Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 03:50 PM EST

PDB ID	:	4GM3
Title	:	Crystal structure of human WD repeat domain 5 with compound MM-101
Authors	:	Karatas, H.; Townsend, E.C.; Chen, Y.; Bernard, D.; Cao, F.; Liu, L.; Lei, M.; Dou, Y.; Wang, S.
Deposited on	:	2012-08-15
Resolution	:	3.39 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:

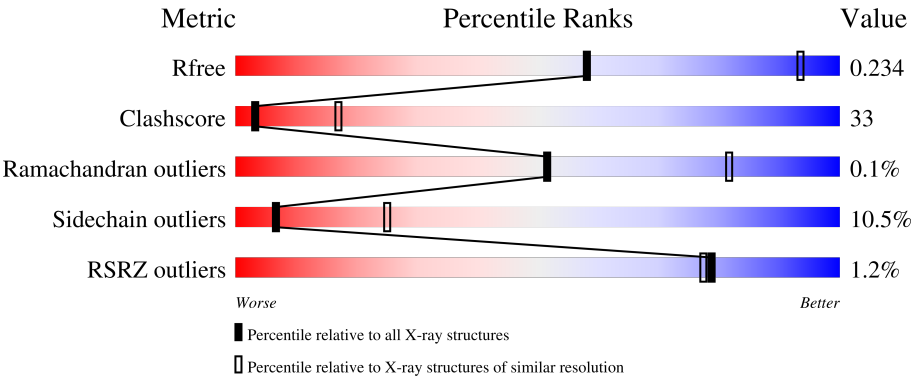
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	313	2% 46% 45% 6%
1	B	313	% 43% 48% 5%
1	C	313	2% 45% 47% 5%
1	D	313	% 43% 47% 6%
1	E	313	% 44% 47% 6%

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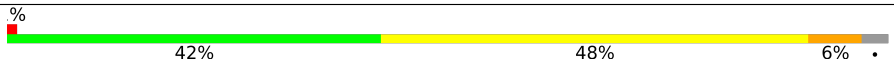
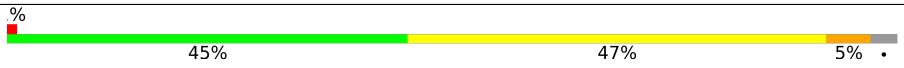
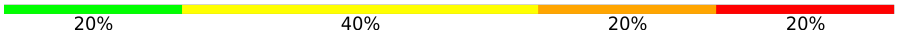
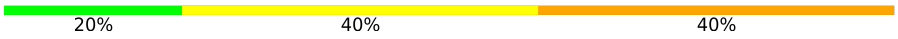
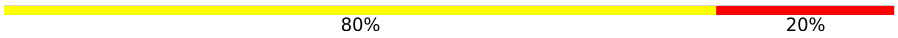
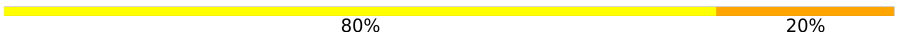
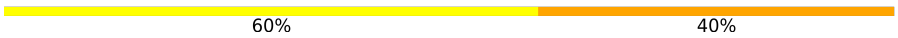
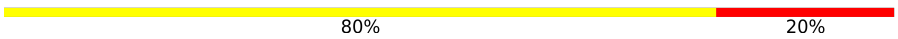
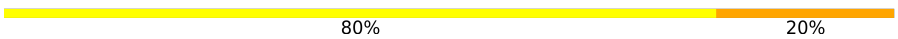
Mol	Chain	Length	Quality of chain
1	F	313	
1	G	313	
1	H	313	
2	I	5	
2	J	5	
2	K	5	
2	L	5	
2	M	5	
2	N	5	
2	O	5	
2	P	5	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AC5	L	4	-	-	X	-
2	AC5	M	4	-	-	X	-
2	AC5	O	4	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19224 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 WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2357	1503	393	451	10			
1	B	304	Total	C	N	O	S	0	0	0
			2357	1503	393	451	10			
1	C	304	Total	C	N	O	S	0	0	0
			2357	1503	393	451	10			
1	D	304	Total	C	N	O	S	0	0	0
			2357	1503	393	451	10			
1	E	304	Total	C	N	O	S	0	0	0
			2357	1503	393	451	10			
1	F	304	Total	C	N	O	S	0	0	0
			2357	1503	393	451	10			
1	G	304	Total	C	N	O	S	0	0	0
			2357	1503	393	451	10			
1	H	304	Total	C	N	O	S	0	0	0
			2357	1503	393	451	10			

- Molecule 2 is a protein called MM-101.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	5	Total	C	N	O	0	0	0
			46	35	7	4			
2	J	5	Total	C	N	O	0	0	0
			46	35	7	4			
2	K	5	Total	C	N	O	0	0	0
			46	35	7	4			
2	L	5	Total	C	N	O	0	0	0
			46	35	7	4			
2	M	5	Total	C	N	O	0	0	0
			46	35	7	4			
2	N	5	Total	C	N	O	0	0	0
			46	35	7	4			

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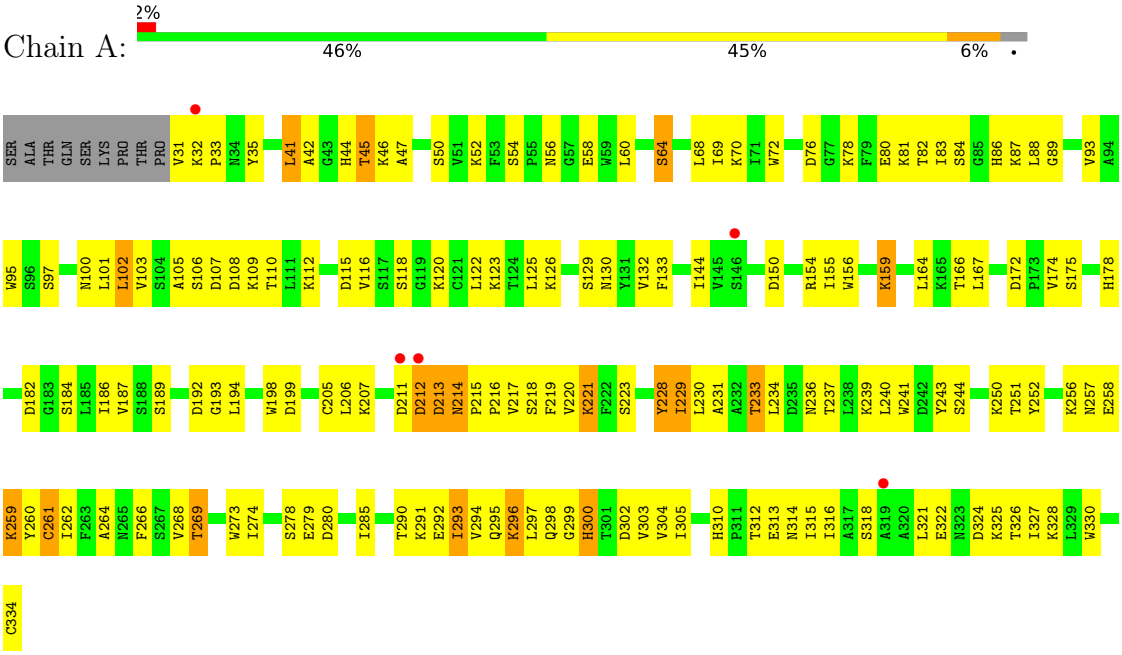
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	5	Total	C	N	O	0	0	0
			46	35	7	4			
2	P	5	Total	C	N	O	0	0	0
			46	35	7	4			

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.

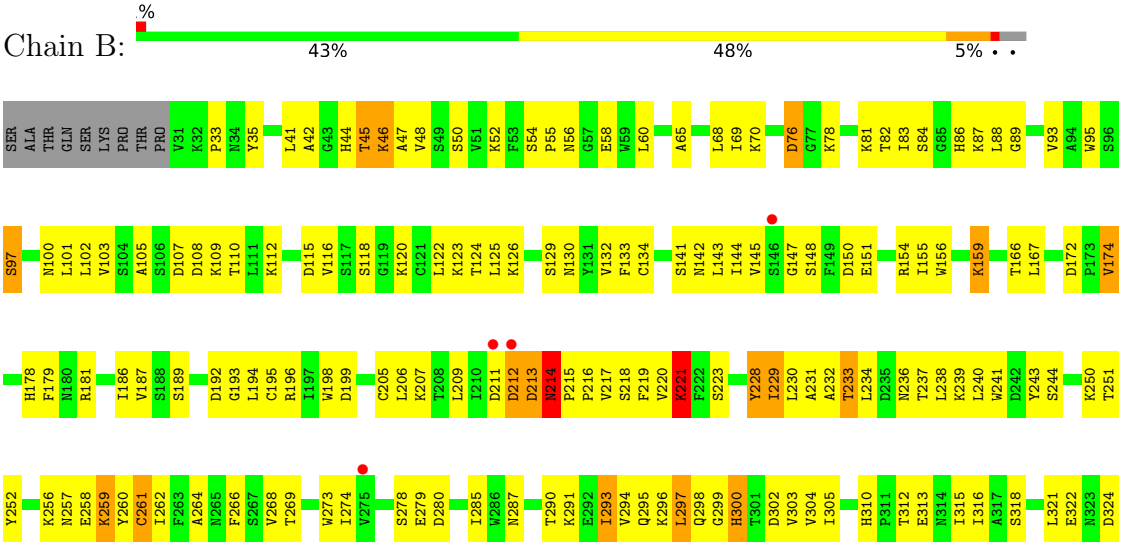
• Molecule 1: WD repeat-containing protein 5

Chain A:

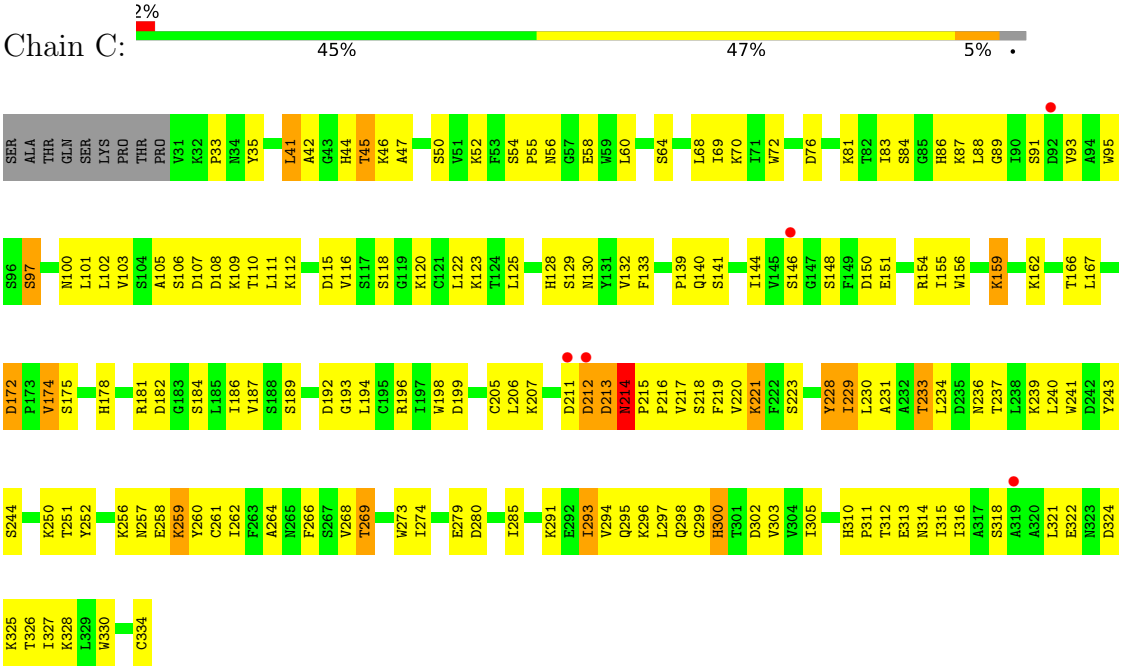


• Molecule 1: WD repeat-containing protein 5

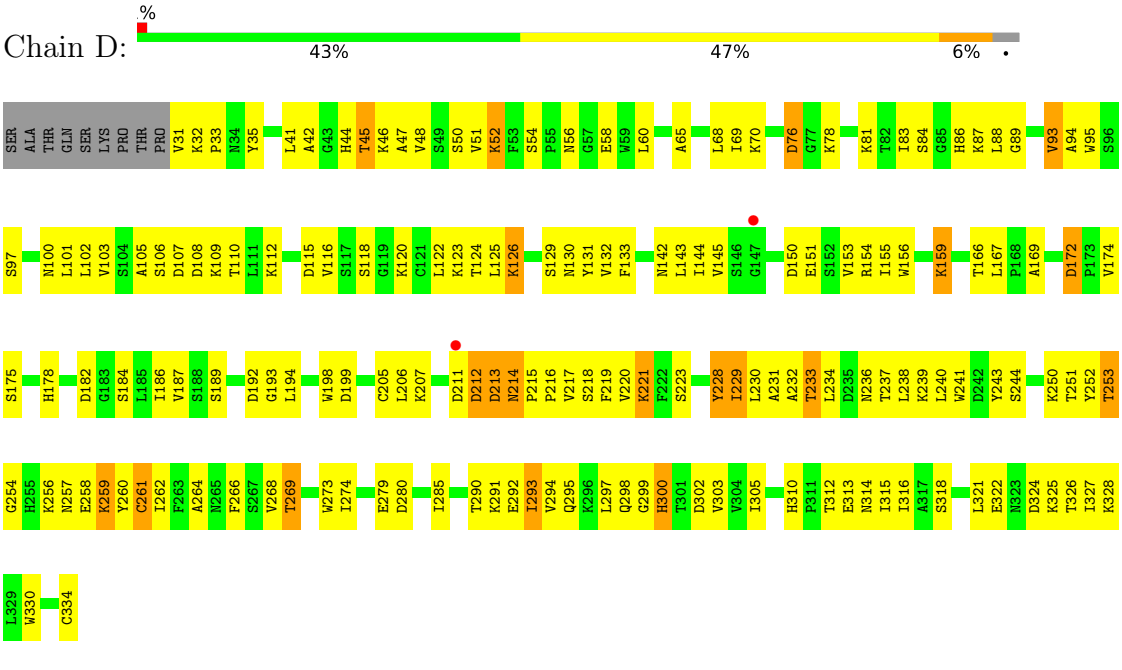
Chain B:



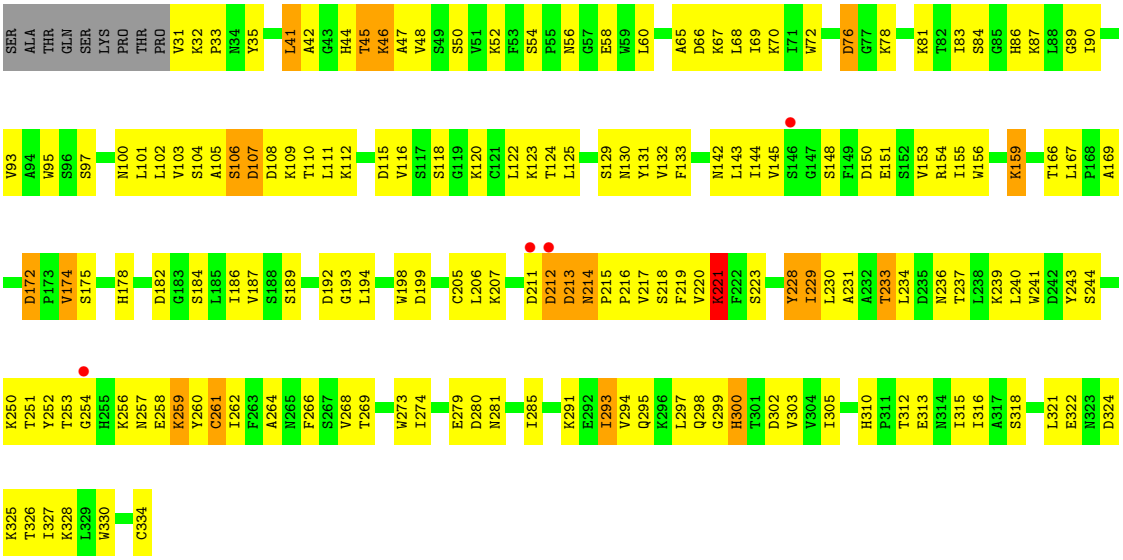
• Molecule 1: WD repeat-containing protein 5



• Molecule 1: WD repeat-containing protein 5

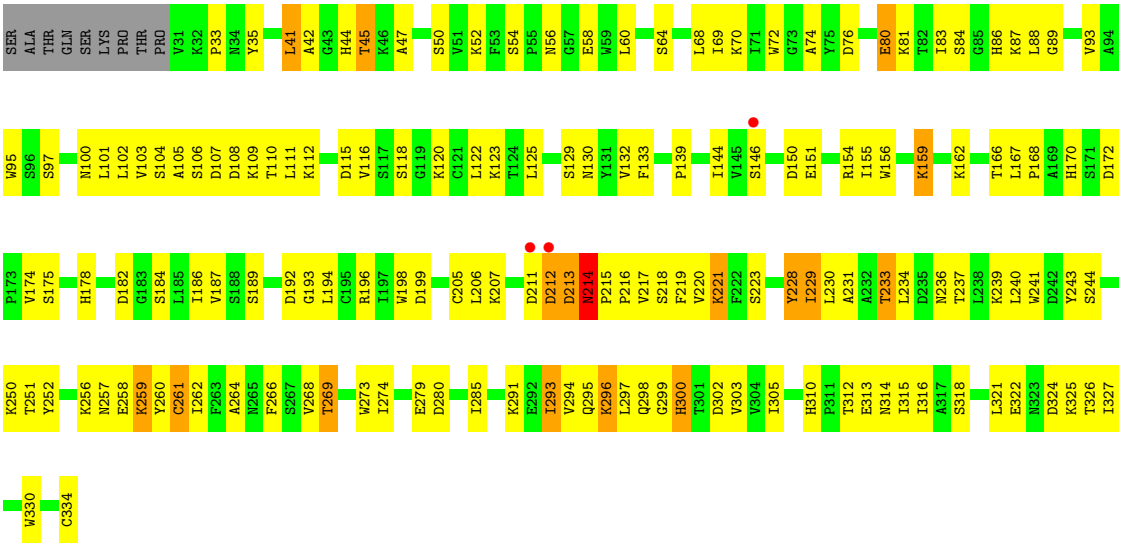


• Molecule 1: WD repeat-containing protein 5



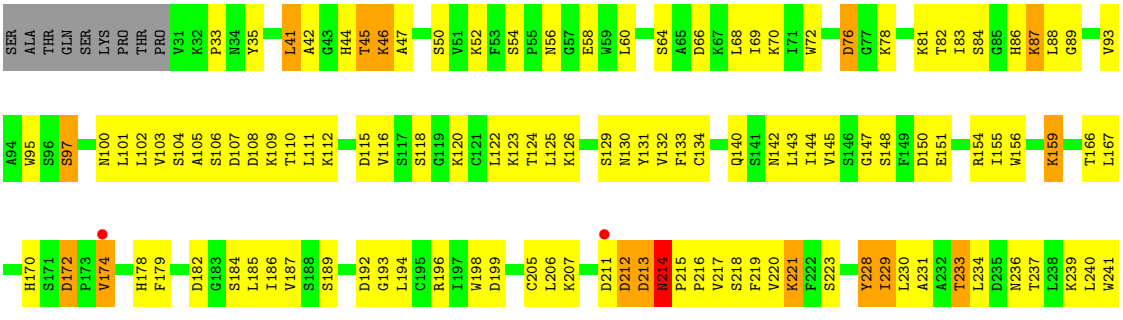
• Molecule 1: WD repeat-containing protein 5

