Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 06:37 AM EDT

PDB ID	:	4EV6
Title	:	The complete structure of CorA magnesium transporter from Methanocaldococcus jannaschii
Authors	:	Guskov, A.; Nordin, N.; Reynaud, A.; Engman, H.; Lundback, A.-K.; Jong, A.J.O.; Cornvik, T.; Phua, T.; Eshaghi, S.
Deposited on	:	2012-04-25
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

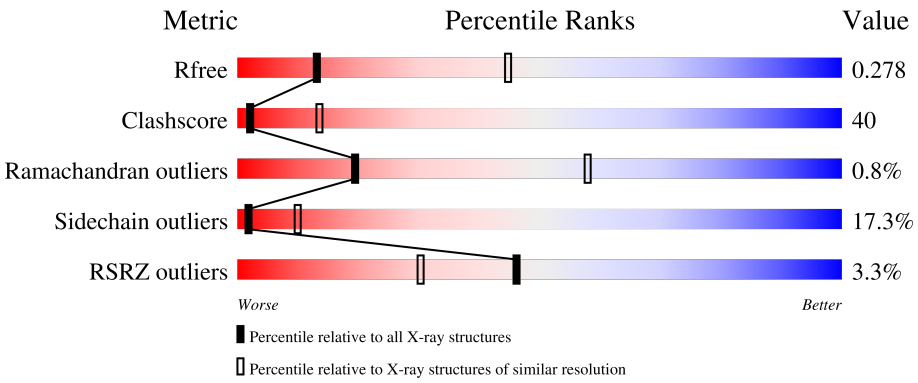
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	339	2%, 38%, 45%, 9%, •, 7%
1	B	339	4%, 36%, 44%, 13%, 7%
1	C	339	3%, 28%, 52%, 12%, 7%
1	D	339	4%, 32%, 50%, 10%, 7%

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Mol	Chain	Length	Quality of chain
1	E	339	3% 39% 45% 9% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMQ	A	402	-	-	-	X
2	UMQ	D	401	-	-	-	X
2	UMQ	E	402	-	-	-	X
3	MG	D	404	-	-	-	X
3	MG	D	406	-	-	-	X
3	MG	D	407	-	-	-	X
3	MG	E	405	-	-	-	X
3	MG	E	407	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13436 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Magnesium transport protein CorA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2596	1695	410	477	14	0	0	0
1	B	314	2589	1691	409	475	14	0	0	0
1	C	314	2589	1691	409	475	14	0	0	0
1	D	314	2589	1691	409	475	14	0	0	0
1	E	317	2618	1710	412	481	15	0	1	0

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q58439
A	-20	HIS	-	expression tag	UNP Q58439
A	-19	HIS	-	expression tag	UNP Q58439
A	-18	HIS	-	expression tag	UNP Q58439
A	-17	HIS	-	expression tag	UNP Q58439
A	-16	HIS	-	expression tag	UNP Q58439
A	-15	HIS	-	expression tag	UNP Q58439
A	-14	SER	-	expression tag	UNP Q58439
A	-13	SER	-	expression tag	UNP Q58439
A	-12	GLY	-	expression tag	UNP Q58439
A	-11	VAL	-	expression tag	UNP Q58439
A	-10	ASP	-	expression tag	UNP Q58439
A	-9	LEU	-	expression tag	UNP Q58439
A	-8	GLY	-	expression tag	UNP Q58439
A	-7	THR	-	expression tag	UNP Q58439
A	-6	GLU	-	expression tag	UNP Q58439
A	-5	ASN	-	expression tag	UNP Q58439
A	-4	LEU	-	expression tag	UNP Q58439
A	-3	TYR	-	expression tag	UNP Q58439

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PHE	-	expression tag	UNP Q58439
A	-1	GLN	-	expression tag	UNP Q58439
A	0	SER	-	expression tag	UNP Q58439
B	-21	MET	-	expression tag	UNP Q58439
B	-20	HIS	-	expression tag	UNP Q58439
B	-19	HIS	-	expression tag	UNP Q58439
B	-18	HIS	-	expression tag	UNP Q58439
B	-17	HIS	-	expression tag	UNP Q58439
B	-16	HIS	-	expression tag	UNP Q58439
B	-15	HIS	-	expression tag	UNP Q58439
B	-14	SER	-	expression tag	UNP Q58439
B	-13	SER	-	expression tag	UNP Q58439
B	-12	GLY	-	expression tag	UNP Q58439
B	-11	VAL	-	expression tag	UNP Q58439
B	-10	ASP	-	expression tag	UNP Q58439
B	-9	LEU	-	expression tag	UNP Q58439
B	-8	GLY	-	expression tag	UNP Q58439
B	-7	THR	-	expression tag	UNP Q58439
B	-6	GLU	-	expression tag	UNP Q58439
B	-5	ASN	-	expression tag	UNP Q58439
B	-4	LEU	-	expression tag	UNP Q58439
B	-3	TYR	-	expression tag	UNP Q58439
B	-2	PHE	-	expression tag	UNP Q58439
B	-1	GLN	-	expression tag	UNP Q58439
B	0	SER	-	expression tag	UNP Q58439
C	-21	MET	-	expression tag	UNP Q58439
C	-20	HIS	-	expression tag	UNP Q58439
C	-19	HIS	-	expression tag	UNP Q58439
C	-18	HIS	-	expression tag	UNP Q58439
C	-17	HIS	-	expression tag	UNP Q58439
C	-16	HIS	-	expression tag	UNP Q58439
C	-15	HIS	-	expression tag	UNP Q58439
C	-14	SER	-	expression tag	UNP Q58439
C	-13	SER	-	expression tag	UNP Q58439
C	-12	GLY	-	expression tag	UNP Q58439
C	-11	VAL	-	expression tag	UNP Q58439
C	-10	ASP	-	expression tag	UNP Q58439
C	-9	LEU	-	expression tag	UNP Q58439
C	-8	GLY	-	expression tag	UNP Q58439
C	-7	THR	-	expression tag	UNP Q58439
C	-6	GLU	-	expression tag	UNP Q58439
C	-5	ASN	-	expression tag	UNP Q58439

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	LEU	-	expression tag	UNP Q58439
C	-3	TYR	-	expression tag	UNP Q58439
C	-2	PHE	-	expression tag	UNP Q58439
C	-1	GLN	-	expression tag	UNP Q58439
C	0	SER	-	expression tag	UNP Q58439
D	-21	MET	-	expression tag	UNP Q58439
D	-20	HIS	-	expression tag	UNP Q58439
D	-19	HIS	-	expression tag	UNP Q58439
D	-18	HIS	-	expression tag	UNP Q58439
D	-17	HIS	-	expression tag	UNP Q58439
D	-16	HIS	-	expression tag	UNP Q58439
D	-15	HIS	-	expression tag	UNP Q58439
D	-14	SER	-	expression tag	UNP Q58439
D	-13	SER	-	expression tag	UNP Q58439
D	-12	GLY	-	expression tag	UNP Q58439
D	-11	VAL	-	expression tag	UNP Q58439
D	-10	ASP	-	expression tag	UNP Q58439
D	-9	LEU	-	expression tag	UNP Q58439
D	-8	GLY	-	expression tag	UNP Q58439
D	-7	THR	-	expression tag	UNP Q58439
D	-6	GLU	-	expression tag	UNP Q58439
D	-5	ASN	-	expression tag	UNP Q58439
D	-4	LEU	-	expression tag	UNP Q58439
D	-3	TYR	-	expression tag	UNP Q58439
D	-2	PHE	-	expression tag	UNP Q58439
D	-1	GLN	-	expression tag	UNP Q58439
D	0	SER	-	expression tag	UNP Q58439
E	-21	MET	-	expression tag	UNP Q58439
E	-20	HIS	-	expression tag	UNP Q58439
E	-19	HIS	-	expression tag	UNP Q58439
E	-18	HIS	-	expression tag	UNP Q58439
E	-17	HIS	-	expression tag	UNP Q58439
E	-16	HIS	-	expression tag	UNP Q58439
E	-15	HIS	-	expression tag	UNP Q58439
E	-14	SER	-	expression tag	UNP Q58439
E	-13	SER	-	expression tag	UNP Q58439
E	-12	GLY	-	expression tag	UNP Q58439
E	-11	VAL	-	expression tag	UNP Q58439
E	-10	ASP	-	expression tag	UNP Q58439
E	-9	LEU	-	expression tag	UNP Q58439
E	-8	GLY	-	expression tag	UNP Q58439
E	-7	THR	-	expression tag	UNP Q58439

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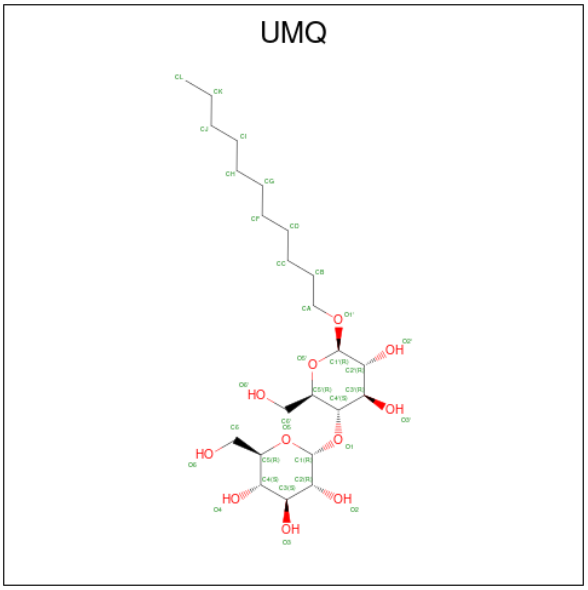
Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	GLU	-	expression tag	UNP Q58439
E	-5	ASN	-	expression tag	UNP Q58439
E	-4	LEU	-	expression tag	UNP Q58439
E	-3	TYR	-	expression tag	UNP Q58439
E	-2	PHE	-	expression tag	UNP Q58439
E	-1	GLN	-	expression tag	UNP Q58439
E	0	SER	-	expression tag	UNP Q58439

- Molecule 2 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	34	23	11	0	0
			Total	C	O		
2	A	1	34	23	11	0	0
			Total	C	O		
2	B	1	30	19	11	0	0
			Total	C			
2	B	1	10	10		0	0
			Total	C	O		
2	C	1	34	23	11	0	0
			Total	C	O		
2	D	1	34	23	11	0	0
			Total	C	O		
2	E	1	34	23	11	0	0
			Total	C	O		
2	E	1	13	12	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	7	7	7	0	0
3	B	3	3	3	0	0
3	C	3	3	3	0	0
3	D	10	10	10	0	0
3	E	9	9	9	0	0

- Molecule 4 is water.

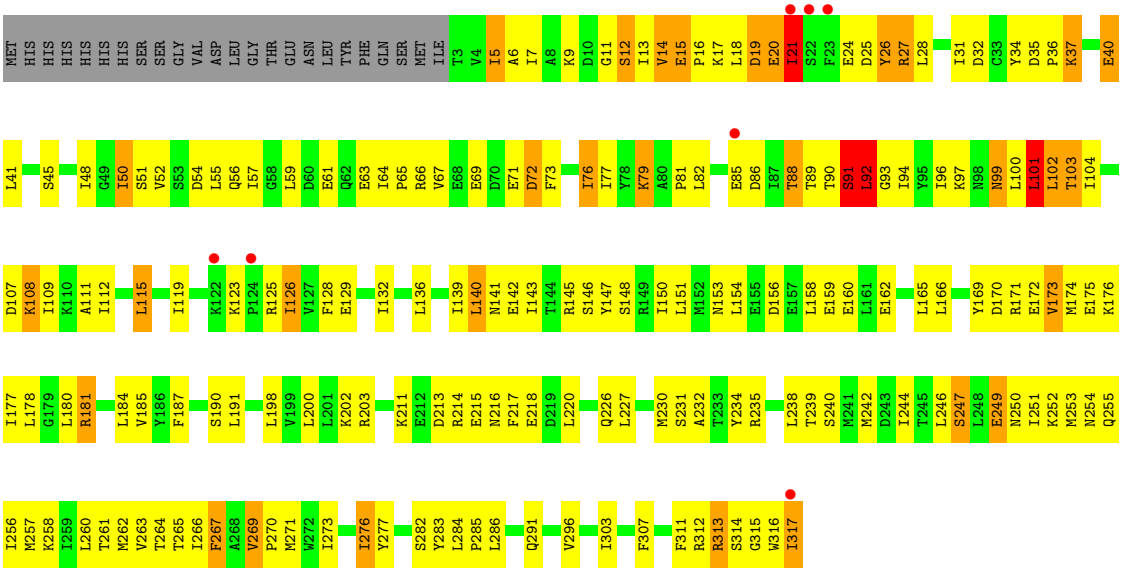
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	40	40	40	0	0
4	B	38	38	38	0	0
4	C	36	36	36	0	0
4	D	23	23	23	0	0
4	E	63	63	63	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

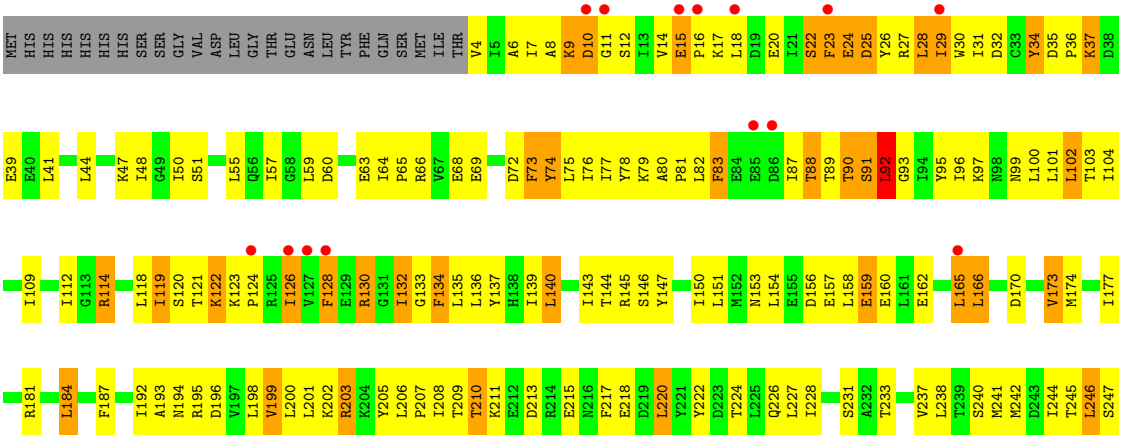
• Molecule 1: Magnesium transport protein CorA

Chain A:



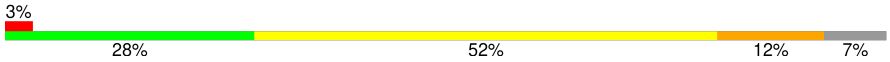
• Molecule 1: Magnesium transport protein CorA

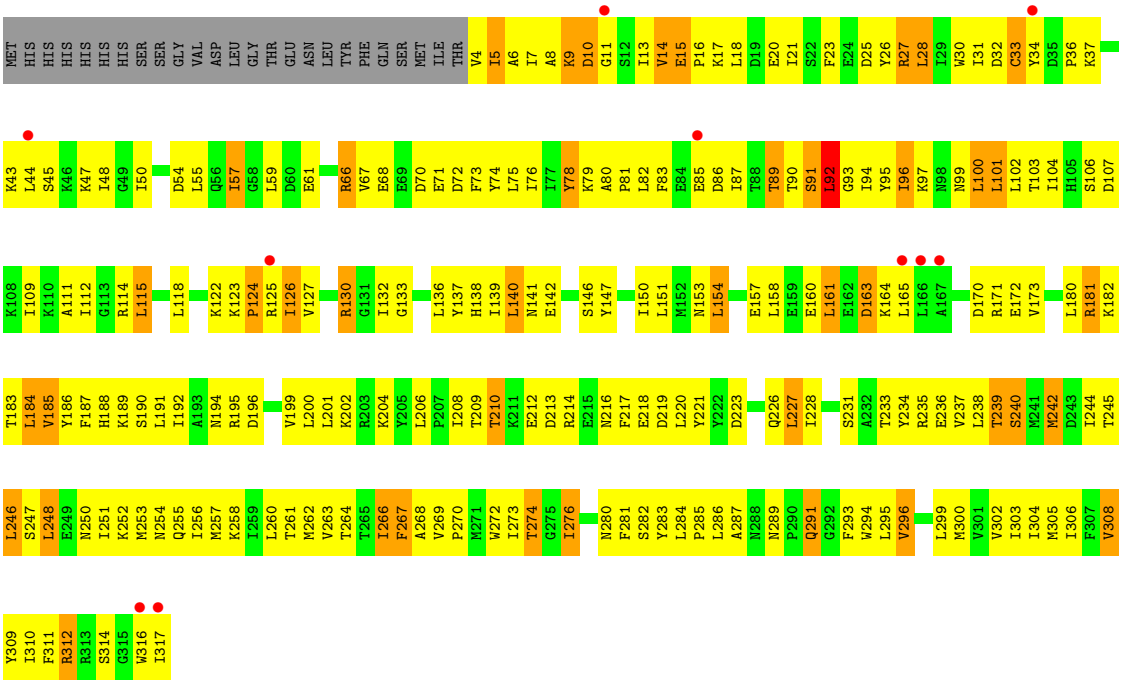
Chain B:



• Molecule 1: Magnesium transport protein CorA

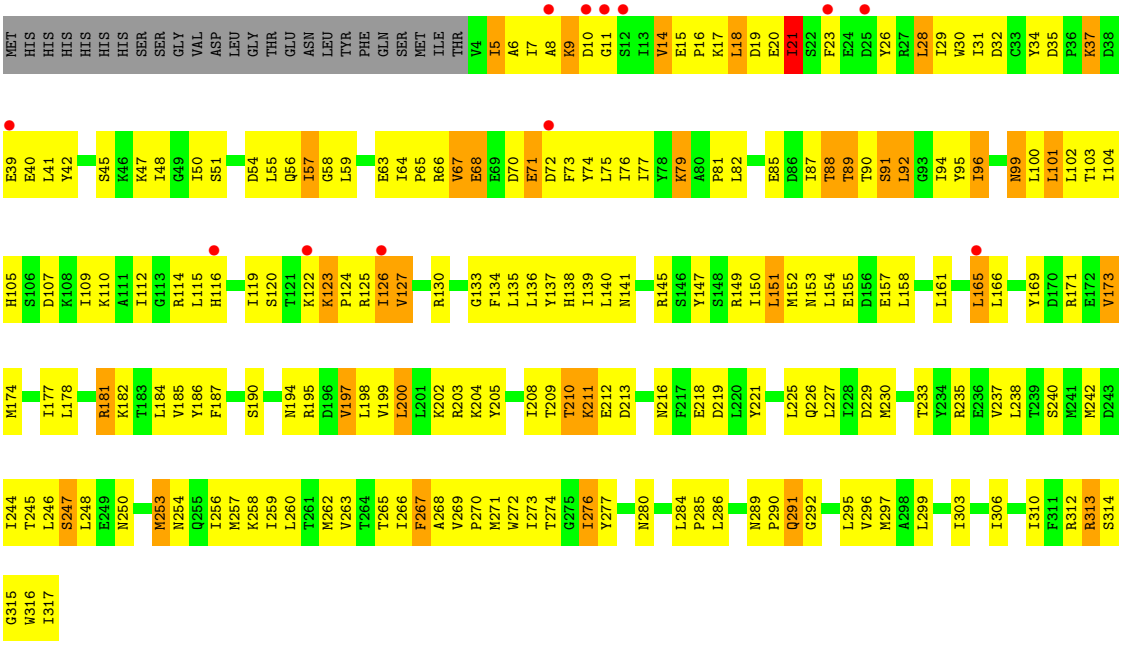
Chain C:





