE2	2.30	0.47
1:B:717:LYS:CE	1:B:721:LEU:HD11	2.45	0.47
1:A:570:GLU:C	1:A:572:ALA:N	2.68	0.46
1:B:705:SER:H	1:B:708:GLU:CB	2.28	0.46
1:B:788:ASP:OD1	1:B:807:ARG:NH1	2.48	0.46
1:A:537:THR:C	1:A:539:GLU:H	2.17	0.46
1:A:642:GLU:CD	1:A:752:LYS:HZ3	2.19	0.46
1:A:654:ASP:HA	1:A:685:HIS:ND1	2.31	0.46
1:B:630:LYS:C	1:B:632:GLY:N	2.67	0.46
1:B:632:GLY:O	1:B:836:SER:OG	2.18	0.46
1:B:692:ILE:HA	1:B:695:SER:OG	2.14	0.46
1:A:793:GLU:CA	1:A:797:LEU:HD23	2.41	0.46
1:B:789:GLN:NE2	1:B:805:MET:SD	2.88	0.46
1:A:732:ARG:HH12	1:A:824:ILE:HA	1.79	0.46
1:A:812:LYS:O	1:A:816:MET:HG3	2.15	0.46
1:B:568:ASP:O	1:B:571:THR:N	2.48	0.46
1:B:632:GLY:HA2	1:B:838:ASP:O	2.15	0.46
1:B:750:HIS:NE2	1:B:754:LEU:HD13	2.30	0.46
1:B:772:TRP:CZ2	1:B:852:LYS:HB3	2.50	0.46
1:B:774:ILE:HG23	1:B:777:ARG:NH2	2.30	0.46
1:B:568:ASP:O	1:B:569:LEU:C	2.53	0.46
1:B:656:ASP:H	1:B:685:HIS:CD2	2.32	0.46
1:B:737:GLU:C	1:B:739:ILE:H	2.18	0.46
1:A:564:PHE:HB2	1:A:777:ARG:NH2	2.31	0.46
1:B:540:LEU:HD21	1:B:597:ARG:HB2	1.97	0.46
1:A:577:ARG:NH1	1:A:581:ASP:OD2	2.44	0.46
1:A:605:ASN:O	1:A:605:ASN:ND2	2.49	0.46
1:A:623:GLN:C	1:A:625:MET:N	2.68	0.46
1:A:735:PHE:CD2	1:A:758:MET:HG2	2.51	0.46
1:A:820:PHE:CE1	4:A:1003:CIA:H11	2.51	0.46
1:A:662:ASN:HD22	1:A:662:ASN:N	2.09	0.46
1:A:685:HIS:O	1:A:689:CYS:N	2.48	0.46
1:B:653:HIS:NE2	1:B:654:ASP:OD2	2.48	0.46
1:B:661:ASN:C	1:B:662:ASN:ND2	2.69	0.46
1:B:732:ARG:HB3	1:B:758:MET:SD	2.56	0.46
1:A:639:THR:O	1:A:643:ILE:HD12	2.16	0.46
1:B:604:LYS:NZ	1:B:604:LYS:CB	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:PHE:HD1	1:B:804:LEU:HG	1.80	0.46
1:B:826:LEU:CD2	1:B:827:GLN:N	2.77	0.46
1:A:695:SER:O	1:A:699:GLN:CG	2.64	0.45
1:B:765:LEU:N	1:B:765:LEU:CD1	2.78	0.45
1:B:549:PRO:CG	1:B:554:LEU:HD21	2.42	0.45
1:A:563:ASP:HB3	1:A:620:ASN:ND2	2.31	0.45
1:A:690:LEU:O	1:A:691:MET:C	2.55	0.45
1:A:554:LEU:HB2	1:A:556:ILE:HG23	1.99	0.45
1:B:784:THR:O	1:B:788:ASP:OD1	2.35	0.45
1:A:603:LYS:O	1:A:605:ASN:N	2.50	0.45
1:A:615:TRP:O	1:A:615:TRP:CE3	2.69	0.45
1:A:701:LEU:HD23	1:A:704:LEU:HD11	1.98	0.45
1:A:783:ALA:HA	4:A:1003:CIA:C29	2.46	0.45
1:B:604:LYS:HB2	1:B:604:LYS:HZ3	1.80	0.45
1:A:781:LEU:O	1:A:784:THR:HB	2.17	0.45
1:B:757:ALA:C	1:B:759:LEU:N	2.70	0.45
1:B:771:PRO:O	1:B:772:TRP:C	2.55	0.45
1:A:598:TRP:O	1:A:601:SER:N	2.50	0.45
1:A:607:ARG:NE	1:A:658:ARG:HE	2.15	0.45
1:B:828:LEU:HD22	1:B:828:LEU:C	2.37	0.45
1:A:622:ALA:HB2	1:A:651:LEU:CD2	2.46	0.45
1:A:843:LEU:HD11	1:A:847:ARG:HE	1.82	0.45
1:A:715:ILE:O	1:A:719:ALA:HB2	2.17	0.45
1:B:813:ILE:HG13	1:B:814:PRO:CD	2.47	0.45
1:A:701:LEU:HD23	1:A:704:LEU:HD12	1.99	0.44
1:A:630:LYS:C	1:A:632:GLY:N	2.67	0.44
1:A:635:GLN:C	1:A:637:LYS:H	2.20	0.44
1:A:727:LEU:HG	1:A:731:ARG:HD2	1.98	0.44
1:A:806:ASN:HD21	1:A:809:LYS:HD3	1.82	0.44
1:B:595:LEU:O	1:B:595:LEU:HD23	2.16	0.44
1:B:732:ARG:CB	1:B:758:MET:SD	3.05	0.44
1:B:786:PHE:CD1	1:B:804:LEU:HG	2.52	0.44
1:A:548:VAL:HG11	1:A:576:ILE:HG21	1.98	0.44
1:B:537:THR:C	1:B:539:GLU:N	2.70	0.44
1:B:584:LEU:HD12	1:B:647:LEU:HD12	1.99	0.44
1:B:605:ASN:O	1:B:605:ASN:ND2	2.50	0.44
1:A:797:LEU:H	1:A:797:LEU:CD2	2.13	0.44
1:B:623:GLN:C	1:B:625:MET:N	2.70	0.44
1:B:686:PHE:O	1:B:689:CYS:N	2.50	0.44
1:B:695:SER:O	1:B:699:GLN:CG	2.65	0.44
1:B:740:ARG:O	1:B:740:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ALA:O	1:A:592:HIS:HE1	2.01	0.44
1:A:559:PHE:CE2	1:A:841:PRO:HB2	2.53	0.44
1:A:788:ASP:OD1	1:A:807:ARG:NH1	2.49	0.44
1:A:814:PRO:O	1:A:817:GLN:HB2	2.17	0.44
1:B:607:ARG:HH21	1:B:658:ARG:NH2	2.09	0.44
1:B:725:LEU:O	1:B:729:ILE:CG1	2.46	0.44
1:B:787:PHE:CB	1:B:807:ARG:HH11	2.31	0.44
1:B:584:LEU:HD13	1:B:644:LEU:HD13	1.98	0.44
1:B:588:PHE:O	1:B:589:GLN:C	2.55	0.44
1:B:615:TRP:CE3	1:B:618:ALA:HB3	2.53	0.44
1:B:820:PHE:O	1:B:824:ILE:N	2.47	0.44
1:A:584:LEU:HD12	1:A:647:LEU:HD12	1.98	0.44
1:A:727:LEU:HD23	1:A:728:TYR:H	1.78	0.44
1:B:646:LEU:O	1:B:650:ALA:CB	2.66	0.44
1:B:857:ALA:C	1:B:859:GLN:H	2.21	0.44
1:A:539:GLU:O	1:A:542:SER:HB3	2.18	0.44
1:A:662:ASN:ND2	1:A:662:ASN:N	2.65	0.44
1:A:741:LYS:O	1:A:743:GLN:N	2.51	0.44
1:B:582:LEU:CD1	1:B:626:PHE:HD1	2.31	0.44
1:B:842:LEU:O	1:B:844:ASP:N	2.51	0.44
1:A:540:LEU:HD11	1:A:596:CYS:HB2	2.00	0.43
1:A:634:ILE:CD1	1:A:836:SER:HB2	2.47	0.43
1:A:681:MET:HG3	1:A:685:HIS:CE1	2.52	0.43
1:B:548:VAL:O	1:B:549:PRO:O	2.36	0.43
1:A:813:ILE:HG13	1:A:814:PRO:HD3	1.98	0.43
1:B:685:HIS:O	1:B:689:CYS:N	2.43	0.43
1:A:612:TYR:O	1:A:614:ASN:N	2.42	0.43
1:A:796:GLU:CB	1:B:717:LYS:HZ3	2.29	0.43
1:B:584:LEU:HB3	1:B:590:MET:HE1	2.00	0.43
1:A:559:PHE:HD2	1:A:842:LEU:CD2	2.31	0.43
1:A:653:HIS:HA	1:A:720:ILE:CG2	2.19	0.43
1:A:734:GLU:O	1:A:736:PHE:N	2.51	0.43
1:A:646:LEU:HD11	1:A:756:LEU:HD22	2.00	0.43
1:A:648:ILE:HG12	1:A:700:ILE:HD11	2.00	0.43
1:A:696:PRO:HA	1:A:699:GLN:NE2	2.27	0.43
1:A:728:TYR:HE2	1:A:824:ILE:CG2	2.32	0.43
1:A:758:MET:HG3	1:A:828:LEU:CD2	2.48	0.43
1:A:768:ILE:HD11	1:A:821:ILE:HD11	2.01	0.43
1:A:771:PRO:O	1:A:772:TRP:C	2.56	0.43
1:A:786:PHE:HE1	1:A:804:LEU:HD21	1.83	0.43
1:B:598:TRP:O	1:B:601:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:ILE:C	1:B:731:ARG:H	2.22	0.43
1:B:787:PHE:CB	1:B:807:ARG:NH1	2.81	0.43
1:B:607:ARG:NE	1:B:658:ARG:NE	2.65	0.43
1:B:740:ARG:HG3	1:B:740:ARG:NH1	2.33	0.43
