



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:57 AM UTC

PDB ID : 8VJJ / pdb_00008vjj
EMDB ID : EMD-43283
Title : Structure of mouse RyR1 (EGTA-only dataset)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2024-01-07
Resolution : 2.53 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

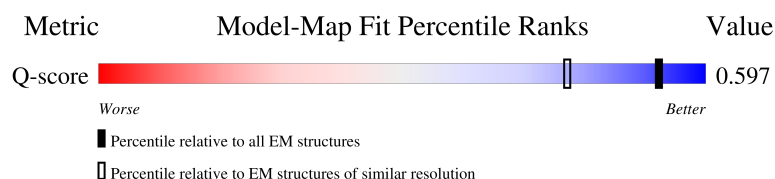
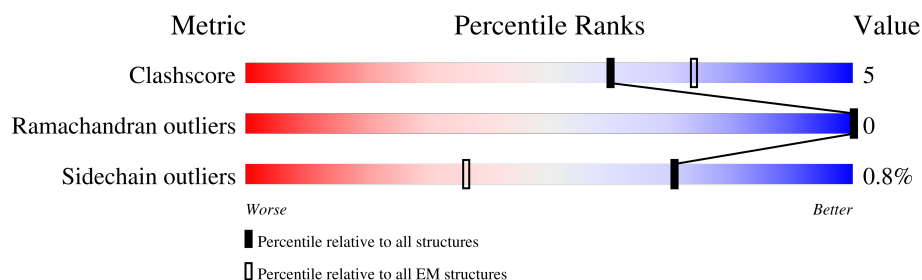
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7309 (2.03 - 3.03)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5035	13% 78% 9% 13%
1	B	5035	13% 78% 8% 13%
1	C	5035	13% 78% 9% 13%
1	D	5035	13% 78% 9% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	95%
2	F	108	95%
2	G	108	94% 5%
2	H	108	94% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 284568 atoms, of which 141580 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	4374	Total	C	H	N	O	S	1	0
			69210	22140	34401	5985	6447	237		
1	D	4374	Total	C	H	N	O	S	1	0
			69210	22140	34401	5985	6447	237		
1	B	4374	Total	C	H	N	O	S	1	0
			69210	22140	34401	5985	6447	237		
1	C	4374	Total	C	H	N	O	S	1	0
			69210	22140	34401	5985	6447	237		

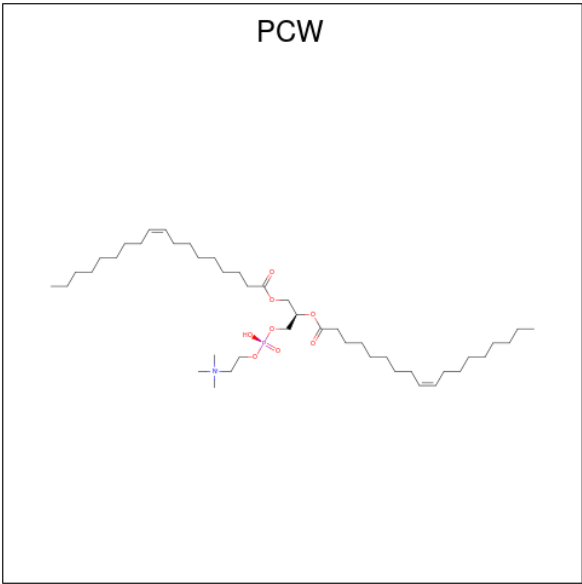
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1655	526	826	145	155	3		
2	H	107	Total	C	H	N	O	S	0	0
			1655	526	826	145	155	3		
2	F	107	Total	C	H	N	O	S	0	0
			1655	526	826	145	155	3		
2	G	107	Total	C	H	N	O	S	0	0
			1655	526	826	145	155	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

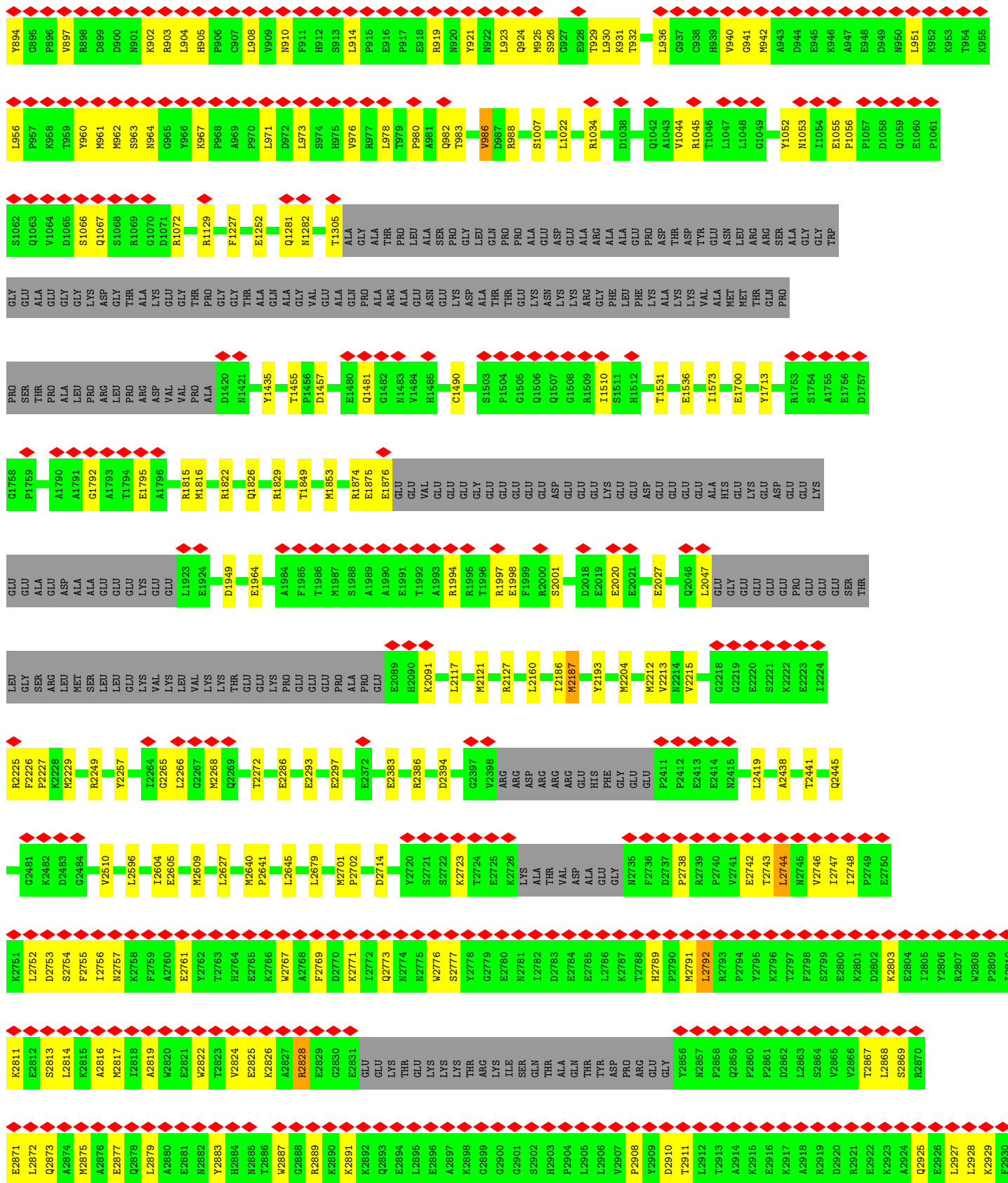
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).

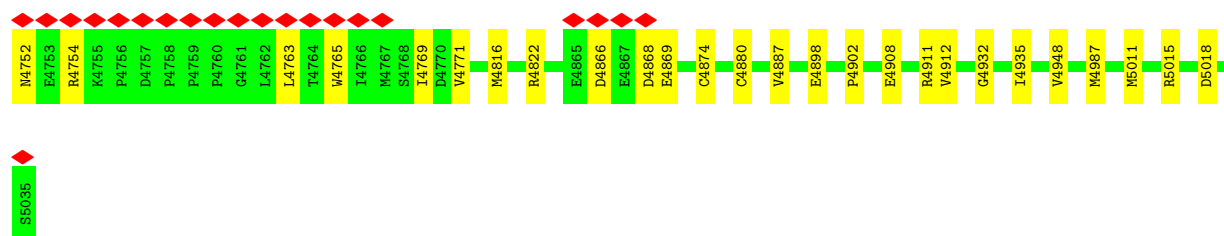


Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	A	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	D	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	D	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	B	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	B	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	C	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	C	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	

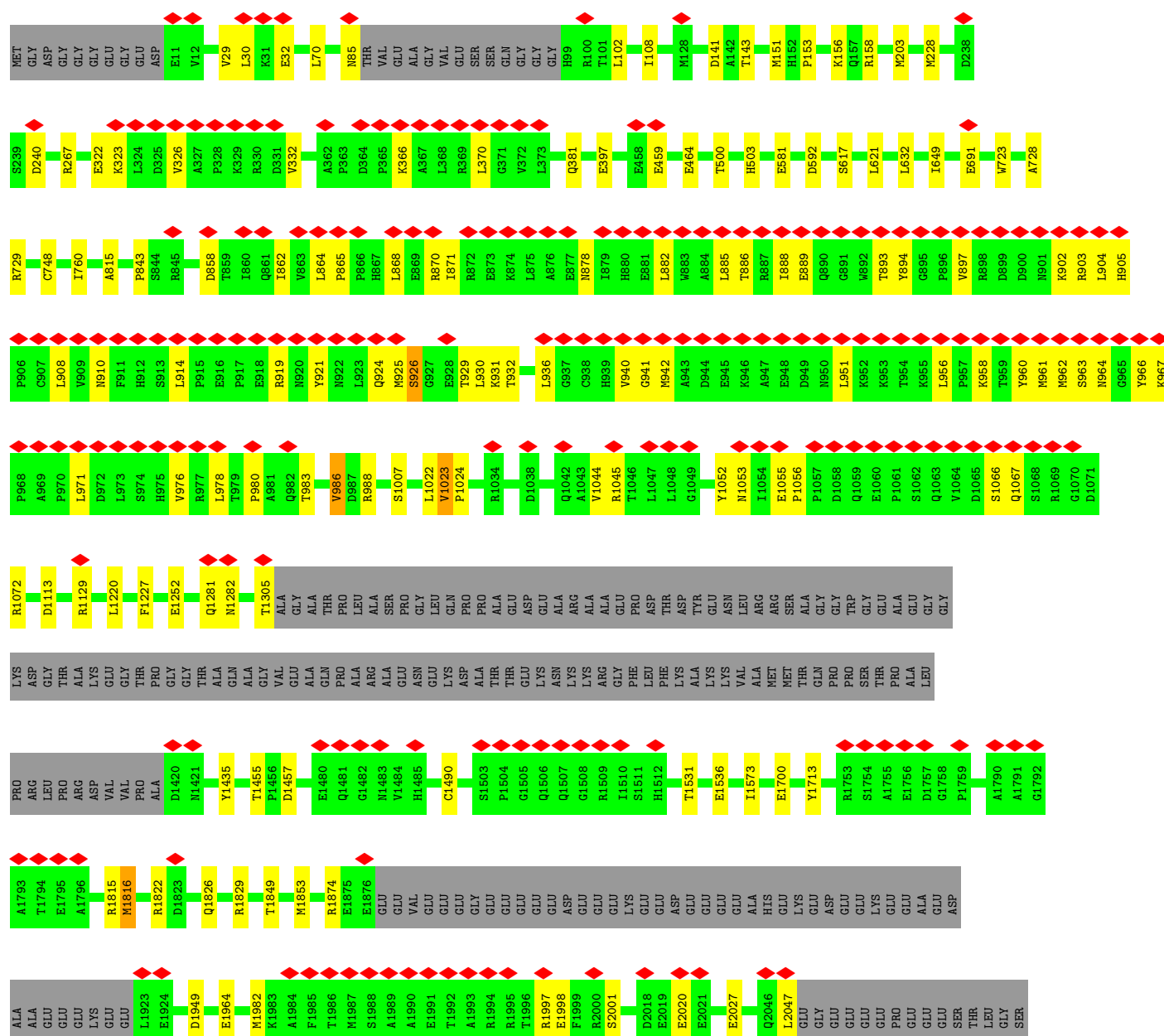
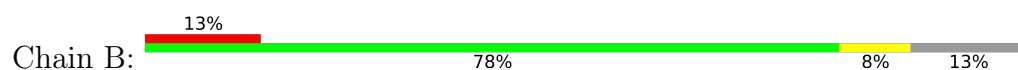




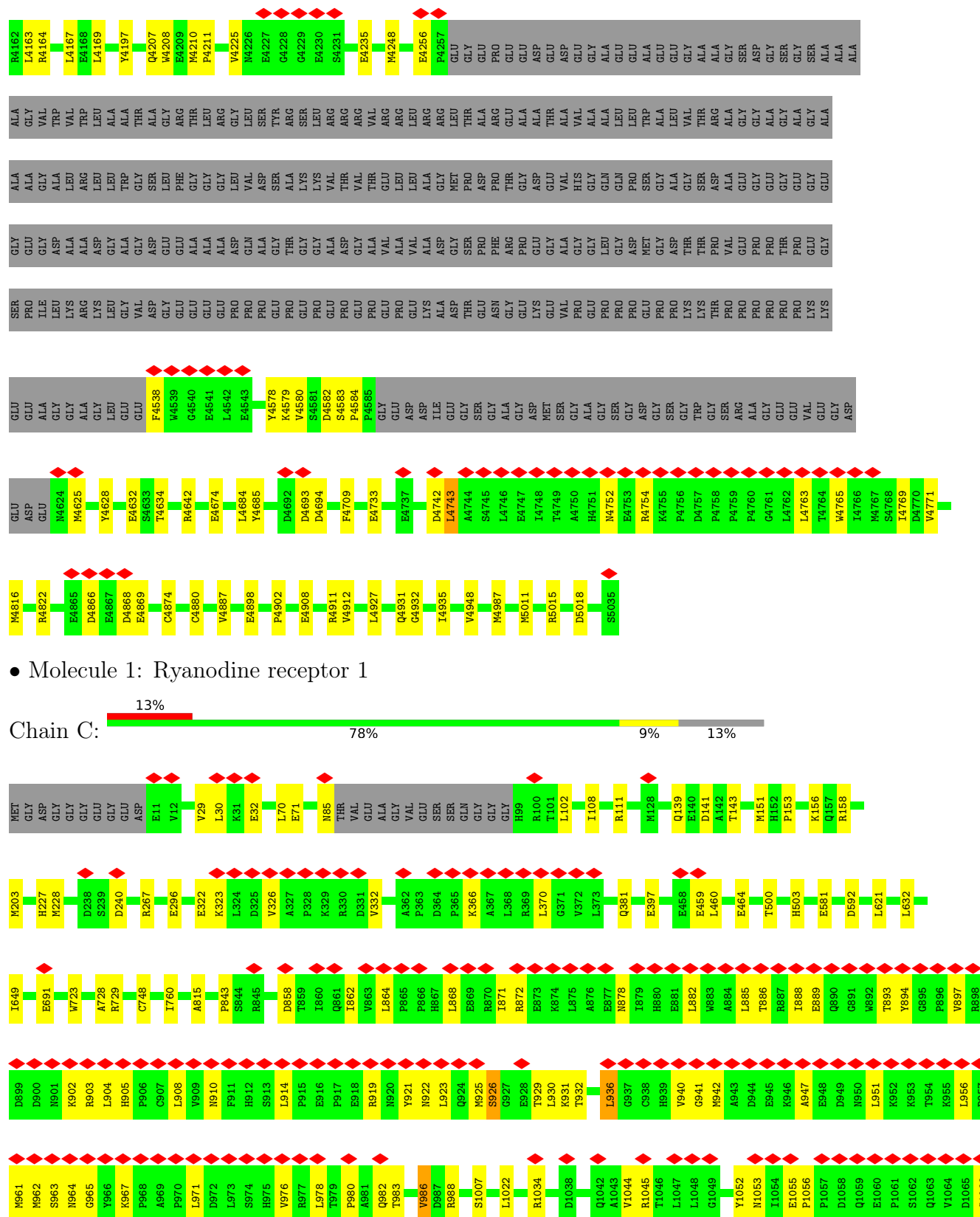


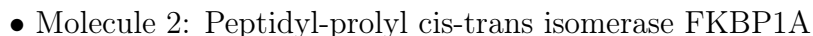


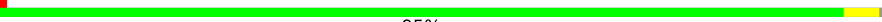
• Molecule 1: Ryanodine receptor 1

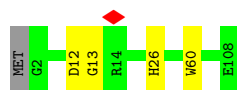


E4059	E3757	HIS	ASP	E3383	H3147	R2940	A2880	W2820	A2760	E2514	ARG
L4071	E3762	LYS	ARG	A3384	L3170	G2941	E2881	E2821	E2761	I2264	LEU
L4072	R3765	LEU	Y3504	K3385	L3176	L2942	E2882	W2822	Y2762	G2265	MET
D4073	L3766	SER	S3505	A3386	R3180	K2943	Y2883	T2823	T2763	L2266	LEU
G4076	C3789	LYS	Q3507	E3387	Y3183	D2944	W2884	V2824	H2764	G2267	LEU
S4077	N3809	GLN	T3508	E3388	V3184	M2945	W2885	E2825	E2765	M2268	GLU
E4078	N3809	ARG	S3509	E3389	E2946	E2946	T2886	K2826	K2766	Q2269	LYS
F4079	S3834	ALA	N3524	E3390	L2947	L2947	W2887	A2827	W2767	T2272	VAL
F4080	G3860	VAL	K3525	G3391	D2948	D2948	Q2888	R2828	F2768	E2286	LEU
Q4081	M3861	C3636	C3526	L3393	S2950	S2950	W2889	E2829	A2769	E2286	VAL
Y4082	V3862	F3637	D3532	D3405	K2954	K2954	E2891	G2830	L2641	E2283	LYS
Y4083	R3863	R3638	L3543	L3406	S2971	S2971	W2890	E2831	L2645	E2283	LYS
Y4084	N3864	N3639	N3556	Y3410	F2974	F2974	E2891	E2831	L2645	E2283	THR
T4085	E3864	M3639	N3557	P3411	L2978	L2978	W2891	E2831	L2645	E2283	GLU
D4086	D3865	C3651	N3558	H3450	V2981	V2981	E2892	E2831	L2645	E2283	PRO
P4087	T3867	Q3651	L3560	Q3457	W2982	W2982	E2893	E2831	L2645	E2283	GLU
R4088	V3868	Q3684	L3561	E3464	D3236	D3236	E2894	E2831	L2645	E2283	GLU
G4089	I3869	E3685	G3562	E3464	E3239	E3239	E2895	E2831	L2645	E2283	PRO
K4094	N3870	E3686	K3563	E3464	D3243	D3243	E2896	E2831	L2645	E2283	GLU
D4095	R3871	E3687	V3564	E3464	I3230	I3230	E2897	E2831	L2645	E2283	GLU
F4096	Q3872	E3688	G3565	E3464	L3231	L3231	E2898	E2831	L2645	E2283	ALA
Q4097	N3873	E3689	G3566	E3464	S3236	S3236	E2899	E2831	L2645	E2283	ALA
K4098	G3874	E3690	S3567	E3464	V2982	V2982	E2899	E2831	L2645	E2283	PRO
A4099	F3002	E3691	P3568	E3471	E3291	E3291	E2899	E2831	L2645	E2283	GLU
M4100	I3919	E3692	S3569	E3472	P3294	P3294	E2899	E2831	L2645	E2283	GLU
S4101	D3844	E3693	G3582	E3472	P3295	P3295	E2899	E2831	L2645	E2283	GLU
S4102	V3945	E3693	R3583	E3472	A3296	A3296	E2899	E2831	L2645	E2283	GLU
Q4103	R3952	E3693	E3584	E3472	L3297	L3297	E2899	E2831	L2645	E2283	GLU
Q4105	S3955	E3693	E3585	E3472	P3298	P3298	E2899	E2831	L2645	E2283	GLU
Q4108	I3972	E3693	E3586	E3472	A3299	A3299	E2899	E2831	L2645	E2283	GLU
P4109	Q3973	E3693	E3587	E3472	G3300	G3300	E2899	E2831	L2645	E2283	GLU
E4110	G3974	E3693	E3588	E3472	A3301	A3301	E2899	E2831	L2645	E2283	GLU
I4111	P3975	E3693	E3591	E3472	L3316	L3316	E2899	E2831	L2645	E2283	GLU
F4113	Q3981	E3693	V3594	E3472	V3325	V3325	E2899	E2831	L2645	E2283	GLU
L4114	S3982	E3693	V3600	E3472	T3362	T3362	E2899	E2831	L2645	E2283	GLU
A4120	L3983	E3693	D3608	E3472	L3366	L3366	E2899	E2831	L2645	E2283	GLU
D4121	V3992	E3693	E3611	E3472	R3369	R3369	E2899	E2831	L2645	E2283	GLU
N4123	D4009	E3693	H3612	E3472	V3373	V3373	E2899	E2831	L2645	E2283	GLU
E4124	S4010	E3693	P3613	E3472	E3378	E3378	E2899	E2831	L2645	E2283	GLU
N4125	E4018	E3693	S3613	E3472	Q3379	Q3379	E2899	E2831	L2645	E2283	GLU
E4129	M4042	E3693	T3613	E3472	L3380	L3380	E2899	E2831	L2645	E2283	GLU
A4132	A4132	E3693	LYS	E3472	R3381	R3381	E2899	E2831	L2645	E2283	GLU
L4142	M4050	E3693	ALA	E3472	L3382	L3382	E2899	E2831	L2645	E2283	GLU
S4154		E3693	TRP	E3472			E2899	E2831	L2645	E2283	GLU
E4155		E3693		E3472			E2899	E2831	L2645	E2283	GLU
P4161		E3693		E3472			E2899	E2831	L2645	E2283	GLU





Chain E:  95% . .



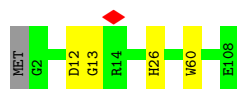
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:  94% 6% .



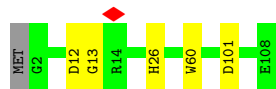
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:  95% . .



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G:  94% 5% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	336237	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.804	Depositor
Minimum map value	0.000	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/35601	0.31	2/48224 (0.0%)
1	B	0.16	0/35601	0.31	1/48224 (0.0%)
1	C	0.16	0/35601	0.31	1/48224 (0.0%)
1	D	0.16	0/35601	0.31	1/48224 (0.0%)
2	E	0.14	0/847	0.27	0/1142
2	F	0.13	0/847	0.26	0/1142
2	G	0.14	0/847	0.27	0/1142
2	H	0.14	0/847	0.27	0/1142
All	All	0.16	0/145792	0.31	5/197464 (0.0%)

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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	4584	PRO	CA-N-CD	-9.53	98.66	112.00
1	C	4584	PRO	CA-N-CD	-9.46	98.76	112.00
1	B	4584	PRO	CA-N-CD	-9.35	98.91	112.00
1	A	4584	PRO	CA-N-CD	-9.29	98.99	112.00
1	A	3568	PRO	CA-N-CD	-5.55	104.22	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	3230	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34809	34401	34401	325	0
1	B	34809	34401	34401	311	0
1	C	34809	34401	34401	327	0
1	D	34809	34401	34401	321	0
2	E	829	826	826	1	0
2	F	829	826	826	1	0
2	G	829	826	826	2	0
2	H	829	826	826	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	108	168	167	0	0
4	B	108	168	167	3	0
4	C	108	168	168	3	0
4	D	108	168	167	1	0
All	All	142988	141580	141577	1291	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 5.

