



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:25 PM GMT

PDB ID : 4LL0  
Title : EGFR L858R/T790M in complex with PD168393  
Authors : Yun, C.H.; Eck, M.J.  
Deposited on : 2013-07-09  
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

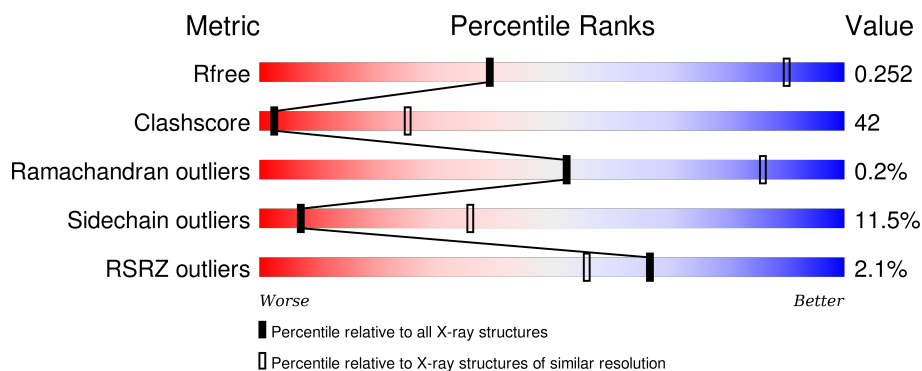
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
$R_{free}$	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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

Mol	Chain	Length	Quality of chain
1	A	331	<div> <div>41%</div> <div>39%</div> <div>7%</div> <div>12%</div> </div>
1	B	331	<div> <div>40%</div> <div>37%</div> <div>7%</div> <div>15%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	YUN	A	1101	-	-	X	X
2	YUN	B	1101	-	-	X	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4552 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.

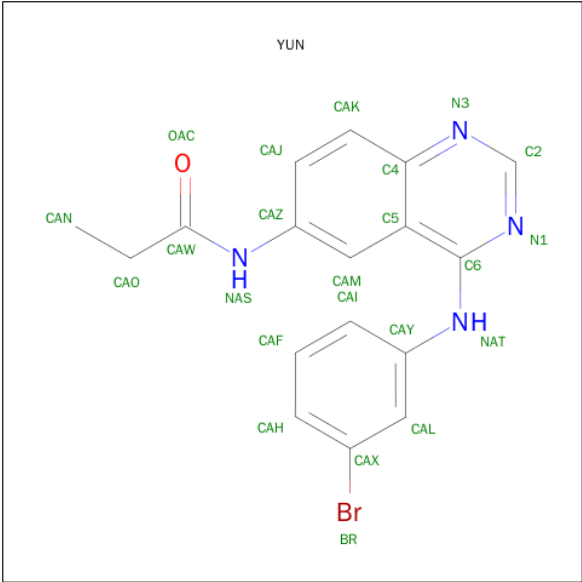
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2287	1471	383	418	15			
1	B	281	Total	C	N	O	S	0	0	0
			2219	1434	371	399	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	EXPRESSION TAG	UNP P00533
A	693	SER	-	EXPRESSION TAG	UNP P00533
A	790	MET	THR	ENGINEERED MUTATION	UNP P00533
A	858	ARG	LEU	ENGINEERED MUTATION	UNP P00533
B	692	GLY	-	EXPRESSION TAG	UNP P00533
B	693	SER	-	EXPRESSION TAG	UNP P00533
B	790	MET	THR	ENGINEERED MUTATION	UNP P00533
B	858	ARG	LEU	ENGINEERED MUTATION	UNP P00533

- Molecule 2 is N-{4-[(3-BROMOPHENYL)AMINO]QUINAZOLIN-6-YL}PROPANAMIDE (three-letter code: YUN) (formula: C<sub>17</sub>H<sub>15</sub>BrN<sub>4</sub>O).

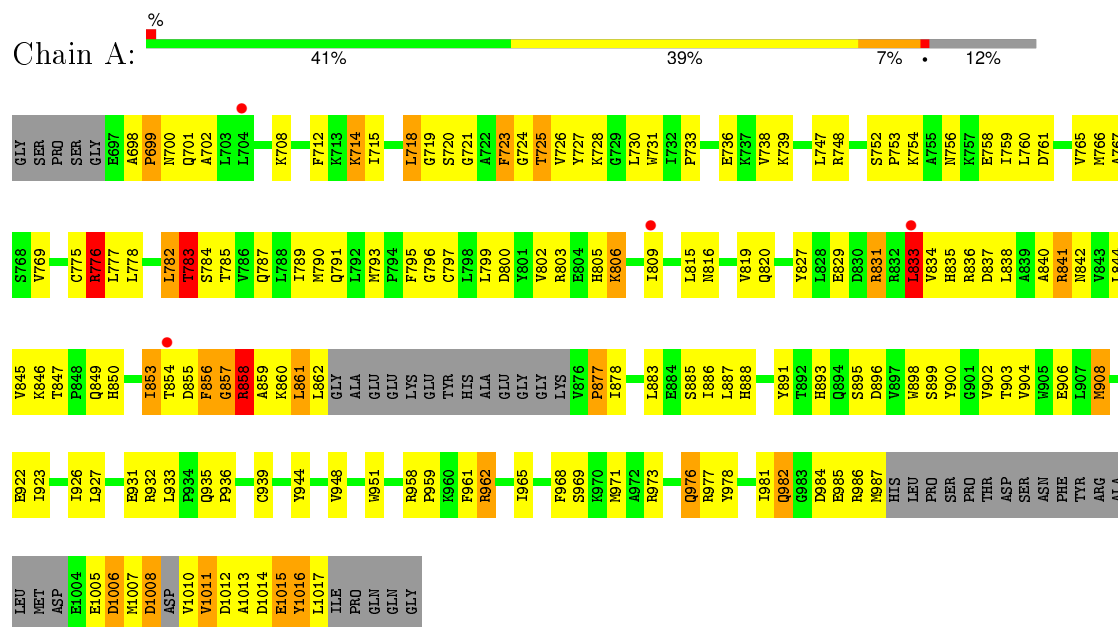


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			23	1	17	4	1		
2	B	1	Total	Br	C	N	O	0	0
			23	1	17	4	1		