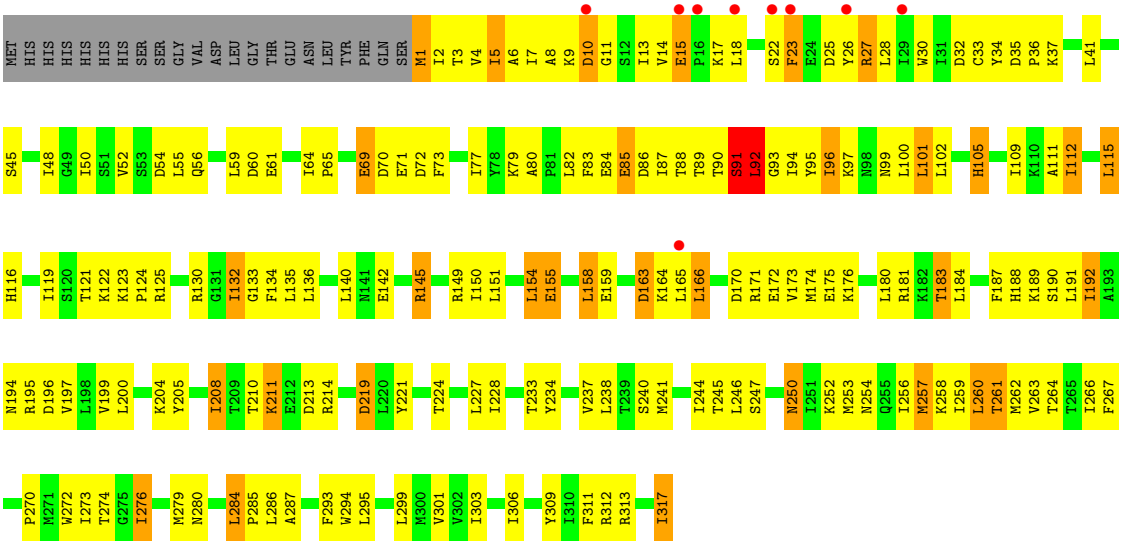
• Molecule 1: Magnesium transport protein CorA

Chain D:



• Molecule 1: Magnesium transport protein CorA

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.11Å 124.83Å 111.88Å 90.00° 90.76° 90.00°	Depositor
Resolution (Å)	49.44 – 3.20 49.44 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.44-3.20) 99.9 (49.44-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.205 , 0.282 0.205 , 0.278	Depositor DCC
R_{free} test set	2344 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	82.1	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 83.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13436	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.50	0/2645	0.75	4/3574 (0.1%)
1	B	0.47	0/2638	0.68	3/3564 (0.1%)
1	C	0.48	0/2638	0.69	3/3564 (0.1%)
1	D	0.43	0/2638	0.62	1/3564 (0.0%)
1	E	0.56	1/2670 (0.0%)	0.79	4/3607 (0.1%)
All	All	0.49	1/13229 (0.0%)	0.71	15/17873 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	1
1	D	0	1
1	E	0	3
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	92	LEU	N-CA	5.93	1.58	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	91	SER	N-CA-C	8.22	133.18	111.00
1	A	91	SER	N-CA-C	8.13	132.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	23	PHE	N-CA-C	7.91	132.35	111.00
1	C	91	SER	N-CA-C	7.82	132.11	111.00
1	B	91	SER	N-CA-C	7.39	130.94	111.00
1	E	92	LEU	N-CA-C	7.30	130.71	111.00
1	C	92	LEU	N-CA-C	6.89	129.62	111.00
1	A	101	LEU	CA-CB-CG	6.66	130.61	115.30
1	D	92	LEU	N-CA-C	6.08	127.41	111.00
1	A	92	LEU	N-CA-C	5.70	126.38	111.00
1	B	10	ASP	N-CA-C	5.62	126.17	111.00
1	C	10	ASP	N-CA-C	5.53	125.94	111.00
1	E	94	ILE	CB-CA-C	-5.48	100.65	111.60
1	B	92	LEU	N-CA-C	5.12	124.81	111.00
1	A	12	SER	N-CA-C	5.07	124.69	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	ILE	Peptide
1	A	91	SER	Peptide
1	B	18	LEU	Peptide
1	B	314	SER	Peptide
1	B	91	SER	Peptide
1	C	91	SER	Peptide
1	D	91	SER	Peptide
1	E	123	LYS	Peptide
1	E	22	SER	Peptide
1	E	91	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2596	0	2681	230	0
1	B	2589	0	2674	231	0
1	C	2589	0	2674	256	1
1	D	2589	0	2674	252	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2618	0	2710	207	0
2	A	68	0	88	20	0
2	B	40	0	52	2	0
2	C	34	0	44	5	0
2	D	34	0	44	3	0
2	E	47	0	67	4	0
3	A	7	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	10	0	0	0	0
3	E	9	0	0	0	0
4	A	40	0	0	2	0
4	B	38	0	0	3	0
4	C	36	0	0	2	0
4	D	23	0	0	2	0
4	E	63	0	0	6	0
All	All	13436	0	13708	1081	1

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 40.

