



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2021 – 04:09 PM JST

PDB ID : 7CFD  
Title : Drosophila melanogaster Krimper eTud2-AubR15me2 complex  
Authors : Hu, H.; Li, S.  
Deposited on : 2020-06-25  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
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) : 2.23.1

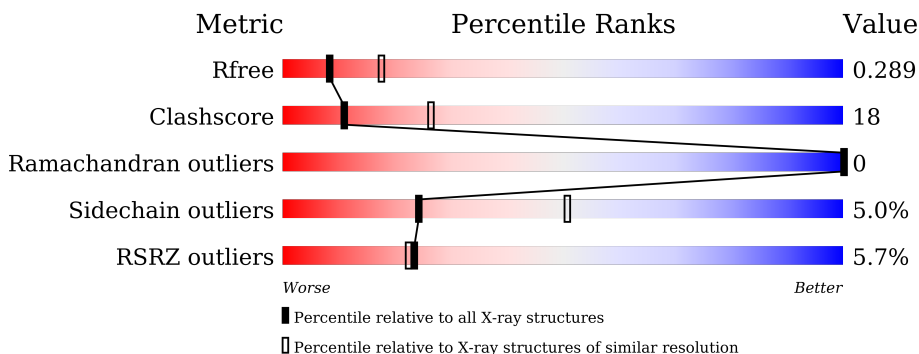
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	186	 3% 72% 23% 5%
1	B	186	 % 76% 19% 5%
1	C	186	 % 69% 26% 5%
1	D	186	 12% 65% 30% 5%
1	E	186	 7% 67% 28% 5%
1	F	186	 % 73% 20% 5%

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Mol	Chain	Length	Quality of chain
1	G	186	
1	H	186	
2	I	13	
2	J	13	
2	K	13	
2	L	13	
2	M	13	
2	N	13	
2	O	13	
2	Z	13	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12199 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 FI20010p1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	178	1460	952	238	264	6	0	0	0
1	C	179	1469	957	239	267	6	0	0	0
1	D	178	1460	952	238	264	6	0	0	0
1	E	180	1484	969	241	268	6	0	0	0
1	F	182	1497	977	244	270	6	0	0	0
1	A	176	1448	944	236	262	6	0	0	0
1	G	181	1490	972	243	269	6	0	0	0
1	H	181	1490	972	243	269	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	561	SER	-	expression tag	UNP A1ZAC4
C	561	SER	-	expression tag	UNP A1ZAC4
D	561	SER	-	expression tag	UNP A1ZAC4
E	561	SER	-	expression tag	UNP A1ZAC4
F	561	SER	-	expression tag	UNP A1ZAC4
A	561	SER	-	expression tag	UNP A1ZAC4
G	561	SER	-	expression tag	UNP A1ZAC4
H	561	SER	-	expression tag	UNP A1ZAC4

- Molecule 2 is a protein called Protein aubergine.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	4	Total	C	N	O	0	0	0
			32	18	10	4			
2	J	7	Total	C	N	O	0	0	0
			56	32	17	7			
2	K	8	Total	C	N	O	0	0	0
			67	38	21	8			
2	L	4	Total	C	N	O	0	0	0
			32	18	10	4			
2	N	6	Total	C	N	O	0	0	0
			47	26	15	6			
2	M	6	Total	C	N	O	0	0	0
			52	30	16	6			
2	Z	3	Total	C	N	O	0	0	0
			28	16	9	3			
2	O	1	Total	C	N	O	0	0	0
			13	8	4	1			

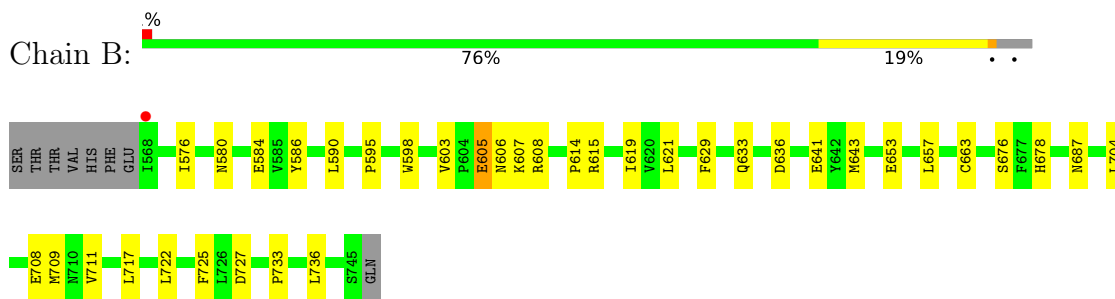
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	10	Total	O	0	0
			10	10		
3	C	12	Total	O	0	0
			12	12		
3	D	11	Total	O	0	0
			11	11		
3	E	9	Total	O	0	0
			9	9		
3	F	5	Total	O	0	0
			5	5		
3	A	15	Total	O	0	0
			15	15		
3	G	12	Total	O	0	0
			12	12		

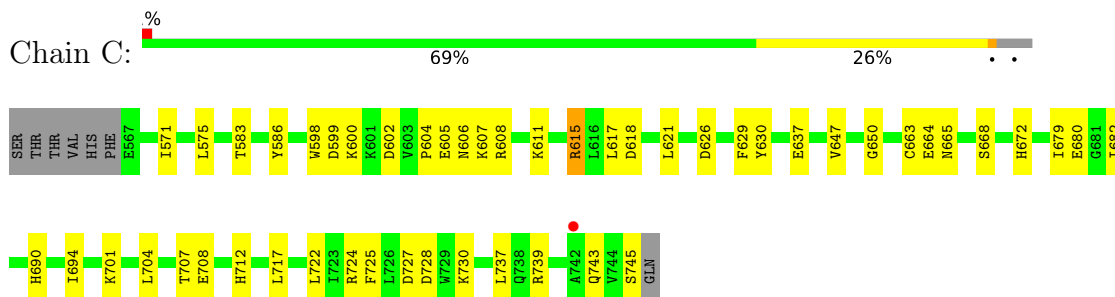
### 3 Residue-property plots [i](#)

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.

