



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:12 AM GMT

PDB ID : 3DQV  
Title : Structural Insights into NEDD8 Activation of Cullin-RING Ligases: Conformational Control of Conjugation  
Authors : Duda, D.M.; Borg, L.A.; Scott, D.C.; Hunt, H.W.; Hammel, M.; Schulman, B.A.  
Deposited on : 2008-07-09  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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

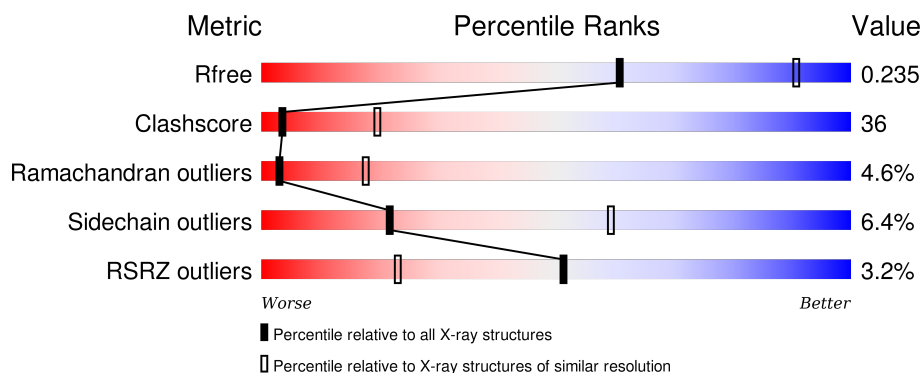
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	81	
1	B	81	
2	C	382	
2	D	382	
3	R	106	

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Mol	Chain	Length	Quality of chain
3	Y	106	<div><div></div><div>18%</div><div>41%</div><div>30%</div><div>9%</div><div>20%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8839 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 NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	Se	1	0	0
			609	382	106	118	3			
1	B	77	Total	C	N	O	Se	0	0	0
			605	380	105	117	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLY	-	INSERTION	UNP Q15843
A	97	SER	-	INSERTION	UNP Q15843
A	98	GLY	-	INSERTION	UNP Q15843
A	99	GLY	-	INSERTION	UNP Q15843
A	100	SER	-	INSERTION	UNP Q15843
A	162	MSE	LEU	CONFLICT	UNP Q15843
B	96	GLY	-	INSERTION	UNP Q15843
B	97	SER	-	INSERTION	UNP Q15843
B	98	GLY	-	INSERTION	UNP Q15843
B	99	GLY	-	INSERTION	UNP Q15843
B	100	SER	-	INSERTION	UNP Q15843
B	162	MSE	LEU	CONFLICT	UNP Q15843

- Molecule 2 is a protein called Cullin-5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	376	Total	C	N	O	S	Se	0	0	0
			3116	1991	540	570	2	13			
2	D	378	Total	C	N	O	S	Se	0	0	0
			3132	1999	544	574	2	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1399	GLY	-	INSERTION	UNP Q93034
C	1400	SER	-	INSERTION	UNP Q93034
C	1407	GLU	LEU	CONFLICT	UNP Q93034
C	1439	LYS	LEU	CONFLICT	UNP Q93034
C	1440	LYS	VAL	CONFLICT	UNP Q93034
D	1399	GLY	-	INSERTION	UNP Q93034
D	1400	SER	-	INSERTION	UNP Q93034
D	1407	GLU	LEU	CONFLICT	UNP Q93034
D	1439	LYS	LEU	CONFLICT	UNP Q93034
D	1440	LYS	VAL	CONFLICT	UNP Q93034

- Molecule 3 is a protein called Rbx1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	R	86	Total	C	N	O	S	Se	10	0	0
			707	448	130	120	8	1			
3	Y	85	Total	C	N	O	S	Se	64	0	0
			664	426	121	108	8	1			

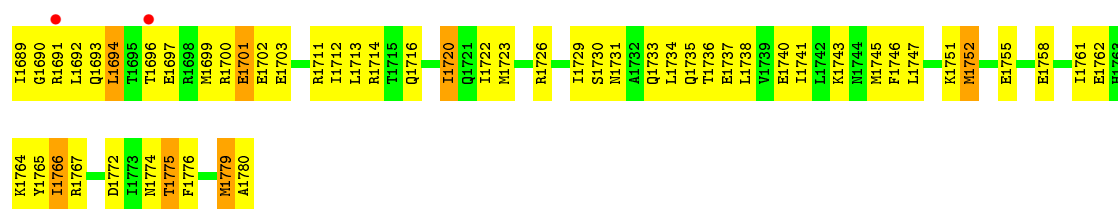
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	3	GLY	-	INSERTION	UNP P62877
R	4	SER	-	INSERTION	UNP P62877
Y	3	GLY	-	INSERTION	UNP P62877
Y	4	SER	-	INSERTION	UNP P62877

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

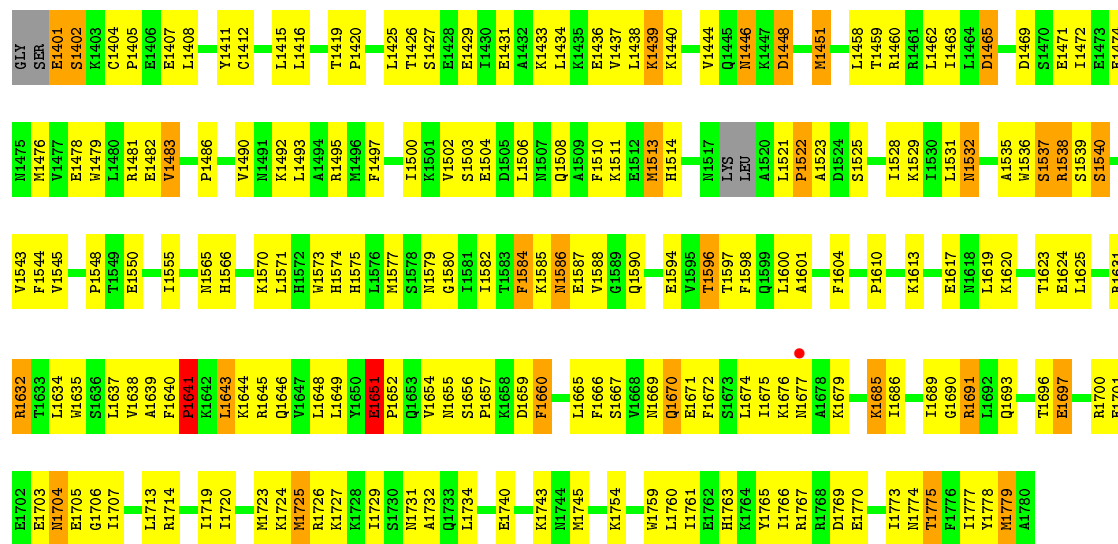
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	3	Total	Zn	0	0
			3	3		
4	Y	3	Total	Zn	0	0
			3	3		





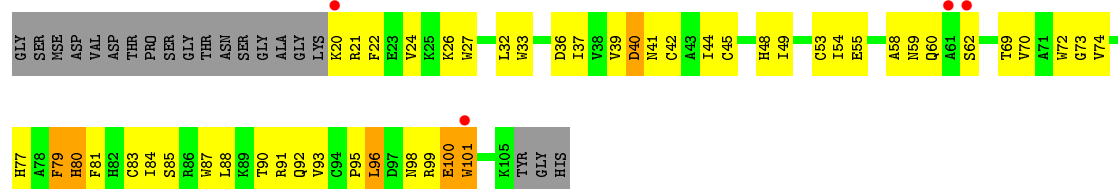
• Molecule 2: Cullin-5

Chain D: 48% 43% 7% ..



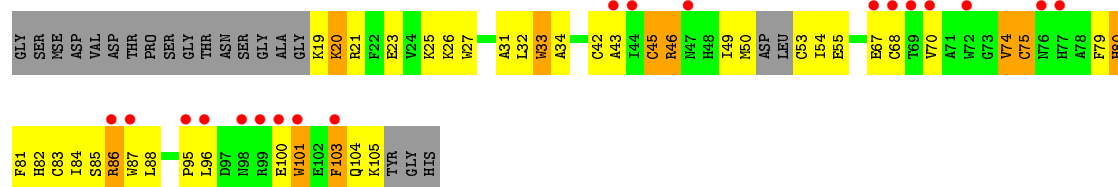
• Molecule 3: Rbx1

Chain R: 4% 35% 41% 6% 19%



• Molecule 3: Rbx1

Chain Y: 18% 41% 30% 9% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.31Å 122.44Å 128.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 29.84 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-3.00) 98.9 (29.84-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.249 , 0.299 0.246 , 0.235	Depositor DCC
$R_{free}$ test set	1439 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.8	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 43.3	EDS
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 28564 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8839	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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 [i](#)

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

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

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	0.48	0/611	0.70	0/811
1	B	0.48	0/607	0.74	0/806
2	C	0.47	0/3157	0.69	0/4220
2	D	0.47	1/3173 (0.0%)	0.69	0/4242
3	R	0.54	0/726	0.71	1/984 (0.1%)
3	Y	0.56	1/681 (0.1%)	0.62	0/923
All	All	0.49	2/8955 (0.0%)	0.69	1/11986 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	101	TRP	CZ3-CH2	-6.42	1.29	1.40
2	D	1724	LYS	CE-NZ	-5.14	1.36	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	40	ASP	CB-CG-OD2	5.41	123.16	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	609	0	641	55	0
1	B	605	0	638	55	0
2	C	3116	0	3205	249	0
2	D	3132	0	3218	198	0
3	R	707	0	659	65	0
3	Y	664	0	605	67	0
4	R	3	0	0	0	0
4	Y	3	0	0	0	0
All	All	8839	0	8966	639	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 36.

