



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:39 PM UTC

PDB ID : 7CFD / pdb_00007cfd
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

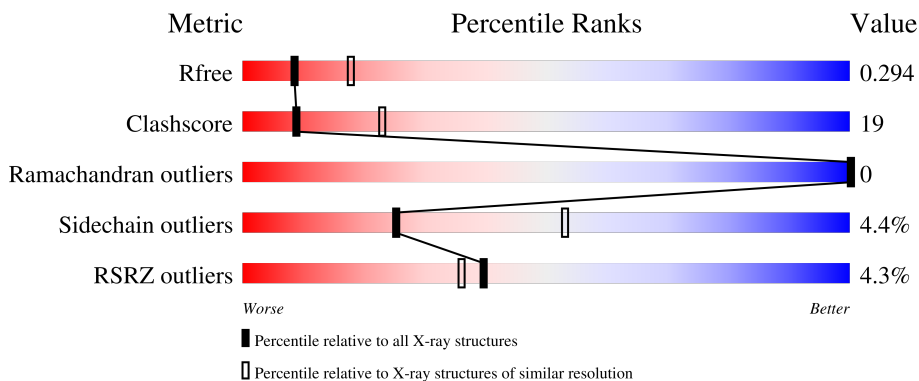
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	 2% 73% 22% • 5%
1	B	186	 2% 77% 18% •
1	C	186	 % 67% 26% • •
1	D	186	 7% 64% 28% • •
1	E	186	 5% 62% 33% • •

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Mol	Chain	Length	Quality of chain
1	F	186	<p>3% 74% 19% 5%</p>
1	G	186	<p>% 77% 20%</p>
1	H	186	<p>13% 44% 46% 8%</p>
2	I	13	<p>8% 23% 69%</p>
2	J	13	<p>23% 23% 8% 46%</p>
2	K	13	<p>8% 23% 15% 23% 38%</p>
2	L	13	<p>15% 8% 8% 69%</p>
2	M	13	<p>23% 15% 8% 54%</p>
2	N	13	<p>31% 8% 8% 54%</p>
2	O	13	<p>8% 92%</p>
2	Z	13	<p>8% 8% 8% 77%</p>

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			

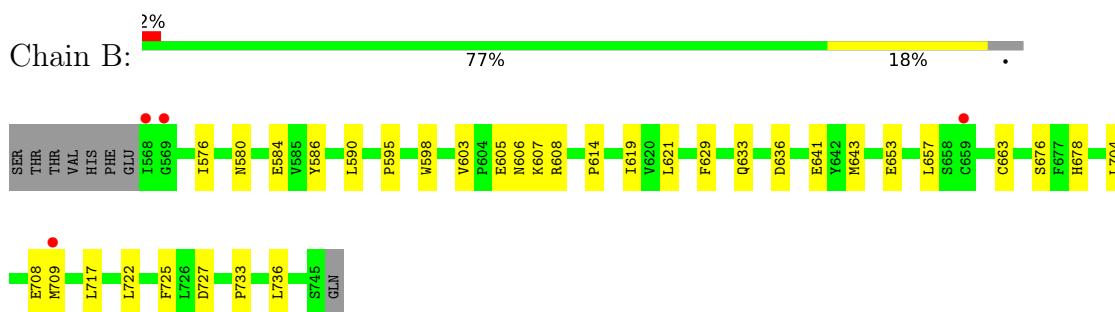
- Molecule 3 is water.