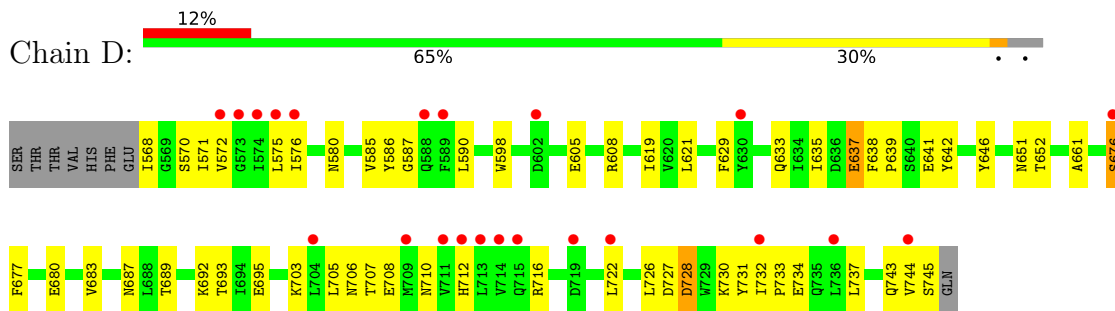
- Molecule 1: FI20010p1



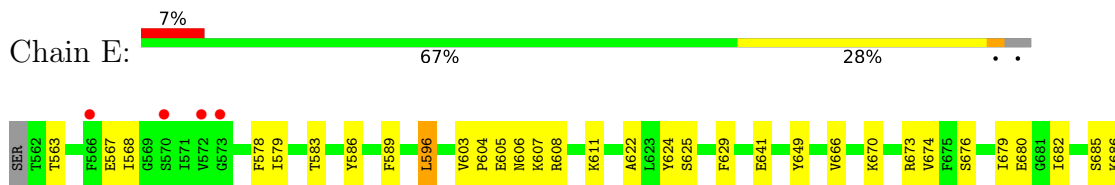
- Molecule 1: FI20010p1



- Molecule 1: FI20010p1



- Molecule 1: FI20010p1

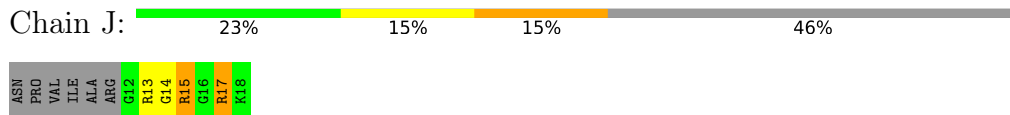




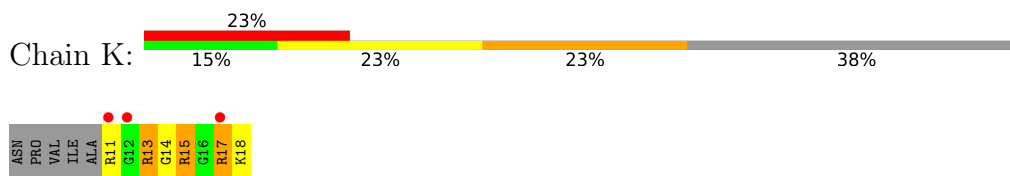
- Molecule 2: Protein aubergine



- Molecule 2: Protein aubergine



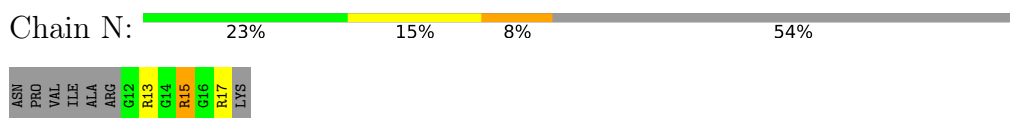
- Molecule 2: Protein aubergine



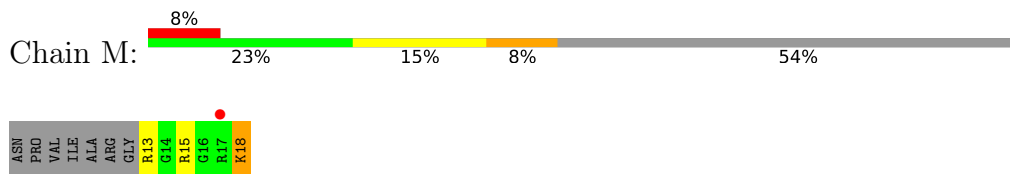
- Molecule 2: Protein aubergine



- Molecule 2: Protein aubergine



- Molecule 2: Protein aubergine



- Molecule 2: Protein aubergine



- Molecule 2: Protein aubergine





ASN	PRO	VAL	ILE	ALA	ARG	GLY	ARG	GLY	<b>RIS</b>	GLY	ARG	LYS
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## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.12Å 101.36Å 191.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.99 – 2.70 48.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.99-2.70) 95.4 (48.99-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.14 3260	Depositor
R, $R_{free}$	0.243 , 0.290 0.243 , 0.289	Depositor DCC
$R_{free}$ test set	2533 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtrriage
Anisotropy	0.994	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12199	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9942e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR

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	0.42	0/1487	0.55	0/2018
1	B	0.31	0/1499	0.50	0/2034
1	C	0.42	0/1508	0.60	0/2046
1	D	0.47	0/1499	0.61	0/2034
1	E	0.40	0/1525	0.65	0/2070
1	F	0.46	0/1538	0.69	0/2087
1	G	0.36	0/1531	0.55	0/2077
1	H	0.54	0/1531	0.74	0/2077
2	I	0.62	0/17	1.00	0/18
2	J	0.64	0/41	1.65	0/48
2	K	0.67	0/52	1.11	0/62
2	L	0.63	0/17	0.72	0/18
2	M	0.59	0/37	1.00	0/43
2	N	0.85	0/32	0.93	0/37
2	Z	0.64	0/14	1.44	0/16
All	All	0.43	0/12328	0.63	0/16685

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	1448	0	1440	39	0
1	B	1460	0	1454	32	0
1	C	1469	0	1460	46	0
1	D	1460	0	1454	56	0
1	E	1484	0	1472	48	0
1	F	1497	0	1485	43	0
1	G	1490	0	1476	24	0
1	H	1490	0	1476	149	0
2	I	32	0	34	5	0
2	J	56	0	63	8	0
2	K	67	0	76	7	0
2	L	32	0	34	3	0
2	M	52	0	60	5	0
2	N	47	0	50	1	0
2	O	13	0	17	3	0
2	Z	28	0	33	7	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	C	12	0	0	0	0
3	D	11	0	0	2	0
3	E	9	0	0	1	0
3	F	5	0	0	0	0
3	G	12	0	0	0	0
All	All	12199	0	12084	437	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 18.