All (1081) 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:E:92:LEU:HA	4:E:519:HOH:O	1.28	1.26
1:C:257:MET:HG3	1:D:257:MET:CE	1.76	1.13
1:C:257:MET:HG3	1:D:257:MET:HE2	1.37	1.07
1:D:9:LYS:HD3	1:D:119:ILE:HG21	1.37	1.06
1:A:253:MET:HG3	1:B:257:MET:HE1	1.40	1.03
1:C:11:GLY:H	1:C:16:PRO:HD2	1.25	1.02
1:E:91:SER:O	4:E:539:HOH:O	1.80	0.99
1:D:73:PHE:HZ	1:D:95:TYR:CD2	1.80	0.98
1:A:52:VAL:HG12	1:A:56:GLN:HE21	1.26	0.98
1:A:125:ARG:HG2	1:A:126:ILE:H	1.25	0.98
1:C:4:VAL:N	1:C:34:TYR:O	1.97	0.98
1:B:202:LYS:HE3	1:B:218:GLU:HG3	1.43	0.97
1:A:5:ILE:HG22	1:A:7:ILE:HG13	1.48	0.96
1:C:11:GLY:HA2	1:C:26:TYR:CD1	2.01	0.95
1:D:73:PHE:CZ	1:D:95:TYR:HD2	1.83	0.95
1:D:109:ILE:HG21	1:D:112:ILE:HG13	1.45	0.95
1:B:11:GLY:H	1:B:16:PRO:HD2	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HD11	1:A:238:LEU:HD21	1.49	0.93
1:D:18:LEU:HD13	1:D:19:ASP:H	1.34	0.92
1:E:79:LYS:HD2	1:E:90:THR:HB	1.53	0.91
1:B:69:GLU:HG2	1:B:74:TYR:HE1	1.34	0.90
1:C:208:ILE:HG13	1:C:209:THR:HG23	1.53	0.90
1:E:14:VAL:HG22	1:E:15:GLU:H	1.35	0.90
1:A:48:ILE:HG13	1:A:50:ILE:HG13	1.54	0.89
1:A:250:ASN:HB3	1:E:250:ASN:HD21	1.37	0.89
1:D:150:ILE:HA	1:D:153:ASN:HD22	1.35	0.89
1:D:79:LYS:HD3	1:D:90:THR:HB	1.53	0.89
1:D:58:GLY:N	1:D:95:TYR:OH	2.05	0.88
1:D:81:PRO:HB2	1:D:150:ILE:HD11	1.55	0.88
1:A:52:VAL:HG12	1:A:56:GLN:NE2	1.88	0.88
1:B:253:MET:HB2	1:C:254:ASN:OD1	1.73	0.87
1:C:257:MET:HG3	1:D:257:MET:HE1	1.54	0.87
1:E:17:LYS:O	1:E:18:LEU:HD23	1.75	0.86
1:B:262:MET:HG2	1:B:311:PHE:CD2	2.11	0.86
1:D:90:THR:O	1:D:91:SER:OG	1.93	0.86
1:B:69:GLU:HG2	1:B:74:TYR:CE1	2.11	0.86
1:B:28:LEU:HA	1:B:99:ASN:HB2	1.59	0.85
1:A:15:GLU:HB3	1:A:123:LYS:O	1.77	0.85
1:A:96:ILE:HG22	1:A:101:LEU:HA	1.59	0.84
1:D:79:LYS:HD3	1:D:90:THR:CB	2.06	0.84
1:D:73:PHE:HZ	1:D:95:TYR:HD2	0.93	0.84
1:D:109:ILE:HG22	1:D:112:ILE:H	1.43	0.84
1:C:187:PHE:O	1:C:191:LEU:HB2	1.78	0.83
1:D:246:LEU:HD12	1:E:247:SER:HB3	1.61	0.83
1:A:263:VAL:HG21	1:B:265:THR:OG1	1.78	0.83
1:B:10:ASP:HA	1:B:15:GLU:HA	1.60	0.83
1:E:80:ALA:O	1:E:90:THR:HA	1.78	0.82
1:E:89:THR:CG2	1:E:90:THR:H	1.92	0.82
1:B:270:PRO:O	1:B:274:THR:HG23	1.79	0.82
1:E:158:LEU:HD11	1:E:238:LEU:HD21	1.61	0.82
1:D:89:THR:HG22	1:D:90:THR:H	1.45	0.82
2:B:401:UMQ:H5'1	2:B:401:UMQ:O5	1.80	0.82
1:E:9:LYS:HB2	1:E:30:TRP:H	1.44	0.81
1:B:11:GLY:H	1:B:16:PRO:CD	1.94	0.81
1:C:158:LEU:HD21	1:C:238:LEU:CD2	2.10	0.81
1:C:8:ALA:O	1:C:9:LYS:HE3	1.81	0.81
1:E:11:GLY:HA2	1:E:27:ARG:H	1.44	0.80
1:A:5:ILE:HG12	1:A:40:GLU:HG3	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ILE:O	1:C:310:ILE:HG12	1.81	0.80
1:E:82:LEU:HB3	1:E:89:THR:HB	1.64	0.80
1:D:110:LYS:O	1:D:114:ARG:HG3	1.82	0.80
1:A:81:PRO:HD3	1:A:147:TYR:CE1	2.17	0.79
1:E:27:ARG:HG3	1:E:27:ARG:HH11	1.47	0.79
1:C:70:ASP:OD1	1:C:71:GLU:N	2.15	0.79
1:B:192:ILE:HD13	1:B:228:ILE:HD13	1.63	0.79
1:B:205:TYR:OH	4:B:517:HOH:O	2.01	0.79
1:D:11:GLY:H	1:D:16:PRO:HG2	1.48	0.79
1:E:233:THR:O	1:E:237:VAL:HG23	1.83	0.78
1:E:10:ASP:OD1	1:E:11:GLY:N	2.16	0.78
1:C:192:ILE:HG13	1:C:195:ARG:NH1	1.99	0.78
1:B:74:TYR:HB2	1:B:96:ILE:HG23	1.64	0.78
1:B:31:ILE:HD12	1:B:100:LEU:HD21	1.65	0.78
1:E:79:LYS:CD	1:E:90:THR:HB	2.13	0.77
1:C:20:GLU:HG2	1:C:47:LYS:NZ	1.99	0.77
1:D:37:LYS:HG2	1:D:40:GLU:HG2	1.66	0.77
1:B:177:ILE:HG23	1:B:238:LEU:HD22	1.66	0.77
1:C:76:ILE:HD12	1:C:136:LEU:HD21	1.66	0.77
1:A:5:ILE:HG12	1:A:36:PRO:HA	1.67	0.77
1:A:88:THR:HG22	1:A:187:PHE:HZ	1.50	0.77
1:E:89:THR:HG22	1:E:90:THR:N	1.99	0.77
1:C:20:GLU:HB3	1:C:21:ILE:HG13	1.67	0.77
1:C:125:ARG:HB2	1:C:126:ILE:HA	1.65	0.77
1:C:123:LYS:N	1:C:124:PRO:HD2	2.00	0.76
1:A:108:LYS:H	1:A:108:LYS:HD2	1.51	0.76
1:D:26:TYR:HD2	1:D:29:ILE:HG12	1.50	0.76
1:A:181:ARG:HH12	1:B:244:ILE:HD11	1.51	0.76
1:B:208:ILE:HG13	1:B:209:THR:HG23	1.68	0.75
1:C:163:ASP:OD1	1:C:164:LYS:N	2.19	0.75
1:A:79:LYS:HB3	1:A:90:THR:HB	1.67	0.75
1:E:199:VAL:HG22	1:E:221:TYR:CE2	2.21	0.75
1:B:24:GLU:CG	1:B:25:ASP:H	1.99	0.75
1:D:7:ILE:HG22	1:D:9:LYS:HZ1	1.52	0.75
1:C:44:LEU:HD23	1:C:55:LEU:HD13	1.68	0.75
1:A:250:ASN:HB3	1:E:250:ASN:ND2	2.02	0.75
1:D:10:ASP:HA	1:D:16:PRO:HD2	1.69	0.75
1:A:24:GLU:HA	1:A:25:ASP:O	1.87	0.74
1:D:8:ALA:O	1:D:9:LYS:NZ	2.20	0.74
1:A:24:GLU:HA	1:A:25:ASP:C	2.06	0.74
1:B:137:TYR:CE1	1:B:220:LEU:HD13	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:H	1:A:6:ALA:HA	1.52	0.74
1:D:262:MET:O	1:D:266:ILE:HG12	1.88	0.74
1:D:260:LEU:HD22	1:E:260:LEU:HD21	1.70	0.74
1:B:256:ILE:HD11	1:C:258:LYS:HG2	1.69	0.74
1:A:125:ARG:HG2	1:A:126:ILE:N	2.03	0.73
1:A:141:ASN:HA	1:A:220:LEU:HD11	1.68	0.73
1:C:284:LEU:HB3	1:C:287:ALA:HB2	1.70	0.73
1:E:199:VAL:HG22	1:E:221:TYR:CD2	2.23	0.73
1:E:14:VAL:HG22	1:E:15:GLU:N	2.03	0.73
1:B:12:SER:HA	1:B:27:ARG:HG2	1.70	0.73
1:A:198:LEU:CD2	1:A:220:LEU:HD23	2.19	0.73
1:A:154:LEU:CD1	1:A:184:LEU:HD13	2.19	0.73
1:C:147:TYR:HB3	1:C:227:LEU:HD12	1.70	0.72
1:C:246:LEU:HD12	1:D:247:SER:HB3	1.71	0.72
1:B:9:LYS:O	1:B:29:ILE:HG22	1.89	0.72
1:C:257:MET:CG	1:D:257:MET:HE1	2.19	0.72
1:E:89:THR:HG22	1:E:90:THR:H	1.50	0.72
1:E:10:ASP:HB2	1:E:15:GLU:HB3	1.71	0.72
1:D:125:ARG:HG3	1:D:126:ILE:H	1.55	0.71
1:A:200:LEU:HA	1:A:203:ARG:HH21	1.54	0.71
1:B:249:GLU:HG2	1:C:251:ILE:HD13	1.73	0.71
1:C:158:LEU:HD21	1:C:238:LEU:HD21	1.71	0.71
1:E:89:THR:CG2	1:E:90:THR:N	2.53	0.71
1:A:67:VAL:HG22	1:A:76:ILE:HG23	1.72	0.71
1:E:170:ASP:HB3	1:E:173:VAL:HG12	1.73	0.71
1:A:12:SER:OG	1:A:13:ILE:N	2.24	0.71
1:E:92:LEU:HD12	1:E:93:GLY:N	2.05	0.71
1:B:198:LEU:O	1:B:202:LYS:HG2	1.90	0.71
1:A:181:ARG:HH22	1:B:244:ILE:HD11	1.56	0.71
1:B:256:ILE:HG21	1:C:257:MET:HB3	1.72	0.71
1:C:6:ALA:HA	1:C:32:ASP:O	1.90	0.71
1:D:18:LEU:CD1	1:D:19:ASP:H	2.03	0.70
1:D:65:PRO:HA	1:D:77:ILE:HB	1.73	0.70
1:D:260:LEU:HB2	1:E:261:THR:OG1	1.91	0.70
1:E:30:TRP:HB2	1:E:135:LEU:HD21	1.72	0.70
1:A:226:GLN:HG2	1:E:192:ILE:HG23	1.73	0.70
1:B:206:LEU:HB3	1:B:207:PRO:HD2	1.72	0.70
1:C:73:PHE:CB	1:C:97:LYS:HB3	2.22	0.70
1:A:154:LEU:O	1:A:154:LEU:HD23	1.92	0.70
1:D:119:ILE:O	1:D:124:PRO:HG3	1.90	0.70
1:D:154:LEU:HD11	1:D:184:LEU:HD22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:GLU:OE1	1:D:66:ARG:NH2	2.17	0.69
2:E:401:UMQ:HC1	2:E:401:UMQ:O2'	1.92	0.69
1:C:125:ARG:CB	1:C:126:ILE:HA	2.22	0.69
1:C:273:ILE:HD12	2:C:401:UMQ:HL1	1.73	0.69
1:C:96:ILE:HA	1:C:100:LEU:O	1.93	0.69
1:B:24:GLU:HA	1:B:26:TYR:CE2	2.28	0.69
1:C:73:PHE:HB3	1:C:97:LYS:HB3	1.73	0.69
1:A:5:ILE:N	1:A:6:ALA:HA	2.08	0.69
1:A:313:ARG:HA	1:A:314:SER:C	2.12	0.69
1:C:96:ILE:HG21	1:C:101:LEU:HD22	1.73	0.69
1:D:272:TRP:O	1:D:276:ILE:HG23	1.93	0.68
1:A:255:GLN:HA	1:A:258:LYS:HD3	1.75	0.68
1:A:262:MET:CE	1:A:317:ILE:HB	2.23	0.68
1:D:210:THR:HG23	1:D:213:ASP:H	1.57	0.68
1:A:269:VAL:HG23	4:A:522:HOH:O	1.93	0.68
1:D:90:THR:HG21	1:D:190:SER:OG	1.93	0.68
1:E:7:ILE:HG22	1:E:8:ALA:H	1.59	0.68
1:B:122:LYS:HA	1:B:123:LYS:HD2	1.75	0.68
1:D:123:LYS:HB3	1:D:125:ARG:HB3	1.76	0.68
1:A:79:LYS:HD3	1:A:90:THR:HB	1.76	0.68
1:E:130:ARG:NH1	1:E:130:ARG:HB3	2.09	0.68
1:A:79:LYS:HD3	1:A:90:THR:CB	2.24	0.68
1:C:109:ILE:HB	1:C:112:ILE:HD12	1.76	0.68
2:D:401:UMQ:HO21	2:D:401:UMQ:HO6'	1.36	0.68
1:D:14:VAL:O	1:D:16:PRO:HD3	1.94	0.68
1:A:20:GLU:O	1:A:21:ILE:HG23	1.93	0.68
1:A:242:MET:HE1	1:B:244:ILE:HG12	1.75	0.68
1:B:242:MET:SD	1:C:244:ILE:HD11	2.34	0.68
1:D:123:LYS:HE3	1:D:123:LYS:HA	1.76	0.67
1:A:156:ASP:O	1:A:159:GLU:HB3	1.95	0.67
1:C:210:THR:HG23	1:C:213:ASP:OD2	1.93	0.67
1:B:11:GLY:N	1:B:16:PRO:HD2	2.08	0.67
1:B:28:LEU:HD13	1:B:132:ILE:HG13	1.75	0.67
1:E:130:ARG:HB3	1:E:130:ARG:HH11	1.59	0.67
1:E:263:VAL:HG12	1:E:264:THR:N	2.10	0.67
1:D:96:ILE:HG22	1:D:101:LEU:HD13	1.77	0.67
1:A:176:LYS:NZ	2:A:401:UMQ:O3'	2.26	0.67
1:B:6:ALA:HA	1:B:32:ASP:O	1.95	0.67
1:A:99:ASN:OD1	1:A:99:ASN:N	2.26	0.67
1:B:256:ILE:CD1	1:C:258:LYS:HG2	2.25	0.67
1:C:170:ASP:OD1	1:C:172:GLU:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ILE:HA	1:D:153:ASN:ND2	2.09	0.67
1:D:297:MET:CE	1:E:276:ILE:HD12	2.24	0.67
1:D:73:PHE:CE1	1:D:95:TYR:HB3	2.29	0.66
1:B:137:TYR:HE1	1:B:220:LEU:HD13	1.60	0.66
1:C:165:LEU:HD21	1:C:244:ILE:HB	1.77	0.66
1:D:54:ASP:O	1:D:57:ILE:HB	1.95	0.66
1:D:137:TYR:CD2	1:D:216:ASN:HB3	2.29	0.66
1:D:70:ASP:OD1	1:D:71:GLU:N	2.29	0.66
1:D:105:HIS:ND1	1:D:109:ILE:HG12	2.10	0.66
1:C:76:ILE:HD13	1:C:201:LEU:HD11	1.77	0.66
1:D:81:PRO:CB	1:D:150:ILE:HD11	2.25	0.66
1:E:317:ILE:OXT	1:E:317:ILE:HG13	1.94	0.66
1:A:171:ARG:NH1	1:A:175:GLU:OE1	2.28	0.66
1:B:130:ARG:HB2	1:B:134:PHE:CD2	2.30	0.66
1:D:20:GLU:HB3	1:D:47:LYS:HE3	1.78	0.66
1:D:269:VAL:HG11	1:D:303:ILE:HD12	1.76	0.66
1:A:125:ARG:O	1:A:126:ILE:HG22	1.96	0.66
1:B:24:GLU:CD	1:B:25:ASP:H	2.00	0.65
1:A:27:ARG:HH11	1:A:27:ARG:HB3	1.60	0.65
1:B:44:LEU:O	1:B:48:ILE:HG12	1.95	0.65
1:B:316:TRP:O	1:B:317:ILE:HG13	1.95	0.65
1:D:23:PHE:O	1:D:23:PHE:CD1	2.49	0.65
1:E:211:LYS:HB2	4:E:533:HOH:O	1.96	0.65
1:D:48:ILE:HD12	1:D:50:ILE:HD12	1.79	0.65
1:A:198:LEU:HD21	1:A:220:LEU:HD23	1.79	0.65
1:D:233:THR:O	1:D:237:VAL:HG23	1.96	0.65
1:D:247:SER:OG	4:D:520:HOH:O	2.15	0.65
1:B:92:LEU:HG	1:B:93:GLY:N	2.11	0.65
1:D:253:MET:HG2	1:E:257:MET:HE2	1.78	0.65
1:D:313:ARG:HA	1:D:314:SER:C	2.15	0.65
1:B:95:TYR:HB2	1:B:102:LEU:HD12	1.77	0.65
1:D:134:PHE:HE1	1:D:138:HIS:NE2	1.95	0.65
1:E:172:GLU:O	1:E:175:GLU:HB2	1.96	0.65
1:B:81:PRO:HD3	1:B:147:TYR:CE2	2.31	0.65
1:A:111:ALA:HB1	1:A:142:GLU:HB3	1.78	0.65
1:A:258:LYS:O	1:A:262:MET:HG3	1.97	0.65
1:B:130:ARG:HH11	1:B:130:ARG:HB3	1.62	0.65
1:C:285:PRO:O	1:C:286:LEU:HB2	1.97	0.64
1:D:126:ILE:O	1:D:127:VAL:HG13	1.97	0.64
1:B:6:ALA:O	1:B:7:ILE:HG12	1.98	0.64
1:B:11:GLY:HA2	1:B:26:TYR:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ILE:CG2	1:D:112:ILE:HG13	2.25	0.64
1:A:253:MET:HB2	1:B:254:ASN:OD1	1.96	0.64
1:C:59:LEU:O	1:C:106:SER:OG	2.14	0.64
1:C:165:LEU:O	1:C:245:THR:HG22	1.97	0.64
1:C:67:VAL:HB	1:C:200:LEU:HD13	1.79	0.64
1:B:92:LEU:C	1:B:92:LEU:HD23	2.17	0.64
1:A:109:ILE:HB	1:A:112:ILE:HG13	1.79	0.64
1:C:196:ASP:HB2	1:D:226:GLN:NE2	2.13	0.64
1:C:14:VAL:HG22	1:C:15:GLU:N	2.13	0.64
1:D:79:LYS:HD3	1:D:90:THR:CG2	2.27	0.64
1:C:115:LEU:HD13	1:C:142:GLU:HG3	1.79	0.63
1:A:12:SER:HB2	1:A:26:TYR:HA	1.79	0.63
1:C:20:GLU:HG2	1:C:47:LYS:HZ2	1.62	0.63
1:C:118:LEU:HD12	1:C:118:LEU:O	1.98	0.63
1:E:27:ARG:HG3	1:E:27:ARG:NH1	2.13	0.63
1:C:268:ALA:H	1:C:270:PRO:HD2	1.64	0.63
1:D:82:LEU:O	1:D:88:THR:HB	1.97	0.63
1:E:240:SER:OG	1:E:244:ILE:HD11	1.98	0.63
1:C:192:ILE:HG13	1:C:195:ARG:HH12	1.64	0.63
1:B:130:ARG:HB3	1:B:130:ARG:NH1	2.14	0.63
1:A:154:LEU:HB2	2:A:401:UMQ:HB1	1.81	0.63
1:B:128:PHE:CE1	1:B:134:PHE:HD2	2.16	0.63
1:E:28:LEU:HA	1:E:99:ASN:HB2	1.81	0.63
1:C:314:SER:O	1:C:316:TRP:HB2	1.99	0.63
1:E:96:ILE:CG2	1:E:101:LEU:HD13	2.29	0.63
1:B:17:LYS:NZ	1:B:123:LYS:HE2	2.14	0.62
1:C:76:ILE:O	1:C:94:ILE:HB	1.99	0.62
1:B:83:PHE:CD1	1:B:83:PHE:N	2.67	0.62
1:B:293:PHE:O	1:B:297:MET:HB2	1.99	0.62
1:E:132:ILE:HG22	1:E:133:GLY:N	2.14	0.62
1:E:294:TRP:HH2	2:E:401:UMQ:HH1	1.64	0.62
1:A:191:LEU:HD11	2:A:401:UMQ:HL1	1.82	0.62
1:C:79:LYS:HD2	1:C:90:THR:HB	1.80	0.62
1:A:264:THR:HG22	1:E:263:VAL:HG11	1.82	0.62
1:C:253:MET:HB2	1:D:254:ASN:OD1	1.99	0.62
1:A:230:MET:CE	1:E:188:HIS:HD2	2.13	0.62
1:B:157:GLU:O	1:B:160:GLU:HG2	2.00	0.62
1:D:276:ILE:HD11	1:D:277:TYR:CE1	2.35	0.62
1:D:39:GLU:O	1:D:42:TYR:HB3	1.99	0.61
1:C:137:TYR:CD1	1:C:216:ASN:HB3	2.35	0.61
1:D:285:PRO:O	1:D:286:LEU:HB2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:GLN:O	1:D:295:LEU:HG	2.01	0.61
1:C:14:VAL:HG22	1:C:15:GLU:H	1.66	0.61
1:D:210:THR:OG1	1:D:211:LYS:N	2.33	0.61
1:E:82:LEU:O	1:E:88:THR:HA	2.00	0.61
1:A:37:LYS:O	1:A:40:GLU:HG2	2.01	0.61
1:B:8:ALA:HA	1:B:30:TRP:O	2.01	0.61
1:C:262:MET:HG3	1:C:316:TRP:HE1	1.65	0.61
1:E:122:LYS:O	1:E:125:ARG:HA	2.00	0.61
1:A:251:ILE:O	1:A:254:ASN:HB2	2.00	0.61
1:B:253:MET:HG3	1:C:257:MET:HE3	1.83	0.61
1:A:5:ILE:CG1	1:A:36:PRO:HA	2.29	0.61
1:A:203:ARG:NH1	1:B:222:TYR:HD2	1.99	0.61
1:D:11:GLY:O	1:D:26:TYR:HA	2.01	0.61
1:D:199:VAL:HA	1:D:202:LYS:HG2	1.82	0.61
1:A:41:LEU:HG	1:A:52:VAL:HG13	1.83	0.61
1:D:37:LYS:HE3	1:D:40:GLU:HG3	1.83	0.61
1:D:130:ARG:HH12	1:D:210:THR:HG21	1.65	0.61
1:C:4:VAL:O	1:C:5:ILE:HG23	2.01	0.60
1:C:81:PRO:HD3	1:C:147:TYR:CZ	2.36	0.60
1:C:96:ILE:HB	1:C:132:ILE:CD1	2.31	0.60
1:D:126:ILE:HG23	1:D:127:VAL:H	1.66	0.60
1:E:210:THR:H	1:E:213:ASP:HB2	1.66	0.60
1:C:76:ILE:CD1	1:C:136:LEU:HD21	2.31	0.60
1:C:257:MET:CG	1:D:257:MET:CE	2.65	0.60
1:D:70:ASP:HB3	1:D:73:PHE:HB3	1.83	0.60
1:E:105:HIS:CD2	1:E:105:HIS:N	2.69	0.60
1:C:78:TYR:CE2	1:C:140:LEU:HG	2.37	0.60
1:D:152:MET:O	1:D:155:GLU:HB2	2.01	0.60
1:B:69:GLU:HA	1:B:74:TYR:CE1	2.37	0.60
1:B:72:ASP:O	1:B:73:PHE:HB3	2.02	0.60
1:D:208:ILE:HG13	1:D:209:THR:HG23	1.83	0.60
1:E:96:ILE:HD11	1:E:208:ILE:HD12	1.84	0.60
1:E:96:ILE:HG22	1:E:101:LEU:HD13	1.84	0.60
1:C:92:LEU:HG	1:C:93:GLY:N	2.16	0.60
1:E:262:MET:SD	1:E:317:ILE:HG22	2.42	0.60
1:A:97:LYS:O	1:A:97:LYS:HG3	2.00	0.60
1:D:253:MET:HG2	1:E:257:MET:CE	2.32	0.60
1:A:88:THR:HG22	1:A:187:PHE:CZ	2.36	0.59
1:A:90:THR:O	1:A:91:SER:OG	2.18	0.59
1:C:92:LEU:O	1:C:92:LEU:HD23	2.03	0.59
1:C:115:LEU:HD23	1:C:139:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LEU:HD23	1:D:245:THR:HG22	1.84	0.59
1:B:59:LEU:HD21	1:B:104:ILE:HG12	1.84	0.59
1:C:157:GLU:O	1:C:160:GLU:HG2	2.03	0.59
1:A:260:LEU:CD2	1:B:260:LEU:HD23	2.33	0.59
1:B:198:LEU:HD22	1:B:220:LEU:HB3	1.85	0.59
1:C:263:VAL:HG12	1:C:264:THR:N	2.17	0.59
1:B:134:PHE:O	1:B:137:TYR:HB3	2.02	0.59
1:A:96:ILE:HA	1:A:100:LEU:O	2.02	0.59
1:A:211:LYS:CG	1:A:214:ARG:HH22	2.16	0.59
1:A:247:SER:HB3	1:E:246:LEU:HD13	1.85	0.59
1:B:17:LYS:HZ3	1:B:123:LYS:HE2	1.67	0.59
1:E:5:ILE:HG23	1:E:6:ALA:H	1.68	0.59
1:B:68:GLU:HB2	1:B:75:LEU:HB3	1.83	0.59
1:C:16:PRO:HG2	1:C:18:LEU:HD21	1.84	0.59
1:D:126:ILE:HG23	1:D:127:VAL:N	2.18	0.59
1:E:10:ASP:HB2	1:E:15:GLU:CB	2.32	0.59
1:A:267:PHE:N	1:A:267:PHE:CD1	2.70	0.59
1:B:154:LEU:O	1:B:158:LEU:HB2	2.03	0.59
1:C:253:MET:HG2	1:C:257:MET:HE2	1.85	0.59
1:D:7:ILE:HD12	1:D:116:HIS:CD2	2.38	0.59
1:A:203:ARG:NH1	1:B:222:TYR:CD2	2.71	0.58
1:B:92:LEU:CG	1:B:93:GLY:N	2.65	0.58
1:C:54:ASP:O	1:C:57:ILE:HG13	2.03	0.58
1:D:11:GLY:H	1:D:16:PRO:CG	2.15	0.58
1:A:198:LEU:HD22	1:A:220:LEU:HD23	1.84	0.58
1:C:210:THR:O	1:C:213:ASP:HB2	2.03	0.58
1:B:80:ALA:O	1:B:90:THR:HA	2.04	0.58
1:E:276:ILE:O	1:E:279:MET:HE2	2.02	0.58
1:A:181:ARG:NH1	1:B:244:ILE:HD11	2.18	0.58
1:D:269:VAL:O	1:D:273:ILE:HG12	2.03	0.58
1:D:267:PHE:CD1	1:D:267:PHE:N	2.71	0.58
1:A:154:LEU:HA	2:A:401:UMQ:HA1	1.86	0.58
1:A:202:LYS:O	1:A:214:ARG:HG2	2.03	0.58
1:B:245:THR:OG1	1:B:246:LEU:N	2.34	0.58
1:E:11:GLY:HA3	1:E:26:TYR:HD1	1.68	0.58
1:E:165:LEU:HD12	1:E:241:MET:HB3	1.86	0.58
1:C:5:ILE:HG13	1:C:34:TYR:HB3	1.85	0.58
1:E:69:GLU:O	1:E:73:PHE:O	2.22	0.58
1:C:82:LEU:HD22	1:C:107:ASP:HB3	1.85	0.58
1:C:223:ASP:O	1:C:227:LEU:HD23	2.04	0.58
1:D:199:VAL:O	1:D:203:ARG:CB	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:GLU:OE1	1:E:145:ARG:NH1	2.36	0.58
1:B:262:MET:HG2	1:B:311:PHE:CE2	2.39	0.57
1:D:5:ILE:HG22	1:D:6:ALA:H	1.69	0.57
1:D:5:ILE:HG22	1:D:6:ALA:N	2.18	0.57
1:E:32:ASP:OD2	1:E:112:ILE:HG21	2.04	0.57
1:A:72:ASP:O	1:A:73:PHE:HB3	2.03	0.57
1:C:92:LEU:HD13	1:C:112:ILE:HD11	1.85	0.57
1:E:1:MET:O	1:E:1:MET:HG2	2.03	0.57
1:B:83:PHE:HD1	1:B:83:PHE:H	1.52	0.57
1:B:196:ASP:HB2	1:C:226:GLN:NE2	2.19	0.57
1:A:17:LYS:HG2	1:A:18:LEU:H	1.69	0.57
1:A:14:VAL:HG12	1:A:15:GLU:H	1.69	0.57
1:C:289:ASN:HD22	2:C:401:UMQ:H51	1.70	0.57
1:D:92:LEU:HD23	1:D:92:LEU:O	2.04	0.57
1:E:124:PRO:O	1:E:125:ARG:HB2	2.05	0.57
1:A:181:ARG:HH12	1:B:244:ILE:CD1	2.15	0.57
1:A:254:ASN:OD1	1:E:253:MET:HG2	2.05	0.57
1:B:75:LEU:HD12	1:B:76:ILE:N	2.19	0.57
1:D:246:LEU:CD1	1:E:247:SER:HB3	2.30	0.57
1:A:65:PRO:HA	1:A:77:ILE:HG22	1.85	0.57
1:C:158:LEU:HD21	1:C:238:LEU:HD22	1.84	0.57
1:D:37:LYS:HG2	1:D:40:GLU:CG	2.35	0.57
1:B:260:LEU:HD13	1:C:261:THR:HA	1.87	0.57
1:E:5:ILE:HG23	1:E:6:ALA:N	2.20	0.57
1:A:145:ARG:O	1:A:148:SER:HB2	2.04	0.56
1:B:24:GLU:HA	1:B:26:TYR:CZ	2.40	0.56
1:B:128:PHE:CE1	1:B:134:PHE:CD2	2.93	0.56
1:D:15:GLU:OE1	1:D:124:PRO:HD2	2.05	0.56
1:D:297:MET:HE3	1:E:276:ILE:HD12	1.87	0.56
1:E:88:THR:HB	1:E:183:THR:OG1	2.05	0.56
1:B:205:TYR:CD1	1:B:205:TYR:C	2.78	0.56
1:E:200:LEU:HD11	1:E:204:LYS:HD3	1.87	0.56
1:A:5:ILE:HD11	1:A:37:LYS:HD3	1.88	0.56
1:A:54:ASP:O	1:A:57:ILE:HG13	2.05	0.56
1:A:65:PRO:HA	1:A:77:ILE:O	2.05	0.56
1:D:67:VAL:HB	1:D:200:LEU:HD13	1.87	0.56
1:E:79:LYS:HD2	1:E:90:THR:CB	2.32	0.56
1:D:9:LYS:NZ	1:D:9:LYS:HB2	2.21	0.56
1:E:10:ASP:OD1	1:E:10:ASP:C	2.43	0.56
1:D:32:ASP:HA	1:D:103:THR:O	2.06	0.56
1:D:124:PRO:CB	1:D:125:ARG:HA	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LEU:CD2	1:E:260:LEU:HD21	2.35	0.56
1:A:230:MET:HE1	1:E:188:HIS:HD2	1.69	0.56
1:C:195:ARG:O	1:C:199:VAL:HG23	2.06	0.56
1:D:184:LEU:HG	1:D:235:ARG:HG2	1.87	0.56
1:D:199:VAL:O	1:D:203:ARG:HB3	2.06	0.56
1:E:4:VAL:HG23	4:E:527:HOH:O	2.05	0.56
1:D:296:VAL:O	1:D:299:LEU:HB3	2.06	0.56
1:B:202:LYS:HE2	4:B:533:HOH:O	2.06	0.56
1:B:210:THR:HG23	1:B:213:ASP:CG	2.27	0.56
1:C:180:LEU:HD12	1:C:238:LEU:HD11	1.87	0.56
1:D:31:ILE:O	1:D:102:LEU:HD22	2.06	0.56
1:E:105:HIS:ND1	1:E:109:ILE:HG12	2.21	0.56
1:E:309:TYR:OH	1:E:313:ARG:NH1	2.39	0.56
1:A:230:MET:HG3	1:E:189:LYS:HG3	1.89	0.55
1:B:96:ILE:HD11	1:B:132:ILE:HG21	1.86	0.55
1:C:96:ILE:HB	1:C:132:ILE:HD11	1.88	0.55
1:A:56:GLN:HA	1:A:59:LEU:HD12	1.88	0.55
1:B:65:PRO:HG3	1:B:79:LYS:HG3	1.88	0.55
1:A:126:ILE:HG23	1:A:126:ILE:O	2.07	0.55
1:A:200:LEU:CA	1:A:203:ARG:HH21	2.20	0.55
1:B:165:LEU:HG	1:B:245:THR:HG22	1.88	0.55
1:B:196:ASP:HB2	1:C:226:GLN:HE21	1.72	0.55
1:C:95:TYR:HE1	1:C:104:ILE:HG21	1.71	0.55
1:C:188:HIS:O	1:C:192:ILE:HG22	2.06	0.55
1:D:124:PRO:N	1:D:125:ARG:HA	2.21	0.55
1:D:181:ARG:O	1:D:185:VAL:HG23	2.06	0.55
1:D:64:ILE:HD12	1:D:65:PRO:O	2.06	0.55
1:A:154:LEU:CD2	1:A:158:LEU:HD13	2.36	0.55
1:B:246:LEU:HD12	1:C:247:SER:OG	2.07	0.55
1:E:210:THR:O	1:E:213:ASP:N	2.39	0.55
1:A:262:MET:HE1	1:A:317:ILE:HB	1.88	0.55
1:E:14:VAL:CG2	1:E:15:GLU:H	2.14	0.55
1:A:9:LYS:HG2	1:A:31:ILE:HG12	1.89	0.55
1:D:73:PHE:CZ	1:D:95:TYR:CD2	2.73	0.55
1:A:81:PRO:HB2	1:A:150:ILE:HD11	1.89	0.55
1:A:115:LEU:HD22	1:A:142:GLU:HG3	1.89	0.55
1:A:154:LEU:HD12	1:A:184:LEU:HD13	1.89	0.55
1:B:34:TYR:HD1	1:B:35:ASP:N	2.03	0.55
1:B:130:ARG:NH1	1:B:213:ASP:OD1	2.37	0.55
1:D:270:PRO:O	1:D:274:THR:HG23	2.06	0.55
1:B:158:LEU:HD11	1:B:238:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:THR:O	1:B:228:ILE:HG13	2.06	0.55
1:C:96:ILE:HD11	1:C:208:ILE:HB	1.89	0.55
1:D:134:PHE:CE1	1:D:138:HIS:NE2	2.75	0.55
1:A:96:ILE:HG21	1:A:101:LEU:HD22	1.89	0.54
1:B:11:GLY:HA2	1:B:26:TYR:CB	2.37	0.54
1:C:10:ASP:HA	1:C:15:GLU:HA	1.89	0.54
1:C:111:ALA:HB1	1:C:142:GLU:HB3	1.88	0.54
1:C:242:MET:HE1	1:D:244:ILE:HD11	1.89	0.54
1:D:260:LEU:HD22	1:E:260:LEU:CD2	2.35	0.54
1:A:5:ILE:HD11	1:A:37:LYS:CD	2.38	0.54
1:A:262:MET:HE3	1:A:317:ILE:HB	1.87	0.54
1:D:256:ILE:HD13	1:E:258:LYS:HG3	1.89	0.54
1:E:10:ASP:HB3	2:E:402:UMQ:HL3	1.88	0.54
1:E:240:SER:O	1:E:244:ILE:HG13	2.07	0.54
1:B:74:TYR:CD2	1:B:208:ILE:HD13	2.42	0.54
1:C:11:GLY:N	1:C:16:PRO:HD2	2.09	0.54
1:C:284:LEU:HD23	1:D:280:ASN:HB2	1.90	0.54
1:D:32:ASP:HB3	1:D:116:HIS:NE2	2.22	0.54
1:E:11:GLY:HA3	1:E:26:TYR:CD1	2.43	0.54
1:B:60:ASP:HB3	1:B:63:GLU:HB2	1.89	0.54
1:C:92:LEU:HD23	1:C:92:LEU:C	2.28	0.54
1:D:313:ARG:HA	1:D:315:GLY:N	2.21	0.54
1:D:48:ILE:HD11	1:D:55:LEU:HD11	1.90	0.54
1:D:57:ILE:HG21	1:D:75:LEU:HD21	1.89	0.54
1:D:95:TYR:HD1	1:D:102:LEU:HD12	1.72	0.54
1:A:79:LYS:HD3	1:A:90:THR:OG1	2.08	0.54
1:A:173:VAL:HG12	1:A:174:MET:N	2.22	0.54
1:A:256:ILE:HG22	1:A:257:MET:N	2.23	0.54
1:C:269:VAL:HB	1:C:270:PRO:HD3	1.90	0.54
1:D:181:ARG:HH12	1:E:244:ILE:HD11	1.73	0.54
1:E:6:ALA:C	1:E:7:ILE:HG12	2.28	0.54
1:B:74:TYR:HD2	1:B:208:ILE:HD13	1.72	0.54
1:A:140:LEU:HB3	1:A:220:LEU:HD21	1.90	0.54
1:A:226:GLN:HG2	1:E:192:ILE:CG2	2.36	0.54
1:C:256:ILE:HG12	1:D:258:LYS:HG2	1.90	0.54
1:D:79:LYS:HD3	1:D:90:THR:HG21	1.90	0.54
1:E:101:LEU:HD12	1:E:101:LEU:C	2.28	0.54
1:A:276:ILE:HD12	1:E:293:PHE:CE1	2.43	0.53
1:B:82:LEU:O	1:B:88:THR:HA	2.08	0.53
1:C:170:ASP:OD1	1:C:170:ASP:C	2.45	0.53
1:C:206:LEU:HB3	1:C:208:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ILE:HG23	1:C:304:ILE:HG23	1.89	0.53
1:D:79:LYS:CD	1:D:90:THR:HB	2.31	0.53
1:E:260:LEU:HD23	1:E:261:THR:N	2.23	0.53
1:E:170:ASP:HB3	1:E:173:VAL:CG1	2.37	0.53
1:D:30:TRP:CZ2	1:D:112:ILE:HG23	2.43	0.53
1:D:81:PRO:HB2	1:D:150:ILE:CD1	2.33	0.53
1:E:154:LEU:HD11	1:E:180:LEU:HD22	1.90	0.53
1:B:24:GLU:CG	1:B:25:ASP:N	2.66	0.53
1:B:200:LEU:HA	1:B:203:ARG:HH21	1.74	0.53
1:B:314:SER:N	1:B:315:GLY:HA2	2.23	0.53
1:D:30:TRP:HZ2	1:D:112:ILE:HG23	1.73	0.53
1:A:181:ARG:NH2	1:B:244:ILE:HD11	2.22	0.53
1:A:267:PHE:N	1:A:267:PHE:HD1	2.07	0.53
1:E:89:THR:HG23	1:E:90:THR:H	1.73	0.53
1:A:37:LYS:HD2	1:A:37:LYS:N	2.23	0.53
1:C:181:ARG:NH2	1:D:240:SER:OG	2.42	0.53
1:D:133:GLY:O	1:D:136:LEU:HB3	2.09	0.53
1:E:65:PRO:HA	1:E:77:ILE:HB	1.89	0.53
1:C:7:ILE:HB	1:C:32:ASP:HB3	1.91	0.53
1:E:89:THR:O	1:E:90:THR:HG23	2.09	0.53
1:A:284:LEU:O	1:A:285:PRO:C	2.46	0.53
1:C:79:LYS:HG3	1:C:190:SER:OG	2.08	0.53
1:C:75:LEU:HD13	1:C:95:TYR:CE2	2.44	0.53
1:D:50:ILE:HG22	1:D:54:ASP:HB2	1.90	0.53
1:D:92:LEU:CD1	1:D:109:ILE:HG13	2.39	0.53
1:D:297:MET:HE1	1:E:276:ILE:HD12	1.91	0.53
1:B:34:TYR:CD1	1:B:34:TYR:C	2.82	0.52
1:B:92:LEU:HG	1:B:93:GLY:H	1.73	0.52
1:A:276:ILE:HG13	1:A:277:TYR:N	2.16	0.52
1:B:96:ILE:HG13	1:B:132:ILE:HD13	1.91	0.52
1:B:256:ILE:CG2	1:C:257:MET:HB3	2.39	0.52
1:C:242:MET:O	1:C:246:LEU:HD23	2.10	0.52
1:E:92:LEU:HD12	1:E:93:GLY:CA	2.39	0.52
1:A:20:GLU:O	1:A:20:GLU:OE1	2.28	0.52
1:B:83:PHE:O	1:B:87:ILE:O	2.27	0.52
1:C:218:GLU:O	1:C:221:TYR:HB3	2.09	0.52
1:E:65:PRO:HA	1:E:77:ILE:O	2.08	0.52
1:E:85:GLU:O	1:E:87:ILE:N	2.43	0.52
1:A:172:GLU:O	1:A:175:GLU:HG2	2.09	0.52
1:C:285:PRO:HB2	2:C:401:UMQ:HF2	1.91	0.52
1:C:267:PHE:N	1:C:267:PHE:CD1	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:PHE:CZ	1:D:95:TYR:HB3	2.45	0.52
1:D:205:TYR:CD1	1:D:205:TYR:C	2.82	0.52
1:E:48:ILE:HD11	1:E:55:LEU:HD11	1.92	0.52
1:B:109:ILE:HB	1:B:112:ILE:HD12	1.91	0.52
1:C:28:LEU:HA	1:C:99:ASN:HB2	1.91	0.52
1:C:302:VAL:O	1:C:305:MET:HB2	2.10	0.52
1:C:104:ILE:O	1:C:104:ILE:HG23	2.09	0.52
1:E:90:THR:HG21	1:E:190:SER:OG	2.10	0.52
1:A:313:ARG:O	1:A:313:ARG:HD3	2.10	0.52
1:B:48:ILE:HD11	1:B:55:LEU:HD11	1.92	0.52
1:C:213:ASP:O	1:C:216:ASN:HB2	2.09	0.52
1:D:95:TYR:CD1	1:D:102:LEU:HD12	2.45	0.52
1:E:253:MET:O	1:E:257:MET:HG3	2.09	0.52
1:A:45:SER:OG	1:A:50:ILE:O	2.19	0.51
1:A:154:LEU:HD23	1:A:158:LEU:HD13	1.92	0.51
1:C:269:VAL:HG12	1:C:303:ILE:HD13	1.92	0.51
1:D:102:LEU:C	1:D:102:LEU:HD13	2.30	0.51
1:E:155:GLU:HB2	1:E:234:TYR:CZ	2.45	0.51
1:A:115:LEU:O	1:A:119:ILE:HG13	2.10	0.51
1:A:270:PRO:O	1:A:273:ILE:HB	2.10	0.51
1:A:145:ARG:HG3	1:A:145:ARG:HH11	1.75	0.51
1:A:211:LYS:HG3	1:A:214:ARG:HH22	1.75	0.51
1:B:22:SER:H	1:B:47:LYS:HZ2	1.58	0.51
1:E:48:ILE:HG13	1:E:50:ILE:H	1.74	0.51
1:A:104:ILE:HG23	1:A:104:ILE:O	2.10	0.51
1:B:257:MET:HG3	1:C:257:MET:SD	2.51	0.51
1:C:68:GLU:HB3	1:C:75:LEU:HB3	1.91	0.51
1:E:10:ASP:CB	1:E:15:GLU:HB3	2.39	0.51
1:B:14:VAL:O	1:B:16:PRO:HD3	2.11	0.51
1:C:11:GLY:CA	1:C:26:TYR:CD1	2.87	0.51
1:C:252:LYS:O	1:C:256:ILE:HD12	2.10	0.51