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		

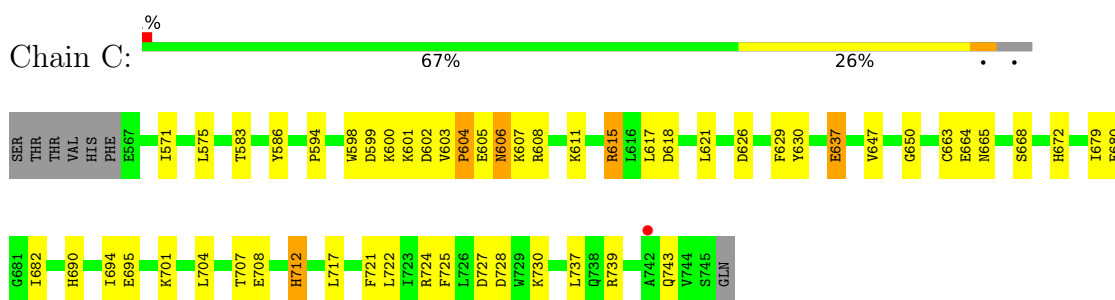
3 Residue-property plots [i](#)

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.

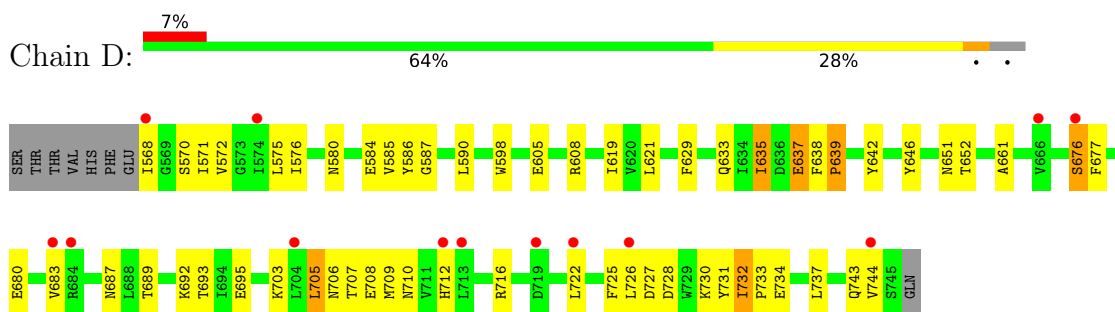
- Molecule 1: FI20010p1



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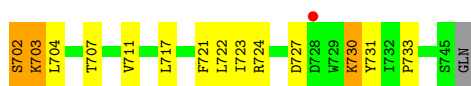
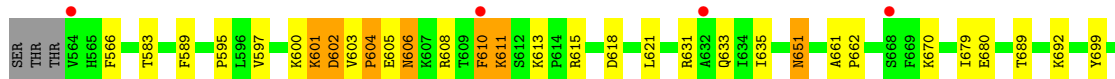
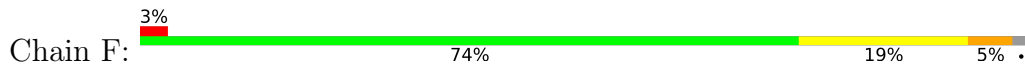


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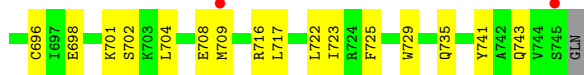




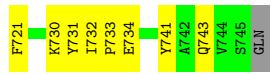
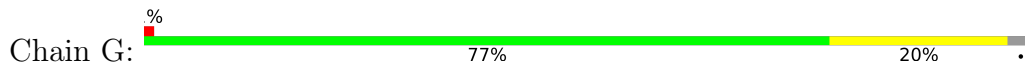
● Molecule 1: FI20010p1