1:B:810:LYS:O	1:B:813:ILE:HG23	2.18	0.43
1:A:582:LEU:CD1	1:A:626:PHE:CD1	3.02	0.43
1:A:820:PHE:HE1	1:A:824:ILE:HD12	1.83	0.43
1:A:636:ASN:HD22	1:A:637:LYS:HG3	1.77	0.43
1:A:645:ALA:O	1:A:649:ALA:CB	2.66	0.43
1:A:656:ASP:HB3	1:A:684:HIS:NE2	2.33	0.43
1:A:830:GLU:CG	1:A:831:ALA:H	2.31	0.43
1:B:571:THR:O	1:B:619:PHE:CE1	2.72	0.43
1:B:580:THR:O	1:B:582:LEU:N	2.52	0.43
1:A:562:SER:OG	1:A:777:ARG:NH2	2.33	0.43
1:A:578:MET:HA	1:A:626:PHE:CE1	2.53	0.43
1:A:584:LEU:HD12	1:A:647:LEU:HD13	2.00	0.43
1:A:719:ALA:HB1	1:A:760:MET:HE3	2.01	0.43
1:B:556:ILE:HG13	1:B:626:PHE:CE2	2.53	0.43
1:B:612:TYR:O	1:B:614:ASN:N	2.46	0.43
1:B:808:GLU:C	1:B:810:LYS:H	2.21	0.43
1:A:690:LEU:HD12	1:A:690:LEU:HA	1.87	0.43
1:A:810:LYS:O	1:A:813:ILE:HG23	2.19	0.42
1:B:779:ALA:CB	1:B:817:GLN:HE22	2.29	0.42
1:B:840:PHE:N	1:B:841:PRO:HD2	2.34	0.42
1:B:590:MET:HE1	1:B:644:LEU:HD11	1.99	0.42
1:B:808:GLU:C	1:B:810:LYS:N	2.73	0.42
1:B:830:GLU:O	1:B:831:ALA:C	2.56	0.42
1:A:676:TYR:CZ	1:A:678:HIS:HA	2.54	0.42
1:A:825:CYS:O	1:A:826:LEU:C	2.57	0.42
1:B:543:LEU:HD22	1:B:576:ILE:CD1	2.49	0.42
1:B:584:LEU:CD1	1:B:647:LEU:HD12	2.49	0.42
1:B:717:LYS:O	1:B:718:GLN:C	2.54	0.42
1:A:622:ALA:HB2	1:A:651:LEU:HD23	2.00	0.42
1:A:722:ALA:HA	1:A:727:LEU:HD22	2.01	0.42
1:A:735:PHE:CD2	1:A:735:PHE:O	2.72	0.42
1:A:840:PHE:N	1:A:841:PRO:HD2	2.34	0.42
1:A:735:PHE:CE1	1:A:755:PHE:HA	2.54	0.42
1:A:740:ARG:HG3	1:A:740:ARG:NH1	2.34	0.42
1:B:714:LYS:O	1:B:718:GLN:HB2	2.20	0.42
1:B:849:ASN:C	1:B:851:GLN:H	2.23	0.42
1:A:779:ALA:CB	1:A:817:GLN:HE22	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:PHE:HB3	1:A:807:ARG:HH11	1.82	0.42
1:A:757:ALA:C	1:A:759:LEU:N	2.72	0.42
1:B:663:SER:OG	1:B:664:TYR:HD1	2.03	0.42
1:B:735:PHE:O	1:B:735:PHE:CG	2.73	0.42
1:A:537:THR:C	1:A:539:GLU:N	2.73	0.42
1:A:623:GLN:C	1:A:625:MET:H	2.23	0.42
1:A:663:SER:HG	1:A:664:TYR:HD1	1.62	0.42
1:A:832:LEU:O	1:A:835:VAL:N	2.41	0.42
1:A:849:ASN:C	1:A:851:GLN:H	2.23	0.42
1:A:711:THR:O	1:A:715:ILE:CG1	2.66	0.42
1:B:642:GLU:OE2	1:B:752:LYS:HE2	2.20	0.42
1:B:690:LEU:HA	1:B:690:LEU:HD12	1.82	0.42
1:B:690:LEU:O	1:B:691:MET:C	2.58	0.42
1:B:771:PRO:O	1:B:773:PRO:N	2.53	0.42
1:B:821:ILE:HA	1:B:825:CYS:SG	2.60	0.42
1:B:843:LEU:HD12	1:B:843:LEU:O	2.20	0.42
1:A:574:CYS:HB2	1:A:619:PHE:CZ	2.55	0.42
1:A:586:GLN:HE21	1:A:586:GLN:CA	2.17	0.42
1:A:750:HIS:NE2	1:A:754:LEU:HD13	2.35	0.42
1:B:652:SER:CB	1:B:655:LEU:CD1	2.96	0.42
1:B:758:MET:HG3	1:B:828:LEU:CD2	2.48	0.42
1:A:646:LEU:CD2	1:A:646:LEU:N	2.83	0.41
1:B:653:HIS:CD2	1:B:764:ASP:OD2	2.72	0.41
1:B:830:GLU:HB3	1:B:843:LEU:HD13	2.03	0.41
1:A:686:PHE:O	1:A:689:CYS:N	2.53	0.41
1:A:717:LYS:NZ	1:B:796:GLU:CG	2.82	0.41
1:B:648:ILE:HD13	1:B:700:ILE:HD11	2.02	0.41
1:A:717:LYS:HZ3	1:B:796:GLU:HG2	1.86	0.41
1:A:771:PRO:C	1:A:773:PRO:CD	2.89	0.41
1:B:765:LEU:N	1:B:765:LEU:HD12	2.34	0.41
1:A:692:ILE:O	1:A:693:LEU:C	2.59	0.41
1:A:720:ILE:O	1:A:722:ALA:N	2.53	0.41
1:A:715:ILE:O	1:A:719:ALA:CB	2.69	0.41
1:A:770:LYS:O	1:A:775:GLN:HB3	2.20	0.41
1:A:830:GLU:CG	1:A:831:ALA:N	2.84	0.41
1:A:830:GLU:HG3	1:A:831:ALA:N	2.36	0.41
1:B:564:PHE:HB2	1:B:777:ARG:NH2	2.35	0.41
1:B:639:THR:HG23	1:B:642:GLU:CD	2.39	0.41
1:B:662:ASN:ND2	1:B:662:ASN:N	2.68	0.41
1:B:711:THR:O	1:B:715:ILE:CG1	2.66	0.41
1:B:717:LYS:O	1:B:721:LEU:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:ILE:HA	1:B:781:LEU:CD1	2.48	0.41
1:B:801:PRO:CB	1:B:806:ASN:HB3	2.26	0.41
1:A:634:ILE:CD1	1:A:836:SER:CB	2.99	0.41
1:A:724:ASP:O	1:A:726:ALA:N	2.53	0.41
1:A:725:LEU:HA	1:A:728:TYR:HB3	2.02	0.41
1:A:797:LEU:CD1	1:B:718:GLN:HE21	2.34	0.41
1:A:813:ILE:HG13	1:A:814:PRO:CD	2.50	0.41
1:B:591:LYS:O	1:B:592:HIS:C	2.57	0.41
1:B:658:ARG:HD2	1:B:658:ARG:HA	1.79	0.41
1:A:603:LYS:O	1:A:606:TYR:N	2.54	0.41
1:A:639:THR:HG23	1:A:642:GLU:OE1	2.20	0.41
1:A:756:LEU:HD23	1:A:756:LEU:HA	1.85	0.41
1:B:847:ARG:O	1:B:851:GLN:CG	2.69	0.41
1:B:850:ARG:HH21	1:B:854:GLN:NE2	2.19	0.41
1:B:540:LEU:O	1:B:541:GLN:C	2.59	0.41
1:B:629:LEU:O	1:B:635:GLN:HB2	2.21	0.41
1:A:603:LYS:O	1:A:604:LYS:C	2.59	0.41
1:A:630:LYS:O	1:A:633:LYS:N	2.41	0.41
1:A:717:LYS:CG	1:A:721:LEU:HD11	2.46	0.41
1:A:787:PHE:HB2	1:A:807:ARG:HH11	1.77	0.41
1:B:624:CYS:O	1:B:624:CYS:SG	2.78	0.41
1:B:730:LYS:O	1:B:730:LYS:HG2	2.21	0.41
1:B:580:THR:C	1:B:582:LEU:N	2.73	0.40
1:B:756:LEU:HD23	1:B:756:LEU:HA	1.90	0.40
1:B:839:CYS:C	1:B:841:PRO:CD	2.88	0.40
1:A:687:ASP:O	1:A:691:MET:HB2	2.21	0.40
1:A:759:LEU:HD12	1:A:763:CYS:HG	1.86	0.40
1:A:796:GLU:HB2	1:B:717:LYS:NZ	2.33	0.40
1:A:821:ILE:CA	1:A:825:CYS:HB2	2.35	0.40
1:B:582:LEU:HD11	1:B:626:PHE:CD1	2.53	0.40
1:A:540:LEU:O	1:A:541:GLN:C	2.58	0.40
1:A:549:PRO:CG	1:A:554:LEU:HD21	2.48	0.40
1:A:612:TYR:CZ	4:A:1003:CIA:H2	2.56	0.40
1:A:612:TYR:C	1:A:614:ASN:H	2.24	0.40
1:B:752:LYS:O	1:B:756:LEU:HB2	2.21	0.40
1:A:566:LEU:HD23	1:A:566:LEU:N	2.26	0.40
1:A:645:ALA:O	1:A:649:ALA:N	2.39	0.40
1:A:646:LEU:O	1:A:650:ALA:HB3	2.21	0.40
1:A:658:ARG:NH1	1:A:658:ARG:CG	2.76	0.40
1:B:732:ARG:HH12	1:B:824:ILE:HA	1.85	0.40
1:B:712:THR:HA	1:B:715:ILE:CD1	2.49	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	309/324 (95%)	194 (63%)	78 (25%)	37 (12%)	0 0
1	B	309/324 (95%)	196 (63%)	79 (26%)	34 (11%)	0 0
All	All	618/648 (95%)	390 (63%)	157 (25%)	71 (12%)	0 0