1:D:81:PRO:HD3	1:D:147:TYR:CE2	2.45	0.51
1:D:200:LEU:HD23	1:D:204:LYS:HG2	1.93	0.51
1:E:130:ARG:HB2	1:E:134:PHE:CD2	2.46	0.51
1:A:176:LYS:HD3	2:A:401:UMQ:O4	2.11	0.51
1:B:63:GLU:CD	1:B:66:ARG:HH12	2.12	0.51
1:C:160:GLU:HG2	1:C:161:LEU:HD23	1.92	0.51
1:A:27:ARG:HB3	1:A:27:ARG:NH1	2.23	0.51
1:B:78:TYR:CZ	1:B:194:ASN:HB3	2.46	0.51
1:C:234:TYR:O	1:C:238:LEU:HD23	2.11	0.51
1:D:158:LEU:HD21	1:D:238:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:MET:CE	1:E:189:LYS:HA	2.41	0.51
1:B:36:PRO:HG3	1:B:104:ILE:HD11	1.92	0.51
1:C:9:LYS:HB2	1:C:9:LYS:NZ	2.25	0.51
1:C:311:PHE:CD1	1:C:316:TRP:CD1	2.99	0.51
1:D:312:ARG:O	1:D:315:GLY:HA2	2.11	0.51
1:E:303:ILE:HA	1:E:306:ILE:HD12	1.93	0.51
1:C:20:GLU:HG2	1:C:47:LYS:HZ1	1.76	0.50
1:A:7:ILE:HG21	1:A:9:LYS:HE3	1.92	0.50
1:C:133:GLY:HA3	1:C:213:ASP:OD2	2.12	0.50
1:C:183:THR:O	1:C:186:TYR:HB2	2.11	0.50
1:D:244:ILE:O	1:D:247:SER:N	2.44	0.50
1:A:260:LEU:HD21	1:B:260:LEU:HD23	1.92	0.50
1:B:101:LEU:HD12	1:B:135:LEU:HD21	1.94	0.50
1:C:90:THR:HG21	1:C:190:SER:OG	2.10	0.50
1:C:255:GLN:HA	1:C:258:LYS:HG3	1.92	0.50
1:C:218:GLU:O	1:C:221:TYR:N	2.45	0.50
1:C:272:TRP:O	1:C:276:ILE:HG23	2.12	0.50
1:D:57:ILE:HB	1:D:95:TYR:OH	2.11	0.50
1:B:24:GLU:HG3	1:B:25:ASP:H	1.77	0.50
1:D:134:PHE:CE1	1:D:138:HIS:CD2	2.98	0.50
1:B:24:GLU:HG3	1:B:25:ASP:N	2.27	0.50
1:C:92:LEU:CD1	1:C:112:ILE:HD11	2.40	0.50
1:C:115:LEU:CD1	1:C:142:GLU:HG3	2.42	0.50
1:D:72:ASP:O	1:D:73:PHE:HB2	2.10	0.50
1:D:92:LEU:HD12	1:D:109:ILE:HG13	1.94	0.50
1:D:268:ALA:H	1:D:270:PRO:HD2	1.76	0.50
1:E:1:MET:O	1:E:1:MET:CG	2.60	0.50
1:E:5:ILE:O	1:E:33:CYS:HA	2.11	0.50
1:E:180:LEU:O	1:E:183:THR:HG22	2.11	0.50
1:A:191:LEU:HD11	2:A:401:UMQ:CL	2.42	0.50
1:D:37:LYS:O	1:D:40:GLU:N	2.45	0.50
1:B:114:ARG:O	1:B:118:LEU:HB2	2.11	0.50
1:B:128:PHE:HE1	1:B:134:PHE:HD2	1.57	0.50
1:B:202:LYS:HE3	1:B:218:GLU:CG	2.29	0.50
1:C:199:VAL:O	1:C:202:LYS:HG2	2.12	0.50
1:C:244:ILE:O	1:C:248:LEU:HB2	2.12	0.50
1:D:20:GLU:O	1:D:21:ILE:HD12	2.12	0.50
1:E:237:VAL:O	1:E:240:SER:HB3	2.11	0.50
1:A:15:GLU:OE1	1:A:15:GLU:HA	2.07	0.50
1:C:20:GLU:CB	1:C:21:ILE:HG13	2.39	0.50
1:D:157:GLU:O	1:D:161:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:LYS:HB2	4:E:552:HOH:O	2.11	0.50
1:E:155:GLU:HB2	1:E:234:TYR:OH	2.12	0.50
1:B:7:ILE:HG22	1:B:8:ALA:N	2.27	0.49
1:C:200:LEU:HD21	1:C:204:LYS:NZ	2.26	0.49
1:C:235:ARG:HD2	4:C:502:HOH:O	2.12	0.49
1:D:9:LYS:HB2	1:D:9:LYS:HZ3	1.76	0.49
1:D:14:VAL:HG13	1:D:15:GLU:N	2.27	0.49
1:E:165:LEU:HG	1:E:245:THR:CG2	2.42	0.49
1:A:154:LEU:CD1	1:A:184:LEU:CD1	2.90	0.49
1:D:73:PHE:HE1	1:D:95:TYR:HB3	1.76	0.49
1:A:5:ILE:CG1	1:A:40:GLU:HG3	2.37	0.49
1:B:119:ILE:HG22	1:B:120:SER:N	2.27	0.49
1:C:311:PHE:HD1	1:C:316:TRP:CD1	2.29	0.49
1:A:96:ILE:CG2	1:A:101:LEU:HD22	2.43	0.49
1:A:154:LEU:HD11	1:A:184:LEU:HD13	1.90	0.49
1:A:170:ASP:OD1	1:A:170:ASP:C	2.49	0.49
1:B:10:ASP:HA	1:B:16:PRO:HD2	1.94	0.49
1:B:196:ASP:OD2	1:C:226:GLN:HG3	2.13	0.49
1:C:185:VAL:CG1	1:C:186:TYR:N	2.73	0.49
1:A:81:PRO:HB2	1:A:150:ILE:CD1	2.43	0.49
1:A:261:THR:OG1	1:E:260:LEU:HB2	2.12	0.49
1:B:260:LEU:HB2	1:C:261:THR:OG1	2.12	0.49
1:D:200:LEU:HD21	1:D:204:LYS:HE3	1.94	0.49
1:B:237:VAL:O	1:B:240:SER:HB3	2.12	0.49
1:C:96:ILE:HG22	1:C:101:LEU:HD13	1.93	0.49
1:D:11:GLY:N	1:D:16:PRO:HG2	2.22	0.49
1:E:158:LEU:CD1	1:E:238:LEU:HD21	2.37	0.49
1:B:25:ASP:OD1	1:B:25:ASP:C	2.50	0.49
1:C:187:PHE:HB3	1:C:191:LEU:HD12	1.94	0.49
1:C:199:VAL:HA	1:C:202:LYS:HD3	1.93	0.49
1:E:60:ASP:OD1	1:E:60:ASP:C	2.50	0.49
1:A:5:ILE:HD12	1:A:5:ILE:O	2.13	0.49
1:A:7:ILE:HA	1:A:32:ASP:O	2.13	0.49
1:A:211:LYS:HA	1:A:214:ARG:NH2	2.27	0.49
1:B:199:VAL:HG12	1:B:200:LEU:N	2.27	0.49
1:E:150:ILE:HG21	1:E:187:PHE:HZ	1.77	0.49
1:A:255:GLN:O	1:A:258:LYS:HB2	2.12	0.49
1:E:72:ASP:CG	1:E:72:ASP:O	2.50	0.49
1:E:299:LEU:O	1:E:303:ILE:HG12	2.13	0.49
1:A:181:ARG:O	1:A:185:VAL:HG23	2.13	0.49
1:B:69:GLU:CG	1:B:74:TYR:HE1	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:HD23	1:B:166:LEU:N	2.28	0.49
1:D:124:PRO:CD	1:D:125:ARG:HA	2.42	0.49
1:A:215:GLU:O	1:A:218:GLU:HB3	2.13	0.48
1:A:250:ASN:O	1:A:253:MET:HB3	2.12	0.48
1:B:315:GLY:H	1:B:316:TRP:HE3	1.60	0.48
1:C:48:ILE:HG13	1:C:50:ILE:H	1.78	0.48
1:D:39:GLU:OE1	1:D:39:GLU:N	2.34	0.48
1:D:246:LEU:N	1:D:246:LEU:HD23	2.27	0.48
1:E:165:LEU:HG	1:E:245:THR:HG23	1.94	0.48
1:E:18:LEU:HD22	1:E:26:TYR:CZ	2.47	0.48
1:B:8:ALA:C	1:B:9:LYS:NZ	2.67	0.48
1:B:63:GLU:OE1	1:B:66:ARG:NH1	2.32	0.48
1:B:69:GLU:HA	1:B:74:TYR:CD1	2.48	0.48
1:B:165:LEU:HD12	1:B:241:MET:HB3	1.95	0.48
1:C:10:ASP:HA	1:C:15:GLU:HB3	1.95	0.48
1:C:270:PRO:O	1:C:274:THR:HG23	2.13	0.48
1:D:276:ILE:HG13	1:D:277:TYR:N	2.29	0.48
1:A:154:LEU:HB2	2:A:401:UMQ:HD2	1.94	0.48
1:C:79:LYS:HG3	1:C:190:SER:CB	2.43	0.48
1:E:54:ASP:O	1:E:95:TYR:OH	2.13	0.48
1:B:150:ILE:O	1:B:153:ASN:HB2	2.14	0.48
1:B:253:MET:HG3	1:C:257:MET:CE	2.44	0.48
1:A:154:LEU:HD12	2:A:401:UMQ:CF	2.43	0.48
1:A:174:MET:HG3	1:A:178:LEU:CD1	2.44	0.48
1:A:312:ARG:O	1:A:315:GLY:HA2	2.13	0.48
1:D:96:ILE:HD11	1:D:208:ILE:HD12	1.96	0.48
1:A:37:LYS:HG2	1:A:40:GLU:OE1	2.13	0.48
1:C:21:ILE:HG12	1:C:47:LYS:HG3	1.96	0.48
1:E:262:MET:O	1:E:266:ILE:HG13	2.14	0.48
1:E:136:LEU:HD12	1:E:140:LEU:HD13	1.96	0.48
1:B:26:TYR:CD2	1:B:29:ILE:HG21	2.49	0.48
1:B:159:GLU:O	1:B:162:GLU:HB2	2.14	0.48
1:C:15:GLU:OE1	1:C:122:LYS:HD3	2.14	0.48
1:C:123:LYS:N	1:C:124:PRO:CD	2.72	0.48
1:C:163:ASP:OD1	1:C:164:LYS:HG3	2.13	0.48
1:D:256:ILE:O	1:D:259:ILE:N	2.46	0.48
1:A:154:LEU:HD12	2:A:401:UMQ:CG	2.43	0.48
1:B:15:GLU:CD	1:B:15:GLU:O	2.53	0.48
1:B:316:TRP:HE3	1:B:316:TRP:N	2.12	0.48
1:D:31:ILE:CD1	1:D:100:LEU:HD21	2.44	0.48
1:A:9:LYS:HZ3	1:A:20:GLU:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:NZ	2:A:401:UMQ:HO3'	2.11	0.47
1:A:260:LEU:HD21	1:B:260:LEU:CD2	2.44	0.47
1:A:296:VAL:HG21	1:B:281:PHE:HZ	1.79	0.47
1:C:75:LEU:HD12	1:C:94:ILE:O	2.14	0.47
1:C:266:ILE:HD13	1:C:308:VAL:HG23	1.95	0.47
1:D:37:LYS:H	1:D:37:LYS:HD3	1.79	0.47
1:A:317:ILE:HG12	1:A:317:ILE:O	2.14	0.47
1:B:8:ALA:O	1:B:9:LYS:HG3	2.14	0.47
1:B:242:MET:O	1:B:246:LEU:HB2	2.14	0.47
1:D:306:ILE:O	1:D:310:ILE:HG12	2.14	0.47
1:A:94:ILE:HG12	1:A:103:THR:HG22	1.96	0.47
1:B:192:ILE:CD1	1:B:228:ILE:HD13	2.40	0.47
1:D:18:LEU:HD12	1:D:19:ASP:O	2.14	0.47
1:D:145:ARG:NH2	1:D:149:ARG:HH22	2.12	0.47
1:D:151:LEU:HD11	1:D:230:MET:HB3	1.96	0.47
1:C:181:ARG:O	1:C:182:LYS:C	2.53	0.47
1:E:61:GLU:HB2	1:E:91:SER:HB3	1.96	0.47
1:A:153:ASN:HB3	2:A:401:UMQ:HA2	1.96	0.47
1:B:51:SER:O	1:B:55:LEU:HG	2.13	0.47
1:B:249:GLU:HA	1:B:249:GLU:OE1	2.13	0.47
1:C:66:ARG:HG2	1:C:66:ARG:HH11	1.79	0.47
1:A:31:ILE:O	1:A:102:LEU:HD23	2.14	0.47
1:C:182:LYS:O	1:C:185:VAL:HG12	2.14	0.47
1:D:82:LEU:HD12	1:D:82:LEU:HA	1.49	0.47
1:D:90:THR:CG2	1:D:190:SER:OG	2.62	0.47
1:D:124:PRO:HB2	1:D:125:ARG:HA	1.96	0.47
1:E:91:SER:C	4:E:519:HOH:O	2.52	0.47
1:E:115:LEU:O	1:E:119:ILE:HG13	2.14	0.47
1:A:154:LEU:HD23	1:A:154:LEU:C	2.35	0.47
1:B:14:VAL:HG22	1:B:15:GLU:H	1.80	0.47
1:B:75:LEU:HD12	1:B:76:ILE:H	1.79	0.47
1:B:173:VAL:HG12	1:B:174:MET:N	2.30	0.47
1:C:14:VAL:CG2	1:C:15:GLU:H	2.27	0.47
1:C:103:THR:HG21	1:C:139:ILE:HD13	1.97	0.47
1:D:130:ARG:NH2	1:D:212:GLU:HB3	2.29	0.47
1:A:173:VAL:CG1	1:A:174:MET:N	2.77	0.47
1:E:34:TYR:CE1	1:E:35:ASP:HB2	2.50	0.47
1:E:83:PHE:O	1:E:84:GLU:C	2.54	0.47
1:A:154:LEU:CA	2:A:401:UMQ:HA1	2.43	0.47
1:A:187:PHE:CG	2:A:401:UMQ:HH2	2.50	0.47
1:D:141:ASN:OD1	1:D:141:ASN:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:ASP:OD2	1:E:112:ILE:HD12	2.15	0.47
1:E:71:GLU:O	1:E:72:ASP:HB3	2.15	0.47
1:C:123:LYS:H	1:C:124:PRO:HD2	1.76	0.47
1:D:101:LEU:HD12	1:D:101:LEU:C	2.36	0.47
1:E:72:ASP:O	1:E:73:PHE:HB3	2.15	0.47
1:E:159:GLU:O	1:E:159:GLU:HG3	2.14	0.47
1:A:191:LEU:HD11	2:A:401:UMQ:CK	2.46	0.46
1:B:23:PHE:N	1:B:23:PHE:CD1	2.82	0.46
1:B:184:LEU:HA	1:B:184:LEU:HD12	1.66	0.46
1:D:34:TYR:CD1	1:D:35:ASP:N	2.83	0.46
1:D:99:ASN:O	1:D:99:ASN:ND2	2.47	0.46
1:D:289:ASN:OD1	1:D:290:PRO:HD2	2.15	0.46
1:B:165:LEU:CD1	1:B:241:MET:HB3	2.45	0.46
1:B:289:ASN:HA	1:B:290:PRO:HD2	1.77	0.46
1:C:17:LYS:C	1:C:18:LEU:HD22	2.35	0.46
1:C:258:LYS:HE2	1:C:316:TRP:CE2	2.50	0.46
1:E:263:VAL:CG1	1:E:264:THR:N	2.77	0.46
1:D:177:ILE:HG21	1:D:242:MET:HG3	1.97	0.46
1:E:171:ARG:O	1:E:175:GLU:HG2	2.15	0.46
1:E:195:ARG:HB2	1:E:224:THR:HG21	1.97	0.46
1:A:246:LEU:HD13	1:B:247:SER:HB3	1.95	0.46
1:B:254:ASN:HA	1:B:257:MET:HE2	1.96	0.46
1:D:67:VAL:O	1:D:67:VAL:HG12	2.14	0.46
1:E:36:PRO:HG2	1:E:59:LEU:HD11	1.96	0.46
1:A:63:GLU:CG	1:A:66:ARG:HH12	2.28	0.46
1:A:276:ILE:HD12	1:E:293:PHE:HE1	1.80	0.46
1:B:9:LYS:HD3	1:B:119:ILE:HG21	1.98	0.46
1:D:100:LEU:HD22	1:D:101:LEU:H	1.81	0.46
1:E:109:ILE:HB	1:E:112:ILE:HG13	1.98	0.46
1:A:48:ILE:O	1:A:97:LYS:HE3	2.15	0.46
1:A:177:ILE:HG21	1:A:242:MET:CG	2.46	0.46
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.79	0.46
2:B:401:UMQ:O6'	2:B:401:UMQ:H11	2.15	0.46
1:C:78:TYR:CZ	1:C:140:LEU:HG	2.51	0.46
1:E:11:GLY:HA2	1:E:27:ARG:N	2.22	0.46
1:A:7:ILE:CG2	1:A:9:LYS:HE3	2.46	0.46
1:E:79:LYS:HD3	1:E:90:THR:HB	1.96	0.46
1:A:257:MET:HB2	1:E:256:ILE:HG21	1.98	0.46
1:C:170:ASP:OD1	1:C:171:ARG:N	2.49	0.46
1:D:23:PHE:HZ	1:D:100:LEU:HB2	1.81	0.46
1:D:218:GLU:O	1:D:219:ASP:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HB2	1:B:261:THR:OG1	2.16	0.46
1:B:4:VAL:O	1:B:4:VAL:HG22	2.14	0.46
1:B:123:LYS:NZ	1:B:124:PRO:HA	2.31	0.46
1:D:57:ILE:HB	1:D:95:TYR:HH	1.79	0.46
1:D:253:MET:HG3	1:E:254:ASN:OD1	2.16	0.46
1:C:73:PHE:HB2	1:C:97:LYS:HB3	1.97	0.46
1:C:99:ASN:OD1	1:C:99:ASN:N	2.48	0.46
1:B:203:ARG:HE	1:B:203:ARG:HB3	1.42	0.45
1:B:246:LEU:HD11	1:C:248:LEU:CD2	2.46	0.45
1:B:284:LEU:HB2	1:B:287:ALA:HB2	1.99	0.45
1:C:96:ILE:HB	1:C:132:ILE:HD13	1.98	0.45
1:A:71:GLU:O	1:A:72:ASP:OD1	2.34	0.45
1:A:150:ILE:O	1:A:153:ASN:HB2	2.16	0.45
1:B:7:ILE:HG22	1:B:8:ALA:H	1.81	0.45
1:B:245:THR:O	1:B:248:LEU:N	2.48	0.45
1:C:311:PHE:O	1:C:312:ARG:C	2.55	0.45
1:C:316:TRP:O	1:C:317:ILE:C	2.54	0.45
1:D:18:LEU:HD11	1:D:26:TYR:OH	2.16	0.45
1:D:114:ARG:NH1	1:D:149:ARG:HH11	2.14	0.45
1:D:194:ASN:O	1:D:195:ARG:C	2.53	0.45
1:E:7:ILE:HG22	1:E:8:ALA:N	2.30	0.45
1:A:177:ILE:HG22	1:A:178:LEU:N	2.30	0.45
1:B:249:GLU:OE1	1:B:249:GLU:CA	2.64	0.45
1:B:309:TYR:CZ	1:B:313:ARG:HD3	2.52	0.45
1:D:262:MET:CG	1:D:316:TRP:HE3	2.29	0.45
1:A:141:ASN:O	1:A:145:ARG:HG2	2.16	0.45
1:A:169:TYR:CD1	1:A:170:ASP:N	2.84	0.45
1:A:170:ASP:OD1	1:A:171:ARG:N	2.50	0.45
1:A:254:ASN:O	1:A:258:LYS:HG3	2.16	0.45
1:B:192:ILE:O	1:B:195:ARG:HB3	2.16	0.45
1:B:210:THR:OG1	1:B:211:LYS:N	2.49	0.45
1:B:251:ILE:HD13	1:B:251:ILE:N	2.30	0.45
1:C:27:ARG:CZ	1:C:27:ARG:HB3	2.41	0.45
1:C:48:ILE:HD11	1:C:55:LEU:HD21	1.98	0.45
1:C:96:ILE:CG2	1:C:101:LEU:HD22	2.43	0.45
1:D:257:MET:HG2	1:E:257:MET:SD	2.57	0.45
1:A:230:MET:HE1	1:E:188:HIS:CD2	2.50	0.45
1:E:96:ILE:HG22	1:E:101:LEU:HA	1.99	0.45
1:A:11:GLY:O	1:A:16:PRO:HD2	2.17	0.45
1:B:34:TYR:HD1	1:B:34:TYR:C	2.20	0.45
1:C:4:VAL:C	1:C:5:ILE:HG12	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:PRO:O	1:C:125:ARG:C	2.53	0.45
1:C:150:ILE:O	1:C:153:ASN:HB2	2.17	0.45
1:D:28:LEU:HA	1:D:99:ASN:HD22	1.81	0.45
1:E:294:TRP:CH2	2:E:401:UMQ:HH1	2.48	0.45
1:A:92:LEU:HG	1:A:93:GLY:N	2.29	0.45
1:B:256:ILE:HD11	1:C:258:LYS:HE3	1.98	0.45
1:C:21:ILE:HG13	1:C:47:LYS:HE3	1.99	0.45
1:C:89:THR:O	1:C:90:THR:HG23	2.17	0.45
1:C:289:ASN:ND2	2:C:401:UMQ:H51	2.32	0.45
1:D:54:ASP:O	1:D:95:TYR:CE2	2.70	0.45
1:E:270:PRO:O	1:E:274:THR:HG23	2.17	0.45
1:A:234:TYR:O	1:A:238:LEU:HG	2.17	0.45
1:B:151:LEU:HD12	1:B:227:LEU:HD22	1.99	0.45
1:C:18:LEU:HD22	1:C:18:LEU:N	2.32	0.45
1:C:45:SER:HB2	1:C:55:LEU:HD12	1.99	0.45
1:D:178:LEU:HD21	1:E:244:ILE:HG21	1.99	0.45
1:E:56:GLN:HA	1:E:59:LEU:HB2	1.99	0.45
1:A:270:PRO:HD3	1:A:303:ILE:HG21	1.98	0.45
1:B:293:PHE:N	1:C:281:PHE:CE1	2.85	0.45
1:D:87:ILE:O	1:D:87:ILE:HG22	2.17	0.45
1:E:151:LEU:HD23	1:E:151:LEU:HA	1.79	0.45
1:C:263:VAL:HG21	1:D:265:THR:OG1	2.17	0.44
1:E:8:ALA:O	1:E:9:LYS:NZ	2.28	0.44
1:E:158:LEU:HD12	1:E:158:LEU:HA	1.70	0.44
1:A:86:ASP:HB2	2:A:401:UMQ:O5	2.18	0.44
1:C:80:ALA:O	1:C:90:THR:HA	2.18	0.44
1:C:137:TYR:HA	1:C:217:PHE:CE1	2.53	0.44
1:C:161:LEU:HD13	1:C:173:VAL:HG13	1.98	0.44
1:C:192:ILE:HD12	1:D:229:ASP:OD2	2.17	0.44
1:E:2:ILE:HG13	1:E:3:THR:N	2.30	0.44
1:E:284:LEU:HA	1:E:284:LEU:HD12	1.45	0.44
1:B:79:LYS:HD3	1:B:90:THR:HB	1.99	0.44
1:B:196:ASP:CB	1:C:226:GLN:HE21	2.29	0.44
1:C:239:THR:HG22	1:C:240:SER:N	2.31	0.44
1:C:284:LEU:O	1:C:285:PRO:C	2.55	0.44
1:D:122:LYS:HB3	1:D:123:LYS:H	1.63	0.44
1:E:273:ILE:HD13	1:E:299:LEU:HD23	1.99	0.44
1:A:158:LEU:HA	1:A:158:LEU:HD12	1.76	0.44
1:B:246:LEU:HD22	1:B:246:LEU:HA	1.79	0.44
1:C:79:LYS:HB2	1:C:194:ASN:OD1	2.18	0.44
1:D:34:TYR:CD1	1:D:34:TYR:C	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:LEU:HD13	1:D:95:TYR:CD2	2.53	0.44
1:D:125:ARG:HG3	1:D:126:ILE:N	2.27	0.44
1:D:177:ILE:HG23	1:D:238:LEU:HD22	1.98	0.44
1:E:150:ILE:HG21	1:E:187:PHE:CZ	2.52	0.44
1:A:261:THR:O	1:A:265:THR:HB	2.17	0.44
1:B:133:GLY:O	1:B:136:LEU:HB3	2.17	0.44
1:B:145:ARG:HG2	4:B:512:HOH:O	2.16	0.44
1:C:218:GLU:O	1:C:219:ASP:C	2.56	0.44
1:D:23:PHE:CZ	1:D:100:LEU:HB2	2.53	0.44
1:D:68:GLU:HB3	1:D:75:LEU:HB3	1.99	0.44
1:D:151:LEU:O	1:D:155:GLU:HG3	2.17	0.44
1:E:36:PRO:CG	1:E:59:LEU:HD11	2.48	0.44
1:E:284:LEU:HB3	1:E:287:ALA:HB2	1.99	0.44
1:A:169:TYR:HB2	1:A:249:GLU:HG2	2.00	0.44
1:B:17:LYS:HE3	1:B:17:LYS:HB2	1.77	0.44
1:C:141:ASN:HA	1:C:220:LEU:HD11	1.98	0.44
1:A:154:LEU:N	2:A:401:UMQ:HA1	2.32	0.44
1:C:140:LEU:HD12	1:C:140:LEU:HA	1.84	0.44
1:D:11:GLY:H	1:D:16:PRO:CD	2.30	0.44
1:E:210:THR:O	1:E:211:LYS:C	2.55	0.44
1:A:67:VAL:HG21	1:A:200:LEU:HD22	1.98	0.44
1:A:170:ASP:HB3	1:A:173:VAL:HB	1.99	0.44
1:C:262:MET:SD	1:C:316:TRP:HD1	2.41	0.44
1:D:29:ILE:HB	1:D:100:LEU:HD23	1.98	0.44
1:E:132:ILE:CG2	1:E:133:GLY:N	2.76	0.44
1:E:262:MET:HG2	1:E:311:PHE:CE2	2.52	0.44
1:A:271:MET:SD	1:B:272:TRP:HD1	2.41	0.44
1:B:57:ILE:C	1:B:59:LEU:N	2.72	0.44
1:C:14:VAL:CG2	1:C:15:GLU:N	2.78	0.44
1:C:83:PHE:CD1	1:C:83:PHE:N	2.85	0.44
1:A:261:THR:CG2	1:E:259:ILE:HG22	2.48	0.43
1:C:9:LYS:HG3	1:C:10:ASP:N	2.32	0.43
1:D:124:PRO:HB2	1:D:125:ARG:CA	2.48	0.43
1:E:194:ASN:O	1:E:197:VAL:HB	2.18	0.43
1:A:71:GLU:HB3	4:A:519:HOH:O	2.19	0.43
1:D:173:VAL:HG12	1:D:174:MET:N	2.33	0.43
1:B:96:ILE:HD11	1:B:132:ILE:CG2	2.48	0.43
1:D:96:ILE:O	1:D:96:ILE:CG1	2.66	0.43
1:A:82:LEU:O	1:A:88:THR:HG23	2.19	0.43
1:A:213:ASP:O	1:A:216:ASN:HB2	2.19	0.43
1:B:173:VAL:CG1	1:B:174:MET:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ILE:HD12	1:C:21:ILE:N	2.34	0.43
1:C:192:ILE:HA	1:C:228:ILE:HD11	2.01	0.43
1:C:233:THR:O	1:C:237:VAL:HG23	2.19	0.43
1:D:32:ASP:OD1	1:D:105:HIS:NE2	2.51	0.43
1:D:135:LEU:O	1:D:139:ILE:HG13	2.19	0.43
1:E:10:ASP:HB2	1:E:15:GLU:CG	2.48	0.43
1:E:166:LEU:HD23	1:E:166:LEU:HA	1.76	0.43
1:A:158:LEU:O	1:A:162:GLU:HG3	2.18	0.43
1:B:65:PRO:HA	1:B:77:ILE:O	2.18	0.43
1:B:130:ARG:HB2	1:B:134:PHE:HD2	1.83	0.43
1:C:20:GLU:HA	1:C:21:ILE:HA	1.69	0.43
1:C:43:LYS:O	1:C:47:LYS:HB2	2.18	0.43
1:C:48:ILE:HD12	1:C:50:ILE:HD12	1.99	0.43
1:E:188:HIS:O	1:E:189:LYS:C	2.56	0.43
1:A:34:TYR:O	1:A:35:ASP:C	2.56	0.43
1:A:170:ASP:OD1	1:A:172:GLU:N	2.51	0.43
1:B:140:LEU:HD12	1:B:140:LEU:HA	1.82	0.43
1:C:83:PHE:O	1:C:87:ILE:O	2.36	0.43
1:C:85:GLU:O	1:C:87:ILE:HG12	2.19	0.43
1:D:289:ASN:O	1:D:292:GLY:N	2.43	0.43
1:E:165:LEU:C	1:E:165:LEU:HD23	2.39	0.43
1:A:266:ILE:HG12	1:A:307:PHE:HB3	2.00	0.43
1:B:48:ILE:HB	1:B:50:ILE:HD12	2.01	0.43
1:C:114:ARG:HD2	1:C:142:GLU:OE1	2.18	0.43
1:C:147:TYR:CB	1:C:227:LEU:HD12	2.44	0.43
1:D:41:LEU:O	1:D:45:SER:HB2	2.19	0.43
1:D:75:LEU:HD12	1:D:94:ILE:O	2.18	0.43
1:E:204:LYS:HE2	1:E:204:LYS:HB3	1.80	0.43
1:A:136:LEU:HD23	1:A:217:PHE:CZ	2.54	0.43
1:A:230:MET:HE2	1:E:188:HIS:HD2	1.83	0.43
1:B:73:PHE:HA	1:B:97:LYS:HB3	2.00	0.43
1:C:74:TYR:O	1:C:95:TYR:HA	2.19	0.43
1:D:41:LEU:HD22	1:D:59:LEU:CD1	2.48	0.43
1:D:73:PHE:CD1	1:D:74:TYR:N	2.86	0.43
1:D:197:VAL:HG12	1:D:198:LEU:N	2.33	0.43
1:E:219:ASP:OD1	1:E:219:ASP:N	2.37	0.43
1:A:20:GLU:O	1:A:20:GLU:CG	2.67	0.43
1:D:227:LEU:HD23	1:D:227:LEU:HA	1.89	0.43
1:E:82:LEU:HD12	1:E:82:LEU:HA	1.62	0.43
1:A:165:LEU:HD21	1:A:244:ILE:HD13	2.01	0.43
1:B:65:PRO:HG2	1:B:193:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLU:HA	1:B:74:TYR:HE1	1.83	0.43
1:B:135:LEU:HD11	1:B:139:ILE:HD11	2.01	0.43
1:B:246:LEU:HD11	1:C:248:LEU:HD22	2.01	0.43
1:C:125:ARG:CB	1:C:126:ILE:CA	2.95	0.43
1:C:192:ILE:HD11	4:C:509:HOH:O	2.19	0.43
1:C:253:MET:HE1	1:D:253:MET:HE2	2.01	0.43
1:C:269:VAL:CG1	1:C:303:ILE:HD13	2.49	0.43
1:D:7:ILE:O	1:D:31:ILE:HA	2.18	0.43
1:D:115:LEU:HD12	1:D:115:LEU:HA	1.71	0.43
1:D:151:LEU:HD22	1:D:151:LEU:HA	1.86	0.43
1:D:17:LYS:HE3	1:D:120:SER:OG	2.19	0.42
1:D:145:ARG:HH22	1:D:149:ARG:HH22	1.67	0.42
1:E:70:ASP:OD1	1:E:70:ASP:C	2.57	0.42
1:E:262:MET:HG2	1:E:311:PHE:CD2	2.54	0.42
1:B:92:LEU:HD23	1:B:93:GLY:N	2.35	0.42
1:A:191:LEU:HD11	2:A:401:UMQ:HK1	2.01	0.42
1:A:249:GLU:HG3	1:B:251:ILE:HD12	2.00	0.42
2:A:401:UMQ:O3'	2:A:401:UMQ:O5	2.31	0.42
1:B:260:LEU:HD22	1:C:260:LEU:HD23	2.00	0.42
1:C:189:LYS:O	1:C:192:ILE:HG22	2.19	0.42
1:C:274:THR:HG22	1:C:300:MET:SD	2.60	0.42
1:D:11:GLY:O	1:D:26:TYR:CD1	2.72	0.42
1:E:9:LYS:HA	1:E:9:LYS:HD3	1.81	0.42
1:A:108:LYS:HD2	1:A:108:LYS:N	2.28	0.42
1:A:252:LYS:C	1:A:254:ASN:N	2.72	0.42
1:C:308:VAL:HG12	1:C:309:TYR:N	2.33	0.42
1:D:39:GLU:H	1:D:39:GLU:CD	2.22	0.42
1:D:199:VAL:O	1:D:203:ARG:HB2	2.19	0.42
1:D:244:ILE:O	1:D:245:THR:C	2.57	0.42
1:A:94:ILE:HA	1:A:102:LEU:O	2.20	0.42
1:A:146:SER:O	1:A:147:TYR:C	2.57	0.42
1:A:191:LEU:HD21	2:A:401:UMQ:HL1	2.01	0.42
1:A:226:GLN:NE2	1:E:196:ASP:HB2	2.35	0.42
1:B:72:ASP:O	1:B:97:LYS:HD2	2.19	0.42
1:B:96:ILE:CD1	1:B:132:ILE:HD13	2.50	0.42
1:C:212:GLU:H	1:C:212:GLU:CD	2.21	0.42
1:D:166:LEU:HA	1:D:248:LEU:HD11	2.01	0.42
1:E:191:LEU:HD13	1:E:227:LEU:HB3	2.01	0.42
1:A:232:ALA:O	1:A:235:ARG:HB2	2.20	0.42
1:B:242:MET:SD	1:C:244:ILE:CD1	3.06	0.42
1:C:283:TYR:C	1:C:283:TYR:CD1	2.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LEU:HD12	1:E:264:THR:HG21	2.01	0.42
1:D:284:LEU:HD13	1:D:284:LEU:HA	1.84	0.42
1:D:295:LEU:HD23	1:D:295:LEU:HA	1.86	0.42
1:A:159:GLU:O	1:A:162:GLU:HB2	2.19	0.42
1:A:291:GLN:HA	1:A:291:GLN:OE1	2.20	0.42
1:C:238:LEU:HD22	1:C:238:LEU:N	2.35	0.42
1:C:253:MET:HB2	1:D:254:ASN:CG	2.39	0.42
1:C:294:TRP:HE1	2:D:401:UMQ:H4'1	1.85	0.42
1:D:182:LYS:HE2	1:E:237:VAL:CG1	2.49	0.42
1:B:192:ILE:HD13	1:B:192:ILE:HA	1.68	0.42
1:C:262:MET:HG2	1:C:311:PHE:CE1	2.55	0.42
1:D:39:GLU:N	1:D:39:GLU:CD	2.73	0.42
1:D:262:MET:HE2	1:D:317:ILE:HD13	2.02	0.42
1:C:130:ARG:HH11	1:C:130:ARG:HB3	1.85	0.42
1:C:293:PHE:CE2	1:D:285:PRO:HG2	2.55	0.42
1:D:184:LEU:CG	1:D:235:ARG:HG2	2.50	0.42
1:E:205:TYR:CD1	1:E:205:TYR:C	2.93	0.42
1:E:273:ILE:O	1:E:276:ILE:HG12	2.20	0.42
1:A:260:LEU:HG	1:E:260:LEU:HD12	2.01	0.42
1:C:185:VAL:HG12	1:C:186:TYR:N	2.35	0.42
1:E:55:LEU:HA	1:E:55:LEU:HD23	1.72	0.42
1:A:139:ILE:O	1:A:143:ILE:HG13	2.19	0.41
1:D:195:ARG:HD2	1:D:225:LEU:HD21	2.01	0.41
1:E:176:LYS:HA	1:E:176:LYS:HD2	1.89	0.41
1:E:284:LEU:HA	1:E:285:PRO:HD3	1.91	0.41
1:B:201:LEU:HD13	1:B:217:PHE:CE1	2.55	0.41
1:B:263:VAL:HG12	1:B:264:THR:N	2.35	0.41
1:A:203:ARG:HE	1:A:203:ARG:HB3	1.54	0.41
1:A:238:LEU:O	1:A:239:THR:C	2.57	0.41
1:B:37:LYS:NZ	1:B:37:LYS:CB	2.84	0.41
1:B:74:TYR:HD1	1:B:74:TYR:HA	1.75	0.41
1:B:255:GLN:O	1:B:255:GLN:HG3	2.12	0.41
1:C:95:TYR:HE1	1:C:104:ILE:CG2	2.31	0.41
1:C:256:ILE:HG12	1:D:258:LYS:CG	2.51	0.41
1:D:218:GLU:O	1:D:221:TYR:HB3	2.21	0.41
1:E:111:ALA:HB1	1:E:142:GLU:HB3	2.03	0.41
2:A:401:UMQ:HL3	2:A:401:UMQ:HI2	1.74	0.41
1:B:269:VAL:O	1:B:270:PRO:C	2.58	0.41
1:C:79:LYS:HD3	1:C:79:LYS:HA	1.66	0.41
1:C:86:ASP:O	1:C:87:ILE:HD13	2.20	0.41
1:D:67:VAL:HG22	1:D:76:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:MET:SD	1:E:272:TRP:HA	2.61	0.41
1:B:15:GLU:HA	1:B:16:PRO:HD2	1.98	0.41
1:B:139:ILE:O	1:B:143:ILE:HG13	2.21	0.41
1:B:313:ARG:O	1:B:314:SER:OG	2.32	0.41
1:C:20:GLU:H	1:C:20:GLU:HG3	1.64	0.41
1:C:82:LEU:HD22	1:C:107:ASP:CB	2.49	0.41
1:D:169:TYR:CD1	1:D:169:TYR:C	2.93	0.41
1:A:311:PHE:HD1	1:A:311:PHE:HA	1.76	0.41
1:B:22:SER:H	1:B:47:LYS:NZ	2.18	0.41
1:B:284:LEU:O	1:B:285:PRO:C	2.58	0.41
1:C:30:TRP:HZ2	1:C:112:ILE:HG23	1.86	0.41
1:D:90:THR:C	1:D:91:SER:OG	2.59	0.41
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.94	0.41
1:B:4:VAL:HA	1:B:34:TYR:O	2.21	0.41
1:B:119:ILE:CG2	1:B:120:SER:N	2.83	0.41
1:B:122:LYS:HA	1:B:123:LYS:HA	1.74	0.41
1:B:200:LEU:HD23	1:B:200:LEU:C	2.41	0.41
1:C:227:LEU:N	1:C:227:LEU:CD2	2.83	0.41
1:D:137:TYR:CE2	1:D:216:ASN:HB3	2.55	0.41
1:E:130:ARG:HB2	1:E:134:PHE:HD2	1.85	0.41
1:E:213:ASP:O	1:E:214:ARG:C	2.58	0.41
1:A:145:ARG:HG3	1:A:145:ARG:NH1	2.36	0.41
1:A:169:TYR:HB2	1:A:249:GLU:CG	2.49	0.41
1:B:14:VAL:HG13	1:B:15:GLU:N	2.35	0.41
1:E:13:ILE:HG13	1:E:14:VAL:HG12	2.02	0.41
1:E:163:ASP:OD1	1:E:164:LYS:N	2.53	0.41
1:A:230:MET:CG	1:E:189:LYS:HG3	2.51	0.41
1:B:24:GLU:HA	1:B:26:TYR:CD2	2.56	0.41
1:B:41:LEU:O	1:B:44:LEU:HB3	2.21	0.41
1:B:126:ILE:O	1:B:126:ILE:HG23	2.21	0.41
1:B:237:VAL:O	1:B:241:MET:HG3	2.20	0.41
1:C:15:GLU:N	1:C:15:GLU:OE1	2.44	0.41
1:C:291:GLN:HG3	2:D:401:UMQ:O4	2.21	0.41
1:D:20:GLU:OE1	1:D:20:GLU:N	2.54	0.41
1:D:92:LEU:HD11	1:D:112:ILE:HD11	2.03	0.41
1:D:199:VAL:HG22	1:D:221:TYR:CE1	2.55	0.41
1:E:101:LEU:HD23	1:E:135:LEU:HD23	2.02	0.41
1:E:174:MET:HE2	1:E:174:MET:HB2	1.92	0.41
1:E:192:ILE:CD1	1:E:228:ILE:HG12	2.49	0.41
1:E:195:ARG:HB2	1:E:224:THR:CG2	2.51	0.41
1:E:252:LYS:C	1:E:254:ASN:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:HB2	1:A:55:LEU:HD12	2.03	0.41
1:B:122:LYS:HG2	1:B:123:LYS:HB2	2.03	0.41
1:C:61:GLU:H	1:C:61:GLU:CD	2.25	0.41
1:C:96:ILE:HG22	1:C:101:LEU:HA	2.01	0.41
1:C:154:LEU:HD22	1:C:184:LEU:HD11	2.03	0.41
1:C:253:MET:HG2	1:C:257:MET:CE	2.48	0.41
1:C:284:LEU:HD12	1:C:284:LEU:HA	1.82	0.41
2:C:401:UMQ:O5'	2:C:401:UMQ:HB2	2.21	0.41
1:A:159:GLU:O	1:A:160:GLU:C	2.60	0.40
1:A:262:MET:HA	1:A:311:PHE:CE2	2.56	0.40
1:B:137:TYR:O	1:B:140:LEU:N	2.54	0.40
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.89	0.40
1:B:293:PHE:CD2	1:C:284:LEU:HD12	2.57	0.40
1:C:7:ILE:O	1:C:31:ILE:HA	2.21	0.40
1:C:33:CYS:HB3	1:C:36:PRO:HG3	2.03	0.40
1:A:18:LEU:HD12	1:A:19:ASP:H	1.85	0.40
1:A:184:LEU:HD12	1:A:184:LEU:HA	1.78	0.40
1:B:65:PRO:HG2	1:B:193:ALA:HB3	2.02	0.40
1:B:317:ILE:OXT	1:B:317:ILE:HG22	2.20	0.40
1:C:188:HIS:O	1:C:189:LYS:C	2.59	0.40
1:C:262:MET:HG3	1:C:316:TRP:NE1	2.31	0.40
1:D:55:LEU:C	1:D:57:ILE:N	2.72	0.40
1:A:5:ILE:HG22	1:A:7:ILE:CG1	2.34	0.40
1:A:178:LEU:HD21	1:B:244:ILE:HG21	2.02	0.40
1:C:296:VAL:O	1:C:299:LEU:HB3	2.22	0.40
1:D:105:HIS:CD2	1:D:105:HIS:N	2.90	0.40
1:E:284:LEU:HB3	1:E:287:ALA:CB	2.51	0.40
1:A:59:LEU:HD11	1:A:104:ILE:HD11	2.04	0.40
1:B:57:ILE:C	1:B:59:LEU:H	2.23	0.40
1:D:59:LEU:HA	1:D:59:LEU:HD23	1.82	0.40
1:E:36:PRO:HG3	1:E:41:LEU:HD13	2.04	0.40
1:A:227:LEU:HA	1:A:227:LEU:HD23	1.83	0.40
1:C:87:ILE:HG23	1:C:182:LYS:NZ	2.36	0.40
1:C:201:LEU:O	1:C:214:ARG:HG2	2.22	0.40
1:D:51:SER:HB2	4:D:513:HOH:O	2.22	0.40
1:D:102:LEU:CD1	1:D:104:ILE:HG22	2.52	0.40
1:D:105:HIS:ND1	1:D:107:ASP:O	2.42	0.40
1:D:134:PHE:CD1	1:D:138:HIS:CD2	3.09	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ASP:N	1:D:42:TYR:OH[2_455]	2.06	0.14