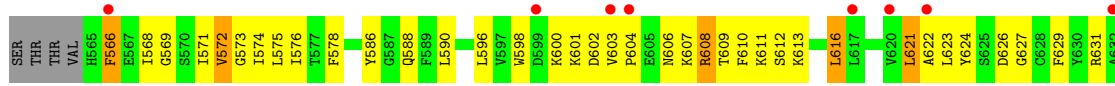
● Molecule 1: FI20010p1

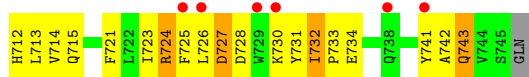


● Molecule 1: FI20010p1

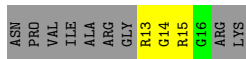


● Molecule 1: FI20010p1





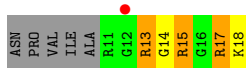
- Molecule 2: Protein aubergine



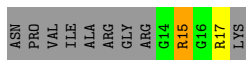
- Molecule 2: Protein aubergine



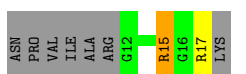
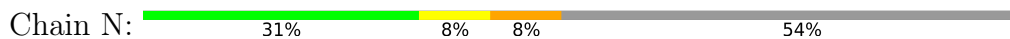
- Molecule 2: Protein aubergine



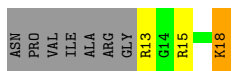
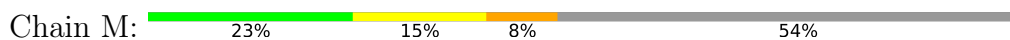
- Molecule 2: Protein aubergine



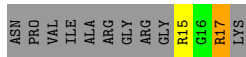
- Molecule 2: Protein aubergine



- Molecule 2: Protein aubergine



- Molecule 2: Protein aubergine



- Molecule 2: Protein aubergine

Chain O:  

ASN	PRO	VAL	ILE	ALA	ARG	GLY	ARG	GLY	R15	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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.14 3260	Depositor
R, R_{free}	0.243 , 0.290 0.244 , 0.294	Depositor DCC
R_{free} test set	2533 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtrriage
Anisotropy	0.994	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

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	0.50	0/1487	0.57	0/2018
1	B	0.26	0/1499	0.47	0/2034
1	C	0.54	2/1508 (0.1%)	0.70	3/2046 (0.1%)
1	D	0.59	2/1499 (0.1%)	0.73	2/2034 (0.1%)
1	E	0.47	0/1525	0.87	6/2070 (0.3%)
1	F	0.60	0/1538	0.89	4/2087 (0.2%)
1	G	0.40	0/1531	0.60	0/2077
1	H	0.75	0/1531	1.11	2/2077 (0.1%)
2	I	0.66	0/17	1.07	0/18
2	J	0.79	0/41	1.86	0/48
2	K	0.90	0/52	1.53	1/62 (1.6%)
2	L	0.71	0/17	0.86	0/18
2	M	0.74	0/37	1.47	0/43
2	N	0.94	0/32	1.29	0/37
2	Z	0.67	0/14	1.45	0/16
All	All	0.54	4/12328 (0.0%)	0.78	18/16685 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	732	ILE	CA-CB	-6.72	1.50	1.54
1	C	594	PRO	CA-C	6.20	1.57	1.52
1	C	604	PRO	C-O	-5.49	1.16	1.23
1	D	639	PRO	C-O	-5.03	1.17	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	686	LYS	N-CA-C	-9.87	98.60	112.13
1	E	602	ASP	CA-C-N	-9.75	115.97	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	602	ASP	C-N-CA	-9.75	115.97	122.60
1	E	565	HIS	CA-CB-CG	-8.42	105.38	113.80
1	E	565	HIS	CA-C-N	-8.29	111.33	122.85
1	E	565	HIS	C-N-CA	-8.29	111.33	122.85
1	H	613	LYS	N-CA-C	-6.64	99.60	109.42
1	F	604	PRO	CA-C-N	6.43	128.90	120.28
1	F	604	PRO	C-N-CA	6.43	128.90	120.28
1	C	604	PRO	CA-C-N	6.41	129.19	120.54
1	C	604	PRO	C-N-CA	6.41	129.19	120.54
1	D	584	GLU	CB-CA-C	-5.65	100.42	109.75
1	C	712	HIS	CB-CA-C	-5.29	101.61	110.19
1	D	584	GLU	N-CA-C	5.08	117.53	109.24
1	F	702	SER	CA-C-N	-5.06	113.81	122.11
1	F	702	SER	C-N-CA	-5.06	113.81	122.11
2	K	13	ARG	CB-CG-CD	5.02	122.85	111.30
1	E	566	PHE	CA-CB-CG	-5.01	108.79	113.80