All (1291) 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:D:2828:ARG:NH1	1:D:2935:GLY:O	1.99	0.93
1:C:4110:GLU:O	1:C:4114:LEU:HD12	1.70	0.91
1:B:4110:GLU:O	1:B:4114:LEU:HD12	1.70	0.90
1:A:4110:GLU:O	1:A:4114:LEU:HD12	1.70	0.90
1:C:893:THR:HG23	1:C:904:LEU:HD23	1.50	0.89
1:D:4110:GLU:O	1:D:4114:LEU:HD12	1.71	0.89
1:B:893:THR:HG23	1:B:904:LEU:HD23	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:893:THR:HG23	1:D:904:LEU:HD23	1.55	0.88
1:B:2813:SER:OG	1:B:2883:TYR:OH	1.91	0.87
1:C:2813:SER:OG	1:C:2883:TYR:OH	1.92	0.85
1:B:32:GLU:OE1	1:B:32:GLU:N	2.11	0.84
1:D:108:ILE:HG23	1:D:151:MET:HE2	1.61	0.83
1:B:2215:VAL:HG21	1:B:2229:MET:HE2	1.61	0.83
1:A:2948:ASP:O	1:A:2949:THR:OG1	1.98	0.82
1:B:2828:ARG:NH1	1:B:2935:GLY:O	2.12	0.82
1:C:2813:SER:HG	1:C:2883:TYR:HH	1.26	0.82
1:C:2215:VAL:HG21	1:C:2229:MET:HE2	1.61	0.82
1:A:2215:VAL:HG21	1:A:2229:MET:HE2	1.61	0.82
1:A:893:THR:HG23	1:A:904:LEU:HD23	1.62	0.81
1:A:2813:SER:OG	1:A:2883:TYR:OH	1.93	0.81
1:D:2813:SER:OG	1:D:2883:TYR:OH	1.95	0.81
1:C:108:ILE:HG23	1:C:151:MET:HE2	1.62	0.81
1:B:108:ILE:HG23	1:B:151:MET:HE2	1.62	0.81
1:A:1700:GLU:OE2	1:A:1815:ARG:NH1	2.14	0.81
1:D:1700:GLU:OE2	1:D:1815:ARG:NH1	2.14	0.80
1:C:1700:GLU:OE2	1:C:1815:ARG:NH1	2.14	0.80
1:B:1700:GLU:OE2	1:B:1815:ARG:NH1	2.15	0.80
1:C:3944:ASP:OD1	1:C:3945:VAL:N	2.15	0.80
1:B:3944:ASP:OD1	1:B:3945:VAL:N	2.15	0.80
1:A:3944:ASP:OD1	1:A:3945:VAL:N	2.15	0.80
1:D:2187:MET:O	1:D:2193:TYR:OH	2.00	0.80
1:D:3944:ASP:OD1	1:D:3945:VAL:N	2.15	0.80
1:A:108:ILE:HG23	1:A:151:MET:HE2	1.63	0.79
1:D:2215:VAL:HG21	1:D:2229:MET:HE2	1.61	0.79
1:B:1252:GLU:N	1:B:1252:GLU:OE1	2.15	0.79
1:B:3608:ASP:OD1	1:B:3612:HIS:NE2	2.15	0.79
1:D:4009:ASP:OD1	1:D:4010:SER:N	2.16	0.79
1:C:3608:ASP:OD1	1:C:3612:HIS:NE2	2.15	0.79
1:C:2187:MET:O	1:C:2193:TYR:OH	1.99	0.79
1:A:4009:ASP:OD1	1:A:4010:SER:N	2.16	0.79
1:A:3608:ASP:OD2	1:A:3612:HIS:NE2	2.16	0.79
1:B:2872:LEU:HD22	1:B:2928:LEU:HD11	1.65	0.79
1:D:1252:GLU:N	1:D:1252:GLU:OE1	2.17	0.78
1:C:4009:ASP:OD1	1:C:4010:SER:N	2.16	0.78
1:A:1252:GLU:OE1	1:A:1252:GLU:N	2.17	0.78
1:C:2825:GLU:O	1:C:2828:ARG:NH1	2.17	0.78
1:B:4009:ASP:OD1	1:B:4010:SER:N	2.16	0.78
1:C:1252:GLU:OE1	1:C:1252:GLU:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2828:ARG:NH1	1:C:2935:GLY:O	2.16	0.78
1:D:3608:ASP:OD1	1:D:3612:HIS:NE2	2.17	0.77
1:A:3861:MET:HE1	1:A:3868:VAL:HG22	1.67	0.77
1:C:2872:LEU:HD22	1:C:2928:LEU:HD11	1.66	0.77
1:C:894:TYR:O	1:C:904:LEU:HD22	1.84	0.77
1:A:2187:MET:O	1:A:2193:TYR:OH	2.00	0.77
1:C:3861:MET:HE1	1:C:3868:VAL:HG22	1.67	0.76
1:B:894:TYR:O	1:B:904:LEU:HD22	1.86	0.76
1:B:2187:MET:O	1:B:2193:TYR:OH	2.00	0.76
1:D:894:TYR:O	1:D:904:LEU:HD22	1.85	0.76
1:D:2383:GLU:OE1	1:D:2386:ARG:NH1	2.19	0.76
1:A:2828:ARG:NH1	1:A:2935:GLY:O	2.18	0.75
1:D:897:VAL:O	1:D:902:LYS:NZ	2.18	0.75
1:B:2383:GLU:OE1	1:B:2386:ARG:NH1	2.19	0.75
1:C:3556:ASN:OD1	1:C:3557:ASN:N	2.19	0.75
1:D:3556:ASN:OD1	1:D:3557:ASN:N	2.20	0.75
1:C:2383:GLU:OE1	1:C:2386:ARG:NH1	2.20	0.75
1:A:2383:GLU:OE1	1:A:2386:ARG:NH1	2.20	0.75
1:A:3556:ASN:OD1	1:A:3557:ASN:N	2.20	0.75
1:A:2871:GLU:O	1:A:2940:ARG:NH1	2.20	0.74
1:B:3556:ASN:OD1	1:B:3557:ASN:N	2.20	0.74
1:A:894:TYR:O	1:A:904:LEU:HD22	1.86	0.74
1:D:460:LEU:HD13	1:D:464:GLU:OE2	1.88	0.73
1:A:2027:GLU:OE1	1:A:2027:GLU:N	2.20	0.73
1:A:4100:MET:HE2	1:A:4100:MET:N	2.03	0.73
1:D:2938:VAL:O	1:D:2940:ARG:NH2	2.22	0.73
1:B:897:VAL:O	1:B:902:LYS:NZ	2.18	0.73
1:B:4100:MET:N	1:B:4100:MET:HE2	2.03	0.72
1:C:897:VAL:O	1:C:902:LYS:NZ	2.19	0.71
1:A:897:VAL:O	1:A:902:LYS:NZ	2.22	0.71
1:C:141:ASP:OD2	1:C:143:THR:OG1	2.04	0.71
1:B:1998:GLU:O	1:B:2001:SER:OG	2.09	0.71
1:A:2825:GLU:O	1:A:2828:ARG:NH1	2.23	0.70
1:D:956:LEU:O	1:D:967:LYS:NZ	2.20	0.70
1:D:2872:LEU:HD22	1:D:2928:LEU:HD11	1.72	0.69
1:C:1998:GLU:O	1:C:2001:SER:OG	2.11	0.69
1:D:4100:MET:N	1:D:4100:MET:HE2	2.08	0.69
1:A:951:LEU:HD23	1:A:971:LEU:HD11	1.75	0.69
1:D:3088:ILE:HD12	1:D:3088:ILE:H	1.58	0.69
1:B:2825:GLU:O	1:B:2828:ARG:NH1	2.26	0.69
1:B:3088:ILE:HD12	1:B:3088:ILE:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3088:ILE:HD12	1:C:3088:ILE:H	1.58	0.69
1:C:4100:MET:HE2	1:C:4100:MET:N	2.08	0.69
1:D:951:LEU:HD23	1:D:971:LEU:HD11	1.75	0.69
1:D:1998:GLU:O	1:D:2001:SER:OG	2.09	0.69
1:D:2948:ASP:O	1:D:2949:THR:OG1	2.09	0.68
1:B:2948:ASP:O	1:B:2949:THR:OG1	2.09	0.68
1:D:2027:GLU:OE1	1:D:2027:GLU:N	2.20	0.68
1:D:2875:MET:SD	1:D:2940:ARG:NE	2.66	0.68
1:C:3861:MET:HE1	1:C:3868:VAL:CG2	2.23	0.68
1:A:3088:ILE:H	1:A:3088:ILE:HD12	1.58	0.68
1:A:3861:MET:HE1	1:A:3868:VAL:CG2	2.23	0.68
1:B:951:LEU:HD23	1:B:971:LEU:HD11	1.74	0.68
1:A:878:ASN:HD22	1:A:878:ASN:C	1.98	0.68
1:B:2027:GLU:OE1	1:B:2027:GLU:N	2.22	0.67
1:C:2027:GLU:OE1	1:C:2027:GLU:N	2.22	0.67
1:A:956:LEU:O	1:A:967:LYS:NZ	2.20	0.67
1:A:2868:LEU:HD12	1:A:2873:GLN:HG3	1.77	0.67
1:D:4908:GLU:O	1:D:4912:VAL:HG13	1.95	0.67
1:B:956:LEU:O	1:B:967:LYS:NZ	2.22	0.67
1:A:2268:MET:SD	1:A:2268:MET:N	2.68	0.67
1:A:1998:GLU:O	1:A:2001:SER:OG	2.11	0.67
1:C:70:LEU:HD21	1:C:203:MET:CE	2.25	0.67
1:A:3690:GLU:N	1:A:3690:GLU:OE1	2.28	0.67
1:C:1055:GLU:N	1:C:1055:GLU:OE1	2.27	0.67
1:C:4816:MET:SD	1:C:4816:MET:N	2.68	0.67
1:C:926:SER:O	1:C:930:LEU:HD22	1.95	0.67
1:B:1023:VAL:HG22	1:B:1024:PRO:HD2	1.77	0.66
1:B:1055:GLU:N	1:B:1055:GLU:OE1	2.27	0.66
1:C:4908:GLU:O	1:C:4912:VAL:HG13	1.95	0.66
1:A:141:ASP:OD2	1:A:143:THR:OG1	2.08	0.66
1:D:4816:MET:SD	1:D:4816:MET:N	2.68	0.66
1:C:885:LEU:HD12	1:C:886:THR:N	2.11	0.66
1:D:2817:MET:HE1	1:D:2938:VAL:HG21	1.76	0.66
1:A:4908:GLU:O	1:A:4912:VAL:HG13	1.95	0.66
1:D:2771:LYS:HE3	1:D:2791:MET:HE1	1.76	0.66
1:A:102:LEU:HB3	1:A:151:MET:HE1	1.78	0.66
1:D:1055:GLU:OE1	1:D:1055:GLU:N	2.29	0.66
1:B:885:LEU:HD12	1:B:886:THR:N	2.11	0.66
1:B:4816:MET:SD	1:B:4816:MET:N	2.68	0.66
1:A:2868:LEU:HD13	1:A:2869:SER:N	2.11	0.65
1:C:942:MET:HA	1:C:942:MET:HE3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:VAL:HG22	1:A:1024:PRO:HD2	1.77	0.65
1:B:2868:LEU:HD13	1:B:2869:SER:O	1.97	0.65
1:B:3690:GLU:N	1:B:3690:GLU:OE1	2.29	0.65
1:B:102:LEU:HB3	1:B:151:MET:HE1	1.78	0.65
1:B:4908:GLU:O	1:B:4912:VAL:HG13	1.95	0.65
1:C:102:LEU:HB3	1:C:151:MET:HE1	1.78	0.65
1:C:951:LEU:HD23	1:C:971:LEU:HD11	1.78	0.65
1:A:2249:ARG:NH2	1:A:2286:GLU:OE2	2.29	0.65
1:C:925:MET:O	1:C:929:THR:HG23	1.97	0.65
1:A:2872:LEU:HD13	1:A:2928:LEU:HD11	1.78	0.65
1:A:893:THR:O	1:A:905:HIS:N	2.29	0.65
1:C:2868:LEU:HD13	1:C:2869:SER:O	1.97	0.65
1:D:3690:GLU:N	1:D:3690:GLU:OE1	2.29	0.65
1:B:925:MET:HA	1:B:925:MET:HE2	1.78	0.65
1:B:926:SER:O	1:B:930:LEU:HD22	1.97	0.65
1:D:2645:LEU:HD13	1:D:2679:LEU:HD21	1.79	0.65
1:A:70:LEU:HD21	1:A:203:MET:CE	2.26	0.64
1:A:2645:LEU:HD13	1:A:2679:LEU:HD21	1.79	0.64
1:A:3548:GLU:OE1	1:A:3551:ARG:NH1	2.30	0.64
1:C:2875:MET:SD	1:C:2940:ARG:NE	2.71	0.64
1:D:2249:ARG:NH2	1:D:2286:GLU:OE2	2.30	0.64
1:D:2868:LEU:HD13	1:D:2869:SER:O	1.97	0.64
1:A:2868:LEU:HD21	1:A:2928:LEU:HD12	1.79	0.64
1:B:141:ASP:OD2	1:B:143:THR:OG1	2.11	0.64
1:A:885:LEU:HD12	1:A:886:THR:N	2.12	0.64
1:D:3548:GLU:OE1	1:D:3551:ARG:NH1	2.31	0.64
1:B:2742:GLU:OE1	1:B:2742:GLU:N	2.30	0.64
1:D:885:LEU:HD12	1:D:886:THR:N	2.11	0.64
1:B:2771:LYS:HE3	1:B:2791:MET:HE1	1.80	0.64
1:C:2249:ARG:NH2	1:C:2286:GLU:OE2	2.30	0.64
1:C:2645:LEU:HD13	1:C:2679:LEU:HD21	1.80	0.64
1:C:962:MET:SD	1:C:963:SER:N	2.71	0.64
1:B:70:LEU:HD21	1:B:203:MET:CE	2.27	0.64
1:C:2742:GLU:N	1:C:2742:GLU:OE1	2.30	0.64
1:A:1055:GLU:OE1	1:A:1055:GLU:N	2.30	0.64
1:B:3972:ILE:HG21	1:B:3983:LEU:HD12	1.79	0.64
1:C:3369:ARG:NH2	1:C:3405:ASP:OD2	2.31	0.64
1:B:2645:LEU:HD13	1:B:2679:LEU:HD21	1.79	0.64
1:A:925:MET:HE2	1:A:925:MET:HA	1.80	0.63
1:C:2789:HIS:HB2	1:C:2792:LEU:HD23	1.79	0.63
1:D:3972:ILE:HG21	1:D:3983:LEU:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:926:SER:O	1:D:930:LEU:HD22	1.98	0.63
1:A:926:SER:O	1:A:930:LEU:HD22	1.97	0.63
1:B:2938:VAL:O	1:B:2940:ARG:NH2	2.31	0.63
1:D:141:ASP:OD2	1:D:143:THR:OG1	2.07	0.63
1:B:2761:GLU:OE1	1:B:2803:LYS:NZ	2.31	0.63
1:C:3972:ILE:HG21	1:C:3983:LEU:HD12	1.79	0.63
1:D:2742:GLU:OE1	1:D:2742:GLU:N	2.32	0.63
1:B:3230:ILE:HD12	1:B:3231:LEU:HD12	1.81	0.63
1:D:3369:ARG:NH2	1:D:3405:ASP:OD2	2.32	0.62
1:B:2268:MET:SD	1:B:2268:MET:N	2.72	0.62
1:B:2789:HIS:HB2	1:B:2792:LEU:HD23	1.81	0.62
1:C:2817:MET:HE3	1:C:2822:TRP:HE3	1.63	0.62
1:D:925:MET:HA	1:D:925:MET:HE2	1.80	0.62
1:D:102:LEU:HB3	1:D:151:MET:HE1	1.82	0.62
1:D:108:ILE:CG2	1:D:151:MET:HE2	2.28	0.62
1:D:942:MET:HE3	1:D:942:MET:HA	1.81	0.62
1:C:893:THR:O	1:C:905:HIS:N	2.33	0.62
1:D:381:GLN:N	1:D:381:GLN:OE1	2.33	0.62
1:B:2875:MET:SD	1:B:2940:ARG:NE	2.72	0.62
1:A:3962:LYS:NZ	1:A:4021:ASP:OD2	2.28	0.62
1:B:2293:GLU:O	1:B:2297:GLU:HG3	1.99	0.62
4:C:5103:PCW:O4P	4:C:5103:PCW:H63	2.00	0.62
1:D:2789:HIS:ND1	1:D:2791:MET:HE3	2.13	0.62
1:D:2824:VAL:CG1	1:D:2938:VAL:HG22	2.30	0.62
1:B:2817:MET:HE3	1:B:2822:TRP:HE3	1.64	0.62
1:C:2268:MET:SD	1:C:2268:MET:N	2.73	0.62
1:A:3972:ILE:HG21	1:A:3983:LEU:HD12	1.80	0.61
1:A:942:MET:HE3	1:A:942:MET:HA	1.82	0.61
1:D:2268:MET:N	1:D:2268:MET:SD	2.73	0.61
1:B:942:MET:HE3	1:B:942:MET:HA	1.81	0.61
1:B:2249:ARG:NH2	1:B:2286:GLU:OE2	2.30	0.61
1:A:2742:GLU:N	1:A:2742:GLU:OE1	2.33	0.61
1:A:2782:ILE:HD12	1:A:2789:HIS:CE1	2.35	0.61
1:D:460:LEU:HD22	1:D:464:GLU:OE2	1.99	0.61
1:A:108:ILE:CG2	1:A:151:MET:HE2	2.31	0.61
1:A:2293:GLU:O	1:A:2297:GLU:HG3	2.01	0.60
1:D:2789:HIS:HB2	1:D:2792:LEU:HD23	1.83	0.60
1:C:2938:VAL:O	1:C:2940:ARG:NH2	2.34	0.60
1:D:70:LEU:HD21	1:D:203:MET:HE1	1.81	0.60
1:D:4235:GLU:OE2	1:D:5015:ARG:NH2	2.35	0.60
1:A:3468:MET:HA	1:A:3468:MET:HE3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4235:GLU:OE2	1:A:5015:ARG:NH2	2.34	0.60
1:A:893:THR:CG2	1:A:904:LEU:HD23	2.32	0.60
1:C:381:GLN:OE1	1:C:381:GLN:N	2.33	0.60
1:B:108:ILE:CG2	1:B:151:MET:HE2	2.32	0.59
1:C:2293:GLU:O	1:C:2297:GLU:HG3	2.02	0.59
1:C:3468:MET:HE3	1:C:3468:MET:HA	1.83	0.59
1:C:2948:ASP:O	1:C:2949:THR:OG1	2.09	0.59
1:D:3468:MET:HE3	1:D:3468:MET:HA	1.84	0.59
1:B:4235:GLU:OE2	1:B:5015:ARG:NH2	2.35	0.59
1:A:3730:MET:O	1:A:3733:SER:OG	2.20	0.59
1:C:4235:GLU:OE2	1:C:5015:ARG:NH2	2.35	0.59
1:C:902:LYS:HZ2	1:C:904:LEU:HB2	1.67	0.59
1:B:381:GLN:OE1	1:B:381:GLN:N	2.33	0.59
1:D:71:GLU:OE1	1:D:111:ARG:NE	2.35	0.59
1:A:941:GLY:O	1:A:1053:ASN:ND2	2.36	0.59
1:C:71:GLU:OE1	1:C:111:ARG:NE	2.35	0.59
1:D:3865:ASP:OD2	1:D:3870:ASN:ND2	2.35	0.58
1:D:4632:GLU:OE2	1:D:4634:THR:OG1	2.18	0.58
1:B:2117:LEU:O	1:B:2121:MET:HG3	2.03	0.58
1:B:3865:ASP:OD2	1:B:3870:ASN:ND2	2.35	0.58
1:D:3730:MET:O	1:D:3733:SER:OG	2.20	0.58
1:B:908:LEU:HD23	1:B:964:ASN:OD1	2.02	0.58
1:C:2817:MET:HE1	1:C:2938:VAL:HG21	1.85	0.58
1:A:2738:PRO:O	1:A:2889:ARG:NH2	2.36	0.58
1:D:691:GLU:OE1	1:D:691:GLU:HA	2.03	0.58
1:C:460:LEU:HD22	1:C:464:GLU:OE1	2.02	0.58
1:A:4887:VAL:HG12	1:A:4898:GLU:HG3	1.84	0.58
1:D:956:LEU:HD22	1:D:960:TYR:CD2	2.38	0.58
1:B:3568:PRO:HD2	1:B:3569:SER:H	1.68	0.58
1:B:3730:MET:O	1:B:3733:SER:OG	2.22	0.58
1:C:4887:VAL:HG12	1:C:4898:GLU:HG3	1.84	0.58
1:B:2817:MET:HE1	1:B:2938:VAL:HG21	1.86	0.58
1:C:2761:GLU:OE1	1:C:2803:LYS:NZ	2.27	0.58
1:C:3457:GLN:O	1:C:3461:VAL:HG12	2.03	0.58
1:A:1069:ARG:NE	1:A:1115:GLU:OE1	2.36	0.58
1:C:2789:HIS:CB	1:C:2792:LEU:HD23	2.33	0.58
1:C:3568:PRO:HD2	1:C:3569:SER:H	1.69	0.58
1:D:893:THR:O	1:D:905:HIS:N	2.37	0.58
1:C:4816:MET:O	1:C:4822:ARG:NH1	2.37	0.58
1:A:1562:VAL:HG12	1:A:1563:VAL:HG13	1.86	0.57
1:B:893:THR:O	1:B:905:HIS:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2117:LEU:O	1:A:2121:MET:HG3	2.04	0.57
1:C:1949:ASP:OD1	1:C:2127:ARG:NH2	2.37	0.57
1:C:2117:LEU:O	1:C:2121:MET:HG3	2.03	0.57
4:B:8002:PCW:O4P	4:B:8002:PCW:H63	2.05	0.57
1:A:3176:LEU:HD13	1:A:3176:LEU:C	2.30	0.57
1:D:4887:VAL:HG12	1:D:4898:GLU:HG3	1.85	0.57
1:B:4887:VAL:HG12	1:B:4898:GLU:HG3	1.84	0.57
1:C:3369:ARG:O	1:C:3373:VAL:HG23	2.05	0.57
1:A:956:LEU:HD22	1:A:960:TYR:CD2	2.39	0.57
1:A:2978:LEU:HD22	1:A:3057:LEU:HD21	1.85	0.57
1:D:3457:GLN:O	1:D:3461:VAL:HG12	2.04	0.57
1:C:108:ILE:CG2	1:C:151:MET:HE2	2.32	0.57
1:D:2931:LEU:O	1:D:2936:TYR:N	2.36	0.57
1:B:2929:LYS:O	1:B:2933:MET:SD	2.63	0.57
1:C:2929:LYS:O	1:C:2933:MET:SD	2.63	0.57
1:A:3590:PRO:O	1:A:3594:VAL:HG23	2.05	0.57
1:D:2117:LEU:O	1:D:2121:MET:HG3	2.03	0.57
1:D:3369:ARG:O	1:D:3373:VAL:HG23	2.05	0.57
1:D:3639:MET:HE2	1:D:3639:MET:HA	1.87	0.57
1:B:581:GLU:HG3	1:B:621:LEU:HD22	1.87	0.57
1:C:3730:MET:O	1:C:3733:SER:OG	2.21	0.57
1:A:581:GLU:HG3	1:A:621:LEU:HD22	1.86	0.56
1:D:581:GLU:HG3	1:D:621:LEU:HD22	1.86	0.56
1:C:581:GLU:HG3	1:C:621:LEU:HD22	1.86	0.56
1:C:2978:LEU:HD22	1:C:3057:LEU:HD21	1.86	0.56
1:B:956:LEU:HD22	1:B:960:TYR:CD2	2.40	0.56
1:B:1949:ASP:OD1	1:B:2127:ARG:NH2	2.37	0.56
1:A:2753:ASP:HA	1:A:2756:ILE:HD12	1.88	0.56
1:A:381:GLN:OE1	1:A:381:GLN:N	2.33	0.56
1:D:1949:ASP:OD1	1:D:2127:ARG:NH2	2.37	0.56
1:D:3568:PRO:HD2	1:D:3569:SER:H	1.69	0.56
1:B:2978:LEU:HD22	1:B:3057:LEU:HD21	1.87	0.56
1:B:3369:ARG:O	1:B:3373:VAL:HG23	2.06	0.56
1:C:936:LEU:HD12	1:C:988:ARG:NH2	2.21	0.56
1:D:2929:LYS:O	1:D:2933:MET:SD	2.64	0.56
1:B:4578:TYR:HE2	1:B:4628:TYR:HB3	1.70	0.56
1:D:4816:MET:O	1:D:4822:ARG:NH1	2.36	0.56
1:C:2743:THR:OG1	1:C:2816:ALA:N	2.39	0.56
1:B:3639:MET:HE2	1:B:3639:MET:HA	1.87	0.56
1:A:4874:CYS:HA	1:A:4880:CYS:HB2	1.87	0.56
1:B:3076:LEU:O	1:B:3147:HIS:NE2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4874:CYS:HA	1:B:4880:CYS:HB2	1.88	0.56
1:C:4578:TYR:HE2	1:C:4628:TYR:HB3	1.70	0.56
1:A:3076:LEU:O	1:A:3147:HIS:NE2	2.36	0.55
1:C:4874:CYS:HA	1:C:4880:CYS:HB2	1.88	0.55
1:D:3590:PRO:O	1:D:3594:VAL:HG23	2.05	0.55
1:A:61:PRO:HG2	1:A:63:LEU:HD13	1.88	0.55
1:A:4578:TYR:HE2	1:A:4628:TYR:HB3	1.70	0.55
1:B:2743:THR:OG1	1:B:2816:ALA:N	2.38	0.55
1:D:2756:ILE:HD13	1:D:2811:LYS:HG2	1.89	0.55
1:D:2978:LEU:HD22	1:D:3057:LEU:HD21	1.87	0.55
1:B:3088:ILE:HD12	1:B:3088:ILE:N	2.22	0.55
1:C:2824:VAL:CG1	1:C:2938:VAL:HG22	2.37	0.55
1:A:1949:ASP:OD1	1:A:2127:ARG:NH2	2.37	0.55
1:A:3369:ARG:O	1:A:3373:VAL:HG23	2.06	0.55
1:B:3041:THR:HA	1:B:3076:LEU:HD11	1.89	0.55
1:A:3981:GLN:OE1	1:A:4042:MET:HE1	2.07	0.55
1:A:4582:ASP:OD1	1:A:4583:SER:N	2.40	0.55
1:C:2887:TRP:CD1	1:C:2891:LYS:HZ1	2.25	0.55
1:C:3041:THR:HA	1:C:3076:LEU:HD11	1.89	0.55
1:C:3981:GLN:OE1	1:C:4042:MET:HE1	2.07	0.55
1:A:862:ILE:O	1:A:931:LYS:NZ	2.40	0.55
1:B:3981:GLN:OE1	1:B:4042:MET:HE1	2.07	0.55
1:C:4765:TRP:O	1:C:4769:ILE:HG23	2.06	0.55
1:C:908:LEU:HD22	1:C:962:MET:CE	2.37	0.55
1:C:4163:LEU:O	1:C:4167:LEU:HD23	2.07	0.55
1:D:4256:GLU:N	1:D:4256:GLU:OE1	2.40	0.54
1:B:936:LEU:HD12	1:B:988:ARG:NH2	2.22	0.54
1:C:2753:ASP:HA	1:C:2756:ILE:HD12	1.89	0.54
1:C:3524:ASN:O	1:C:3583:ARG:NH1	2.40	0.54
1:A:936:LEU:HD12	1:A:988:ARG:NH2	2.22	0.54
1:A:2089:GLU:OE2	1:A:2090:HIS:ND1	2.40	0.54
1:D:3541:TYR:OH	1:D:3547:ASP:OD1	2.15	0.54
1:B:3524:ASN:O	1:B:3583:ARG:NH1	2.41	0.54
1:C:3088:ILE:HD12	1:C:3088:ILE:N	2.22	0.54
1:D:902:LYS:HZ2	1:D:904:LEU:HB2	1.71	0.54
1:D:3524:ASN:O	1:D:3583:ARG:NH1	2.41	0.54
1:B:2753:ASP:HA	1:B:2756:ILE:HD12	1.88	0.54
1:B:3378:GLU:OE2	1:B:3378:GLU:HA	2.08	0.54
1:C:3170:LEU:HD12	1:C:3195:LEU:HD11	1.88	0.54
1:D:3981:GLN:OE1	1:D:4042:MET:HE1	2.06	0.54
1:B:4163:LEU:O	1:B:4167:LEU:HD23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4582:ASP:OD1	1:B:4583:SER:N	2.41	0.54
1:C:3378:GLU:HA	1:C:3378:GLU:OE2	2.08	0.54
1:C:4155:GLU:OE1	1:C:4197:TYR:OH	2.17	0.54
1:C:4582:ASP:OD1	1:C:4583:SER:N	2.40	0.54
1:A:1874:ARG:HB3	1:A:1874:ARG:CZ	2.38	0.54
1:A:2929:LYS:O	1:A:2933:MET:SD	2.65	0.54
1:D:3378:GLU:OE2	1:D:3378:GLU:HA	2.08	0.54
1:C:2738:PRO:O	1:C:2889:ARG:NH2	2.40	0.54
1:D:936:LEU:HD12	1:D:988:ARG:NH2	2.23	0.54
1:D:3170:LEU:HD12	1:D:3195:LEU:HD11	1.88	0.54
1:D:4163:LEU:O	1:D:4167:LEU:HD23	2.07	0.54
1:C:2756:ILE:HD13	1:C:2811:LYS:HG2	1.90	0.54
1:C:3683:GLU:HB3	1:C:3686:GLU:HB3	1.89	0.54
1:D:868:LEU:HD21	1:D:940:VAL:HG21	1.88	0.54
1:D:2753:ASP:HA	1:D:2756:ILE:HD12	1.90	0.54
1:B:366:LYS:NZ	1:B:370:LEU:HD11	2.23	0.54
1:B:902:LYS:HZ2	1:B:904:LEU:HB2	1.73	0.54
1:B:2746:VAL:HG21	1:B:2819:ALA:HB2	1.88	0.54
1:B:4816:MET:O	1:B:4822:ARG:NH1	2.40	0.54
1:B:2738:PRO:O	1:B:2889:ARG:NH2	2.40	0.54
1:B:2756:ILE:HD13	1:B:2811:LYS:HG2	1.89	0.54
1:C:366:LYS:NZ	1:C:370:LEU:HD11	2.23	0.54
1:A:4163:LEU:O	1:A:4167:LEU:HD23	2.07	0.54
1:B:2824:VAL:CG1	1:B:2938:VAL:HG22	2.38	0.54
1:A:2822:TRP:CG	1:A:2875:MET:HE1	2.43	0.53
1:D:3088:ILE:HD12	1:D:3088:ILE:N	2.22	0.53
1:D:4582:ASP:OD1	1:D:4583:SER:N	2.41	0.53
1:C:956:LEU:O	1:C:967:LYS:NZ	2.31	0.53
1:A:2746:VAL:HG21	1:A:2819:ALA:HB2	1.90	0.53
1:A:3236:SER:OG	1:A:3239:GLU:OE2	2.20	0.53
1:B:3325:VAL:HG12	1:B:3362:THR:HG23	1.90	0.53
1:B:3468:MET:HE3	1:B:3468:MET:HA	1.89	0.53
1:D:1510:ILE:HD12	1:D:1510:ILE:H	1.73	0.53
1:D:1874:ARG:CZ	1:D:1874:ARG:HB3	2.38	0.53
1:C:2746:VAL:HG21	1:C:2819:ALA:HB2	1.89	0.53
1:C:4868:ASP:OD1	1:C:4869:GLU:N	2.42	0.53
1:A:3524:ASN:O	1:A:3583:ARG:NH1	2.41	0.53
1:D:3041:THR:HA	1:D:3076:LEU:HD11	1.89	0.53
1:B:228:MET:SD	1:B:228:MET:N	2.81	0.53
1:D:2738:PRO:O	1:D:2889:ARG:NH2	2.40	0.53
1:A:2823:THR:HG1	1:A:2939:THR:HG1	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:862:ILE:O	1:B:931:LYS:NZ	2.41	0.53
1:B:4902:PRO:HB3	1:B:4911:ARG:HG2	1.91	0.53
1:A:2678:LYS:NZ	1:A:2910:ASP:OD2	2.42	0.53
1:D:366:LYS:NZ	1:D:370:LEU:HD11	2.23	0.53
1:D:4868:ASP:OD1	1:D:4869:GLU:N	2.41	0.53
4:D:5103:PCW:O4P	4:D:5103:PCW:H63	2.07	0.53
1:A:4816:MET:O	1:A:4822:ARG:NH1	2.39	0.53
1:B:2089:GLU:OE2	1:B:2090:HIS:ND1	2.41	0.53
1:B:2887:TRP:CD1	1:B:2891:LYS:HZ1	2.27	0.53
1:B:4868:ASP:OD1	1:B:4869:GLU:N	2.42	0.53
1:A:2789:HIS:HB3	1:A:2792:LEU:HD23	1.90	0.53
1:A:3556:ASN:OD1	1:A:3556:ASN:C	2.52	0.53
1:A:3568:PRO:HD2	1:A:3569:SER:H	1.72	0.53
1:C:862:ILE:O	1:C:931:LYS:NZ	2.42	0.53
1:C:3556:ASN:OD1	1:C:3556:ASN:C	2.52	0.53
1:C:3639:MET:HE2	1:C:3639:MET:HA	1.91	0.53
1:A:4112:GLN:OE1	1:A:4112:GLN:HA	2.08	0.52
1:D:925:MET:O	1:D:929:THR:HG23	2.08	0.52
1:B:926:SER:O	1:B:929:THR:OG1	2.25	0.52
1:C:3076:LEU:O	1:C:3147:HIS:NE2	2.36	0.52
1:A:4248:MET:HE1	1:A:4987:MET:HE1	1.91	0.52
1:A:4868:ASP:OD1	1:A:4869:GLU:N	2.42	0.52
1:A:4902:PRO:HB3	1:A:4911:ARG:HG2	1.91	0.52
1:D:3076:LEU:O	1:D:3147:HIS:NE2	2.36	0.52
1:C:922:ASN:HA	1:C:925:MET:HE2	1.91	0.52
1:A:3041:THR:HA	1:A:3076:LEU:HD11	1.89	0.52
1:A:3325:VAL:HG12	1:A:3362:THR:HG23	1.90	0.52
1:D:2761:GLU:OE1	1:D:2803:LYS:NZ	2.38	0.52
1:D:3556:ASN:OD1	1:D:3556:ASN:C	2.52	0.52
1:B:925:MET:O	1:B:929:THR:HG23	2.09	0.52
1:C:2887:TRP:CG	1:C:2891:LYS:HZ1	2.27	0.52
1:C:4256:GLU:OE1	1:C:4256:GLU:N	2.40	0.52
1:D:910:ASN:O	1:D:914:LEU:N	2.43	0.52
1:A:4256:GLU:OE1	1:A:4256:GLU:N	2.40	0.52
1:B:2767:TRP:C	1:B:2771:LYS:HZ2	2.18	0.52
1:B:3170:LEU:HD12	1:B:3195:LEU:HD11	1.91	0.52
1:D:2268:MET:HE2	1:D:2272:THR:HG22	1.92	0.52
1:C:868:LEU:HD21	1:C:940:VAL:HG21	1.91	0.52
1:C:4902:PRO:HB3	1:C:4911:ARG:HG2	1.91	0.52
1:A:240:ASP:OD2	1:A:240:ASP:N	2.41	0.52
1:A:3378:GLU:HA	1:A:3378:GLU:OE2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4902:PRO:HB3	1:D:4911:ARG:HG2	1.92	0.52
1:A:925:MET:O	1:A:929:THR:HG23	2.09	0.52
1:A:3683:GLU:O	1:A:3686:GLU:N	2.43	0.52
1:B:2020:GLU:OE1	1:B:2020:GLU:HA	2.10	0.52
1:C:322:GLU:OE1	1:C:322:GLU:HA	2.10	0.52
1:A:366:LYS:NZ	1:A:370:LEU:HD11	2.24	0.51
1:A:3088:ILE:HD12	1:A:3088:ILE:N	2.22	0.51
1:D:2908:PRO:O	1:D:2911:THR:OG1	2.28	0.51
1:B:2887:TRP:CG	1:B:2891:LYS:HZ1	2.27	0.51
1:A:2413:GLU:OE1	1:A:2413:GLU:O	2.28	0.51
1:A:2756:ILE:HD13	1:A:2811:LYS:HG2	1.91	0.51
1:D:2771:LYS:HB3	1:D:2776:TRP:HB2	1.92	0.51
1:B:3556:ASN:OD1	1:B:3556:ASN:C	2.53	0.51
1:D:3236:SER:OG	1:D:3239:GLU:OE2	2.19	0.51
1:A:366:LYS:HZ2	1:A:370:LEU:HD11	1.75	0.51
1:B:322:GLU:HA	1:B:322:GLU:OE1	2.10	0.51
1:C:2767:TRP:O	1:C:2771:LYS:HG3	2.10	0.51
1:A:878:ASN:C	1:A:878:ASN:ND2	2.67	0.51
1:A:4742:ASP:OD1	1:A:4742:ASP:C	2.54	0.51
1:B:4742:ASP:C	1:B:4742:ASP:OD1	2.53	0.51
1:B:868:LEU:HD21	1:B:940:VAL:HG21	1.91	0.51
1:C:2817:MET:HE1	1:C:2938:VAL:HG11	1.93	0.51
1:D:4742:ASP:OD1	1:D:4742:ASP:C	2.54	0.51
1:B:4733:GLU:OE2	1:B:4733:GLU:HA	2.11	0.51
1:B:4743:LEU:HD22	1:B:4743:LEU:H	1.76	0.51
1:C:961:MET:HE3	1:C:962:MET:H	1.76	0.51
1:C:2268:MET:HE2	1:C:2272:THR:HG22	1.92	0.51
1:A:2020:GLU:OE1	1:A:2020:GLU:HA	2.11	0.51
1:A:2747:ILE:C	1:A:2747:ILE:HD12	2.36	0.51
1:D:893:THR:CG2	1:D:904:LEU:HD23	2.35	0.51
1:D:2944:ASP:OD1	1:D:2945:MET:N	2.44	0.51
1:D:4733:GLU:OE2	1:D:4733:GLU:HA	2.11	0.51
1:C:2020:GLU:OE2	1:C:2020:GLU:HA	2.09	0.51
1:B:2944:ASP:OD1	1:B:2945:MET:N	2.44	0.51
1:B:4256:GLU:OE1	1:B:4256:GLU:N	2.40	0.51
1:C:240:ASP:OD1	1:C:240:ASP:N	2.44	0.51
1:A:2743:THR:OG1	1:A:2816:ALA:N	2.44	0.50
1:B:1874:ARG:CZ	1:B:1874:ARG:HB3	2.41	0.50
1:D:864:LEU:HD13	1:D:865:PRO:O	2.12	0.50
1:B:2817:MET:HE1	1:B:2938:VAL:HG11	1.92	0.50
1:C:910:ASN:O	1:C:914:LEU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4112:GLN:HA	1:C:4112:GLN:OE1	2.11	0.50
1:C:4742:ASP:OD1	1:C:4742:ASP:C	2.54	0.50
1:D:1066:SER:OG	1:D:1067:GLN:OE1	2.29	0.50
1:B:4142:ILE:HD12	1:B:4142:ILE:H	1.77	0.50
1:A:4733:GLU:OE2	1:A:4733:GLU:HA	2.11	0.50
1:B:3683:GLU:HB3	1:B:3686:GLU:HB3	1.94	0.50
1:C:2944:ASP:OD1	1:C:2945:MET:N	2.43	0.50
1:C:4733:GLU:HA	1:C:4733:GLU:OE2	2.11	0.50
1:A:2874:ALA:HB3	1:A:2940:ARG:HH12	1.76	0.50
1:B:2268:MET:HE2	1:B:2272:THR:HG22	1.92	0.50
1:A:2868:LEU:HD21	1:A:2928:LEU:CD1	2.40	0.50
1:C:2186:ILE:HG21	1:C:2204:MET:HE1	1.93	0.50
1:C:3282:LEU:HD12	1:C:3316:LEU:HD22	1.94	0.50
1:A:32:GLU:OE2	1:A:32:GLU:HA	2.12	0.50
1:A:926:SER:O	1:A:929:THR:OG1	2.25	0.50
1:D:4625:MET:HE3	1:D:4625:MET:HA	1.94	0.50
1:B:4112:GLN:OE1	1:B:4112:GLN:HA	2.11	0.50
1:C:32:GLU:OE2	1:C:32:GLU:HA	2.12	0.50
1:A:3362:THR:HG21	1:A:3409:LEU:HD22	1.94	0.50
1:A:4743:LEU:H	1:A:4743:LEU:HD22	1.76	0.50
1:D:4112:GLN:OE1	1:D:4112:GLN:HA	2.11	0.50
1:B:3362:THR:HG21	1:B:3409:LEU:HD22	1.94	0.50
1:C:3828:GLU:OE1	1:C:3828:GLU:N	2.37	0.50
1:D:926:SER:O	1:D:929:THR:OG1	2.25	0.50
1:B:2817:MET:HE3	1:B:2822:TRP:CE3	2.45	0.50
1:C:3380:LEU:C	1:C:3380:LEU:HD23	2.37	0.50
1:A:908:LEU:HD23	1:A:964:ASN:OD1	2.12	0.49
1:A:910:ASN:O	1:A:914:LEU:N	2.44	0.49
1:A:2870:ARG:NH2	1:A:2873:GLN:OE1	2.45	0.49
1:D:2813:SER:O	1:D:2817:MET:HG3	2.12	0.49
1:B:4625:MET:HA	1:B:4625:MET:HE3	1.94	0.49
1:C:2817:MET:HE3	1:C:2822:TRP:CE3	2.44	0.49
1:C:2908:PRO:O	1:C:2911:THR:OG1	2.28	0.49
1:C:4142:ILE:HD12	1:C:4142:ILE:H	1.77	0.49
1:A:2974:PHE:CD1	1:A:2974:PHE:C	2.90	0.49
1:D:276:ARG:NH1	1:D:339:GLU:OE2	2.45	0.49
1:D:4142:ILE:HD12	1:D:4142:ILE:H	1.77	0.49
1:B:868:LEU:HD23	1:B:871:ILE:HD11	1.93	0.49
1:C:1874:ARG:CZ	1:C:1874:ARG:HB3	2.42	0.49
1:C:4743:LEU:HD22	1:C:4743:LEU:H	1.76	0.49
1:A:3282:LEU:HD12	1:A:3316:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2755:PHE:HD2	1:D:2814:LEU:HD11	1.77	0.49
1:B:3683:GLU:O	1:B:3686:GLU:N	2.45	0.49
1:D:2828:ARG:HH12	1:D:2936:TYR:HA	1.76	0.49
1:D:3282:LEU:HD12	1:D:3316:LEU:HD22	1.94	0.49
1:D:4765:TRP:O	1:D:4769:ILE:HG23	2.12	0.49
1:C:926:SER:O	1:C:929:THR:OG1	2.26	0.49
1:C:2091:LYS:HD2	1:C:2091:LYS:N	2.28	0.49
1:A:276:ARG:NH1	1:A:339:GLU:OE2	2.45	0.49
1:A:2771:LYS:CE	1:A:2791:MET:HE1	2.42	0.49
1:A:4142:ILE:HD12	1:A:4142:ILE:H	1.77	0.49
1:A:4765:TRP:O	1:A:4769:ILE:HG23	2.13	0.49
1:D:3683:GLU:O	1:D:3686:GLU:N	2.45	0.49
1:B:1849:THR:O	1:B:1853:MET:HG3	2.13	0.49
1:B:4632:GLU:OE2	1:B:4634:THR:OG1	2.25	0.49
1:C:1066:SER:OG	1:C:1067:GLN:OE1	2.31	0.49
1:D:2747:ILE:HD12	1:D:2747:ILE:C	2.38	0.49
1:D:4866:ASP:N	1:D:4866:ASP:OD1	2.46	0.49
1:B:2596:LEU:HD21	1:B:2604:ILE:CD1	2.43	0.49
1:B:2747:ILE:HD12	1:B:2747:ILE:C	2.38	0.49
1:B:3282:LEU:HD12	1:B:3316:LEU:HD22	1.94	0.49
1:C:894:TYR:CB	1:C:962:MET:HE1	2.43	0.49
1:C:908:LEU:HD23	1:C:964:ASN:OD1	2.13	0.49
1:C:4625:MET:HE3	1:C:4625:MET:HA	1.94	0.49
1:A:902:LYS:HZ2	1:A:904:LEU:HB2	1.76	0.49
1:A:962:MET:O	1:A:964:ASN:N	2.45	0.49
1:A:2887:TRP:CG	1:A:2891:LYS:HZ1	2.30	0.49
1:A:3683:GLU:HB3	1:A:3686:GLU:HB3	1.94	0.49
1:D:2746:VAL:HG21	1:D:2819:ALA:HB2	1.94	0.49
1:C:1849:THR:O	1:C:1853:MET:HG3	2.13	0.49
1:C:2974:PHE:CD1	1:C:2974:PHE:C	2.90	0.49
1:A:2982:VAL:O	1:A:2986:ARG:NE	2.46	0.49
1:D:4743:LEU:H	1:D:4743:LEU:HD22	1.76	0.49
1:B:4765:TRP:O	1:B:4769:ILE:HG23	2.12	0.49
1:C:2747:ILE:C	1:C:2747:ILE:HD12	2.38	0.49
1:C:4210:MET:HE3	1:C:4211:PRO:HD2	1.95	0.49
1:A:1227:PHE:O	1:A:1829:ARG:NH2	2.45	0.49
1:D:29:VAL:HG12	1:D:30:LEU:HD22	1.94	0.49
1:D:2974:PHE:CD1	1:D:2974:PHE:C	2.90	0.49
1:B:1227:PHE:O	1:B:1829:ARG:NH2	2.45	0.49
1:B:2091:LYS:N	1:B:2091:LYS:HD2	2.28	0.49
1:B:2826:LYS:NZ	1:B:2934:ASN:O	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3590:PRO:O	1:B:3594:VAL:HG23	2.13	0.49
1:B:4099:ALA:C	1:B:4100:MET:HE2	2.38	0.49
1:B:4866:ASP:N	1:B:4866:ASP:OD1	2.46	0.49
1:C:4769:ILE:HD11	1:C:4771:VAL:HG23	1.94	0.49
1:A:2767:TRP:CG	1:A:2771:LYS:HZ2	2.31	0.49
1:D:2791:MET:SD	1:D:2792:LEU:N	2.86	0.49
1:D:3683:GLU:HB3	1:D:3686:GLU:HB3	1.94	0.49
1:D:4874:CYS:HA	1:D:4880:CYS:HB2	1.93	0.49
1:B:240:ASP:OD1	1:B:240:ASP:N	2.44	0.49
4:B:8002:PCW:H20	4:B:8002:PCW:H462	1.95	0.49
1:C:70:LEU:HD21	1:C:203:MET:HE1	1.95	0.49
1:A:691:GLU:OE2	1:A:691:GLU:HA	2.12	0.48
1:A:2091:LYS:HD2	1:A:2091:LYS:N	2.27	0.48
1:A:2789:HIS:CB	1:A:2792:LEU:HD23	2.43	0.48
1:A:3170:LEU:HD12	1:A:3195:LEU:HD11	1.94	0.48
1:D:961:MET:HE3	1:D:962:MET:N	2.28	0.48
1:D:2887:TRP:CG	1:D:2891:LYS:HZ1	2.30	0.48
1:A:961:MET:HE3	1:A:962:MET:N	2.28	0.48
1:A:1113:ASP:OD1	1:A:1113:ASP:N	2.45	0.48
1:D:1822:ARG:NH1	1:D:1822:ARG:HB3	2.28	0.48
1:D:3789:CYS:SG	1:D:3834:SER:OG	2.71	0.48
1:B:1066:SER:OG	1:B:1067:GLN:OE1	2.31	0.48
1:B:3789:CYS:SG	1:B:3834:SER:OG	2.71	0.48
1:C:868:LEU:HD23	1:C:871:ILE:HD11	1.93	0.48
1:C:2791:MET:SD	1:C:2792:LEU:N	2.86	0.48
1:A:4210:MET:HE3	1:A:4211:PRO:HD2	1.95	0.48
1:D:2743:THR:OG1	1:D:2816:ALA:N	2.46	0.48
1:B:2974:PHE:CD1	1:B:2974:PHE:C	2.90	0.48
1:C:1822:ARG:HB3	1:C:1822:ARG:NH1	2.28	0.48
1:A:70:LEU:HD21	1:A:203:MET:HE1	1.95	0.48
1:A:2753:ASP:O	1:A:2757:ASN:OD1	2.31	0.48
1:A:4099:ALA:C	1:A:4100:MET:HE2	2.38	0.48
1:B:29:VAL:HG12	1:B:30:LEU:HD22	1.94	0.48
1:C:1227:PHE:O	1:C:1829:ARG:NH2	2.44	0.48
1:C:3789:CYS:SG	1:C:3834:SER:OG	2.71	0.48
1:A:4866:ASP:OD1	1:A:4866:ASP:N	2.46	0.48
1:D:366:LYS:HZ3	1:D:370:LEU:HD11	1.78	0.48
1:D:862:ILE:O	1:D:931:LYS:NZ	2.46	0.48
1:D:3861:MET:HE2	1:D:3870:ASN:OD1	2.14	0.48
1:B:366:LYS:HZ2	1:B:370:LEU:HD11	1.78	0.48
1:B:1822:ARG:HB3	1:B:1822:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3230:ILE:CD1	1:B:3231:LEU:HD12	2.42	0.48
1:C:592:ASP:HA	1:C:632:LEU:HD21	1.95	0.48
1:D:240:ASP:OD2	1:D:240:ASP:N	2.45	0.48
1:D:1849:THR:O	1:D:1853:MET:HG3	2.13	0.48
1:B:2767:TRP:CH2	1:B:2791:MET:HE2	2.48	0.48
1:C:2771:LYS:HE2	1:C:2791:MET:HE1	1.96	0.48
1:A:2822:TRP:CD2	1:A:2875:MET:HE1	2.49	0.48
1:D:2910:ASP:OD1	1:D:2911:THR:N	2.47	0.48
1:B:3869:ILE:HD11	1:B:3872:GLN:O	2.14	0.48
1:A:3789:CYS:SG	1:A:3834:SER:OG	2.72	0.48
1:D:4210:MET:HE3	1:D:4211:PRO:HD2	1.94	0.48
1:C:3590:PRO:O	1:C:3594:VAL:HG23	2.13	0.48
1:A:5011:MET:HE1	1:A:5018:ASP:HB2	1.95	0.48
1:D:941:GLY:O	1:D:1053:ASN:ND2	2.47	0.48
1:D:2752:LEU:HD13	1:D:2814:LEU:HD13	1.96	0.48
1:B:910:ASN:O	1:B:914:LEU:N	2.46	0.48
1:B:941:GLY:O	1:B:1053:ASN:ND2	2.47	0.48
1:B:962:MET:HG3	1:B:963:SER:H	1.78	0.48
1:C:871:ILE:HD13	1:C:1052:TYR:CZ	2.49	0.48
1:A:1822:ARG:HB3	1:A:1822:ARG:NH1	2.28	0.48
1:A:2944:ASP:OD1	1:A:2945:MET:N	2.47	0.48
1:A:3240:MET:HA	1:A:3240:MET:HE2	1.94	0.48
1:D:858:ASP:OD1	1:D:858:ASP:N	2.47	0.48
1:D:1227:PHE:O	1:D:1829:ARG:NH2	2.45	0.48
1:D:2091:LYS:N	1:D:2091:LYS:HD2	2.29	0.48
1:D:4207:GLN:HB3	1:D:4248:MET:HG2	1.96	0.48
1:C:941:GLY:O	1:C:1053:ASN:ND2	2.47	0.48
1:A:592:ASP:HA	1:A:632:LEU:HD21	1.96	0.47
1:A:1849:THR:O	1:A:1853:MET:HG3	2.13	0.47
1:A:2265:GLY:C	1:A:2266:LEU:HD12	2.38	0.47
1:A:2927:LEU:C	1:A:2927:LEU:HD23	2.39	0.47
1:D:2265:GLY:C	1:D:2266:LEU:HD12	2.39	0.47
1:D:3869:ILE:HD11	1:D:3872:GLN:O	2.14	0.47
1:A:1066:SER:OG	1:A:1067:GLN:OE1	2.32	0.47
2:H:12:ASP:OD1	2:H:13:GLY:N	2.47	0.47
1:D:2879:LEU:CD1	1:D:2883:TYR:CE2	2.97	0.47
1:D:5011:MET:HE1	1:D:5018:ASP:HB2	1.95	0.47
1:B:2265:GLY:C	1:B:2266:LEU:HD12	2.39	0.47
1:B:3861:MET:HE2	1:B:3870:ASN:OD1	2.14	0.47
1:C:2777:SER:C	1:C:2792:LEU:HD21	2.38	0.47
1:C:3108:VAL:HG13	1:C:3176:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2978:LEU:O	1:A:2978:LEU:HD23	2.14	0.47
1:D:592:ASP:HA	1:D:632:LEU:HD21	1.97	0.47
1:B:592:ASP:HA	1:B:632:LEU:HD21	1.96	0.47
1:B:1455:THR:OG1	1:B:1457:ASP:OD1	2.31	0.47
1:B:2910:ASP:OD1	1:B:2911:THR:N	2.47	0.47
1:B:2927:LEU:C	1:B:2927:LEU:HD23	2.40	0.47
1:B:3714:LYS:NZ	1:B:3716:LYS:O	2.47	0.47
1:A:1055:GLU:O	1:A:1056:PRO:C	2.57	0.47
2:E:12:ASP:OD1	2:E:13:GLY:N	2.47	0.47
1:D:921:TYR:O	1:D:924:GLN:HG3	2.15	0.47
1:D:2824:VAL:HG11	1:D:2938:VAL:HG22	1.95	0.47
1:B:1055:GLU:O	1:B:1056:PRO:C	2.57	0.47
1:B:5011:MET:HE1	1:B:5018:ASP:HB2	1.95	0.47
1:C:2265:GLY:C	1:C:2266:LEU:HD12	2.39	0.47
1:C:2771:LYS:CE	1:C:2791:MET:HE1	2.44	0.47
1:A:893:THR:HA	1:A:962:MET:SD	2.55	0.47
1:A:2887:TRP:CD1	1:A:2891:LYS:HZ1	2.33	0.47
1:D:1055:GLU:O	1:D:1056:PRO:C	2.57	0.47
1:D:1455:THR:OG1	1:D:1457:ASP:OD1	2.32	0.47
1:B:70:LEU:HD21	1:B:203:MET:HE1	1.96	0.47
1:C:2047:LEU:N	1:C:2047:LEU:HD22	2.29	0.47
1:C:4752:ASN:O	1:C:4754:ARG:NH1	2.47	0.47
1:A:858:ASP:OD1	1:A:858:ASP:N	2.46	0.47
1:A:2047:LEU:N	1:A:2047:LEU:HD22	2.30	0.47