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	313/339 (92%)	279 (89%)	30 (10%)	4 (1%)	12	47
1	B	312/339 (92%)	271 (87%)	40 (13%)	1 (0%)	41	74
1	C	312/339 (92%)	277 (89%)	32 (10%)	3 (1%)	15	54
1	D	312/339 (92%)	275 (88%)	33 (11%)	4 (1%)	12	47
1	E	316/339 (93%)	276 (87%)	40 (13%)	0	100	100
All	All	1565/1695 (92%)	1378 (88%)	175 (11%)	12 (1%)	19	58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	13	ILE
1	A	21	ILE
1	C	14	VAL
1	D	5	ILE
1	D	21	ILE
1	D	126	ILE
1	A	26	TYR
1	C	124	PRO
1	A	14	VAL
1	B	126	ILE
1	D	57	ILE
1	A	126	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	292/314 (93%)	244 (84%)	48 (16%)	2 11
1	B	291/314 (93%)	232 (80%)	59 (20%)	1 6
1	C	291/314 (93%)	237 (81%)	54 (19%)	1 8
1	D	291/314 (93%)	252 (87%)	39 (13%)	4 18
1	E	295/314 (94%)	242 (82%)	53 (18%)	1 9
All	All	1460/1570 (93%)	1207 (83%)	253 (17%)	2 10