All (639) 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)
3:Y:84:ILE:HD13	3:Y:103:PHE:CZ	1.87	1.08
3:Y:49:ILE:HG23	3:Y:70:VAL:HG21	1.35	1.07
2:C:1481:ARG:HB2	2:C:1490:VAL:HG11	1.37	1.06
1:A:152:ASP:H	2:D:1774:ASN:HD21	1.06	1.01
2:C:1689:ILE:HG22	2:C:1690:GLY:H	1.28	0.97
2:C:1403:LYS:HD3	2:C:1404:CYS:N	1.80	0.96
2:D:1462:LEU:HB3	2:D:1500:ILE:HD11	1.47	0.95
2:C:1651:GLU:HB3	2:C:1652:PRO:CD	1.97	0.94
3:Y:74:VAL:HG12	3:Y:75:CYS:H	1.34	0.93
2:D:1654:VAL:HG12	2:D:1656:SER:H	1.30	0.93
2:D:1463:ILE:CD1	2:D:1577:MSE:HE3	2.01	0.91
2:D:1463:ILE:HD12	2:D:1577:MSE:HE3	1.50	0.91
3:Y:55:GLU:HG2	3:Y:86:ARG:NH1	1.87	0.90
2:C:1649:LEU:HG	2:C:1669:ASN:HB2	1.54	0.89
2:D:1570:LYS:HD3	2:D:1571:LEU:N	1.87	0.89
2:C:1730:SER:HA	2:C:1775:THR:HA	1.54	0.87
3:Y:25:LYS:HG2	3:Y:26:LYS:HG2	1.57	0.86
2:C:1569:ARG:CZ	3:R:33:TRP:HE1	1.87	0.86
2:C:1651:GLU:HB3	2:C:1652:PRO:HD2	1.57	0.86
2:D:1532:ASN:HB3	3:Y:33:TRP:CZ3	2.11	0.86
2:D:1434:LEU:HD13	2:D:1476:MSE:HE2	1.58	0.85
3:Y:88:LEU:HD11	3:Y:101:TRP:CD1	2.11	0.85
3:R:40:ASP:O	3:R:49:ILE:HG13	1.75	0.84
2:C:1438:LEU:HB3	2:C:1483:VAL:HG21	1.58	0.84
2:C:1594:GLU:HB2	2:C:1687:ASN:HA	1.61	0.82
2:C:1693:GLN:HB2	2:C:1697:GLU:OE1	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1729:ILE:HD12	2:D:1734:LEU:HB2	1.60	0.82
2:D:1411:TYR:OH	2:D:1433:LYS:HE3	1.80	0.82
2:C:1460:ARG:HH21	2:C:1692:LEU:HG	1.45	0.81
2:C:1562:TYR:HH	3:R:33:TRP:HD1	1.25	0.80
2:C:1723:MSE:SE	2:C:1766:ILE:HD11	2.32	0.80
1:B:168:HIS:CE1	2:D:1745:MSE:HE1	2.17	0.79
3:Y:81:PHE:O	3:Y:84:ILE:HG22	1.83	0.79
2:D:1434:LEU:HD22	2:D:1476:MSE:HE1	1.62	0.79
2:C:1623:THR:HG22	2:C:1625:LEU:HG	1.65	0.79
3:Y:49:ILE:CG2	3:Y:70:VAL:HG21	2.13	0.78
2:D:1532:ASN:C	2:D:1532:ASN:HD22	1.87	0.78
2:C:1674:LEU:HD21	2:C:1686:ILE:HG21	1.66	0.77
3:Y:84:ILE:CD1	3:Y:103:PHE:CZ	2.67	0.77
1:A:123:VAL:CG2	1:A:152:ASP:HA	2.15	0.77
2:C:1569:ARG:NH1	3:R:33:TRP:HE1	1.84	0.76
2:C:1566:HIS:HB2	2:C:1569:ARG:HD2	1.67	0.76
3:Y:45:CYS:SG	3:Y:53:CYS:HB2	2.25	0.76
2:C:1458:LEU:HD12	2:C:1461:ARG:HH11	1.50	0.76
2:C:1576:LEU:HD21	2:C:1694:LEU:HD21	1.67	0.76
2:C:1711:ARG:HB3	2:C:1752:MSE:HE3	1.65	0.76
2:C:1488:ASP:O	2:C:1492:LYS:HB2	1.84	0.76
2:D:1654:VAL:HG11	2:D:1659:ASP:HB2	1.67	0.75
1:B:173:LEU:C	1:B:175:GLY:H	1.88	0.75
2:C:1711:ARG:HB3	2:C:1752:MSE:CE	2.15	0.75
2:C:1448:ASP:HA	2:C:1451:MSE:HE3	1.69	0.75
2:C:1559:GLU:O	2:C:1563:LYS:HG3	1.87	0.75
2:D:1434:LEU:HD13	2:D:1476:MSE:CE	2.17	0.75
1:A:168:HIS:HD2	2:C:1714:ARG:HH21	1.34	0.74
2:C:1649:LEU:HD11	2:C:1669:ASN:HD22	1.52	0.74
2:D:1538:ARG:HE	2:D:1538:ARG:HA	1.52	0.74
1:B:126:ILE:O	1:B:130:VAL:HG23	1.88	0.74
2:C:1772:ASP:O	2:C:1774:ASN:O	2.05	0.74
2:D:1426:THR:CG2	2:D:1429:GLU:HG3	2.17	0.74
3:Y:84:ILE:HD11	3:Y:101:TRP:HE1	1.53	0.74
3:R:77:HIS:CE1	3:R:96:LEU:HD22	2.22	0.74
2:D:1431:GLU:HG3	2:D:1479:TRP:CH2	2.23	0.74
1:B:144:ILE:HD13	2:D:1713:LEU:HD12	1.68	0.73
1:A:168:HIS:CD2	2:C:1714:ARG:HH21	2.06	0.73
2:D:1644:LYS:HG3	2:D:1675:ILE:HD12	1.68	0.73
2:C:1689:ILE:HG22	2:C:1690:GLY:N	2.01	0.73
2:C:1576:LEU:HD11	2:C:1694:LEU:HG	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:80:HIS:HB2	3:Y:83:CYS:SG	2.28	0.73
1:A:143:LEU:HB2	1:A:150:MSE:HG3	1.70	0.73
2:C:1692:LEU:HD22	2:C:1693:GLN:HG2	1.69	0.72
2:D:1405:PRO:HG3	2:D:1444:VAL:HG13	1.70	0.72
1:A:121:ASP:OD1	1:A:125:ARG:HD3	1.88	0.72
1:A:123:VAL:HG22	1:A:152:ASP:HA	1.70	0.72
1:B:128:GLU:O	1:B:132:GLU:HG2	1.89	0.71
3:Y:88:LEU:HD11	3:Y:101:TRP:NE1	2.04	0.71
2:D:1696:THR:O	2:D:1700:ARG:HG2	1.91	0.71
3:Y:84:ILE:HD11	3:Y:101:TRP:NE1	2.06	0.71
2:C:1529:LYS:HG2	2:C:1531:LEU:HD21	1.72	0.71
1:A:121:ASP:O	1:A:155:THR:HG23	1.91	0.71
1:A:153:GLU:HG2	2:D:1754:LYS:HD2	1.72	0.71
1:A:127:LYS:HE2	1:A:141:GLN:O	1.91	0.71
2:D:1459:THR:CG2	2:D:1577:MSE:HE1	2.21	0.70
2:C:1462:LEU:HD12	2:C:1496:MSE:HE2	1.72	0.70
1:B:101:MSE:HE3	1:B:119:PRO:HG3	1.73	0.70
2:C:1555:ILE:HG23	2:C:1573:TRP:CE2	2.27	0.70
2:D:1463:ILE:HD12	2:D:1577:MSE:CE	2.20	0.70
2:C:1462:LEU:HB3	2:C:1500:ILE:HD11	1.73	0.69
2:C:1462:LEU:HD22	2:C:1500:ILE:HD12	1.74	0.69
2:D:1623:THR:HG21	2:D:1625:LEU:HD12	1.74	0.69
2:D:1740:GLU:O	2:D:1743:LYS:HB2	1.92	0.69
2:C:1723:MSE:HE1	2:C:1729:ILE:HG22	1.74	0.69
1:B:143:LEU:HB3	1:B:150:MSE:CE	2.23	0.68
3:Y:84:ILE:HD13	3:Y:103:PHE:HZ	1.53	0.68
2:C:1452:ARG:NH2	2:C:1701:GLU:HB2	2.09	0.68
1:B:150:MSE:HE1	1:B:167:LEU:HD13	1.75	0.68
2:C:1649:LEU:CG	2:C:1669:ASN:HB2	2.23	0.68
2:C:1436:GLU:HG3	2:C:1437:VAL:N	2.08	0.68
2:C:1582:ILE:HG21	2:C:1600:LEU:HD13	1.74	0.68
1:A:150:MSE:CE	1:A:167:LEU:HD13	2.23	0.67
2:D:1613:LYS:HG2	2:D:1667:SER:HB3	1.76	0.67
2:C:1740:GLU:HG3	2:C:1743:LYS:HE2	1.76	0.67
3:Y:103:PHE:H	3:Y:103:PHE:HD1	1.40	0.67
2:C:1651:GLU:CB	2:C:1652:PRO:CD	2.72	0.67
2:C:1674:LEU:HD21	2:C:1686:ILE:CG2	2.25	0.67
3:R:21:ARG:HH11	3:R:21:ARG:HG3	1.58	0.67
1:A:155:THR:HG22	1:A:156:ALA:N	2.10	0.66
2:D:1654:VAL:CG1	2:D:1659:ASP:HB2	2.25	0.66
2:D:1532:ASN:ND2	2:D:1532:ASN:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1640:PHE:N	2:D:1646:GLN:HE22	1.94	0.65
2:C:1586:ASN:OD1	2:C:1670:GLN:HA	1.95	0.65
1:B:144:ILE:CD1	2:D:1713:LEU:HD12	2.26	0.65
1:A:152:ASP:H	2:D:1774:ASN:ND2	1.88	0.65
2:C:1623:THR:CG2	2:C:1625:LEU:HG	2.25	0.65
2:C:1485:MSE:HA	2:C:1485:MSE:CE	2.27	0.65
2:C:1638:VAL:HG12	2:C:1648:LEU:O	1.96	0.65
2:D:1632:ARG:HH12	2:D:1691:ARG:HG3	1.60	0.65
1:A:126:ILE:O	1:A:130:VAL:HG23	1.96	0.65
2:C:1472:ILE:O	2:C:1476:MSE:N	2.20	0.65
2:D:1588:VAL:O	2:D:1588:VAL:HG12	1.97	0.64
2:D:1525:SER:OG	3:Y:26:LYS:HD3	1.98	0.64
2:D:1674:LEU:HD11	2:D:1685:LYS:H	1.62	0.64
2:D:1704:ASN:HA	2:D:1707:ILE:HG12	1.79	0.64
2:C:1405:PRO:HG3	2:C:1444:VAL:HG13	1.78	0.64
2:D:1594:GLU:OE2	2:D:1685:LYS:HE2	1.98	0.64
2:D:1574:HIS:CG	2:D:1577:MSE:HG2	2.32	0.64
1:B:143:LEU:HB3	1:B:150:MSE:HE3	1.78	0.64
2:C:1498:GLN:O	2:C:1502:VAL:HG23	1.98	0.64
1:A:129:ARG:HG2	1:A:129:ARG:HH11	1.61	0.63
2:D:1462:LEU:HB3	2:D:1500:ILE:CD1	2.24	0.63
1:A:152:ASP:N	2:D:1774:ASN:HD21	1.88	0.63
3:R:69:THR:HG22	3:R:70:VAL:H	1.64	0.63
3:Y:74:VAL:HG12	3:Y:75:CYS:N	2.11	0.62
2:C:1445:GLN:HE21	2:C:1445:GLN:HA	1.64	0.62
1:A:150:MSE:HE2	1:A:167:LEU:HD13	1.81	0.62
3:Y:74:VAL:O	3:Y:75:CYS:C	2.38	0.62
2:D:1434:LEU:HD22	2:D:1476:MSE:CE	2.30	0.62
2:C:1528:ILE:HG22	2:C:1529:LYS:N	2.15	0.62
1:A:109:THR:HG23	1:A:111:LYS:H	1.65	0.62
2:C:1677:ASN:O	2:C:1679:LYS:HG2	2.00	0.62
1:A:120:THR:HA	1:A:155:THR:HG21	1.82	0.62
2:D:1651:GLU:HB2	2:D:1665:LEU:HB2	1.79	0.62
2:C:1458:LEU:HD12	2:C:1461:ARG:NH1	2.15	0.61
3:Y:105:LYS:HG3	3:Y:105:LYS:O	1.99	0.61
1:B:117:ILE:HG23	1:B:121:ASP:HB2	1.81	0.61
2:D:1634:LEU:HD13	2:D:1666:PHE:CZ	2.35	0.61
2:C:1767:ARG:HB2	2:C:1779:MSE:HE3	1.81	0.61
1:A:102:LEU:HD21	1:A:114:GLU:OE2	2.00	0.61
2:C:1693:GLN:HB2	2:C:1697:GLU:CD	2.21	0.61
1:A:118:GLU:O	1:A:121:ASP:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1649:LEU:HG	2:D:1669:ASN:HB2	1.82	0.61
1:B:136:ILE:HD13	1:B:169:LEU:HD21	1.81	0.61
2:C:1569:ARG:NH1	3:R:33:TRP:NE1	2.49	0.60
2:C:1416:LEU:HD11	2:C:1476:MSE:HG3	1.82	0.60
1:B:168:HIS:HE1	2:D:1745:MSE:HE1	1.63	0.60
2:D:1701:GLU:O	2:D:1705:GLU:HG3	2.00	0.60
2:C:1601:ALA:HB1	2:C:1623:THR:HG23	1.82	0.60
2:D:1637:LEU:HB3	2:D:1648:LEU:HD12	1.83	0.60
3:R:73:GLY:HA3	3:R:101:TRP:CZ3	2.36	0.60