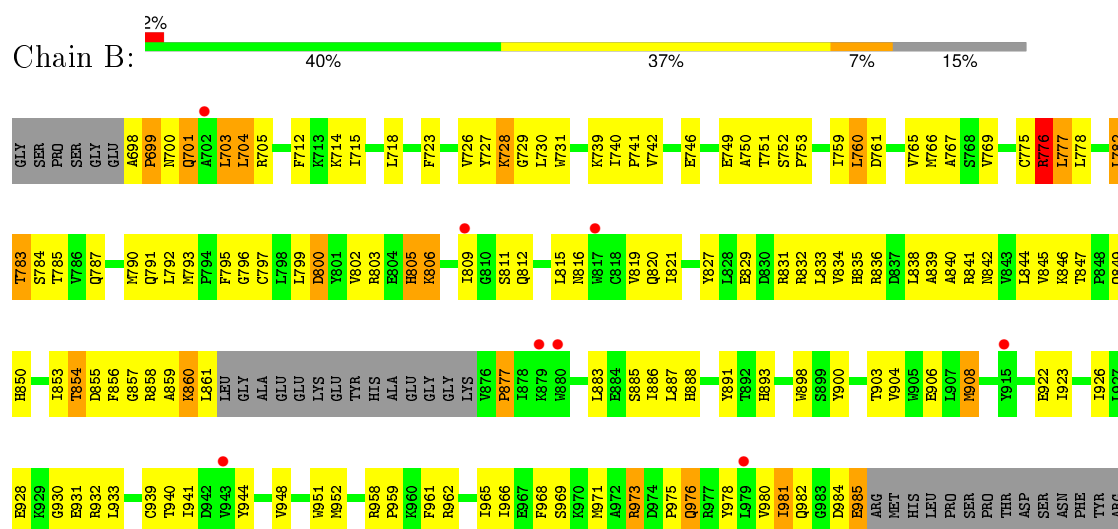
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Epidermal growth factor receptor



#### • Molecule 1: Epidermal growth factor receptor



ALA	LEU	MET	ASP	GLU	GLU	ASP	MET	ASP	ASP	ASP	VAL	V1011	D1012	A1013	D1014	E1015	Y1016	L1017	I1E	PRO	GLN	GLN	GLY
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.64Å 72.71Å 167.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 4.00 49.59 – 3.99	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.60-4.00) 95.5 (49.59-3.99)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 4.00Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.238 , 0.257 0.236 , 0.252	Depositor DCC
$R_{free}$ test set	334 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	200.5	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 231.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 6485 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	257.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