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	1448	0	1440	39	0
1	B	1460	0	1454	32	0
1	C	1469	0	1460	50	0
1	D	1460	0	1454	58	0
1	E	1484	0	1472	52	0
1	F	1497	0	1485	43	0
1	G	1490	0	1476	27	0
1	H	1490	0	1476	151	0
2	I	32	0	34	5	0
2	J	56	0	63	8	0
2	K	67	0	76	6	0
2	L	32	0	34	3	0
2	M	52	0	60	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	449	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 19.

All (449) 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:B:709:MET:HE1	1:B:725:PHE:CE1	1.78	1.19
1:A:709:MET:HE1	1:A:725:PHE:CD1	1.80	1.15
1:H:704:LEU:HD21	1:H:732:ILE:CD1	1.76	1.15
1:H:709:MET:HE1	1:H:725:PHE:HE1	1.13	1.14
1:H:709:MET:HE1	1:H:725:PHE:CE1	1.84	1.13
1:E:695:GLU:HG2	1:H:643:MET:HE1	1.21	1.12
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: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
1:H:604:PRO:HG2	1:H:607:LYS:HB2	1.35	1.06
1:B:709:MET:HE1	1:B:725:PHE:CD1	1.90	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:H:598:TRP:CZ3	1:H:621:LEU:HD11	1.93	1.03
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:695:GLU:CG	1:H:643:MET:HE1	2.00	0.92
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: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: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:B:709:MET:CE	1:B:725:PHE:HE1	1.86	0.87
1:A:709:MET:HE1	1:A:725:PHE:HD1	1.27	0.87
1:H:685:SER:HB2	1:H:688:LEU:HD13	1.54	0.87
1:A:709:MET:HE1	1:A:725:PHE:CE1	2.10	0.87
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
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:H:680:GLU:CD	1:H:724:ARG:HG3	2.02	0.83
1:B:709:MET:CE	1:B:725:PHE:CD1	2.63	0.82
1:A:709:MET:CE	1:A:725:PHE:CD1	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:600:LYS:HE2	1:F:608:ARG:HH12	1.45	0.81
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: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:A:709:MET:CE	1:A:725:PHE:HD1	1.96	0.77
1:F:602:ASP:O	1:F:604:PRO:CD	2.34	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:B:636:ASP:HB2	1:B:643:MET:HE3	1.68	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
1:H:616:LEU:H	1:H:616:LEU:CD1	2.03	0.71
1:D:726:LEU:C	1:D:730:LYS:HG3	2.15	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:B:709:MET:HE2	1:B:725:PHE:HE1	1.54	0.70
1:D:689:THR:HG1	1:D:692:LYS:H	1.37	0.70
1:B:641:GLU:OE1	1:C:739:ARG:NH2	2.23	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:685:SER:O	1:H:743:GLN:CG	2.43	0.67
1:B:580:ASN:ND2	1:B:584:GLU:OE2	2.22	0.66
1:B:643:MET:HE2	1:C:695:GLU:OE2	1.96	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:680:GLU:CD	1:H:724:ARG:HD3	2.21	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:H:709:MET:CE	1:H:725:PHE:CE1	2.66	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
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:709:MET:HE1	1:H:725:PHE:CD1	2.32	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:680:GLU:CD	1:H:724:ARG:CG	2.71	0.62
1:H:588:GLN:HG2	1:H:673:ARG:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:664:GLU:CD	1:C:664:GLU:H	2.08	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: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:D:709:MET:HE1	1:D:725:PHE:CE2	2.37	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:651:ASN:CG	2:Z:15:2MR:CQ1	2.75	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:E:695:GLU:CG	1:H:643:MET:CE	2.68	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
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:B:605:GLU:HG2	1:B:608:ARG:HB2	1.87	0.56
1:B:636:ASP:CB	1:B:643:MET:HE3	2.34	0.56
1:G:731:TYR:HA	1:G:734:GLU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:605:GLU:H	1:D:605:GLU:CD	2.13	0.55
1:F:633:GLN:HG2	1:F:635:ILE:HD12	1.89	0.55