1:A:3004:LEU:HB2	1:A:3005:PRO:HD3	1.97	0.47
1:D:2020:GLU:HA	1:D:2020:GLU:OE2	2.14	0.47
1:D:2047:LEU:HD22	1:D:2047:LEU:N	2.30	0.47
1:D:2887:TRP:CD1	1:D:2891:LYS:HZ1	2.33	0.47
1:B:878:ASN:C	1:B:878:ASN:HD22	2.22	0.47
1:B:2047:LEU:N	1:B:2047:LEU:HD22	2.29	0.47
1:B:3955:SER:OG	1:B:4018:GLU:OE1	2.28	0.47
1:B:4752:ASN:O	1:B:4754:ARG:NH1	2.48	0.47
1:C:858:ASP:OD1	1:C:858:ASP:N	2.47	0.47
2:F:12:ASP:OD1	2:F:13:GLY:N	2.47	0.47
1:D:925:MET:HE2	1:D:925:MET:CA	2.43	0.47
1:D:2927:LEU:C	1:D:2927:LEU:HD23	2.40	0.47
1:B:858:ASP:OD1	1:B:858:ASP:N	2.47	0.47
1:B:2767:TRP:CG	1:B:2771:LYS:HZ1	2.32	0.47
1:C:3457:GLN:HA	1:C:3457:GLN:OE1	2.14	0.47
1:C:4207:GLN:HB3	1:C:4248:MET:HG2	1.97	0.47
1:D:2769:PHE:O	1:D:2773:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3004:LEU:HB2	1:D:3005:PRO:HD3	1.97	0.47
1:D:3588:ASP:OD1	1:D:3588:ASP:N	2.48	0.47
1:B:871:ILE:HD13	1:B:1052:TYR:CZ	2.50	0.47
1:B:893:THR:CG2	1:B:904:LEU:HD23	2.36	0.47
1:B:4208:TRP:CE3	1:B:4987:MET:HE2	2.50	0.47
1:A:228:MET:SD	1:A:228:MET:N	2.88	0.47
1:A:942:MET:HE3	1:A:943:ALA:H	1.80	0.47
1:A:3457:GLN:OE1	1:A:3457:GLN:HA	2.14	0.47
1:D:914:LEU:O	1:D:919:ARG:NH2	2.41	0.47
1:B:2769:PHE:O	1:B:2773:GLN:HG2	2.15	0.47
1:C:3362:THR:HG21	1:C:3409:LEU:HD22	1.97	0.47
1:C:3588:ASP:N	1:C:3588:ASP:OD1	2.48	0.47
1:C:4769:ILE:C	1:C:4769:ILE:HD12	2.40	0.47
1:C:5011:MET:HE1	1:C:5018:ASP:HB2	1.97	0.47
1:A:908:LEU:O	1:A:966:TYR:OH	2.20	0.46
1:A:2767:TRP:O	1:A:2771:LYS:HG3	2.15	0.46
1:A:2879:LEU:CD1	1:A:2883:TYR:CE2	2.98	0.46
1:D:3559:ASN:O	1:D:3560:LEU:HB2	2.15	0.46
1:B:921:TYR:O	1:B:924:GLN:HG3	2.15	0.46
1:B:2978:LEU:HD23	1:B:2978:LEU:O	2.15	0.46
1:B:3559:ASN:O	1:B:3560:LEU:HB2	2.15	0.46
1:C:1510:ILE:HD12	1:C:1510:ILE:H	1.80	0.46
1:C:4208:TRP:CE3	1:C:4987:MET:HE2	2.50	0.46
1:C:4579:LYS:HG2	1:C:4580:VAL:N	2.30	0.46
1:A:460:LEU:HD22	1:A:464:GLU:OE2	2.15	0.46
1:D:980:PRO:O	1:D:983:THR:OG1	2.28	0.46
1:C:2978:LEU:O	1:C:2978:LEU:HD23	2.15	0.46
1:C:3559:ASN:O	1:C:3560:LEU:HB2	2.15	0.46
1:C:3714:LYS:NZ	1:C:3716:LYS:O	2.46	0.46
1:A:29:VAL:HG12	1:A:30:LEU:HD22	1.98	0.46
1:D:228:MET:SD	1:D:228:MET:N	2.88	0.46
1:D:3828:GLU:OE1	1:D:3828:GLU:N	2.40	0.46
1:B:3004:LEU:HB2	1:B:3005:PRO:HD3	1.97	0.46
1:B:3369:ARG:NH2	1:B:3405:ASP:OD2	2.48	0.46
1:B:3457:GLN:HA	1:B:3457:GLN:OE1	2.14	0.46
1:C:961:MET:HE1	1:C:965:GLY:C	2.40	0.46
1:C:1792:GLY:N	1:C:1795:GLU:OE2	2.43	0.46
1:C:3004:LEU:HB2	1:C:3005:PRO:HD3	1.97	0.46
1:A:903:ARG:O	1:A:904:LEU:HD23	2.14	0.46
1:A:980:PRO:O	1:A:983:THR:OG1	2.26	0.46
1:B:2755:PHE:HD2	1:B:2814:LEU:HD11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4207:GLN:HB3	1:B:4248:MET:HG2	1.97	0.46
1:C:878:ASN:C	1:C:878:ASN:HD22	2.22	0.46
1:C:894:TYR:HA	1:C:905:HIS:O	2.14	0.46
1:C:3955:SER:OG	1:C:4018:GLU:OE1	2.28	0.46
1:A:3541:TYR:OH	1:A:3547:ASP:OD1	2.16	0.46
1:D:3714:LYS:NZ	1:D:3716:LYS:O	2.47	0.46
1:B:3112:ARG:HG3	1:B:3112:ARG:HH11	1.81	0.46
1:C:1055:GLU:O	1:C:1056:PRO:C	2.57	0.46
1:A:2863:LEU:CD2	1:A:2933:MET:HE1	2.45	0.46
1:A:3588:ASP:OD1	1:A:3588:ASP:N	2.48	0.46
1:A:4207:GLN:HB3	1:A:4248:MET:HG2	1.96	0.46
1:D:2978:LEU:HD23	1:D:2978:LEU:O	2.15	0.46
1:C:2927:LEU:C	1:C:2927:LEU:HD23	2.40	0.46
1:C:3526:CYS:SG	1:C:3600:VAL:HG21	2.56	0.46
1:C:4099:ALA:C	1:C:4100:MET:HE2	2.40	0.46
1:D:908:LEU:HD23	1:D:964:ASN:OD1	2.16	0.46
1:D:3112:ARG:HH11	1:D:3112:ARG:HG3	1.81	0.46
1:D:3362:THR:HG21	1:D:3409:LEU:HD22	1.97	0.46
1:D:3952:ARG:CZ	1:D:3952:ARG:HB3	2.46	0.46
1:B:3762:GLU:OE2	1:B:3765:ARG:NH2	2.49	0.46
1:C:2910:ASP:OD1	1:C:2911:THR:N	2.47	0.46
1:C:4866:ASP:OD1	1:C:4866:ASP:N	2.46	0.46
1:D:3457:GLN:OE1	1:D:3457:GLN:HA	2.15	0.46
1:B:2753:ASP:O	1:B:2757:ASN:OD1	2.34	0.46
1:C:1455:THR:OG1	1:C:1457:ASP:OD1	2.32	0.46
1:A:2756:ILE:HD11	1:A:2814:LEU:HD12	1.98	0.46
1:A:3559:ASN:O	1:A:3560:LEU:HB2	2.15	0.46
1:D:460:LEU:CD1	1:D:464:GLU:OE2	2.61	0.46
1:D:3762:GLU:OE2	1:D:3765:ARG:NH2	2.49	0.46
1:C:2755:PHE:HD2	1:C:2814:LEU:HD11	1.81	0.46
2:G:12:ASP:OD1	2:G:13:GLY:N	2.49	0.46
1:D:2826:LYS:NZ	1:D:2934:ASN:O	2.46	0.46
1:D:3944:ASP:OD1	1:D:3944:ASP:C	2.59	0.46
1:D:4099:ALA:C	1:D:4100:MET:HE2	2.40	0.46
1:B:2394:ASP:OD1	1:B:2419:LEU:N	2.48	0.46
1:B:2879:LEU:CD1	1:B:2883:TYR:CE2	2.99	0.46
1:C:885:LEU:O	1:C:889:GLU:HG2	2.16	0.46
1:A:153:PRO:HB3	1:A:158:ARG:HB2	1.98	0.45
1:A:921:TYR:O	1:A:924:GLN:HG3	2.17	0.45
1:A:3369:ARG:NH2	1:A:3405:ASP:OD2	2.49	0.45
1:A:3944:ASP:OD1	1:A:3944:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3952:ARG:CZ	1:A:3952:ARG:HB3	2.46	0.45
1:C:2879:LEU:CD1	1:C:2883:TYR:CE2	2.99	0.45
1:C:2971:SER:HA	1:C:2974:PHE:CE2	2.51	0.45
1:A:1875:GLU:OE1	1:A:1876:GLU:N	2.49	0.45
1:D:2872:LEU:HD13	1:D:2928:LEU:HD11	1.98	0.45
1:B:3526:CYS:SG	1:B:3600:VAL:HG21	2.56	0.45
1:B:4155:GLU:OE1	1:B:4197:TYR:OH	2.16	0.45
1:C:366:LYS:HZ2	1:C:370:LEU:HD11	1.81	0.45
1:A:1455:THR:OG1	1:A:1457:ASP:OD1	2.32	0.45
1:A:2931:LEU:O	1:A:2936:TYR:N	2.45	0.45
1:D:962:MET:O	1:D:964:ASN:N	2.49	0.45
1:D:973:LEU:HD13	1:D:1045:ARG:HB3	1.97	0.45
1:D:3526:CYS:SG	1:D:3600:VAL:HG21	2.56	0.45
1:C:1281:GLN:O	1:C:1282:ASN:OD1	2.35	0.45
1:C:3944:ASP:OD1	1:C:3944:ASP:C	2.59	0.45
1:A:885:LEU:HA	1:A:888:ILE:HG12	1.98	0.45
1:A:2761:GLU:OE1	1:A:2803:LYS:NZ	2.36	0.45
1:A:4752:ASN:O	1:A:4754:ARG:NH1	2.49	0.45
1:D:1129:ARG:HB2	1:D:1129:ARG:NH1	2.32	0.45
1:D:1875:GLU:OE1	1:D:1876:GLU:N	2.49	0.45
1:B:2931:LEU:O	1:B:2936:TYR:N	2.45	0.45
1:C:2871:GLU:O	1:C:2875:MET:HG2	2.16	0.45
1:C:3112:ARG:HG3	1:C:3112:ARG:HH11	1.81	0.45
1:A:2441:THR:O	1:A:2445:GLN:HG2	2.16	0.45
1:A:2627:LEU:HD22	1:A:2641:PRO:HB3	1.98	0.45
1:A:4579:LYS:HG2	1:A:4580:VAL:N	2.30	0.45
1:D:885:LEU:HA	1:D:888:ILE:HG12	1.97	0.45
1:D:1281:GLN:O	1:D:1282:ASN:OD1	2.35	0.45
1:D:3955:SER:OG	1:D:4018:GLU:OE1	2.28	0.45
1:B:3108:VAL:HG22	1:B:3176:LEU:HB2	1.99	0.45
1:C:227:HIS:H	1:C:228:MET:HE2	1.81	0.45
1:A:2394:ASP:OD1	1:A:2419:LEU:N	2.50	0.45
1:D:903:ARG:CZ	1:D:903:ARG:HA	2.46	0.45
1:D:1826:GLN:OE1	1:D:1826:GLN:HA	2.17	0.45
1:B:3588:ASP:OD1	1:B:3588:ASP:N	2.48	0.45
1:C:4763:LEU:HD13	1:C:4763:LEU:C	2.41	0.45
1:A:1129:ARG:NH1	1:A:1129:ARG:HB2	2.32	0.45
1:A:2213:VAL:HG11	1:A:2257:TYR:OH	2.17	0.45
1:A:2978:LEU:HD23	1:A:2982:VAL:HG23	1.99	0.45
1:D:885:LEU:O	1:D:889:GLU:HG2	2.15	0.45
1:D:978:LEU:CD1	1:D:982:GLN:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:LEU:HA	1:B:888:ILE:HG12	1.99	0.45
1:B:894:TYR:HA	1:B:905:HIS:O	2.17	0.45
1:B:3683:GLU:O	1:B:3687:GLU:OE2	2.34	0.45
1:B:3952:ARG:CZ	1:B:3952:ARG:HB3	2.46	0.45
1:C:3762:GLU:OE2	1:C:3765:ARG:NH2	2.49	0.45
1:A:3526:CYS:SG	1:A:3600:VAL:HG21	2.56	0.45
1:B:2441:THR:O	1:B:2445:GLN:HG2	2.17	0.45
1:B:2822:TRP:CD2	1:B:2875:MET:HE1	2.52	0.45
1:C:29:VAL:HG12	1:C:30:LEU:HD22	1.98	0.45
1:C:3952:ARG:CZ	1:C:3952:ARG:HB3	2.46	0.45
1:A:85:ASN:OD1	1:A:85:ASN:C	2.60	0.45
1:A:2771:LYS:HB3	1:A:2776:TRP:HB2	1.99	0.45
1:A:3955:SER:OG	1:A:4018:GLU:OE1	2.28	0.45
1:A:4763:LEU:HD13	1:A:4763:LEU:C	2.42	0.45
1:D:894:TYR:HA	1:D:905:HIS:O	2.16	0.45
1:A:882:LEU:HD23	1:A:885:LEU:HD21	1.99	0.45
1:A:988:ARG:HG3	1:A:988:ARG:HH11	1.82	0.45
1:A:2971:SER:HA	1:A:2974:PHE:CE2	2.52	0.45
1:D:2394:ASP:OD1	1:D:2419:LEU:N	2.50	0.45
1:D:2441:THR:O	1:D:2445:GLN:HG2	2.16	0.45
1:D:2971:SER:HA	1:D:2974:PHE:CE2	2.52	0.45
1:D:4752:ASN:O	1:D:4754:ARG:NH1	2.50	0.45
1:B:85:ASN:C	1:B:85:ASN:OD1	2.60	0.45
1:B:885:LEU:O	1:B:889:GLU:HG2	2.16	0.45
1:B:4769:ILE:HD11	1:B:4771:VAL:HG23	1.99	0.45
1:C:2441:THR:O	1:C:2445:GLN:HG2	2.17	0.45
1:A:925:MET:HE2	1:A:925:MET:CA	2.46	0.44
1:D:988:ARG:HG3	1:D:988:ARG:HH11	1.82	0.44
1:D:3861:MET:SD	1:D:3868:VAL:CG2	3.06	0.44
1:B:988:ARG:HG3	1:B:988:ARG:HH11	1.82	0.44
1:B:1113:ASP:OD1	1:B:1113:ASP:N	2.45	0.44
1:B:2944:ASP:OD1	1:B:2945:MET:SD	2.76	0.44
1:A:894:TYR:HA	1:A:905:HIS:O	2.17	0.44
1:D:267:ARG:NH2	1:D:332:VAL:O	2.47	0.44
1:D:3683:GLU:O	1:D:3687:GLU:OE2	2.34	0.44
1:B:1281:GLN:O	1:B:1282:ASN:OD1	2.35	0.44
1:A:2246:GLN:OE1	1:A:3868:VAL:HG12	2.17	0.44
1:A:3683:GLU:O	1:A:3687:GLU:OE2	2.34	0.44
1:A:4155:GLU:OE1	1:A:4197:TYR:OH	2.16	0.44
1:D:3447:SER:O	1:D:3453:LYS:NZ	2.44	0.44
1:B:153:PRO:HB3	1:B:158:ARG:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1713:TYR:OH	1:B:1816:MET:HE3	2.18	0.44
1:C:3088:ILE:H	1:C:3088:ILE:CD1	2.28	0.44
1:A:864:LEU:HD13	1:A:865:PRO:O	2.18	0.44
1:A:3714:LYS:NZ	1:A:3716:LYS:O	2.47	0.44
1:D:153:PRO:HB3	1:D:158:ARG:HB2	1.98	0.44
1:D:2944:ASP:OD1	1:D:2945:MET:SD	2.76	0.44
1:B:2971:SER:HA	1:B:2974:PHE:CE2	2.52	0.44
1:D:882:LEU:HD23	1:D:885:LEU:HD21	1.98	0.44
1:D:2226:PHE:N	1:D:2227:PRO:HD3	2.33	0.44
1:D:3736:LEU:HD12	1:D:3766:LEU:HD22	2.00	0.44
1:D:4684:LEU:HD12	1:D:4685:TYR:CE2	2.53	0.44
1:B:908:LEU:O	1:B:966:TYR:OH	2.30	0.44
1:B:2627:LEU:HD22	1:B:2641:PRO:HB3	1.99	0.44
1:C:153:PRO:HB3	1:C:158:ARG:HB2	1.99	0.44
1:C:885:LEU:HA	1:C:888:ILE:HG12	2.00	0.44
1:C:2944:ASP:OD1	1:C:2945:MET:SD	2.76	0.44
1:A:2438:ALA:HB2	1:A:2510:VAL:HG22	1.99	0.44
1:B:4579:LYS:HG2	1:B:4580:VAL:N	2.30	0.44
1:C:85:ASN:OD1	1:C:85:ASN:C	2.60	0.44
1:C:893:THR:CG2	1:C:904:LEU:HD23	2.35	0.44
1:C:988:ARG:HG3	1:C:988:ARG:HH11	1.82	0.44
1:C:2438:ALA:HB2	1:C:2510:VAL:HG22	1.99	0.44
1:A:1826:GLN:OE1	1:A:1826:GLN:HA	2.17	0.44
1:D:1007:SER:C	1:D:1022:LEU:HD23	2.43	0.44
1:B:3088:ILE:H	1:B:3088:ILE:CD1	2.29	0.44
1:B:3861:MET:SD	1:B:3868:VAL:CG2	3.05	0.44
1:C:3160:ASP:OD2	1:C:3223:LYS:NZ	2.51	0.44
1:D:2627:LEU:HD22	1:D:2641:PRO:HB3	1.99	0.44
1:D:4763:LEU:HD13	1:D:4763:LEU:C	2.42	0.44
1:D:4769:ILE:HD11	1:D:4771:VAL:HG23	1.99	0.44
1:C:3410:TYR:N	1:C:3411:PRO:HD2	2.33	0.44
1:D:2701:MET:HE3	1:D:2701:MET:HB3	1.95	0.44
1:B:1007:SER:C	1:B:1022:LEU:HD23	2.43	0.44
1:B:3684:GLN:HA	1:B:3687:GLU:OE2	2.18	0.44
1:B:3944:ASP:OD1	1:B:3944:ASP:C	2.59	0.44
1:C:956:LEU:HD22	1:C:960:TYR:CD2	2.52	0.44
1:C:2949:THR:OG1	1:C:2954:LYS:NZ	2.51	0.44
1:A:974:SER:O	1:A:977:ARG:NH2	2.50	0.43
1:D:878:ASN:HD22	1:D:878:ASN:C	2.24	0.43
1:B:2213:VAL:HG11	1:B:2257:TYR:OH	2.18	0.43
1:B:4684:LEU:HD12	1:B:4685:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2394:ASP:OD1	1:C:2419:LEU:N	2.51	0.43
1:C:2822:TRP:CD2	1:C:2875:MET:HE1	2.53	0.43
1:C:4684:LEU:HD12	1:C:4685:TYR:CE2	2.53	0.43
1:A:1713:TYR:OH	1:A:1816:MET:HE3	2.18	0.43
1:D:85:ASN:OD1	1:D:85:ASN:C	2.60	0.43
1:D:868:LEU:HD23	1:D:871:ILE:HD11	1.99	0.43
1:B:980:PRO:O	1:B:983:THR:OG1	2.27	0.43
1:B:3176:LEU:HD11	1:B:3184:VAL:HG22	2.00	0.43
4:B:8003:PCW:H483	4:C:5103:PCW:H271	1.99	0.43
1:C:882:LEU:HD23	1:C:885:LEU:HD21	2.00	0.43
1:C:2226:PHE:N	1:C:2227:PRO:HD3	2.33	0.43
1:C:2246:GLN:OE1	1:C:3868:VAL:HG12	2.18	0.43
1:D:893:THR:HA	1:D:962:MET:SD	2.58	0.43
1:D:2822:TRP:CE2	1:D:2875:MET:HE1	2.54	0.43
1:D:3684:GLN:HA	1:D:3687:GLU:OE2	2.18	0.43
1:B:1129:ARG:HB2	1:B:1129:ARG:NH1	2.32	0.43
1:B:1826:GLN:HA	1:B:1826:GLN:OE1	2.18	0.43
1:B:4090:LEU:N	1:B:4090:LEU:HD12	2.33	0.43
1:C:926:SER:O	1:C:930:LEU:CD2	2.66	0.43
1:C:1129:ARG:NH1	1:C:1129:ARG:HB2	2.32	0.43
1:C:1826:GLN:HA	1:C:1826:GLN:OE1	2.17	0.43
1:C:2940:ARG:CB	1:C:2944:ASP:HB3	2.48	0.43
1:C:4090:LEU:HD12	1:C:4090:LEU:N	2.33	0.43
1:C:4210:MET:HE3	1:C:4211:PRO:CD	2.49	0.43
1:A:973:LEU:HD13	1:A:1045:ARG:HB3	2.00	0.43
1:A:978:LEU:CD2	1:A:1045:ARG:HD3	2.48	0.43
1:A:978:LEU:HD23	1:A:1045:ARG:HD3	1.98	0.43
1:A:1007:SER:C	1:A:1022:LEU:HD23	2.43	0.43
1:A:2755:PHE:HD2	1:A:2814:LEU:HD11	1.83	0.43
1:D:2212:MET:HE2	1:D:2212:MET:HB3	1.96	0.43
1:D:2978:LEU:HD23	1:D:2982:VAL:HG23	2.01	0.43
1:A:1435:TYR:HB2	1:A:1573:ILE:HG21	2.00	0.43
1:A:1964:GLU:HA	1:A:3651:CYS:SG	2.59	0.43
1:A:4684:LEU:HD12	1:A:4685:TYR:CE2	2.54	0.43
1:D:723:TRP:CZ2	1:D:728:ALA:HB2	2.54	0.43
1:B:1435:TYR:HB2	1:B:1573:ILE:HG21	2.01	0.43
1:B:2226:PHE:N	1:B:2227:PRO:HD3	2.33	0.43
1:B:2871:GLU:O	1:B:2875:MET:HG2	2.17	0.43
1:B:3236:SER:OG	1:B:3239:GLU:OE2	2.34	0.43
1:B:4763:LEU:C	1:B:4763:LEU:HD13	2.42	0.43
1:C:872:ARG:NH2	1:C:923:LEU:O	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2596:LEU:HD21	1:C:2604:ILE:CD1	2.49	0.43
1:C:2627:LEU:HD22	1:C:2641:PRO:HB3	1.98	0.43
1:C:2931:LEU:O	1:C:2936:TYR:N	2.49	0.43
1:C:3974:GLY:N	1:C:3975:PRO:HA	2.34	0.43
1:A:723:TRP:CZ2	1:A:728:ALA:HB2	2.54	0.43
1:A:1171:MET:HE3	1:A:1171:MET:HB2	1.97	0.43
1:A:3684:GLN:HA	1:A:3687:GLU:OE2	2.18	0.43
1:D:843:PRO:HG2	1:D:1072:ARG:O	2.19	0.43
1:D:1964:GLU:HA	1:D:3651:CYS:SG	2.59	0.43
1:D:2213:VAL:HG11	1:D:2257:TYR:OH	2.18	0.43
1:D:3380:LEU:C	1:D:3380:LEU:HD23	2.43	0.43
1:D:3410:TYR:N	1:D:3411:PRO:HD2	2.34	0.43
1:D:3992:VAL:HG11	1:D:4050:MET:HE2	2.01	0.43
1:B:3974:GLY:N	1:B:3975:PRO:HA	2.33	0.43
1:D:2438:ALA:HB2	1:D:2510:VAL:HG22	1.99	0.43
1:D:4932:GLY:HA2	1:C:4935:ILE:HG12	2.01	0.43
1:B:729:ARG:NH2	1:B:1490:CYS:SG	2.92	0.43
1:B:1964:GLU:HA	1:B:3651:CYS:SG	2.59	0.43
1:C:4225:VAL:HG11	1:C:4948:VAL:HA	2.00	0.43
1:A:1531:THR:HG22	1:A:1536:GLU:HA	2.00	0.43
1:A:3410:TYR:N	1:A:3411:PRO:HD2	2.33	0.43
1:A:3761:MET:HA	1:A:3761:MET:HE2	2.01	0.43
1:A:4090:LEU:N	1:A:4090:LEU:HD12	2.33	0.43
1:A:4932:GLY:HA2	1:D:4935:ILE:HG12	2.01	0.43
1:D:2767:TRP:CH2	1:D:2791:MET:HE2	2.54	0.43
1:D:2940:ARG:CB	1:D:2944:ASP:HB3	2.49	0.43
1:B:2940:ARG:CB	1:B:2944:ASP:HB3	2.48	0.43
1:B:4225:VAL:HG11	1:B:4948:VAL:HA	1.99	0.43
1:C:1964:GLU:HA	1:C:3651:CYS:SG	2.59	0.43
1:A:2922:GLU:OE1	1:A:2925:GLN:NE2	2.50	0.43
1:A:2950:SER:OG	1:A:2951:SER:N	2.52	0.43
1:A:3974:GLY:N	1:A:3975:PRO:HA	2.33	0.43
1:D:872:ARG:HE	1:D:923:LEU:HB3	1.84	0.43
1:D:3952:ARG:HB3	1:D:3952:ARG:NH1	2.34	0.43
1:B:500:THR:HG23	1:B:503:HIS:H	1.84	0.43
1:B:2949:THR:OG1	1:B:2954:LYS:NZ	2.51	0.43
1:C:2868:LEU:HD21	1:C:2928:LEU:HD12	2.01	0.43
1:C:2950:SER:OG	1:C:2951:SER:N	2.52	0.43
1:A:843:PRO:HG2	1:A:1072:ARG:O	2.19	0.43
1:A:932:THR:O	1:A:936:LEU:HD23	2.19	0.43
1:A:962:MET:HE3	1:A:963:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2226:PHE:N	1:A:2227:PRO:HD3	2.33	0.43
1:A:4935:ILE:HG12	1:B:4932:GLY:HA2	2.01	0.43
1:D:2186:ILE:HG21	1:D:2204:MET:HE1	2.01	0.43
1:D:3088:ILE:H	1:D:3088:ILE:CD1	2.29	0.43
1:B:267:ARG:NH2	1:B:332:VAL:O	2.48	0.43
1:B:2868:LEU:HD21	1:B:2928:LEU:HD12	2.00	0.43
1:B:3410:TYR:N	1:B:3411:PRO:HD2	2.34	0.43
1:B:3992:VAL:HG11	1:B:4050:MET:HE2	2.01	0.43
1:C:872:ARG:HD3	1:C:923:LEU:HD22	2.01	0.43
1:C:1113:ASP:OD1	1:C:1113:ASP:N	2.45	0.43
1:D:871:ILE:HD13	1:D:1052:TYR:CZ	2.54	0.42
1:D:2723:LYS:H	1:D:2723:LYS:HD3	1.84	0.42
1:D:2822:TRP:CD2	1:D:2875:MET:HE1	2.54	0.42
1:D:2949:THR:OG1	1:D:2954:LYS:NZ	2.51	0.42
1:B:2723:LYS:HD3	1:B:2723:LYS:H	1.84	0.42
1:C:323:LYS:NZ	1:C:326:VAL:HG13	2.34	0.42
1:C:649:ILE:HG23	1:C:815:ALA:HB3	2.01	0.42
1:C:2929:LYS:HB3	1:C:2933:MET:HE1	2.01	0.42
1:C:3992:VAL:HG11	1:C:4050:MET:HE2	2.01	0.42
1:A:893:THR:HG23	1:A:904:LEU:CD2	2.38	0.42
1:A:2445:GLN:HA	1:A:2445:GLN:OE1	2.19	0.42
1:A:2723:LYS:H	1:A:2723:LYS:HD3	1.85	0.42
1:A:4059:GLU:HG2	1:A:4169:LEU:HD13	2.01	0.42
1:D:729:ARG:NH2	1:D:1490:CYS:SG	2.92	0.42
1:D:1713:TYR:OH	1:D:1816:MET:HE3	2.20	0.42
1:D:4059:GLU:HG2	1:D:4169:LEU:HD13	2.01	0.42
1:B:760:ILE:O	1:B:760:ILE:HG23	2.19	0.42
1:B:2825:GLU:O	1:B:2828:ARG:CZ	2.66	0.42
1:B:2872:LEU:HD13	1:B:2928:LEU:HD11	2.00	0.42
1:B:3952:ARG:HB3	1:B:3952:ARG:NH1	2.34	0.42
1:B:4769:ILE:HD12	1:B:4769:ILE:C	2.44	0.42
1:C:500:THR:HG23	1:C:503:HIS:H	1.84	0.42
1:C:1007:SER:C	1:C:1022:LEU:HD23	2.43	0.42
1:C:2605:GLU:O	1:C:2609:MET:HG2	2.20	0.42
1:C:3736:LEU:HD12	1:C:3766:LEU:HD22	2.01	0.42
1:A:3108:VAL:HG22	1:A:3176:LEU:HB2	2.01	0.42
1:A:3952:ARG:HB3	1:A:3952:ARG:NH1	2.34	0.42
1:D:760:ILE:O	1:D:760:ILE:HG23	2.19	0.42
1:D:2871:GLU:O	1:D:2875:MET:HG2	2.19	0.42
1:D:3736:LEU:HD13	1:D:3809:ASN:HB3	2.02	0.42
1:B:1982:MET:HE2	1:B:1982:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:723:TRP:CZ2	1:C:728:ALA:HB2	2.54	0.42
1:C:2771:LYS:HB3	1:C:2776:TRP:HB2	2.01	0.42
1:C:2978:LEU:HD23	1:C:2982:VAL:HG23	2.01	0.42
1:C:4161:PRO:N	1:C:4164:ARG:NH2	2.67	0.42
1:A:460:LEU:HD13	1:A:464:GLU:HG2	2.02	0.42
1:A:978:LEU:CD1	1:A:982:GLN:HB3	2.50	0.42
1:A:2186:ILE:HG21	1:A:2204:MET:HE1	2.01	0.42
1:A:3108:VAL:HG13	1:A:3176:LEU:HB2	2.00	0.42
1:A:4161:PRO:N	1:A:4164:ARG:NH2	2.67	0.42
1:B:864:LEU:HD21	1:B:868:LEU:HB3	2.01	0.42
1:B:882:LEU:HD23	1:B:885:LEU:HD21	2.00	0.42
1:B:2438:ALA:HB2	1:B:2510:VAL:HG22	2.00	0.42
1:C:228:MET:SD	1:C:228:MET:N	2.93	0.42
1:C:921:TYR:CE2	1:C:925:MET:HE1	2.54	0.42
1:C:1713:TYR:OH	1:C:1816:MET:HE3	2.20	0.42
1:C:2744:LEU:HD13	1:C:2744:LEU:O	2.20	0.42
1:C:3227:GLU:O	1:C:3228:ARG:HB2	2.19	0.42
1:C:3952:ARG:HB3	1:C:3952:ARG:NH1	2.34	0.42
1:A:2605:GLU:O	1:A:2609:MET:HG2	2.20	0.42
1:A:3736:LEU:HD12	1:A:3766:LEU:HD22	2.01	0.42
1:D:649:ILE:HG23	1:D:815:ALA:HB3	2.01	0.42
1:D:864:LEU:HD21	1:D:868:LEU:HB3	2.01	0.42
1:D:1822:ARG:HB3	1:D:1822:ARG:HH11	1.85	0.42
1:D:2605:GLU:O	1:D:2609:MET:HG2	2.20	0.42
1:D:4090:LEU:N	1:D:4090:LEU:HD12	2.33	0.42
1:D:4769:ILE:C	1:D:4769:ILE:HD12	2.44	0.42
1:B:691:GLU:OE1	1:B:691:GLU:HA	2.20	0.42
1:B:2445:GLN:OE1	1:B:2445:GLN:HA	2.19	0.42
1:B:4935:ILE:HG12	1:C:4932:GLY:HA2	2.01	0.42
1:C:978:LEU:CD2	1:C:1045:ARG:HD3	2.50	0.42
1:C:1822:ARG:HB3	1:C:1822:ARG:HH11	1.85	0.42
1:C:1982:MET:HA	1:C:1982:MET:HE2	2.01	0.42
1:C:2215:VAL:HG21	1:C:2229:MET:CE	2.42	0.42
1:C:2872:LEU:HD13	1:C:2928:LEU:HD11	2.00	0.42
1:A:156:LYS:HE2	1:A:156:LYS:HA	2.02	0.42
1:A:760:ILE:HG23	1:A:760:ILE:O	2.19	0.42
1:A:983:THR:O	1:A:986:VAL:HG12	2.19	0.42
1:A:3227:GLU:O	1:A:3228:ARG:HB2	2.19	0.42
1:A:3861:MET:SD	1:A:3870:ASN:OD1	2.78	0.42
1:A:4769:ILE:HD11	1:A:4771:VAL:HG23	2.02	0.42
1:D:323:LYS:NZ	1:D:326:VAL:HG13	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LYS:NZ	1:B:326:VAL:HG13	2.34	0.42
1:B:2605:GLU:O	1:B:2609:MET:HG2	2.20	0.42
1:C:843:PRO:HG2	1:C:1072:ARG:O	2.19	0.42
1:C:914:LEU:O	1:C:919:ARG:NH2	2.41	0.42
1:C:980:PRO:O	1:C:983:THR:OG1	2.27	0.42
1:C:1435:TYR:HB2	1:C:1573:ILE:HG21	2.01	0.42
1:C:2445:GLN:HA	1:C:2445:GLN:OE1	2.19	0.42
1:C:3869:ILE:HD11	1:C:3872:GLN:O	2.20	0.42
1:A:2940:ARG:HB2	1:A:2944:ASP:HB3	2.00	0.42
1:D:932:THR:O	1:D:936:LEU:HD23	2.20	0.42
1:D:983:THR:O	1:D:986:VAL:HG12	2.20	0.42
1:D:986:VAL:HG23	1:D:1044:VAL:HG21	2.02	0.42
1:D:2950:SER:OG	1:D:2951:SER:N	2.53	0.42
1:D:3176:LEU:HD11	1:D:3184:VAL:HG22	2.02	0.42
1:B:723:TRP:CZ2	1:B:728:ALA:HB2	2.54	0.42
1:B:3227:GLU:O	1:B:3228:ARG:HB2	2.20	0.42
1:B:4161:PRO:N	1:B:4164:ARG:NH2	2.67	0.42
1:C:2938:VAL:HB	1:C:2940:ARG:NH2	2.35	0.42
1:C:4632:GLU:OE2	1:C:4634:THR:OG1	2.25	0.42
1:A:961:MET:HG2	1:A:967:LYS:HE2	2.01	0.42
1:A:2944:ASP:OD1	1:A:2945:MET:SD	2.78	0.42
1:A:3160:ASP:OD2	1:A:3223:LYS:NZ	2.52	0.42
1:A:4210:MET:HE3	1:A:4211:PRO:CD	2.49	0.42
1:A:4225:VAL:HG11	1:A:4948:VAL:HA	2.00	0.42
1:D:276:ARG:HG2	1:D:276:ARG:HH11	1.84	0.42
1:D:870:ARG:NH2	1:D:1052:TYR:OH	2.53	0.42
1:D:2225:ARG:HD3	1:D:2225:ARG:N	2.34	0.42
1:D:2596:LEU:HD21	1:D:2604:ILE:CD1	2.50	0.42
1:D:3227:GLU:O	1:D:3228:ARG:HB2	2.19	0.42
1:D:4225:VAL:HG11	1:D:4948:VAL:HA	2.01	0.42
1:B:2817:MET:HE1	1:B:2938:VAL:CG2	2.50	0.42
1:B:2978:LEU:HD23	1:B:2982:VAL:HG23	2.01	0.42
1:B:4210:MET:HE3	1:B:4211:PRO:HD2	2.02	0.42
1:C:296:GLU:H	1:C:296:GLU:CD	2.27	0.42
1:C:729:ARG:NH2	1:C:1490:CYS:SG	2.93	0.42
1:C:760:ILE:HG23	1:C:760:ILE:O	2.20	0.42
1:A:3736:LEU:HD13	1:A:3809:ASN:HB3	2.02	0.42
1:D:961:MET:HG2	1:D:967:LYS:HE2	2.01	0.42
1:D:2825:GLU:O	1:D:2828:ARG:CZ	2.68	0.42
1:D:3974:GLY:N	1:D:3975:PRO:HA	2.33	0.42
1:B:156:LYS:HE2	1:B:156:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:868:LEU:HD13	1:B:930:LEU:HB3	2.02	0.42
1:B:932:THR:O	1:B:936:LEU:HD23	2.20	0.42
1:B:2938:VAL:HB	1:B:2940:ARG:NH2	2.35	0.42
1:B:2950:SER:OG	1:B:2951:SER:N	2.52	0.42
1:C:1531:THR:HG22	1:C:1536:GLU:HA	2.01	0.42
1:C:1987:MET:N	1:C:1987:MET:HE2	2.35	0.42
1:C:4893:GLY:N	1:C:4897:ASP:OD2	2.46	0.42
1:A:500:THR:HG23	1:A:503:HIS:H	1.84	0.42
1:A:673:ALA:O	1:A:681:THR:OG1	2.36	0.42
1:A:2225:ARG:HD3	1:A:2225:ARG:N	2.35	0.42
1:A:4769:ILE:C	1:A:4769:ILE:HD12	2.45	0.42
1:D:978:LEU:HD23	1:D:1045:ARG:HD3	2.01	0.42
1:D:1435:TYR:HB2	1:D:1573:ILE:HG21	2.01	0.42
1:D:2293:GLU:O	1:D:2297:GLU:HG3	2.20	0.42
1:D:2714:ASP:OD1	1:D:2714:ASP:N	2.50	0.42
1:D:3366:LEU:HD13	1:D:3406:LEU:HD23	2.02	0.42
1:D:4155:GLU:OE1	1:D:4197:TYR:OH	2.35	0.42
1:D:4161:PRO:N	1:D:4164:ARG:NH2	2.67	0.42
1:D:4248:MET:HE1	1:D:4987:MET:HE1	2.01	0.42
1:C:864:LEU:HD21	1:C:868:LEU:HB3	2.01	0.42
1:C:2213:VAL:HG11	1:C:2257:TYR:OH	2.19	0.42
4:C:5103:PCW:H20	4:C:5103:PCW:H462	2.01	0.42
1:D:500:THR:HG23	1:D:503:HIS:H	1.84	0.41
1:D:2744:LEU:HD13	1:D:2744:LEU:O	2.20	0.41
1:C:3861:MET:SD	1:C:3870:ASN:OD1	2.78	0.41
1:A:276:ARG:HG2	1:A:276:ARG:HH11	1.85	0.41
1:A:2701:MET:HE3	1:A:2701:MET:HB3	1.95	0.41
1:D:4210:MET:HE3	1:D:4211:PRO:CD	2.49	0.41
1:B:1531:THR:HG22	1:B:1536:GLU:HA	2.01	0.41
1:B:2866:VAL:HG21	1:B:2933:MET:HE3	2.02	0.41
1:C:156:LYS:HA	1:C:156:LYS:HE2	2.02	0.41
1:C:932:THR:O	1:C:936:LEU:HD23	2.20	0.41
1:C:947:ALA:O	1:C:951:LEU:HD13	2.18	0.41
1:C:2723:LYS:H	1:C:2723:LYS:HD3	1.84	0.41
1:A:885:LEU:O	1:A:889:GLU:HG2	2.21	0.41
1:A:2872:LEU:HD22	1:A:2928:LEU:HD11	2.02	0.41
1:D:1481:GLN:O	1:D:1481:GLN:HG2	2.20	0.41
1:D:1531:THR:HG22	1:D:1536:GLU:HA	2.01	0.41
1:D:2640:MET:HE3	1:D:2640:MET:HB3	1.96	0.41
1:D:2868:LEU:HD21	1:D:2928:LEU:HD12	2.02	0.41
1:B:843:PRO:HG2	1:B:1072:ARG:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:870:ARG:NH2	1:B:1052:TYR:OH	2.53	0.41
1:B:914:LEU:O	1:B:919:ARG:NH2	2.41	0.41
1:B:2215:VAL:HG21	1:B:2229:MET:CE	2.42	0.41
1:C:139:GLN:NE2	1:C:141:ASP:O	2.53	0.41
1:A:2769:PHE:O	1:A:2773:GLN:HG2	2.21	0.41
1:A:4833:LYS:O	1:A:4837:MET:HG2	2.19	0.41
1:D:32:GLU:OE1	1:D:32:GLU:N	2.54	0.41
1:D:2160:LEU:HD13	1:D:2204:MET:HG2	2.02	0.41
1:D:2771:LYS:CE	1:D:2791:MET:HE1	2.47	0.41
1:B:2480:LEU:HD23	1:B:2480:LEU:HA	1.96	0.41
1:B:2768:ALA:O	1:B:2772:ILE:HG12	2.21	0.41
1:C:1481:GLN:HG2	1:C:1481:GLN:O	2.20	0.41
1:C:3919:ILE:N	1:C:3919:ILE:HD12	2.36	0.41
2:G:101:ASP:OD1	2:G:101:ASP:C	2.64	0.41
1:D:882:LEU:O	1:D:885:LEU:HG	2.21	0.41
1:D:2777:SER:C	1:D:2792:LEU:HD21	2.45	0.41
1:B:1822:ARG:HB3	1:B:1822:ARG:HH11	1.85	0.41
1:B:2225:ARG:HD3	1:B:2225:ARG:N	2.35	0.41
1:C:691:GLU:HA	1:C:691:GLU:OE1	2.20	0.41
1:C:2225:ARG:HD3	1:C:2225:ARG:N	2.35	0.41
1:C:2752:LEU:HD13	1:C:2814:LEU:HD13	2.01	0.41
1:A:227:HIS:H	1:A:228:MET:HE2	1.85	0.41
1:A:887:ARG:HA	1:A:887:ARG:NE	2.36	0.41
1:A:2609:MET:HE3	1:A:2609:MET:HB3	1.98	0.41
1:A:2825:GLU:O	1:A:2828:ARG:CZ	2.68	0.41
1:A:3365:ARG:HE	1:A:3365:ARG:HB3	1.77	0.41
1:B:2791:MET:SD	1:B:2792:LEU:N	2.93	0.41
1:B:3757:GLU:HA	1:B:3757:GLU:OE1	2.21	0.41
1:B:3919:ILE:HD12	1:B:3919:ILE:N	2.36	0.41
1:C:868:LEU:HD13	1:C:930:LEU:HB3	2.03	0.41
1:C:2754:SER:HA	1:C:2757:ASN:OD1	2.20	0.41
1:C:4578:TYR:CE2	1:C:4628:TYR:HB3	2.53	0.41
1:A:1987:MET:HE2	1:A:1987:MET:N	2.35	0.41
1:A:3291:GLU:O	1:A:3291:GLU:CG	2.68	0.41
1:D:461:GLN:O	1:D:465:LYS:HB2	2.20	0.41
1:D:2445:GLN:OE1	1:D:2445:GLN:HA	2.20	0.41
1:D:2931:LEU:HD22	1:D:2936:TYR:CB	2.51	0.41
1:D:3291:GLU:O	1:D:3291:GLU:CG	2.68	0.41
1:B:962:MET:O	1:B:964:ASN:N	2.54	0.41
1:B:3111:LEU:HD21	1:B:3187:LEU:HD22	2.03	0.41
1:B:4059:GLU:HG2	1:B:4169:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:903:ARG:O	1:C:904:LEU:HD23	2.20	0.41
1:C:962:MET:SD	1:C:962:MET:C	3.03	0.41
1:C:3366:LEU:HD13	1:C:3406:LEU:HD23	2.03	0.41
1:C:3736:LEU:HD13	1:C:3809:ASN:HB3	2.02	0.41
1:C:3757:GLU:OE1	1:C:3757:GLU:HA	2.21	0.41
1:A:649:ILE:HG23	1:A:815:ALA:HB3	2.01	0.41
1:A:908:LEU:HD22	1:A:962:MET:HE1	2.02	0.41
1:A:2701:MET:HB3	1:A:2702:PRO:HD3	2.03	0.41
1:A:3919:ILE:HD12	1:A:3919:ILE:N	2.36	0.41
2:H:101:ASP:OD1	2:H:101:ASP:C	2.64	0.41
1:D:156:LYS:HE2	1:D:156:LYS:HA	2.02	0.41
1:D:1874:ARG:HB3	1:D:1874:ARG:NH1	2.36	0.41
1:D:2701:MET:HB3	1:D:2702:PRO:HD3	2.03	0.41
1:B:903:ARG:O	1:B:904:LEU:HD23	2.21	0.41
1:B:2767:TRP:O	1:B:2771:LYS:HG3	2.20	0.41
1:B:3291:GLU:O	1:B:3291:GLU:CG	2.68	0.41
1:C:921:TYR:CD2	1:C:925:MET:HE1	2.56	0.41
1:C:2791:MET:SD	1:C:2791:MET:C	3.04	0.41
1:C:4059:GLU:HG2	1:C:4169:LEU:HD13	2.02	0.41
1:A:958:LYS:HA	1:A:961:MET:HB2	2.02	0.41
1:A:986:VAL:HG21	1:A:1041:CYS:HA	2.02	0.41
1:A:3294:PRO:HB2	1:A:3297:LEU:HB2	2.03	0.41
1:A:3366:LEU:HD13	1:A:3406:LEU:HD23	2.03	0.41
1:D:903:ARG:O	1:D:904:LEU:HD23	2.20	0.41
1:D:2789:HIS:CB	1:D:2792:LEU:HD23	2.50	0.41
1:B:459:GLU:OE1	1:B:459:GLU:C	2.64	0.41
1:B:649:ILE:HG23	1:B:815:ALA:HB3	2.02	0.41
1:B:882:LEU:O	1:B:885:LEU:HG	2.21	0.41
1:B:958:LYS:HA	1:B:961:MET:HB2	2.02	0.41
1:B:986:VAL:HG23	1:B:1044:VAL:HG21	2.02	0.41
1:B:2883:TYR:CE2	1:B:2923:LYS:HE3	2.56	0.41
1:B:3076:LEU:HD12	1:B:3076:LEU:HA	1.96	0.41
1:B:3366:LEU:HD13	1:B:3406:LEU:HD23	2.03	0.41
1:B:3736:LEU:HD12	1:B:3766:LEU:HD22	2.02	0.41
1:B:4927:LEU:O	1:B:4931:GLN:OE1	2.39	0.41
1:B:4987:MET:HE3	1:B:4987:MET:HB3	1.94	0.41
1:C:459:GLU:C	1:C:459:GLU:OE1	2.64	0.41
1:C:2701:MET:HB3	1:C:2702:PRO:HD3	2.03	0.41
1:C:2748:ILE:O	1:C:2748:ILE:HG23	2.21	0.41
1:C:2817:MET:CE	1:C:2938:VAL:HG11	2.50	0.41
1:C:2873:GLN:O	1:C:2877:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3294:PRO:HB2	1:C:3297:LEU:HB2	2.03	0.41
1:C:4575:LEU:O	1:C:4578:TYR:HB2	2.21	0.41
1:C:4709:PHE:CD1	1:C:4709:PHE:C	2.99	0.41
1:A:869:GLU:O	1:A:869:GLU:OE2	2.39	0.41
1:A:882:LEU:O	1:A:885:LEU:HG	2.21	0.41
1:A:1034:ARG:HH11	1:A:1034:ARG:HB3	1.86	0.41
1:A:2941:GLY:O	1:A:2945:MET:SD	2.79	0.41
1:A:3828:GLU:OE1	1:A:3828:GLU:N	2.40	0.41
1:A:4578:TYR:CE2	1:A:4628:TYR:HB3	2.53	0.41
1:A:4642:ARG:NH1	1:A:4642:ARG:HG2	2.36	0.41
1:D:2754:SER:HA	1:D:2757:ASN:OD1	2.21	0.41
1:D:2873:GLN:O	1:D:2877:GLU:HG2	2.21	0.41
1:D:3160:ASP:OD2	1:D:3223:LYS:NZ	2.52	0.41
1:B:1997:ARG:HB2	1:B:1997:ARG:NH1	2.36	0.41
1:B:2873:GLN:O	1:B:2877:GLU:HG2	2.21	0.41
1:B:3294:PRO:HB2	1:B:3297:LEU:HB2	2.03	0.41
1:B:3736:LEU:HD13	1:B:3809:ASN:HB3	2.03	0.41
1:C:986:VAL:HG23	1:C:1044:VAL:HG21	2.02	0.41
1:C:1034:ARG:HB3	1:C:1034:ARG:HH11	1.86	0.41
1:C:1997:ARG:HB2	1:C:1997:ARG:NH1	2.36	0.41
1:C:2160:LEU:HD13	1:C:2204:MET:HG2	2.03	0.41
1:C:3037:LYS:O	1:C:3040:ILE:HG22	2.21	0.41
1:C:4869:GLU:OE2	1:C:4869:GLU:HA	2.21	0.41
1:A:323:LYS:NZ	1:A:326:VAL:HG13	2.35	0.40
1:A:961:MET:HE1	1:A:965:GLY:CA	2.50	0.40
1:A:3037:LYS:O	1:A:3040:ILE:HG22	2.21	0.40
1:A:3568:PRO:HD2	1:A:3569:SER:N	2.36	0.40
1:A:3576:LEU:HD23	1:B:1220:LEU:HD22	2.03	0.40
1:A:4869:GLU:HA	1:A:4869:GLU:OE2	2.22	0.40
1:D:1034:ARG:HH11	1:D:1034:ARG:HB3	1.86	0.40
1:D:2748:ILE:HG23	1:D:2748:ILE:O	2.21	0.40
1:B:2514:GLU:OE1	1:B:2514:GLU:N	2.49	0.40
1:B:2817:MET:CE	1:B:2938:VAL:HG11	2.50	0.40
1:C:2769:PHE:O	1:C:2773:GLN:HG2	2.21	0.40
1:A:1874:ARG:HB3	1:A:1874:ARG:NH1	2.36	0.40
1:A:2160:LEU:HD13	1:A:2204:MET:HG2	2.02	0.40
1:A:2948:ASP:C	1:A:2949:THR:HG1	2.10	0.40
1:A:3545:ASP:OD2	1:A:3550:VAL:HG23	2.22	0.40
1:A:3757:GLU:OE1	1:A:3757:GLU:CA	2.70	0.40
1:A:3757:GLU:OE1	1:A:3757:GLU:HA	2.21	0.40
1:A:3869:ILE:HD11	1:A:3872:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4009:ASP:OD1	1:D:4009:ASP:C	2.64	0.40
1:B:865:PRO:HD2	1:B:868:LEU:HD12	2.03	0.40
1:B:2701:MET:HB3	1:B:2702:PRO:HD3	2.03	0.40
1:B:3176:LEU:HD12	1:B:3176:LEU:O	2.21	0.40
1:B:4869:GLU:OE2	1:B:4869:GLU:HA	2.21	0.40
1:C:882:LEU:O	1:C:885:LEU:HG	2.21	0.40
1:C:1156:LEU:HD22	1:C:1185:ILE:HD12	2.03	0.40
1:C:1793:ALA:O	1:C:1794:THR:OG1	2.35	0.40
1:C:2701:MET:HB3	1:C:2701:MET:HE3	1.95	0.40
1:C:2866:VAL:HG21	1:C:2933:MET:CE	2.51	0.40
1:C:3291:GLU:O	1:C:3291:GLU:CG	2.68	0.40
1:C:4927:LEU:O	1:C:4931:GLN:OE1	2.39	0.40
1:A:2922:GLU:O	1:A:2926:GLU:HG2	2.22	0.40
1:D:1792:GLY:N	1:D:1795:GLU:OE2	2.43	0.40
1:D:1994:ARG:HA	1:D:1997:ARG:HH12	1.86	0.40
1:D:2755:PHE:CD2	1:D:2814:LEU:HD11	2.55	0.40
1:D:3757:GLU:HA	1:D:3757:GLU:OE1	2.21	0.40
1:D:3919:ILE:HD12	1:D:3919:ILE:N	2.36	0.40
1:D:4869:GLU:HA	1:D:4869:GLU:OE2	2.21	0.40
1:B:978:LEU:CD2	1:B:1045:ARG:HD3	2.50	0.40
1:B:2229:MET:HE3	1:B:2229:MET:HB3	2.00	0.40
1:B:4578:TYR:CE2	1:B:4628:TYR:HB3	2.53	0.40
1:B:4709:PHE:CD1	1:B:4709:PHE:C	2.99	0.40
1:C:978:LEU:CD1	1:C:982:GLN:HB3	2.52	0.40
1:C:2767:TRP:CZ3	1:C:2791:MET:HE2	2.56	0.40
1:C:4009:ASP:OD1	1:C:4009:ASP:C	2.64	0.40
1:C:4642:ARG:NH1	1:C:4642:ARG:HG2	2.36	0.40
1:C:4693:ASP:OD1	1:C:4694:ASP:N	2.54	0.40
1:A:2789:HIS:CE1	1:A:2791:MET:HE3	2.56	0.40
1:A:2910:ASP:OD1	1:A:2911:THR:N	2.54	0.40
1:A:2931:LEU:HD22	1:A:2936:TYR:CB	2.52	0.40
1:A:4687:THR:HG22	1:A:4730:PHE:CZ	2.57	0.40
1:D:962:MET:HE3	1:D:963:SER:OG	2.20	0.40
1:D:3037:LYS:O	1:D:3040:ILE:HG22	2.21	0.40
1:D:3294:PRO:HB2	1:D:3297:LEU:HB2	2.03	0.40
1:D:3545:ASP:OD2	1:D:3550:VAL:HG23	2.22	0.40
1:D:4575:LEU:O	1:D:4578:TYR:HB2	2.21	0.40
1:B:29:VAL:HG12	1:B:30:LEU:CD2	2.52	0.40
1:B:2609:MET:HE3	1:B:2609:MET:HB3	1.98	0.40
1:B:2941:GLY:O	1:B:2942:LEU:C	2.64	0.40
1:B:4693:ASP:OD1	1:B:4694:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ARG:NH2	1:C:332:VAL:O	2.49	0.40
1:C:2824:VAL:HG11	1:C:2938:VAL:HG22	2.03	0.40
1:C:3732:LYS:HE2	1:C:3732:LYS:HB3	1.98	0.40
1:A:17:THR:O	1:A:18:ASP:HB2	2.22	0.40
1:A:1281:GLN:O	1:A:1282:ASN:OD1	2.40	0.40
1:A:2480:LEU:HD23	1:A:2480:LEU:HA	1.95	0.40
1:A:2640:MET:HE3	1:A:2640:MET:HB3	1.95	0.40
1:D:673:ALA:O	1:D:681:THR:OG1	2.37	0.40
1:D:3757:GLU:OE1	1:D:3757:GLU:CA	2.70	0.40
1:B:1007:SER:CA	1:B:1022:LEU:HD23	2.52	0.40
1:B:4642:ARG:NH1	1:B:4642:ARG:HG2	2.36	0.40
1:C:1466:ASP:OD1	1:C:1466:ASP:C	2.65	0.40
1:C:4133:ASN:OD1	1:C:4133:ASN:O	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 PDB entries followed by that with respect to all EM entries.