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	0.69	1/2334 (0.0%)	1.10	20/3163 (0.6%)
1	B	0.66	0/2267	1.00	13/3073 (0.4%)
All	All	0.68	1/4601 (0.0%)	1.05	33/6236 (0.5%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	858	ARG	N-CA	-5.18	1.35	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	776	ARG	NE-CZ-NH2	-13.49	113.55	120.30
1	A	962	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	A	831	ARG	NE-CZ-NH1	-12.82	113.89	120.30
1	B	776	ARG	NE-CZ-NH1	-12.52	114.04	120.30
1	A	962	ARG	NE-CZ-NH1	11.95	126.27	120.30
1	A	831	ARG	NE-CZ-NH2	11.65	126.12	120.30
1	A	776	ARG	NE-CZ-NH1	11.56	126.08	120.30
1	B	841	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	B	776	ARG	NE-CZ-NH2	11.07	125.83	120.30
1	B	841	ARG	NE-CZ-NH1	11.00	125.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	841	ARG	NE-CZ-NH1	-9.10	115.75	120.30
1	A	841	ARG	NE-CZ-NH2	8.46	124.53	120.30
1	A	833	LEU	CB-CG-CD2	-7.10	98.94	111.00
1	A	857	GLY	N-CA-C	-6.93	95.78	113.10
1	A	962	ARG	CD-NE-CZ	6.71	132.99	123.60
1	A	861	LEU	CA-CB-CG	6.55	130.37	115.30
1	A	831	ARG	CD-NE-CZ	6.45	132.63	123.60
1	B	704	LEU	CB-CG-CD1	-6.44	100.06	111.00
1	A	783	THR	N-CA-C	-6.05	94.66	111.00
1	A	857	GLY	C-N-CA	-5.85	107.07	121.70
1	A	782	LEU	CA-CB-CG	-5.66	102.29	115.30
1	B	841	ARG	CD-NE-CZ	5.61	131.46	123.60
1	B	782	LEU	CA-CB-CG	-5.59	102.43	115.30
1	A	776	ARG	CD-NE-CZ	5.54	131.36	123.60
1	B	760	LEU	CA-CB-CG	-5.33	103.04	115.30
1	B	776	ARG	CD-NE-CZ	5.32	131.04	123.60
1	B	728	LYS	N-CA-C	-5.30	96.68	111.00
1	A	718	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	A	721	GLY	N-CA-C	-5.14	100.24	113.10
1	B	783	THR	N-CA-C	-5.13	97.14	111.00
1	A	728	LYS	N-CA-C	-5.09	97.27	111.00
1	B	704	LEU	CA-CB-CG	-5.04	103.70	115.30
1	B	854	THR	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	856	PHE	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2287	0	2278	207	0
1	B	2219	0	2241	171	0
2	A	23	0	14	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	23	0	14	7	0
All	All	4552	0	4547	379	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 42.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:ARG:CB	1:B:860:LYS:HE2	1.60	1.32
1:B:860:LYS:HE3	1:B:891:TYR:CD2	1.69	1.27
1:B:836:ARG:CB	1:B:860:LYS:CE	2.25	1.14
1:A:982:GLN:OE1	1:A:982:GLN:HA	1.44	1.13
1:A:860:LYS:NZ	1:A:891:TYR:HD2	1.46	1.12
1:B:698:ALA:CB	1:B:699:PRO:CD	2.29	1.10
1:A:833:LEU:HD23	1:A:834:VAL:N	1.66	1.10
1:B:698:ALA:HB1	1:B:699:PRO:HD3	1.26	1.08
1:B:698:ALA:CB	1:B:699:PRO:HD3	1.88	1.00
1:A:724:GLY:O	1:A:725:THR:HG22	1.60	1.00
1:B:1012:ASP:HB2	1:B:1015:GLU:HG3	1.45	0.98
1:A:860:LYS:NZ	1:A:891:TYR:CD2	2.23	0.98
1:B:860:LYS:CE	1:B:891:TYR:CD2	2.49	0.96
1:A:718:LEU:HB2	1:A:726:VAL:CG1	1.95	0.96
1:A:853:ILE:N	1:A:853:ILE:CD1	2.30	0.95
1:A:853:ILE:HD12	1:A:853:ILE:N	1.80	0.94
1:A:726:VAL:CG1	1:A:727:TYR:N	2.30	0.94
1:B:833:LEU:HG	1:B:861:LEU:HD13	1.48	0.93
1:A:1011:VAL:CG1	1:A:1015:GLU:HG2	1.98	0.93
1:A:708:LYS:HB3	1:B:931:GLU:HB2	1.51	0.92
2:A:1101:YUN:H1	2:A:1101:YUN:N1	1.84	0.91
2:B:1101:YUN:H1	2:B:1101:YUN:N1	1.84	0.91
1:A:1011:VAL:HG11	1:A:1015:GLU:HG2	1.50	0.90
1:A:718:LEU:CB	1:A:726:VAL:HG11	2.01	0.90
1:B:795:PHE:HB2	1:B:845:VAL:HB	1.54	0.90
1:B:698:ALA:HB3	1:B:699:PRO:CD	2.02	0.89
1:A:739:LYS:O	1:A:1010:VAL:HA	1.73	0.89
1:A:753:PRO:CD	1:A:754:LYS:H	1.86	0.88
1:B:1016:TYR:O	1:B:1017:LEU:HD23	1.74	0.88
1:B:698:ALA:HB1	1:B:699:PRO:CD	1.98	0.87
1:B:698:ALA:HB3	1:B:699:PRO:HD2	1.56	0.86
2:A:1101:YUN:H6	2:A:1101:YUN:OAC	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1101:YUN:H6	2:B:1101:YUN:OAC	1.76	0.85
1:B:923:ILE:HA	1:B:926:ILE:HD12	1.59	0.85
1:A:726:VAL:O	1:A:727:TYR:CD1	2.29	0.85
1:A:923:ILE:HA	1:A:926:ILE:HD12	1.59	0.84
1:A:795:PHE:HB2	1:A:845:VAL:HB	1.59	0.84
1:A:712:PHE:HB3	1:A:731:TRP:HA	1.59	0.84
1:A:833:LEU:HD23	1:A:833:LEU:C	1.96	0.83
1:A:854:THR:O	1:A:854:THR:HG23	1.79	0.82
1:A:718:LEU:HB2	1:A:726:VAL:HG12	1.62	0.81
1:B:712:PHE:HB3	1:B:731:TRP:HA	1.60	0.81
1:B:793:MET:H	2:B:1101:YUN:H8	1.46	0.81
1:A:718:LEU:HB2	1:A:726:VAL:HG11	1.59	0.81
1:A:1015:GLU:OE2	1:A:1015:GLU:CA	2.30	0.80
1:B:797:CYS:H	2:B:1101:YUN:H15	1.45	0.80
1:A:726:VAL:HG12	1:A:727:TYR:N	1.96	0.79
1:B:1016:TYR:O	1:B:1017:LEU:CD2	2.30	0.79
1:A:723:PHE:CD1	1:A:723:PHE:N	2.44	0.79
1:B:1016:TYR:O	1:B:1017:LEU:CG	2.30	0.79
1:A:835:HIS:CE1	1:A:855:ASP:O	2.35	0.79
1:A:797:CYS:H	2:A:1101:YUN:H15	1.47	0.79
1:A:753:PRO:HD2	1:A:754:LYS:H	1.46	0.78
1:A:936:PRO:HG2	1:A:939:CYS:SG	2.22	0.78
1:A:877:PRO:HG2	1:A:877:PRO:O	1.81	0.78
1:B:833:LEU:HD23	1:B:834:VAL:N	1.97	0.78
1:B:856:PHE:HD1	1:B:859:ALA:CB	1.97	0.77
1:B:883:LEU:HD12	1:B:886:ILE:HD12	1.66	0.77
1:A:860:LYS:HZ1	1:A:891:TYR:HD2	0.80	0.77
1:A:723:PHE:HB2	1:A:748:ARG:CB	2.15	0.77