All (437) 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:H:711:VAL:CG1	1:H:723:ILE:HD11	1.47	1.41
1:H:604:PRO:CG	1:H:607:LYS:HB2	1.63	1.28
1:F:610:PHE:CD2	1:F:662:PRO:HG3	1.76	1.19
1:H:704:LEU:HD21	1:H:732:ILE:CD1	1.76	1.15
1:H:711:VAL:CG1	1:H:723:ILE:CD1	2.27	1.12
1:H:711:VAL:CG2	1:H:723:ILE:HD11	1.81	1.10
1:A:709:MET:HE1	1:A:725:PHE:CD1	1.86	1.10
1:D:727:ASP:HA	1:D:730:LYS:CD	1.82	1.09
2:Z:17:ARG:HA	2:Z:17:ARG:HE	1.17	1.08
1:H:657:LEU:H	1:H:657:LEU:HD23	1.15	1.07
1:H:704:LEU:HD21	1:H:732:ILE:HD12	1.13	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:604:PRO:HG2	1:H:607:LYS:HB2	1.35	1.06
1:H:679:ILE:HB	1:H:682:ILE:HD11	1.31	1.05
1:H:711:VAL:CB	1:H:723:ILE:HD11	1.86	1.05
1:E:695:GLU:HG2	1:H:643:MET:CE	1.85	1.05
1:B:709:MET:HE2	1:B:725:PHE:HE1	1.21	1.03
1:H:598:TRP:CZ3	1:H:621:LEU:HD11	1.93	1.03
1:B:709:MET:HE1	1:B:725:PHE:CD1	1.95	1.02
1:H:637:GLU:HG2	1:H:642:TYR:CD1	1.97	1.00
1:H:711:VAL:HG11	1:H:723:ILE:CD1	1.90	0.99
1:B:709:MET:CE	1:B:725:PHE:CE1	2.45	0.99
1:H:711:VAL:HG11	1:H:723:ILE:HD11	1.42	0.99
1:D:727:ASP:HA	1:D:730:LYS:HD2	1.44	0.99
1:H:616:LEU:HD12	1:H:616:LEU:H	1.28	0.98
1:H:726:LEU:HD13	1:H:727:ASP:N	1.78	0.98
1:H:711:VAL:HG13	1:H:723:ILE:HD11	1.41	0.97
1:H:667:ASP:HA	1:H:670:LYS:HE3	1.48	0.95
1:D:727:ASP:HA	1:D:730:LYS:CG	1.95	0.95
1:H:711:VAL:CG2	1:H:723:ILE:CD1	2.44	0.94
1:H:603:VAL:HG21	1:H:629:PHE:HE2	1.30	0.93
1:H:596:LEU:HG	1:H:673:ARG:HH12	1.32	0.93
1:F:602:ASP:O	1:F:604:PRO:HD3	1.67	0.93
1:C:604:PRO:HG2	1:C:607:LYS:CG	1.99	0.93
1:D:683:VAL:HG12	1:D:743:GLN:O	1.68	0.92
1:B:709:MET:HE2	1:B:725:PHE:CE1	2.04	0.91
1:A:709:MET:HE1	1:A:725:PHE:HD1	1.24	0.91
1:E:695:GLU:HG2	1:H:643:MET:HE2	1.52	0.91
1:H:623:LEU:N	1:H:659:CYS:SG	2.43	0.91
1:H:709:MET:CE	1:H:725:PHE:HE1	1.84	0.91
1:B:709:MET:HE1	1:B:725:PHE:CE1	2.06	0.90
1:H:604:PRO:HG3	1:H:607:LYS:HB2	1.49	0.90
1:H:711:VAL:HG22	1:H:723:ILE:CG1	2.01	0.90
1:C:704:LEU:O	1:C:707:THR:HG22	1.69	0.90
1:H:709:MET:HE2	1:H:725:PHE:CE1	2.07	0.90
1:E:695:GLU:HG2	1:H:643:MET:HE1	1.54	0.89
1:H:685:SER:O	1:H:743:GLN:HG2	1.73	0.88
1:F:610:PHE:HD2	1:F:662:PRO:HG3	1.38	0.88
1:E:606:ASN:OD1	1:E:607:LYS:N	2.07	0.87
1:H:685:SER:HB2	1:H:688:LEU:HD13	1.54	0.87
1:H:709:MET:HE2	1:H:725:PHE:HE1	1.37	0.86
1:H:724:ARG:HB3	1:H:724:ARG:NH1	1.91	0.86
1:F:595:PRO:HG2	2:M:13:ARG:HD3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:704:LEU:CD2	1:H:732:ILE:CD1	2.53	0.85
1:H:711:VAL:CG2	1:H:723:ILE:CG1	2.54	0.85
1:H:603:VAL:HG21	1:H:629:PHE:CE2	2.12	0.84
1:H:623:LEU:CB	1:H:659:CYS:SG	2.66	0.84
1:F:602:ASP:OD1	1:F:602:ASP:N	2.11	0.84
1:A:709:MET:CE	1:A:725:PHE:CD1	2.61	0.83
1:B:709:MET:CE	1:B:725:PHE:CD1	2.63	0.82
1:D:727:ASP:HA	1:D:730:LYS:HG3	1.60	0.82
1:C:604:PRO:HG2	1:C:607:LYS:HG3	1.62	0.82
1:F:615:ARG:HB2	1:F:618:ASP:OD2	1.78	0.81
1:H:711:VAL:CG2	1:H:723:ILE:HG12	2.10	0.81
1:F:600:LYS:HE2	1:F:608:ARG:HH12	1.45	0.81
1:H:680:GLU:CD	1:H:724:ARG:HG3	2.02	0.80
1:H:704:LEU:CD2	1:H:732:ILE:HD12	2.06	0.80
2:K:17:ARG:HG2	2:K:17:ARG:HH11	1.45	0.80
1:H:711:VAL:HG21	1:H:723:ILE:CD1	2.10	0.80
1:F:680:GLU:OE2	1:F:724:ARG:HD2	1.81	0.80
1:E:695:GLU:CG	1:H:643:MET:HE2	2.11	0.79
1:C:604:PRO:HG2	1:C:607:LYS:HG2	1.66	0.77
1:H:637:GLU:HG2	1:H:642:TYR:HD1	1.45	0.77
2:M:18:LYS:O	2:M:18:LYS:HD3	1.83	0.77
1:B:709:MET:CE	1:B:725:PHE:HE1	1.86	0.76
1:F:602:ASP:O	1:F:604:PRO:CD	2.34	0.76
1:H:709:MET:CE	1:H:725:PHE:CE1	2.66	0.76
1:H:616:LEU:HD12	1:H:616:LEU:N	2.00	0.76
1:H:679:ILE:HB	1:H:682:ILE:CD1	2.14	0.76
1:A:709:MET:CE	1:A:725:PHE:HD1	1.96	0.76
2:K:17:ARG:HG2	2:K:17:ARG:NH1	2.01	0.75
1:C:615:ARG:HD2	1:C:618:ASP:OD1	1.86	0.75
1:H:724:ARG:HB3	1:H:724:ARG:HH11	1.50	0.75
1:H:711:VAL:HG13	1:H:723:ILE:CD1	2.07	0.75
1:H:679:ILE:CB	1:H:682:ILE:HD11	2.13	0.74
1:H:603:VAL:CG2	1:H:629:PHE:CE2	2.71	0.74
1:C:604:PRO:CG	1:C:607:LYS:HG3	2.18	0.74
1:F:606:ASN:OD1	1:F:606:ASN:N	2.19	0.73
1:C:575:LEU:CD1	1:C:708:GLU:HG3	2.19	0.73
1:H:651:ASN:OD1	2:Z:15:2MR:CQ1	2.36	0.73
1:H:657:LEU:H	1:H:657:LEU:CD2	1.95	0.72
1:C:606:ASN:ND2	1:C:607:LYS:HE3	2.04	0.72
1:C:615:ARG:CD	1:C:618:ASP:OD1	2.37	0.71
1:H:623:LEU:HB3	1:H:659:CYS:SG	2.29	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:616:LEU:H	1:H:616:LEU:CD1	2.03	0.71
1:C:575:LEU:HD12	1:C:708:GLU:HG3	1.73	0.71
1:D:727:ASP:CA	1:D:730:LYS:HG3	2.20	0.71
1:G:604:PRO:HG2	1:G:607:LYS:HB2	1.72	0.71
2:Z:17:ARG:HA	2:Z:17:ARG:NE	1.96	0.71
1:D:689:THR:HG1	1:D:692:LYS:H	1.38	0.70
1:B:641:GLU:OE1	1:C:739:ARG:NH2	2.23	0.70
1:A:709:MET:HE1	1:A:725:PHE:CE1	2.27	0.69
1:H:623:LEU:HB2	1:H:659:CYS:SG	2.32	0.69
1:H:685:SER:HB3	1:H:688:LEU:HD22	1.74	0.69
1:H:621:LEU:O	1:H:661:ALA:N	2.26	0.69
1:H:712:HIS:ND1	1:H:724:ARG:NH2	2.41	0.69
1:A:709:MET:SD	1:A:729:TRP:CD1	2.87	0.68
1:H:637:GLU:CG	1:H:642:TYR:CD1	2.76	0.68
1:E:603:VAL:O	1:E:608:ARG:NH2	2.25	0.68
1:E:567:GLU:OE1	1:E:567:GLU:HA	1.91	0.68
1:H:711:VAL:HG21	1:H:723:ILE:HG12	1.75	0.68
1:H:657:LEU:HD23	1:H:657:LEU:N	2.00	0.68
1:H:706:ASN:OD1	2:Z:15:2MR:HB3	1.92	0.68
1:A:709:MET:CE	1:A:725:PHE:CE1	2.76	0.68
1:D:726:LEU:C	1:D:730:LYS:HG3	2.15	0.67
1:H:685:SER:O	1:H:743:GLN:CG	2.43	0.67
1:E:695:GLU:CG	1:H:643:MET:CE	2.68	0.66
1:B:580:ASN:ND2	1:B:584:GLU:OE2	2.22	0.66
1:H:657:LEU:HA	1:H:660:LEU:HD12	1.76	0.66
1:E:727:ASP:HA	1:E:730:LYS:HD3	1.77	0.66
1:E:717:LEU:HD12	1:E:719:ASP:H	1.61	0.66
1:D:726:LEU:O	1:D:730:LYS:HG3	1.96	0.65
1:A:604:PRO:HD2	1:A:607:LYS:HD3	1.78	0.65
1:G:605:GLU:OE2	1:G:605:GLU:N	2.28	0.65
1:G:642:TYR:HE1	1:G:657:LEU:HG	1.62	0.65
1:H:624:TYR:HB3	1:H:626:ASP:OD1	1.95	0.65
1:D:689:THR:O	1:D:693:THR:HG23	1.97	0.65
1:H:598:TRP:CE3	1:H:621:LEU:HD21	2.32	0.64
1:E:596:LEU:HD21	1:E:670:LYS:HD2	1.79	0.64
1:E:641:GLU:OE2	1:H:703:LYS:NZ	2.23	0.64
2:I:13:ARG:HG3	2:I:14:GLY:N	2.12	0.64
2:I:13:ARG:HG3	2:I:14:GLY:H	1.62	0.64
1:D:731:TYR:HD2	3:D:804:HOH:O	1.78	0.64
1:A:685:SER:HB3	1:A:688:LEU:HD13	1.79	0.64
1:E:604:PRO:O	1:E:608:ARG:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:680:GLU:OE2	1:F:724:ARG:CD	2.46	0.64
1:H:680:GLU:OE1	1:H:724:ARG:HD3	1.98	0.64
1:E:703:LYS:NZ	1:H:641:GLU:HG3	2.13	0.64
1:F:595:PRO:O	2:M:13:ARG:NH1	2.32	0.63
1:F:651:ASN:OD1	1:F:651:ASN:N	2.21	0.63
1:C:737:LEU:HD21	1:C:743:GLN:HA	1.81	0.63
1:H:726:LEU:HD13	1:H:727:ASP:H	1.60	0.62
1:D:727:ASP:N	1:D:730:LYS:HE3	2.14	0.62
1:F:601:LYS:HD2	1:F:602:ASP:OD1	2.00	0.62
1:H:588:GLN:HG2	1:H:673:ARG:HB3	1.80	0.62
1:H:608:ARG:NH1	1:H:659:CYS:O	2.33	0.62
1:C:599:ASP:OD1	1:C:600:LYS:N	2.32	0.62
1:H:711:VAL:HG21	1:H:723:ILE:CG1	2.27	0.62
1:C:728:ASP:OD1	1:C:728:ASP:N	2.33	0.61
1:B:576:ILE:HD12	1:B:704:LEU:HB3	1.81	0.61
1:G:642:TYR:CE1	1:G:657:LEU:HG	2.35	0.61
1:H:680:GLU:N	1:H:723:ILE:O	2.30	0.61
1:D:635:ILE:HD13	1:D:635:ILE:N	2.13	0.61
1:H:711:VAL:HG22	1:H:723:ILE:HG12	1.75	0.61
1:E:589:PHE:O	1:E:673:ARG:NH2	2.34	0.60
1:H:680:GLU:CD	1:H:724:ARG:HD3	2.21	0.60