1:H:598:TRP:O	1:H:629:PHE:N	2.31	0.55
1:G:731:TYR:O	1:G:732:ILE:C	2.49	0.55
1:F:610:PHE:CD2	1:F:662:PRO:CG	2.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:G:603:VAL:HG12	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:A:636:ASP:HB2	1:A:643:MET:HE2	1.92	0.51
1:D:709:MET:HE1	1:D:725:PHE:HE2	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: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:H:680:GLU:CD	1:H:724:ARG:CD	2.83	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: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:E:574:ILE:HD11	1:E:709:MET:HE2	1.94	0.49
1:E:695:GLU:CD	1:H:643:MET:HE1	2.35	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
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:E:695:GLU:OE2	1:H:643:MET:HE1	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:TRP:HB2	1:B:629:PHE:HB2	1.96	0.48
1:A:584:GLU:CD	1:A:678:HIS:HE2	2.21	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:B:709:MET:HE2	1:B:725:PHE:CE1	2.34	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:D:730:LYS:C	1:D:733:PRO:HD2	2.39	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:F:731:TYR:CD1	1:F:731:TYR:C	2.93	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:631:ARG:HH21	1:H:648:ASP:CG	2.23	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:641:GLU:N	1:H:641:GLU:CD	2.73	0.46
1:H:680:GLU:OE2	1:H:724:ARG:CD	2.63	0.46
1:H:726:LEU:HD13	1:H:726:LEU:C	2.36	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: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: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:A:709:MET:CE	1:A:725:PHE:HE1	2.29	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:E:717:LEU:HD12	1:E:717:LEU:C	2.42	0.44
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:E:704:LEU:O	1:E:707:THR:OG1	2.36	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: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:573:GLY:C	1:H:590:LEU:HD12	2.43	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:B:709:MET:CE	1:B:725:PHE:HD1	2.23	0.43
1:C:571:ILE:HD11	1:C:712:HIS:HE1	1.83	0.43
1:C:601:LYS:NZ	3:C:804:HOH:O	2.43	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:G:646:TYR:OH	1:G:653:GLU:OE1	2.29	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:G:685:SER:HB2	1:G:741:TYR:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:659:CYS:SG	1:H:660:LEU:N	2.92	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: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
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:C:717:LEU:HD12	1:C:721:PHE:C	2.46	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:C:704:LEU:C	1:C:707:THR:HG22	2.39	0.41
1:E:686:LYS:NZ	3:E:802:HOH:O	2.53	0.41
1:G:591:ASP:OD1	1:G:593:SER:OG	2.34	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
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: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:689:THR:O	1:H:690:HIS:C	2.64	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: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%)	163 (99%)	1 (1%)	78	91
1	B	165/173 (95%)	165 (100%)	0	100	100
1	C	166/173 (96%)	159 (96%)	7 (4%)	26	55
1	D	165/173 (95%)	160 (97%)	5 (3%)	36	66
1	E	168/173 (97%)	163 (97%)	5 (3%)	36	66
1	F	169/173 (98%)	160 (95%)	9 (5%)	20	46
1	G	168/173 (97%)	167 (99%)	1 (1%)	78	91
1	H	168/173 (97%)	142 (84%)	26 (16%)	2	7
2	I	1/8 (12%)	1 (100%)	0	100	100
2	J	3/8 (38%)	3 (100%)	0	100	100
2	K	4/8 (50%)	3 (75%)	1 (25%)	0	2
2	L	1/8 (12%)	0	1 (100%)	0	0
2	M	3/8 (38%)	2 (67%)	1 (33%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	2/8 (25%)	1 (50%)	1 (50%)	0	0
2	Z	1/8 (12%)	0	1 (100%)	0	0
All	All	1348/1440 (94%)	1289 (96%)	59 (4%)	25	53