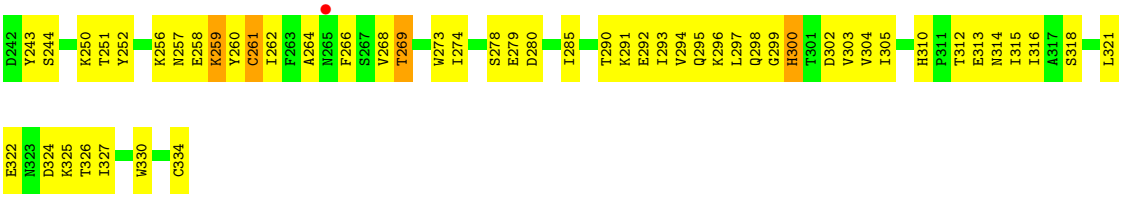
Chain F:



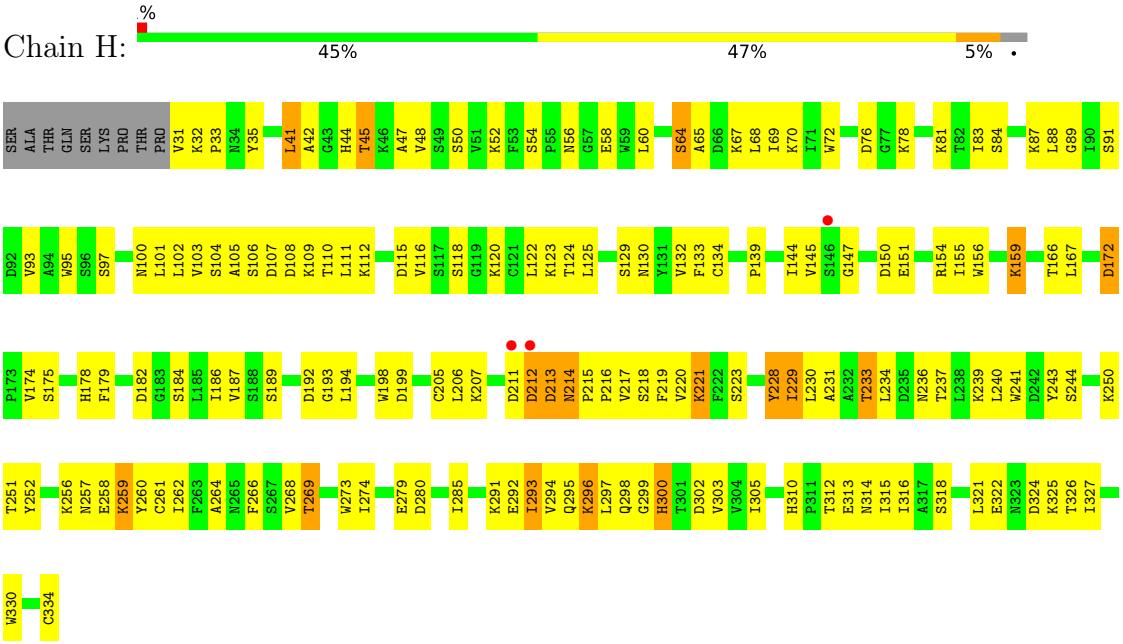
• Molecule 1: WD repeat-containing protein 5

Chain G:

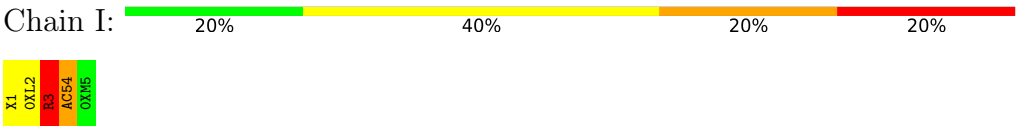




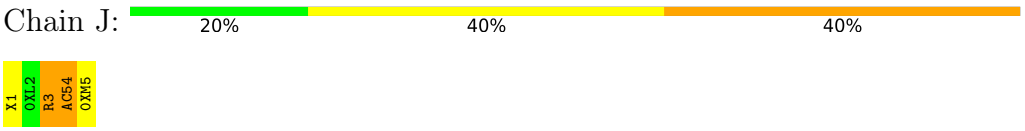
• Molecule 1: WD repeat-containing protein 5



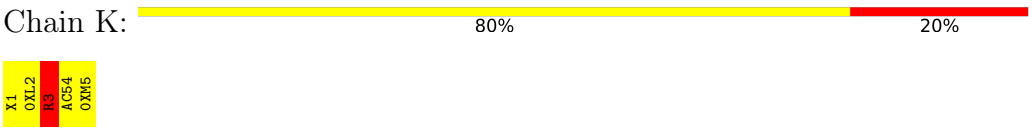
• Molecule 2: MM-101



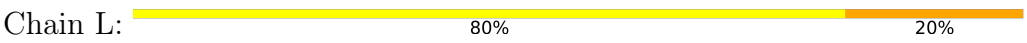
• Molecule 2: MM-101



• Molecule 2: MM-101

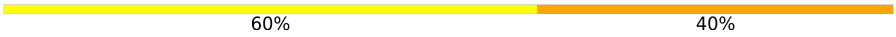


• Molecule 2: MM-101



- Molecule 2: MM-101

Chain M:



- Molecule 2: MM-101

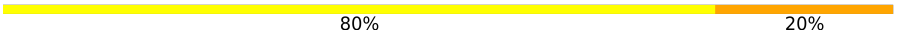
Chain N:

- Molecule 2: MM-101

Chain O:

- Molecule 2: MM-101

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.94Å 105.98Å 120.91Å 90.00° 89.76° 90.03°	Depositor
Resolution (Å)	48.54 – 3.39 48.54 – 3.39	Depositor EDS
% Data completeness (in resolution range)	89.8 (48.54-3.39) 89.4 (48.54-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.28 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.195 , 0.226 0.199 , 0.234	Depositor DCC
R_{free} test set	1554 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	1.547	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 27.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.409 for h,-k,-l 0.409 for -h,k,-l 0.409 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19224	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.32 % 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 1.3439e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0XM, AC5, ALQ, 0XL

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	0.61	3/2413 (0.1%)	0.76	2/3272 (0.1%)
1	B	0.59	2/2413 (0.1%)	0.78	6/3272 (0.2%)
1	C	0.62	2/2413 (0.1%)	0.76	2/3272 (0.1%)
1	D	0.60	4/2413 (0.2%)	0.77	3/3272 (0.1%)
1	E	0.64	4/2413 (0.2%)	0.78	5/3272 (0.2%)
1	F	0.61	3/2413 (0.1%)	0.74	1/3272 (0.0%)
1	G	0.59	3/2413 (0.1%)	0.74	1/3272 (0.0%)
1	H	0.57	2/2413 (0.1%)	0.74	1/3272 (0.0%)
2	I	3.66	2/10 (20.0%)	6.98	2/11 (18.2%)
2	J	3.88	2/10 (20.0%)	6.62	2/11 (18.2%)
2	K	3.82	1/10 (10.0%)	6.32	2/11 (18.2%)
2	L	3.64	1/10 (10.0%)	6.63	2/11 (18.2%)
2	M	3.60	1/10 (10.0%)	6.46	2/11 (18.2%)
2	N	3.46	2/10 (20.0%)	7.11	2/11 (18.2%)
2	O	3.97	1/10 (10.0%)	5.89	2/11 (18.2%)
2	P	4.04	1/10 (10.0%)	7.02	2/11 (18.2%)
All	All	0.65	34/19384 (0.2%)	0.85	37/26264 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	3	ARG	NE-CZ	10.94	1.47	1.33
2	P	3	ARG	NE-CZ	10.90	1.47	1.33
2	L	3	ARG	NE-CZ	10.49	1.46	1.33
2	K	3	ARG	NE-CZ	9.94	1.46	1.33
2	M	3	ARG	NE-CZ	9.84	1.45	1.33
2	J	3	ARG	NE-CZ	8.95	1.44	1.33
1	B	214	ASN	CG-ND2	-7.41	1.14	1.32
1	G	214	ASN	CG-ND2	-7.30	1.14	1.32
1	C	214	ASN	CG-ND2	-7.16	1.15	1.32
1	F	80	GLU	CG-CD	7.15	1.62	1.51
2	I	3	ARG	NE-CZ	7.10	1.42	1.33
2	N	3	ARG	NE-CZ	7.08	1.42	1.33
2	J	3	ARG	CZ-NH2	6.97	1.42	1.33
1	E	214	ASN	CG-OD1	-6.97	1.08	1.24
1	D	214	ASN	CG-OD1	-6.96	1.08	1.24
1	D	214	ASN	CG-ND2	-6.96	1.15	1.32
2	I	3	ARG	CZ-NH2	6.88	1.42	1.33
1	E	214	ASN	CG-ND2	-6.87	1.15	1.32
1	F	214	ASN	CG-ND2	-6.86	1.15	1.32
1	A	214	ASN	CG-OD1	-6.77	1.09	1.24
1	A	214	ASN	CG-ND2	-6.75	1.16	1.32
1	B	214	ASN	CG-OD1	-6.69	1.09	1.24
1	H	214	ASN	CG-OD1	-6.68	1.09	1.24
1	G	214	ASN	CG-OD1	-6.60	1.09	1.24
1	H	214	ASN	CG-ND2	-6.50	1.16	1.32
1	C	214	ASN	CG-OD1	-6.41	1.09	1.24
2	N	3	ARG	CZ-NH2	6.18	1.41	1.33
1	F	214	ASN	CG-OD1	-6.01	1.10	1.24
1	A	80	GLU	CD-OE1	5.72	1.31	1.25
1	E	107	ASP	CB-CG	-5.72	1.39	1.51
1	G	46	LYS	CD-CE	5.33	1.64	1.51
1	D	46	LYS	CD-CE	5.30	1.64	1.51
1	E	46	LYS	CD-CE	5.16	1.64	1.51
1	D	46	LYS	CE-NZ	5.10	1.61	1.49

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	3	ARG	NE-CZ-NH1	18.96	129.78	120.30
2	J	3	ARG	NE-CZ-NH1	18.83	129.72	120.30
2	I	3	ARG	NE-CZ-NH1	18.41	129.51	120.30
2	P	3	ARG	NE-CZ-NH1	17.59	129.09	120.30
2	L	3	ARG	NE-CZ-NH1	17.47	129.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	3	ARG	NE-CZ-NH1	16.53	128.57	120.30
2	K	3	ARG	NE-CZ-NH1	16.02	128.31	120.30
2	O	3	ARG	NE-CZ-NH1	15.96	128.28	120.30
2	P	3	ARG	NE-CZ-NH2	-14.26	113.17	120.30
2	N	3	ARG	NE-CZ-NH2	-12.63	113.98	120.30
2	I	3	ARG	NE-CZ-NH2	-12.52	114.04	120.30
2	M	3	ARG	NE-CZ-NH2	-12.52	114.04	120.30
2	L	3	ARG	NE-CZ-NH2	-12.22	114.19	120.30
2	K	3	ARG	NE-CZ-NH2	-11.95	114.32	120.30
2	J	3	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	D	87	LYS	CD-CE-NZ	9.45	133.43	111.70
1	B	46	LYS	CB-CG-CD	9.42	136.09	111.60
2	O	3	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	E	107	ASP	CB-CG-OD1	-9.04	110.17	118.30
1	A	87	LYS	CD-CE-NZ	8.72	131.76	111.70
1	B	87	LYS	CD-CE-NZ	8.54	131.34	111.70
1	E	87	LYS	CD-CE-NZ	8.47	131.19	111.70
1	G	87	LYS	CD-CE-NZ	8.34	130.88	111.70
1	E	107	ASP	CB-CG-OD2	7.94	125.45	118.30
1	B	46	LYS	CD-CE-NZ	7.71	129.42	111.70
1	H	87	LYS	CD-CE-NZ	6.71	127.13	111.70
1	D	126	LYS	CD-CE-NZ	6.62	126.92	111.70
1	C	87	LYS	CD-CE-NZ	6.59	126.86	111.70
1	B	46	LYS	CA-CB-CG	6.45	127.58	113.40
1	F	87	LYS	CD-CE-NZ	6.25	126.09	111.70
1	B	46	LYS	CG-CD-CE	5.38	128.04	111.90
1	E	46	LYS	CD-CE-NZ	5.33	123.97	111.70
1	B	221	LYS	CD-CE-NZ	5.23	123.72	111.70
1	D	46	LYS	CD-CE-NZ	5.21	123.68	111.70
1	E	221	LYS	CD-CE-NZ	5.13	123.49	111.70
1	C	46	LYS	CD-CE-NZ	5.03	123.27	111.70
1	A	46	LYS	CD-CE-NZ	5.01	123.22	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	LYS	Mainchain
1	B	126	LYS	Mainchain

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	2357	0	2339	149	0
1	B	2357	0	2339	146	0
1	C	2357	0	2339	156	0
1	D	2357	0	2339	168	0
1	E	2357	0	2338	169	0
1	F	2357	0	2339	157	0
1	G	2357	0	2339	164	0
1	H	2357	0	2339	155	0
2	I	46	0	38	18	0
2	J	46	0	38	12	0
2	K	46	0	39	24	0
2	L	46	0	39	23	0
2	M	46	0	39	24	0
2	N	46	0	39	19	0
2	O	46	0	39	24	0
2	P	46	0	39	28	0
All	All	19224	0	19021	1265	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 33.