2:C:1537:SER:HB2	3:R:32:LEU:HD11	1.82	0.60
2:C:1696:THR:HA	2:C:1699:MSE:HE2	1.81	0.60
2:D:1632:ARG:NH1	2:D:1691:ARG:HG3	2.17	0.60
1:A:105:VAL:CG2	1:A:113:ILE:HB	2.31	0.60
1:B:129:ARG:O	1:B:132:GLU:HB2	2.02	0.60
3:Y:70:VAL:HG13	3:Y:79:PHE:O	2.00	0.60
2:D:1532:ASN:HB3	3:Y:33:TRP:CE3	2.36	0.60
1:A:119:PRO:O	1:A:155:THR:CG2	2.49	0.60
2:C:1528:ILE:CG2	2:C:1529:LYS:N	2.65	0.60
3:R:88:LEU:C	3:R:90:THR:H	2.05	0.60
2:C:1649:LEU:HD21	2:C:1669:ASN:ND2	2.17	0.60
2:D:1723:MSE:HE1	2:D:1729:ILE:HG12	1.84	0.60
2:D:1714:ARG:HE	2:D:1745:MSE:HE2	1.67	0.60
2:D:1767:ARG:HH21	2:D:1777:ILE:HD12	1.67	0.60
2:C:1512:GLU:C	2:C:1514:HIS:H	2.05	0.60
1:A:127:LYS:HD3	1:A:141:GLN:HB2	1.83	0.59
2:D:1503:SER:OG	2:D:1529:LYS:HA	2.02	0.59
1:B:115:ILE:HG22	1:B:117:ILE:HG13	1.84	0.59
2:D:1438:LEU:HB3	2:D:1483:VAL:HG21	1.83	0.59
3:Y:55:GLU:HG2	3:Y:86:ARG:HH11	1.64	0.59
1:B:173:LEU:C	1:B:175:GLY:N	2.56	0.59
1:A:115:ILE:HG22	1:A:117:ILE:HG23	1.85	0.59
2:D:1769:ASP:HB2	2:D:1775:THR:HG22	1.83	0.59
2:C:1674:LEU:HD12	2:C:1684:GLY:HA3	1.85	0.58
2:D:1767:ARG:HH21	2:D:1777:ILE:CD1	2.16	0.58
3:Y:88:LEU:HD11	3:Y:101:TRP:HE1	1.67	0.58
2:C:1740:GLU:O	2:C:1743:LYS:HB2	2.04	0.58
2:D:1651:GLU:HB3	2:D:1652:PRO:CD	2.34	0.58
2:D:1408:LEU:HD22	2:D:1437:VAL:HG13	1.84	0.58
1:B:107:THR:OG1	1:B:109:THR:HG22	2.03	0.58
3:R:90:THR:HG22	3:R:91:ARG:N	2.18	0.58
2:D:1426:THR:HG23	2:D:1429:GLU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:21:ARG:NH1	3:R:21:ARG:HG3	2.17	0.58
3:R:45:CYS:HB3	3:R:83:CYS:SG	2.42	0.58
2:D:1574:HIS:ND1	2:D:1577:MSE:HG2	2.19	0.58
2:C:1569:ARG:CZ	3:R:33:TRP:NE1	2.64	0.58
2:C:1438:LEU:HD11	2:C:1476:MSE:HE1	1.85	0.58
3:R:77:HIS:ND1	3:R:96:LEU:HD13	2.18	0.58
1:A:105:VAL:HG22	1:A:113:ILE:HB	1.85	0.58
3:Y:104:GLN:O	3:Y:105:LYS:HB3	2.03	0.58
1:B:109:THR:HG23	1:B:111:LYS:H	1.69	0.58
3:Y:20:LYS:H	3:Y:20:LYS:HD2	1.69	0.58
3:Y:43:ALA:HB1	3:Y:96:LEU:HD21	1.86	0.57
3:Y:43:ALA:HB2	3:Y:96:LEU:HD11	1.86	0.57
2:D:1635:TRP:CD2	2:D:1657:PRO:HG3	2.39	0.57
2:D:1436:GLU:HA	2:D:1439:LYS:HE3	1.85	0.57
2:C:1645:ARG:HH12	2:C:1675:ILE:HD11	1.70	0.57
2:D:1654:VAL:HG12	2:D:1655:ASN:N	2.20	0.57
2:C:1433:LYS:O	2:C:1436:GLU:HG2	2.05	0.57
2:D:1460:ARG:NH1	2:D:1690:GLY:HA2	2.20	0.57
2:C:1541:GLU:HG2	2:C:1541:GLU:O	2.04	0.57
2:C:1651:GLU:OE1	2:C:1651:GLU:HA	2.04	0.57
2:D:1689:ILE:HG22	2:D:1690:GLY:N	2.20	0.57
1:A:129:ARG:HA	1:A:132:GLU:HG2	1.87	0.57
3:Y:45:CYS:O	3:Y:45:CYS:SG	2.62	0.57
2:D:1623:THR:HG22	2:D:1623:THR:O	2.06	0.56
2:D:1596:THR:HG22	2:D:1598:PHE:N	2.20	0.56
2:C:1594:GLU:OE1	2:C:1687:ASN:HB2	2.05	0.56
2:C:1460:ARG:NH2	2:C:1692:LEU:HG	2.17	0.56
2:D:1550:GLU:H	2:D:1550:GLU:CD	2.08	0.56
2:C:1642:LYS:HE3	2:D:1482:GLU:OE1	2.05	0.56
3:Y:82:HIS:O	3:Y:86:ARG:HG2	2.06	0.56
2:D:1725:MSE:O	2:D:1727:LYS:HD3	2.06	0.56
2:C:1689:ILE:CG2	2:C:1690:GLY:H	2.10	0.55
2:C:1433:LYS:C	2:C:1436:GLU:HG2	2.27	0.55
2:D:1640:PHE:CD1	2:D:1641:PRO:HD2	2.40	0.55
2:D:1531:LEU:O	3:Y:32:LEU:HA	2.07	0.55
2:C:1574:HIS:CE1	2:C:1576:LEU:HB2	2.42	0.55
2:D:1638:VAL:O	2:D:1646:GLN:HG3	2.05	0.55
2:D:1404:CYS:HB3	2:D:1407:GLU:HB2	1.88	0.55
1:B:137:PRO:HG2	1:B:140:GLN:HG2	1.89	0.55
2:D:1638:VAL:HG12	2:D:1648:LEU:O	2.07	0.55
2:D:1767:ARG:NH2	2:D:1777:ILE:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1478:GLU:OE2	2:D:1481:ARG:NH1	2.37	0.55
2:D:1532:ASN:ND2	2:D:1532:ASN:C	2.56	0.55
1:B:144:ILE:HD12	1:B:170:VAL:CG2	2.37	0.55
2:C:1493:LEU:O	2:C:1496:MSE:HB2	2.07	0.55
2:C:1479:TRP:O	2:C:1483:VAL:HG23	2.07	0.55
2:C:1576:LEU:HD21	2:C:1694:LEU:CD2	2.37	0.55
2:D:1767:ARG:HD3	2:D:1779:MSE:HE3	1.88	0.55
2:C:1551:LEU:HD21	3:R:27:TRP:CG	2.42	0.55
2:D:1675:ILE:HA	2:D:1679:LYS:O	2.07	0.55
2:C:1638:VAL:O	2:C:1646:GLN:HG3	2.07	0.55
2:C:1485:MSE:HE2	2:C:1486:PRO:CD	2.36	0.54
3:R:101:TRP:CE3	3:R:101:TRP:HA	2.42	0.54
2:C:1569:ARG:NE	3:R:33:TRP:HE1	2.04	0.54
2:D:1640:PHE:N	2:D:1646:GLN:NE2	2.55	0.54
2:D:1483:VAL:O	2:D:1483:VAL:HG12	2.07	0.54
2:C:1635:TRP:HB2	2:C:1657:PRO:HG3	1.90	0.54
2:C:1584:PHE:CG	2:C:1584:PHE:O	2.61	0.54
2:D:1670:GLN:HE22	3:Y:21:ARG:NH1	2.05	0.54
2:C:1420:PRO:O	2:C:1424:LYS:HG3	2.07	0.54
2:C:1640:PHE:CD1	2:C:1641:PRO:HD2	2.42	0.54
2:D:1586:ASN:HD21	2:D:1672:PHE:H	1.54	0.54
2:C:1460:ARG:HH21	2:C:1692:LEU:CG	2.16	0.54
2:D:1725:MSE:CE	2:D:1726:ARG:HH21	2.21	0.54
2:C:1452:ARG:NH1	2:C:1701:GLU:HB3	2.22	0.54
2:C:1485:MSE:HA	2:C:1485:MSE:HE2	1.88	0.54
2:D:1531:LEU:HB2	3:Y:32:LEU:HD23	1.90	0.54
2:D:1601:ALA:HB1	2:D:1623:THR:HG23	1.89	0.53
1:A:155:THR:HG22	1:A:157:ALA:H	1.73	0.53
2:C:1511:LYS:HD3	2:C:1524:ASP:OD2	2.08	0.53
2:C:1606:TRP:CE2	2:C:1614:ILE:HD12	2.43	0.53
2:D:1631:ARG:NH1	2:D:1660:PHE:HB2	2.22	0.53
1:B:125:ARG:O	1:B:128:GLU:HB2	2.09	0.53
2:C:1645:ARG:HH12	2:C:1675:ILE:CD1	2.20	0.53
3:Y:84:ILE:CD1	3:Y:101:TRP:HE1	2.19	0.53
2:D:1463:ILE:HD11	2:D:1577:MSE:HE3	1.84	0.53
2:D:1596:THR:HG22	2:D:1598:PHE:H	1.73	0.53
2:D:1565:ASN:HB2	2:D:1566:HIS:CD2	2.44	0.53
2:D:1434:LEU:HB3	2:D:1476:MSE:HE1	1.90	0.53
2:D:1640:PHE:CG	2:D:1641:PRO:HD2	2.44	0.53
1:A:99:GLY:HA2	1:A:118:GLU:OE2	2.08	0.53
2:D:1575:HIS:O	2:D:1597:THR:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1458:LEU:HD23	2:D:1493:LEU:HD22	1.91	0.53
2:D:1674:LEU:HD22	2:D:1686:ILE:HG21	1.91	0.53
2:C:1767:ARG:CB	2:C:1779:MSE:HE3	2.39	0.53
2:C:1592:ASP:HB2	2:C:1685:LYS:HG2	1.90	0.52
2:C:1693:GLN:HG3	2:C:1693:GLN:O	2.10	0.52
3:R:101:TRP:HE3	3:R:101:TRP:HA	1.74	0.52
2:D:1759:TRP:O	2:D:1763:HIS:HD2	1.93	0.52
2:C:1734:LEU:O	2:C:1738:LEU:HB2	2.10	0.52
3:Y:43:ALA:HB3	3:Y:79:PHE:CE2	2.44	0.52
1:B:117:ILE:HG23	1:B:121:ASP:OD1	2.09	0.52
1:A:119:PRO:O	1:A:155:THR:HG21	2.10	0.52
2:D:1433:LYS:O	2:D:1436:GLU:HG2	2.10	0.52
2:C:1460:ARG:NH2	2:C:1692:LEU:CD2	2.73	0.52
1:A:153:GLU:HG2	2:D:1754:LYS:CD	2.39	0.52
2:D:1690:GLY:C	2:D:1691:ARG:HG2	2.30	0.52
2:C:1762:GLU:C	2:C:1764:LYS:H	2.13	0.52
3:Y:85:SER:C	3:Y:87:TRP:H	2.14	0.52
3:Y:45:CYS:O	3:Y:46:ARG:C	2.48	0.52
2:C:1565:ASN:HB3	2:C:1566:HIS:CD2	2.45	0.52
1:A:101:MSE:CE	1:A:119:PRO:HB3	2.40	0.52
2:C:1701:GLU:O	2:C:1702:GLU:C	2.48	0.52
3:R:87:TRP:CD1	3:R:87:TRP:O	2.62	0.52
2:C:1711:ARG:CB	2:C:1752:MSE:HE1	2.39	0.51
1:A:150:MSE:HE1	1:A:167:LEU:HD13	1.92	0.51
2:C:1436:GLU:HG3	2:C:1437:VAL:H	1.73	0.51
3:R:88:LEU:C	3:R:90:THR:N	2.63	0.51
2:C:1731:ASN:HD22	2:C:1776:PHE:HZ	1.58	0.51
3:R:49:ILE:HG22	3:R:70:VAL:HG12	1.91	0.51
1:B:173:LEU:O	1:B:175:GLY:N	2.41	0.51
3:R:95:PRO:O	3:R:96:LEU:HB2	2.09	0.51
1:B:145:TYR:O	1:B:146:SER:C	2.49	0.51
2:D:1644:LYS:CG	2:D:1675:ILE:HD12	2.37	0.51
2:D:1582:ILE:HG21	2:D:1600:LEU:HD13	1.92	0.51
3:R:36:ASP:OD1	3:R:37:ILE:N	2.41	0.51
1:A:155:THR:HB	1:A:158:ASP:OD1	2.10	0.51
2:C:1419:THR:OG1	2:C:1420:PRO:HD2	2.11	0.51
3:R:73:GLY:HA3	3:R:101:TRP:CH2	2.46	0.51
2:D:1767:ARG:HD3	2:D:1779:MSE:CE	2.39	0.51
3:R:44:ILE:HD13	3:R:83:CYS:O	2.11	0.51
1:A:142:ARG:HB2	1:A:170:VAL:O	2.10	0.51
3:Y:19:LYS:HD3	3:Y:23:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1723:MSE:HG2	2:C:1766:ILE:HD11	1.92	0.51
3:R:90:THR:O	3:R:92:GLN:HG3	2.09	0.51
2:C:1464:LEU:O	2:C:1466:ILE:HG23	2.11	0.51
2:C:1649:LEU:HD21	2:C:1669:ASN:HD22	1.76	0.51
3:R:41:ASN:ND2	3:R:48:HIS:HA	2.25	0.51
1:A:114:GLU:O	1:A:133:LYS:HE3	2.10	0.51
2:D:1510:PHE:CD2	2:D:1528:ILE:HD11	2.46	0.51
2:D:1522:PRO:HB2	2:D:1525:SER:CB	2.40	0.51