1:F:595:PRO:HG2	2:M:13:ARG:CD	2.29	0.60
1:B:606:ASN:OD1	1:B:607:LYS:HG3	2.02	0.60
2:J:15:2MR:CQ1	1:A:630:TYR:CG	2.85	0.60
2:J:15:2MR:CQ1	1:A:630:TYR:CD1	2.85	0.60
2:K:17:ARG:HH11	2:K:17:ARG:CG	2.11	0.59
1:E:605:GLU:OE1	1:E:605:GLU:N	2.34	0.59
1:H:642:TYR:HE2	1:H:657:LEU:HB3	1.67	0.59
1:H:685:SER:CB	1:H:688:LEU:HD13	2.30	0.59
1:H:604:PRO:CB	1:H:607:LYS:HB2	2.32	0.59
1:H:711:VAL:HG22	1:H:723:ILE:CD1	2.26	0.59
1:F:704:LEU:O	1:F:707:THR:OG1	2.20	0.59
1:H:680:GLU:CD	1:H:724:ARG:CG	2.71	0.59
1:A:580:ASN:HB3	1:A:584:GLU:HG2	1.83	0.59
1:H:685:SER:O	1:H:743:GLN:NE2	2.32	0.59
1:D:605:GLU:HA	1:D:608:ARG:HD2	1.85	0.58
1:H:566:PHE:HB3	1:H:572:VAL:HG11	1.83	0.58
1:B:653:GLU:OE1	2:K:18:LYS:NZ	2.28	0.58
1:D:575:LEU:HD13	1:D:708:GLU:HG3	1.85	0.58
1:H:680:GLU:OE2	1:H:724:ARG:HD3	2.03	0.58
1:E:679:ILE:HG22	1:E:680:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:ASN:OD1	1:C:606:ASN:N	2.28	0.57
1:D:680:GLU:HG3	1:D:722:LEU:HD21	1.86	0.57
1:F:600:LYS:HE2	1:F:608:ARG:NH1	2.15	0.57
1:C:586:TYR:HD2	1:C:650:GLY:HA3	1.69	0.57
1:F:717:LEU:HD11	1:F:722:LEU:HB2	1.87	0.57
1:C:664:GLU:H	1:C:664:GLU:CD	2.08	0.57
1:B:605:GLU:HG2	1:B:608:ARG:HB2	1.87	0.56
1:G:731:TYR:HA	1:G:734:GLU:HB2	1.87	0.56
1:H:573:GLY:HA3	1:H:590:LEU:HD12	1.86	0.56
2:Z:17:ARG:HE	2:Z:17:ARG:CA	2.04	0.56
1:D:638:PHE:HB3	1:D:639:PRO:HD2	1.87	0.56
1:E:696:CYS:HB2	1:E:741:TYR:CD1	2.40	0.56
1:A:590:LEU:HD21	1:A:708:GLU:HG2	1.86	0.56
1:E:699:TYR:HB2	1:H:654:PHE:CE1	2.41	0.56
1:E:666:VAL:HG21	1:A:716:ARG:HE	1.69	0.56
1:F:605:GLU:HA	1:F:608:ARG:HG3	1.87	0.56
1:F:699:TYR:O	1:F:702:SER:HB3	2.06	0.56
1:C:680:GLU:OE1	1:C:724:ARG:NH1	2.39	0.55
1:F:633:GLN:HG2	1:F:635:ILE:HD12	1.89	0.55
1:A:709:MET:HE2	1:A:725:PHE:CE1	2.41	0.55
1:H:598:TRP:O	1:H:629:PHE:N	2.31	0.55
1:F:610:PHE:CD2	1:F:662:PRO:CG	2.70	0.55
1:H:651:ASN:CG	2:Z:15:2MR:CQ1	2.75	0.55
2:L:15:2MR:CD	2:L:15:2MR:CQ1	2.85	0.55
1:H:604:PRO:HG3	1:H:607:LYS:CB	2.28	0.54
2:J:14:GLY:O	2:J:15:2MR:C	2.54	0.54
1:H:712:HIS:CE1	1:H:724:ARG:NH2	2.75	0.54
1:C:664:GLU:OE2	1:C:664:GLU:N	2.32	0.54
1:G:706:ASN:OD1	2:N:15:2MR:HB3	2.07	0.54
1:H:576:ILE:HD12	1:H:704:LEU:HB3	1.90	0.54
1:E:568:ILE:HG23	1:E:568:ILE:O	2.08	0.54
1:H:732:ILE:HB	1:H:733:PRO:HD3	1.90	0.54
1:C:575:LEU:CD1	1:C:708:GLU:CG	2.85	0.54
2:J:15:2MR:CD	2:J:15:2MR:CQ2	2.85	0.54
1:C:615:ARG:NH2	1:E:674:VAL:O	2.40	0.54
1:H:711:VAL:HG22	1:H:723:ILE:HD11	1.78	0.54
1:E:735:GLN:O	1:E:739:ARG:HB2	2.07	0.53
1:F:566:PHE:CZ	1:F:589:PHE:HB3	2.44	0.53
1:D:727:ASP:CA	1:D:730:LYS:CD	2.73	0.53
1:H:604:PRO:CG	1:H:607:LYS:CB	2.59	0.53
1:A:696:CYS:HB2	1:A:741:TYR:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:17:ARG:NH2	1:A:701:LYS:O	2.41	0.53
1:F:610:PHE:CD1	1:F:610:PHE:N	2.76	0.53
1:D:730:LYS:O	1:D:733:PRO:HD2	2.08	0.53
1:F:611:LYS:CD	1:F:611:LYS:H	2.22	0.53
1:A:619:ILE:HD13	1:A:633:GLN:HB2	1.89	0.53
1:E:685:SER:HA	1:E:686:LYS:HE2	1.91	0.53
1:G:704:LEU:HD21	1:G:732:ILE:HG13	1.91	0.53
1:G:576:ILE:HD12	1:G:704:LEU:HB3	1.90	0.52
1:C:575:LEU:HD13	1:C:708:GLU:CG	2.40	0.52
1:D:732:ILE:N	1:D:733:PRO:HD2	2.23	0.52
1:F:611:LYS:CD	1:F:611:LYS:N	2.72	0.52
1:C:665:ASN:HA	1:C:668:SER:OG	2.10	0.52
1:A:680:GLU:HG3	1:A:722:LEU:HD21	1.90	0.52
1:G:730:LYS:O	1:G:733:PRO:HD2	2.09	0.52
1:H:711:VAL:HG22	1:H:723:ILE:HG13	1.90	0.52
1:C:737:LEU:HD21	1:C:743:GLN:CA	2.39	0.52
1:D:727:ASP:CA	1:D:730:LYS:HD2	2.27	0.52
1:G:603:VAL:HG12	1:G:603:VAL:O	2.10	0.52
1:B:603:VAL:HG12	1:B:608:ARG:HG2	1.93	0.51
1:F:621:LEU:HB2	1:F:661:ALA:HB3	1.90	0.51
1:F:689:THR:HG23	1:F:692:LYS:H	1.75	0.51
1:E:699:TYR:O	1:E:702:SER:HB3	2.10	0.51
1:H:637:GLU:CG	1:H:642:TYR:HD1	2.18	0.51
1:B:709:MET:HE1	1:B:725:PHE:HD1	1.63	0.51
1:D:605:GLU:H	1:D:605:GLU:CD	2.13	0.51
1:D:716:ARG:HH21	1:D:716:ARG:HB3	1.75	0.51
1:E:563:THR:HG23	1:E:563:THR:O	2.10	0.51
1:E:682:ILE:HG22	1:E:737:LEU:HD11	1.92	0.50
1:G:731:TYR:O	1:G:732:ILE:C	2.49	0.50
2:I:13:ARG:CG	2:I:14:GLY:H	2.20	0.50
1:D:572:VAL:O	1:D:710:ASN:HA	2.11	0.50
1:B:636:ASP:HB2	1:B:643:MET:HE3	1.93	0.50
1:H:634:ILE:HG21	1:H:637:GLU:OE2	2.10	0.50
1:B:614:PRO:HD2	1:B:657:LEU:HD11	1.93	0.50
1:H:638:PHE:HB3	1:H:639:PRO:HD2	1.93	0.50
1:B:678:HIS:HB2	1:B:722:LEU:HD12	1.94	0.50
1:C:690:HIS:O	1:C:694:ILE:HG12	2.11	0.49
1:A:709:MET:HE2	1:A:725:PHE:HE1	1.76	0.49
1:F:631:ARG:NH2	1:F:670:LYS:O	2.45	0.49
1:F:689:THR:HG22	1:F:692:LYS:HB2	1.95	0.49
1:D:692:LYS:HA	1:D:695:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:711:VAL:HG11	1:H:723:ILE:HD13	1.89	0.49
1:D:586:TYR:HE1	1:D:676:SER:HB3	1.76	0.49
1:C:621:LEU:HD13	1:C:663:CYS:HB2	1.93	0.49
1:F:597:VAL:HG11	2:M:13:ARG:HA	1.93	0.49
1:F:703:LYS:HE3	1:G:641:GLU:HG2	1.93	0.48
1:H:598:TRP:CH2	1:H:621:LEU:HD11	2.45	0.48
1:H:569:GLY:O	1:H:712:HIS:NE2	2.47	0.48
1:B:598:TRP:HB2	1:B:629:PHE:HB2	1.96	0.48
1:A:685:SER:HA	1:A:743:GLN:OE1	2.13	0.48
1:C:583:THR:HA	1:C:679:ILE:HD12	1.95	0.48
1:C:598:TRP:HB2	1:C:629:PHE:HB2	1.95	0.48
1:A:686:LYS:N	1:A:743:GLN:OE1	2.35	0.48
1:H:644:ILE:HD13	1:H:655:VAL:HG21	1.95	0.48
1:H:680:GLU:CB	1:H:724:ARG:HG3	2.44	0.48
1:D:568:ILE:HG23	1:D:570:SER:H	1.78	0.48
1:G:732:ILE:HB	1:G:733:PRO:HD3	1.96	0.48
1:C:626:ASP:OD2	1:C:630:TYR:OH	2.24	0.47
1:F:702:SER:OG	1:F:703:LYS:HE2	2.14	0.47
1:A:611:LYS:NZ	1:G:618:ASP:HA	2.29	0.47
1:F:730:LYS:O	1:F:733:PRO:HD2	2.14	0.47
1:B:621:LEU:HG	1:B:663:CYS:HB2	1.97	0.47
1:D:706:ASN:ND2	2:O:15:2MR:HA	2.29	0.47
1:G:686:LYS:N	1:G:743:GLN:OE1	2.47	0.47
1:D:576:ILE:HD13	1:D:585:VAL:HG21	1.95	0.47
1:C:602:ASP:O	1:C:604:PRO:HD3	2.15	0.47
1:D:571:ILE:HG22	1:D:712:HIS:ND1	2.29	0.47
1:D:705:LEU:O	1:D:707:THR:HG23	2.14	0.47
1:D:716:ARG:HB3	1:D:716:ARG:NH2	2.30	0.47
1:E:682:ILE:HD12	1:E:736:LEU:HD12	1.97	0.47
1:G:647:VAL:O	1:G:674:VAL:HG12	2.15	0.47
1:H:684:ARG:O	1:H:684:ARG:HG2	2.07	0.47
1:B:727:ASP:OD2	1:A:735:GLN:NE2	2.45	0.47
2:K:14:GLY:O	2:K:15:2MR:C	2.62	0.47
1:E:579:ILE:HD13	1:E:701:LYS:HG2	1.97	0.47
1:E:703:LYS:HZ1	1:H:641:GLU:HG3	1.78	0.47
1:H:573:GLY:CA	1:H:590:LEU:HD12	2.44	0.46
1:C:615:ARG:HD3	1:C:618:ASP:OD1	2.14	0.46
1:H:566:PHE:HB3	1:H:572:VAL:CG1	2.46	0.46
1:D:637:GLU:HB2	1:D:642:TYR:CD1	2.50	0.46
1:H:680:GLU:OE2	1:H:724:ARG:CD	2.63	0.46
1:D:703:LYS:O	1:D:707:THR:HG21	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:688:LEU:HD12	1:H:688:LEU:HA	1.73	0.46
1:H:709:MET:HE1	1:H:725:PHE:CE1	2.50	0.46
1:D:727:ASP:CA	1:D:730:LYS:HE3	2.45	0.46
1:D:727:ASP:HA	1:D:730:LYS:CE	2.44	0.46
1:H:600:LYS:HG3	1:H:627:GLY:O	2.15	0.46
1:H:680:GLU:CD	1:H:724:ARG:CD	2.83	0.46
1:G:578:PHE:HB3	1:G:586:TYR:HB2	1.98	0.46
1:C:617:LEU:HD13	1:E:720:GLY:HA2	1.98	0.46
1:D:687:ASN:O	1:D:687:ASN:ND2	2.49	0.45
1:E:691:GLN:NE2	1:E:695:GLU:OE1	2.36	0.45
1:H:713:LEU:HD11	1:H:721:PHE:HB3	1.98	0.45
1:E:649:TYR:CD1	2:L:15:2MR:HD3	2.51	0.45
1:A:630:TYR:CD2	1:A:649:TYR:CE2	3.04	0.45
1:H:705:LEU:HD23	1:H:705:LEU:HA	1.81	0.45
1:B:717:LEU:HD11	1:B:722:LEU:HB2	1.99	0.45