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	19	ASP
1	A	20	GLU
1	A	21	ILE
1	A	27	ARG
1	A	28	LEU
1	A	37	LYS
1	A	40	GLU
1	A	50	ILE
1	A	51	SER
1	A	61	GLU
1	A	64	ILE
1	A	69	GLU
1	A	72	ASP
1	A	76	ILE
1	A	79	LYS
1	A	85	GLU
1	A	88	THR
1	A	89	THR
1	A	92	LEU
1	A	99	ASN
1	A	101	LEU
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	103	THR
1	A	107	ASP
1	A	108	LYS
1	A	115	LEU
1	A	128	PHE
1	A	129	GLU
1	A	132	ILE
1	A	140	LEU
1	A	151	LEU
1	A	173	VAL
1	A	181	ARG
1	A	190	SER
1	A	231	SER
1	A	240	SER
1	A	247	SER
1	A	249	GLU
1	A	267	PHE
1	A	269	VAL
1	A	276	ILE
1	A	282	SER
1	A	283	TYR
1	A	286	LEU
1	A	313	ARG
1	A	316	TRP
1	A	317	ILE
1	B	9	LYS
1	B	15	GLU
1	B	20	GLU
1	B	22	SER
1	B	23	PHE
1	B	24	GLU
1	B	25	ASP
1	B	28	LEU
1	B	29	ILE
1	B	34	TYR
1	B	37	LYS
1	B	39	GLU
1	B	64	ILE
1	B	73	PHE
1	B	74	TYR
1	B	83	PHE
1	B	88	THR