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	4347/5035 (86%)	4240 (98%)	107 (2%)	0	100	100
1	B	4347/5035 (86%)	4238 (98%)	109 (2%)	0	100	100
1	C	4347/5035 (86%)	4236 (97%)	111 (3%)	0	100	100
1	D	4347/5035 (86%)	4241 (98%)	106 (2%)	0	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17808/20572 (87%)	17363 (98%)	445 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	3808/4296 (89%)	3783 (99%)	25 (1%)	76	89
1	B	3808/4296 (89%)	3780 (99%)	28 (1%)	76	89
1	C	3808/4296 (89%)	3780 (99%)	28 (1%)	76	89
1	D	3808/4296 (89%)	3781 (99%)	27 (1%)	76	89
2	E	89/90 (99%)	87 (98%)	2 (2%)	45	71
2	F	89/90 (99%)	87 (98%)	2 (2%)	45	71
2	G	89/90 (99%)	87 (98%)	2 (2%)	45	71
2	H	89/90 (99%)	86 (97%)	3 (3%)	32	57
All	All	15588/17544 (89%)	15471 (99%)	117 (1%)	70	88

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	GLU
1	A	748	CYS
1	A	976	VAL
1	A	985	LEU
1	A	986	VAL
1	A	1023	VAL
1	A	1816	MET
1	A	2297	GLU
1	A	2744	LEU
1	A	2828	ARG
1	A	2902	SER
1	A	2984	SER
1	A	3076	LEU
1	A	3241	CYS
1	A	3385	LYS
1	A	3509	SER