1:C:637:GLU:O	1:C:637:GLU:HG2	2.17	0.45
1:C:679:ILE:HG12	1:C:725:PHE:HE2	1.82	0.45
1:C:571:ILE:HG12	1:C:712:HIS:ND1	2.32	0.45
1:D:575:LEU:HB2	1:D:590:LEU:HD21	1.99	0.45
1:E:703:LYS:HZ3	1:H:641:GLU:HG3	1.80	0.45
1:C:737:LEU:HD23	1:C:737:LEU:HA	1.67	0.45
1:A:584:GLU:OE2	1:A:678:HIS:NE2	2.45	0.45
1:H:727:ASP:O	1:H:728:ASP:CB	2.65	0.45
1:D:638:PHE:HB3	1:D:639:PRO:CD	2.47	0.45
1:D:727:ASP:N	1:D:730:LYS:HG3	2.32	0.45
1:E:578:PHE:HB3	1:E:586:TYR:HB2	1.99	0.45
1:G:673:ARG:HG2	1:G:673:ARG:HH11	1.82	0.45
1:H:598:TRP:CD2	1:H:621:LEU:HD21	2.51	0.44
1:E:711:VAL:HG22	1:E:712:HIS:H	1.82	0.44
1:H:574:ILE:HD13	1:H:711:VAL:HG11	1.98	0.44
1:F:603:VAL:O	1:F:608:ARG:NH2	2.36	0.44
1:A:616:LEU:HD13	1:G:721:PHE:HZ	1.82	0.44
1:F:711:VAL:HG13	1:F:723:ILE:HB	1.98	0.44
1:E:589:PHE:HZ	1:E:721:PHE:CE2	2.36	0.44
2:J:17:ARG:HA	2:J:17:ARG:HD2	1.51	0.44
1:G:686:LYS:HB2	1:G:743:GLN:OE1	2.17	0.44
1:C:679:ILE:HG12	1:C:725:PHE:CE2	2.53	0.44
1:C:727:ASP:OD1	1:C:730:LYS:HE3	2.18	0.44
1:D:706:ASN:HD21	2:O:15:2MR:HA	1.83	0.44
1:F:613:LYS:O	1:F:613:LYS:HG3	2.17	0.44
1:G:598:TRP:HB2	1:G:629:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:621:LEU:HB3	1:H:661:ALA:HB3	1.99	0.44
1:H:680:GLU:HB3	1:H:724:ARG:HG3	2.00	0.44
1:B:605:GLU:HA	1:B:608:ARG:HB2	2.00	0.44
2:K:13:ARG:O	2:K:13:ARG:HG3	2.16	0.44
1:D:598:TRP:HB2	1:D:629:PHE:HB2	2.00	0.44
1:D:651:ASN:ND2	2:O:15:2MR:HH2	2.16	0.43
1:E:622:ALA:O	1:E:629:PHE:HA	2.18	0.43
1:A:584:GLU:CD	1:A:678:HIS:HE2	2.21	0.43
1:D:652:THR:O	1:A:698:GLU:HG2	2.18	0.43
1:D:737:LEU:HD11	1:D:744:VAL:HG13	1.99	0.43
1:H:696:CYS:HB2	1:H:741:TYR:CD1	2.53	0.43
1:D:737:LEU:CD1	1:D:744:VAL:HG13	2.49	0.43
1:G:645:PHE:CZ	1:G:650:GLY:HA2	2.54	0.43
1:H:685:SER:H	1:H:742:ALA:HA	1.84	0.43
2:L:15:2MR:CQ1	2:L:15:2MR:HD2	2.48	0.43
1:A:595:PRO:HB2	1:A:597:VAL:HG12	2.01	0.43
2:I:15:2MR:H	2:I:15:2MR:HG3	1.39	0.43
1:D:571:ILE:HG22	1:D:712:HIS:CE1	2.53	0.43
1:D:587:GLY:HA3	1:D:677:PHE:CE2	2.54	0.43
1:G:596:LEU:HD21	1:G:670:LYS:HD2	2.01	0.43
1:B:586:TYR:CE1	1:B:676:SER:HB2	2.53	0.43
1:C:575:LEU:HD13	1:C:708:GLU:HG3	1.98	0.43
1:D:619:ILE:HD13	1:D:633:GLN:HB2	2.00	0.43
1:G:703:LYS:HA	1:G:703:LYS:HD3	1.76	0.43
1:H:714:VAL:HG12	1:H:715:GLN:HB2	1.99	0.43
1:D:730:LYS:C	1:D:733:PRO:HD2	2.39	0.43
1:C:571:ILE:HD11	1:C:712:HIS:HE1	1.83	0.43
1:C:617:LEU:HD11	1:E:721:PHE:CE1	2.53	0.43
2:J:13:ARG:HA	2:J:13:ARG:HD3	1.66	0.43
1:D:726:LEU:HD23	1:D:728:ASP:H	1.83	0.43
1:E:679:ILE:HG22	1:E:680:GLU:CG	2.46	0.43
1:C:647:VAL:HB	1:C:672:HIS:CG	2.54	0.42
1:D:621:LEU:HB2	1:D:661:ALA:HB3	2.01	0.42
1:D:646:TYR:HB2	1:D:651:ASN:OD1	2.18	0.42
1:A:677:PHE:HB3	1:A:723:ILE:HG12	2.01	0.42
1:H:732:ILE:N	1:H:733:PRO:CD	2.81	0.42
1:A:630:TYR:HD2	1:A:649:TYR:CE2	2.37	0.42
1:B:709:MET:CE	1:B:725:PHE:HD1	2.23	0.42
1:B:733:PRO:HA	1:B:736:LEU:HD12	2.01	0.42
1:C:717:LEU:HD11	1:C:722:LEU:HB2	2.01	0.42
1:A:576:ILE:HD12	1:A:704:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:659:CYS:SG	1:H:660:LEU:N	2.92	0.42
1:F:731:TYR:CD1	1:F:731:TYR:C	2.93	0.42
1:H:685:SER:HB2	1:H:688:LEU:CD1	2.37	0.42
1:H:731:TYR:HA	1:H:734:GLU:HB2	2.01	0.42
1:H:578:PHE:HB3	1:H:586:TYR:HB2	2.02	0.42
1:H:631:ARG:HH21	1:H:648:ASP:CG	2.23	0.42
1:H:703:LYS:HA	1:H:703:LYS:HD3	1.73	0.42
1:A:621:LEU:HG	1:A:663:CYS:HB2	2.02	0.42
1:B:619:ILE:HD13	1:B:633:GLN:HB2	2.01	0.42
1:E:688:LEU:HD11	1:E:692:LYS:HB3	2.02	0.42
1:E:700:LEU:HD23	1:E:700:LEU:HA	1.90	0.42
1:H:680:GLU:OE1	1:H:724:ARG:CG	2.68	0.42
1:B:590:LEU:HD21	1:B:708:GLU:HG2	2.01	0.41
1:C:617:LEU:HD21	1:E:716:ARG:HG3	2.00	0.41
1:F:583:THR:O	1:F:679:ILE:HG13	2.20	0.41
1:A:686:LYS:HB2	1:A:686:LYS:HE2	1.72	0.41
1:H:641:GLU:CD	1:H:641:GLU:N	2.73	0.41
1:H:726:LEU:HD13	1:H:726:LEU:C	2.36	0.41
2:J:17:ARG:HH22	1:A:702:SER:HA	1.85	0.41
1:F:711:VAL:CG1	1:F:723:ILE:HB	2.50	0.41
1:D:580:ASN:HA	3:D:805:HOH:O	2.20	0.41
1:E:583:THR:O	1:E:679:ILE:HG13	2.20	0.41
1:H:575:LEU:HD13	1:H:708:GLU:HG3	2.01	0.41
1:H:611:LYS:HD2	1:H:611:LYS:HA	1.71	0.41
1:C:682:ILE:HG22	1:C:737:LEU:HD11	2.00	0.41
1:D:568:ILE:CG2	1:D:570:SER:H	2.33	0.41
1:A:716:ARG:O	1:A:717:LEU:HD23	2.21	0.41
1:H:608:ARG:O	1:H:608:ARG:CD	2.69	0.41
1:E:686:LYS:NZ	3:E:802:HOH:O	2.53	0.41
1:H:596:LEU:HG	1:H:673:ARG:NH1	2.15	0.41
1:H:637:GLU:HB3	1:H:642:TYR:CE1	2.55	0.41
2:K:13:ARG:O	2:K:13:ARG:CG	2.68	0.41
1:E:624:TYR:CG	1:E:625:SER:N	2.89	0.41
1:E:727:ASP:HA	1:E:730:LYS:CD	2.47	0.41
1:H:608:ARG:O	1:H:608:ARG:CG	2.69	0.41
1:H:647:VAL:O	1:H:674:VAL:HG12	2.20	0.41
1:C:604:PRO:O	1:C:608:ARG:HG3	2.21	0.41
1:E:611:LYS:O	1:E:611:LYS:HD3	2.21	0.41
1:A:709:MET:SD	1:A:729:TRP:CG	3.14	0.41
1:H:596:LEU:HD23	1:H:596:LEU:HA	1.79	0.41
1:H:604:PRO:HG2	1:H:607:LYS:CB	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:637:GLU:CB	1:H:642:TYR:CD1	3.04	0.41
1:B:584:GLU:OE1	1:B:678:HIS:NE2	2.54	0.41
1:H:622:ALA:O	1:H:629:PHE:HA	2.21	0.41
1:H:724:ARG:NH1	1:H:724:ARG:CB	2.72	0.41
1:B:603:VAL:HG12	1:B:608:ARG:CG	2.51	0.41
1:D:575:LEU:HD12	1:D:707:THR:O	2.21	0.41
1:H:637:GLU:CB	1:H:642:TYR:HD1	2.34	0.40
1:B:595:PRO:HG2	2:I:13:ARG:HD3	2.03	0.40
1:F:610:PHE:CG	1:F:662:PRO:HG3	2.45	0.40
1:H:606:ASN:O	1:H:609:THR:HG22	2.21	0.40
2:Z:17:ARG:NE	2:Z:17:ARG:CA	2.73	0.40
1:F:601:LYS:HG2	1:F:602:ASP:OD1	2.22	0.40
1:A:688:LEU:HD23	1:A:693:THR:HA	2.03	0.40
1:H:604:PRO:HB2	1:H:607:LYS:CG	2.51	0.40
1:B:709:MET:HE3	1:B:711:VAL:HG12	2.03	0.40
1:F:589:PHE:HZ	1:F:721:PHE:CE2	2.40	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	174/186 (94%)	171 (98%)	3 (2%)	0	100	100
1	B	176/186 (95%)	173 (98%)	3 (2%)	0	100	100
1	C	177/186 (95%)	170 (96%)	7 (4%)	0	100	100
1	D	176/186 (95%)	174 (99%)	2 (1%)	0	100	100
1	E	178/186 (96%)	175 (98%)	3 (2%)	0	100	100
1	F	180/186 (97%)	175 (97%)	5 (3%)	0	100	100
1	G	179/186 (96%)	176 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	179/186 (96%)	167 (93%)	12 (7%)	0	100	100
2	I	1/13 (8%)	1 (100%)	0	0	100	100
2	J	4/13 (31%)	4 (100%)	0	0	100	100
2	K	5/13 (38%)	5 (100%)	0	0	100	100
2	L	1/13 (8%)	1 (100%)	0	0	100	100
2	M	3/13 (23%)	3 (100%)	0	0	100	100
2	N	3/13 (23%)	3 (100%)	0	0	100	100
2	Z	1/13 (8%)	1 (100%)	0	0	100	100
All	All	1437/1579 (91%)	1399 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	164/173 (95%)	161 (98%)	3 (2%)	59	83
1	B	165/173 (95%)	162 (98%)	3 (2%)	59	83
1	C	166/173 (96%)	161 (97%)	5 (3%)	41	70
1	D	165/173 (95%)	159 (96%)	6 (4%)	35	64
1	E	168/173 (97%)	164 (98%)	4 (2%)	49	77
1	F	169/173 (98%)	159 (94%)	10 (6%)	19	43
1	G	168/173 (97%)	166 (99%)	2 (1%)	71	88
1	H	168/173 (97%)	143 (85%)	25 (15%)	3	7
2	I	1/8 (12%)	1 (100%)	0	100	100
2	J	3/8 (38%)	2 (67%)	1 (33%)	0	0
2	K	4/8 (50%)	1 (25%)	3 (75%)	0	0
2	L	1/8 (12%)	0	1 (100%)	0	0
2	M	3/8 (38%)	2 (67%)	1 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	2/8 (25%)	0	2 (100%)	0	0
2	Z	1/8 (12%)	0	1 (100%)	0	0
All	All	1348/1440 (94%)	1281 (95%)	67 (5%)	24	51