2:D:1416:LEU:HD11	2:D:1476:MSE:HE3	1.93	0.51
2:C:1401:GLU:O	2:C:1402:SER:HB2	2.11	0.51
2:C:1445:GLN:HE21	2:C:1445:GLN:CA	2.24	0.50
2:C:1565:ASN:HB3	2:C:1566:HIS:NE2	2.27	0.50
1:B:144:ILE:HD12	1:B:170:VAL:HG21	1.91	0.50
1:B:131:GLU:HG2	1:B:131:GLU:O	2.11	0.50
2:C:1761:ILE:HG12	2:C:1766:ILE:HG22	1.92	0.50
1:B:143:LEU:CB	1:B:150:MSE:HE3	2.40	0.50
2:C:1581:ILE:HD12	3:R:26:LYS:HB3	1.92	0.50
2:D:1635:TRP:CG	2:D:1657:PRO:HG3	2.46	0.50
2:D:1522:PRO:HB2	2:D:1525:SER:HB2	1.92	0.50
2:C:1677:ASN:ND2	2:D:1426:THR:OG1	2.44	0.50
2:C:1711:ARG:HB3	2:C:1752:MSE:HE1	1.92	0.50
2:D:1719:ILE:HG21	2:D:1760:LEU:CD1	2.41	0.50
2:C:1610:PRO:HB3	3:R:20:LYS:HG2	1.93	0.50
3:Y:53:CYS:HB3	3:Y:80:HIS:CD2	2.46	0.50
2:C:1539:SER:OG	2:C:1697:GLU:OE1	2.27	0.50
2:C:1583:THR:HG22	2:C:1584:PHE:N	2.25	0.50
1:A:106:LYS:HD3	2:C:1745:MSE:HE1	1.93	0.50
2:C:1562:TYR:OH	3:R:33:TRP:HD1	1.88	0.50
2:D:1401:GLU:O	2:D:1402:SER:C	2.50	0.50
2:C:1513:MSE:O	2:C:1513:MSE:SE	2.80	0.50
2:C:1693:GLN:O	2:C:1694:LEU:C	2.50	0.50
2:D:1651:GLU:HB3	2:D:1652:PRO:HD3	1.94	0.50
2:D:1440:LYS:HG3	2:D:1440:LYS:O	2.12	0.50
3:R:69:THR:O	3:R:81:PHE:HB2	2.12	0.49
2:C:1403:LYS:HD3	2:C:1404:CYS:H	1.73	0.49
2:C:1462:LEU:CD1	2:C:1496:MSE:HE2	2.42	0.49
2:D:1639:ALA:HA	2:D:1646:GLN:NE2	2.28	0.49
2:C:1418:LYS:HE3	2:C:1467:SER:O	2.12	0.49
3:R:45:CYS:O	3:R:54:ILE:HD11	2.12	0.49
2:D:1429:GLU:O	2:D:1433:LYS:HG3	2.12	0.49
2:C:1614:ILE:HG22	2:C:1619:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:69:THR:HG22	3:R:70:VAL:N	2.27	0.49
2:C:1635:TRP:CG	2:C:1657:PRO:HG3	2.47	0.49
2:C:1451:MSE:HG2	2:C:1489:TYR:CE2	2.48	0.49
2:D:1474:GLU:HG3	2:D:1497:PHE:CE2	2.48	0.49
3:R:49:ILE:HG22	3:R:70:VAL:CG1	2.42	0.49
1:A:113:ILE:HD13	1:A:134:GLU:HG3	1.94	0.49
2:C:1477:VAL:O	2:C:1480:LEU:HB3	2.13	0.49
1:B:123:VAL:HG23	1:B:154:LYS:O	2.12	0.49
2:D:1570:LYS:HD3	2:D:1571:LEU:H	1.70	0.49
2:D:1426:THR:HG22	2:D:1429:GLU:OE1	2.13	0.49
2:D:1469:ASP:CG	2:D:1472:ILE:HG13	2.32	0.49
2:C:1650:TYR:CE2	2:C:1653:GLN:HA	2.47	0.48
1:B:117:ILE:CG2	1:B:118:GLU:N	2.76	0.48
1:B:117:ILE:CG2	1:B:121:ASP:HB2	2.43	0.48
3:R:77:HIS:HE1	3:R:96:LEU:HD22	1.73	0.48
1:B:145:TYR:HD2	1:B:146:SER:HG	1.58	0.48
1:A:129:ARG:NH1	1:A:132:GLU:OE2	2.46	0.48
2:C:1634:LEU:HD13	2:C:1666:PHE:CZ	2.48	0.48
1:A:136:ILE:HD13	1:A:169:LEU:HD21	1.95	0.48
2:C:1445:GLN:NE2	2:C:1445:GLN:HA	2.28	0.48
2:D:1438:LEU:O	2:D:1483:VAL:HG11	2.13	0.48
2:C:1751:LYS:HG2	2:C:1755:GLU:OE1	2.14	0.48
2:C:1409:ALA:HA	2:C:1450:PHE:CE1	2.49	0.48
1:A:155:THR:CG2	1:A:156:ALA:N	2.76	0.48
1:A:106:LYS:HG3	1:A:112:GLU:HG2	1.94	0.48
2:D:1492:LYS:HD3	2:D:1535:ALA:HA	1.96	0.48
2:D:1623:THR:HG22	2:D:1625:LEU:HG	1.95	0.48
1:B:117:ILE:HG23	1:B:121:ASP:CB	2.42	0.48
2:C:1550:GLU:CD	2:C:1550:GLU:H	2.16	0.48
2:C:1532:ASN:ND2	3:R:33:TRP:CZ3	2.81	0.48
2:C:1723:MSE:CG	2:C:1766:ILE:HD11	2.44	0.48
2:D:1704:ASN:O	2:D:1705:GLU:C	2.52	0.48
3:R:85:SER:C	3:R:87:TRP:H	2.16	0.48
2:D:1725:MSE:O	2:D:1726:ARG:C	2.52	0.48
2:C:1629:GLU:CD	2:C:1694:LEU:HD22	2.34	0.47
1:B:175:GLY:O	1:B:176:GLY:C	2.51	0.47
1:B:117:ILE:HG22	1:B:118:GLU:N	2.29	0.47
1:A:119:PRO:O	1:A:155:THR:HG22	2.13	0.47
2:D:1586:ASN:HD21	2:D:1672:PHE:N	2.12	0.47
2:C:1614:ILE:CG2	2:C:1619:LEU:HG	2.43	0.47
2:C:1568:GLY:HA3	3:R:72:TRP:CH2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.78	0.47
2:D:1545:VAL:HG22	2:D:1625:LEU:CD2	2.44	0.47
2:D:1586:ASN:ND2	2:D:1672:PHE:HB3	2.29	0.47
3:Y:49:ILE:HG22	3:Y:50:MSE:HE2	1.96	0.47
2:D:1426:THR:HG22	2:D:1429:GLU:HG3	1.96	0.47
2:D:1548:PRO:HB2	2:D:1550:GLU:OE1	2.14	0.47
2:C:1609:ARG:N	2:C:1610:PRO:HD3	2.30	0.47
2:D:1469:ASP:HB3	2:D:1472:ILE:HD12	1.95	0.47
1:A:150:MSE:HA	1:A:159:TYR:CZ	2.49	0.47
2:C:1485:MSE:HE2	2:C:1486:PRO:HD2	1.95	0.47
2:C:1596:THR:CG2	2:C:1597:THR:N	2.77	0.47
2:C:1596:THR:HG22	2:C:1597:THR:N	2.28	0.47
2:C:1631:ARG:NH1	2:C:1660:PHE:HB2	2.29	0.47
2:C:1731:ASN:HA	2:C:1776:PHE:HE1	1.80	0.47
2:D:1532:ASN:ND2	2:D:1535:ALA:H	2.12	0.47
2:C:1467:SER:OG	2:C:1473:GLU:OE1	2.28	0.47
3:R:41:ASN:HD22	3:R:48:HIS:HA	1.79	0.47
2:D:1531:LEU:HD13	2:D:1536:TRP:CE3	2.49	0.47
1:B:159:TYR:C	1:B:160:LYS:HG2	2.35	0.47
2:C:1485:MSE:HE2	2:C:1486:PRO:HD3	1.97	0.47
3:R:90:THR:HG22	3:R:91:ARG:H	1.80	0.47
3:R:99:ARG:O	3:R:100:GLU:O	2.33	0.47
1:B:145:TYR:HD1	1:B:167:LEU:HD23	1.79	0.47
1:A:129:ARG:NH1	1:A:129:ARG:HG2	2.30	0.47
2:C:1444:VAL:O	2:C:1445:GLN:C	2.53	0.46
2:C:1672:PHE:O	2:C:1673:SER:HB3	2.15	0.46
2:C:1452:ARG:CZ	2:C:1701:GLU:HB2	2.45	0.46
2:C:1586:ASN:CG	2:C:1587:GLU:H	2.19	0.46
2:D:1674:LEU:HD22	2:D:1686:ILE:CG2	2.45	0.46
2:D:1669:ASN:C	2:D:1671:GLU:H	2.17	0.46
2:C:1405:PRO:HG3	2:C:1444:VAL:CG1	2.44	0.46
2:C:1438:LEU:CB	2:C:1483:VAL:HG21	2.37	0.46
1:B:117:ILE:HD13	1:B:126:ILE:HG12	1.96	0.46
3:R:79:PHE:HB2	3:R:84:ILE:HD11	1.98	0.46
3:R:99:ARG:O	3:R:100:GLU:C	2.53	0.46
2:C:1663:GLY:O	2:C:1665:LEU:HG	2.15	0.46
2:C:1598:PHE:CD1	2:C:1598:PHE:N	2.82	0.46
2:D:1584:PHE:C	2:D:1584:PHE:CD1	2.86	0.46
3:R:84:ILE:O	3:R:88:LEU:HG	2.15	0.46
3:R:77:HIS:CE1	3:R:96:LEU:HD13	2.50	0.46
2:C:1537:SER:HB2	3:R:32:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1566:HIS:CB	2:C:1569:ARG:HD2	2.41	0.46
2:C:1611:ARG:HE	3:R:20:LYS:HE2	1.79	0.46
2:D:1654:VAL:CG1	2:D:1655:ASN:N	2.78	0.46
2:D:1528:ILE:HG22	2:D:1529:LYS:N	2.31	0.46
1:B:131:GLU:O	1:B:134:GLU:O	2.34	0.46
2:C:1544:PHE:N	2:C:1544:PHE:CD1	2.83	0.46
2:C:1469:ASP:CG	2:C:1472:ILE:HG13	2.36	0.46
3:R:87:TRP:O	3:R:88:LEU:HD23	2.16	0.46
2:D:1555:ILE:HG23	2:D:1573:TRP:CE2	2.51	0.46
2:D:1723:MSE:HG3	2:D:1778:TYR:HB2	1.96	0.45
2:C:1420:PRO:HB3	2:C:1424:LYS:HE3	1.98	0.45
2:D:1761:ILE:HG12	2:D:1766:ILE:HG22	1.97	0.45
2:C:1569:ARG:CD	3:R:33:TRP:HE1	2.29	0.45
2:C:1512:GLU:C	2:C:1514:HIS:N	2.70	0.45
3:Y:84:ILE:CG1	3:Y:101:TRP:HE1	2.27	0.45
2:C:1693:GLN:HG2	2:C:1693:GLN:H	1.48	0.45
2:C:1697:GLU:O	2:C:1700:ARG:HB3	2.15	0.45
2:D:1674:LEU:CD1	2:D:1685:LYS:H	2.28	0.45
2:C:1508:GLN:O	2:C:1512:GLU:HG3	2.16	0.45
2:D:1573:TRP:CZ3	3:Y:31:ALA:HB2	2.52	0.45
1:B:145:TYR:CD1	1:B:167:LEU:HD23	2.51	0.45
1:A:150:MSE:HE1	1:A:167:LEU:CD1	2.47	0.45
2:D:1600:LEU:HD11	2:D:1604:PHE:CE1	2.52	0.45
2:C:1615:SER:HA	2:C:1665:LEU:HD23	1.97	0.45
2:C:1429:GLU:O	2:C:1432:ALA:HB3	2.16	0.45
2:C:1463:ILE:C	2:C:1465:ASP:H	2.19	0.45
2:C:1696:THR:HA	2:C:1699:MSE:CE	2.47	0.45
2:C:1774:ASN:O	2:C:1775:THR:HB	2.17	0.45
2:C:1569:ARG:HD3	3:R:33:TRP:HE1	1.80	0.45
2:C:1512:GLU:O	2:C:1514:HIS:N	2.50	0.45
2:C:1598:PHE:N	2:C:1598:PHE:HD1	2.14	0.45
3:R:74:VAL:O	3:R:74:VAL:HG12	2.16	0.45
2:D:1729:ILE:CD1	2:D:1734:LEU:HD13	2.46	0.45
2:D:1426:THR:HG22	2:D:1429:GLU:CG	2.47	0.45
3:Y:87:TRP:CZ2	3:Y:95:PRO:HD3	2.52	0.45
1:A:144:ILE:HD13	2:C:1713:LEU:HD13	1.98	0.45
2:C:1607:ASN:HD21	3:R:22:PHE:N	2.15	0.45
2:C:1489:TYR:O	2:C:1492:LYS:HB3	2.17	0.45
2:D:1675:ILE:HG23	2:D:1679:LYS:N	2.32	0.45
2:C:1779:MSE:O	2:C:1780:ALA:OXT	2.35	0.45
3:Y:84:ILE:CD1	3:Y:103:PHE:CE1	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1672:PHE:O	2:C:1673:SER:CB	2.65	0.45
2:C:1520:ALA:O	2:C:1521:LEU:HG	2.17	0.45
2:C:1712:ILE:O	2:C:1716:GLN:HB2	2.17	0.45
2:C:1620:LYS:HE3	2:C:1620:LYS:HB2	1.68	0.45
3:Y:81:PHE:O	3:Y:84:ILE:CG2	2.62	0.44
2:C:1472:ILE:O	2:C:1473:GLU:C	2.55	0.44
2:C:1560:GLU:HA	2:C:1563:LYS:HD2	1.99	0.44