1:A:753:PRO:CG	1:A:754:LYS:N	2.48	0.77
1:B:877:PRO:O	1:B:877:PRO:HG2	1.84	0.77
1:B:1012:ASP:HB2	1:B:1015:GLU:CG	2.16	0.76
1:A:853:ILE:CD1	1:A:853:ILE:H	1.97	0.75
1:A:724:GLY:C	1:A:725:THR:CG2	2.54	0.75
1:A:718:LEU:HD22	2:A:1101:YUN:CAO	2.16	0.75
1:A:723:PHE:HD1	1:A:723:PHE:H	1.34	0.74
1:A:853:ILE:HD13	1:A:853:ILE:H	1.52	0.74
1:B:836:ARG:CB	1:B:860:LYS:NZ	2.51	0.74
1:A:726:VAL:HG13	1:A:727:TYR:N	2.01	0.74
1:A:793:MET:H	2:A:1101:YUN:H8	1.51	0.74
1:A:718:LEU:CB	1:A:726:VAL:CG1	2.64	0.74
1:A:833:LEU:CD2	1:A:833:LEU:C	2.56	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1101:YUN:CAL	2:B:1101:YUN:N1	2.47	0.73
1:B:836:ARG:CB	1:B:860:LYS:HZ3	2.03	0.72
1:A:753:PRO:HG2	1:A:754:LYS:N	2.05	0.72
1:B:1016:TYR:O	1:B:1017:LEU:HG	1.89	0.72
1:B:860:LYS:HE3	1:B:891:TYR:HD2	1.49	0.72
1:A:715:ILE:HD11	1:A:730:LEU:HG	1.72	0.71
1:B:715:ILE:HD11	1:B:730:LEU:HG	1.73	0.71
1:A:724:GLY:O	1:A:725:THR:CG2	2.39	0.71
1:A:753:PRO:CD	1:A:754:LYS:N	2.52	0.71
1:A:883:LEU:HD12	1:A:886:ILE:HD12	1.70	0.71
1:A:753:PRO:CG	1:A:754:LYS:H	2.02	0.71
1:A:718:LEU:HB3	1:A:726:VAL:HG11	1.72	0.71
1:B:802:VAL:O	1:B:806:LYS:HB3	1.91	0.70
2:A:1101:YUN:CAL	2:A:1101:YUN:N1	2.47	0.70
1:B:984:ASP:OD1	1:B:984:ASP:C	2.30	0.70
1:A:1015:GLU:OE2	1:A:1015:GLU:HA	1.90	0.69
1:B:819:VAL:HG22	1:B:968:PHE:HB3	1.74	0.69
1:A:976:GLN:NE2	1:A:984:ASP:OD2	2.26	0.69
1:A:738:VAL:CG2	1:A:1011:VAL:HG23	2.24	0.68
1:A:1011:VAL:HG11	1:A:1015:GLU:CG	2.21	0.68
1:B:803:ARG:O	1:B:806:LYS:HG2	1.93	0.68
1:A:877:PRO:CG	1:A:877:PRO:O	2.42	0.68
1:A:819:VAL:HG22	1:A:968:PHE:HB3	1.76	0.68
1:A:835:HIS:O	1:A:836:ARG:CB	2.43	0.67
1:A:783:THR:OG1	1:A:787:GLN:NE2	2.27	0.67
1:A:856:PHE:HB3	1:A:859:ALA:HB2	1.76	0.66
1:A:724:GLY:C	1:A:725:THR:HG22	2.16	0.66
1:B:778:LEU:HD11	1:B:791:GLN:HG2	1.76	0.66
1:A:982:GLN:CA	1:A:982:GLN:OE1	2.30	0.66
1:A:833:LEU:HD23	1:A:834:VAL:H	1.58	0.66
1:A:1016:TYR:O	1:A:1017:LEU:C	2.34	0.66
1:A:802:VAL:O	1:A:806:LYS:HB3	1.96	0.66
1:A:803:ARG:O	1:A:806:LYS:HG2	1.96	0.65
1:A:985:GLU:OE1	1:A:985:GLU:N	2.30	0.65
1:A:726:VAL:HG13	1:A:727:TYR:H	1.61	0.65
1:A:856:PHE:O	1:A:859:ALA:N	2.30	0.65
1:A:1015:GLU:OE2	1:A:1015:GLU:N	2.30	0.65
1:A:791:GLN:CG	1:A:1013:ALA:HB2	2.27	0.65
1:B:858:ARG:HD2	1:B:860:LYS:HZ2	1.61	0.64
1:B:877:PRO:O	1:B:877:PRO:CG	2.45	0.64
1:A:856:PHE:O	1:A:857:GLY:C	2.35	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:LEU:HA	1:A:790:MET:HG3	1.80	0.64
1:B:835:HIS:CE1	1:B:855:ASP:O	2.52	0.63
1:B:856:PHE:HB3	1:B:859:ALA:HB2	1.80	0.63
1:A:815:LEU:O	1:A:819:VAL:HG23	1.99	0.63
1:A:805:HIS:O	1:A:809:ILE:HG13	2.00	0.62
1:B:860:LYS:CE	1:B:891:TYR:HD2	2.09	0.62
1:B:856:PHE:HD1	1:B:859:ALA:HB2	1.64	0.62
1:A:736:GLU:CD	1:A:1016:TYR:HH	2.03	0.61
1:A:833:LEU:CD2	1:A:834:VAL:N	2.54	0.61
1:B:968:PHE:HA	1:B:971:MET:HE3	1.83	0.61
1:A:791:GLN:HB2	1:A:1013:ALA:HB2	1.82	0.61
1:A:933:LEU:HB2	1:A:951:TRP:CH2	2.35	0.61
1:A:1011:VAL:HG12	1:A:1015:GLU:HG2	1.81	0.61
1:A:968:PHE:HA	1:A:971:MET:HE3	1.82	0.61
1:B:856:PHE:CD1	1:B:859:ALA:HB2	2.35	0.61
1:A:738:VAL:HG21	1:A:1011:VAL:HG23	1.83	0.61
1:B:712:PHE:CB	1:B:731:TRP:HA	2.31	0.61
1:A:856:PHE:O	1:A:859:ALA:HB2	2.01	0.60
1:A:844:LEU:CD1	1:A:854:THR:HG21	2.31	0.60
1:A:1014:ASP:OD2	1:A:1014:ASP:N	2.33	0.60
1:B:858:ARG:O	1:B:859:ALA:HB3	2.01	0.60
1:B:903:THR:O	1:B:906:GLU:HB2	2.02	0.59
1:A:835:HIS:NE2	1:A:855:ASP:O	2.35	0.59
1:A:856:PHE:O	1:A:858:ARG:N	2.36	0.59
1:B:749:GLU:O	1:B:750:ALA:C	2.41	0.59
1:B:815:LEU:O	1:B:819:VAL:HG23	2.03	0.59
1:B:819:VAL:HG22	1:B:968:PHE:CB	2.33	0.59
1:B:856:PHE:HD1	1:B:859:ALA:HB1	1.65	0.59
1:B:751:THR:O	1:B:751:THR:HG23	2.02	0.59
1:B:718:LEU:HD11	1:B:728:LYS:HB2	1.85	0.59
1:B:829:GLU:HA	1:B:893:HIS:CE1	2.38	0.58
1:B:699:PRO:O	1:B:699:PRO:CG	2.51	0.58
1:A:723:PHE:CD1	1:A:723:PHE:O	2.56	0.58
1:B:777:LEU:HA	1:B:790:MET:HG3	1.85	0.58
1:B:844:LEU:CD1	1:B:854:THR:HG21	2.33	0.58
1:A:908:MET:HG2	1:A:939:CYS:SG	2.43	0.58
1:B:860:LYS:NZ	1:B:891:TYR:CE2	2.72	0.58
1:A:753:PRO:HG2	1:A:754:LYS:H	1.65	0.58
1:B:831:ARG:C	1:B:832:ARG:HG2	2.24	0.58
1:A:718:LEU:HD22	2:A:1101:YUN:H12	1.86	0.58
1:A:791:GLN:CD	1:A:1013:ALA:HB3	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:HIS:O	1:B:809:ILE:HG13	2.02	0.58
1:B:933:LEU:HB2	1:B:951:TRP:CH2	2.38	0.57
1:A:712:PHE:CB	1:A:731:TRP:HA	2.32	0.57
1:A:931:GLU:O	1:A:932:ARG:HG2	2.05	0.57
1:A:791:GLN:CD	1:A:1013:ALA:CB	2.74	0.57
1:B:699:PRO:O	1:B:699:PRO:CD	2.52	0.56
1:B:833:LEU:HG	1:B:861:LEU:CD1	2.30	0.56
1:A:923:ILE:HD13	1:A:926:ILE:HD12	1.86	0.56
1:A:855:ASP:C	1:A:856:PHE:HD2	2.08	0.56
1:A:778:LEU:HD11	1:A:791:GLN:HB2	1.87	0.56
1:A:853:ILE:HG22	1:A:854:THR:N	2.20	0.56
1:A:736:GLU:O	1:A:738:VAL:HG12	2.06	0.56
1:A:922:GLU:O	1:A:926:ILE:HG13	2.06	0.56
1:B:746:GLU:HA	1:B:787:GLN:HG2	1.87	0.56