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Mol	Chain	Res	Type
1	A	3902	PHE
1	A	3955	SER
1	A	4067	MET
1	A	4073	ASP
1	A	4154	SER
1	A	4186	ILE
1	A	4538	PHE
1	A	4674	GLU
1	A	4743	LEU
2	E	26	HIS
2	E	60	TRP
2	H	26	HIS
2	H	60	TRP
2	H	61	GLU
2	F	26	HIS
2	F	60	TRP
2	G	26	HIS
2	G	60	TRP
1	D	397	GLU
1	D	748	CYS
1	D	846	CYS
1	D	976	VAL
1	D	986	VAL
1	D	1305	THR
1	D	2187	MET
1	D	2744	LEU
1	D	2792	LEU
1	D	2828	ARG
1	D	2867	THR
1	D	2925	GLN
1	D	2984	SER
1	D	3009	GLN
1	D	3076	LEU
1	D	3170	LEU
1	D	3175	SER
1	D	3273	ILE
1	D	3385	LYS
1	D	3509	SER
1	D	3902	PHE
1	D	3955	SER
1	D	4073	ASP
1	D	4116	SER

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Mol	Chain	Res	Type
1	D	4154	SER
1	D	4538	PHE
1	D	4743	LEU
1	B	397	GLU
1	B	464	GLU
1	B	617	SER
1	B	748	CYS
1	B	926	SER
1	B	976	VAL
1	B	986	VAL
1	B	1023	VAL
1	B	1305	THR
1	B	1816	MET
1	B	2297	GLU
1	B	2514	GLU
1	B	2596	LEU
1	B	2744	LEU
1	B	2828	ARG
1	B	2867	THR
1	B	2925	GLN
1	B	3076	LEU
1	B	3273	ILE
1	B	3385	LYS
1	B	3509	SER
1	B	3902	PHE
1	B	3955	SER
1	B	4073	ASP
1	B	4154	SER
1	B	4538	PHE
1	B	4674	GLU
1	B	4743	LEU
1	C	397	GLU
1	C	748	CYS
1	C	926	SER
1	C	936	LEU
1	C	976	VAL
1	C	986	VAL
1	C	1305	THR
1	C	2187	MET
1	C	2297	GLU
1	C	2744	LEU
1	C	2761	GLU

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Mol	Chain	Res	Type
1	C	2792	LEU
1	C	2828	ARG
1	C	2867	THR
1	C	2925	GLN
1	C	3009	GLN
1	C	3076	LEU
1	C	3170	LEU
1	C	3273	ILE
1	C	3385	LYS
1	C	3509	SER
1	C	3902	PHE
1	C	3955	SER
1	C	4073	ASP
1	C	4116	SER
1	C	4154	SER
1	C	4538	PHE
1	C	4743	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	157	GLN
1	A	219	HIS
1	A	350	GLN
1	A	878	ASN
1	A	890	GLN
1	A	922	ASN
1	A	1059	GLN
1	A	1512	HIS
1	A	1546	ASN
1	A	1939	GLN
1	A	1950	GLN
1	A	2162	GLN
1	A	2284	ASN
1	A	2757	ASN
1	A	2992	HIS
1	A	3431	ASN
1	A	3450	HIS
1	A	3557	ASN
1	A	3606	HIS
1	A	3873	ASN

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Mol	Chain	Res	Type
1	A	3898	HIS
1	A	3930	GLN
1	A	4159	HIS
1	A	4226	ASN
1	A	4660	ASN
1	A	5013	GLN
1	D	114	HIS
1	D	157	GLN
1	D	219	HIS
1	D	309	HIS
1	D	922	ASN
1	D	1059	GLN
1	D	1126	ASN
1	D	1512	HIS
1	D	1546	ASN
1	D	1939	GLN
1	D	1950	GLN
1	D	2284	ASN
1	D	2992	HIS
1	D	3557	ASN
1	D	3606	HIS
1	D	3735	HIS
1	D	3873	ASN
1	D	3898	HIS
1	D	4159	HIS
1	D	4226	ASN
1	D	4660	ASN
1	D	4945	GLN
1	D	5013	GLN
1	B	114	HIS
1	B	157	GLN
1	B	219	HIS
1	B	350	GLN
1	B	922	ASN
1	B	1059	GLN
1	B	1301	HIS
1	B	1512	HIS
1	B	1939	GLN
1	B	1950	GLN
1	B	2162	GLN
1	B	2284	ASN
1	B	2992	HIS

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Mol	Chain	Res	Type
1	B	3431	ASN
1	B	3450	HIS
1	B	3557	ASN
1	B	3606	HIS
1	B	3873	ASN
1	B	3898	HIS
1	B	3930	GLN
1	B	4159	HIS
1	B	4226	ASN
1	B	4660	ASN
1	B	4945	GLN
1	B	5013	GLN
1	C	114	HIS
1	C	157	GLN
1	C	219	HIS
1	C	350	GLN
1	C	922	ASN
1	C	1059	GLN
1	C	1301	HIS
1	C	1512	HIS
1	C	1939	GLN
1	C	1950	GLN
1	C	2284	ASN
1	C	2442	HIS
1	C	2992	HIS
1	C	3431	ASN
1	C	3557	ASN
1	C	3606	HIS
1	C	3735	HIS
1	C	3873	ASN
1	C	3930	GLN
1	C	4159	HIS
1	C	4226	ASN
1	C	4660	ASN
1	C	4945	GLN
1	C	5013	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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$
4	PCW	A	8003	-	53,53,53	1.17	5 (9%)	59,61,61	2.27	9 (15%)
4	PCW	D	5103	-	53,53,53	1.18	6 (11%)	59,61,61	2.37	10 (16%)
4	PCW	A	8002	-	53,53,53	1.17	4 (7%)	59,61,61	2.34	9 (15%)
4	PCW	C	5103	-	53,53,53	1.17	5 (9%)	59,61,61	2.36	9 (15%)
4	PCW	C	5101	-	53,53,53	1.18	5 (9%)	59,61,61	2.27	9 (15%)
4	PCW	B	8002	-	53,53,53	1.16	5 (9%)	59,61,61	2.39	9 (15%)
4	PCW	B	8003	-	53,53,53	1.18	5 (9%)	59,61,61	2.28	9 (15%)
4	PCW	D	5101	-	53,53,53	1.18	5 (9%)	59,61,61	2.29	9 (15%)

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
4	PCW	A	8003	-	-	22/57/57/57	-
4	PCW	D	5103	-	-	25/57/57/57	-
4	PCW	A	8002	-	-	25/57/57/57	-
4	PCW	C	5103	-	-	24/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	C	5101	-	-	26/57/57/57	-
4	PCW	B	8002	-	-	22/57/57/57	-
4	PCW	B	8003	-	-	23/57/57/57	-
4	PCW	D	5101	-	-	20/57/57/57	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5103	PCW	O3-C11	3.12	1.42	1.33
4	B	8002	PCW	O3-C11	3.10	1.42	1.33
4	C	5103	PCW	O3-C11	3.09	1.42	1.33
4	D	5101	PCW	O3-C11	3.04	1.42	1.33
4	B	8003	PCW	O3-C11	3.04	1.42	1.33
4	A	8002	PCW	O3-C11	3.00	1.42	1.33
4	C	5101	PCW	O3-C11	3.00	1.42	1.33
4	A	8003	PCW	O3-C11	3.00	1.42	1.33
4	B	8002	PCW	O2-C2	-2.85	1.39	1.46
4	A	8003	PCW	O2-C31	2.84	1.42	1.34
4	D	5103	PCW	O2-C2	-2.84	1.39	1.46
4	C	5101	PCW	O2-C31	2.83	1.42	1.34
4	B	8003	PCW	O2-C31	2.83	1.42	1.34
4	D	5101	PCW	O2-C31	2.82	1.42	1.34
4	C	5103	PCW	O2-C2	-2.80	1.40	1.46
4	C	5103	PCW	O2-C31	2.80	1.42	1.34
4	D	5101	PCW	O2-C2	-2.80	1.40	1.46
4	A	8002	PCW	O2-C2	-2.80	1.40	1.46
4	B	8003	PCW	O2-C2	-2.78	1.40	1.46
4	C	5101	PCW	O2-C2	-2.77	1.40	1.46
4	A	8002	PCW	O2-C31	2.75	1.42	1.34
4	A	8003	PCW	O2-C2	-2.73	1.40	1.46
4	B	8002	PCW	O2-C31	2.72	1.42	1.34
4	D	5103	PCW	O2-C31	2.68	1.41	1.34
4	B	8002	PCW	C5-C4	2.10	1.57	1.51
4	C	5103	PCW	C5-C4	2.10	1.57	1.51
4	D	5103	PCW	C5-C4	2.07	1.57	1.51
4	B	8003	PCW	P-O4P	2.07	1.67	1.59
4	A	8002	PCW	P-O4P	2.07	1.67	1.59
4	C	5101	PCW	P-O4P	2.05	1.67	1.59
4	C	5103	PCW	P-O4P	2.05	1.67	1.59
4	A	8003	PCW	C5-C4	2.04	1.57	1.51
4	D	5101	PCW	P-O4P	2.04	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5103	PCW	P-O4P	2.04	1.67	1.59
4	D	5101	PCW	C5-C4	2.04	1.57	1.51
4	B	8003	PCW	C5-C4	2.03	1.57	1.51
4	A	8003	PCW	P-O4P	2.02	1.67	1.59
4	B	8002	PCW	P-O4P	2.02	1.67	1.59
4	C	5101	PCW	C5-C4	2.01	1.57	1.51
4	D	5103	PCW	P-O3P	2.01	1.67	1.59