2:D:1697:GLU:O	2:D:1700:ARG:HB2	2.16	0.44
2:C:1607:ASN:HD21	3:R:22:PHE:H	1.65	0.44
3:Y:49:ILE:HG23	3:Y:70:VAL:CG2	2.27	0.44
2:C:1404:CYS:HB3	2:C:1407:GLU:HG3	1.98	0.44
2:D:1676:LYS:O	2:D:1677:ASN:HB2	2.17	0.44
2:C:1723:MSE:CE	2:C:1729:ILE:HG22	2.43	0.44
2:C:1735:GLN:OE1	2:C:1735:GLN:HA	2.17	0.44
2:C:1623:THR:O	2:C:1623:THR:HG22	2.17	0.44
2:C:1448:ASP:CA	2:C:1451:MSE:HE3	2.42	0.44
1:B:105:VAL:HA	1:B:167:LEU:O	2.17	0.44
2:C:1436:GLU:HG3	2:C:1437:VAL:HG23	2.00	0.44
2:D:1669:ASN:O	2:D:1671:GLU:N	2.50	0.44
2:C:1419:THR:OG1	2:C:1420:PRO:CD	2.65	0.44
2:C:1677:ASN:HA	2:D:1427:SER:HB3	1.99	0.44
3:R:80:HIS:HB2	3:R:83:CYS:HB2	2.00	0.44
3:Y:84:ILE:CD1	3:Y:101:TRP:CZ2	3.00	0.44
2:C:1560:GLU:HA	2:C:1563:LYS:CD	2.48	0.44
2:D:1632:ARG:NH2	2:D:1693:GLN:O	2.50	0.44
2:C:1672:PHE:CG	2:C:1673:SER:N	2.86	0.44
3:R:70:VAL:HG23	3:R:72:TRP:CZ3	2.53	0.44
2:C:1492:LYS:HZ3	2:C:1538:ARG:HH22	1.66	0.44
1:B:123:VAL:HB	1:B:152:ASP:HA	1.99	0.44
2:D:1502:VAL:O	2:D:1506:LEU:HB2	2.18	0.44
3:Y:49:ILE:HA	3:Y:80:HIS:CE1	2.52	0.44
2:C:1404:CYS:HA	2:C:1405:PRO:HD3	1.84	0.44
2:C:1694:LEU:HA	2:C:1694:LEU:HD23	1.65	0.44
1:A:113:ILE:CD1	1:A:134:GLU:HG3	2.48	0.44
2:C:1452:ARG:CZ	2:C:1701:GLU:CB	2.96	0.44
3:R:53:CYS:SG	3:R:55:GLU:HB2	2.58	0.44
2:D:1631:ARG:HH11	2:D:1660:PHE:HB2	1.82	0.44
1:B:136:ILE:CD1	1:B:169:LEU:HD21	2.46	0.44
2:D:1539:SER:OG	2:D:1540:SER:N	2.46	0.44
1:B:118:GLU:O	1:B:119:PRO:C	2.53	0.43
3:R:93:VAL:HA	3:R:100:GLU:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:58:ALA:O	3:R:59:ASN:C	2.56	0.43
2:C:1699:MSE:O	2:C:1703:GLU:HB2	2.18	0.43
2:D:1481:ARG:HB2	2:D:1490:VAL:HG11	1.99	0.43
2:C:1424:LYS:O	2:C:1425:LEU:HD23	2.18	0.43
2:C:1722:ILE:HD13	2:C:1737:GLU:HG3	2.00	0.43
1:B:106:LYS:HD3	1:B:112:GLU:HG2	1.99	0.43
3:Y:81:PHE:C	3:Y:83:CYS:H	2.20	0.43
1:B:168:HIS:CE1	2:D:1745:MSE:CE	2.95	0.43
2:C:1492:LYS:HZ1	2:C:1538:ARG:NH1	2.17	0.43
1:B:118:GLU:C	1:B:120:THR:N	2.69	0.43
2:D:1536:TRP:O	2:D:1537:SER:C	2.56	0.43
3:Y:55:GLU:CG	3:Y:86:ARG:NH1	2.72	0.43
1:B:101:MSE:SE	1:B:161:ILE:O	2.86	0.43
1:A:105:VAL:HA	1:A:167:LEU:O	2.18	0.43
2:D:1508:GLN:O	2:D:1511:LYS:HB2	2.19	0.43
2:D:1415:LEU:HD22	2:D:1425:LEU:HD12	2.00	0.43
2:D:1703:GLU:O	2:D:1703:GLU:CG	2.66	0.43
2:D:1731:ASN:O	2:D:1732:ALA:C	2.55	0.43
2:C:1645:ARG:HG2	2:C:1645:ARG:HH11	1.83	0.43
3:Y:42:CYS:SG	3:Y:79:PHE:CD2	3.11	0.43
3:Y:55:GLU:CG	3:Y:86:ARG:HH11	2.30	0.43
2:C:1650:TYR:CZ	2:C:1653:GLN:HA	2.54	0.43
2:C:1623:THR:O	2:C:1624:GLU:HB2	2.19	0.43
2:D:1582:ILE:HG13	2:D:1582:ILE:O	2.18	0.43
2:C:1691:ARG:HD3	2:C:1691:ARG:HA	1.77	0.43
2:D:1643:LEU:HG	2:D:1645:ARG:O	2.19	0.43
2:C:1649:LEU:CD2	2:C:1669:ASN:HB2	2.49	0.43
2:D:1523:ALA:C	2:D:1525:SER:H	2.22	0.43
2:D:1769:ASP:OD1	2:D:1770:GLU:N	2.52	0.43
2:C:1632:ARG:HD2	2:C:1691:ARG:CZ	2.49	0.43
2:C:1660:PHE:CD2	2:C:1664:THR:HG21	2.54	0.43
1:A:105:VAL:O	1:A:105:VAL:HG23	2.19	0.43
2:C:1551:LEU:HD21	3:R:27:TRP:CD2	2.54	0.43
2:C:1403:LYS:HD3	2:C:1404:CYS:CA	2.48	0.42
2:C:1726:ARG:NH1	2:C:1733:GLN:OE1	2.52	0.42
3:Y:100:GLU:OE1	3:Y:100:GLU:HA	2.19	0.42
1:A:155:THR:HG22	1:A:156:ALA:H	1.83	0.42
2:D:1588:VAL:O	2:D:1588:VAL:CG1	2.66	0.42
2:D:1521:LEU:HB3	2:D:1522:PRO:HD2	2.01	0.42
3:Y:20:LYS:O	3:Y:21:ARG:HG2	2.19	0.42
2:D:1495:ARG:HA	2:D:1495:ARG:HD2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG22	1:A:152:ASP:CA	2.45	0.42
3:Y:33:TRP:CD1	3:Y:34:ALA:N	2.87	0.42
3:R:40:ASP:OD1	3:R:41:ASN:N	2.52	0.42
3:Y:105:LYS:CG	3:Y:105:LYS:O	2.63	0.42
2:D:1543:VAL:HG11	2:D:1598:PHE:HZ	1.83	0.42
2:D:1704:ASN:C	2:D:1706:GLY:N	2.69	0.42
2:D:1531:LEU:HD13	2:D:1536:TRP:CZ3	2.53	0.42
2:C:1635:TRP:CB	2:C:1657:PRO:HG3	2.49	0.42
1:B:129:ARG:HA	1:B:132:GLU:CG	2.50	0.42
3:R:42:CYS:C	3:R:44:ILE:H	2.22	0.42
2:D:1585:LYS:HB2	3:Y:21:ARG:HA	2.02	0.42
2:C:1548:PRO:HB3	2:C:1604:PHE:HD2	1.83	0.42
2:D:1573:TRP:CE3	3:Y:31:ALA:HB2	2.54	0.42
1:B:104:LYS:HA	1:B:113:ILE:O	2.20	0.42
2:C:1481:ARG:HB2	2:C:1490:VAL:CG1	2.27	0.42
2:C:1565:ASN:HB3	2:C:1566:HIS:CE1	2.55	0.42
2:C:1472:ILE:O	2:C:1475:ASN:N	2.52	0.42
2:C:1720:ILE:HD11	2:C:1765:TYR:HB3	2.00	0.42
3:Y:42:CYS:SG	3:Y:79:PHE:HD2	2.42	0.42
2:C:1650:TYR:CD2	2:C:1660:PHE:HE2	2.37	0.42
2:D:1674:LEU:HD11	2:D:1685:LYS:N	2.32	0.42
2:D:1481:ARG:NH2	2:D:1490:VAL:HG12	2.34	0.42
2:D:1656:SER:HA	2:D:1657:PRO:HD3	1.87	0.42
2:D:1521:LEU:HB3	2:D:1522:PRO:CD	2.50	0.42
2:C:1640:PHE:CD2	2:C:1688:LEU:HD23	2.55	0.42
2:D:1617:GLU:O	2:D:1620:LYS:HB2	2.20	0.42
3:Y:82:HIS:N	3:Y:82:HIS:CD2	2.87	0.41
1:B:118:GLU:O	1:B:120:THR:N	2.53	0.41
3:Y:84:ILE:HD12	3:Y:101:TRP:HZ2	1.85	0.41
3:Y:45:CYS:HB2	3:Y:54:ILE:CD1	2.50	0.41
2:C:1730:SER:O	2:C:1731:ASN:C	2.57	0.41
2:C:1723:MSE:O	2:C:1726:ARG:O	2.37	0.41
2:C:1569:ARG:HD3	3:R:33:TRP:NE1	2.36	0.41
2:D:1580:GLY:HA3	3:Y:27:TRP:CE3	2.55	0.41
2:C:1481:ARG:HA	2:C:1490:VAL:HG21	2.02	0.41
1:A:150:MSE:HG2	1:A:150:MSE:H	1.65	0.41
2:D:1451:MSE:HE1	2:D:1486:PRO:HG2	2.02	0.41
2:C:1470:SER:O	2:C:1474:GLU:HG3	2.20	0.41
2:C:1651:GLU:O	2:C:1652:PRO:C	2.58	0.41
1:B:142:ARG:HB2	1:B:170:VAL:O	2.20	0.41
2:D:1463:ILE:C	2:D:1465:ASP:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1669:ASN:OD1	2:C:1672:PHE:N	2.53	0.41
2:C:1438:LEU:HD11	2:C:1476:MSE:CE	2.49	0.41
2:D:1623:THR:O	2:D:1624:GLU:HB2	2.21	0.41
2:D:1412:CYS:SG	2:D:1437:VAL:HG11	2.61	0.41
2:D:1670:GLN:HE22	3:Y:21:ARG:HH11	1.68	0.41
3:Y:81:PHE:C	3:Y:83:CYS:N	2.74	0.41
2:C:1729:ILE:HD13	2:C:1734:LEU:HB2	2.03	0.41
2:D:1408:LEU:HD23	2:D:1408:LEU:HA	1.94	0.41
1:B:143:LEU:C	1:B:144:ILE:HG13	2.41	0.41
2:C:1666:PHE:CD1	2:C:1666:PHE:N	2.89	0.41
2:C:1607:ASN:HD22	2:C:1607:ASN:HA	1.64	0.41
2:C:1661:THR:H	2:C:1664:THR:HG1	1.65	0.41
2:D:1574:HIS:CE1	2:D:1577:MSE:HG2	2.54	0.41
2:C:1594:GLU:CD	2:C:1687:ASN:HD22	2.24	0.41
2:D:1426:THR:CG2	2:D:1429:GLU:CG	2.95	0.41
2:C:1446:ASN:HB2	2:C:1448:ASP:OD1	2.21	0.41
1:A:143:LEU:CB	1:A:150:MSE:HG3	2.46	0.41
2:D:1586:ASN:HD21	2:D:1672:PHE:HB3	1.86	0.41
2:D:1462:LEU:HD22	2:D:1500:ILE:HD12	2.01	0.41
2:C:1684:GLY:C	2:C:1685:LYS:HG3	2.42	0.41
1:A:105:VAL:HG12	1:A:167:LEU:HB2	2.03	0.41
2:C:1495:ARG:HA	2:C:1498:GLN:HG3	2.02	0.41
2:C:1521:LEU:HD11	3:R:24:VAL:HG11	2.02	0.41
2:C:1711:ARG:HB2	2:C:1752:MSE:HE1	2.03	0.40
2:D:1644:LYS:CB	2:D:1675:ILE:HD12	2.51	0.40
2:C:1745:MSE:O	2:C:1746:PHE:HB3	2.20	0.40
2:D:1419:THR:HB	2:D:1420:PRO:HD2	2.02	0.40
2:D:1446:ASN:ND2	2:D:1448:ASP:OD1	2.54	0.40
2:C:1651:GLU:O	2:C:1653:GLN:N	2.55	0.40
1:B:150:MSE:HE1	1:B:167:LEU:HD22	2.02	0.40
2:D:1513:MSE:HE1	2:D:1514:HIS:CE1	2.57	0.40
2:C:1711:ARG:CB	2:C:1752:MSE:CE	2.91	0.40
2:D:1619:LEU:HD13	2:D:1634:LEU:HD21	2.02	0.40
1:B:122:LYS:HD2	1:B:124:GLU:OE1	2.21	0.40
2:D:1631:ARG:HD3	2:D:1657:PRO:O	2.22	0.40
2:C:1485:MSE:HA	2:C:1485:MSE:HE3	2.01	0.40
2:D:1720:ILE:HD11	2:D:1765:TYR:HB3	2.03	0.40
3:Y:45:CYS:HB2	3:Y:54:ILE:HG13	2.04	0.40
2:C:1462:LEU:HD23	2:C:1462:LEU:HA	1.82	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	76/81 (94%)	66 (87%)	8 (10%)	2 (3%)	7	33
1	B	75/81 (93%)	67 (89%)	5 (7%)	3 (4%)	4	21
2	C	372/382 (97%)	305 (82%)	54 (14%)	13 (4%)	4	24
2	D	374/382 (98%)	315 (84%)	43 (12%)	16 (4%)	3	19
3	R	84/106 (79%)	61 (73%)	17 (20%)	6 (7%)	1	7
3	Y	81/106 (76%)	50 (62%)	22 (27%)	9 (11%)	0	2
All	All	1062/1138 (93%)	864 (81%)	149 (14%)	49 (5%)	3	18