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	603	VAL
1	C	605	GLU
1	C	606	ASN
1	C	611	LYS
1	C	615	ARG
1	C	637	GLU
1	C	701	LYS
2	K	17	ARG
1	D	635	ILE
1	D	637	GLU
1	D	676	SER
1	D	705	LEU
1	D	734	GLU
1	E	603	VAL
1	E	695	GLU
1	E	738	GLN
1	E	739	ARG
1	E	740	ASN
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	703	LYS
1	F	727	ASP
1	F	730	LYS
1	A	686	LYS
1	G	599	ASP
2	N	17	ARG
1	H	566	PHE
1	H	568	ILE
1	H	571	ILE

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Mol	Chain	Res	Type
1	H	572	VAL
1	H	601	LYS
1	H	602	ASP
1	H	608	ARG
1	H	610	PHE
1	H	612	SER
1	H	616	LEU
1	H	621	LEU
1	H	635	ILE
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	732	ILE
1	H	743	GLN
2	M	18	LYS
2	Z	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	691	GLN
1	C	687	ASN
1	C	706	ASN
1	C	712	HIS
1	D	580	ASN
1	D	633	GLN
1	D	687	ASN
1	D	706	ASN
1	E	672	HIS
1	E	710	ASN
1	F	580	ASN
1	F	710	ASN
1	G	651	ASN