All (1265) 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)
2:M:1:ALQ:HM1	2:M:4:AC5:HB22	1.27	1.10
1:H:321:LEU:HD22	2:P:4:AC5:HG12	1.24	1.08
1:E:321:LEU:HD22	2:M:4:AC5:CG1	1.84	1.07
2:L:1:ALQ:HM1	2:L:4:AC5:HB22	1.35	1.06
1:D:253:THR:HG21	1:E:253:THR:HG21	1.05	1.05
1:C:250:LYS:HB3	1:C:291:LYS:HD3	1.37	1.04
1:E:321:LEU:HD22	2:M:4:AC5:HG11	1.40	1.03
1:G:89:GLY:HA3	2:O:1:ALQ:HB3	1.41	1.03
1:A:213:ASP:HB2	1:A:215:PRO:HD3	1.41	1.02
2:L:5:0XM:H32	2:L:5:0XM:H27	1.39	1.02
1:B:250:LYS:HB3	1:B:291:LYS:HD3	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:LYS:HB3	1:G:291:LYS:HD3	1.40	1.01
1:E:250:LYS:HB3	1:E:291:LYS:HD3	1.40	1.00
1:F:250:LYS:HB3	1:F:291:LYS:HD3	1.42	0.99
1:B:213:ASP:HB2	1:B:215:PRO:HD3	1.41	0.99
1:H:213:ASP:HB2	1:H:215:PRO:HD3	1.43	0.99
1:D:250:LYS:HB3	1:D:291:LYS:HD3	1.42	0.99
1:C:213:ASP:HB2	1:C:215:PRO:HD3	1.40	0.99
1:B:293:ILE:H	1:B:293:ILE:HD12	1.27	0.99
1:D:321:LEU:CD2	2:L:4:AC5:HG12	1.94	0.97
1:H:89:GLY:HA3	2:P:1:ALQ:HB3	1.46	0.97
2:J:1:ALQ:HM1	2:J:4:AC5:HB22	1.47	0.96
1:E:321:LEU:CD2	2:M:4:AC5:HG11	1.96	0.94
1:H:250:LYS:HB3	1:H:291:LYS:HD3	1.47	0.94
1:A:250:LYS:HB3	1:A:291:LYS:HD3	1.47	0.94
1:E:293:ILE:HD12	1:E:293:ILE:H	1.31	0.94
2:P:5:0XM:H36	2:P:5:0XM:CBM	1.96	0.93
1:C:321:LEU:CD2	2:K:4:AC5:HG12	1.98	0.93
1:D:213:ASP:HB2	1:D:215:PRO:HD3	1.50	0.93
1:D:293:ILE:HD12	1:D:293:ILE:H	1.32	0.93
1:D:256:LYS:HE2	1:E:256:LYS:HE2	1.48	0.92
1:G:89:GLY:HA3	2:O:1:ALQ:CB	1.97	0.92
1:C:91:SER:O	2:K:3:ARG:HD2	1.69	0.92
1:C:100:ASN:HB3	1:C:101:LEU:HG	1.50	0.92
1:E:213:ASP:HB2	1:E:215:PRO:HD3	1.52	0.92
2:L:5:0XM:H32	2:L:5:0XM:CBI	1.98	0.92
1:B:256:LYS:HD2	1:B:280:ASP:HB3	1.52	0.92
1:A:298:GLN:HG2	1:A:299:GLY:H	1.34	0.91
1:G:321:LEU:HD22	2:O:4:AC5:HG12	1.52	0.91
1:D:253:THR:HG21	1:E:253:THR:CG2	1.97	0.91
1:G:293:ILE:HD12	1:G:293:ILE:H	1.31	0.91
1:H:100:ASN:HB3	1:H:101:LEU:HG	1.50	0.91
1:C:321:LEU:HD22	2:K:4:AC5:HG12	1.53	0.91
1:D:237:THR:HG21	1:D:239:LYS:HE3	1.50	0.91
1:F:213:ASP:HB2	1:F:215:PRO:HD3	1.53	0.91
1:F:100:ASN:HB3	1:F:101:LEU:HG	1.52	0.91
1:C:293:ILE:HD12	1:C:293:ILE:H	1.36	0.90
1:H:133:PHE:CE2	2:P:3:ARG:HA	2.06	0.90
1:G:100:ASN:HB3	1:G:101:LEU:HG	1.52	0.90
1:C:240:LEU:HD12	1:C:241:TRP:H	1.37	0.90
1:A:100:ASN:HB3	1:A:101:LEU:HG	1.52	0.89
1:A:293:ILE:HD12	1:A:293:ILE:H	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:ILE:HD12	1:F:293:ILE:H	1.37	0.89
1:G:298:GLN:HG2	1:G:299:GLY:H	1.37	0.89
1:E:100:ASN:HB3	1:E:101:LEU:HG	1.53	0.89
1:G:213:ASP:HB2	1:G:215:PRO:HD3	1.53	0.89
1:A:89:GLY:HA3	2:I:1:ALQ:HB3	1.53	0.89
1:D:129:SER:HB3	1:D:150:ASP:HB3	1.54	0.89
1:E:259:LYS:HD3	2:M:5:0XM:H29	1.54	0.89
1:D:100:ASN:HB3	1:D:101:LEU:HG	1.52	0.88
1:H:298:GLN:HG2	1:H:299:GLY:H	1.37	0.88
1:B:100:ASN:HB3	1:B:101:LEU:HG	1.52	0.88
1:H:256:LYS:HD2	1:H:280:ASP:HB3	1.54	0.88
1:D:298:GLN:HG2	1:D:299:GLY:H	1.36	0.88
1:G:129:SER:HB3	1:G:150:ASP:HB3	1.54	0.88
1:G:256:LYS:HD2	1:G:280:ASP:HB3	1.56	0.88
1:A:237:THR:HG21	1:A:239:LYS:HE3	1.56	0.88
1:H:240:LEU:HD12	1:H:241:TRP:H	1.36	0.88
1:G:237:THR:HG21	1:G:239:LYS:HE3	1.55	0.88
1:E:237:THR:HG21	1:E:239:LYS:HE3	1.53	0.88
1:B:192:ASP:OD1	1:B:194:LEU:HD12	1.73	0.88
1:C:129:SER:HB3	1:C:150:ASP:HB3	1.56	0.88
1:C:298:GLN:HG2	1:C:299:GLY:H	1.35	0.87
1:H:293:ILE:HD12	1:H:293:ILE:H	1.36	0.87
1:A:192:ASP:OD1	1:A:194:LEU:HD12	1.73	0.87
1:H:237:THR:HG21	1:H:239:LYS:HE3	1.55	0.87
1:F:298:GLN:HG2	1:F:299:GLY:H	1.36	0.87
1:D:89:GLY:HA3	2:L:1:ALQ:HB3	1.57	0.87
1:E:298:GLN:HG2	1:E:299:GLY:H	1.37	0.87
1:B:237:THR:HG21	1:B:239:LYS:HE3	1.56	0.87
1:D:321:LEU:HD22	2:L:4:AC5:HG12	1.54	0.87
1:A:240:LEU:HD12	1:A:241:TRP:H	1.37	0.86
1:D:256:LYS:HD2	1:D:280:ASP:HB3	1.57	0.86
1:E:256:LYS:HD2	1:E:280:ASP:HB3	1.57	0.86
1:F:129:SER:HB3	1:F:150:ASP:HB3	1.57	0.86
1:B:298:GLN:HG2	1:B:299:GLY:H	1.40	0.86
1:D:240:LEU:HD12	1:D:241:TRP:H	1.40	0.86
1:C:237:THR:HG21	1:C:239:LYS:HE3	1.55	0.86
1:F:240:LEU:HD12	1:F:241:TRP:H	1.40	0.86
1:E:129:SER:HB3	1:E:150:ASP:HB3	1.57	0.86
1:C:256:LYS:HD2	1:C:280:ASP:HB3	1.57	0.86
1:E:240:LEU:HD12	1:E:241:TRP:H	1.41	0.86
1:E:321:LEU:HD22	2:M:4:AC5:HG12	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:LEU:HD12	1:G:241:TRP:H	1.39	0.85
1:H:321:LEU:HD22	2:P:4:AC5:CG1	2.05	0.85
1:B:129:SER:HB3	1:B:150:ASP:HB3	1.58	0.85
1:D:199:ASP:HB2	1:D:206:LEU:HD11	1.58	0.85
1:F:192:ASP:OD1	1:F:194:LEU:HD12	1.75	0.85
1:F:237:THR:HG21	1:F:239:LYS:HE3	1.57	0.85
1:B:89:GLY:HA3	2:J:1:ALQ:CB	2.07	0.85
1:D:89:GLY:HA3	2:L:1:ALQ:CB	2.07	0.85
1:A:129:SER:HB3	1:A:150:ASP:HB3	1.57	0.84
1:A:256:LYS:HD2	1:A:280:ASP:HB3	1.58	0.84
1:A:107:ASP:OD2	2:I:1:ALQ:HB1	1.78	0.84
1:B:240:LEU:HD12	1:B:241:TRP:H	1.40	0.84
1:D:133:PHE:CE2	2:L:3:ARG:HA	2.12	0.84
1:G:211:ASP:O	1:G:213:ASP:OD1	1.94	0.84
1:C:192:ASP:OD1	1:C:194:LEU:HD12	1.77	0.84
1:A:199:ASP:HB2	1:A:206:LEU:HD11	1.60	0.84
1:D:192:ASP:OD1	1:D:194:LEU:HD12	1.77	0.84
1:H:192:ASP:OD1	1:H:194:LEU:HD12	1.78	0.83
1:G:192:ASP:OD1	1:G:194:LEU:HD12	1.77	0.83
1:B:211:ASP:O	1:B:213:ASP:OD1	1.95	0.83
1:D:256:LYS:HE2	1:E:256:LYS:CE	2.08	0.83
1:H:129:SER:HB3	1:H:150:ASP:HB3	1.59	0.83
1:D:298:GLN:HG2	1:D:299:GLY:N	1.94	0.83
1:A:298:GLN:HG2	1:A:299:GLY:N	1.95	0.82
1:H:91:SER:O	2:P:3:ARG:HD2	1.79	0.82
1:E:211:ASP:O	1:E:213:ASP:OD1	1.96	0.82
1:F:199:ASP:HB2	1:F:206:LEU:HD11	1.61	0.82
1:C:298:GLN:HG2	1:C:299:GLY:N	1.94	0.82
1:D:211:ASP:O	1:D:213:ASP:OD1	1.96	0.82
1:G:298:GLN:HG2	1:G:299:GLY:N	1.95	0.82
1:B:65:ALA:HB2	2:J:1:ALQ:HM2	1.62	0.81
1:C:133:PHE:CE2	2:K:3:ARG:HA	2.14	0.81
1:C:259:LYS:HD3	2:K:5:0XM:H29	1.60	0.81
1:D:256:LYS:CE	1:E:256:LYS:HE2	2.10	0.81
1:E:192:ASP:OD1	1:E:194:LEU:HD12	1.80	0.81
1:B:219:PHE:HZ	1:B:221:LYS:HZ2	1.26	0.81
1:B:298:GLN:HG2	1:B:299:GLY:N	1.96	0.81
1:H:298:GLN:HG2	1:H:299:GLY:N	1.96	0.81
1:A:211:ASP:O	1:A:213:ASP:OD1	1.99	0.81
1:E:298:GLN:HG2	1:E:299:GLY:N	1.96	0.81
1:F:196:ARG:HH22	1:G:194:LEU:CD1	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3:ARG:HH21	2:I:3:ARG:HG3	1.45	0.80
1:F:298:GLN:HG2	1:F:299:GLY:N	1.95	0.80
1:G:129:SER:HB3	1:G:150:ASP:CB	2.12	0.80
1:C:239:LYS:HG2	1:C:251:THR:HG22	1.61	0.80
1:F:211:ASP:O	1:F:213:ASP:OD1	1.99	0.79
1:B:199:ASP:HB2	1:B:206:LEU:HD11	1.64	0.79
1:A:129:SER:HB3	1:A:150:ASP:CB	2.12	0.79
1:G:133:PHE:CE2	2:O:3:ARG:HB2	2.18	0.79
1:H:211:ASP:O	1:H:213:ASP:OD1	2.01	0.79
1:H:199:ASP:HB2	1:H:206:LEU:HD11	1.64	0.79
1:H:321:LEU:CD2	2:P:4:AC5:HG12	2.11	0.79
1:B:115:ASP:HB2	1:B:122:LEU:HD11	1.64	0.79
1:E:199:ASP:HB2	1:E:206:LEU:HD11	1.65	0.79
1:C:199:ASP:HB2	1:C:206:LEU:HD11	1.65	0.78
1:D:129:SER:HB3	1:D:150:ASP:CB	2.13	0.78
1:A:239:LYS:HG2	1:A:251:THR:HG22	1.66	0.78
1:B:129:SER:HB3	1:B:150:ASP:CB	2.13	0.78
1:B:89:GLY:HA3	2:J:1:ALQ:HB3	1.66	0.78
1:C:211:ASP:O	1:C:213:ASP:OD1	2.02	0.78
1:F:256:LYS:HD2	1:F:280:ASP:HB3	1.64	0.78
1:G:199:ASP:HB2	1:G:206:LEU:HD11	1.66	0.77
1:E:115:ASP:HB2	1:E:122:LEU:HD11	1.65	0.77
1:A:133:PHE:HE2	2:I:3:ARG:N	1.82	0.77
1:C:129:SER:HB3	1:C:150:ASP:CB	2.13	0.77
1:G:239:LYS:HG2	1:G:251:THR:HG22	1.66	0.77
1:D:256:LYS:HZ3	1:E:256:LYS:NZ	1.82	0.77
1:F:129:SER:HB3	1:F:150:ASP:CB	2.14	0.77
1:E:129:SER:HB3	1:E:150:ASP:CB	2.14	0.77
1:B:239:LYS:HG2	1:B:251:THR:HG22	1.67	0.77
1:D:253:THR:CG2	1:E:253:THR:HG21	2.01	0.77
2:K:3:ARG:NH2	2:K:3:ARG:HG3	2.00	0.77
1:E:239:LYS:HG2	1:E:251:THR:HG22	1.66	0.76
1:G:321:LEU:CD2	2:O:4:AC5:HG12	2.15	0.76
1:D:115:ASP:HB2	1:D:122:LEU:HD11	1.65	0.76
1:H:239:LYS:HG2	1:H:251:THR:HG22	1.68	0.75
1:C:115:ASP:HB2	1:C:122:LEU:HD11	1.67	0.75
1:G:115:ASP:HB2	1:G:122:LEU:HD11	1.67	0.75
1:D:239:LYS:HG2	1:D:251:THR:HG22	1.68	0.75
1:D:133:PHE:HE2	2:L:3:ARG:HA	1.48	0.75
1:F:115:ASP:HB2	1:F:122:LEU:HD11	1.68	0.75
1:H:129:SER:HB3	1:H:150:ASP:CB	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:5:0XM:H36	2:P:5:0XM:H31	1.69	0.75
1:D:256:LYS:NZ	1:E:256:LYS:NZ	2.33	0.74
1:B:133:PHE:CE2	2:J:3:ARG:HA	2.22	0.74
1:G:125:LEU:HB3	1:G:156:TRP:CZ3	2.23	0.74
2:I:3:ARG:HG3	2:I:3:ARG:NH2	2.02	0.74
1:G:172:ASP:HB2	1:G:192:ASP:HB3	1.69	0.74
1:E:172:ASP:HB2	1:E:192:ASP:HB3	1.69	0.74
1:E:214:ASN:N	1:E:215:PRO:HD3	2.03	0.74
2:M:1:ALQ:HM1	2:M:4:AC5:CB2	2.14	0.74
1:E:33:PRO:HD3	1:E:273:TRP:CH2	2.23	0.73
1:H:115:ASP:HB2	1:H:122:LEU:HD11	1.68	0.73
1:H:133:PHE:HE2	2:P:3:ARG:HA	1.53	0.73
2:K:3:ARG:CG	2:K:3:ARG:HH21	2.01	0.73
1:E:89:GLY:HA3	2:M:1:ALQ:CB	2.18	0.73
1:D:108:ASP:O	1:D:109:LYS:HB2	1.86	0.73
1:B:133:PHE:HE2	2:J:3:ARG:HA	1.52	0.73
1:F:239:LYS:HG2	1:F:251:THR:HG22	1.69	0.73
1:H:219:PHE:HZ	1:H:221:LYS:HZ2	1.36	0.73
1:D:172:ASP:HB2	1:D:192:ASP:HB3	1.70	0.73
1:C:172:ASP:HB2	1:C:192:ASP:HB3	1.70	0.73
1:B:172:ASP:HB2	1:B:192:ASP:HB3	1.71	0.72
1:D:214:ASN:N	1:D:215:PRO:HD3	2.05	0.72
1:A:115:ASP:HB2	1:A:122:LEU:HD11	1.69	0.72
1:B:108:ASP:O	1:B:109:LYS:HB2	1.87	0.72
1:C:89:GLY:HA3	2:K:1:ALQ:HB3	1.70	0.72
1:H:172:ASP:HB2	1:H:192:ASP:HB3	1.72	0.72
1:C:313:GLU:HB2	1:C:315:ILE:CD1	2.20	0.72
1:A:125:LEU:HB3	1:A:156:TRP:CZ3	2.25	0.72
1:A:108:ASP:O	1:A:109:LYS:HB2	1.88	0.71
1:F:125:LEU:HB3	1:F:156:TRP:CZ3	2.26	0.71
1:D:219:PHE:HZ	1:D:221:LYS:HZ2	1.38	0.71
1:E:133:PHE:CE2	2:M:3:ARG:HA	2.26	0.71
1:A:172:ASP:HB2	1:A:192:ASP:HB3	1.73	0.70
1:C:250:LYS:CB	1:C:291:LYS:HD3	2.19	0.70
1:D:187:VAL:HG22	1:D:220:VAL:HG21	1.71	0.70
1:F:89:GLY:HA3	2:N:1:ALQ:HM2	1.71	0.70
1:F:214:ASN:N	1:F:215:PRO:HD3	2.06	0.70
1:F:313:GLU:HB2	1:F:315:ILE:CD1	2.21	0.70
1:G:108:ASP:O	1:G:109:LYS:HB2	1.88	0.70
1:D:105:ALA:HB1	1:D:132:VAL:HG12	1.72	0.70
1:E:108:ASP:O	1:E:109:LYS:HB2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:VAL:HG22	1:E:220:VAL:HG21	1.71	0.70
1:C:125:LEU:HB3	1:C:156:TRP:CZ3	2.27	0.70
1:E:103:VAL:HG21	1:E:144:ILE:HD13	1.73	0.70
1:H:214:ASN:N	1:H:215:PRO:HD3	2.06	0.70
1:C:33:PRO:HD3	1:C:273:TRP:CH2	2.27	0.70
1:B:33:PRO:HD3	1:B:273:TRP:CH2	2.27	0.70
1:D:33:PRO:HD3	1:D:273:TRP:CH2	2.27	0.70
1:G:214:ASN:N	1:G:215:PRO:HD3	2.07	0.70
1:H:108:ASP:O	1:H:109:LYS:HB2	1.90	0.70
1:D:103:VAL:HG21	1:D:144:ILE:HD13	1.73	0.69
1:F:105:ALA:HB1	1:F:132:VAL:HG12	1.73	0.69
1:A:103:VAL:HG21	1:A:144:ILE:HD13	1.73	0.69
1:B:214:ASN:N	1:B:215:PRO:HD3	2.07	0.69
1:E:250:LYS:CB	1:E:291:LYS:HD3	2.21	0.69
1:F:103:VAL:HG21	1:F:144:ILE:HD13	1.74	0.69
1:H:133:PHE:CE2	2:P:3:ARG:CA	2.75	0.69
1:C:214:ASN:N	1:C:215:PRO:HD3	2.08	0.69
1:D:42:ALA:HB2	1:D:326:THR:HG22	1.75	0.69
1:D:223:SER:HA	1:D:266:PHE:CE2	2.27	0.69
1:F:108:ASP:O	1:F:109:LYS:HB2	1.90	0.69
1:F:187:VAL:HG22	1:F:220:VAL:HG21	1.74	0.69
1:A:313:GLU:HB2	1:A:315:ILE:CD1	2.22	0.69
1:G:33:PRO:HD3	1:G:273:TRP:CH2	2.28	0.69
1:B:187:VAL:HG22	1:B:220:VAL:HG21	1.74	0.68
1:C:103:VAL:HG21	1:C:144:ILE:HD13	1.75	0.68
1:G:187:VAL:HG22	1:G:220:VAL:HG21	1.74	0.68
1:H:313:GLU:HB2	1:H:315:ILE:CD1	2.23	0.68
2:P:5:0XM:CBM	2:P:5:0XM:CBR	2.67	0.68
1:D:125:LEU:HB3	1:D:156:TRP:CZ3	2.28	0.68
1:E:259:LYS:CD	2:M:5:0XM:H29	2.22	0.68
2:N:1:ALQ:O	2:N:2:0XL:C	2.42	0.68
1:A:187:VAL:HG22	1:A:220:VAL:HG21	1.74	0.68
1:H:103:VAL:HG21	1:H:144:ILE:HD13	1.74	0.68
1:C:159:LYS:HE3	1:C:159:LYS:HA	1.75	0.68
1:F:125:LEU:HB3	1:F:156:TRP:CE3	2.29	0.68
1:A:214:ASN:N	1:A:215:PRO:HD3	2.09	0.68
1:C:54:SER:HB3	1:C:95:TRP:CE2	2.28	0.68
1:C:187:VAL:HG22	1:C:220:VAL:HG21	1.74	0.68
1:A:321:LEU:HD22	2:I:4:AC5:HB12	1.76	0.68
1:F:33:PRO:HD3	1:F:273:TRP:CH2	2.29	0.68
1:G:125:LEU:HB3	1:G:156:TRP:CE3	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:TRP:CD2	1:H:102:LEU:HD21	2.29	0.67
1:H:240:LEU:HD12	1:H:241:TRP:N	2.09	0.67
1:A:125:LEU:HB3	1:A:156:TRP:CE3	2.29	0.67
1:F:219:PHE:HZ	1:F:221:LYS:HZ2	1.42	0.67
2:P:5:0XM:H31	2:P:5:0XM:CBR	2.24	0.67
2:O:3:ARG:HG2	2:O:3:ARG:O	1.92	0.67
2:K:3:ARG:HG3	2:K:3:ARG:HH21	1.55	0.67
1:E:42:ALA:HB2	1:E:326:THR:HG22	1.77	0.67
1:H:125:LEU:HB3	1:H:156:TRP:CZ3	2.30	0.67
1:D:256:LYS:HZ3	1:E:256:LYS:HZ3	1.41	0.67
1:F:212:ASP:C	1:F:213:ASP:OD1	2.33	0.67
1:E:68:LEU:CD2	1:E:84:SER:HB3	2.25	0.67
1:H:33:PRO:HD3	1:H:273:TRP:CH2	2.30	0.67
1:D:68:LEU:CD2	1:D:84:SER:HB3	2.25	0.67
1:E:223:SER:HA	1:E:266:PHE:CE2	2.30	0.67
1:A:33:PRO:HD3	1:A:273:TRP:CH2	2.30	0.67
1:A:105:ALA:HB1	1:A:132:VAL:HG12	1.76	0.67
1:B:223:SER:HA	1:B:266:PHE:CE2	2.30	0.67
1:F:223:SER:HA	1:F:266:PHE:CE2	2.30	0.67
1:G:103:VAL:HG21	1:G:144:ILE:HD13	1.76	0.67
1:G:219:PHE:HZ	1:G:221:LYS:HZ2	1.43	0.67
1:B:125:LEU:HB3	1:B:156:TRP:CZ3	2.30	0.66
1:B:167:LEU:HD13	1:B:198:TRP:CE3	2.30	0.66
1:B:194:LEU:CD1	1:C:196:ARG:HH22	2.08	0.66
1:C:125:LEU:HB3	1:C:156:TRP:CE3	2.30	0.66
1:E:89:GLY:HA3	2:M:1:ALQ:HB3	1.77	0.66
1:H:105:ALA:HB1	1:H:132:VAL:HG12	1.76	0.66
1:A:240:LEU:HD12	1:A:241:TRP:N	2.09	0.66
1:D:250:LYS:CB	1:D:291:LYS:HD3	2.23	0.66
1:C:95:TRP:CD2	1:C:102:LEU:HD21	2.31	0.66
1:D:313:GLU:HB2	1:D:315:ILE:CD1	2.26	0.66
1:H:89:GLY:CA	2:P:1:ALQ:HB3	2.23	0.66
1:C:108:ASP:O	1:C:109:LYS:HB2	1.94	0.66
1:F:321:LEU:HD22	2:N:4:AC5:HB12	1.76	0.66
1:F:133:PHE:HE2	2:N:3:ARG:N	1.94	0.66
1:H:187:VAL:HG22	1:H:220:VAL:HG21	1.76	0.66
1:A:95:TRP:CD2	1:A:102:LEU:HD21	2.31	0.66
1:G:105:ALA:HB1	1:G:132:VAL:HG12	1.77	0.66
1:B:95:TRP:CD2	1:B:102:LEU:HD21	2.30	0.66
1:E:125:LEU:HB3	1:E:156:TRP:CZ3	2.31	0.66
1:F:250:LYS:CB	1:F:291:LYS:HD3	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:TRP:CD2	1:G:102:LEU:HD21	2.30	0.65
1:D:95:TRP:CD2	1:D:102:LEU:HD21	2.31	0.65
1:F:54:SER:HB3	1:F:95:TRP:CE2	2.31	0.65
1:F:172:ASP:HB2	1:F:192:ASP:HB3	1.77	0.65
1:E:106:SER:OG	1:E:107:ASP:N	2.30	0.65
1:F:230:LEU:HD12	1:F:231:ALA:H	1.61	0.65
1:G:68:LEU:CD2	1:G:84:SER:HB3	2.27	0.65
1:C:240:LEU:HD12	1:C:241:TRP:N	2.09	0.65
1:E:219:PHE:HZ	1:E:221:LYS:HZ2	1.44	0.65
1:H:223:SER:HA	1:H:266:PHE:CE2	2.31	0.65
1:B:212:ASP:C	1:B:213:ASP:OD1	2.35	0.65
1:B:321:LEU:CD2	2:J:4:AC5:HG12	2.27	0.65
1:C:123:LYS:NZ	1:H:292:GLU:HG2	2.12	0.65
1:D:256:LYS:NZ	1:E:256:LYS:HZ3	1.95	0.65
1:G:240:LEU:HD12	1:G:241:TRP:N	2.11	0.65
1:G:223:SER:HA	1:G:266:PHE:CE2	2.32	0.65
2:L:5:0XM:CBI	2:L:5:0XM:CBN	2.75	0.64
2:P:1:ALQ:O	2:P:2:0XL:C	2.45	0.64
1:A:219:PHE:HZ	1:A:221:LYS:HZ2	1.43	0.64
1:E:212:ASP:C	1:E:213:ASP:OD1	2.36	0.64
1:E:313:GLU:HB2	1:E:315:ILE:CD1	2.28	0.64
1:G:313:GLU:HB2	1:G:315:ILE:CD1	2.26	0.64
2:J:1:ALQ:HM1	2:J:4:AC5:CB2	2.25	0.64
1:B:230:LEU:HD12	1:B:231:ALA:H	1.63	0.64
1:E:259:LYS:HD3	2:M:5:0XM:CBK	2.26	0.64
1:G:212:ASP:C	1:G:213:ASP:OD1	2.36	0.64
1:C:60:LEU:HD21	1:C:327:ILE:HG21	1.79	0.64
1:A:223:SER:HA	1:A:266:PHE:CE2	2.32	0.64
1:B:42:ALA:HB2	1:B:326:THR:HG22	1.79	0.64
1:H:54:SER:HB3	1:H:95:TRP:CE2	2.32	0.64
1:D:212:ASP:C	1:D:213:ASP:OD1	2.36	0.64
1:A:60:LEU:HD21	1:A:327:ILE:HG21	1.79	0.63
1:F:303:VAL:HB	1:F:321:LEU:HD12	1.80	0.63
1:F:60:LEU:HD21	1:F:327:ILE:HG21	1.79	0.63
1:H:262:ILE:HG12	1:H:305:ILE:HD12	1.80	0.63
1:H:60:LEU:HD21	1:H:327:ILE:HG21	1.79	0.63
1:F:220:VAL:HA	1:F:230:LEU:O	1.99	0.63
1:A:54:SER:HB3	1:A:95:TRP:CE2	2.34	0.63
1:E:259:LYS:HE3	1:H:259:LYS:HE3	1.80	0.63
1:B:240:LEU:HD12	1:B:241:TRP:N	2.13	0.63
1:B:68:LEU:CD2	1:B:84:SER:HB3	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:SER:HB2	1:D:261:CYS:HB3	1.80	0.63
1:H:125:LEU:HB3	1:H:156:TRP:CE3	2.34	0.63
1:H:133:PHE:CZ	2:P:3:ARG:HA	2.34	0.63
2:M:5:0XM:CBM	2:M:5:0XM:H36	2.29	0.63
1:B:103:VAL:HG21	1:B:144:ILE:HD13	1.79	0.62
1:B:313:GLU:HB2	1:B:315:ILE:CD1	2.28	0.62
1:G:42:ALA:HB2	1:G:326:THR:HG22	1.80	0.62
1:H:133:PHE:HE2	2:P:3:ARG:CA	2.11	0.62
1:A:292:GLU:HG2	1:F:123:LYS:NZ	2.14	0.62
1:E:95:TRP:CD2	1:E:102:LEU:HD21	2.34	0.62
1:F:95:TRP:CD2	1:F:102:LEU:HD21	2.35	0.62
1:C:223:SER:HA	1:C:266:PHE:CE2	2.34	0.62
1:D:154:ARG:CG	1:D:166:THR:HG23	2.29	0.62
1:C:133:PHE:HE2	2:K:3:ARG:HA	1.64	0.62
1:C:321:LEU:HD22	2:K:4:AC5:CG1	2.28	0.62
1:C:154:ARG:CG	1:C:166:THR:HG23	2.29	0.62
1:D:313:GLU:HB2	1:D:315:ILE:HD12	1.82	0.62
1:C:230:LEU:HD12	1:C:231:ALA:H	1.65	0.62
1:D:240:LEU:HD12	1:D:241:TRP:N	2.12	0.62
1:E:125:LEU:HB3	1:E:156:TRP:CE3	2.35	0.62
2:I:1:ALQ:O	2:I:2:0XL:C	2.47	0.62
1:A:262:ILE:HG12	1:A:305:ILE:HD12	1.82	0.62
1:D:125:LEU:HB3	1:D:156:TRP:CE3	2.35	0.62
1:E:313:GLU:HB2	1:E:315:ILE:HD12	1.82	0.62
1:F:196:ARG:NH1	1:G:196:ARG:NH1	2.47	0.62
1:H:321:LEU:CD2	2:P:4:AC5:CG1	2.73	0.62
1:C:105:ALA:HB1	1:C:132:VAL:HG12	1.81	0.62
1:G:313:GLU:HB2	1:G:315:ILE:HD12	1.81	0.62
1:B:159:LYS:HE3	1:B:159:LYS:HA	1.81	0.62
1:C:219:PHE:HZ	1:C:221:LYS:HZ2	1.47	0.62
1:D:230:LEU:HD12	1:D:231:ALA:H	1.65	0.61
2:K:1:ALQ:O	2:K:2:0XL:C	2.48	0.61
1:C:100:ASN:CB	1:C:101:LEU:HG	2.28	0.61
1:D:54:SER:HB3	1:D:95:TRP:CE2	2.34	0.61
1:F:196:ARG:HH12	1:G:194:LEU:HD11	1.65	0.61
1:C:52:LYS:HG3	1:C:93:VAL:O	2.00	0.61
1:F:240:LEU:HD12	1:F:241:TRP:N	2.13	0.61
1:B:52:LYS:HG3	1:B:93:VAL:O	2.01	0.61
1:G:250:LYS:CB	1:G:291:LYS:HD3	2.23	0.61
1:H:100:ASN:CB	1:H:101:LEU:HG	2.28	0.61
1:C:313:GLU:HB2	1:C:315:ILE:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ALA:HB1	1:B:132:VAL:HG12	1.81	0.61
1:E:240:LEU:HD12	1:E:241:TRP:N	2.14	0.61
1:B:220:VAL:HA	1:B:230:LEU:O	2.01	0.61
1:E:218:SER:HB2	1:E:261:CYS:HB3	1.82	0.61
1:F:100:ASN:CB	1:F:101:LEU:HG	2.29	0.61
1:G:47:ALA:HB2	1:G:322:GLU:HB3	1.82	0.60
1:G:52:LYS:HG3	1:G:93:VAL:O	2.02	0.60
1:G:262:ILE:HG12	1:G:305:ILE:HD12	1.83	0.60
1:H:154:ARG:CG	1:H:166:THR:HG23	2.31	0.60
1:C:68:LEU:CD2	1:C:84:SER:HB3	2.31	0.60
1:G:303:VAL:HB	1:G:321:LEU:HD12	1.83	0.60
1:F:218:SER:HB2	1:F:261:CYS:HA	1.84	0.60
1:A:107:ASP:CG	2:I:1:ALQ:HB1	2.21	0.60
1:E:230:LEU:HD12	1:E:231:ALA:H	1.67	0.60
1:E:133:PHE:HE2	2:M:3:ARG:HA	1.65	0.60
1:G:154:ARG:CG	1:G:166:THR:HG23	2.32	0.60
1:A:230:LEU:HD12	1:A:231:ALA:H	1.67	0.60
1:A:303:VAL:HB	1:A:321:LEU:HD12	1.83	0.60
1:B:293:ILE:H	1:B:293:ILE:CD1	2.02	0.60
1:G:100:ASN:CB	1:G:101:LEU:HG	2.29	0.60
1:H:42:ALA:HB2	1:H:326:THR:HG22	1.84	0.60
2:P:3:ARG:NH2	2:P:3:ARG:HG3	2.17	0.60
1:B:250:LYS:CB	1:B:291:LYS:HD3	2.23	0.60
1:C:218:SER:HB2	1:C:261:CYS:HA	1.84	0.60
1:B:35:TYR:CE2	1:B:316:ILE:HG13	2.37	0.60
1:A:220:VAL:HA	1:A:230:LEU:O	2.02	0.59
1:B:125:LEU:HB3	1:B:156:TRP:CE3	2.37	0.59
1:B:300:HIS:ND1	1:B:324:ASP:OD2	2.35	0.59
1:G:60:LEU:HD21	1:G:327:ILE:HG21	1.82	0.59
1:G:133:PHE:HE2	2:O:3:ARG:HA	1.67	0.59
2:O:1:ALQ:HM1	2:O:4:AC5:HB22	1.84	0.59
1:E:47:ALA:HB2	1:E:322:GLU:HB3	1.84	0.59
1:E:100:ASN:O	1:E:116:VAL:HG23	2.01	0.59
1:E:154:ARG:CG	1:E:166:THR:HG23	2.31	0.59
1:E:159:LYS:HE3	1:E:159:LYS:HA	1.83	0.59
1:E:262:ILE:HG12	1:E:305:ILE:HD12	1.84	0.59
1:H:218:SER:HB2	1:H:261:CYS:HA	1.84	0.59
1:E:60:LEU:HD21	1:E:327:ILE:HG21	1.84	0.59
1:B:100:ASN:O	1:B:116:VAL:HG23	2.02	0.59
1:D:220:VAL:HA	1:D:230:LEU:O	2.02	0.59
1:C:133:PHE:CZ	2:K:3:ARG:HA	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:TYR:CE2	1:H:316:ILE:HG13	2.36	0.59
1:G:218:SER:HB2	1:G:261:CYS:HB3	1.84	0.59
1:G:300:HIS:ND1	1:G:324:ASP:OD2	2.35	0.59