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	549	PRO
1	A	564	PHE
1	A	631	ALA
1	A	693	LEU
1	A	732	ARG
1	A	826	LEU
1	B	549	PRO
1	B	631	ALA
1	B	650	ALA
1	B	732	ARG
1	B	743	GLN
1	B	826	LEU
1	A	589	GLN
1	A	598	TRP
1	A	599	ILE
1	A	624	CYS
1	A	721	LEU
1	A	742	ASN
1	A	743	GLN
1	A	745	ASN
1	A	794	ARG
1	B	589	GLN

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Mol	Chain	Res	Type
1	B	649	ALA
1	B	663	SER
1	B	693	LEU
1	B	721	LEU
1	B	725	LEU
1	B	742	ASN
1	B	744	PHE
1	B	745	ASN
1	B	794	ARG
1	A	602	VAL
1	A	604	LYS
1	A	612	TYR
1	A	650	ALA
1	A	663	SER
1	A	725	LEU
1	A	744	PHE
1	A	803	ASP
1	B	581	ASP
1	B	604	LYS
1	B	612	TYR
1	B	735	PHE
1	B	803	ASP
1	A	601	SER
1	A	623	GLN
1	A	703	GLY
1	A	756	LEU
1	A	772	TRP
1	A	809	LYS
1	B	564	PHE
1	B	642	GLU
1	B	703	GLY
1	B	717	LYS
1	B	773	PRO
1	A	649	ALA
1	A	692	ILE
1	A	717	LYS
1	A	733	GLY
1	A	735	PHE
1	A	773	PRO
1	B	758	MET
1	B	843	LEU
1	A	755	PHE