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	605	GLU
1	B	615	ARG
1	B	687	ASN
1	C	605	GLU
1	C	611	LYS
1	C	615	ARG
1	C	701	LYS
1	C	745	SER
2	J	17	ARG
2	K	11	ARG
2	K	13	ARG
2	K	17	ARG
1	D	637	GLU
1	D	641	GLU
1	D	676	SER
1	D	728	ASP
1	D	734	GLU
1	D	745	SER
1	E	596	LEU
1	E	676	SER
1	E	695	GLU
1	E	739	ARG
2	L	17	ARG
1	F	601	LYS
1	F	602	ASP
1	F	606	ASN
1	F	610	PHE
1	F	611	LYS
1	F	651	ASN
1	F	658	SER
1	F	676	SER
1	F	703	LYS
1	F	730	LYS
1	A	570	SER

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Mol	Chain	Res	Type
1	A	640	SER
1	A	676	SER
1	G	599	ASP
1	G	606	ASN
2	N	13	ARG
2	N	17	ARG
1	H	566	PHE
1	H	568	ILE
1	H	571	ILE
1	H	572	VAL
1	H	593	SER
1	H	601	LYS
1	H	608	ARG
1	H	610	PHE
1	H	612	SER
1	H	618	ASP
1	H	636	ASP
1	H	641	GLU
1	H	657	LEU
1	H	658	SER
1	H	668	SER
1	H	682	ILE
1	H	684	ARG
1	H	687	ASN
1	H	688	LEU
1	H	724	ARG
1	H	727	ASP
1	H	730	LYS
1	H	740	ASN
1	H	743	GLN
1	H	745	SER
2	M	18	LYS
2	Z	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2MR	I	15	2	10,12,13	0.79	0	5,13,15	0.79	0
2	2MR	L	15	2	10,12,13	1.23	1 (10%)	5,13,15	1.90	1 (20%)
2	2MR	M	15	2	10,12,13	0.59	0	5,13,15	1.89	1 (20%)
2	2MR	N	15	2	10,12,13	1.11	1 (10%)	5,13,15	2.32	3 (60%)
2	2MR	O	15	-	10,12,13	0.57	0	5,13,15	0.73	0
2	2MR	J	15	2	10,12,13	1.34	1 (10%)	5,13,15	1.48	1 (20%)
2	2MR	Z	15	2	10,12,13	0.69	0	5,13,15	0.52	0
2	2MR	K	15	2	10,12,13	0.52	0	5,13,15	1.63	1 (20%)