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5103	PCW	C8-N-C6	12.12	140.80	108.98
4	B	8002	PCW	C8-N-C6	12.05	140.63	108.98
4	C	5103	PCW	C8-N-C6	11.88	140.18	108.98
4	A	8002	PCW	C8-N-C6	11.74	139.82	108.98
4	D	5101	PCW	C8-N-C6	10.63	136.90	108.98
4	B	8003	PCW	C8-N-C6	10.62	136.87	108.98
4	C	5101	PCW	C8-N-C6	10.61	136.84	108.98
4	A	8003	PCW	C8-N-C6	10.51	136.59	108.98
4	B	8003	PCW	C7-N-C5	7.90	141.30	109.91
4	D	5101	PCW	C7-N-C5	7.89	141.28	109.91
4	C	5101	PCW	C7-N-C5	7.87	141.20	109.91
4	A	8003	PCW	C7-N-C5	7.76	140.78	109.91
4	A	8002	PCW	C7-N-C5	7.39	139.29	109.91
4	B	8002	PCW	C7-N-C5	7.16	138.37	109.91
4	C	5103	PCW	C7-N-C5	7.13	138.26	109.91
4	D	5103	PCW	C7-N-C5	7.12	138.20	109.91
4	C	5103	PCW	C8-N-C7	-5.81	93.71	108.98
4	D	5103	PCW	C8-N-C7	-5.60	94.26	108.98
4	B	8002	PCW	C8-N-C7	-5.59	94.28	108.98
4	A	8002	PCW	C8-N-C7	-5.37	94.86	108.98
4	A	8003	PCW	C8-N-C7	-5.23	95.24	108.98
4	C	5103	PCW	C7-N-C6	-5.05	95.72	108.98
4	B	8003	PCW	C8-N-C7	-4.98	95.90	108.98
4	D	5101	PCW	C8-N-C7	-4.97	95.92	108.98
4	C	5101	PCW	C8-N-C7	-4.96	95.94	108.98
4	B	8002	PCW	C7-N-C6	-4.89	96.13	108.98
4	D	5103	PCW	C7-N-C6	-4.85	96.23	108.98
4	A	8003	PCW	C7-N-C6	-4.82	96.32	108.98
4	B	8003	PCW	C7-N-C6	-4.76	96.47	108.98
4	D	5101	PCW	C7-N-C6	-4.76	96.47	108.98
4	C	5101	PCW	C7-N-C6	-4.76	96.47	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	8002	PCW	C7-N-C6	-4.69	96.66	108.98
4	D	5101	PCW	C21-C20-C19	4.21	156.35	124.83
4	B	8003	PCW	C21-C20-C19	4.11	155.64	124.83
4	A	8003	PCW	C21-C20-C19	3.98	154.69	124.83
4	A	8002	PCW	C21-C20-C19	3.93	154.24	124.83
4	C	5101	PCW	C21-C20-C19	3.84	153.63	124.83
4	C	5103	PCW	C21-C20-C19	3.84	153.57	124.83
4	D	5103	PCW	O2-C31-C32	3.83	119.76	111.48
4	B	8002	PCW	C21-C20-C19	3.80	153.31	124.83
4	B	8002	PCW	O2-C31-C32	3.77	119.63	111.48
4	D	5103	PCW	C21-C20-C19	3.75	152.92	124.83
4	A	8002	PCW	O2-C31-C32	3.75	119.59	111.48
4	C	5103	PCW	O2-C31-C32	3.64	119.35	111.48
4	B	8003	PCW	C8-N-C5	-3.57	95.71	109.91
4	D	5101	PCW	C8-N-C5	-3.57	95.72	109.91
4	A	8003	PCW	C8-N-C5	-3.56	95.75	109.91
4	C	5101	PCW	O2-C31-C32	3.56	119.18	111.48
4	C	5101	PCW	C8-N-C5	-3.55	95.81	109.91
4	D	5101	PCW	O2-C31-C32	3.40	118.84	111.48
4	A	8003	PCW	O2-C31-C32	3.37	118.76	111.48
4	A	8002	PCW	C8-N-C5	-3.33	96.65	109.91
4	B	8003	PCW	O2-C31-C32	3.32	118.65	111.48
4	D	5103	PCW	C8-N-C5	-3.16	97.34	109.91
4	B	8002	PCW	C8-N-C5	-3.13	97.47	109.91
4	C	5103	PCW	C8-N-C5	-3.02	97.89	109.91
4	C	5101	PCW	O3-C11-C12	2.79	120.36	111.83
4	D	5101	PCW	O3-C11-C12	2.79	120.33	111.83
4	A	8002	PCW	C6-N-C5	-2.70	99.19	109.91
4	A	8003	PCW	O3-C11-C12	2.67	119.97	111.83
4	B	8002	PCW	C6-N-C5	-2.62	99.48	109.91
4	D	5103	PCW	C6-N-C5	-2.61	99.54	109.91
4	B	8003	PCW	O3-C11-C12	2.58	119.71	111.83
4	C	5101	PCW	C6-N-C5	-2.55	99.78	109.91
4	D	5101	PCW	C6-N-C5	-2.55	99.79	109.91
4	B	8003	PCW	C6-N-C5	-2.54	99.83	109.91
4	C	5103	PCW	C6-N-C5	-2.41	100.33	109.91
4	C	5103	PCW	O3-C11-C12	2.34	118.97	111.83
4	B	8002	PCW	O3-C11-C12	2.34	118.97	111.83
4	A	8002	PCW	O3-C11-C12	2.29	118.81	111.83
4	D	5103	PCW	O3-C11-C12	2.27	118.75	111.83
4	A	8003	PCW	C6-N-C5	-2.23	101.06	109.91
4	D	5103	PCW	C2-O2-C31	-2.16	112.62	117.80

There are no chirality outliers.

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	8002	PCW	O4P-C4-C5-N
4	A	8002	PCW	C1-O3P-P-O4P
4	D	5101	PCW	O4P-C4-C5-N
4	D	5103	PCW	O4P-C4-C5-N
4	D	5103	PCW	C1-O3P-P-O4P
4	B	8002	PCW	O4P-C4-C5-N
4	B	8002	PCW	C1-O3P-P-O4P
4	B	8002	PCW	C4-O4P-P-O2P
4	B	8003	PCW	O4P-C4-C5-N
4	C	5101	PCW	O4P-C4-C5-N
4	C	5103	PCW	O4P-C4-C5-N
4	C	5103	PCW	C1-O3P-P-O1P
4	C	5103	PCW	C1-O3P-P-O4P
4	C	5103	PCW	C4-O4P-P-O2P
4	A	8002	PCW	C13-C14-C15-C16
4	D	5103	PCW	C13-C14-C15-C16
4	D	5101	PCW	C11-C12-C13-C14
4	C	5103	PCW	C13-C14-C15-C16
4	B	8003	PCW	C44-C45-C46-C47
4	A	8002	PCW	C33-C34-C35-C36
4	C	5103	PCW	C44-C45-C46-C47
4	B	8003	PCW	C11-C12-C13-C14
4	D	5103	PCW	C32-C31-O2-C2
4	A	8003	PCW	C41-C42-C43-C44
4	B	8003	PCW	C32-C33-C34-C35
4	C	5103	PCW	C11-C12-C13-C14
4	A	8002	PCW	C35-C36-C37-C38
4	B	8002	PCW	C44-C45-C46-C47
4	C	5103	PCW	C32-C33-C34-C35
4	A	8003	PCW	C21-C22-C23-C24
4	D	5103	PCW	C44-C45-C46-C47
4	D	5103	PCW	C22-C23-C24-C25
4	B	8002	PCW	C35-C36-C37-C38
4	C	5101	PCW	C41-C42-C43-C44
4	B	8002	PCW	C32-C31-O2-C2
4	C	5103	PCW	C32-C31-O2-C2
4	A	8002	PCW	C40-C41-C42-C43
4	D	5101	PCW	C20-C21-C22-C23
4	B	8003	PCW	C15-C16-C17-C18
4	D	5103	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
4	D	5101	PCW	C43-C44-C45-C46
4	A	8003	PCW	C43-C44-C45-C46
4	C	5101	PCW	C43-C44-C45-C46
4	A	8003	PCW	C24-C25-C26-C27
4	A	8002	PCW	C32-C31-O2-C2
4	B	8003	PCW	C32-C31-O2-C2
4	A	8002	PCW	O31-C31-O2-C2
4	B	8002	PCW	O31-C31-O2-C2
4	B	8003	PCW	O31-C31-O2-C2
4	B	8003	PCW	C20-C21-C22-C23
4	A	8002	PCW	C44-C45-C46-C47
4	C	5103	PCW	C43-C44-C45-C46
4	C	5103	PCW	O31-C31-O2-C2
4	A	8002	PCW	C43-C44-C45-C46
4	C	5101	PCW	C13-C14-C15-C16
4	D	5101	PCW	C16-C17-C18-C19
4	B	8003	PCW	C13-C14-C15-C16
4	C	5101	PCW	C2-C1-O3P-P
4	B	8003	PCW	C35-C36-C37-C38
4	B	8003	PCW	C12-C13-C14-C15
4	A	8002	PCW	C24-C25-C26-C27
4	D	5101	PCW	C35-C36-C37-C38
4	A	8003	PCW	O3P-C1-C2-C3
4	C	5101	PCW	O3P-C1-C2-C3
4	B	8002	PCW	C15-C16-C17-C18
4	C	5101	PCW	C24-C25-C26-C27
4	C	5101	PCW	C20-C21-C22-C23
4	C	5103	PCW	C15-C16-C17-C18
4	D	5101	PCW	C12-C11-O3-C3
4	D	5103	PCW	C33-C34-C35-C36
4	A	8002	PCW	C11-C12-C13-C14
4	C	5101	PCW	C42-C43-C44-C45
4	B	8002	PCW	C24-C25-C26-C27
4	A	8003	PCW	C20-C21-C22-C23
4	C	5101	PCW	C16-C17-C18-C19
4	B	8002	PCW	C33-C34-C35-C36
4	C	5101	PCW	C35-C36-C37-C38
4	C	5101	PCW	C11-C12-C13-C14
4	A	8002	PCW	C32-C33-C34-C35
4	C	5103	PCW	C40-C41-C42-C43
4	A	8002	PCW	C12-C11-O3-C3
4	B	8002	PCW	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	C	5103	PCW	C41-C42-C43-C44
4	B	8003	PCW	C19-C20-C21-C22
4	B	8003	PCW	C2-C1-O3P-P
4	D	5101	PCW	C14-C15-C16-C17
4	C	5103	PCW	C24-C25-C26-C27
4	B	8003	PCW	O3P-C1-C2-C3
4	D	5101	PCW	O11-C11-O3-C3
4	B	8002	PCW	C32-C33-C34-C35
4	B	8003	PCW	C41-C42-C43-C44
4	D	5103	PCW	C32-C33-C34-C35
4	A	8002	PCW	C1-C2-C3-O3
4	B	8002	PCW	C1-C2-C3-O3
4	C	5103	PCW	C1-C2-C3-O3
4	A	8003	PCW	C35-C36-C37-C38
4	A	8003	PCW	C4-C5-N-C8
4	D	5103	PCW	O2-C2-C3-O3
4	B	8002	PCW	O2-C2-C3-O3
4	D	5103	PCW	C11-C12-C13-C14
4	C	5101	PCW	C21-C22-C23-C24
4	D	5103	PCW	C12-C11-O3-C3
4	B	8003	PCW	C12-C11-O3-C3
4	D	5101	PCW	O3P-C1-C2-C3
4	A	8002	PCW	O11-C11-O3-C3
4	D	5103	PCW	O11-C11-O3-C3
4	B	8003	PCW	O11-C11-O3-C3
4	B	8003	PCW	C1-C2-O2-C31
4	D	5101	PCW	C44-C45-C46-C47
4	A	8003	PCW	O3P-C1-C2-O2
4	C	5101	PCW	O3P-C1-C2-O2
4	A	8002	PCW	O2-C2-C3-O3
4	D	5103	PCW	C40-C41-C42-C43
4	C	5103	PCW	O2-C2-C3-O3
4	D	5103	PCW	C35-C36-C37-C38
4	D	5101	PCW	C13-C14-C15-C16
4	A	8003	PCW	C45-C46-C47-C48
4	D	5101	PCW	C19-C20-C21-C22
4	D	5101	PCW	O3P-C1-C2-O2
4	B	8003	PCW	O3P-C1-C2-O2
4	C	5101	PCW	C4-C5-N-C8
4	D	5103	PCW	C1-C2-C3-O3
4	A	8002	PCW	C1-O3P-P-O2P
4	D	5103	PCW	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
4	D	5103	PCW	C4-O4P-P-O2P
4	B	8002	PCW	C1-O3P-P-O2P
4	C	5103	PCW	C1-O3P-P-O2P
4	C	5101	PCW	C45-C46-C47-C48
4	A	8003	PCW	C2-C1-O3P-P
4	D	5101	PCW	C2-C1-O3P-P
4	C	5103	PCW	C2-C1-O3P-P
4	A	8003	PCW	C1-C2-O2-C31
4	D	5103	PCW	C24-C25-C26-C27
4	D	5101	PCW	C4-C5-N-C8
4	B	8003	PCW	C4-C5-N-C8
4	C	5103	PCW	O3P-C1-C2-C3
4	A	8003	PCW	C15-C16-C17-C18
4	A	8003	PCW	O11-C11-O3-C3
4	D	5101	PCW	C12-C13-C14-C15
4	A	8003	PCW	C12-C11-O3-C3
4	B	8002	PCW	C37-C38-C39-C40
4	C	5101	PCW	C19-C20-C21-C22
4	D	5103	PCW	C25-C26-C27-C28
4	A	8002	PCW	C2-C1-O3P-P
4	B	8002	PCW	C41-C42-C43-C44
4	C	5103	PCW	C25-C26-C27-C28
4	A	8003	PCW	C17-C18-C19-C20
4	D	5101	PCW	C3-C2-O2-C31
4	C	5101	PCW	C1-C2-O2-C31
4	C	5101	PCW	C3-C2-O2-C31
4	D	5103	PCW	C41-C42-C43-C44
4	A	8003	PCW	C19-C20-C21-C22
4	B	8003	PCW	C37-C38-C39-C40
4	A	8002	PCW	C45-C46-C47-C48
4	C	5101	PCW	O31-C31-O2-C2
4	C	5103	PCW	O3P-C1-C2-O2
4	D	5103	PCW	C19-C20-C21-C22
4	C	5101	PCW	C32-C31-O2-C2
4	A	8002	PCW	C25-C26-C27-C28
4	A	8003	PCW	C42-C43-C44-C45
4	B	8003	PCW	C17-C18-C19-C20
4	C	5101	PCW	O11-C11-O3-C3
4	D	5101	PCW	C1-C2-O2-C31
4	B	8002	PCW	C19-C20-C21-C22
4	C	5103	PCW	C37-C38-C39-C40
4	A	8003	PCW	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
4	A	8002	PCW	C37-C38-C39-C40
4	B	8003	PCW	C14-C15-C16-C17
4	B	8002	PCW	C2-C1-O3P-P
4	C	5101	PCW	C12-C11-O3-C3
4	D	5103	PCW	C39-C40-C41-C42
4	A	8002	PCW	C4-C5-N-C8
4	C	5103	PCW	C19-C20-C21-C22
4	B	8002	PCW	C40-C41-C42-C43
4	A	8002	PCW	C17-C18-C19-C20
4	A	8003	PCW	C11-C12-C13-C14
4	A	8003	PCW	C39-C40-C41-C42
4	D	5101	PCW	C15-C16-C17-C18
4	C	5101	PCW	C44-C45-C46-C47
4	A	8003	PCW	C3-C2-O2-C31
4	A	8002	PCW	C23-C24-C25-C26
4	C	5101	PCW	C37-C38-C39-C40
4	C	5101	PCW	C33-C34-C35-C36
4	B	8002	PCW	O3P-C1-C2-C3
4	D	5103	PCW	C45-C46-C47-C48
4	B	8002	PCW	C13-C14-C15-C16
4	D	5103	PCW	C17-C18-C19-C20

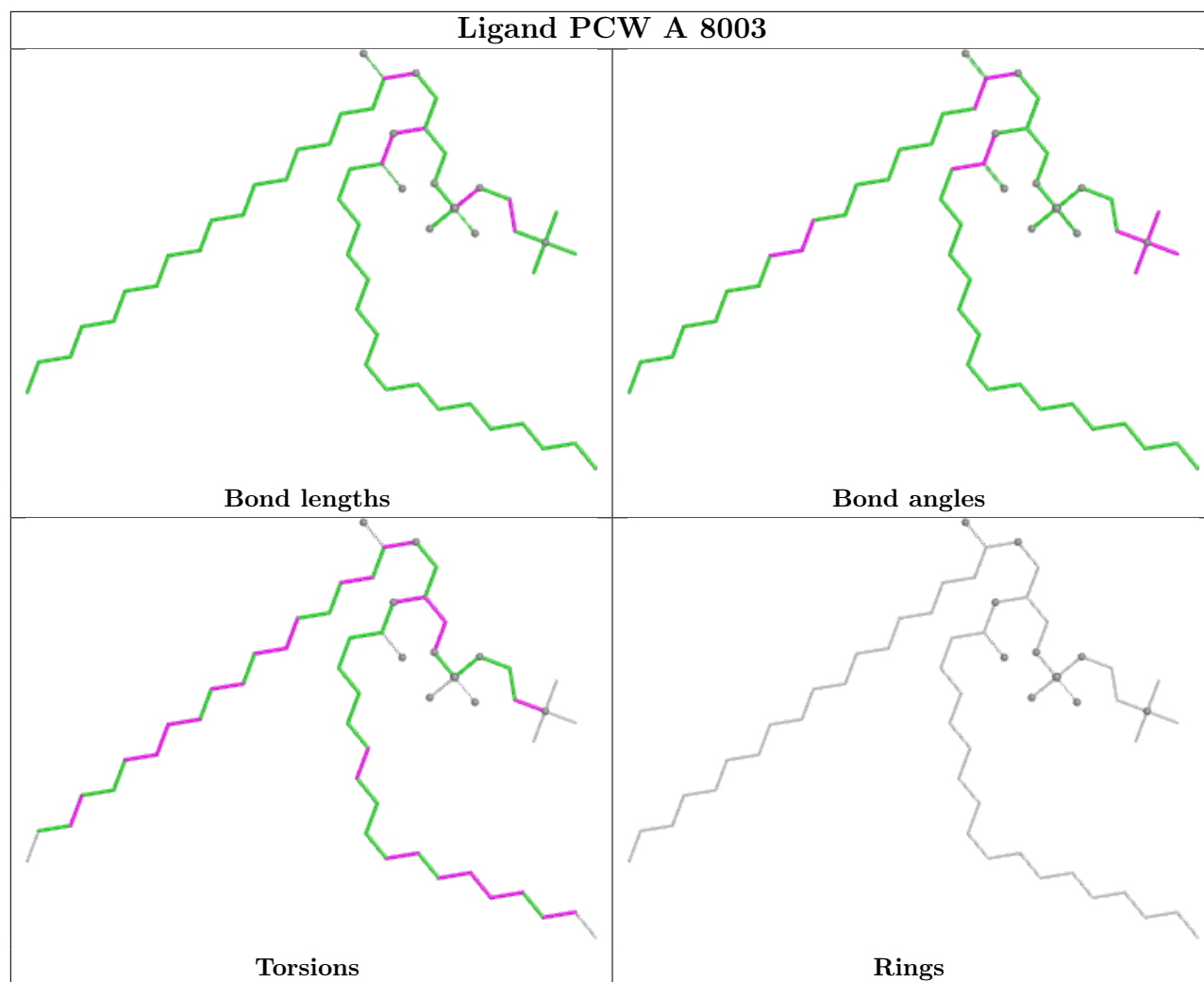
There are no ring outliers.

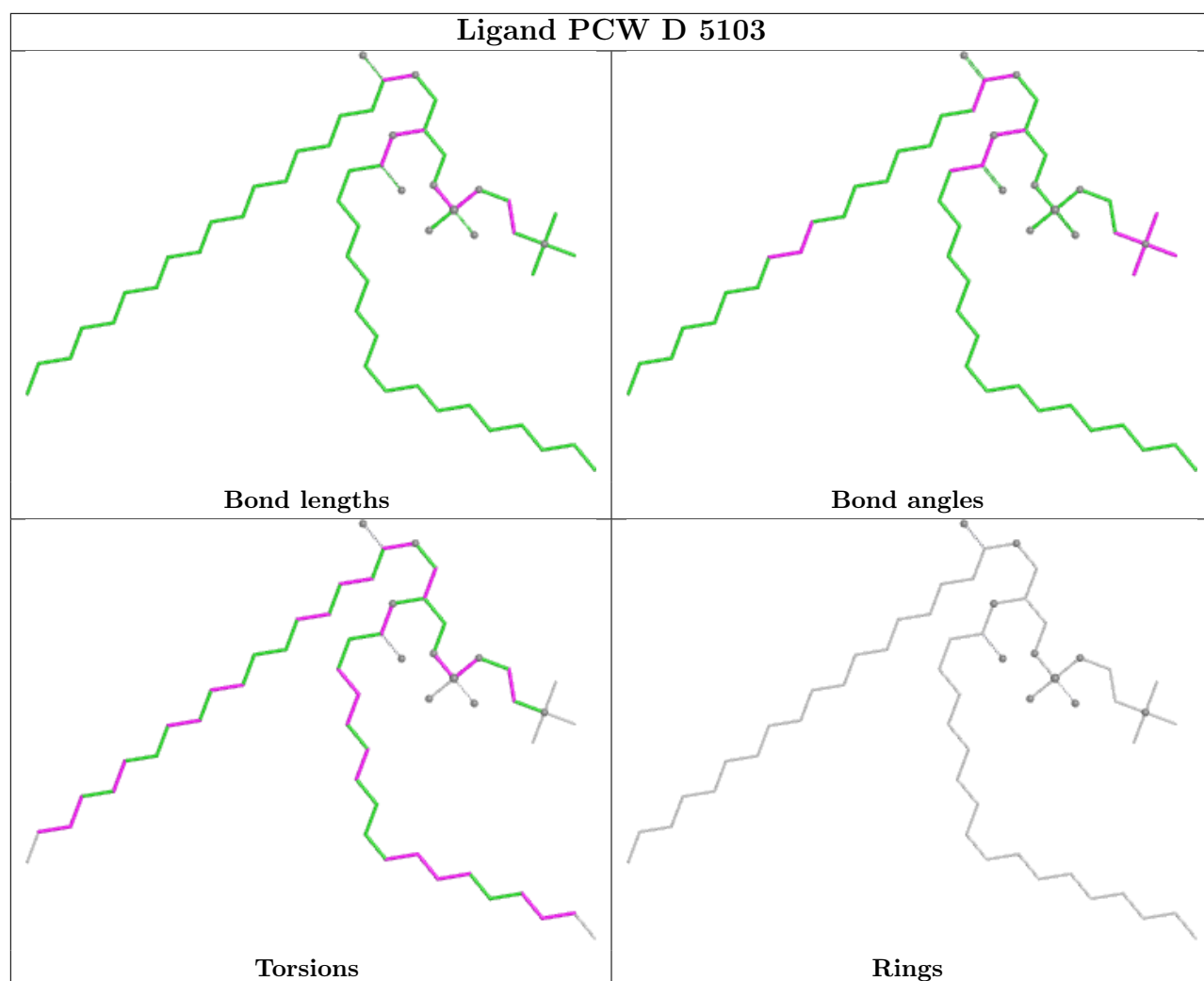
4 monomers are involved in 6 short contacts:

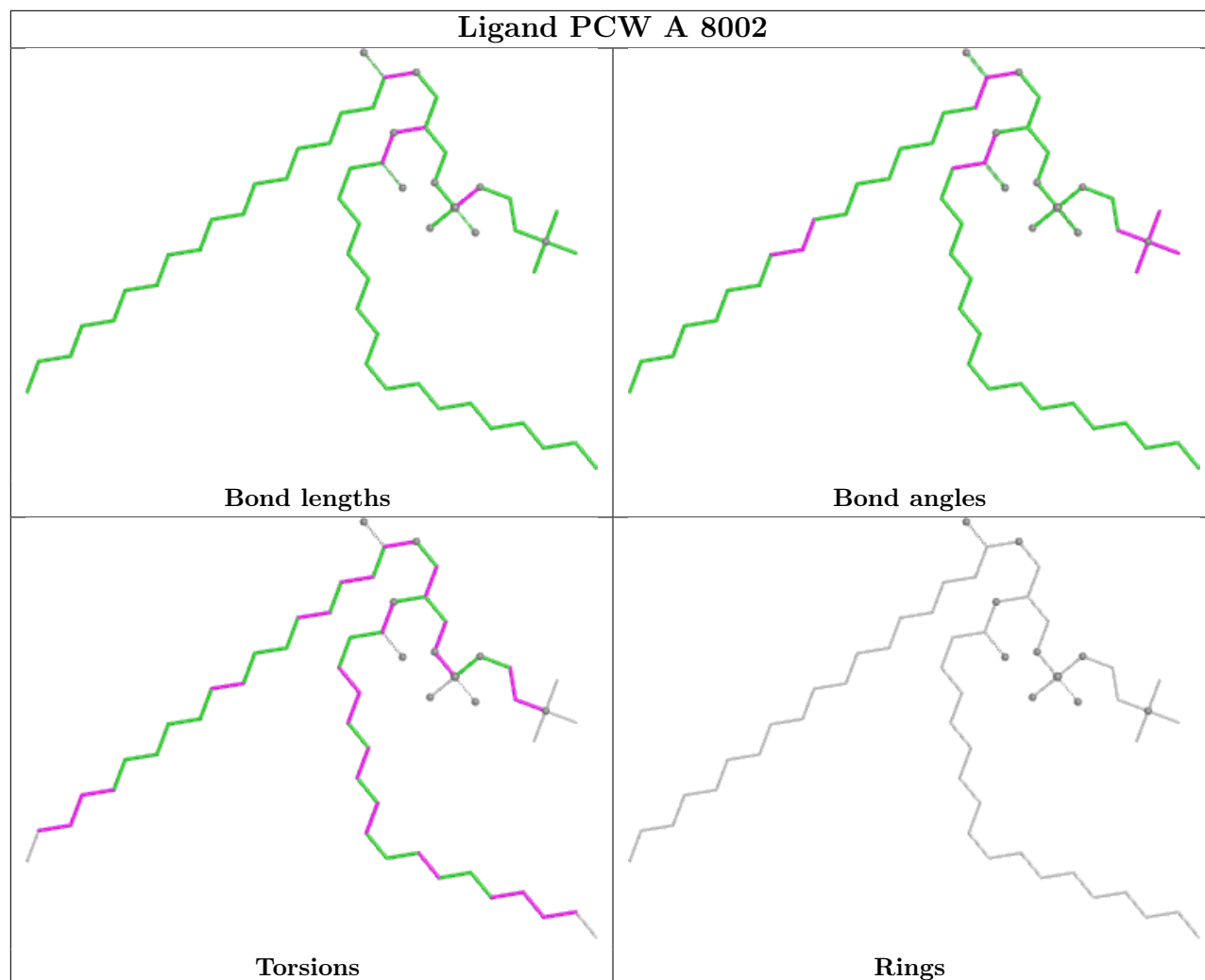
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5103	PCW	1	0
4	C	5103	PCW	3	0
4	B	8002	PCW	2	0
4	B	8003	PCW	1	0