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Mol	Chain	Res	Type
1	B	542	SER
1	B	593	GLU
1	B	624	CYS
1	B	814	PRO
1	B	733	GLY
1	B	716	ILE
1	A	814	PRO

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	279/289 (96%)	239 (86%)	40 (14%)	3	6
1	B	279/289 (96%)	240 (86%)	39 (14%)	3	6
All	All	558/578 (96%)	479 (86%)	79 (14%)	3	6

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	543	LEU
1	A	558	ASP
1	A	559	PHE
1	A	564	PHE
1	A	566	LEU
1	A	569	LEU
1	A	586	GLN
1	A	589	GLN
1	A	591	LYS
1	A	601	SER
1	A	620	ASN
1	A	636	ASN
1	A	655	LEU
1	A	658	ARG
1	A	661	ASN
1	A	682	GLU

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Mol	Chain	Res	Type
1	A	687	ASP
1	A	691	MET
1	A	698	ASN
1	A	713	LEU
1	A	727	LEU
1	A	747	GLU
1	A	752	LYS
1	A	759	LEU
1	A	760	MET
1	A	765	LEU
1	A	775	GLN
1	A	782	VAL
1	A	788	ASP
1	A	795	LYS
1	A	797	LEU
1	A	798	ASN
1	A	809	LYS
1	A	812	LYS
1	A	818	VAL
1	A	828	LEU
1	A	833	THR
1	A	838	ASP
1	A	850	ARG
1	A	858	GLU
1	B	543	LEU
1	B	558	ASP
1	B	559	PHE
1	B	566	LEU
1	B	569	LEU
1	B	586	GLN
1	B	589	GLN
1	B	601	SER
1	B	609	ASN
1	B	615	TRP
1	B	620	ASN
1	B	636	ASN
1	B	655	LEU
1	B	658	ARG
1	B	661	ASN
1	B	682	GLU
1	B	687	ASP
1	B	691	MET