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	2MR	I	15	2	-	4/10/13/15	-
2	2MR	L	15	2	-	3/10/13/15	-
2	2MR	M	15	2	-	4/10/13/15	-
2	2MR	N	15	2	-	4/10/13/15	-
2	2MR	O	15	-	-	1/10/13/15	-
2	2MR	J	15	2	-	6/10/13/15	-
2	2MR	Z	15	2	-	2/10/13/15	-
2	2MR	K	15	2	-	4/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	15	2MR	CZ-NH2	-3.10	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	15	2MR	CZ-NH2	-2.97	1.26	1.33
2	N	15	2MR	CZ-NH2	-2.59	1.27	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	15	2MR	CG-CD-NE	4.11	123.95	112.21
2	L	15	2MR	CD-NE-CZ	3.67	130.28	123.41
2	N	15	2MR	CQ2-NH2-CZ	-2.96	117.33	123.86
2	N	15	2MR	CB-CG-CD	2.56	119.74	112.05
2	K	15	2MR	CG-CD-NE	2.40	119.06	112.21
2	J	15	2MR	NE-CZ-NH2	2.36	121.65	119.48
2	N	15	2MR	NE-CZ-NH2	2.27	121.56	119.48

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	15	2MR	N-CA-CB-CG
2	I	15	2MR	C-CA-CB-CG
2	J	15	2MR	C-CA-CB-CG
2	J	15	2MR	NE-CZ-NH2-CQ2
2	J	15	2MR	NH1-CZ-NH2-CQ2
2	K	15	2MR	N-CA-CB-CG
2	K	15	2MR	C-CA-CB-CG
2	L	15	2MR	NH1-CZ-NE-CD
2	L	15	2MR	NH2-CZ-NE-CD
2	N	15	2MR	NH1-CZ-NE-CD
2	N	15	2MR	NH2-CZ-NE-CD
2	M	15	2MR	O-C-CA-CB
2	M	15	2MR	NH1-CZ-NH2-CQ2
2	Z	15	2MR	NE-CZ-NH2-CQ2
2	Z	15	2MR	NH1-CZ-NH2-CQ2
2	O	15	2MR	NE-CD-CG-CB
2	I	15	2MR	NE-CD-CG-CB
2	L	15	2MR	NE-CD-CG-CB
2	K	15	2MR	NE-CD-CG-CB
2	N	15	2MR	NE-CD-CG-CB
2	I	15	2MR	CA-CB-CG-CD
2	K	15	2MR	CA-CB-CG-CD
2	M	15	2MR	CA-CB-CG-CD
2	M	15	2MR	NE-CZ-NH2-CQ2