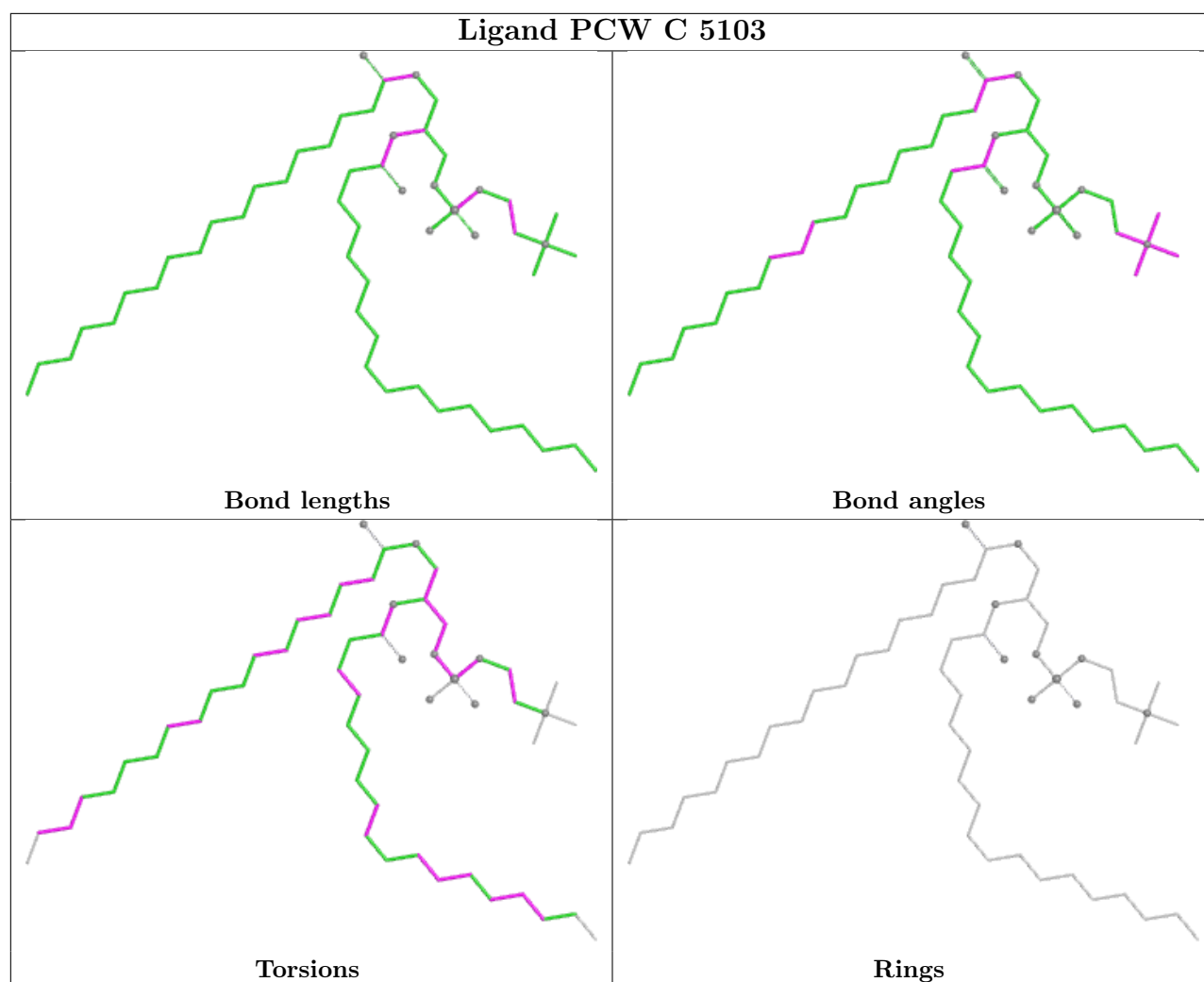
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

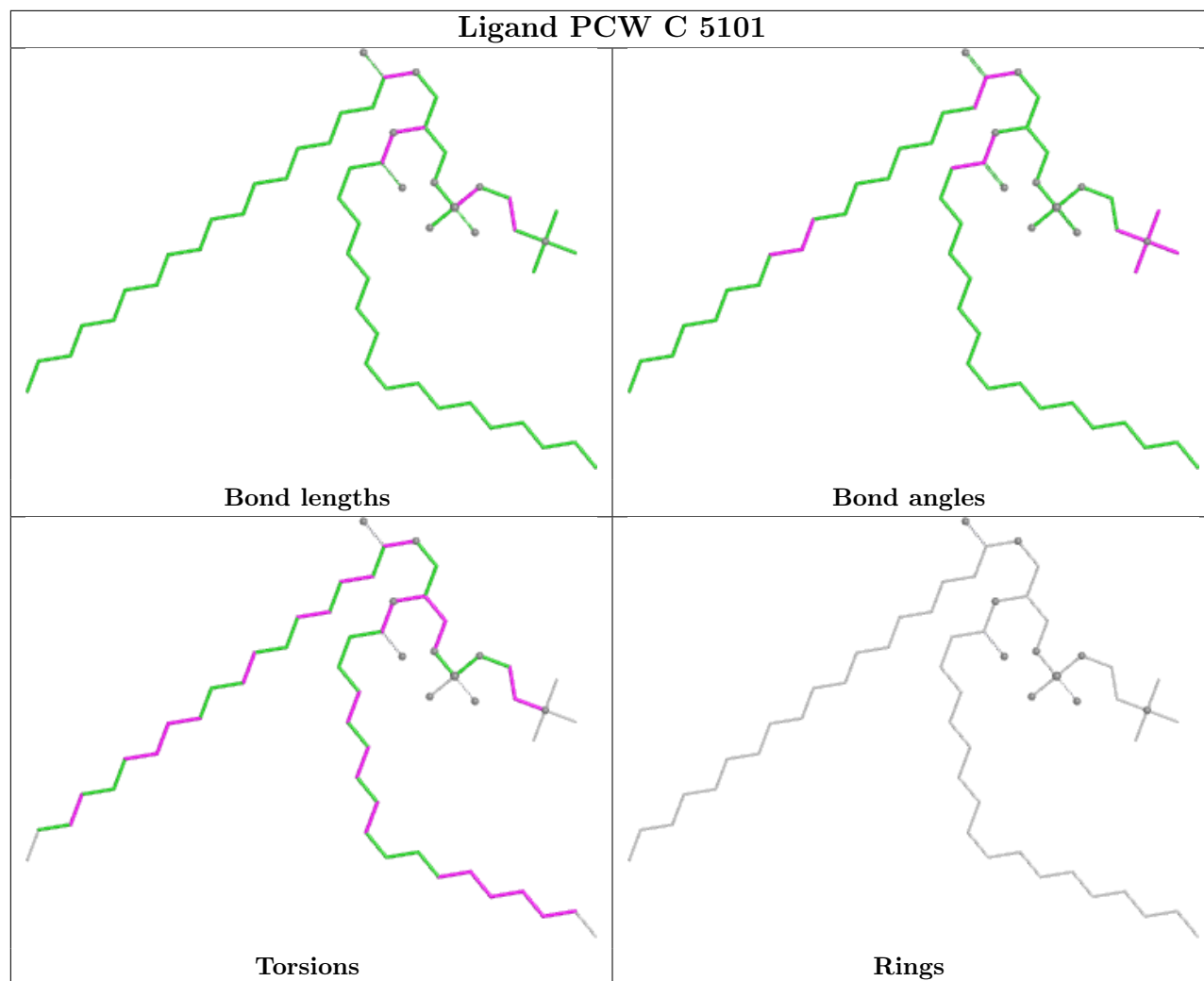
equivalents in the CSD to analyse the geometry.

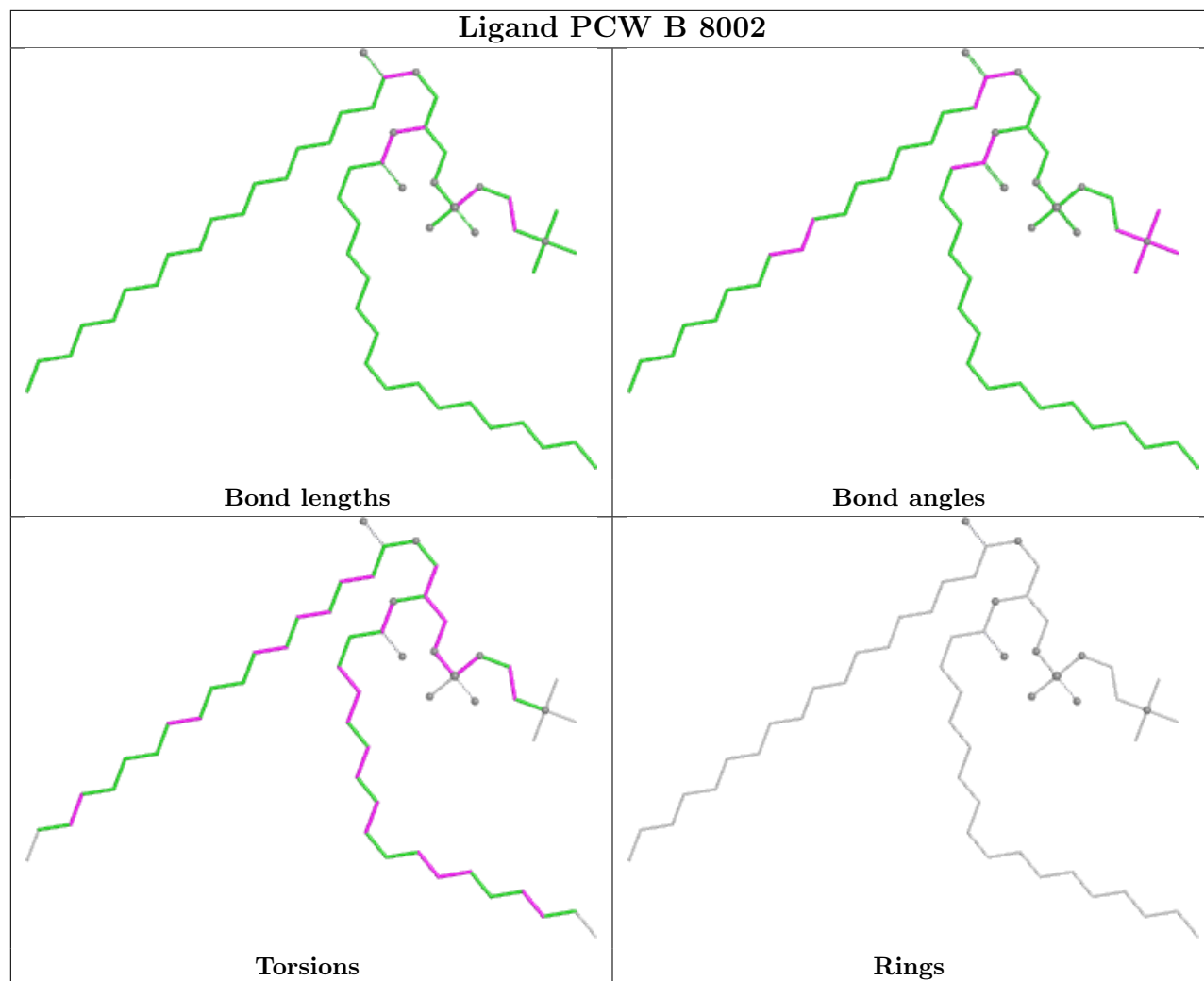


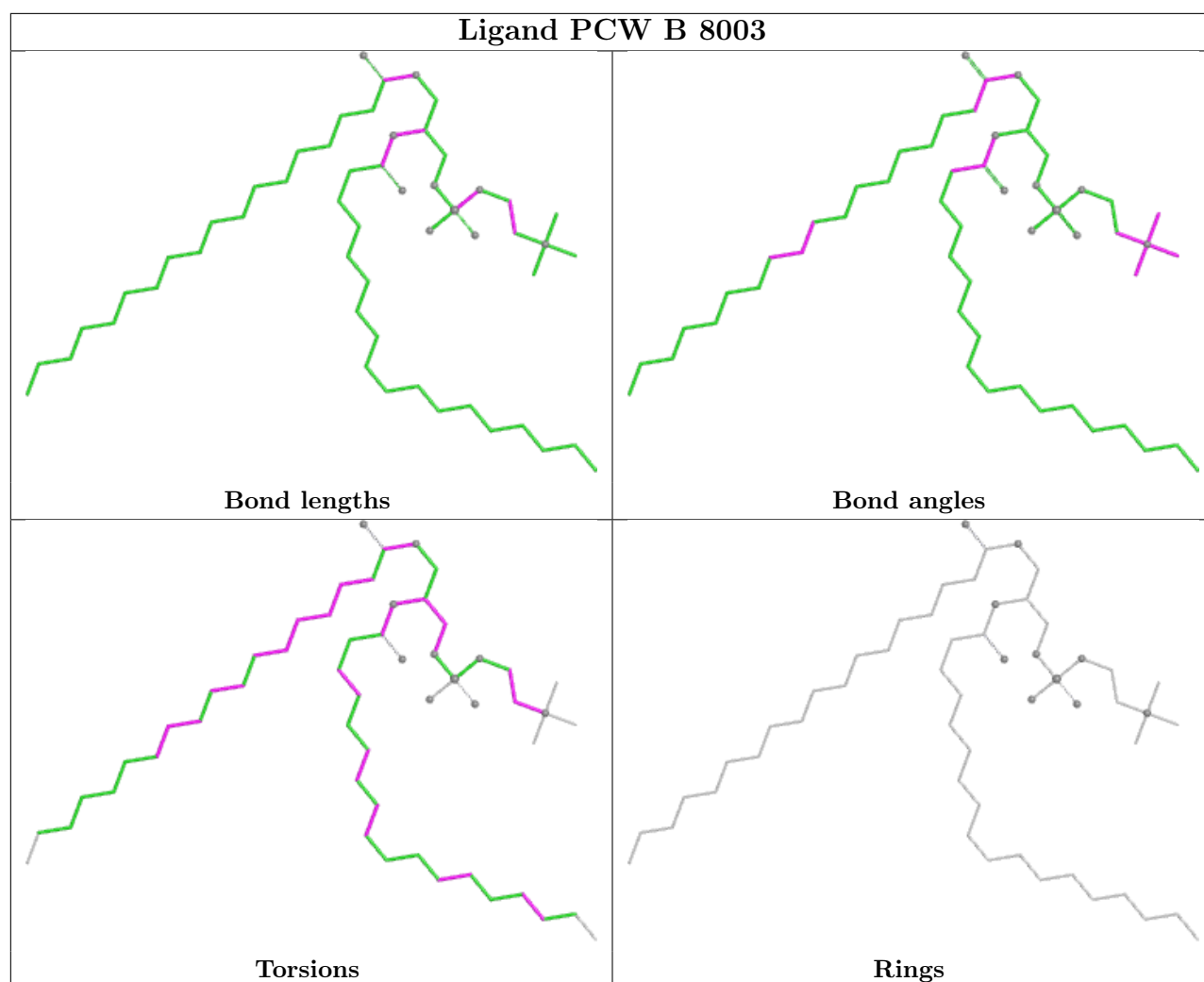


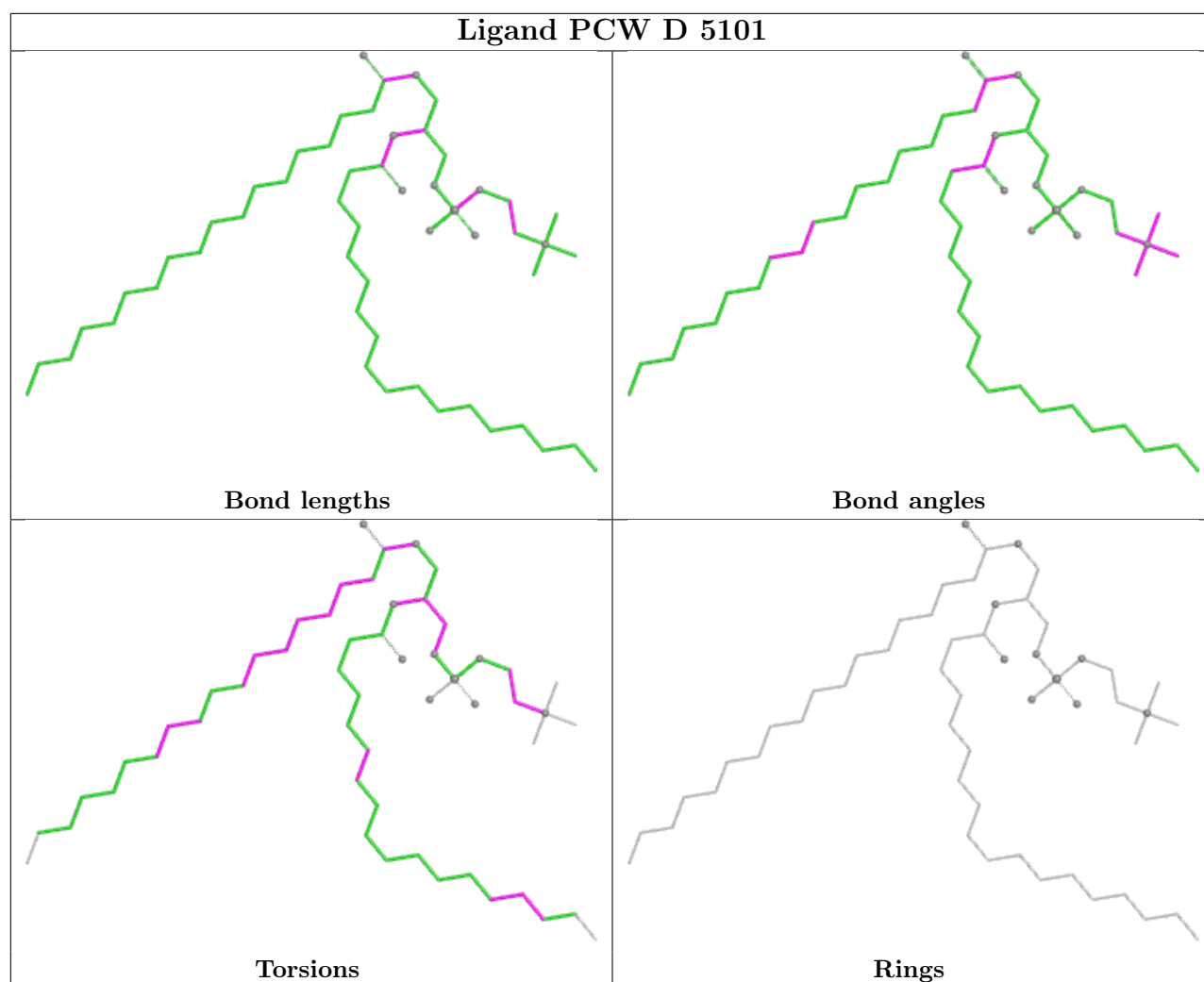












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

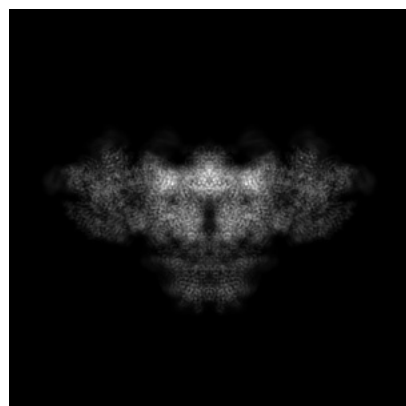
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43283. These allow visual inspection of the internal detail of the map and identification of artifacts.

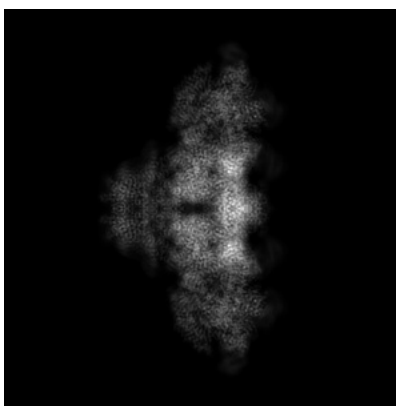
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

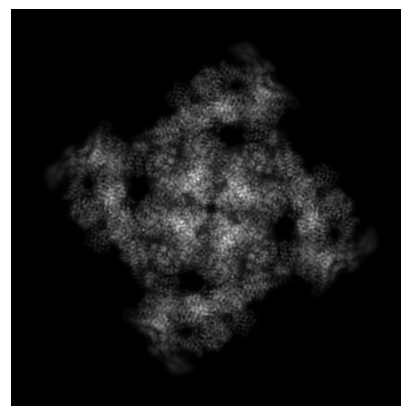
6.1.1 Primary map



X

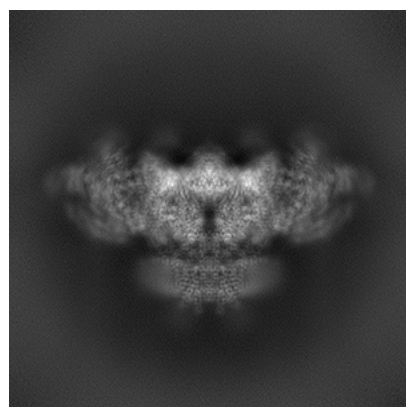


Y

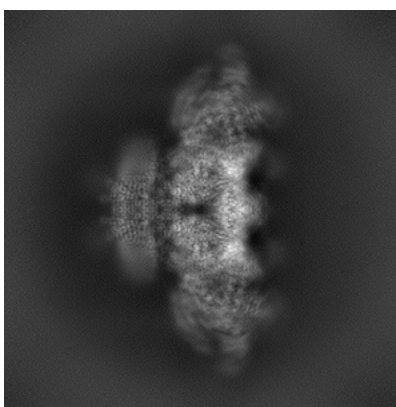


Z

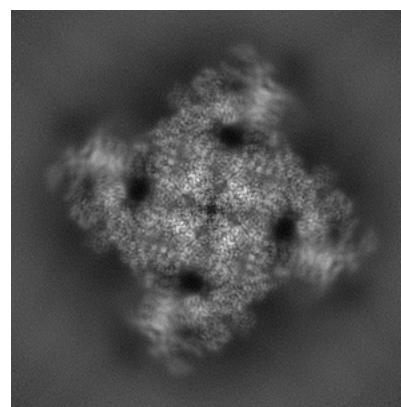
6.1.2 Raw map



X



Y



Z

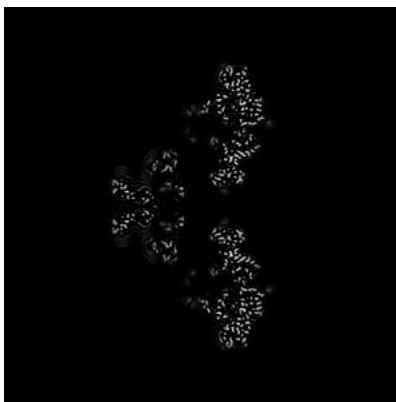
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

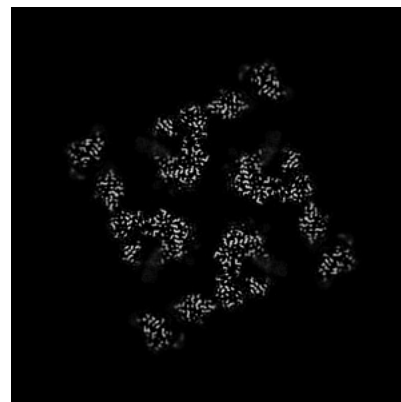
6.2.1 Primary map



X Index: 256

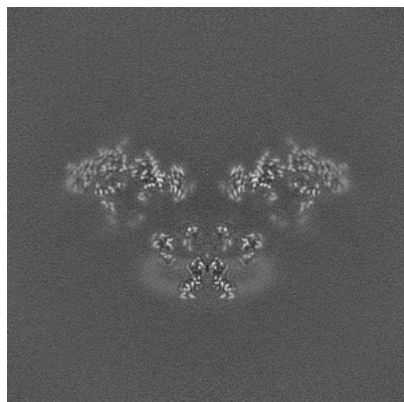


Y Index: 256

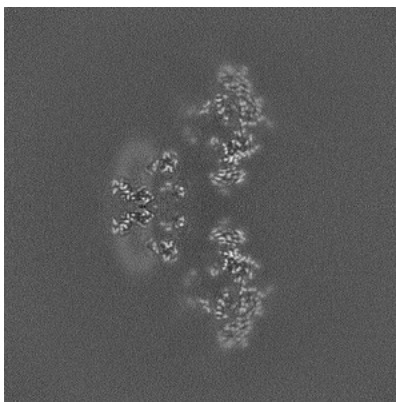


Z Index: 256

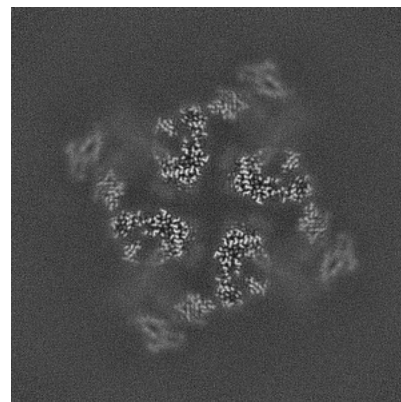
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

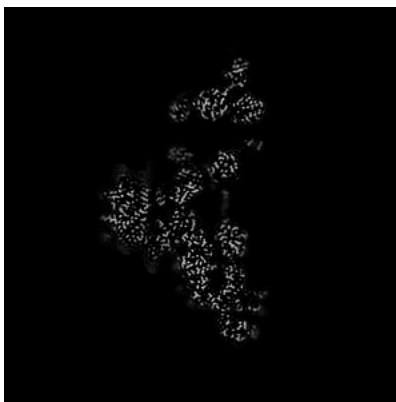
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

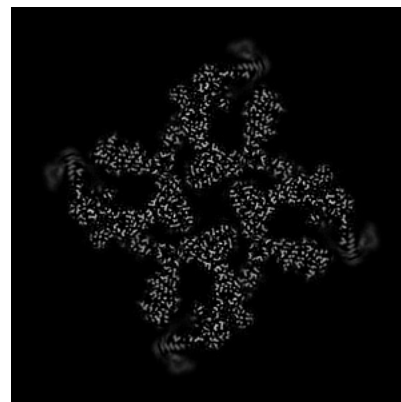
6.3.1 Primary map



X Index: 238

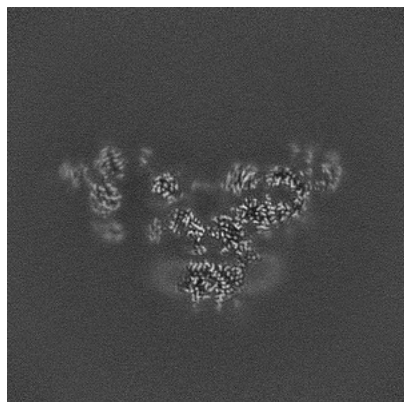


Y Index: 238

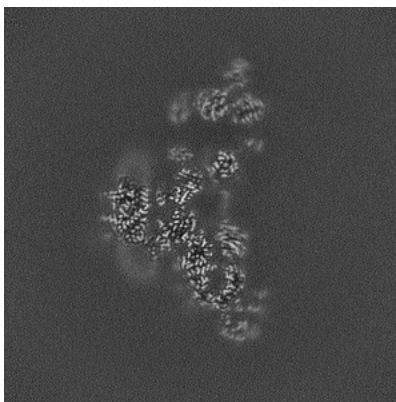


Z Index: 289

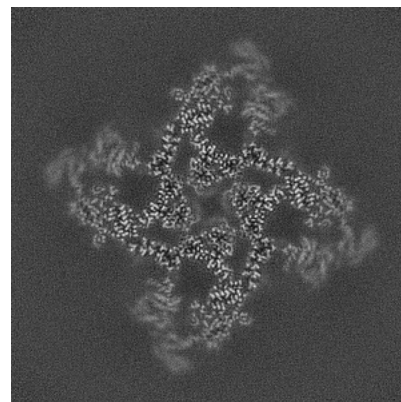
6.3.2 Raw map



X Index: 238



Y Index: 238

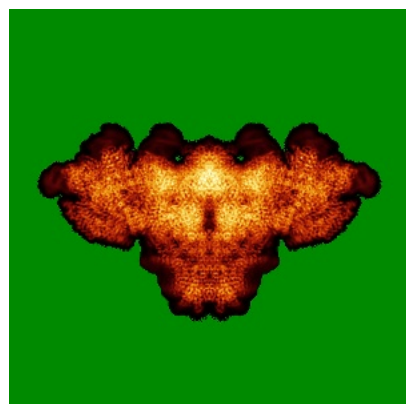


Z Index: 285

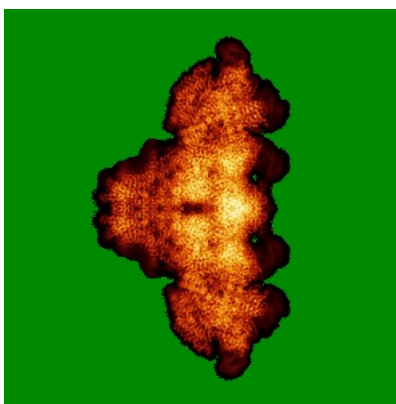
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