1:B:313:GLU:HB2	1:B:315:ILE:HD12	1.84	0.59
1:E:35:TYR:CE2	1:E:316:ILE:HG13	2.36	0.59
1:G:159:LYS:HE3	1:G:159:LYS:HA	1.83	0.59
1:F:68:LEU:CD2	1:F:84:SER:HB3	2.33	0.59
1:G:220:VAL:HA	1:G:230:LEU:O	2.03	0.59
1:C:68:LEU:HD13	1:C:70:LYS:HE3	1.85	0.59
1:D:100:ASN:O	1:D:116:VAL:HG23	2.02	0.59
1:C:42:ALA:HB2	1:C:326:THR:HG22	1.85	0.59
1:D:262:ILE:HG12	1:D:305:ILE:HD12	1.84	0.59
1:A:68:LEU:HD13	1:A:70:LYS:HE3	1.85	0.58
1:A:154:ARG:CG	1:A:166:THR:HG23	2.32	0.58
1:G:133:PHE:HE2	2:O:3:ARG:CA	2.16	0.58
1:D:159:LYS:HE3	1:D:159:LYS:HA	1.84	0.58
1:F:194:LEU:CD1	1:G:196:ARG:HH22	2.16	0.58
1:G:100:ASN:O	1:G:116:VAL:HG23	2.03	0.58
1:A:42:ALA:HB2	1:A:326:THR:HG22	1.85	0.58
1:C:35:TYR:CE2	1:C:316:ILE:HG13	2.37	0.58
1:C:133:PHE:CE2	2:K:3:ARG:CA	2.84	0.58
1:D:60:LEU:HD21	1:D:327:ILE:HG21	1.85	0.58
1:F:262:ILE:HG12	1:F:305:ILE:HD12	1.85	0.58
1:B:262:ILE:HG12	1:B:305:ILE:HD12	1.86	0.58
1:D:303:VAL:HB	1:D:321:LEU:HD12	1.86	0.58
1:F:42:ALA:HB2	1:F:326:THR:HG22	1.85	0.58
1:F:154:ARG:CG	1:F:166:THR:HG23	2.33	0.58
1:A:159:LYS:HA	1:A:159:LYS:HE3	1.84	0.58
1:D:100:ASN:CB	1:D:101:LEU:HG	2.31	0.58
1:E:105:ALA:HB1	1:E:132:VAL:HG12	1.84	0.58
1:A:313:GLU:HB2	1:A:315:ILE:HD12	1.85	0.58
1:H:220:VAL:HA	1:H:230:LEU:O	2.04	0.58
1:B:118:SER:OG	1:B:120:LYS:HG2	2.04	0.58
1:B:196:ARG:HH22	1:C:194:LEU:CD1	2.17	0.58
1:F:47:ALA:HB2	1:F:322:GLU:HB3	1.86	0.58
2:K:2:0XL:O	2:K:5:0XM:NAV	2.37	0.58
2:O:1:ALQ:O	2:O:4:AC5:HB22	2.04	0.58
1:B:47:ALA:HB2	1:B:322:GLU:HB3	1.85	0.57
1:C:89:GLY:CA	2:K:1:ALQ:HB3	2.33	0.57
1:G:35:TYR:CE2	1:G:316:ILE:HG13	2.39	0.57
1:C:262:ILE:HG12	1:C:305:ILE:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ALA:HB2	2:L:1:ALQ:HM2	1.86	0.57
1:E:218:SER:HB2	1:E:261:CYS:HA	1.86	0.57
1:F:313:GLU:HB2	1:F:315:ILE:HD12	1.86	0.57
1:B:60:LEU:HD21	1:B:327:ILE:HG21	1.84	0.57
1:C:315:ILE:HA	1:C:330:TRP:O	2.03	0.57
1:E:300:HIS:ND1	1:E:324:ASP:OD2	2.37	0.57
1:F:35:TYR:CE2	1:F:316:ILE:HG13	2.38	0.57
1:A:218:SER:HB2	1:A:261:CYS:HB3	1.86	0.57
1:E:129:SER:O	1:H:67:LYS:HE2	2.05	0.57
1:D:47:ALA:HB2	1:D:322:GLU:HB3	1.87	0.57
1:D:321:LEU:HD22	2:L:4:AC5:CG1	2.29	0.57
1:F:196:ARG:HH22	1:G:194:LEU:HD12	1.69	0.57
2:P:2:0XL:O	2:P:5:0XM:NAV	2.37	0.57
1:B:54:SER:HB3	1:B:95:TRP:CE2	2.40	0.57
1:E:54:SER:HB3	1:E:95:TRP:CE2	2.39	0.57
1:F:133:PHE:CE2	2:N:3:ARG:HA	2.39	0.57
1:A:100:ASN:O	1:A:116:VAL:HG23	2.05	0.57
1:D:300:HIS:ND1	1:D:324:ASP:OD2	2.37	0.57
1:H:52:LYS:HG3	1:H:93:VAL:O	2.05	0.57
1:H:230:LEU:HD12	1:H:231:ALA:H	1.70	0.57
1:B:303:VAL:HB	1:B:321:LEU:HD12	1.87	0.57
1:H:100:ASN:O	1:H:116:VAL:HG23	2.05	0.57
1:E:52:LYS:HG3	1:E:93:VAL:O	2.04	0.57
1:F:159:LYS:HA	1:F:159:LYS:HE3	1.86	0.57
1:A:68:LEU:CD2	1:A:84:SER:HB3	2.35	0.56
1:F:80:GLU:OE1	1:F:80:GLU:HA	2.05	0.56
1:F:88:LEU:HB3	1:F:107:ASP:HB2	1.87	0.56
1:E:220:VAL:HA	1:E:230:LEU:O	2.04	0.56
1:F:218:SER:HB2	1:F:261:CYS:HB3	1.86	0.56
1:H:261:CYS:O	2:P:3:ARG:NH2	2.36	0.56
1:A:218:SER:HB2	1:A:261:CYS:HA	1.87	0.56
1:A:250:LYS:CB	1:A:291:LYS:HD3	2.28	0.56
1:C:88:LEU:HB3	1:C:107:ASP:HB2	1.87	0.56
1:C:189:SER:OG	1:C:220:VAL:HG22	2.05	0.56
1:D:321:LEU:HD21	2:L:4:AC5:HG12	1.83	0.56
1:H:159:LYS:HE3	1:H:159:LYS:HA	1.86	0.56
1:B:154:ARG:CG	1:B:166:THR:HG23	2.36	0.56
1:D:218:SER:HB2	1:D:261:CYS:HA	1.88	0.56
1:E:100:ASN:CB	1:E:101:LEU:HG	2.33	0.56
1:A:69:ILE:HB	1:A:83:ILE:HB	1.88	0.56
1:E:67:LYS:HE2	1:H:129:SER:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:LEU:HD13	1:F:70:LYS:HE3	1.88	0.56
1:F:100:ASN:O	1:F:116:VAL:HG23	2.05	0.56
1:A:52:LYS:HG3	1:A:93:VAL:O	2.06	0.56
1:B:218:SER:HB2	1:B:261:CYS:HA	1.88	0.56
1:D:131:TYR:CG	2:L:2:0XL:CBD	2.88	0.56
1:D:167:LEU:HD13	1:D:198:TRP:CE3	2.41	0.56
1:G:218:SER:HB2	1:G:261:CYS:HA	1.88	0.56
1:C:220:VAL:HA	1:C:230:LEU:O	2.05	0.56
1:C:162:LYS:CE	1:H:32:LYS:HZ2	2.19	0.56
1:D:69:ILE:HB	1:D:83:ILE:HB	1.88	0.56
1:D:293:ILE:H	1:D:293:ILE:CD1	2.08	0.56
1:E:69:ILE:HB	1:E:83:ILE:HB	1.88	0.56
1:H:69:ILE:HB	1:H:83:ILE:HB	1.88	0.56
1:A:133:PHE:CE2	2:I:3:ARG:N	2.70	0.55
1:A:212:ASP:C	1:A:213:ASP:OD1	2.44	0.55
1:A:315:ILE:HA	1:A:330:TRP:O	2.05	0.55
1:E:167:LEU:HD13	1:E:198:TRP:CE3	2.41	0.55
1:E:293:ILE:H	1:E:293:ILE:CD1	2.07	0.55
1:C:181:ARG:NH2	1:D:58:GLU:HG3	2.21	0.55
2:N:3:ARG:HH21	2:N:3:ARG:HG3	1.70	0.55
1:A:187:VAL:HG21	1:A:229:ILE:HD13	1.88	0.55
1:B:315:ILE:HA	1:B:330:TRP:O	2.06	0.55
1:D:155:ILE:HD11	1:D:186:ILE:CD1	2.36	0.55
1:E:118:SER:OG	1:E:120:LYS:HG2	2.07	0.55
1:A:100:ASN:CB	1:A:101:LEU:HG	2.31	0.55
1:G:230:LEU:HD12	1:G:231:ALA:H	1.72	0.55
1:A:293:ILE:H	1:A:293:ILE:CD1	2.13	0.55
1:D:133:PHE:CE2	2:L:3:ARG:CA	2.87	0.55
1:H:250:LYS:CB	1:H:291:LYS:HD3	2.28	0.55
1:E:133:PHE:CE2	2:M:3:ARG:CA	2.89	0.55
1:H:133:PHE:HE2	2:P:3:ARG:N	2.05	0.55
1:A:47:ALA:HB2	1:A:322:GLU:HB3	1.88	0.55
1:D:256:LYS:CE	1:E:256:LYS:CE	2.78	0.55
1:E:45:THR:O	1:E:325:LYS:HD3	2.07	0.55
1:E:260:TYR:CE1	2:M:4:AC5:HB12	2.42	0.55
1:E:260:TYR:HE1	2:M:4:AC5:HB12	1.72	0.55
1:C:212:ASP:C	1:C:213:ASP:OD1	2.46	0.55
1:A:35:TYR:CE2	1:A:316:ILE:HG13	2.42	0.54
1:C:56:ASN:OD1	1:C:58:GLU:HB2	2.06	0.54
1:D:35:TYR:CE2	1:D:316:ILE:HG13	2.41	0.54
1:H:212:ASP:C	1:H:213:ASP:OD1	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:313:GLU:HB2	1:H:315:ILE:HD12	1.88	0.54
1:B:69:ILE:HB	1:B:83:ILE:HB	1.89	0.54
1:H:259:LYS:HD3	2:P:5:0XM:H29	1.88	0.54
1:A:56:ASN:OD1	1:A:58:GLU:HB2	2.06	0.54
1:D:315:ILE:HA	1:D:330:TRP:O	2.06	0.54
1:F:154:ARG:HG2	1:F:166:THR:HG23	1.88	0.54
1:F:170:HIS:HA	1:G:196:ARG:HH21	1.72	0.54
1:C:154:ARG:HG2	1:C:166:THR:HG23	1.88	0.54
1:G:133:PHE:CE2	2:O:3:ARG:CB	2.91	0.54
1:G:167:LEU:HD13	1:G:198:TRP:CE3	2.42	0.54
1:H:47:ALA:HB2	1:H:322:GLU:HB3	1.89	0.54
1:H:95:TRP:CE3	1:H:102:LEU:HD21	2.43	0.54
1:F:52:LYS:HG3	1:F:93:VAL:O	2.08	0.54
1:G:68:LEU:HD23	1:G:84:SER:HB3	1.88	0.54
2:K:5:0XM:CBM	2:K:5:0XM:CBN	2.84	0.54
1:A:88:LEU:HB3	1:A:107:ASP:HB2	1.89	0.54
1:A:154:ARG:HG2	1:A:166:THR:HG23	1.89	0.54
1:A:300:HIS:ND1	1:A:324:ASP:OD2	2.40	0.54
1:H:56:ASN:OD1	1:H:58:GLU:HB2	2.07	0.54
1:C:228:TYR:CD2	1:C:228:TYR:N	2.76	0.54
1:E:68:LEU:HD23	1:E:84:SER:HB3	1.89	0.54
1:B:65:ALA:CB	2:J:1:ALQ:HM2	2.35	0.54
1:D:68:LEU:HD23	1:D:84:SER:HB3	1.89	0.54
1:F:167:LEU:HD13	1:F:198:TRP:CE3	2.43	0.54
1:F:196:ARG:HH12	1:G:194:LEU:CD1	2.20	0.54
2:P:3:ARG:HG3	2:P:3:ARG:HH21	1.73	0.54
1:A:133:PHE:CE2	2:I:3:ARG:CA	2.91	0.54
1:F:133:PHE:CE2	2:N:3:ARG:CA	2.90	0.54
1:G:69:ILE:HB	1:G:83:ILE:HB	1.90	0.54
1:G:88:LEU:HB3	1:G:107:ASP:HB2	1.89	0.54
1:G:315:ILE:HA	1:G:330:TRP:O	2.07	0.54
2:K:5:0XM:CBM	2:K:5:0XM:H32	2.36	0.54
1:C:133:PHE:HE2	2:K:3:ARG:CA	2.21	0.54
1:C:133:PHE:HE2	2:K:3:ARG:N	2.06	0.54
1:D:118:SER:OG	1:D:120:LYS:HG2	2.08	0.54
1:E:315:ILE:HA	1:E:330:TRP:O	2.06	0.54
1:H:303:VAL:HB	1:H:321:LEU:HD12	1.89	0.54
1:A:32:LYS:HZ2	1:F:162:LYS:CE	2.21	0.53
1:A:44:HIS:CE1	1:A:64:SER:HB3	2.43	0.53
1:E:303:VAL:HB	1:E:321:LEU:HD12	1.91	0.53
1:C:69:ILE:HB	1:C:83:ILE:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:ARG:HG3	1:D:166:THR:HG23	1.91	0.53
1:D:259:LYS:HB3	1:D:260:TYR:CD2	2.44	0.53
1:F:69:ILE:HB	1:F:83:ILE:HB	1.89	0.53
1:G:155:ILE:HD11	1:G:186:ILE:CD1	2.38	0.53
1:A:167:LEU:HD13	1:A:198:TRP:CE3	2.43	0.53
1:C:95:TRP:CE3	1:C:102:LEU:HD21	2.43	0.53
1:C:300:HIS:ND1	1:C:324:ASP:OD2	2.40	0.53
1:H:167:LEU:HD13	1:H:198:TRP:CE3	2.43	0.53
1:H:252:TYR:CE1	1:H:291:LYS:HA	2.44	0.53
1:G:133:PHE:CE2	2:O:3:ARG:CA	2.91	0.53
1:H:154:ARG:HG2	1:H:166:THR:HG23	1.90	0.53
1:A:182:ASP:OD1	1:A:184:SER:HB3	2.09	0.53
1:A:198:TRP:CZ3	1:A:205:CYS:HB2	2.44	0.53
1:F:252:TYR:CE1	1:F:291:LYS:HA	2.44	0.53
1:F:313:GLU:HB2	1:F:315:ILE:HD11	1.89	0.53
1:H:218:SER:HB2	1:H:261:CYS:HB3	1.89	0.53
1:H:315:ILE:HA	1:H:330:TRP:O	2.07	0.53
1:C:47:ALA:HB2	1:C:322:GLU:HB3	1.91	0.53
1:C:303:VAL:HB	1:C:321:LEU:HD12	1.91	0.53
1:F:321:LEU:CD2	2:N:4:AC5:HG12	2.39	0.53
1:B:155:ILE:HD11	1:B:186:ILE:CD1	2.39	0.53
1:B:207:LYS:NZ	1:B:244:SER:O	2.41	0.53
1:C:252:TYR:CE1	1:C:291:LYS:HA	2.44	0.53
1:F:194:LEU:CD1	1:G:196:ARG:HH12	2.22	0.53
1:G:54:SER:HB3	1:G:95:TRP:CE2	2.44	0.53
1:F:315:ILE:HA	1:F:330:TRP:O	2.08	0.53
1:A:95:TRP:CE3	1:A:102:LEU:HD21	2.44	0.53
1:H:88:LEU:HB3	1:H:107:ASP:HB2	1.90	0.53
1:E:86:HIS:CE1	1:E:106:SER:HB3	2.43	0.53
1:C:100:ASN:O	1:C:116:VAL:HG23	2.08	0.52
1:C:198:TRP:CZ3	1:C:205:CYS:HB2	2.43	0.52
1:E:259:LYS:HB3	1:E:260:TYR:CD2	2.45	0.52
1:G:118:SER:OG	1:G:120:LYS:HG2	2.09	0.52
1:G:252:TYR:CE1	1:G:291:LYS:HA	2.44	0.52
1:H:68:LEU:CD2	1:H:84:SER:HB3	2.38	0.52
2:M:5:0XM:CBM	2:M:5:0XM:CBR	2.86	0.52
1:A:133:PHE:HE2	2:I:3:ARG:H	1.54	0.52
1:B:100:ASN:CB	1:B:101:LEU:HG	2.33	0.52
1:D:45:THR:O	1:D:325:LYS:HD3	2.09	0.52
1:D:254:GLY:CA	1:E:236:ASN:HD22	2.23	0.52
1:H:155:ILE:HD11	1:H:186:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:SER:HB2	1:B:261:CYS:HB3	1.91	0.52
1:D:88:LEU:HB3	1:D:107:ASP:HB2	1.92	0.52
1:D:187:VAL:CG2	1:D:220:VAL:HG21	2.40	0.52
1:F:300:HIS:ND1	1:F:324:ASP:OD2	2.42	0.52
1:B:196:ARG:NH1	1:C:196:ARG:NH1	2.57	0.52
1:E:154:ARG:HG2	1:E:166:THR:HG23	1.91	0.52
1:B:293:ILE:HD12	1:B:293:ILE:N	2.10	0.52
1:F:89:GLY:HA3	2:N:1:ALQ:CM	2.39	0.52
1:G:133:PHE:CE2	2:O:3:ARG:HA	2.43	0.52
1:H:313:GLU:HB2	1:H:315:ILE:HD11	1.90	0.52
1:G:107:ASP:OD1	2:O:2:0XL:CBD	2.58	0.52
1:B:56:ASN:OD1	1:B:58:GLU:HB2	2.08	0.52
1:E:252:TYR:CE1	1:E:291:LYS:HA	2.45	0.52
1:F:68:LEU:HD23	1:F:84:SER:HB3	1.92	0.52
1:F:198:TRP:CZ3	1:F:205:CYS:HB2	2.44	0.52
1:G:302:ASP:OD1	1:G:303:VAL:N	2.40	0.52
1:A:313:GLU:HB2	1:A:315:ILE:HD11	1.91	0.52
1:A:155:ILE:HD11	1:A:186:ILE:CD1	2.39	0.52
1:E:133:PHE:HE2	2:M:3:ARG:CA	2.22	0.52
1:G:154:ARG:HG3	1:G:166:THR:HG23	1.91	0.52
1:G:193:GLY:HA2	1:G:215:PRO:O	2.10	0.52
1:H:68:LEU:HD13	1:H:70:LYS:HE3	1.92	0.52
1:D:252:TYR:CE1	1:D:291:LYS:HA	2.45	0.52
1:B:228:TYR:N	1:B:228:TYR:CD2	2.78	0.51
1:C:89:GLY:C	2:K:1:ALQ:HB3	2.31	0.51
1:C:313:GLU:HB2	1:C:315:ILE:HD11	1.92	0.51
1:D:154:ARG:HG2	1:D:166:THR:HG23	1.91	0.51
1:E:68:LEU:HD13	1:E:70:LYS:HE3	1.93	0.51
1:E:310:HIS:CE1	1:E:312:THR:OG1	2.63	0.51
1:G:68:LEU:HD13	1:G:70:LYS:HE3	1.91	0.51
2:P:3:ARG:HH21	2:P:3:ARG:CG	2.22	0.51
1:C:167:LEU:HD13	1:C:198:TRP:CE3	2.46	0.51
1:G:259:LYS:HB3	1:G:260:TYR:CD2	2.45	0.51
1:H:193:GLY:HA2	1:H:215:PRO:O	2.10	0.51
1:A:252:TYR:CE1	1:A:291:LYS:HA	2.46	0.51
1:D:133:PHE:HE2	2:L:3:ARG:CA	2.20	0.51
1:D:189:SER:HB2	1:D:217:VAL:HG12	1.91	0.51
1:F:187:VAL:HG21	1:F:229:ILE:HD13	1.93	0.51
1:A:44:HIS:HD2	1:A:70:LYS:HD2	1.75	0.51
1:D:207:LYS:HD2	1:D:243:TYR:O	2.11	0.51
1:A:259:LYS:HB3	1:A:260:TYR:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLY:HA2	1:B:215:PRO:O	2.11	0.51
1:D:56:ASN:OD1	1:D:58:GLU:HB2	2.10	0.51
1:A:193:GLY:HA2	1:A:215:PRO:O	2.11	0.51
1:C:159:LYS:HA	1:C:159:LYS:CE	2.40	0.51
1:F:228:TYR:N	1:F:228:TYR:CD2	2.79	0.51
2:M:1:ALQ:CM	2:M:4:AC5:HB22	2.20	0.51
1:A:118:SER:OG	1:A:120:LYS:HG2	2.11	0.51
1:C:259:LYS:HB3	1:C:260:TYR:CD2	2.46	0.51
1:E:293:ILE:HD12	1:E:293:ILE:N	2.14	0.51
1:G:95:TRP:CE3	1:G:102:LEU:HD21	2.46	0.51
1:H:300:HIS:ND1	1:H:324:ASP:OD2	2.44	0.51
1:A:41:LEU:HD13	1:A:72:TRP:CE3	2.46	0.51
1:F:133:PHE:HE2	2:N:3:ARG:CA	2.24	0.51
1:F:207:LYS:HD2	1:F:243:TYR:O	2.11	0.51
1:H:189:SER:OG	1:H:220:VAL:HG22	2.11	0.51
1:B:95:TRP:CE3	1:B:102:LEU:HD21	2.46	0.51
1:D:293:ILE:HD12	1:D:293:ILE:N	2.15	0.51
1:E:207:LYS:NZ	1:E:244:SER:O	2.43	0.51
1:F:259:LYS:HB3	1:F:260:TYR:CD2	2.46	0.51
1:G:189:SER:HB2	1:G:217:VAL:HG12	1.91	0.51
1:D:95:TRP:CE3	1:D:102:LEU:HD21	2.46	0.50
1:C:218:SER:HB2	1:C:261:CYS:HB3	1.93	0.50
1:A:217:VAL:HG22	1:A:233:THR:HG23	1.93	0.50
1:A:310:HIS:CE1	1:A:312:THR:OG1	2.64	0.50
1:B:310:HIS:CE1	1:B:312:THR:OG1	2.64	0.50
1:C:154:ARG:HG3	1:C:166:THR:HG23	1.93	0.50
1:H:198:TRP:CZ3	1:H:205:CYS:HB2	2.47	0.50
1:A:189:SER:OG	1:A:220:VAL:HG22	2.12	0.50
1:F:155:ILE:HD11	1:F:186:ILE:CD1	2.42	0.50
1:B:88:LEU:HB3	1:B:107:ASP:HB2	1.92	0.50
1:B:257:ASN:HA	1:B:279:GLU:OE2	2.12	0.50
1:E:189:SER:HB2	1:E:217:VAL:HG12	1.93	0.50
1:E:228:TYR:N	1:E:228:TYR:CD2	2.79	0.50
1:B:207:LYS:HD2	1:B:243:TYR:O	2.12	0.50
1:F:194:LEU:HD11	1:G:196:ARG:HH12	1.76	0.50
1:G:321:LEU:HD22	2:O:4:AC5:CG1	2.34	0.50
1:B:236:ASN:OD1	1:B:258:GLU:HG3	2.11	0.50
1:D:310:HIS:CE1	1:D:312:THR:OG1	2.65	0.50
1:E:154:ARG:HG3	1:E:166:THR:HG23	1.94	0.50
1:G:310:HIS:CE1	1:G:312:THR:OG1	2.65	0.50
1:B:45:THR:O	1:B:325:LYS:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:TYR:CD1	1:C:291:LYS:HA	2.47	0.50
1:G:234:LEU:HD13	1:G:258:GLU:O	2.11	0.50
1:B:259:LYS:HB3	1:B:260:TYR:CD2	2.47	0.49
1:G:228:TYR:N	1:G:228:TYR:CD2	2.80	0.49
1:A:207:LYS:HD2	1:A:243:TYR:O	2.12	0.49
1:E:302:ASP:OD1	1:E:303:VAL:N	2.42	0.49
1:C:189:SER:HB2	1:C:217:VAL:HG12	1.94	0.49
1:C:237:THR:HG22	1:C:239:LYS:HG3	1.95	0.49
1:B:302:ASP:OD1	1:B:303:VAL:N	2.43	0.49
1:C:68:LEU:HD23	1:C:84:SER:HB3	1.93	0.49
1:D:207:LYS:NZ	1:D:244:SER:O	2.45	0.49
1:F:230:LEU:HD12	1:F:231:ALA:N	2.27	0.49
2:N:3:ARG:HG3	2:N:3:ARG:NH2	2.28	0.49
1:A:103:VAL:CG2	1:A:144:ILE:HD13	2.40	0.49
1:B:189:SER:OG	1:B:220:VAL:HG22	2.13	0.49
1:F:107:ASP:OD2	2:N:1:ALQ:HB2	2.11	0.49
1:F:252:TYR:CD1	1:F:291:LYS:HA	2.47	0.49
1:B:187:VAL:CG2	1:B:220:VAL:HG21	2.42	0.49
1:F:217:VAL:HG22	1:F:233:THR:HG23	1.95	0.49
1:G:187:VAL:HG21	1:G:229:ILE:HD13	1.95	0.49
1:G:252:TYR:CD1	1:G:291:LYS:HA	2.47	0.49
1:H:207:LYS:HD2	1:H:243:TYR:O	2.12	0.49
1:B:68:LEU:HD23	1:B:84:SER:HB3	1.93	0.49
1:D:193:GLY:HA2	1:D:215:PRO:O	2.11	0.49
1:D:236:ASN:HD22	1:E:254:GLY:CA	2.26	0.49
1:F:310:HIS:CE1	1:F:312:THR:OG1	2.66	0.49
1:H:236:ASN:OD1	1:H:258:GLU:HG3	2.13	0.49
1:B:252:TYR:CE1	1:B:291:LYS:HA	2.48	0.49
1:C:103:VAL:CG2	1:C:144:ILE:HD13	2.40	0.49
1:C:236:ASN:OD1	1:C:258:GLU:HG3	2.12	0.49
1:D:142:ASN:O	1:D:143:LEU:HD23	2.13	0.49
1:D:236:ASN:OD1	1:D:258:GLU:HG3	2.13	0.49
1:E:56:ASN:OD1	1:E:58:GLU:HB2	2.12	0.49
1:G:216:PRO:O	1:G:233:THR:HG22	2.13	0.49
1:H:252:TYR:CD1	1:H:291:LYS:HA	2.48	0.49
1:H:259:LYS:HB3	1:H:260:TYR:CD2	2.47	0.49
1:A:189:SER:HB2	1:A:217:VAL:HG12	1.93	0.49
1:C:257:ASN:HA	1:C:279:GLU:OE2	2.13	0.49
1:D:237:THR:HG22	1:D:239:LYS:HG3	1.95	0.49
1:F:189:SER:HB2	1:F:217:VAL:HG12	1.94	0.49
1:F:236:ASN:OD1	1:F:258:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:182:ASP:OD1	1:H:184:SER:HB3	2.13	0.49
1:E:252:TYR:CD1	1:E:291:LYS:HA	2.47	0.48
1:F:151:GLU:HG2	1:F:172:ASP:C	2.33	0.48
1:G:112:LYS:HG2	1:G:124:THR:HG23	1.95	0.48
2:I:1:ALQ:HM1	2:I:4:AC5:HB22	1.94	0.48
1:A:68:LEU:HD23	1:A:84:SER:HB3	1.94	0.48
1:B:154:ARG:HG3	1:B:166:THR:HG23	1.94	0.48
1:B:178:HIS:O	1:B:186:ILE:HA	2.12	0.48
1:B:318:SER:O	1:B:327:ILE:HA	2.14	0.48
1:F:45:THR:O	1:F:325:LYS:HD3	2.13	0.48
1:F:103:VAL:CG2	1:F:144:ILE:HD13	2.40	0.48
1:F:187:VAL:CG2	1:F:220:VAL:HG21	2.43	0.48
1:F:234:LEU:HD13	1:F:258:GLU:O	2.12	0.48
1:G:236:ASN:OD1	1:G:258:GLU:HG3	2.13	0.48
1:H:103:VAL:CG2	1:H:144:ILE:HD13	2.41	0.48
1:H:154:ARG:HG3	1:H:166:THR:HG23	1.95	0.48
1:A:228:TYR:N	1:A:228:TYR:CD2	2.80	0.48
1:B:230:LEU:HD12	1:B:231:ALA:N	2.28	0.48
1:H:228:TYR:CD2	1:H:228:TYR:N	2.81	0.48
2:I:3:ARG:HH21	2:I:3:ARG:CG	2.13	0.48
2:N:2:0XL:O	2:N:4:AC5:N	2.46	0.48
1:D:228:TYR:N	1:D:228:TYR:CD2	2.81	0.48
1:B:234:LEU:HD13	1:B:258:GLU:O	2.13	0.48
1:D:302:ASP:OD1	1:D:303:VAL:N	2.43	0.48
1:A:236:ASN:OD1	1:A:258:GLU:HG3	2.14	0.48
1:C:182:ASP:OD1	1:C:184:SER:HB3	2.13	0.48
1:C:219:PHE:CZ	1:C:221:LYS:HG2	2.49	0.48
1:F:182:ASP:OD1	1:F:184:SER:HB3	2.13	0.48
1:A:237:THR:HG22	1:A:239:LYS:HG3	1.96	0.48
1:C:239:LYS:HG2	1:C:251:THR:CG2	2.40	0.48
1:D:198:TRP:CZ3	1:D:205:CYS:HB2	2.49	0.48
1:E:103:VAL:CG2	1:E:144:ILE:HD13	2.42	0.48
1:G:318:SER:O	1:G:327:ILE:HA	2.14	0.48
1:H:310:HIS:CE1	1:H:312:THR:OG1	2.67	0.48
1:E:193:GLY:HA2	1:E:215:PRO:O	2.13	0.48
1:F:95:TRP:CE3	1:F:102:LEU:HD21	2.49	0.48
1:A:45:THR:O	1:A:325:LYS:HD3	2.14	0.48
1:C:207:LYS:HD2	1:C:243:TYR:O	2.14	0.48
1:A:133:PHE:HE2	2:I:3:ARG:CA	2.27	0.47
1:C:118:SER:OG	1:C:120:LYS:HG2	2.14	0.47
1:D:254:GLY:HA3	1:E:236:ASN:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LYS:HE3	1:B:97:SER:OG	2.14	0.47
1:C:207:LYS:NZ	1:C:244:SER:O	2.47	0.47
2:O:1:ALQ:HM1	2:O:4:AC5:HG22	1.94	0.47
1:A:187:VAL:HG21	1:A:229:ILE:CD1	2.45	0.47
1:B:321:LEU:HD22	2:J:4:AC5:HG12	1.97	0.47
1:C:193:GLY:HA2	1:C:215:PRO:O	2.13	0.47
1:E:131:TYR:CG	2:M:2:0XL:CBD	2.96	0.47
1:E:318:SER:O	1:E:327:ILE:HA	2.13	0.47
2:P:1:ALQ:HM1	2:P:4:AC5:HB22	1.96	0.47
1:C:155:ILE:HD11	1:C:186:ILE:CD1	2.44	0.47
1:D:103:VAL:CG2	1:D:144:ILE:HD13	2.42	0.47
1:E:93:VAL:HG21	1:E:102:LEU:HD13	1.96	0.47
1:E:155:ILE:HD11	1:E:186:ILE:CD1	2.45	0.47
1:H:318:SER:O	1:H:327:ILE:HA	2.15	0.47
1:C:187:VAL:HG21	1:C:229:ILE:HD13	1.97	0.47
1:D:216:PRO:O	1:D:233:THR:HG22	2.14	0.47
1:H:187:VAL:HG21	1:H:229:ILE:HD13	1.96	0.47
1:H:219:PHE:CZ	1:H:221:LYS:HG2	2.50	0.47
1:B:123:LYS:HE3	1:B:159:LYS:O	2.14	0.47
1:B:279:GLU:HA	1:B:303:VAL:HG22	1.96	0.47
1:C:230:LEU:HD12	1:C:231:ALA:N	2.29	0.47
1:D:230:LEU:HD12	1:D:231:ALA:N	2.29	0.47
1:D:234:LEU:HD13	1:D:258:GLU:O	2.14	0.47
1:D:256:LYS:CE	1:E:256:LYS:NZ	2.77	0.47
1:E:133:PHE:CZ	2:M:3:ARG:HA	2.49	0.47
1:E:234:LEU:HD13	1:E:258:GLU:O	2.14	0.47
1:G:198:TRP:CZ3	1:G:205:CYS:HB2	2.50	0.47
1:H:189:SER:HB2	1:H:217:VAL:HG12	1.95	0.47
1:A:252:TYR:CD1	1:A:291:LYS:HA	2.49	0.47
1:A:318:SER:O	1:A:327:ILE:HA	2.15	0.47
1:B:217:VAL:HG22	1:B:233:THR:HG23	1.96	0.47
1:D:133:PHE:CZ	2:L:3:ARG:HA	2.49	0.47
1:D:178:HIS:O	1:D:186:ILE:HA	2.14	0.47
1:D:299:GLY:O	1:D:328:LYS:HE3	2.15	0.47
1:B:134:CYS:SG	1:B:147:GLY:HA3	2.55	0.47
1:B:252:TYR:CD1	1:B:291:LYS:HA	2.50	0.47
1:C:302:ASP:OD1	1:C:303:VAL:N	2.45	0.47
1:F:237:THR:HG22	1:F:239:LYS:HG3	1.97	0.47
1:G:187:VAL:CG2	1:G:220:VAL:HG21	2.45	0.47
1:H:217:VAL:HG22	1:H:233:THR:HG23	1.96	0.47
1:A:216:PRO:O	1:A:233:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:HD13	1:B:70:LYS:HE3	1.95	0.47
1:C:219:PHE:HE2	1:C:264:ALA:O	1.96	0.47
1:E:207:LYS:HD2	1:E:243:TYR:O	2.15	0.47
1:A:213:ASP:HB2	1:A:215:PRO:CD	2.30	0.47
1:D:252:TYR:CD1	1:D:291:LYS:HA	2.50	0.47
1:E:236:ASN:OD1	1:E:258:GLU:HG3	2.15	0.46
1:H:45:THR:O	1:H:325:LYS:HD3	2.15	0.46
1:H:216:PRO:O	1:H:233:THR:HG22	2.15	0.46
1:C:261:CYS:O	2:K:3:ARG:NH2	2.45	0.46
1:G:207:LYS:HD2	1:G:243:TYR:O	2.15	0.46
1:H:219:PHE:HE2	1:H:264:ALA:O	1.98	0.46
1:B:219:PHE:CZ	1:B:221:LYS:HG2	2.51	0.46
1:D:217:VAL:HG22	1:D:233:THR:HG23	1.97	0.46
1:E:237:THR:HG22	1:E:239:LYS:HG3	1.97	0.46
1:F:118:SER:OG	1:F:120:LYS:HG2	2.15	0.46
1:F:193:GLY:HA2	1:F:215:PRO:O	2.14	0.46
1:G:56:ASN:OD1	1:G:58:GLU:HB2	2.14	0.46
1:A:321:LEU:CD2	2:I:4:AC5:HG12	2.45	0.46
1:C:217:VAL:HG22	1:C:233:THR:HG23	1.98	0.46
1:E:76:ASP:OD2	1:E:78:LYS:HB2	2.15	0.46
1:E:214:ASN:N	1:E:215:PRO:CD	2.78	0.46
1:F:187:VAL:HG22	1:F:220:VAL:CG2	2.45	0.46
1:G:103:VAL:CG2	1:G:144:ILE:HD13	2.43	0.46