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Mol	Chain	Res	Type
1	B	89	THR
1	B	90	THR
1	B	92	LEU
1	B	102	LEU
1	B	103	THR
1	B	114	ARG
1	B	119	ILE
1	B	121	THR
1	B	122	LYS
1	B	128	PHE
1	B	130	ARG
1	B	132	ILE
1	B	134	PHE
1	B	140	LEU
1	B	144	THR
1	B	146	SER
1	B	156	ASP
1	B	159	GLU
1	B	165	LEU
1	B	166	LEU
1	B	170	ASP
1	B	173	VAL
1	B	181	ARG
1	B	184	LEU
1	B	187	PHE
1	B	199	VAL
1	B	203	ARG
1	B	210	THR
1	B	215	GLU
1	B	220	LEU
1	B	226	GLN
1	B	231	SER
1	B	233	THR
1	B	246	LEU
1	B	249	GLU
1	B	255	GLN
1	B	264	THR
1	B	265	THR
1	B	269	VAL
1	B	276	ILE
1	B	312	ARG
1	B	316	TRP

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Mol	Chain	Res	Type
1	C	5	ILE
1	C	9	LYS
1	C	15	GLU
1	C	23	PHE
1	C	25	ASP
1	C	27	ARG
1	C	28	LEU
1	C	33	CYS
1	C	37	LYS
1	C	57	ILE
1	C	66	ARG
1	C	72	ASP
1	C	78	TYR
1	C	89	THR
1	C	92	LEU
1	C	96	ILE
1	C	100	LEU
1	C	101	LEU
1	C	102	LEU
1	C	115	LEU
1	C	126	ILE
1	C	127	VAL
1	C	130	ARG
1	C	138	HIS
1	C	140	LEU
1	C	146	SER
1	C	151	LEU
1	C	154	LEU
1	C	161	LEU
1	C	163	ASP
1	C	181	ARG
1	C	184	LEU
1	C	185	VAL
1	C	210	THR
1	C	227	LEU
1	C	231	SER
1	C	236	GLU
1	C	239	THR
1	C	240	SER
1	C	242	MET
1	C	246	LEU
1	C	248	LEU

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Mol	Chain	Res	Type
1	C	250	ASN
1	C	266	ILE
1	C	267	PHE
1	C	274	THR
1	C	276	ILE
1	C	280	ASN
1	C	282	SER
1	C	291	GLN
1	C	295	LEU
1	C	296	VAL
1	C	308	VAL
1	C	312	ARG
1	D	9	LYS
1	D	14	VAL
1	D	18	LEU
1	D	21	ILE
1	D	28	LEU
1	D	37	LYS
1	D	56	GLN
1	D	67	VAL
1	D	68	GLU
1	D	71	GLU
1	D	79	LYS
1	D	85	GLU
1	D	88	THR
1	D	89	THR
1	D	96	ILE
1	D	99	ASN
1	D	101	LEU
1	D	123	LYS
1	D	127	VAL
1	D	140	LEU
1	D	151	LEU
1	D	165	LEU
1	D	171	ARG
1	D	173	VAL
1	D	181	ARG
1	D	186	TYR
1	D	187	PHE
1	D	197	VAL
1	D	200	LEU
1	D	210	THR

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Mol	Chain	Res	Type
1	D	211	LYS
1	D	247	SER
1	D	250	ASN
1	D	253	MET
1	D	263	VAL
1	D	267	PHE
1	D	276	ILE
1	D	291	GLN
1	D	313	ARG
1	E	1	MET
1	E	5	ILE
1	E	10	ASP
1	E	15	GLU
1	E	23	PHE
1	E	25	ASP
1	E	27	ARG
1	E	37	LYS
1	E	45	SER
1	E	52	VAL
1	E	64	ILE
1	E	69	GLU
1	E	85	GLU
1	E	86	ASP
1	E	91	SER
1	E	92	LEU
1	E	96	ILE
1	E	100	LEU
1	E	101	LEU
1	E	102	LEU
1	E	105	HIS
1	E	112	ILE
1	E	115	LEU
1	E	116	HIS
1	E	121	THR
1	E	132	ILE
1	E	145	ARG
1	E	149	ARG
1	E	154	LEU
1	E	155	GLU
1	E	158	LEU
1	E	163	ASP
1	E	166	LEU

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Mol	Chain	Res	Type
1	E	181	ARG
1	E	183	THR
1	E	184	LEU
1	E	192	ILE
1	E	208	ILE
1	E	211	LYS
1	E	219	ASP
1	E	250	ASN
1	E	257	MET
1	E	260	LEU
1	E	261	THR
1	E	267	PHE
1	E	276	ILE
1	E	280	ASN
1	E	284	LEU
1	E	286	LEU
1	E	295	LEU
1	E	301	VAL
1	E	312	ARG
1	E	317	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	98	ASN
1	A	226	GLN
1	A	250	ASN
1	B	216	ASN
1	C	62	GLN
1	C	216	ASN
1	C	226	GLN
1	C	250	ASN
1	D	99	ASN
1	D	153	ASN
1	D	291	GLN
1	E	138	HIS
1	E	188	HIS
1	E	226	GLN
1	E	255	GLN
1	E	291	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 40 ligands modelled in this entry, 32 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	$\#\|Z\| > 2$
2	UMQ	E	402	-	12,12,35	0.49	0	11,11,46	1.02	1 (9%)
2	UMQ	C	401	-	35,35,35	1.31	4 (11%)	46,46,46	1.52	7 (15%)
2	UMQ	D	401	-	35,35,35	1.35	6 (17%)	46,46,46	1.24	4 (8%)
2	UMQ	B	401	-	31,31,35	1.39	4 (12%)	42,42,46	1.31	5 (11%)
2	UMQ	E	401	-	35,35,35	1.32	6 (17%)	46,46,46	1.37	6 (13%)
2	UMQ	A	401	-	35,35,35	1.26	4 (11%)	46,46,46	1.44	7 (15%)
2	UMQ	B	402	-	9,9,35	0.33	0	8,8,46	0.69	0
2	UMQ	A	402	-	35,35,35	1.35	5 (14%)	46,46,46	1.36	7 (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
2	UMQ	E	402	-	-	5/10/10/60	-
2	UMQ	C	401	-	-	14/20/60/60	0/2/2/2
2	UMQ	D	401	-	-	10/20/60/60	0/2/2/2
2	UMQ	B	401	-	-	11/16/56/60	0/2/2/2
2	UMQ	E	401	-	-	15/20/60/60	0/2/2/2
2	UMQ	A	401	-	-	14/20/60/60	0/2/2/2
2	UMQ	B	402	-	-	5/7/7/60	-
2	UMQ	A	402	-	-	11/20/60/60	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	UMQ	C3'-C4'	-3.82	1.41	1.52
2	C	401	UMQ	C3'-C4'	-3.81	1.41	1.52
2	B	401	UMQ	C3'-C4'	-3.62	1.42	1.52
2	E	401	UMQ	C3'-C4'	-3.58	1.42	1.52
2	A	402	UMQ	C3'-C4'	-3.48	1.42	1.52
2	A	401	UMQ	C3'-C4'	-3.33	1.43	1.52
2	A	402	UMQ	O5-C1	3.26	1.50	1.41
2	A	401	UMQ	O5-C1	3.22	1.50	1.41
2	B	401	UMQ	O5-C1	2.98	1.49	1.41
2	D	401	UMQ	O5-C1	2.80	1.49	1.41
2	E	401	UMQ	O5-C1	2.79	1.49	1.41
2	C	401	UMQ	O5-C1	2.75	1.48	1.41
2	A	402	UMQ	C3-C4	-2.69	1.45	1.52
2	D	401	UMQ	C3-C4	-2.67	1.45	1.52
2	A	401	UMQ	C3-C4	-2.61	1.45	1.52
2	C	401	UMQ	C3'-C2'	-2.52	1.45	1.52
2	C	401	UMQ	C3-C4	-2.51	1.45	1.52
2	E	401	UMQ	C3-C4	-2.50	1.45	1.52
2	B	401	UMQ	C3-C4	-2.49	1.45	1.52
2	A	402	UMQ	C3'-C2'	-2.42	1.46	1.52
2	E	401	UMQ	C3'-C2'	-2.39	1.46	1.52
2	A	401	UMQ	O1-C4'	2.34	1.49	1.43
2	E	401	UMQ	C3-C2	-2.29	1.46	1.52
2	D	401	UMQ	C3'-C2'	-2.29	1.46	1.52
2	B	401	UMQ	C3'-C2'	-2.23	1.46	1.52
2	E	401	UMQ	C1-C2	-2.22	1.46	1.52
2	A	402	UMQ	C3-C2	-2.16	1.46	1.52
2	D	401	UMQ	C1-C2	-2.08	1.46	1.52
2	D	401	UMQ	C3-C2	-2.06	1.47	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	UMQ	CA-O1'-C1'	4.33	121.07	113.68
2	A	401	UMQ	C1'-C2'-C3'	4.21	118.87	110.01
2	C	401	UMQ	C1-O1-C4'	-4.07	108.34	117.98
2	D	401	UMQ	CA-O1'-C1'	3.88	120.30	113.68
2	E	401	UMQ	CA-O1'-C1'	3.82	120.20	113.68
2	A	402	UMQ	CA-O1'-C1'	3.81	120.19	113.68
2	A	402	UMQ	O5'-C5'-C4'	3.69	117.35	109.72
2	A	401	UMQ	C2'-C3'-C4'	3.67	118.02	109.68
2	A	401	UMQ	O5'-C1'-C2'	3.52	117.60	110.37
2	B	401	UMQ	CA-O1'-C1'	3.44	119.56	113.68
2	C	401	UMQ	O5'-C5'-C4'	3.38	116.72	109.72
2	C	401	UMQ	C1'-O5'-C5'	3.34	120.24	113.72
2	E	401	UMQ	O1'-CA-CB	3.31	120.61	109.37
2	E	401	UMQ	C1-O1-C4'	-3.26	110.26	117.98
2	A	401	UMQ	O1'-CA-CB	2.82	118.95	109.37
2	B	401	UMQ	O1'-CA-CB	2.80	118.86	109.37
2	E	401	UMQ	C3-C4-C5	2.80	115.30	110.23
2	D	401	UMQ	O1'-CA-CB	2.78	118.81	109.37
2	A	401	UMQ	CA-O1'-C1'	2.77	118.41	113.68
2	D	401	UMQ	C1-O1-C4'	-2.77	111.42	117.98
2	A	402	UMQ	C1-O1-C4'	-2.67	111.64	117.98
2	E	401	UMQ	O5-C5-C4	2.64	114.45	109.70
2	C	401	UMQ	O1'-CA-CB	2.64	118.31	109.37
2	A	401	UMQ	O1-C1-C2	2.60	114.50	108.09
2	E	402	UMQ	O1'-CA-CB	2.53	119.72	109.79
2	A	402	UMQ	C1'-O5'-C5'	2.47	118.54	113.72
2	A	402	UMQ	O6-C6-C5	2.33	119.26	111.33
2	A	401	UMQ	O6-C6-C5	2.32	119.25	111.33
2	C	401	UMQ	O5'-C1'-C2'	2.31	115.12	110.37
2	B	401	UMQ	O5'-C5'-C4'	2.25	114.37	109.72
2	A	402	UMQ	O1'-CA-CB	2.25	116.99	109.37
2	B	401	UMQ	C1-O1-C4'	-2.19	112.78	117.98
2	E	401	UMQ	O5'-C5'-C6'	2.12	111.70	106.44
2	B	401	UMQ	O1'-C1'-C2'	2.12	111.48	108.27
2	C	401	UMQ	O5'-C5'-C6'	2.11	111.66	106.44
2	D	401	UMQ	O6-C6-C5	2.04	118.28	111.33
2	A	402	UMQ	C3'-C4'-C5'	2.03	115.43	110.93

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	UMQ	C2'-C1'-O1'-CA
2	A	402	UMQ	O5'-C1'-O1'-CA
2	C	401	UMQ	O5'-C1'-O1'-CA
2	C	401	UMQ	CB-CA-O1'-C1'
2	E	401	UMQ	CB-CA-O1'-C1'
2	B	401	UMQ	C5'-C4'-O1-C1
2	A	401	UMQ	C2-C1-O1-C4'
2	C	401	UMQ	C4'-C5'-C6'-O6'
2	E	401	UMQ	O5-C5-C6-O6
2	B	402	UMQ	CC-CD-CF-CG
2	E	401	UMQ	O5'-C5'-C6'-O6'
2	D	401	UMQ	O5'-C5'-C6'-O6'
2	A	402	UMQ	C4-C5-C6-O6
2	D	401	UMQ	C4'-C5'-C6'-O6'
2	E	401	UMQ	C4'-C5'-C6'-O6'
2	C	401	UMQ	O5'-C5'-C6'-O6'
2	A	401	UMQ	O1'-CA-CB-CC
2	A	401	UMQ	O5-C1-O1-C4'
2	A	402	UMQ	CD-CF-CG-CH
2	E	401	UMQ	C4-C5-C6-O6
2	B	401	UMQ	O1'-CA-CB-CC
2	A	402	UMQ	O5-C5-C6-O6
2	D	401	UMQ	C3'-C4'-O1-C1
2	A	401	UMQ	C5'-C4'-O1-C1
2	E	401	UMQ	C2'-C1'-O1'-CA
2	E	401	UMQ	O1'-CA-CB-CC
2	A	401	UMQ	C3'-C4'-O1-C1
2	A	401	UMQ	O5-C5-C6-O6
2	A	402	UMQ	CI-CJ-CK-CL
2	A	401	UMQ	C4-C5-C6-O6
2	E	401	UMQ	CA-CB-CC-CD
2	D	401	UMQ	C5'-C4'-O1-C1
2	E	402	UMQ	CC-CD-CF-CG
2	A	402	UMQ	CA-CB-CC-CD
2	A	401	UMQ	CB-CC-CD-CF
2	B	401	UMQ	CB-CA-O1'-C1'
2	E	402	UMQ	CH-CI-CJ-CK
2	B	401	UMQ	CA-CB-CC-CD
2	C	401	UMQ	CG-CH-CI-CJ
2	A	401	UMQ	CD-CF-CG-CH
2	A	401	UMQ	CH-CI-CJ-CK
2	B	402	UMQ	CG-CH-CI-CJ
2	A	401	UMQ	CI-CJ-CK-CL

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Mol	Chain	Res	Type	Atoms
2	B	401	UMQ	O5'-C5'-C6'-O6'
2	C	401	UMQ	CI-CJ-CK-CL
2	C	401	UMQ	C4-C5-C6-O6
2	E	401	UMQ	CD-CF-CG-CH
2	C	401	UMQ	CH-CI-CJ-CK
2	B	401	UMQ	C3'-C4'-O1-C1
2	D	401	UMQ	O1'-CA-CB-CC
2	E	401	UMQ	CB-CC-CD-CF
2	D	401	UMQ	CI-CJ-CK-CL
2	C	401	UMQ	CB-CC-CD-CF
2	C	401	UMQ	CA-CB-CC-CD
2	A	401	UMQ	O5'-C5'-C6'-O6'
2	A	401	UMQ	CA-CB-CC-CD
2	B	401	UMQ	CD-CF-CG-CH
2	D	401	UMQ	CH-CI-CJ-CK
2	A	401	UMQ	CB-CA-O1'-C1'
2	A	402	UMQ	CG-CH-CI-CJ
2	D	401	UMQ	CB-CC-CD-CF
2	C	401	UMQ	CC-CD-CF-CG
2	B	401	UMQ	O5-C5-C6-O6
2	E	402	UMQ	O1'-CA-CB-CC
2	D	401	UMQ	CA-CB-CC-CD
2	E	402	UMQ	CB-CC-CD-CF
2	D	401	UMQ	CD-CF-CG-CH
2	A	402	UMQ	C3'-C4'-O1-C1
2	E	401	UMQ	O5'-C1'-O1'-CA
2	E	401	UMQ	CC-CD-CF-CG
2	B	402	UMQ	CH-CI-CJ-CK
2	A	402	UMQ	CC-CD-CF-CG
2	B	402	UMQ	CI-CJ-CK-CL
2	C	401	UMQ	CD-CF-CG-CH
2	B	402	UMQ	CF-CG-CH-CI
2	C	401	UMQ	O5-C5-C6-O6
2	B	401	UMQ	CB-CC-CD-CF
2	A	402	UMQ	C5'-C4'-O1-C1
2	E	402	UMQ	CD-CF-CG-CH
2	E	401	UMQ	CG-CH-CI-CJ
2	E	401	UMQ	CH-CI-CJ-CK
2	C	401	UMQ	C5'-C4'-O1-C1
2	B	401	UMQ	CC-CD-CF-CG
2	B	401	UMQ	C4'-C5'-C6'-O6'
2	E	401	UMQ	C3'-C4'-O1-C1

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	402	UMQ	1	0
2	C	401	UMQ	5	0
2	D	401	UMQ	3	0
2	B	401	UMQ	2	0
2	E	401	UMQ	3	0
2	A	401	UMQ	20	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 then 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.