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Mol	Chain	Res	Type
1	B	698	ASN
1	B	710	LYS
1	B	713	LEU
1	B	727	LEU
1	B	747	GLU
1	B	758	MET
1	B	759	LEU
1	B	760	MET
1	B	765	LEU
1	B	775	GLN
1	B	782	VAL
1	B	788	ASP
1	B	797	LEU
1	B	798	ASN
1	B	812	LYS
1	B	822	ASP
1	B	828	LEU
1	B	833	THR
1	B	838	ASP
1	B	850	ARG
1	B	858	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	583	ASN
1	A	586	GLN
1	A	587	ASN
1	A	592	HIS
1	A	605	ASN
1	A	609	ASN
1	A	617	HIS
1	A	620	ASN
1	A	635	GLN
1	A	636	ASN
1	A	662	ASN
1	A	685	HIS
1	A	698	ASN
1	A	699	GLN
1	A	718	GLN
1	A	743	GLN
1	A	775	GLN

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Mol	Chain	Res	Type
1	A	834	HIS
1	A	849	ASN
1	A	851	GLN
1	B	583	ASN
1	B	586	GLN
1	B	587	ASN
1	B	592	HIS
1	B	605	ASN
1	B	609	ASN
1	B	617	HIS
1	B	620	ASN
1	B	635	GLN
1	B	636	ASN
1	B	662	ASN
1	B	685	HIS
1	B	698	ASN
1	B	699	GLN
1	B	718	GLN
1	B	743	GLN
1	B	775	GLN
1	B	834	HIS
1	B	849	ASN
1	B	851	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	CIA	B	2003	-	30,34,34	3.89	20 (66%)	40,52,52	1.20	3 (7%)
4	CIA	A	1003	-	30,34,34	4.09	19 (63%)	40,52,52	1.42	4 (10%)

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
4	CIA	B	2003	-	-	0/4/42/42	0/6/6/6
4	CIA	A	1003	-	-	0/4/42/42	0/6/6/6

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	CIA	C31-N15	8.54	1.42	1.34
4	A	1003	CIA	C17-N12	7.80	1.42	1.35
4	A	1003	CIA	C22-C13	7.64	1.63	1.52
4	B	2003	CIA	C31-N15	7.42	1.41	1.34
4	B	2003	CIA	C22-C13	7.03	1.62	1.52
4	B	2003	CIA	C16-N15	6.72	1.51	1.45
4	B	2003	CIA	C23-C22	6.49	1.49	1.39
4	A	1003	CIA	C23-C22	6.46	1.49	1.39
4	B	2003	CIA	C11-N12	6.41	1.57	1.47
4	A	1003	CIA	C11-N12	6.33	1.57	1.47
4	A	1003	CIA	C16-N15	6.23	1.51	1.45
4	B	2003	CIA	C11-C31	5.45	1.62	1.51
4	B	2003	CIA	C17-N12	5.45	1.40	1.35
4	A	1003	CIA	C11-C31	5.14	1.61	1.51
4	A	1003	CIA	C10-C7	5.01	1.57	1.51
4	B	2003	CIA	C27-C22	4.93	1.47	1.39
4	B	2003	CIA	C26-C25	4.59	1.49	1.39
4	A	1003	CIA	C26-C25	4.22	1.48	1.39
4	A	1003	CIA	C27-C22	4.01	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2003	CIA	C10-C7	3.84	1.56	1.51
4	A	1003	CIA	C2-C1	3.58	1.44	1.36
4	A	1003	CIA	C7-C8	3.58	1.44	1.39
4	B	2003	CIA	C7-C8	3.52	1.44	1.39
4	A	1003	CIA	C4-C5	3.48	1.47	1.41
4	B	2003	CIA	C2-C1	3.33	1.44	1.36
4	B	2003	CIA	C2-C3	3.13	1.46	1.38
4	B	2003	CIA	C3-C4	3.12	1.43	1.36
4	A	1003	CIA	C3-C4	3.08	1.43	1.36
4	B	2003	CIA	C26-C27	3.05	1.44	1.38
4	A	1003	CIA	C26-C27	2.99	1.44	1.38
4	A	1003	CIA	C1-C6	2.88	1.48	1.42
4	B	2003	CIA	C4-C5	2.86	1.46	1.41
4	A	1003	CIA	C2-C3	2.84	1.45	1.38
4	A	1003	CIA	O32-C31	2.74	1.27	1.22
4	B	2003	CIA	C1-C6	2.39	1.47	1.42
4	B	2003	CIA	C16-C17	2.38	1.55	1.51
4	B	2003	CIA	O32-C31	2.18	1.26	1.22
4	B	2003	CIA	C6-C5	2.10	1.48	1.42
4	A	1003	CIA	C6-C5	2.10	1.48	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1003	CIA	C22-C13-C8	-4.68	104.73	112.78
4	B	2003	CIA	C22-C13-C8	-3.22	107.23	112.78
4	A	1003	CIA	C10-C11-N12	2.84	113.96	109.30
4	A	1003	CIA	C18-N15-C31	2.78	122.42	119.42
4	A	1003	CIA	O20-C17-N12	2.59	125.57	122.28
4	B	2003	CIA	C18-N15-C31	2.32	121.93	119.42
4	B	2003	CIA	C10-C11-C31	-2.25	107.67	110.12

There are no chirality outliers.

There are no torsion outliers.