1:G:187:VAL:HG21	1:G:229:ILE:CD1	2.46	0.46
1:H:106:SER:OG	1:H:107:ASP:N	2.48	0.46
1:H:118:SER:OG	1:H:120:LYS:HG2	2.16	0.46
1:A:44:HIS:CD2	1:A:70:LYS:HD2	2.49	0.46
1:C:310:HIS:CE1	1:C:312:THR:OG1	2.69	0.46
1:H:257:ASN:HA	1:H:279:GLU:OE2	2.16	0.46
1:B:237:THR:HG22	1:B:239:LYS:HG3	1.98	0.46
1:E:230:LEU:HD12	1:E:231:ALA:N	2.30	0.46
1:A:86:HIS:CE1	1:A:112:LYS:HG3	2.51	0.46
1:E:217:VAL:HG22	1:E:233:THR:HG23	1.97	0.46
1:G:76:ASP:OD2	1:G:78:LYS:HB2	2.16	0.46
1:B:213:ASP:OD1	1:B:213:ASP:N	2.48	0.46
1:D:68:LEU:HD13	1:D:70:LYS:HE3	1.98	0.46
1:F:133:PHE:CE2	2:N:3:ARG:N	2.81	0.46
1:F:168:PRO:HB2	1:G:198:TRP:HZ3	1.80	0.46
1:G:45:THR:O	1:G:325:LYS:HD3	2.15	0.46
1:G:207:LYS:NZ	1:G:244:SER:O	2.48	0.46
1:G:237:THR:HG22	1:G:239:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:ILE:HD12	1:G:293:ILE:N	2.14	0.46
1:H:234:LEU:HD13	1:H:258:GLU:O	2.15	0.46
1:A:93:VAL:HG21	1:A:102:LEU:HD13	1.97	0.46
1:A:106:SER:OG	1:A:107:ASP:N	2.47	0.46
1:F:196:ARG:HH21	1:G:170:HIS:HA	1.81	0.46
1:G:133:PHE:CZ	2:O:3:ARG:HB2	2.49	0.46
1:A:106:SER:HB3	1:A:108:ASP:OD1	2.15	0.46
1:D:259:LYS:CD	2:L:5:0XM:H29	2.46	0.46
1:E:95:TRP:CE3	1:E:102:LEU:HD21	2.51	0.46
1:B:216:PRO:O	1:B:233:THR:HG22	2.16	0.45
1:C:123:LYS:HZ1	1:H:292:GLU:HG2	1.81	0.45
1:C:269:THR:HB	1:C:314:ASN:OD1	2.15	0.45
1:D:112:LYS:HG2	1:D:124:THR:HG23	1.98	0.45
1:G:154:ARG:HG2	1:G:166:THR:HG23	1.96	0.45
1:H:207:LYS:NZ	1:H:244:SER:O	2.48	0.45
1:H:269:THR:HB	1:H:314:ASN:OD1	2.17	0.45
1:A:207:LYS:NZ	1:A:244:SER:O	2.48	0.45
1:A:302:ASP:OD1	1:A:303:VAL:N	2.47	0.45
1:B:133:PHE:CE2	2:J:3:ARG:CA	2.98	0.45
1:C:41:LEU:HD13	1:C:72:TRP:CE3	2.51	0.45
1:D:256:LYS:HZ3	1:E:256:LYS:HZ1	1.63	0.45
1:E:230:LEU:HD12	1:E:239:LYS:O	2.16	0.45
1:F:133:PHE:CD1	1:F:175:SER:HA	2.51	0.45
1:G:178:HIS:O	1:G:186:ILE:HA	2.15	0.45
1:H:133:PHE:CD1	1:H:175:SER:HA	2.52	0.45
1:C:103:VAL:HA	1:C:112:LYS:O	2.16	0.45
1:E:216:PRO:O	1:E:233:THR:HG22	2.15	0.45
1:G:321:LEU:CD2	2:O:4:AC5:CG1	2.89	0.45
1:H:302:ASP:OD1	1:H:303:VAL:N	2.47	0.45
1:D:187:VAL:HG21	1:D:229:ILE:HD13	1.98	0.45
1:F:56:ASN:OD1	1:F:58:GLU:HB2	2.15	0.45
1:H:106:SER:HB3	1:H:108:ASP:OD1	2.15	0.45
2:O:2:0XL:CBD	2:O:2:0XL:CBE	2.94	0.45
1:A:133:PHE:CE2	2:I:3:ARG:HA	2.51	0.45
1:F:207:LYS:NZ	1:F:244:SER:O	2.49	0.45
1:F:219:PHE:HE2	1:F:264:ALA:O	1.98	0.45
1:F:269:THR:HG21	1:F:313:GLU:O	2.17	0.45
1:F:274:ILE:O	1:F:285:ILE:HA	2.16	0.45
1:A:133:PHE:CD1	1:A:175:SER:HA	2.52	0.45
1:B:187:VAL:HG22	1:B:220:VAL:CG2	2.45	0.45
1:B:189:SER:HB2	1:B:217:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ARG:HH21	1:D:58:GLU:HG3	1.81	0.45
1:C:237:THR:CG2	1:C:239:LYS:HG3	2.46	0.45
1:E:112:LYS:HG2	1:E:124:THR:HG23	1.98	0.45
1:E:279:GLU:HA	1:E:303:VAL:HG22	1.99	0.45
1:G:134:CYS:SG	1:G:147:GLY:HA3	2.57	0.45
1:H:237:THR:HG22	1:H:239:LYS:HG3	1.99	0.45
1:A:154:ARG:HG3	1:A:166:THR:HG23	1.99	0.45
1:A:187:VAL:HG22	1:A:220:VAL:CG2	2.46	0.45
1:C:123:LYS:HE3	1:C:159:LYS:O	2.17	0.45
1:C:230:LEU:HD12	1:C:239:LYS:O	2.17	0.45
1:F:106:SER:HB3	1:F:108:ASP:OD1	2.17	0.45
1:H:269:THR:HG21	1:H:313:GLU:O	2.17	0.45
1:D:257:ASN:HA	1:D:279:GLU:OE2	2.17	0.45
1:D:318:SER:O	1:D:327:ILE:HA	2.16	0.45
1:B:187:VAL:HG21	1:B:229:ILE:HD13	1.99	0.45
1:B:299:GLY:O	1:B:328:LYS:HE3	2.16	0.45
1:E:187:VAL:CG2	1:E:220:VAL:HG21	2.41	0.45
1:F:259:LYS:HD3	2:N:5:0XM:H28	1.99	0.45
1:B:86:HIS:CE1	1:B:112:LYS:HG3	2.52	0.45
1:D:214:ASN:N	1:D:215:PRO:CD	2.79	0.45
1:D:260:TYR:HE1	2:L:4:AC5:HB12	1.82	0.45
1:E:142:ASN:O	1:E:143:LEU:HD23	2.17	0.45
1:F:106:SER:OG	1:F:107:ASP:N	2.50	0.45
1:G:217:VAL:HG22	1:G:233:THR:HG23	1.98	0.45
1:H:91:SER:HB3	2:P:3:ARG:HB2	1.99	0.45
1:H:93:VAL:HG21	1:H:102:LEU:HD13	1.99	0.45
1:D:51:VAL:C	1:D:52:LYS:HG2	2.36	0.44
1:D:145:VAL:O	1:D:145:VAL:HG13	2.17	0.44
1:D:290:THR:O	1:D:292:GLU:N	2.51	0.44
1:F:257:ASN:HA	1:F:279:GLU:OE2	2.17	0.44
1:G:123:LYS:HE3	1:G:159:LYS:O	2.17	0.44
1:G:257:ASN:HA	1:G:279:GLU:OE2	2.17	0.44
1:G:302:ASP:CG	1:G:303:VAL:H	2.19	0.44
1:A:234:LEU:HD13	1:A:258:GLU:O	2.16	0.44
1:A:274:ILE:O	1:A:285:ILE:HA	2.16	0.44
1:E:145:VAL:O	1:E:145:VAL:HG13	2.18	0.44
1:G:189:SER:OG	1:G:220:VAL:HG22	2.18	0.44
1:G:219:PHE:CZ	1:G:221:LYS:HG2	2.52	0.44
1:G:295:GLN:HG2	1:G:296:LYS:N	2.32	0.44
1:A:133:PHE:CZ	2:I:3:ARG:HA	2.52	0.44
1:B:154:ARG:HG2	1:B:166:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASP:HB2	1:B:215:PRO:CD	2.29	0.44
1:C:228:TYR:CB	1:C:240:LEU:HD11	2.47	0.44
1:C:269:THR:HG21	1:C:313:GLU:O	2.18	0.44
1:C:274:ILE:O	1:C:285:ILE:HA	2.17	0.44
1:D:31:VAL:HG13	1:D:32:LYS:N	2.33	0.44
1:E:219:PHE:HE2	1:E:264:ALA:O	2.00	0.44
1:F:133:PHE:CZ	2:N:3:ARG:HA	2.51	0.44
1:G:97:SER:OG	1:H:78:LYS:HE3	2.18	0.44
1:H:230:LEU:HD12	1:H:239:LYS:O	2.17	0.44
1:D:236:ASN:HD22	1:E:254:GLY:HA3	1.82	0.44
1:E:103:VAL:HA	1:E:112:LYS:O	2.18	0.44
1:F:103:VAL:HA	1:F:112:LYS:O	2.17	0.44
1:F:318:SER:O	1:F:327:ILE:HA	2.17	0.44
1:G:145:VAL:HG12	1:G:179:PHE:CE2	2.52	0.44
1:H:134:CYS:SG	1:H:147:GLY:HA3	2.58	0.44
1:D:76:ASP:OD2	1:D:78:LYS:HB2	2.17	0.44
1:D:213:ASP:HB2	1:D:215:PRO:CD	2.35	0.44
1:E:198:TRP:CZ3	1:E:205:CYS:HB2	2.52	0.44
1:G:86:HIS:CE1	1:G:112:LYS:HG3	2.53	0.44
1:G:219:PHE:HE2	1:G:264:ALA:O	2.01	0.44
1:H:213:ASP:HB2	1:H:215:PRO:CD	2.31	0.44
1:B:76:ASP:OD2	1:B:78:LYS:HB2	2.18	0.44
1:C:318:SER:O	1:C:327:ILE:HA	2.17	0.44
1:D:230:LEU:HD12	1:D:239:LYS:O	2.18	0.44
1:D:256:LYS:NZ	1:E:256:LYS:CE	2.80	0.44
1:E:46:LYS:HB3	1:E:65:ALA:HB3	2.00	0.44
1:E:107:ASP:CG	2:M:2:0XL:CBD	2.85	0.44
1:E:148:SER:O	1:E:174:VAL:HG23	2.18	0.44
1:F:293:ILE:HD12	1:F:293:ILE:N	2.20	0.44
1:H:41:LEU:HD13	1:H:72:TRP:CE3	2.53	0.44
1:B:302:ASP:CG	1:B:303:VAL:H	2.20	0.44
1:D:151:GLU:HG2	1:D:172:ASP:C	2.38	0.44
1:D:274:ILE:O	1:D:285:ILE:HA	2.18	0.44
1:E:299:GLY:O	1:E:328:LYS:HE3	2.18	0.44
1:F:133:PHE:HE2	2:N:3:ARG:H	1.61	0.44
1:D:214:ASN:H	1:D:215:PRO:HD3	1.80	0.44
1:D:259:LYS:HD3	2:L:5:0XM:H29	1.99	0.44
1:A:215:PRO:HG2	1:A:233:THR:HG21	2.00	0.43
1:D:302:ASP:CG	1:D:303:VAL:H	2.19	0.43
1:F:41:LEU:HD13	1:F:72:TRP:CE3	2.53	0.43
1:F:189:SER:OG	1:F:220:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:187:VAL:HG21	1:H:229:ILE:CD1	2.48	0.43
1:C:45:THR:O	1:C:325:LYS:HD3	2.18	0.43
1:E:302:ASP:CG	1:E:303:VAL:H	2.20	0.43
1:F:111:LEU:HD11	1:F:146:SER:CB	2.48	0.43
1:H:228:TYR:CB	1:H:240:LEU:HD11	2.48	0.43
1:D:219:PHE:HE2	1:D:264:ALA:O	2.01	0.43
1:E:46:LYS:H	1:E:66:ASP:HB3	1.82	0.43
1:E:189:SER:OG	1:E:220:VAL:HG22	2.18	0.43
1:F:105:ALA:HB1	1:F:132:VAL:CG1	2.45	0.43
1:F:215:PRO:HG2	1:F:233:THR:HG21	1.99	0.43
1:G:93:VAL:HG21	1:G:102:LEU:HD13	1.99	0.43
1:G:103:VAL:HA	1:G:112:LYS:O	2.18	0.43
1:G:140:GLN:H	1:G:140:GLN:HG3	1.51	0.43
2:L:5:0XM:H27	2:L:5:0XM:CBN	2.27	0.43
1:B:103:VAL:HA	1:B:112:LYS:O	2.17	0.43
1:C:86:HIS:CE1	1:C:112:LYS:HG3	2.53	0.43
1:C:93:VAL:HG21	1:C:102:LEU:HD13	2.00	0.43
1:C:106:SER:OG	1:C:107:ASP:N	2.52	0.43
1:E:178:HIS:O	1:E:186:ILE:HA	2.17	0.43
1:F:302:ASP:OD1	1:F:303:VAL:N	2.48	0.43
1:H:123:LYS:HE3	1:H:159:LYS:O	2.18	0.43
1:H:133:PHE:CE2	2:P:3:ARG:N	2.86	0.43
1:A:219:PHE:HE2	1:A:264:ALA:O	2.01	0.43
1:B:187:VAL:HG21	1:B:229:ILE:CD1	2.49	0.43
1:C:106:SER:HB3	1:C:108:ASP:OD1	2.19	0.43
1:E:310:HIS:HE1	1:E:312:THR:OG1	2.01	0.43
1:F:269:THR:HB	1:F:314:ASN:OD1	2.18	0.43
1:H:219:PHE:HD2	1:H:264:ALA:HB3	1.84	0.43
1:A:103:VAL:HA	1:A:112:LYS:O	2.18	0.43
1:C:54:SER:HA	1:C:55:PRO:HD3	1.93	0.43
1:C:140:GLN:H	1:C:140:GLN:HG3	1.55	0.43
1:D:52:LYS:HE2	1:D:94:ALA:HB2	1.99	0.43
1:D:313:GLU:HB2	1:D:315:ILE:HD11	2.00	0.43
1:F:178:HIS:O	1:F:186:ILE:HA	2.18	0.43
1:F:228:TYR:CB	1:F:240:LEU:HD11	2.48	0.43
1:F:228:TYR:HB3	1:F:240:LEU:HD11	2.00	0.43
1:H:187:VAL:HG22	1:H:220:VAL:CG2	2.47	0.43
2:J:5:0XM:CBI	2:J:5:0XM:H32	2.49	0.43
1:A:257:ASN:HA	1:A:279:GLU:OE2	2.19	0.43
1:B:48:VAL:O	1:B:305:ILE:HG21	2.19	0.43
1:C:215:PRO:HG2	1:C:233:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:PRO:HG2	1:F:182:ASP:C	2.39	0.43
1:F:214:ASN:N	1:F:215:PRO:CD	2.81	0.43
1:F:230:LEU:HD12	1:F:239:LYS:O	2.19	0.43
1:H:48:VAL:HA	1:H:64:SER:HB2	2.01	0.43
1:D:243:TYR:H	1:D:243:TYR:HD2	1.66	0.43
1:F:170:HIS:HA	1:G:196:ARG:NH2	2.34	0.43
1:H:243:TYR:H	1:H:243:TYR:HD2	1.66	0.43
1:B:93:VAL:HG21	1:B:102:LEU:HD13	2.00	0.43
1:B:142:ASN:O	1:B:143:LEU:HD23	2.19	0.43
1:B:232:ALA:HA	1:B:238:LEU:HD23	2.00	0.43
1:D:182:ASP:OD1	1:D:184:SER:HB3	2.19	0.43
1:F:89:GLY:CA	2:N:1:ALQ:HM2	2.46	0.43
1:F:93:VAL:HG21	1:F:102:LEU:HD13	2.01	0.43
1:F:187:VAL:HG21	1:F:229:ILE:CD1	2.47	0.43
1:G:142:ASN:O	1:G:143:LEU:HD23	2.19	0.43
1:G:212:ASP:HB3	1:G:213:ASP:H	1.61	0.43
1:G:215:PRO:HG2	1:G:233:THR:HG21	2.01	0.43
1:G:274:ILE:O	1:G:285:ILE:HA	2.18	0.43
1:H:65:ALA:CB	2:P:1:ALQ:HM2	2.49	0.43
1:B:219:PHE:HE2	1:B:264:ALA:O	2.02	0.43
1:C:133:PHE:CD1	1:C:175:SER:HA	2.54	0.43
1:C:243:TYR:H	1:C:243:TYR:HD2	1.66	0.43
1:E:243:TYR:H	1:E:243:TYR:HD2	1.67	0.43
1:G:239:LYS:HG2	1:G:251:THR:CG2	2.42	0.43
1:A:237:THR:CG2	1:A:239:LYS:HG3	2.49	0.42
1:A:330:TRP:CD1	1:A:330:TRP:N	2.86	0.42
1:D:106:SER:OG	1:D:107:ASP:N	2.52	0.42
1:F:302:ASP:CG	1:F:303:VAL:H	2.20	0.42
1:H:230:LEU:HD12	1:H:231:ALA:N	2.33	0.42
2:O:1:ALQ:HM1	2:O:4:AC5:CG2	2.49	0.42
1:A:178:HIS:O	1:A:186:ILE:HA	2.18	0.42
1:B:103:VAL:CG2	1:B:144:ILE:HD13	2.47	0.42
1:E:86:HIS:CE1	1:E:112:LYS:HG3	2.54	0.42
1:F:219:PHE:CZ	1:F:221:LYS:HG2	2.54	0.42
1:G:41:LEU:HD13	1:G:72:TRP:CE3	2.53	0.42
1:G:189:SER:CB	1:G:217:VAL:HG12	2.49	0.42
1:A:212:ASP:HB3	1:A:213:ASP:H	1.63	0.42
1:A:269:THR:HB	1:A:314:ASN:OD1	2.20	0.42
1:A:302:ASP:CG	1:A:303:VAL:H	2.21	0.42
1:F:243:TYR:H	1:F:243:TYR:HD2	1.67	0.42
1:G:68:LEU:HD22	1:G:82:THR:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:HIS:HE1	1:A:312:THR:OG1	2.02	0.42
1:B:278:SER:H	1:B:304:VAL:HB	1.84	0.42
1:C:151:GLU:HG2	1:C:172:ASP:C	2.39	0.42
1:F:279:GLU:HA	1:F:303:VAL:HG22	2.01	0.42
2:K:2:0XL:O	2:K:2:0XL:CBE	2.67	0.42
1:A:189:SER:CB	1:A:217:VAL:HG12	2.50	0.42
1:A:228:TYR:CB	1:A:240:LEU:HD11	2.49	0.42
1:A:230:LEU:HD12	1:A:239:LYS:O	2.19	0.42
1:B:274:ILE:O	1:B:285:ILE:HA	2.18	0.42
1:D:93:VAL:HG21	1:D:102:LEU:HD13	2.02	0.42
1:E:214:ASN:H	1:E:215:PRO:HD3	1.79	0.42
1:C:148:SER:O	1:C:174:VAL:HG23	2.20	0.42
1:D:103:VAL:HA	1:D:112:LYS:O	2.20	0.42
1:E:31:VAL:HG13	1:E:32:LYS:N	2.35	0.42
1:F:294:VAL:HG23	1:F:295:GLN:N	2.34	0.42
1:F:295:GLN:HG2	1:F:296:LYS:N	2.34	0.42
1:G:182:ASP:OD1	1:G:184:SER:HB3	2.19	0.42
1:G:230:LEU:HD12	1:G:231:ALA:N	2.34	0.42
1:H:68:LEU:HD23	1:H:84:SER:HB3	2.01	0.42
1:H:212:ASP:HB3	1:H:213:ASP:H	1.62	0.42
1:H:295:GLN:HG2	1:H:296:LYS:N	2.34	0.42
1:C:259:LYS:CD	2:K:5:0XM:H29	2.41	0.42
1:H:151:GLU:HG2	1:H:172:ASP:C	2.40	0.42
1:H:294:VAL:HG23	1:H:295:GLN:N	2.34	0.42
1:A:219:PHE:CZ	1:A:221:LYS:HG2	2.55	0.42
1:B:198:TRP:CZ3	1:B:205:CYS:HB2	2.55	0.42
1:D:88:LEU:HD22	1:D:89:GLY:H	1.85	0.42
1:D:189:SER:OG	1:D:220:VAL:HG22	2.20	0.42
1:D:213:ASP:OD1	1:D:213:ASP:N	2.53	0.42
1:E:90:ILE:HA	1:E:106:SER:HA	2.00	0.42
1:F:213:ASP:HB2	1:F:215:PRO:CD	2.38	0.42
1:G:243:TYR:H	1:G:243:TYR:HD2	1.68	0.42
2:O:3:ARG:O	2:O:4:AC5:HB11	2.19	0.42
1:A:68:LEU:HD22	1:A:82:THR:CG2	2.50	0.42
1:A:243:TYR:H	1:A:243:TYR:HD2	1.68	0.42
1:B:297:LEU:HD13	1:B:330:TRP:CE3	2.55	0.42
1:B:310:HIS:HE1	1:B:312:THR:OG1	2.02	0.42
1:C:187:VAL:CG2	1:C:220:VAL:HG21	2.45	0.42
1:C:214:ASN:N	1:C:215:PRO:CD	2.82	0.42
1:C:216:PRO:O	1:C:233:THR:HG22	2.19	0.42
1:C:302:ASP:CG	1:C:303:VAL:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:TYR:CE1	2:L:4:AC5:HB12	2.54	0.42
1:F:58:GLU:O	1:F:74:ALA:CB	2.68	0.42
1:G:107:ASP:OD1	2:O:2:0XL:CBA	2.68	0.42
1:G:294:VAL:HG23	1:G:295:GLN:N	2.34	0.42
1:H:112:LYS:HG2	1:H:124:THR:HG23	2.02	0.42
1:H:228:TYR:HB3	1:H:240:LEU:HD11	2.01	0.42
2:O:3:ARG:O	2:O:3:ARG:CG	2.62	0.42
1:A:230:LEU:HD12	1:A:231:ALA:N	2.32	0.42
1:E:213:ASP:HB2	1:E:215:PRO:CD	2.36	0.42
1:H:274:ILE:O	1:H:285:ILE:HA	2.19	0.42
1:C:54:SER:HB3	1:C:95:TRP:CZ2	2.55	0.41
1:C:128:HIS:ND1	1:C:148:SER:CB	2.83	0.41
1:C:234:LEU:HD13	1:C:258:GLU:O	2.19	0.41
1:D:48:VAL:O	1:D:305:ILE:HG21	2.19	0.41
1:D:294:VAL:HG23	1:D:295:GLN:N	2.34	0.41
1:E:239:LYS:HG2	1:E:251:THR:CG2	2.44	0.41
1:E:257:ASN:HA	1:E:279:GLU:OE2	2.20	0.41
1:F:216:PRO:O	1:F:233:THR:HG22	2.19	0.41
1:H:95:TRP:CE3	1:H:102:LEU:CD2	3.03	0.41
1:A:78:LYS:HE2	1:B:55:PRO:HB3	2.02	0.41
1:C:330:TRP:CD1	1:C:330:TRP:N	2.87	0.41
1:E:65:ALA:HB2	2:M:1:ALQ:HM2	2.02	0.41
1:G:106:SER:OG	1:G:107:ASP:N	2.53	0.41
1:G:213:ASP:OD1	1:G:213:ASP:N	2.52	0.41
1:G:218:SER:HB2	1:G:261:CYS:CB	2.50	0.41
1:A:123:LYS:HE3	1:A:159:LYS:O	2.20	0.41
1:A:155:ILE:HG22	1:A:164:LEU:HD12	2.01	0.41
1:A:295:GLN:HG2	1:A:296:LYS:N	2.35	0.41
1:B:239:LYS:HG2	1:B:251:THR:CG2	2.44	0.41
1:B:294:VAL:HG23	1:B:295:GLN:N	2.35	0.41
1:C:139:PRO:HG2	1:C:182:ASP:C	2.41	0.41
1:C:213:ASP:OD1	1:C:213:ASP:N	2.53	0.41
1:D:232:ALA:HA	1:D:238:LEU:HD23	2.02	0.41
1:D:237:THR:CG2	1:D:239:LYS:HG3	2.50	0.41
1:E:187:VAL:HG21	1:E:229:ILE:HD13	2.02	0.41
1:G:151:GLU:HG2	1:G:172:ASP:C	2.41	0.41
1:G:293:ILE:H	1:G:293:ILE:CD1	2.07	0.41
1:C:213:ASP:HB2	1:C:215:PRO:CD	2.29	0.41
1:D:105:ALA:HB1	1:D:132:VAL:CG1	2.46	0.41
1:F:154:ARG:HG3	1:F:166:THR:HG23	2.02	0.41
1:F:213:ASP:OD1	1:F:213:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:LEU:HD22	1:G:89:GLY:H	1.84	0.41
1:G:278:SER:H	1:G:304:VAL:HB	1.85	0.41
1:G:310:HIS:HE1	1:G:312:THR:OG1	2.02	0.41
1:H:139:PRO:HG2	1:H:182:ASP:C	2.40	0.41
1:B:68:LEU:HD22	1:B:82:THR:CG2	2.51	0.41
1:B:230:LEU:HD12	1:B:239:LYS:O	2.19	0.41
1:C:228:TYR:HB3	1:C:240:LEU:HD11	2.02	0.41
1:C:299:GLY:O	1:C:328:LYS:HE3	2.21	0.41
1:E:187:VAL:HG22	1:E:220:VAL:CG2	2.44	0.41
1:E:213:ASP:OD1	1:E:213:ASP:N	2.53	0.41
1:G:131:TYR:CG	2:O:2:0XL:CBD	3.04	0.41
1:G:148:SER:H	1:G:174:VAL:HG23	1.86	0.41
1:G:185:LEU:HD23	1:G:185:LEU:HA	1.90	0.41
1:G:213:ASP:HB2	1:G:215:PRO:CD	2.38	0.41
1:G:229:ILE:O	1:G:229:ILE:HG13	2.19	0.41
1:A:72:TRP:CD1	1:A:72:TRP:N	2.88	0.41
1:A:213:ASP:OD1	1:A:213:ASP:N	2.54	0.41
1:B:212:ASP:HB3	1:B:213:ASP:H	1.64	0.41
1:F:86:HIS:CE1	1:F:112:LYS:HG3	2.55	0.41
1:G:313:GLU:HB2	1:G:315:ILE:HD11	2.02	0.41
1:H:31:VAL:HG13	1:H:32:LYS:N	2.35	0.41
1:H:279:GLU:HA	1:H:303:VAL:HG22	2.01	0.41
1:A:278:SER:H	1:A:304:VAL:HB	1.85	0.41
1:B:287:ASN:HB3	1:B:290:THR:OG1	2.21	0.41
1:D:269:THR:HB	1:D:314:ASN:OD1	2.20	0.41
1:D:310:HIS:HE1	1:D:312:THR:OG1	2.03	0.41
1:H:178:HIS:O	1:H:186:ILE:HA	2.19	0.41
1:H:302:ASP:CG	1:H:303:VAL:H	2.23	0.41
1:A:228:TYR:HB3	1:A:240:LEU:HD11	2.02	0.41
1:B:112:LYS:HG2	1:B:124:THR:HG23	2.03	0.41
1:B:151:GLU:HG2	1:B:172:ASP:C	2.41	0.41
1:D:131:TYR:CD2	2:L:2:0XL:CBD	3.04	0.41
1:E:41:LEU:HD13	1:E:72:TRP:CE3	2.56	0.41
1:E:133:PHE:CD1	1:E:175:SER:HA	2.56	0.41
1:F:273:TRP:CZ3	1:F:294:VAL:HG11	2.55	0.41
1:G:104:SER:O	1:G:111:LEU:HA	2.21	0.41
1:G:290:THR:O	1:G:292:GLU:N	2.52	0.41
1:H:56:ASN:OD1	1:H:56:ASN:C	2.58	0.41
1:H:330:TRP:CD1	1:H:330:TRP:N	2.87	0.41
1:A:58:GLU:HG3	1:B:181:ARG:NH2	2.35	0.41
1:A:105:ALA:HB1	1:A:132:VAL:CG1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:THR:O	1:A:292:GLU:N	2.53	0.41
1:A:294:VAL:HG23	1:A:295:GLN:N	2.35	0.41
1:A:321:LEU:HD22	2:I:4:AC5:CB1	2.48	0.41
1:B:97:SER:HB2	1:B:141:SER:OG	2.21	0.41
1:B:148:SER:H	1:B:174:VAL:HG23	1.86	0.41
1:B:215:PRO:HG2	1:B:233:THR:HG21	2.03	0.41
1:B:313:GLU:HB2	1:B:315:ILE:HD11	2.02	0.41
1:C:310:HIS:HA	1:C:311:PRO:HD3	1.92	0.41
1:D:187:VAL:HG21	1:D:229:ILE:CD1	2.49	0.41
1:D:218:SER:HB2	1:D:261:CYS:CB	2.47	0.41
1:E:123:LYS:HE3	1:E:159:LYS:O	2.21	0.41
1:E:237:THR:CG2	1:E:239:LYS:HG3	2.51	0.41
1:F:72:TRP:CD1	1:F:72:TRP:N	2.89	0.41
1:F:237:THR:CG2	1:F:239:LYS:HG3	2.51	0.41
1:F:310:HIS:HE1	1:F:312:THR:OG1	2.03	0.41
1:F:321:LEU:HD22	2:N:4:AC5:CB1	2.47	0.41
1:G:46:LYS:H	1:G:66:ASP:HB3	1.85	0.41
1:G:88:LEU:CD2	1:G:89:GLY:H	2.34	0.41
1:G:228:TYR:CB	1:G:240:LEU:HD11	2.51	0.41
1:H:103:VAL:HA	1:H:112:LYS:O	2.21	0.41
1:A:31:VAL:HG13	1:A:32:LYS:N	2.35	0.41
1:A:95:TRP:CE3	1:A:102:LEU:CD2	3.04	0.41
1:B:219:PHE:HD2	1:B:264:ALA:HB3	1.86	0.41
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.91	0.41
1:C:128:HIS:CE1	1:C:148:SER:HB2	2.56	0.41
1:D:86:HIS:CE1	1:D:112:LYS:HG3	2.56	0.41
1:D:153:VAL:HG23	1:D:169:ALA:HB2	2.03	0.41
1:E:153:VAL:HG23	1:E:169:ALA:HB2	2.03	0.41
1:G:279:GLU:HA	1:G:303:VAL:HG22	2.02	0.41
1:H:310:HIS:HB2	1:H:315:ILE:HB	2.02	0.41
1:A:299:GLY:O	1:A:328:LYS:HE3	2.21	0.40
1:B:195:CYS:HB2	1:B:209:LEU:HB2	2.03	0.40
1:C:219:PHE:HD2	1:C:264:ALA:HB3	1.86	0.40
1:E:48:VAL:O	1:E:305:ILE:HG21	2.20	0.40
1:E:280:ASP:O	1:E:281:ASN:HB2	2.21	0.40
1:G:237:THR:CG2	1:G:239:LYS:HG3	2.52	0.40
1:G:269:THR:HB	1:G:314:ASN:OD1	2.21	0.40
1:H:104:SER:O	1:H:111:LEU:HA	2.21	0.40
1:H:105:ALA:HB1	1:H:132:VAL:CG1	2.46	0.40
1:C:56:ASN:OD1	1:C:56:ASN:C	2.59	0.40
1:C:97:SER:HB2	1:C:141:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:PHE:CD1	1:D:175:SER:HA	2.56	0.40
1:D:279:GLU:HA	1:D:303:VAL:HG22	2.03	0.40
1:B:145:VAL:HG12	1:B:179:PHE:CE2	2.56	0.40
1:B:145:VAL:HG13	1:B:145:VAL:O	2.22	0.40
1:B:243:TYR:H	1:B:243:TYR:HD2	1.69	0.40
1:C:111:LEU:HD11	1:C:146:SER:CB	2.51	0.40
1:C:178:HIS:O	1:C:186:ILE:HA	2.21	0.40
1:D:239:LYS:HG2	1:D:251:THR:CG2	2.45	0.40
1:E:151:GLU:HG2	1:E:172:ASP:C	2.41	0.40
1:E:182:ASP:OD1	1:E:184:SER:HB3	2.21	0.40
1:E:294:VAL:HG23	1:E:295:GLN:N	2.36	0.40
1:H:145:VAL:HG12	1:H:179:PHE:CE2	2.56	0.40
1:C:189:SER:CB	1:C:217:VAL:HG12	2.50	0.40
1:C:294:VAL:HG23	1:C:295:GLN:N	2.35	0.40
1:D:123:LYS:HE3	1:D:159:LYS:O	2.22	0.40
1:D:187:VAL:HG22	1:D:220:VAL:CG2	2.45	0.40
1:E:187:VAL:HG21	1:E:229:ILE:CD1	2.50	0.40
1:E:274:ILE:O	1:E:285:ILE:HA	2.22	0.40
1:F:104:SER:O	1:F:111:LEU:HA	2.22	0.40
1:H:189:SER:CB	1:H:217:VAL:HG12	2.52	0.40
1:H:218:SER:HB2	1:H:261:CYS:CB	2.51	0.40
1:B:295:GLN:HG2	1:B:296:LYS:N	2.36	0.40
1:E:104:SER:O	1:E:111:LEU:HA	2.22	0.40
1:H:187:VAL:CG2	1:H:220:VAL:HG21	2.46	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	302/313 (96%)	274 (91%)	28 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	302/313 (96%)	275 (91%)	27 (9%)	0	100 100
1	C	302/313 (96%)	273 (90%)	29 (10%)	0	100 100
1	D	302/313 (96%)	275 (91%)	27 (9%)	0	100 100
1	E	302/313 (96%)	273 (90%)	29 (10%)	0	100 100
1	F	302/313 (96%)	276 (91%)	26 (9%)	0	100 100
1	G	302/313 (96%)	273 (90%)	29 (10%)	0	100 100
1	H	302/313 (96%)	275 (91%)	27 (9%)	0	100 100
2	I	1/5 (20%)	0	0	1 (100%)	0 0
2	J	1/5 (20%)	1 (100%)	0	0	100 100
2	K	1/5 (20%)	0	1 (100%)	0	100 100
2	L	1/5 (20%)	1 (100%)	0	0	100 100
2	M	1/5 (20%)	1 (100%)	0	0	100 100
2	N	1/5 (20%)	0	0	1 (100%)	0 0
2	O	1/5 (20%)	1 (100%)	0	0	100 100
2	P	1/5 (20%)	0	1 (100%)	0	100 100
All	All	2424/2544 (95%)	2198 (91%)	224 (9%)	2 (0%)	51 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	3	ARG
2	N	3	ARG