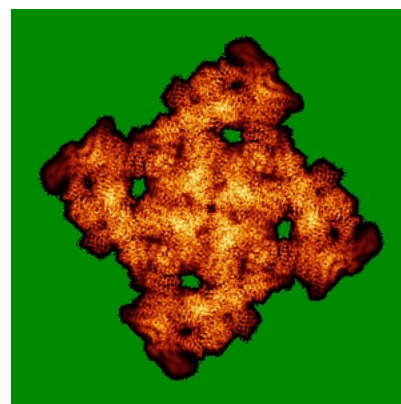
6.4.1 Primary map



X



Y

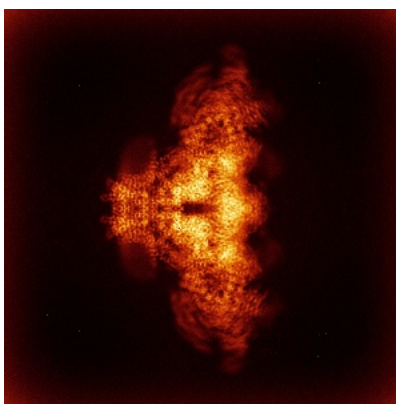


Z

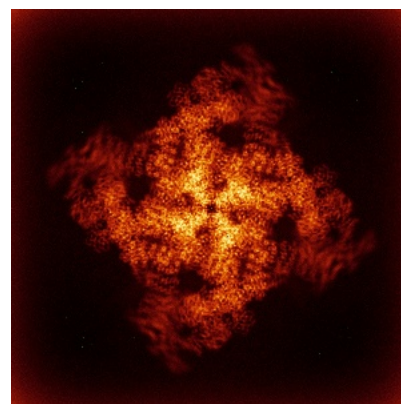
6.4.2 Raw map



X



Y

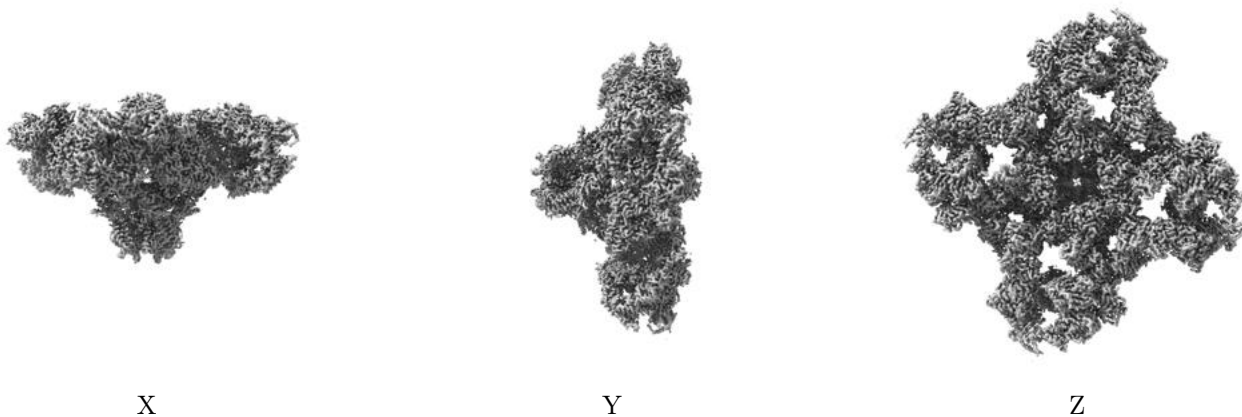


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

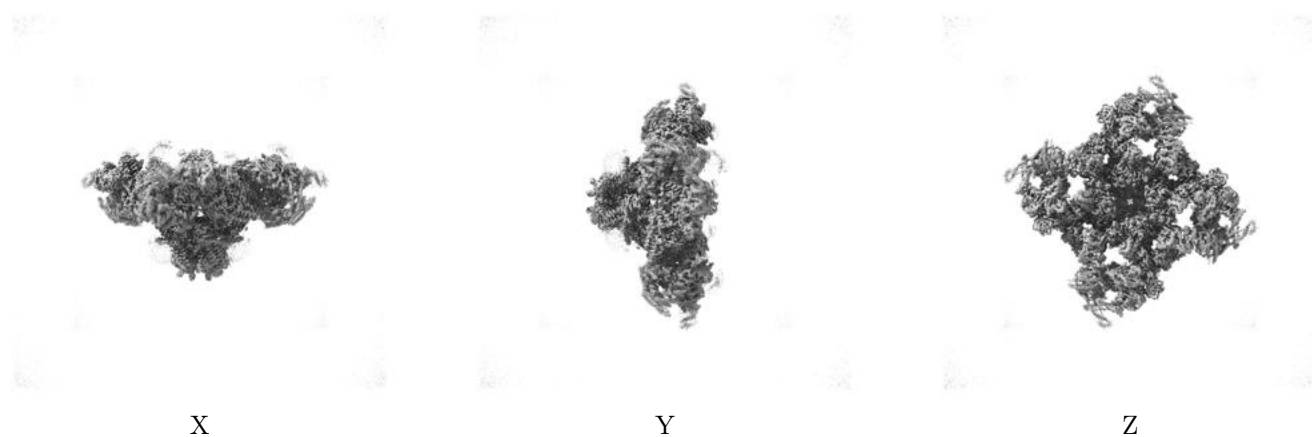
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

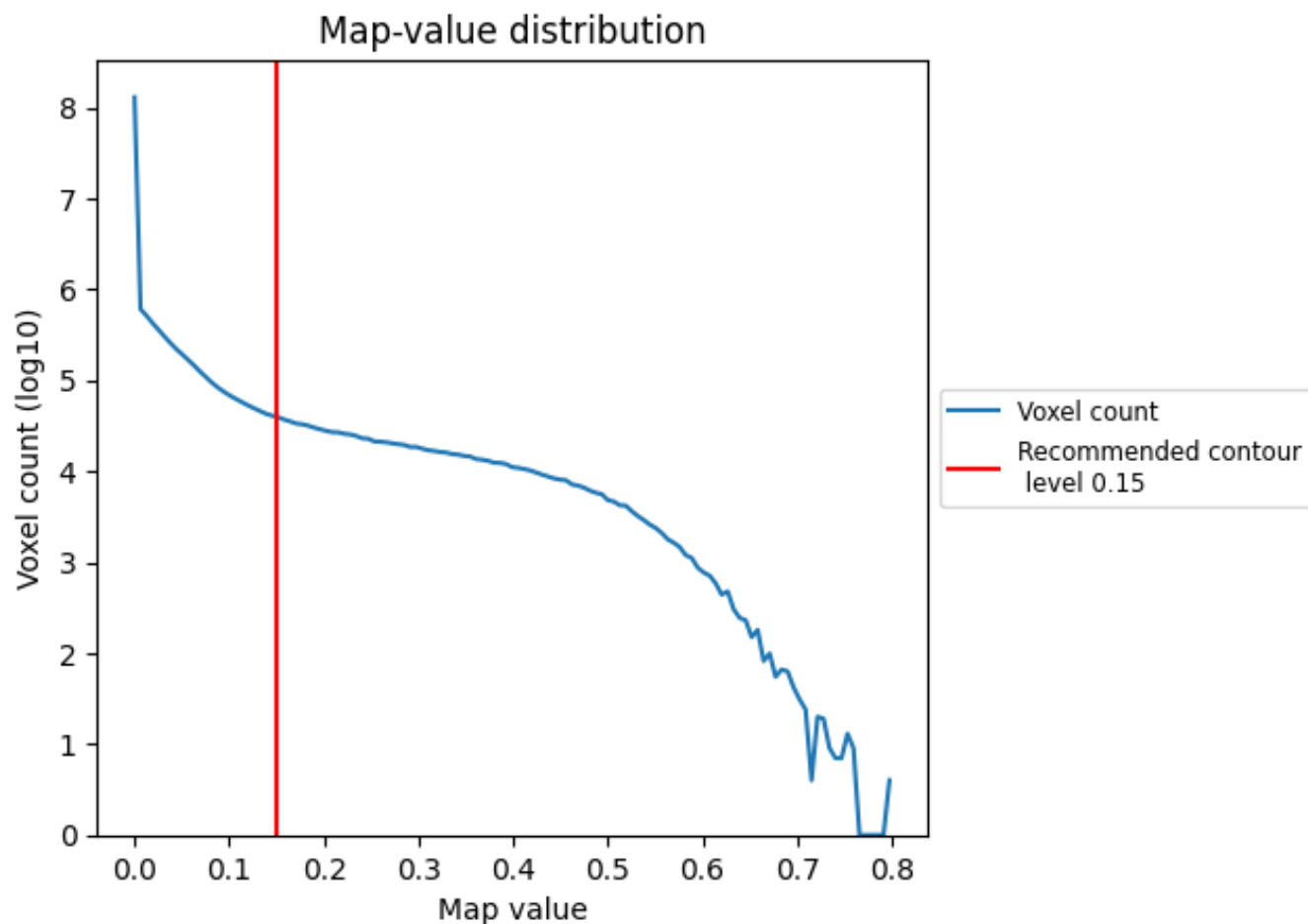
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

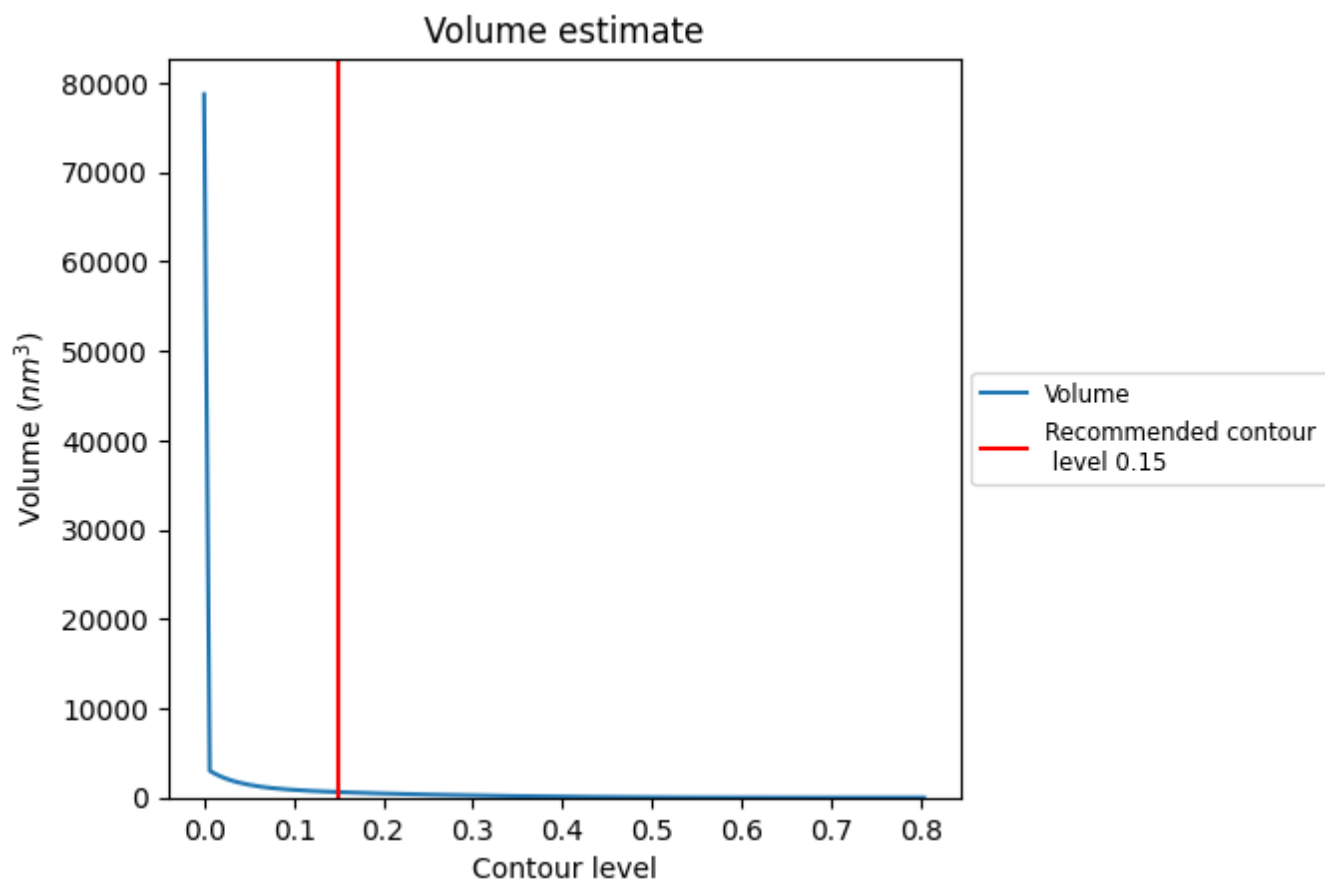
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

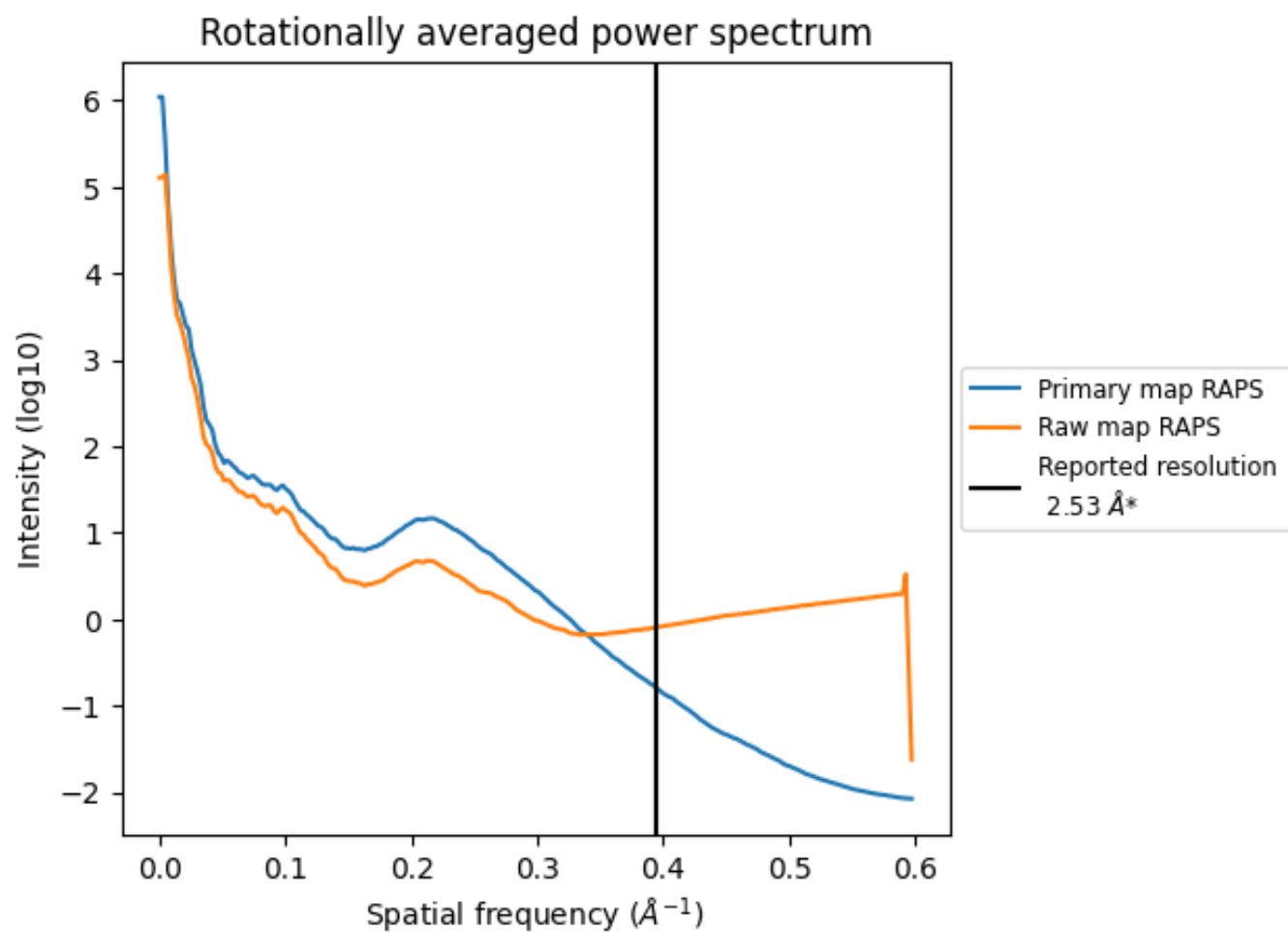
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 612 nm³; this corresponds to an approximate mass of 552 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

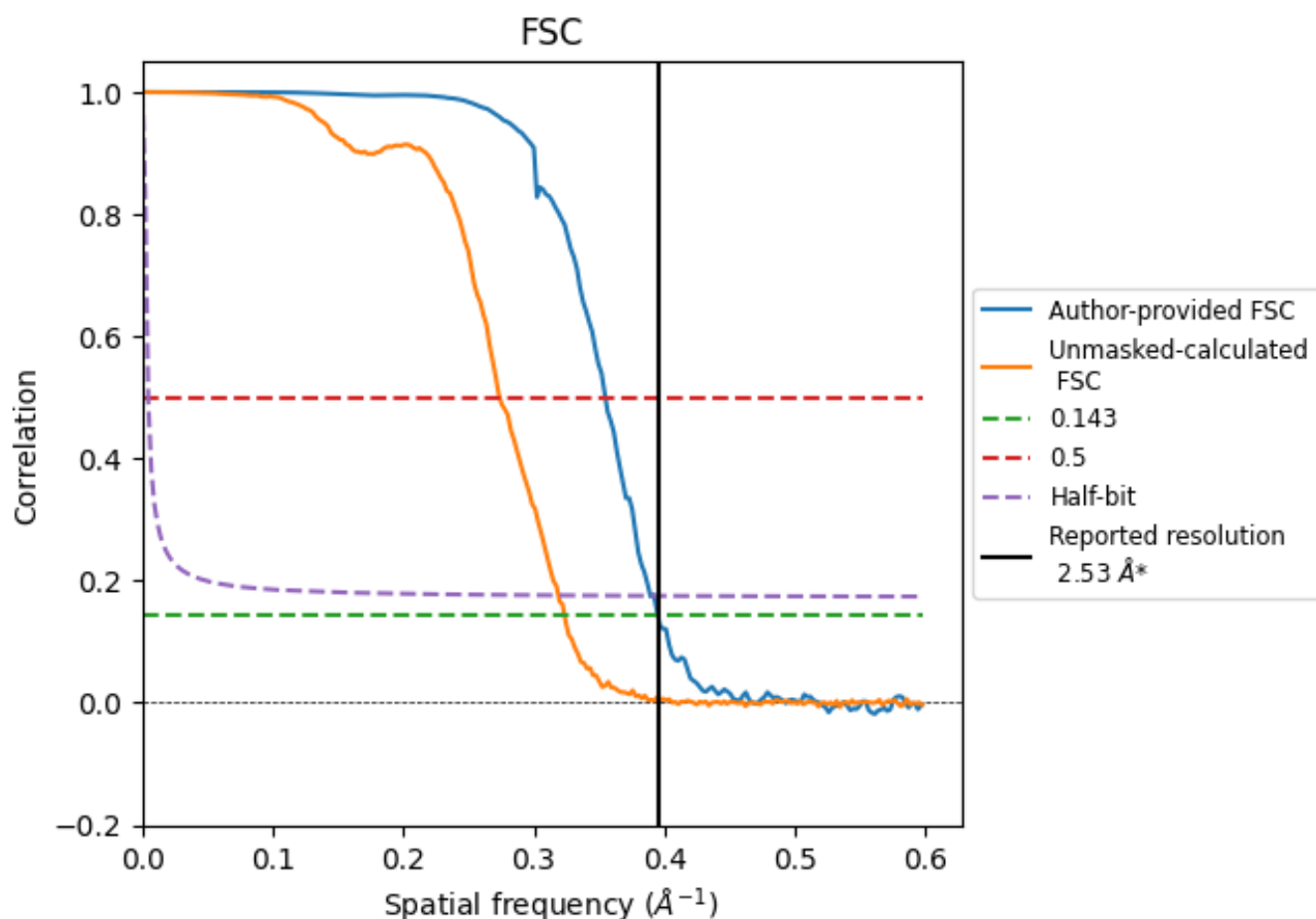


*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.395 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

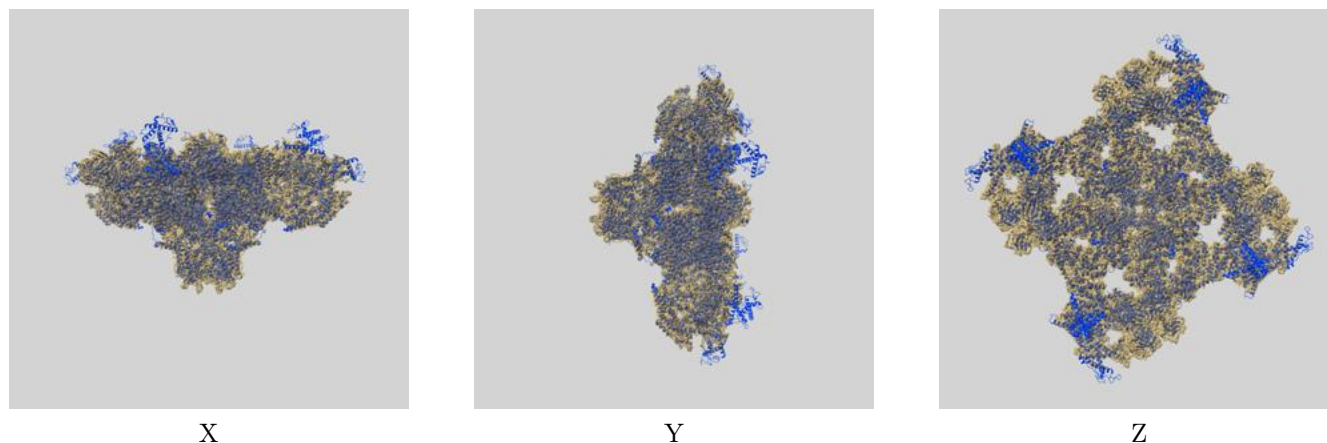
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.53	2.82	2.57
Unmasked-calculated*	3.09	3.65	3.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.53 by more than 10 %

9 Map-model fit [i](#)

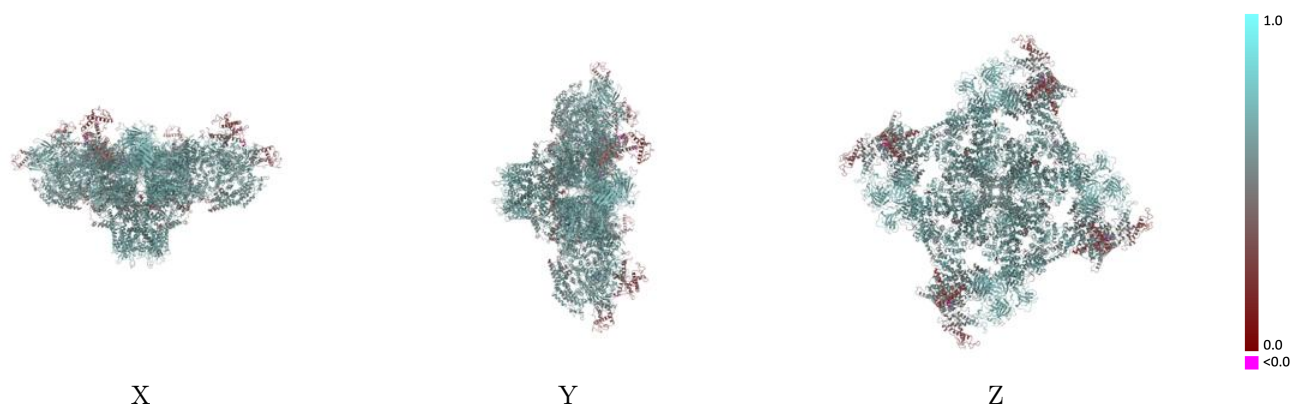
This section contains information regarding the fit between EMDB map EMD-43283 and PDB model 8VJJ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



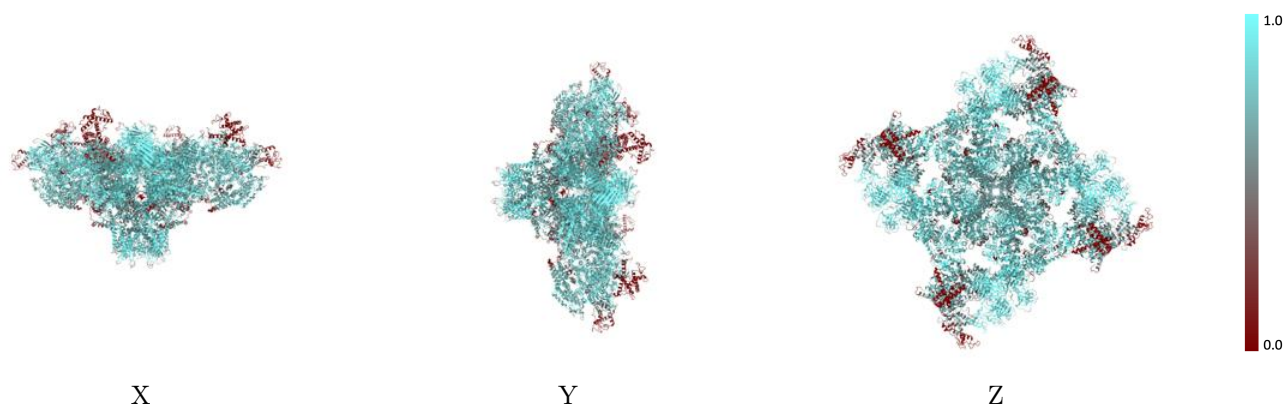
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



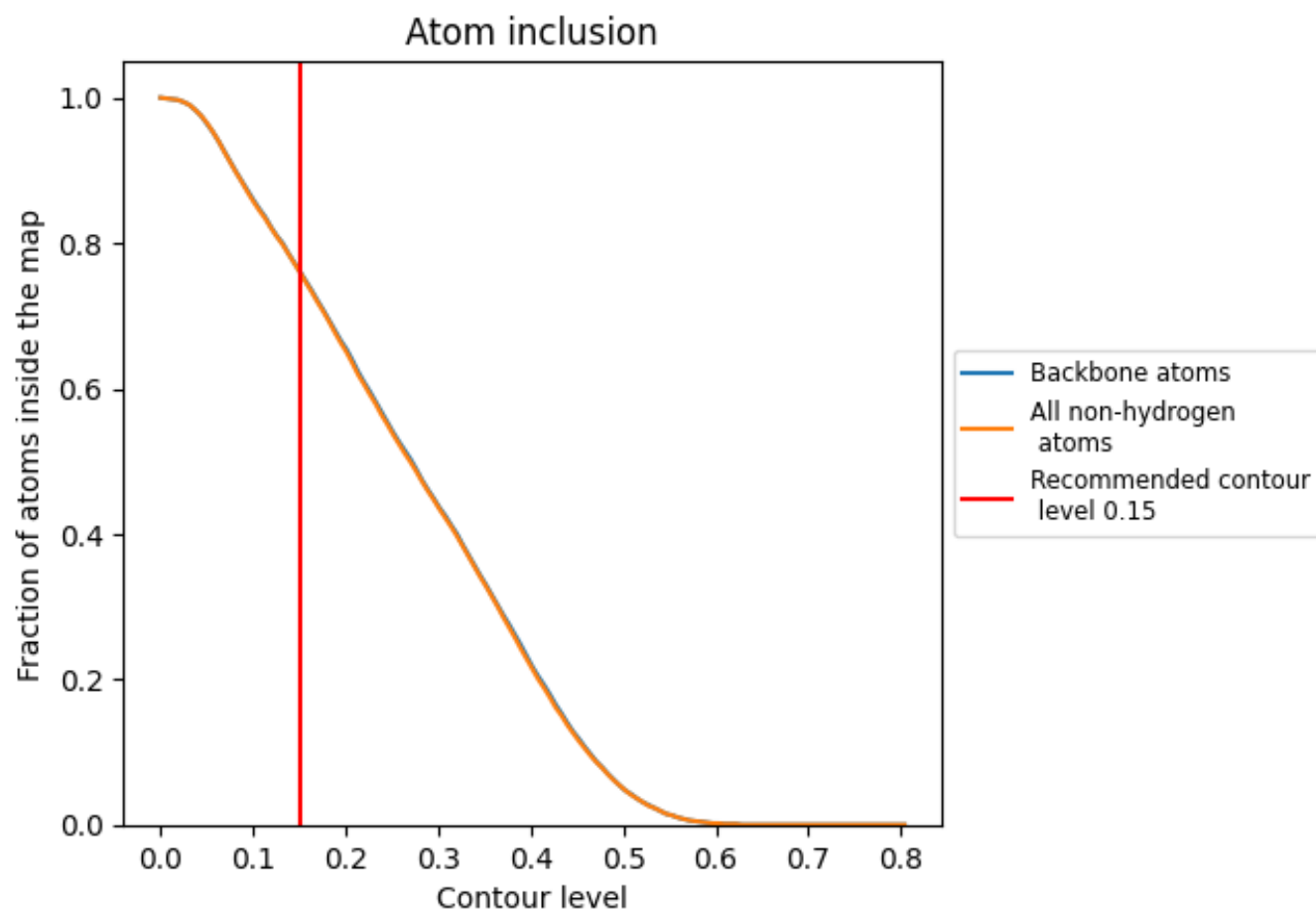
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7610	0.5970
A	0.7630	0.5960
B	0.7640	0.5950
C	0.7630	0.5960
D	0.7640	0.5960
E	0.8670	0.6550
F	0.8660	0.6530
G	0.8650	0.6530
H	0.8680	0.6540

1.0

0.0

<0.0