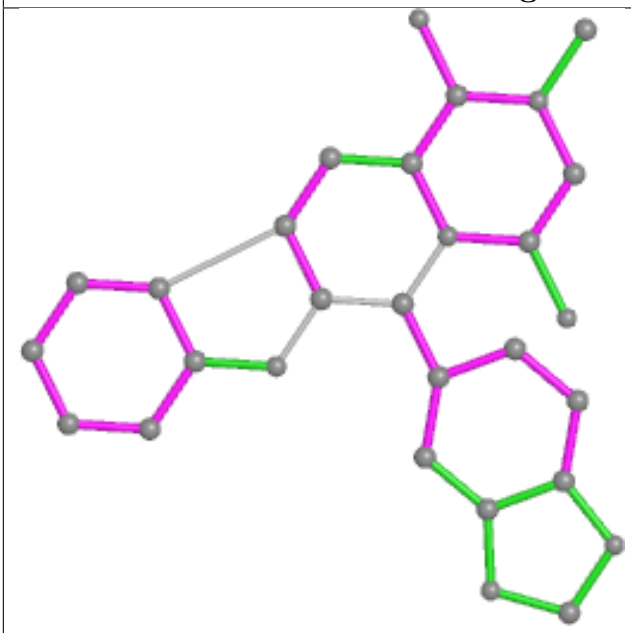
There are no ring outliers.

2 monomers are involved in 9 short contacts:

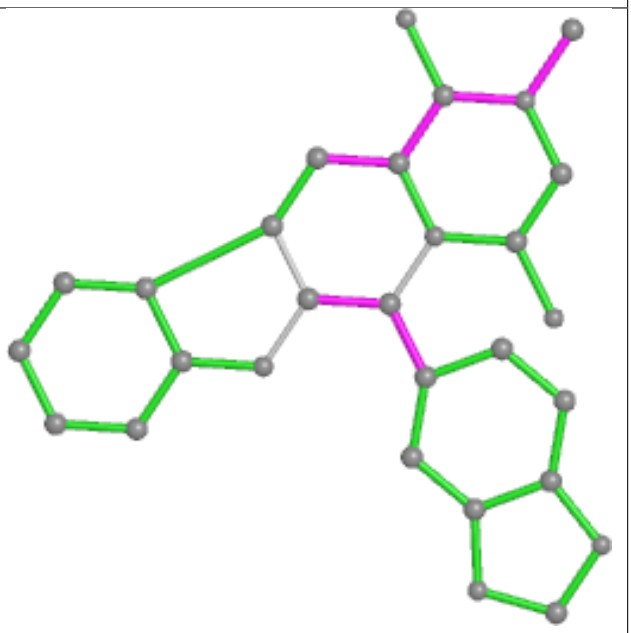
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2003	CIA	1	0
4	A	1003	CIA	8	0