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	266/274 (97%)	239 (90%)	27 (10%)	7 26
1	B	266/274 (97%)	239 (90%)	27 (10%)	7 26
1	C	266/274 (97%)	238 (90%)	28 (10%)	7 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	266/274 (97%)	236 (89%)	30 (11%)	6 21
1	E	266/274 (97%)	239 (90%)	27 (10%)	7 26
1	F	266/274 (97%)	238 (90%)	28 (10%)	7 25
1	G	266/274 (97%)	237 (89%)	29 (11%)	6 23
1	H	266/274 (97%)	239 (90%)	27 (10%)	7 26
2	I	1/1 (100%)	1 (100%)	0	100 100
2	J	1/1 (100%)	1 (100%)	0	100 100
2	K	1/1 (100%)	0	1 (100%)	0 0
2	L	1/1 (100%)	1 (100%)	0	100 100
2	M	1/1 (100%)	1 (100%)	0	100 100
2	N	1/1 (100%)	1 (100%)	0	100 100
2	O	1/1 (100%)	1 (100%)	0	100 100
2	P	1/1 (100%)	1 (100%)	0	100 100
All	All	2136/2200 (97%)	1912 (90%)	224 (10%)	7 25

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	45	THR
1	A	50	SER
1	A	64	SER
1	A	76	ASP
1	A	81	LYS
1	A	97	SER
1	A	102	LEU
1	A	110	THR
1	A	130	ASN
1	A	159	LYS
1	A	174	VAL
1	A	212	ASP
1	A	213	ASP
1	A	221	LYS
1	A	228	TYR
1	A	229	ILE
1	A	233	THR
1	A	259	LYS