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Mol	Chain	Res	Type	Atoms
2	N	15	2MR	CG-CD-NE-CZ
2	J	15	2MR	NH2-CZ-NE-CD
2	J	15	2MR	NH1-CZ-NE-CD
2	J	15	2MR	N-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	15	2MR	1	0
2	L	15	2MR	3	0
2	N	15	2MR	1	0
2	O	15	2MR	3	0
2	J	15	2MR	4	0
2	Z	15	2MR	3	0
2	K	15	2MR	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	176/186 (94%)	0.33	6 (3%) 45 45	32, 48, 72, 89	0
1	B	178/186 (95%)	0.15	1 (0%) 89 91	32, 47, 76, 97	0
1	C	179/186 (96%)	0.15	1 (0%) 89 91	33, 48, 74, 94	0
1	D	178/186 (95%)	0.72	22 (12%) 4 3	40, 63, 85, 99	0
1	E	180/186 (96%)	0.55	13 (7%) 15 13	38, 64, 88, 103	0
1	F	182/186 (97%)	0.10	2 (1%) 80 82	37, 53, 77, 96	0
1	G	181/186 (97%)	0.28	5 (2%) 53 54	37, 53, 80, 91	0
1	H	181/186 (97%)	0.87	28 (15%) 2 1	44, 75, 108, 123	0
2	I	3/13 (23%)	0.88	0 100 100	59, 59, 69, 82	0
2	J	6/13 (46%)	0.80	0 100 100	65, 76, 84, 89	0
2	K	7/13 (53%)	1.96	3 (42%) 0 0	63, 68, 83, 85	0
2	L	3/13 (23%)	1.58	1 (33%) 0 0	82, 82, 83, 100	0
2	M	5/13 (38%)	0.27	1 (20%) 1 0	67, 75, 80, 87	0
2	N	5/13 (38%)	0.20	0 100 100	58, 58, 85, 92	0
2	O	0/13	-	-	-	-
2	Z	2/13 (15%)	0.22	0 100 100	69, 69, 69, 73	0
All	All	1466/1592 (92%)	0.41	83 (5%) 23 22	32, 55, 87, 123	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	699	TYR	4.8
1	H	661	ALA	4.8
2	K	12	GLY	4.3
1	H	642	TYR	4.3
1	D	712	HIS	4.2
1	H	622	ALA	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	659	CYS	4.2
1	H	644	ILE	4.2
1	E	713	LEU	4.1
1	D	573	GLY	3.9
1	D	713	LEU	3.9
2	K	11	ARG	3.9
1	H	598	TRP	3.8
2	K	17	ARG	3.8
1	D	574	ILE	3.7
1	H	623	LEU	3.7
1	H	641	GLU	3.7
1	D	572	VAL	3.7
1	H	599	ASP	3.6
1	H	634	ILE	3.6
1	G	610	PHE	3.4
1	H	637	GLU	3.4
1	G	620	VAL	3.3
1	D	722	LEU	3.2
1	H	638	PHE	3.2
1	D	576	ILE	3.2
1	D	704	LEU	3.2
1	H	660	LEU	3.1
1	A	605	GLU	3.1
1	E	711	VAL	3.1
2	L	17	ARG	3.1
1	E	573	GLY	3.1
1	H	620	VAL	2.9
1	H	566	PHE	2.9
1	A	659	CYS	2.9
1	D	711	VAL	2.8
1	D	589	PHE	2.8
1	F	632	ALA	2.8
1	E	741	TYR	2.8
1	D	719	ASP	2.8
1	E	570	SER	2.7
1	H	663	CYS	2.7
1	A	688	LEU	2.7
1	E	725	PHE	2.7
1	E	687	ASN	2.6
1	D	744	VAL	2.6
1	H	596	LEU	2.6
1	G	634	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	572	VAL	2.6
1	E	566	PHE	2.6
1	H	575	LEU	2.6
1	D	736	LEU	2.5
1	G	644	ILE	2.5
1	A	709	MET	2.5
1	H	565	HIS	2.4
1	E	704	LEU	2.4
1	E	712	HIS	2.4
1	H	708	GLU	2.4
1	D	715	GLN	2.3
1	C	742	ALA	2.3
1	D	676	SER	2.3
1	D	575	LEU	2.3
1	D	732	ILE	2.3
1	A	629	PHE	2.3
1	E	735	GLN	2.3
1	H	600	LYS	2.3
1	A	658	SER	2.2
1	D	630	TYR	2.2
1	H	605	GLU	2.2
1	D	709	MET	2.2
1	F	728	ASP	2.2
2	M	17	ARG	2.2
1	D	588	GLN	2.2
1	H	567	GLU	2.1
1	H	711	VAL	2.1
1	H	643	MET	2.1
1	H	655	VAL	2.1
1	H	621	LEU	2.1
1	D	714	VAL	2.1
1	D	602	ASP	2.1
1	B	568	ILE	2.0
1	G	642	TYR	2.0
1	H	632	ALA	2.0

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

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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2MR	O	15	13/14	0.86	0.24	52,54,72,73	0
2	2MR	Z	15	13/14	0.90	0.20	48,52,74,80	0
2	2MR	J	15	13/14	0.91	0.25	41,45,69,72	0
2	2MR	M	15	13/14	0.91	0.22	33,44,67,67	0
2	2MR	K	15	13/14	0.92	0.21	32,36,59,60	0
2	2MR	N	15	13/14	0.93	0.20	36,43,65,66	0
2	2MR	L	15	13/14	0.93	0.18	34,45,68,74	0
2	2MR	I	15	13/14	0.94	0.20	34,45,60,65	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.