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

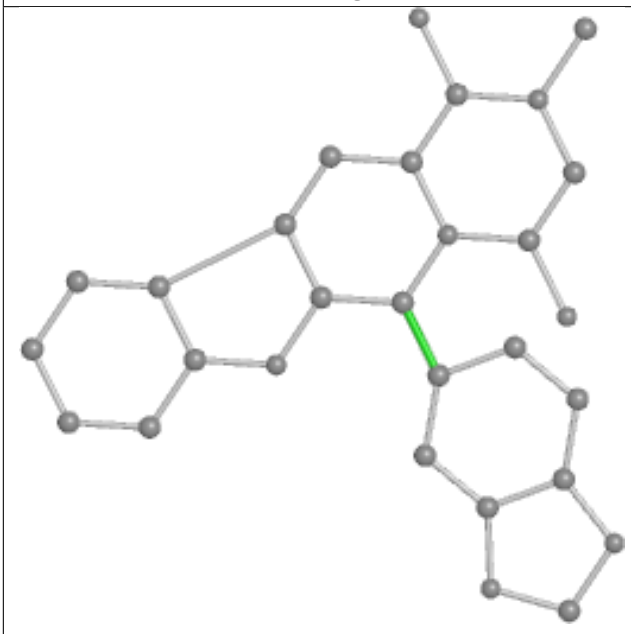
Ligand CIA B 2003



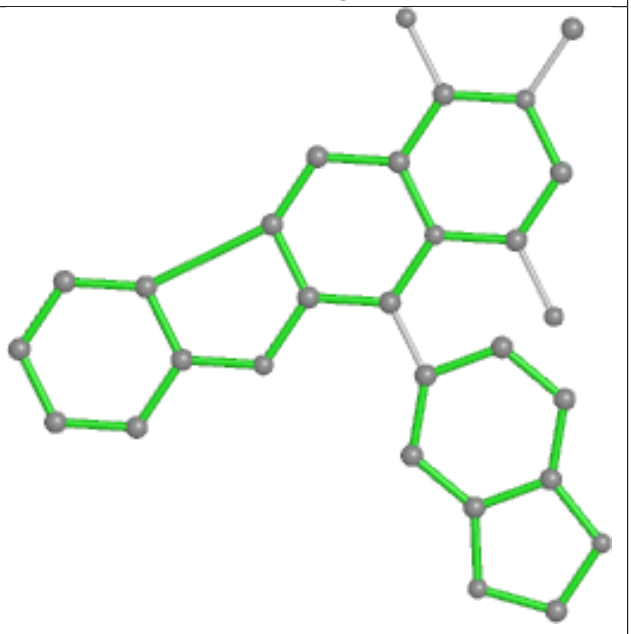
Bond lengths



Bond angles

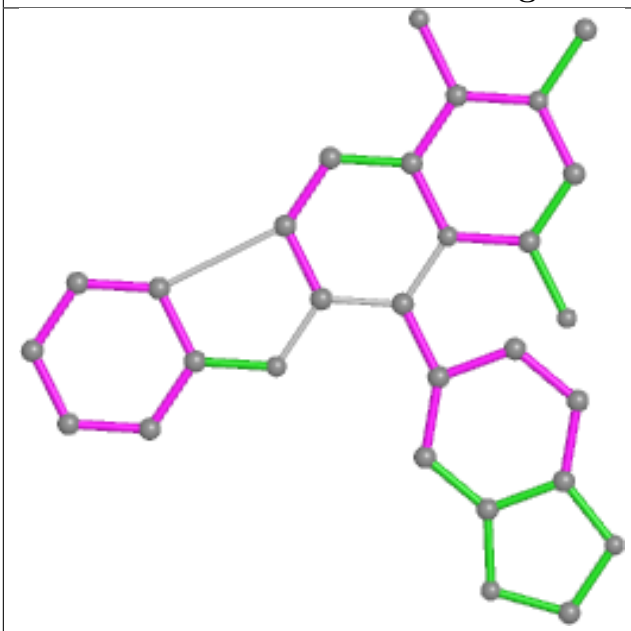


Torsions

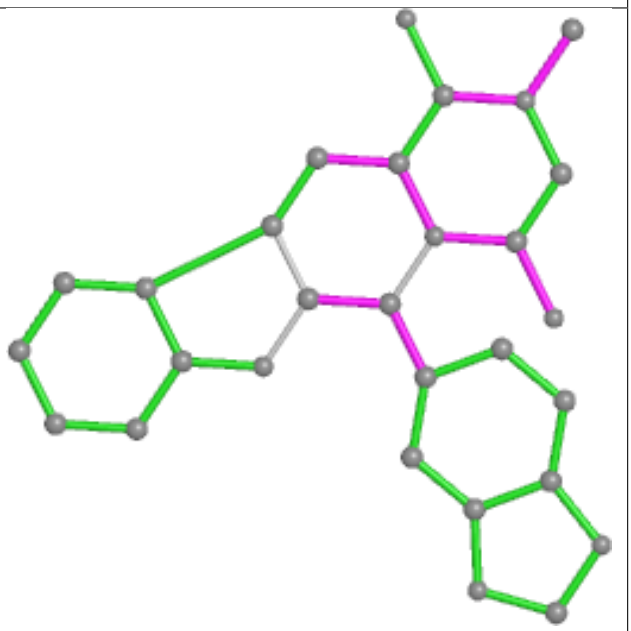


Rings

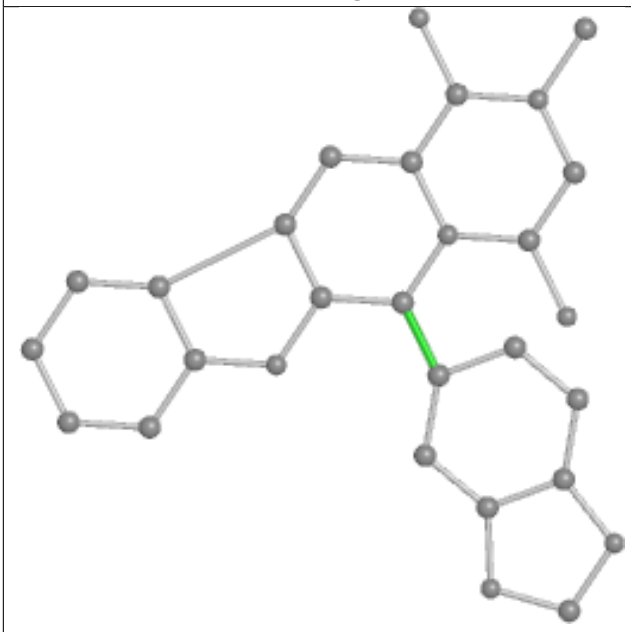
Ligand CIA A 1003



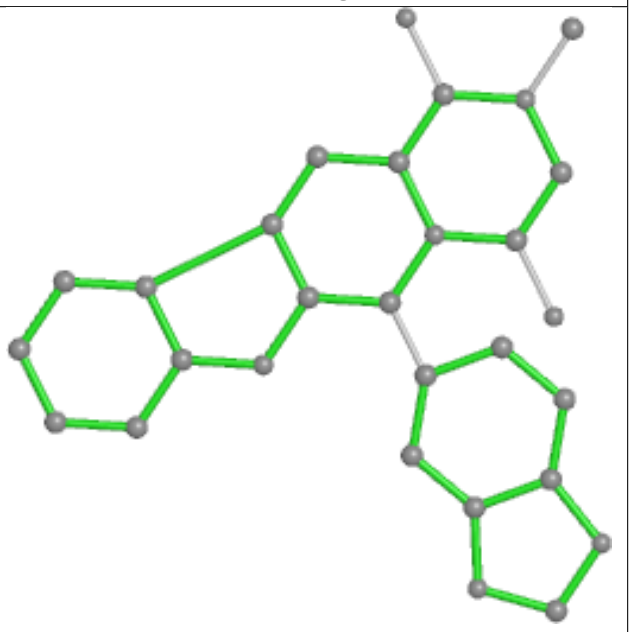
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	313/324 (96%)	-0.24	3 (0%)	82	79	13, 47, 78, 104	0
1	B	313/324 (96%)	-0.20	5 (1%)	72	68	10, 47, 83, 97	0
All	All	626/648 (96%)	-0.22	8 (1%)	77	74	10, 47, 81, 104	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	676	TYR	3.1
1	A	664	TYR	2.8
1	B	608	LYS	2.4
1	B	676	TYR	2.3
1	B	748	ASP	2.2
1	B	706	ILE	2.2
1	A	796	GLU	2.2
1	B	800	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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,

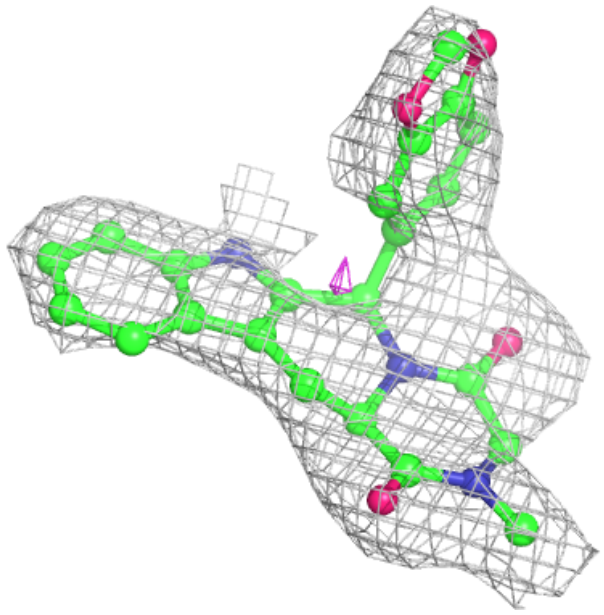
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