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Mol	Chain	Res	Type
1	A	261	CYS
1	A	268	VAL
1	A	269	THR
1	A	293	ILE
1	A	296	LYS
1	A	297	LEU
1	A	300	HIS
1	A	334	CYS
1	B	41	LEU
1	B	44	HIS
1	B	45	THR
1	B	46	LYS
1	B	50	SER
1	B	76	ASP
1	B	81	LYS
1	B	97	SER
1	B	110	THR
1	B	130	ASN
1	B	159	LYS
1	B	174	VAL
1	B	212	ASP
1	B	213	ASP
1	B	214	ASN
1	B	221	LYS
1	B	228	TYR
1	B	229	ILE
1	B	233	THR
1	B	259	LYS
1	B	261	CYS
1	B	268	VAL
1	B	269	THR
1	B	293	ILE
1	B	297	LEU
1	B	300	HIS
1	B	334	CYS
1	C	41	LEU
1	C	44	HIS
1	C	45	THR
1	C	50	SER
1	C	64	SER
1	C	76	ASP
1	C	81	LYS

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Mol	Chain	Res	Type
1	C	97	SER
1	C	110	THR
1	C	130	ASN
1	C	159	LYS
1	C	172	ASP
1	C	174	VAL
1	C	212	ASP
1	C	213	ASP
1	C	214	ASN
1	C	221	LYS
1	C	228	TYR
1	C	229	ILE
1	C	233	THR
1	C	259	LYS
1	C	268	VAL
1	C	269	THR
1	C	293	ILE
1	C	296	LYS
1	C	297	LEU
1	C	300	HIS
1	C	334	CYS
1	D	41	LEU
1	D	44	HIS
1	D	45	THR
1	D	50	SER
1	D	52	LYS
1	D	76	ASP
1	D	81	LYS
1	D	93	VAL
1	D	97	SER
1	D	110	THR
1	D	126	LYS
1	D	130	ASN
1	D	159	LYS
1	D	172	ASP
1	D	174	VAL
1	D	212	ASP
1	D	213	ASP
1	D	221	LYS
1	D	228	TYR
1	D	229	ILE
1	D	233	THR