1:A:898:TRP:CD1	1:A:898:TRP:C	2.79	0.56
1:B:795:PHE:CE1	1:B:847:THR:HA	2.40	0.55
1:A:726:VAL:O	1:A:727:TYR:CG	2.60	0.55
1:B:976:GLN:NE2	1:B:984:ASP:OD2	2.40	0.55
1:A:829:GLU:HA	1:A:893:HIS:CE1	2.42	0.55
1:B:776:ARG:HG3	1:B:776:ARG:O	2.05	0.55
2:B:1101:YUN:CAM	2:B:1101:YUN:OAC	2.46	0.55
1:B:860:LYS:CD	1:B:891:TYR:HD2	2.20	0.55
1:A:819:VAL:HG22	1:A:968:PHE:CB	2.37	0.55
1:B:769:VAL:HB	1:B:827:TYR:HE2	1.70	0.54
1:B:846:LYS:HD3	1:B:850:HIS:ND1	2.23	0.54
1:A:718:LEU:CD2	2:A:1101:YUN:H11	2.36	0.54
1:A:723:PHE:HD1	1:A:723:PHE:N	1.95	0.54
2:A:1101:YUN:CAM	2:A:1101:YUN:OAC	2.46	0.54
1:A:714:LYS:HD3	1:A:727:TYR:CD2	2.42	0.54
1:A:775:CYS:SG	1:A:854:THR:HB	2.47	0.54
1:B:1012:ASP:CB	1:B:1015:GLU:HB2	2.38	0.54
1:B:703:LEU:HD23	1:B:703:LEU:H	1.73	0.54
1:A:718:LEU:HD13	2:A:1101:YUN:CAW	2.38	0.54
1:A:766:MET:HB3	1:A:777:LEU:HB2	1.89	0.54
1:B:699:PRO:O	1:B:699:PRO:HG2	2.06	0.54
1:B:944:TYR:O	1:B:948:VAL:HG23	2.07	0.54
1:A:795:PHE:CE1	1:A:847:THR:HA	2.43	0.53
1:B:969:SER:O	1:B:973:ARG:HG2	2.09	0.53
1:A:791:GLN:CB	1:A:1013:ALA:HB2	2.39	0.53
1:B:898:TRP:C	1:B:898:TRP:CD1	2.81	0.53
1:B:726:VAL:HG12	1:B:727:TYR:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:THR:O	1:A:906:GLU:HB2	2.09	0.53
1:B:858:ARG:HB3	1:B:860:LYS:HG3	1.90	0.52
1:A:723:PHE:CB	1:A:748:ARG:CB	2.86	0.52
1:B:860:LYS:CE	1:B:891:TYR:CE2	2.91	0.52
1:A:723:PHE:HD1	1:A:723:PHE:O	1.93	0.52
1:A:1011:VAL:CG1	1:A:1015:GLU:CG	2.79	0.52
1:A:718:LEU:CD2	2:A:1101:YUN:CAO	2.87	0.52
1:B:887:LEU:HB3	1:B:888:HIS:CE1	2.44	0.52
1:B:1012:ASP:CB	1:B:1015:GLU:HG3	2.31	0.52
1:A:844:LEU:HD11	1:A:854:THR:HG21	1.91	0.52
1:B:767:ALA:HB2	1:B:777:LEU:HD23	1.91	0.52
1:B:829:GLU:HG3	1:B:893:HIS:CD2	2.45	0.52
1:B:923:ILE:HD13	1:B:926:ILE:HD12	1.92	0.52
1:B:856:PHE:CB	1:B:859:ALA:HB2	2.40	0.52
1:A:753:PRO:O	1:A:754:LYS:C	2.48	0.52
1:A:944:TYR:O	1:A:948:VAL:HG23	2.10	0.52
1:B:766:MET:HB3	1:B:777:LEU:HB2	1.91	0.51
1:B:858:ARG:HD2	1:B:860:LYS:NZ	2.25	0.51
1:B:1012:ASP:HB3	1:B:1015:GLU:H	1.75	0.51
1:A:702:ALA:O	1:B:941:ILE:HB	2.11	0.51
1:A:782:LEU:O	1:B:930:GLY:HA2	2.10	0.51
1:A:837:ASP:OD2	1:A:858:ARG:HD3	2.11	0.51
1:A:724:GLY:C	1:A:725:THR:HG23	2.30	0.51
1:B:835:HIS:NE2	1:B:855:ASP:O	2.43	0.51
1:B:740:ILE:HG21	1:B:1013:ALA:HB2	1.93	0.51
1:A:767:ALA:HB2	1:A:777:LEU:HD23	1.93	0.51
1:B:833:LEU:C	1:B:833:LEU:HD23	2.30	0.51
1:B:860:LYS:HD3	1:B:891:TYR:HD2	1.77	0.50
1:A:860:LYS:NZ	1:A:860:LYS:HB2	2.27	0.50
1:B:833:LEU:HA	1:B:861:LEU:HD12	1.93	0.50
1:B:1012:ASP:HB2	1:B:1015:GLU:HB2	1.93	0.50
1:B:984:ASP:O	1:B:984:ASP:OD1	2.29	0.50
1:A:782:LEU:HD21	1:B:952:MET:CE	2.41	0.50
1:A:736:GLU:OE2	1:A:1016:TYR:OH	2.29	0.50
1:B:700:ASN:OD1	1:B:700:ASN:O	2.29	0.50
1:B:701:GLN:O	1:B:701:GLN:OE1	2.30	0.50
1:A:1012:ASP:OD1	1:A:1014:ASP:OD2	2.30	0.50
1:B:829:GLU:HG3	1:B:893:HIS:CG	2.46	0.50
1:B:860:LYS:HE3	1:B:891:TYR:CE2	2.39	0.50
1:A:856:PHE:O	1:A:859:ALA:CB	2.60	0.50
1:A:1011:VAL:HG11	1:A:1015:GLU:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:CYS:SG	1:B:854:THR:HB	2.52	0.50
1:B:1012:ASP:O	1:B:1015:GLU:HB2	2.11	0.49
1:A:1008:ASP:HB2	1:A:1010:VAL:HG23	1.93	0.49
1:A:698:ALA:HB1	1:A:699:PRO:HD2	1.93	0.49
1:A:736:GLU:OE1	1:A:1016:TYR:OH	2.30	0.49
1:B:847:THR:O	1:B:849:GLN:N	2.46	0.49
1:A:829:GLU:HG3	1:A:893:HIS:CD2	2.48	0.49
1:A:986:ARG:O	1:A:987:MET:O	2.30	0.49
1:B:855:ASP:OD2	1:B:856:PHE:N	2.45	0.49
1:A:778:LEU:HG	1:A:790:MET:HA	1.93	0.49
1:A:736:GLU:CD	1:A:1016:TYR:OH	2.49	0.49
1:B:796:GLY:O	1:B:845:VAL:HG23	2.12	0.49
1:A:887:LEU:HB3	1:A:888:HIS:CE1	2.48	0.49
1:A:769:VAL:HB	1:A:827:TYR:HE2	1.78	0.49
1:B:847:THR:C	1:B:849:GLN:N	2.66	0.48
1:A:847:THR:C	1:A:849:GLN:H	2.16	0.48
1:B:1012:ASP:HB2	1:B:1015:GLU:CB	2.43	0.48
1:A:714:LYS:HD3	1:A:727:TYR:HD2	1.79	0.48
1:B:728:LYS:HE2	1:B:792:LEU:HD21	1.95	0.48
1:B:908:MET:HG2	1:B:939:CYS:SG	2.53	0.48
1:A:719:GLY:O	1:A:720:SER:OG	2.30	0.48
1:A:747:LEU:CB	1:A:759:ILE:HD12	2.43	0.48
1:B:847:THR:C	1:B:849:GLN:H	2.15	0.48
1:B:883:LEU:HA	1:B:883:LEU:HD12	1.68	0.48
1:B:740:ILE:CG2	1:B:1013:ALA:HB2	2.44	0.47
1:A:847:THR:C	1:A:849:GLN:N	2.67	0.47
1:B:799:LEU:O	1:B:802:VAL:HG22	2.15	0.47
1:B:704:LEU:HD12	1:B:704:LEU:HA	1.16	0.47
1:B:778:LEU:HD11	1:B:791:GLN:CG	2.44	0.47
1:A:969:SER:O	1:A:973:ARG:HG2	2.13	0.47
1:A:797:CYS:HB2	1:A:800:ASP:OD1	2.14	0.47
1:B:797:CYS:HB2	1:B:800:ASP:OD1	2.13	0.47
1:A:856:PHE:C	1:A:858:ARG:N	2.57	0.47
1:A:837:ASP:HB2	1:A:858:ARG:CG	2.43	0.47
1:B:700:ASN:O	1:B:700:ASN:CG	2.52	0.47
1:B:856:PHE:O	1:B:857:GLY:C	2.52	0.47
1:A:776:ARG:HG3	1:A:776:ARG:O	2.15	0.47
1:B:985:GLU:OE1	1:B:985:GLU:O	2.33	0.47
1:A:1007:MET:O	1:A:1008:ASP:C	2.54	0.47
1:A:827:TYR:O	1:A:831:ARG:HG3	2.15	0.46
1:A:853:ILE:CG2	1:A:854:THR:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:922:GLU:O	1:B:926:ILE:HG13	2.15	0.46