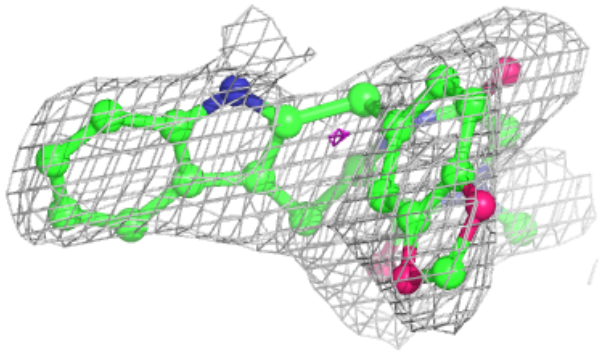
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	2001	1/1	0.81	0.30	105,105,105,105	0
2	ZN	A	1001	1/1	0.93	0.34	105,105,105,105	0
3	MG	B	2002	1/1	0.93	0.14	15,15,15,15	0
4	CIA	A	1003	29/29	0.93	0.18	15,59,81,83	0
4	CIA	B	2003	29/29	0.93	0.19	9,49,77,105	0
3	MG	A	1002	1/1	0.94	0.38	36,36,36,36	0

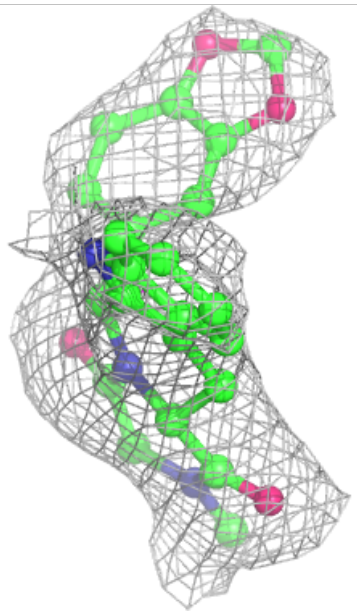
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CIA A 1003:

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

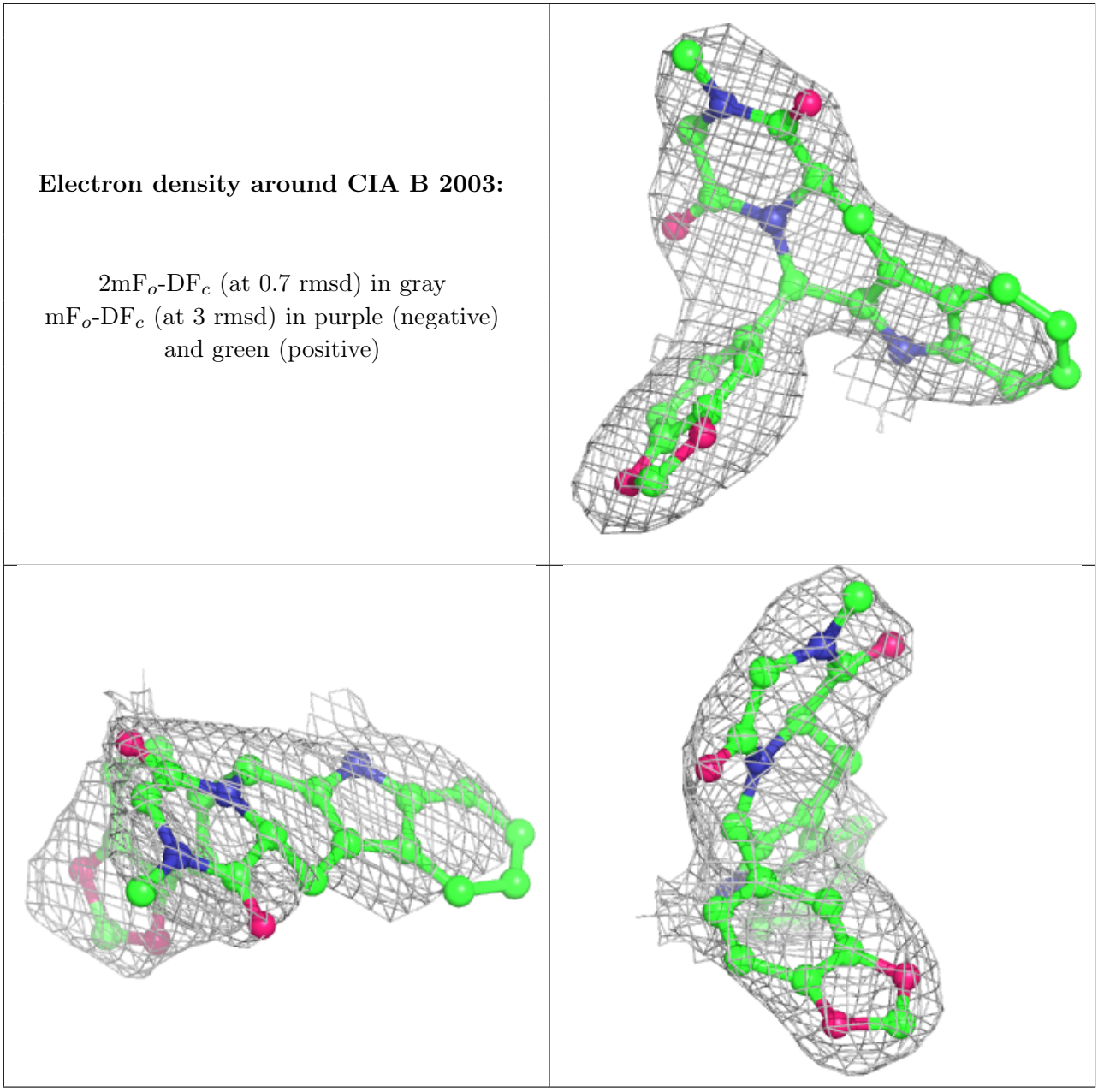






Electron density around CIA B 2003:

$2mF_o$-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

There are no such residues in this entry.