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	LYS
1	A	163	GLY
2	C	1445	GLN
2	C	1536	TRP
2	C	1537	SER
2	C	1651	GLU
3	R	60	GLN
3	R	96	LEU
3	R	100	GLU
2	D	1540	SER
2	D	1641	PRO
2	D	1643	LEU
2	C	1486	PRO
2	C	1513	MSE
2	C	1673	SER
2	C	1694	LEU
3	R	80	HIS
3	R	98	ASN
2	D	1402	SER
2	D	1586	ASN

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Mol	Chain	Res	Type
2	D	1587	GLU
2	D	1670	GLN
2	D	1691	ARG
3	Y	20	LYS
3	Y	46	ARG
3	Y	74	VAL
3	Y	75	CYS
3	Y	80	HIS
3	Y	103	PHE
1	B	146	SER
2	D	1537	SER
2	D	1725	MSE
3	Y	67	GLU
3	Y	68	CYS
3	Y	86	ARG
2	C	1775	THR
3	R	62	SER
1	B	174	ARG
2	D	1465	ASP
2	D	1651	GLU
2	D	1685	LYS
2	C	1535	ALA
2	C	1607	ASN
1	B	121	ASP
2	D	1522	PRO
2	D	1610	PRO
2	C	1490	VAL
2	D	1483	VAL
2	C	1652	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	67/65 (103%)	60 (90%)	7 (10%)	9 32
1	B	67/65 (103%)	66 (98%)	1 (2%)	72 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	347/339 (102%)	322 (93%)	25 (7%)	18	53
2	D	349/339 (103%)	325 (93%)	24 (7%)	19	56
3	R	74/88 (84%)	71 (96%)	3 (4%)	37	76
3	Y	63/88 (72%)	61 (97%)	2 (3%)	46	82
All	All	967/984 (98%)	905 (94%)	62 (6%)	22	59