1:A:789:ILE:HG22	1:A:790:MET:N	2.30	0.46
1:B:844:LEU:HD11	1:B:854:THR:HG21	1.97	0.46
1:A:898:TRP:CD1	1:A:898:TRP:O	2.68	0.46
1:A:756:ASN:HA	1:A:759:ILE:HG22	1.96	0.46
1:A:791:GLN:HB2	1:A:1013:ALA:CB	2.45	0.46
1:A:846:LYS:HD3	1:A:850:HIS:ND1	2.30	0.46
1:B:752:SER:HB2	1:B:753:PRO:CD	2.45	0.46
1:A:854:THR:O	1:A:854:THR:CG2	2.48	0.46
1:A:971:MET:HA	1:A:978:TYR:CE1	2.50	0.46
1:A:799:LEU:O	1:A:802:VAL:HG22	2.15	0.46
1:A:961:PHE:O	1:A:965:ILE:HG13	2.16	0.46
1:A:738:VAL:HG23	1:A:1011:VAL:HG23	1.98	0.46
1:A:986:ARG:O	1:A:987:MET:C	2.54	0.46
1:A:1014:ASP:O	1:A:1015:GLU:C	2.54	0.45
1:A:837:ASP:HB2	1:A:858:ARG:HG2	1.98	0.45
1:B:769:VAL:O	1:B:769:VAL:HG23	2.16	0.45
1:A:861:LEU:O	1:A:862:LEU:CB	2.65	0.45
1:B:985:GLU:CA	1:B:985:GLU:OE1	2.63	0.45
1:A:885:SER:HB3	1:A:891:TYR:HE1	1.81	0.45
1:A:984:ASP:HB3	1:A:985:GLU:OE1	2.16	0.45
1:B:860:LYS:H	1:B:860:LYS:HG3	1.55	0.45
1:B:854:THR:OG1	1:B:854:THR:O	2.26	0.45
1:A:829:GLU:HG3	1:A:893:HIS:CG	2.52	0.45
1:A:736:GLU:O	1:A:738:VAL:N	2.50	0.44
1:A:760:LEU:HD23	1:A:760:LEU:HA	1.79	0.44
1:B:858:ARG:HB3	1:B:860:LYS:CG	2.48	0.44
1:A:789:ILE:N	1:A:789:ILE:HD12	2.32	0.44
1:B:742:VAL:O	1:B:792:LEU:HB2	2.17	0.44
1:A:931:GLU:C	1:A:932:ARG:HG2	2.37	0.44
1:B:1013:ALA:O	1:B:1016:TYR:N	2.49	0.44
1:A:718:LEU:HD21	2:A:1101:YUN:H11	2.00	0.44
1:A:986:ARG:H	1:A:986:ARG:HG3	1.40	0.44
1:A:923:ILE:HD13	1:A:926:ILE:CD1	2.47	0.44
1:A:761:ASP:O	1:A:765:VAL:HG23	2.17	0.44
1:A:733:PRO:HG2	1:A:1016:TYR:HE2	1.82	0.44
1:A:847:THR:O	1:A:849:GLN:N	2.51	0.44
1:A:701:GLN:CD	1:B:980:VAL:HG21	2.38	0.44
1:A:840:ALA:C	1:A:842:ASN:H	2.21	0.44
1:B:700:ASN:OD1	1:B:700:ASN:C	2.55	0.44
1:A:860:LYS:HE2	1:A:891:TYR:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:LYS:O	1:B:1011:VAL:HG22	2.18	0.43
1:A:708:LYS:HD3	1:B:931:GLU:OE2	2.18	0.43
1:A:753:PRO:O	1:A:756:ASN:N	2.51	0.43
1:A:796:GLY:O	1:A:845:VAL:HG23	2.17	0.43
1:B:838:LEU:O	1:B:839:ALA:HB2	2.19	0.43
1:B:816:ASN:O	1:B:820:GLN:HG3	2.18	0.43
1:B:856:PHE:O	1:B:859:ALA:HB2	2.19	0.43
1:B:1012:ASP:CB	1:B:1015:GLU:CG	2.91	0.43
1:A:789:ILE:CG2	1:A:790:MET:N	2.82	0.43
1:A:883:LEU:HA	1:A:883:LEU:HD12	1.72	0.43
1:B:898:TRP:O	1:B:898:TRP:CD1	2.72	0.43
1:A:958:ARG:HA	1:A:959:PRO:HD3	1.85	0.43
1:A:747:LEU:CB	1:A:759:ILE:CD1	2.97	0.42
1:B:726:VAL:CG1	1:B:727:TYR:N	2.83	0.42
1:B:759:ILE:HG23	1:B:760:LEU:N	2.33	0.42
1:B:844:LEU:HD12	1:B:854:THR:HG21	1.99	0.42
1:B:761:ASP:O	1:B:765:VAL:HG23	2.20	0.42
1:B:812:GLN:NE2	1:B:975:PRO:HG3	2.34	0.42
1:A:816:ASN:O	1:A:820:GLN:HG3	2.20	0.42
1:B:931:GLU:O	1:B:932:ARG:HG2	2.19	0.42
1:B:793:MET:N	2:B:1101:YUN:H8	2.25	0.42
1:A:791:GLN:HG3	1:A:1013:ALA:HB2	2.00	0.42
1:A:726:VAL:HG12	1:A:727:TYR:CA	2.50	0.42
1:B:971:MET:HA	1:B:978:TYR:CE1	2.55	0.42
1:B:861:LEU:O	1:B:861:LEU:HG	2.19	0.41
1:B:778:LEU:HG	1:B:790:MET:HA	2.02	0.41
1:B:840:ALA:C	1:B:842:ASN:H	2.23	0.41
1:B:900:TYR:O	1:B:904:VAL:HG23	2.20	0.41
1:B:856:PHE:O	1:B:858:ARG:N	2.53	0.41
1:A:754:LYS:HE2	1:A:758:GLU:OE2	2.20	0.41
1:B:958:ARG:HA	1:B:959:PRO:HD3	1.89	0.41
1:B:961:PHE:O	1:B:965:ILE:HG13	2.20	0.41
1:A:977:ARG:O	1:A:977:ARG:HG2	2.20	0.41
1:A:902:VAL:HG13	1:A:933:LEU:HD11	2.03	0.41
1:A:718:LEU:HD23	1:A:718:LEU:HA	1.51	0.41
1:B:740:ILE:HD12	1:B:740:ILE:N	2.36	0.41
1:B:928:GLU:O	1:B:930:GLY:N	2.53	0.41
1:B:811:SER:N	1:B:981:ILE:HD11	2.36	0.41
1:B:821:ILE:HG23	1:B:853:ILE:HD11	2.03	0.41
1:B:856:PHE:O	1:B:858:ARG:C	2.59	0.41
1:B:760:LEU:HD23	1:B:760:LEU:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:CYS:HA	1:B:844:LEU:HD23	2.01	0.41
1:A:700:ASN:O	1:B:940:THR:HB	2.21	0.41
1:B:856:PHE:O	1:B:859:ALA:CB	2.69	0.41
1:B:885:SER:HG	1:B:891:TYR:HD1	1.66	0.41
1:B:718:LEU:HD23	1:B:718:LEU:HA	1.78	0.41
1:A:769:VAL:HG23	1:A:769:VAL:O	2.21	0.41
1:A:896:ASP:O	1:A:899:SER:N	2.54	0.41
1:A:1011:VAL:CG1	1:A:1015:GLU:HB2	2.51	0.41
1:B:740:ILE:HA	1:B:741:PRO:HD3	1.94	0.41
1:B:931:GLU:C	1:B:932:ARG:HG2	2.41	0.40
1:A:855:ASP:C	1:A:856:PHE:CD2	2.91	0.40
1:B:715:ILE:HG13	1:B:729:GLY:HA2	2.02	0.40
1:A:878:ILE:HD13	1:A:878:ILE:HA	1.80	0.40
1:A:1011:VAL:CG1	1:A:1015:GLU:CB	2.99	0.40
1:A:935:GLN:HA	1:A:936:PRO:HD3	1.87	0.40
1:A:927:LEU:CD2	1:A:932:ARG:HD3	2.51	0.40
1:B:805:HIS:ND1	1:B:805:HIS:N	2.70	0.40
1:B:962:ARG:O	1:B:966:ILE:HD13	2.22	0.40
1:A:900:TYR:O	1:A:904:VAL:HG23	2.21	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	283/331 (86%)	261 (92%)	21 (7%)	1 (0%)	39	79
1	B	275/331 (83%)	256 (93%)	19 (7%)	0	100	100
All	All	558/662 (84%)	517 (93%)	40 (7%)	1 (0%)	52	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1006	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/290 (84%)	217 (89%)	28 (11%)	7	36
1	B	240/290 (83%)	212 (88%)	28 (12%)	7	35
All	All	485/580 (84%)	429 (88%)	56 (12%)	7	36