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Mol	Chain	Res	Type
1	D	253	THR
1	D	259	LYS
1	D	261	CYS
1	D	268	VAL
1	D	269	THR
1	D	293	ILE
1	D	297	LEU
1	D	300	HIS
1	D	334	CYS
1	E	41	LEU
1	E	44	HIS
1	E	45	THR
1	E	50	SER
1	E	76	ASP
1	E	81	LYS
1	E	97	SER
1	E	106	SER
1	E	110	THR
1	E	130	ASN
1	E	159	LYS
1	E	172	ASP
1	E	174	VAL
1	E	212	ASP
1	E	213	ASP
1	E	221	LYS
1	E	228	TYR
1	E	229	ILE
1	E	233	THR
1	E	259	LYS
1	E	261	CYS
1	E	268	VAL
1	E	269	THR
1	E	293	ILE
1	E	297	LEU
1	E	300	HIS
1	E	334	CYS
1	F	41	LEU
1	F	44	HIS
1	F	45	THR
1	F	50	SER
1	F	64	SER
1	F	76	ASP

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Mol	Chain	Res	Type
1	F	81	LYS
1	F	97	SER
1	F	110	THR
1	F	130	ASN
1	F	159	LYS
1	F	174	VAL
1	F	212	ASP
1	F	213	ASP
1	F	214	ASN
1	F	221	LYS
1	F	228	TYR
1	F	229	ILE
1	F	233	THR
1	F	259	LYS
1	F	261	CYS
1	F	268	VAL
1	F	269	THR
1	F	293	ILE
1	F	296	LYS
1	F	297	LEU
1	F	300	HIS
1	F	334	CYS
1	G	41	LEU
1	G	44	HIS
1	G	45	THR
1	G	50	SER
1	G	64	SER
1	G	76	ASP
1	G	81	LYS
1	G	87	LYS
1	G	97	SER
1	G	110	THR
1	G	126	LYS
1	G	130	ASN
1	G	159	LYS
1	G	172	ASP
1	G	174	VAL
1	G	212	ASP
1	G	213	ASP
1	G	214	ASN
1	G	221	LYS
1	G	228	TYR

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Mol	Chain	Res	Type
1	G	229	ILE
1	G	233	THR
1	G	259	LYS
1	G	261	CYS
1	G	268	VAL
1	G	269	THR
1	G	297	LEU
1	G	300	HIS
1	G	334	CYS
1	H	41	LEU
1	H	44	HIS
1	H	45	THR
1	H	50	SER
1	H	64	SER
1	H	76	ASP
1	H	81	LYS
1	H	97	SER
1	H	110	THR
1	H	130	ASN
1	H	159	LYS
1	H	172	ASP
1	H	174	VAL
1	H	212	ASP
1	H	213	ASP
1	H	221	LYS
1	H	228	TYR
1	H	229	ILE
1	H	233	THR
1	H	259	LYS
1	H	268	VAL
1	H	269	THR
1	H	293	ILE
1	H	296	LYS
1	H	297	LEU
1	H	300	HIS
1	H	334	CYS
2	K	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	136	ASN

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Mol	Chain	Res	Type
1	F	214	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

16 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	0XL	N	2	2	3,7,8	0.89	0	1,9,11	0.52	0
2	AC5	P	4	2	6,8,9	0.69	0	5,11,13	0.72	0
2	0XL	K	2	2	3,7,8	0.27	0	1,9,11	0.58	0
2	0XL	P	2	2	3,7,8	0.45	0	1,9,11	1.53	0
2	0XL	L	2	2	3,7,8	0.44	0	1,9,11	1.65	0
2	0XL	I	2	2	3,7,8	0.59	0	1,9,11	0.84	0
2	AC5	N	4	2	6,8,9	0.78	0	5,11,13	1.02	0
2	AC5	K	4	2	6,8,9	0.79	0	5,11,13	0.90	0
2	AC5	J	4	2	6,8,9	1.96	2 (33%)	5,11,13	0.84	0
2	AC5	M	4	2	6,8,9	1.31	1 (16%)	5,11,13	0.76	0
2	0XL	O	2	2	3,7,8	0.45	0	1,9,11	2.07	1 (100%)
2	AC5	I	4	2	6,8,9	1.32	1 (16%)	5,11,13	0.63	0
2	AC5	L	4	2	6,8,9	1.21	0	5,11,13	0.75	0
2	0XL	J	2	2	3,7,8	0.71	0	1,9,11	0.82	0
2	AC5	O	4	2	6,8,9	1.46	1 (16%)	5,11,13	1.33	1 (20%)
2	0XL	M	2	2	3,7,8	0.50	0	1,9,11	0.27	0

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	0XL	N	2	2	-	3/4/9/12	-
2	AC5	P	4	2	-	2/2/12/15	0/1/1/1
2	0XL	K	2	2	-	3/4/9/12	-
2	0XL	P	2	2	-	3/4/9/12	-
2	0XL	L	2	2	-	2/4/9/12	-
2	0XL	I	2	2	-	4/4/9/12	-
2	AC5	N	4	2	-	2/2/12/15	0/1/1/1
2	AC5	K	4	2	-	2/2/12/15	0/1/1/1
2	AC5	J	4	2	-	2/2/12/15	0/1/1/1
2	AC5	M	4	2	-	2/2/12/15	0/1/1/1
2	0XL	O	2	2	-	2/4/9/12	-
2	AC5	I	4	2	-	2/2/12/15	0/1/1/1
2	AC5	L	4	2	-	2/2/12/15	0/1/1/1
2	0XL	J	2	2	-	2/4/9/12	-
2	AC5	O	4	2	-	1/2/12/15	0/1/1/1
2	0XL	M	2	2	-	1/4/9/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	4	AC5	CB1-CA	-3.31	1.50	1.54
2	J	4	AC5	CB2-CA	3.08	1.58	1.54
2	O	4	AC5	CB1-CA	-2.79	1.51	1.54
2	M	4	AC5	CB1-CA	-2.56	1.51	1.54
2	I	4	AC5	CB1-CA	-2.31	1.51	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	4	AC5	CG2-CB2-CA	2.31	108.34	104.03
2	O	2	0XL	CAZ-CA-CBA	2.07	115.15	111.96

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	2	0XL	C-CA-CAZ-CBE
2	I	2	0XL	CBA-CA-CAZ-CBE
2	I	2	0XL	C-CA-CBA-CBD

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Mol	Chain	Res	Type	Atoms
2	I	2	0XL	CAZ-CA-CBA-CBD
2	J	2	0XL	C-CA-CAZ-CBE
2	J	2	0XL	CBA-CA-CAZ-CBE
2	K	2	0XL	CAZ-CA-CBA-CBD
2	L	2	0XL	C-CA-CBA-CBD
2	L	2	0XL	CAZ-CA-CBA-CBD
2	M	2	0XL	CBA-CA-CAZ-CBE
2	N	2	0XL	C-CA-CBA-CBD
2	N	2	0XL	CAZ-CA-CBA-CBD
2	O	2	0XL	C-CA-CBA-CBD
2	O	2	0XL	CAZ-CA-CBA-CBD
2	P	2	0XL	C-CA-CBA-CBD
2	P	2	0XL	CAZ-CA-CBA-CBD
2	I	4	AC5	O-C-CA-CB1
2	I	4	AC5	O-C-CA-CB2
2	J	4	AC5	O-C-CA-CB1
2	J	4	AC5	O-C-CA-CB2
2	K	4	AC5	O-C-CA-CB1
2	K	4	AC5	O-C-CA-CB2
2	L	4	AC5	O-C-CA-CB1
2	L	4	AC5	O-C-CA-CB2
2	M	4	AC5	O-C-CA-CB1
2	M	4	AC5	O-C-CA-CB2
2	N	4	AC5	O-C-CA-CB1
2	N	4	AC5	O-C-CA-CB2
2	P	4	AC5	O-C-CA-CB1
2	P	4	AC5	O-C-CA-CB2
2	K	2	0XL	CBA-CA-CAZ-CBE
2	K	2	0XL	C-CA-CAZ-CBE
2	N	2	0XL	C-CA-CAZ-CBE
2	O	4	AC5	O-C-CA-CB1
2	P	2	0XL	CBA-CA-CAZ-CBE

There are no ring outliers.

15 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	2	0XL	2	0
2	P	4	AC5	5	0
2	K	2	0XL	3	0
2	P	2	0XL	2	0
2	L	2	0XL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	0XL	1	0
2	N	4	AC5	4	0
2	K	4	AC5	3	0
2	J	4	AC5	4	0
2	M	4	AC5	9	0
2	O	2	0XL	4	0
2	I	4	AC5	4	0
2	L	4	AC5	7	0
2	O	4	AC5	9	0
2	M	2	0XL	2	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	304/313 (97%)	0.08	5 (1%)	72	70	34, 53, 85, 128	0
1	B	304/313 (97%)	-0.01	4 (1%)	77	76	32, 53, 84, 132	0
1	C	304/313 (97%)	0.03	5 (1%)	72	70	34, 54, 85, 130	0
1	D	304/313 (97%)	0.02	2 (0%)	87	87	32, 53, 85, 135	0
1	E	304/313 (97%)	-0.02	4 (1%)	77	76	28, 53, 84, 136	0
1	F	304/313 (97%)	0.03	3 (0%)	82	81	34, 54, 84, 130	0
1	G	304/313 (97%)	0.00	3 (0%)	82	81	32, 52, 84, 133	0
1	H	304/313 (97%)	0.03	3 (0%)	82	81	34, 54, 84, 127	0
2	I	1/5 (20%)	0.19	0	100	100	44, 44, 44, 44	0
2	J	1/5 (20%)	-0.50	0	100	100	37, 37, 37, 37	0
2	K	1/5 (20%)	0.17	0	100	100	42, 42, 42, 42	0
2	L	1/5 (20%)	-0.50	0	100	100	34, 34, 34, 34	0
2	M	1/5 (20%)	-0.26	0	100	100	37, 37, 37, 37	0
2	N	1/5 (20%)	-0.58	0	100	100	39, 39, 39, 39	0
2	O	1/5 (20%)	-0.73	0	100	100	36, 36, 36, 36	0
2	P	1/5 (20%)	-0.18	0	100	100	42, 42, 42, 42	0
All	All	2440/2544 (95%)	0.02	29 (1%)	79	77	28, 53, 85, 136	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	211	ASP	4.7
1	D	211	ASP	4.6
1	G	211	ASP	4.3
1	B	211	ASP	4.2
1	C	211	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	211	ASP	3.5
1	A	211	ASP	3.1
1	E	212	ASP	2.9
1	H	212	ASP	2.8
1	F	211	ASP	2.7
1	H	146	SER	2.6
1	C	212	ASP	2.5
1	C	146	SER	2.3
1	F	212	ASP	2.3
1	A	319	ALA	2.3
1	B	146	SER	2.3
1	G	265	ASN	2.2
1	C	319	ALA	2.2
1	A	146	SER	2.2
1	F	146	SER	2.2
1	A	212	ASP	2.2
1	A	32	LYS	2.2
1	B	212	ASP	2.1
1	B	275	VAL	2.1
1	D	147	GLY	2.1
1	E	146	SER	2.1
1	C	92	ASP	2.1
1	G	174	VAL	2.0
1	E	254	GLY	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	0XL	I	2	8/9	0.95	0.24	37,49,57,59	0
2	0XL	P	2	8/9	0.95	0.24	24,42,51,51	0
2	0XL	M	2	8/9	0.96	0.20	39,42,50,55	0
2	0XL	J	2	8/9	0.96	0.25	38,44,48,53	0
2	AC5	M	4	8/9	0.96	0.20	26,33,53,64	0
2	0XL	N	2	8/9	0.97	0.18	40,48,49,52	0
2	0XL	L	2	8/9	0.97	0.20	36,41,46,57	0
2	AC5	I	4	8/9	0.97	0.19	36,45,51,52	0
2	AC5	K	4	8/9	0.97	0.18	40,44,50,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AC5	L	4	8/9	0.97	0.18	27,37,45,55	0
2	0XL	K	2	8/9	0.97	0.21	30,38,50,50	0
2	AC5	P	4	8/9	0.97	0.18	28,42,54,59	0
2	0XL	O	2	8/9	0.98	0.25	36,38,47,52	0
2	AC5	N	4	8/9	0.98	0.19	26,38,45,48	0
2	AC5	O	4	8/9	0.98	0.18	29,38,46,54	0
2	AC5	J	4	8/9	0.98	0.18	20,31,42,53	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.