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	MSE
1	A	116	ASP
1	A	121	ASP
1	A	139	GLN
1	A	150	MSE
1	A	153	GLU
1	A	165	SER
2	C	1403	LYS
2	C	1460	ARG
2	C	1470	SER
2	C	1476	MSE
2	C	1478	GLU
2	C	1485	MSE
2	C	1486	PRO
2	C	1504	GLU
2	C	1505	ASP
2	C	1531	LEU
2	C	1541	GLU
2	C	1544	PHE
2	C	1606	TRP
2	C	1636	SER
2	C	1677	ASN
2	C	1681	GLN
2	C	1701	GLU
2	C	1720	ILE
2	C	1736	THR
2	C	1741	ILE
2	C	1747	LEU
2	C	1752	MSE
2	C	1758	GLU
2	C	1766	ILE
2	C	1779	MSE

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Mol	Chain	Res	Type
3	R	39	VAL
3	R	79	PHE
3	R	101	TRP
1	B	125	ARG
2	D	1401	GLU
2	D	1439	LYS
2	D	1446	ASN
2	D	1448	ASP
2	D	1451	MSE
2	D	1471	GLU
2	D	1504	GLU
2	D	1513	MSE
2	D	1532	ASN
2	D	1538	ARG
2	D	1544	PHE
2	D	1579	ASN
2	D	1584	PHE
2	D	1590	GLN
2	D	1596	THR
2	D	1632	ARG
2	D	1641	PRO
2	D	1651	GLU
2	D	1660	PHE
2	D	1697	GLU
2	D	1704	ASN
2	D	1773	ILE
2	D	1775	THR
2	D	1779	MSE
3	Y	33	TRP
3	Y	45	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	168	HIS
2	C	1410	ASN
2	C	1445	GLN
2	C	1457	HIS
2	C	1527	ASN
2	C	1566	HIS
2	C	1590	GLN