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	699	PRO
1	A	714	LYS
1	A	723	PHE
1	A	725	THR
1	A	752	SER
1	A	776	ARG
1	A	783	THR
1	A	784	SER
1	A	785	THR
1	A	806	LYS
1	A	833	LEU
1	A	838	LEU
1	A	841	ARG
1	A	853	ILE
1	A	858	ARG
1	A	877	PRO
1	A	895	SER
1	A	908	MET
1	A	962	ARG
1	A	976	GLN
1	A	981	ILE
1	A	982	GLN
1	A	1005	GLU

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Mol	Chain	Res	Type
1	A	1006	ASP
1	A	1008	ASP
1	A	1011	VAL
1	A	1015	GLU
1	A	1016	TYR
1	B	699	PRO
1	B	701	GLN
1	B	703	LEU
1	B	705	ARG
1	B	714	LYS
1	B	723	PHE
1	B	776	ARG
1	B	777	LEU
1	B	782	LEU
1	B	783	THR
1	B	784	SER
1	B	785	THR
1	B	800	ASP
1	B	805	HIS
1	B	806	LYS
1	B	860	LYS
1	B	877	PRO
1	B	908	MET
1	B	973	ARG
1	B	976	GLN
1	B	981	ILE
1	B	982	GLN
1	B	985	GLU
1	B	1011	VAL
1	B	1012	ASP
1	B	1014	ASP
1	B	1016	TYR
1	B	1017	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	701	GLN
1	A	773	HIS
1	A	808	ASN
1	A	893	HIS
1	A	976	GLN