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Mol	Chain	Res	Type
1	G	672	HIS
1	G	687	ASN
1	H	710	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	N	15	2	10,12,13	1.16	1 (10%)	5,13,15	2.35	3 (60%)
2	2MR	Z	15	2	10,12,13	0.71	0	5,13,15	0.55	0
2	2MR	O	15	-	10,12,13	0.59	0	5,13,15	0.73	0
2	2MR	K	15	2	10,12,13	0.53	0	5,13,15	1.66	1 (20%)
2	2MR	M	15	2	10,12,13	0.60	0	5,13,15	1.93	1 (20%)
2	2MR	J	15	2	10,12,13	1.39	1 (10%)	5,13,15	1.48	1 (20%)
2	2MR	I	15	2	10,12,13	0.80	0	5,13,15	0.81	0
2	2MR	L	15	2	10,12,13	1.28	1 (10%)	5,13,15	1.90	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2MR	N	15	2	-	4/10/13/15	-
2	2MR	Z	15	2	-	2/10/13/15	-
2	2MR	O	15	-	-	1/10/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2MR	K	15	2	-	4/10/13/15	-
2	2MR	M	15	2	-	4/10/13/15	-
2	2MR	J	15	2	-	6/10/13/15	-
2	2MR	I	15	2	-	4/10/13/15	-
2	2MR	L	15	2	-	3/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	15	2MR	CZ-NH2	-3.28	1.26	1.33
2	L	15	2MR	CZ-NH2	-3.15	1.26	1.33
2	N	15	2MR	CZ-NH2	-2.75	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	4.19	123.95	112.20
2	L	15	2MR	CD-NE-CZ	3.68	130.28	123.36
2	N	15	2MR	CQ2-NH2-CZ	-2.94	117.33	123.65
2	N	15	2MR	CB-CG-CD	2.66	119.74	112.07
2	K	15	2MR	CG-CD-NE	2.45	119.06	112.20
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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	176/186 (94%)	0.19	3 (1%) 69 67	32, 48, 72, 89	0
1	B	178/186 (95%)	0.17	4 (2%) 62 59	32, 48, 76, 97	0
1	C	179/186 (96%)	0.13	1 (0%) 85 85	33, 48, 74, 94	0
1	D	178/186 (95%)	0.68	13 (7%) 21 18	40, 63, 85, 99	0
1	E	180/186 (96%)	0.60	9 (5%) 34 30	38, 64, 88, 103	0
1	F	182/186 (97%)	0.20	5 (2%) 56 53	37, 53, 77, 96	0
1	G	181/186 (97%)	0.33	2 (1%) 78 76	37, 53, 80, 91	0
1	H	181/186 (97%)	0.98	25 (13%) 6 5	44, 75, 108, 123	0
2	I	3/13 (23%)	1.18	0 100 100	59, 59, 69, 82	0
2	J	6/13 (46%)	1.37	0 100 100	65, 76, 84, 89	0
2	K	7/13 (53%)	1.13	1 (14%) 6 5	63, 68, 83, 85	0
2	L	3/13 (23%)	1.13	0 100 100	82, 82, 83, 100	0
2	M	5/13 (38%)	1.04	0 100 100	67, 75, 80, 87	0
2	N	5/13 (38%)	0.65	0 100 100	58, 58, 85, 92	0
2	O	0/13	-	-	-	-
2	Z	2/13 (15%)	0.54	0 100 100	69, 69, 69, 73	0
All	All	1466/1592 (92%)	0.42	63 (4%) 40 36	32, 55, 87, 123	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	722	LEU	3.8
1	E	699	TYR	3.7
1	H	634	ILE	3.5
1	B	568	ILE	3.4
1	A	659	CYS	3.4
1	B	569	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	661	ALA	3.2
1	H	566	PHE	3.1
1	H	637	GLU	3.1
1	H	617	LEU	3.0
1	D	712	HIS	3.0
1	H	726	LEU	3.0
1	H	729	TRP	3.0
1	D	568	ILE	2.9
1	H	730	LYS	2.9
1	A	709	MET	2.8
1	H	603	VAL	2.8
1	F	610	PHE	2.8
1	E	562	THR	2.8
1	D	704	LEU	2.7
2	K	12	GLY	2.6
1	E	687	ASN	2.6
1	F	564	VAL	2.6
1	B	709	MET	2.6
1	D	666	VAL	2.5
1	H	599	ASP	2.5
1	E	682	ILE	2.5
1	H	644	ILE	2.5
1	H	620	VAL	2.5
1	H	738	GLN	2.5
1	H	659	CYS	2.5
1	E	713	LEU	2.5
1	H	741	TYR	2.5
1	F	632	ALA	2.4
1	D	574	ILE	2.4
1	E	741	TYR	2.3
1	H	642	TYR	2.3
1	H	660	LEU	2.3
1	E	737	LEU	2.3
1	H	632	ALA	2.2
1	H	662	PRO	2.2
1	E	681	GLY	2.2
1	G	566	PHE	2.2
1	H	643	MET	2.2
1	C	742	ALA	2.2
1	A	745	SER	2.2
1	H	725	PHE	2.2
1	G	568	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	622	ALA	2.1
1	D	684	ARG	2.1
1	D	676	SER	2.1
1	E	725	PHE	2.1
1	H	711	VAL	2.1
1	D	719	ASP	2.1
1	D	713	LEU	2.1
1	H	688	LEU	2.1
1	B	659	CYS	2.1
1	D	744	VAL	2.1
1	H	604	PRO	2.0
1	D	726	LEU	2.0
1	F	728	ASP	2.0
1	F	668	SER	2.0
1	D	683	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	2MR	Z	15	13/14	0.86	0.12	48,52,74,80	0
2	2MR	O	15	13/14	0.86	0.12	52,54,72,73	0
2	2MR	N	15	13/14	0.87	0.13	36,43,65,66	0
2	2MR	M	15	13/14	0.87	0.13	33,44,67,67	0
2	2MR	K	15	13/14	0.88	0.11	32,36,59,60	0
2	2MR	J	15	13/14	0.89	0.11	41,45,69,72	0
2	2MR	L	15	13/14	0.89	0.10	34,45,68,74	0
2	2MR	I	15	13/14	0.92	0.10	34,45,60,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.