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Mol	Chain	Res	Type
2	C	1607	ASN
2	C	1653	GLN
2	C	1670	GLN
2	C	1677	ASN
2	C	1709	GLN
2	C	1763	HIS
3	R	41	ASN
3	R	77	HIS
3	R	82	HIS
2	D	1446	ASN
2	D	1475	ASN
2	D	1514	HIS
2	D	1532	ASN
2	D	1579	ASN
2	D	1586	ASN
2	D	1655	ASN
2	D	1709	GLN
2	D	1716	GLN
2	D	1733	GLN
2	D	1749	GLN
2	D	1763	HIS
2	D	1774	ASN
3	Y	28	ASN
3	Y	57	GLN
3	Y	80	HIS
3	Y	82	HIS

### 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

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<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	75/81 (92%)	-0.46	0	100	100	38, 62, 75, 85	1 (1%)
1	B	74/81 (91%)	-0.42	0	100	100	35, 64, 81, 91	0
2	C	363/382 (95%)	-0.23	9 (2%)	61	30	32, 71, 112, 132	0
2	D	365/382 (95%)	-0.33	1 (0%)	94	84	29, 59, 100, 127	0
3	R	83/106 (78%)	0.21	4 (4%)	34	14	51, 96, 137, 142	0
3	Y	72/106 (67%)	1.19	19 (26%)	1	1	47, 149, 150, 150	0
All	All	1032/1138 (90%)	-0.16	33 (3%)	51	23	29, 68, 141, 150	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	77	HIS	6.1
3	Y	67	GLU	4.3
3	Y	98	ASN	4.2
2	C	1443	TYR	4.1
3	R	62	SER	3.9
2	C	1515	LYS	3.8
3	R	61	ALA	3.6
3	Y	87	TRP	3.6
3	Y	96	LEU	3.6
3	Y	95	PRO	3.6
3	Y	86	ARG	3.5
3	Y	76	ASN	3.4
3	Y	44	ILE	3.0
3	Y	69	THR	3.0
3	Y	72	TRP	3.0
3	Y	68	CYS	2.8
3	Y	101	TRP	2.8
2	C	1696	THR	2.7
3	Y	100	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	Y	99	ARG	2.6
2	C	1539	SER	2.5
3	Y	70	VAL	2.5
3	Y	43	ALA	2.4
2	C	1403	LYS	2.4
2	D	1677	ASN	2.3
2	C	1402	SER	2.3
3	Y	103	PHE	2.3
2	C	1442	LYS	2.2
2	C	1691	ARG	2.2
3	R	101	TRP	2.1
3	R	20	LYS	2.1
2	C	1421	LEU	2.1
3	Y	47	ASN	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(Å <sup>2</sup> )	Q<0.9
4	ZN	R	4005	1/1	0.98	0.11	-1.28	72,72,72,72	0
4	ZN	R	4004	1/1	0.99	0.12	-1.74	79,79,79,79	0
4	ZN	Y	4001	1/1	0.85	0.09	-1.99	149,149,149,149	0
4	ZN	Y	4002	1/1	0.59	0.05	-2.07	149,149,149,149	0
4	ZN	R	4006	1/1	0.90	0.06	-2.16	105,105,105,105	0
4	ZN	Y	4003	1/1	0.93	0.11	-	149,149,149,149	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.