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Mol	Chain	Res	Type
1	B	701	GLN
1	B	756	ASN
1	B	773	HIS
1	B	808	ASN
1	B	893	HIS
1	B	976	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	YUN	A	1101	1	25,25,25	1.67	3 (12%)	34,34,34	2.97	9 (26%)
2	YUN	B	1101	1	25,25,25	1.64	3 (12%)	34,34,34	2.97	10 (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	YUN	A	1101	1	-	0/10/10/10	0/3/3/3
2	YUN	B	1101	1	-	0/10/10/10	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	YUN	C6-C5	-4.61	1.39	1.44
2	B	1101	YUN	CAZ-NAS	-4.60	1.32	1.41
2	A	1101	YUN	CAZ-NAS	-4.50	1.33	1.41
2	B	1101	YUN	C6-C5	-4.22	1.39	1.44
2	B	1101	YUN	CAY-NAT	-3.37	1.33	1.40
2	A	1101	YUN	CAY-NAT	-3.20	1.33	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	YUN	N3-C2-N1	-9.94	121.28	128.89
2	B	1101	YUN	N3-C2-N1	-9.87	121.34	128.89
2	A	1101	YUN	CAM-C5-C6	-6.79	121.27	124.89
2	B	1101	YUN	CAM-C5-C6	-6.63	121.35	124.89
2	B	1101	YUN	C5-C6-N1	-3.84	118.72	121.46
2	A	1101	YUN	C5-C6-N1	-3.67	118.84	121.46
2	A	1101	YUN	CAZ-NAS-CAW	-3.28	121.26	127.47
2	A	1101	YUN	C5-C4-N3	-3.23	119.44	122.88
2	B	1101	YUN	C5-C4-N3	-3.11	119.57	122.88
2	B	1101	YUN	CAZ-NAS-CAW	-3.08	121.62	127.47
2	B	1101	YUN	CAY-NAT-C6	-2.68	122.48	128.40
2	A	1101	YUN	CAY-NAT-C6	-2.59	122.68	128.40
2	B	1101	YUN	CAY-CAL-CAX	2.20	120.96	118.74
2	B	1101	YUN	C6-C5-C4	4.12	118.12	115.77
2	A	1101	YUN	C6-C5-C4	4.20	118.16	115.77
2	B	1101	YUN	C2-N3-C4	5.92	120.66	115.19
2	A	1101	YUN	C2-N3-C4	6.13	120.85	115.19
2	A	1101	YUN	C2-N1-C6	6.81	121.38	116.48
2	B	1101	YUN	C2-N1-C6	7.02	121.54	116.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 19 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	YUN	12	0
2	B	1101	YUN	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	291/331 (87%)	0.13	4 (1%) 78 68	192, 256, 310, 335	1 (0%)
1	B	281/331 (84%)	0.09	8 (2%) 56 44	201, 255, 301, 327	1 (0%)
All	All	572/662 (86%)	0.11	12 (2%) 67 56	192, 256, 307, 335	2 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	704	LEU	3.6
1	B	915	TYR	2.9
1	B	880	TRP	2.8
1	B	879	LYS	2.7
1	B	817	TRP	2.6
1	A	854	THR	2.6
1	B	979	LEU	2.3
1	B	943	VAL	2.3
1	A	809	ILE	2.2
1	B	702	ALA	2.2
1	B	809	ILE	2.1
1	A	833	LEU	2.1

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	YUN	A	1101	23/23	0.83	0.49	0.52	208,256,288,291	0
2	YUN	B	1101	23/23	0.75	0.43	0.49	211,256,286,297	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.