Ligand UMQ E 402

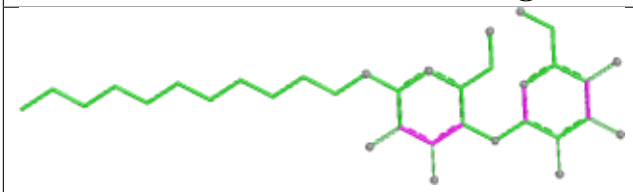
Bond lengths

Bond angles

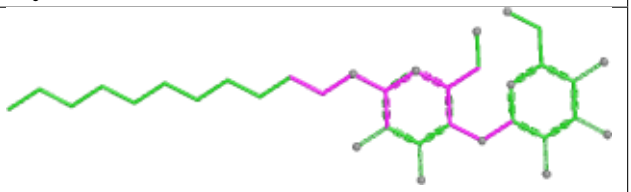
Torsions

Rings

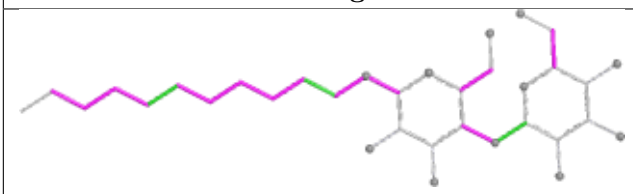
Ligand UMQ C 401



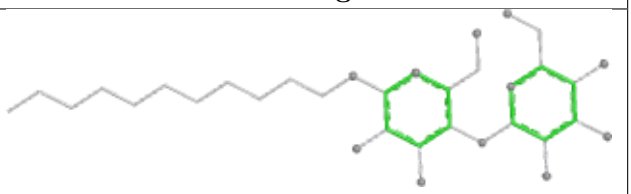
Bond lengths



Bond angles

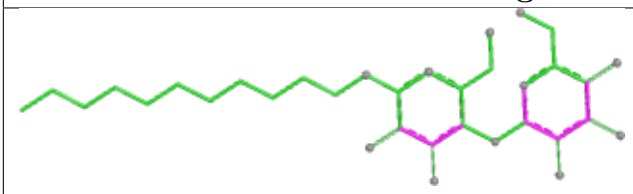


Torsions

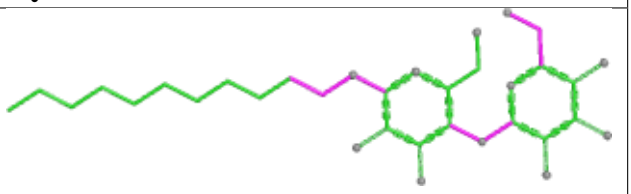


Rings

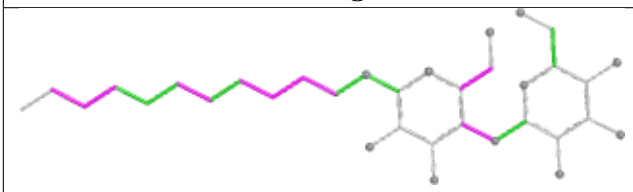
Ligand UMQ D 401



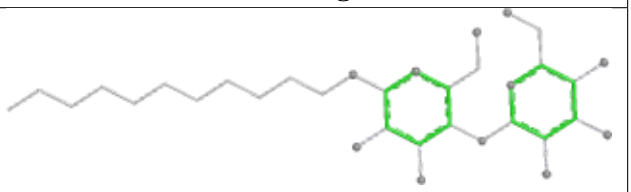
Bond lengths



Bond angles

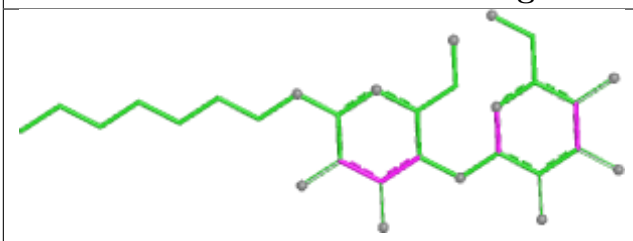


Torsions

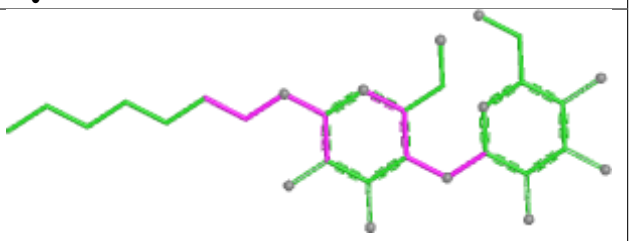


Rings

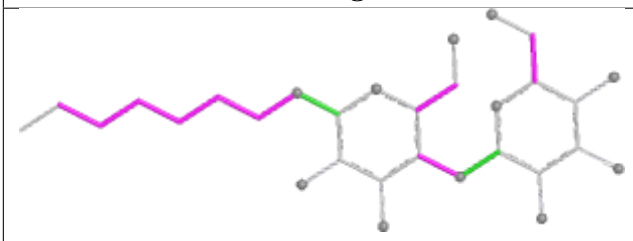
Ligand UMQ B 401



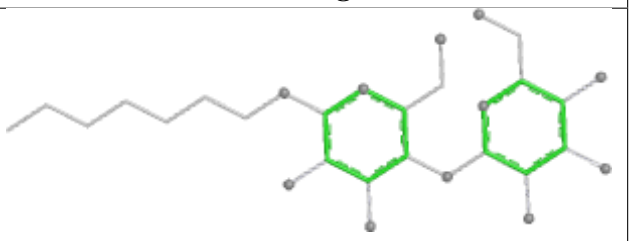
Bond lengths



Bond angles

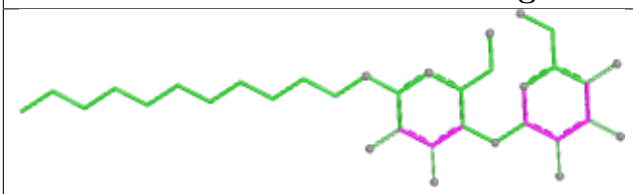


Torsions

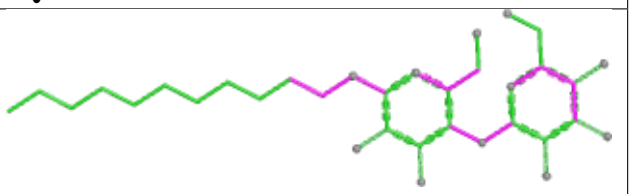


Rings

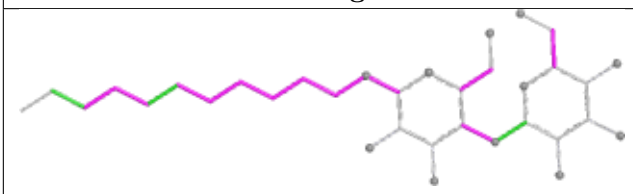
Ligand UMQ E 401



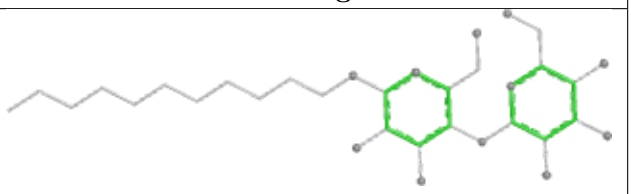
Bond lengths



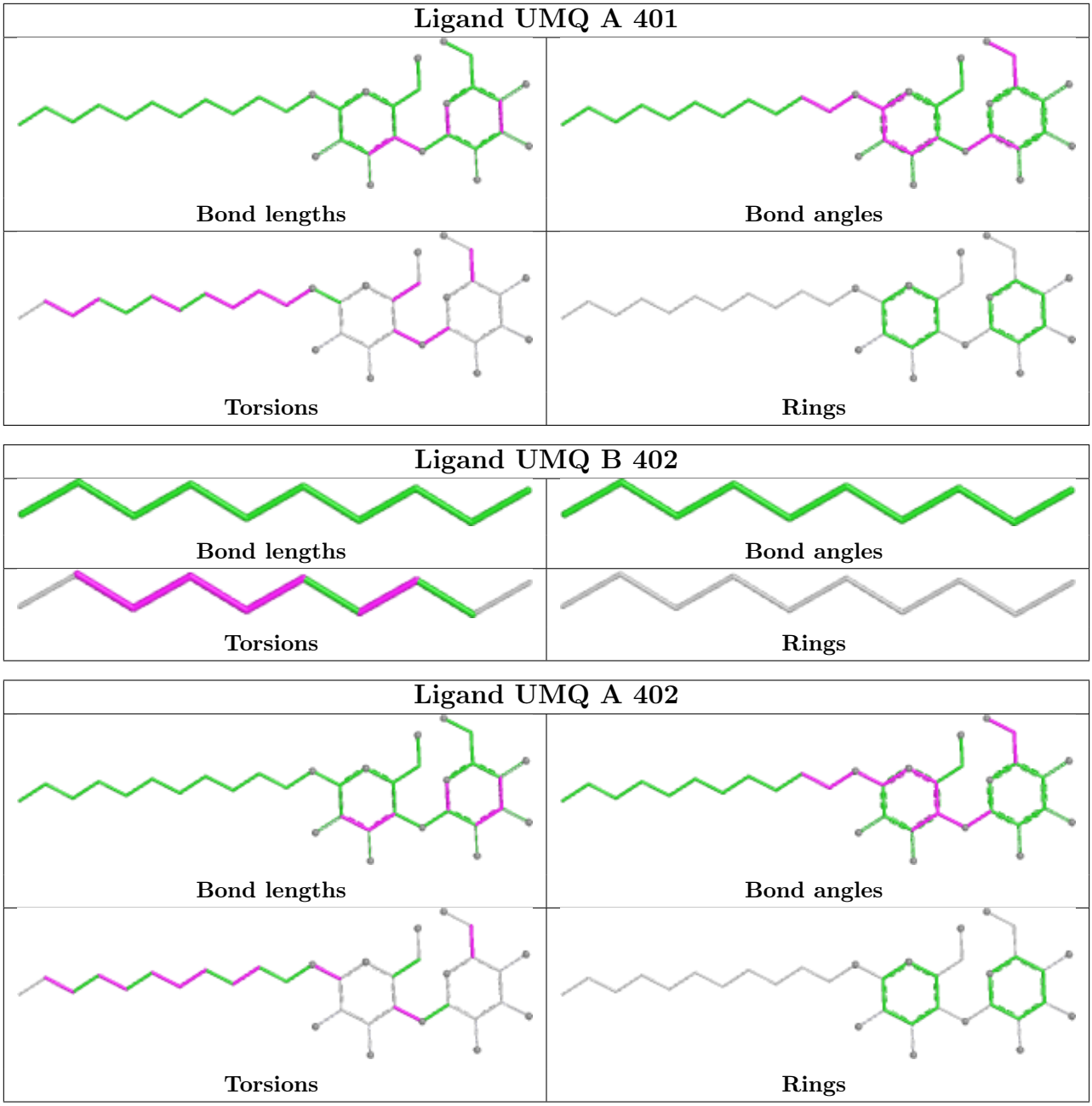
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	315/339 (92%)	-0.37	7 (2%)	62	48	39, 79, 147, 236	0
1	B	314/339 (92%)	-0.22	14 (4%)	33	21	41, 92, 170, 238	0
1	C	314/339 (92%)	-0.24	10 (3%)	47	31	48, 90, 168, 229	0
1	D	314/339 (92%)	-0.13	12 (3%)	40	26	47, 96, 188, 242	0
1	E	317/339 (93%)	-0.39	9 (2%)	53	37	33, 72, 131, 188	0
All	All	1574/1695 (92%)	-0.27	52 (3%)	46	30	33, 85, 168, 242	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	10	ASP	5.9
1	B	126	ILE	5.7
1	D	11	GLY	5.4
1	B	127	VAL	5.1
1	E	165	LEU	4.7
1	B	128	PHE	4.7
1	A	22	SER	4.3
1	D	12	SER	4.3
1	D	122	LYS	4.2
1	B	86	ASP	4.1
1	C	85	GLU	3.9
1	B	18	LEU	3.8
1	B	16	PRO	3.8
1	A	23	PHE	3.8
1	D	8	ALA	3.6
1	C	166	LEU	3.6
1	C	34	TYR	3.4
1	D	116	HIS	3.2
1	A	122	LYS	3.1
1	D	23	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	85	GLU	3.0
1	C	44	LEU	3.0
1	C	125	ARG	3.0
1	B	23	PHE	3.0
1	B	10	ASP	2.9
1	E	29	ILE	2.9
1	E	26	TYR	2.9
1	A	124	PRO	2.8
1	E	16	PRO	2.8
1	C	316	TRP	2.6
1	C	165	LEU	2.6
1	B	85	GLU	2.5
1	B	11	GLY	2.5
1	E	18	LEU	2.5
1	D	39	GLU	2.4
1	C	167	ALA	2.4
1	B	124	PRO	2.3
1	E	15	GLU	2.3
1	D	72	ASP	2.3
1	E	22	SER	2.3
1	C	317	ILE	2.3
1	B	15	GLU	2.2
1	A	21	ILE	2.2
1	A	317	ILE	2.2
1	C	11	GLY	2.2
1	D	10	ASP	2.1
1	D	25	ASP	2.1
1	B	29	ILE	2.1
1	D	165	LEU	2.1
1	B	165	LEU	2.0
1	E	23	PHE	2.0
1	D	126	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	407	1/1	0.64	0.65	127,127,127,127	0
3	MG	E	405	1/1	0.65	0.60	98,98,98,98	0
2	UMQ	A	402	34/34	0.71	0.48	92,165,173,175	0
2	UMQ	E	402	13/34	0.74	0.57	50,54,142,144	0
3	MG	D	409	1/1	0.75	0.38	113,113,113,113	0
3	MG	D	404	1/1	0.75	0.45	77,77,77,77	0
2	UMQ	D	401	34/34	0.76	0.55	80,252,258,261	0
3	MG	E	403	1/1	0.77	0.21	78,78,78,78	0
3	MG	E	407	1/1	0.77	0.43	63,63,63,63	0
3	MG	D	406	1/1	0.78	0.40	85,85,85,85	0
2	UMQ	A	401	34/34	0.80	0.38	75,169,189,190	0
2	UMQ	E	401	34/34	0.81	0.28	59,195,198,199	0
2	UMQ	B	401	30/34	0.83	0.35	105,193,208,210	0
2	UMQ	C	401	34/34	0.84	0.53	113,176,185,186	0
3	MG	E	411	1/1	0.84	0.32	80,80,80,80	0
3	MG	A	404	1/1	0.85	0.26	77,77,77,77	0
3	MG	D	403	1/1	0.85	0.14	84,84,84,84	0
3	MG	B	405	1/1	0.87	0.87	75,75,75,75	0
3	MG	A	409	1/1	0.87	0.21	123,123,123,123	0
3	MG	E	406	1/1	0.88	0.61	82,82,82,82	0
3	MG	D	411	1/1	0.89	0.12	92,92,92,92	0
3	MG	A	403	1/1	0.89	0.20	74,74,74,74	0
3	MG	D	402	1/1	0.90	0.27	106,106,106,106	0
3	MG	E	409	1/1	0.91	0.57	81,81,81,81	0
3	MG	E	410	1/1	0.91	0.25	92,92,92,92	0
3	MG	A	405	1/1	0.91	0.09	93,93,93,93	0
3	MG	A	406	1/1	0.92	0.14	96,96,96,96	0
3	MG	C	404	1/1	0.92	0.10	72,72,72,72	0
2	UMQ	B	402	10/34	0.92	0.97	79,95,96,98	0
3	MG	B	403	1/1	0.92	0.73	76,76,76,76	0
3	MG	D	408	1/1	0.93	0.17	89,89,89,89	0
3	MG	C	403	1/1	0.94	0.18	71,71,71,71	0
3	MG	B	404	1/1	0.94	0.51	61,61,61,61	0
3	MG	A	408	1/1	0.94	0.13	94,94,94,94	0
3	MG	D	410	1/1	0.94	0.16	87,87,87,87	0
3	MG	D	405	1/1	0.95	0.15	49,49,49,49	0
3	MG	A	407	1/1	0.95	0.18	66,66,66,66	0

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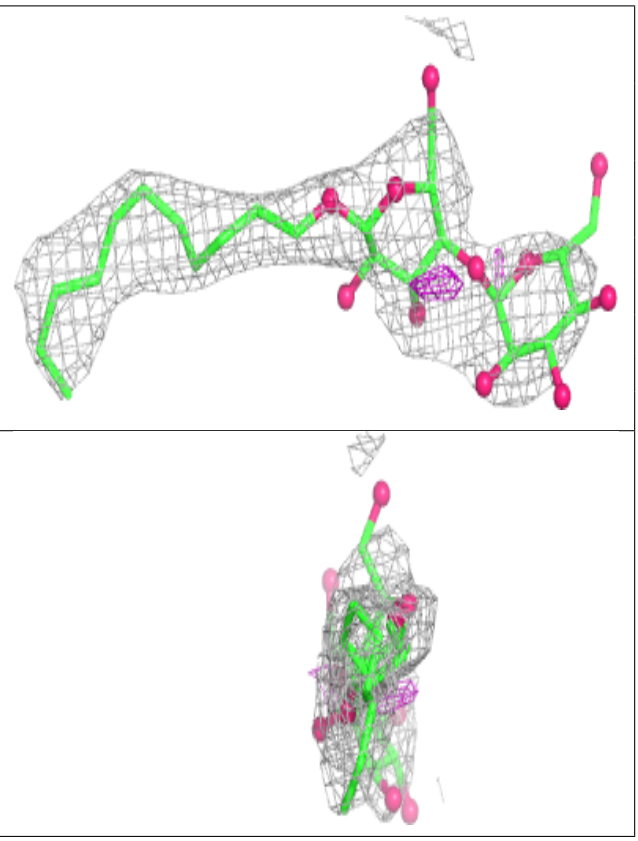
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	E	404	1/1	0.95	0.23	75,75,75,75	0
3	MG	E	408	1/1	0.96	0.11	89,89,89,89	0
3	MG	C	402	1/1	0.97	0.30	55,55,55,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

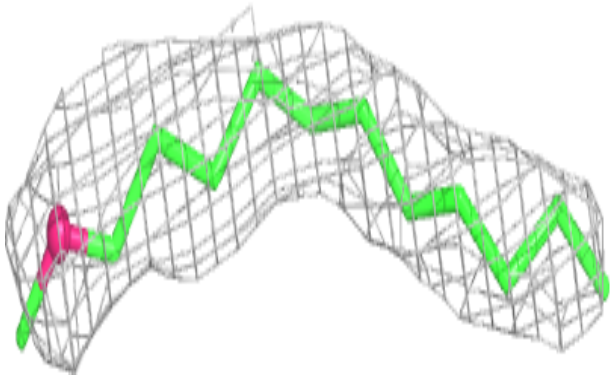
Electron density around UMQ A 402:

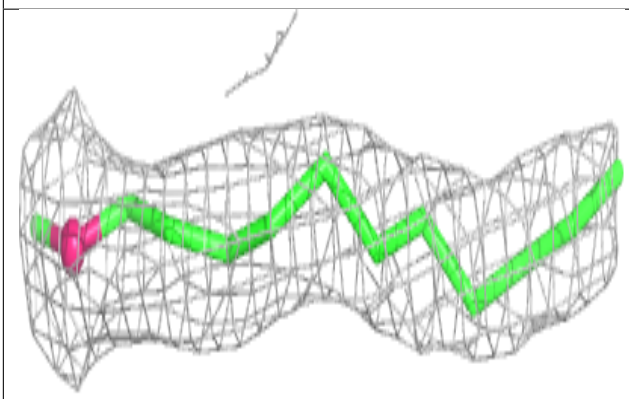
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around UMQ E 402:

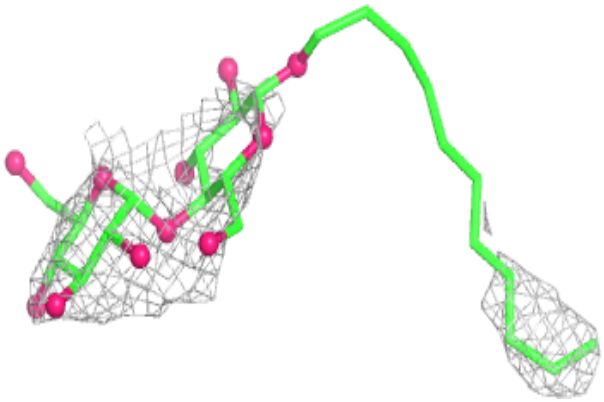
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

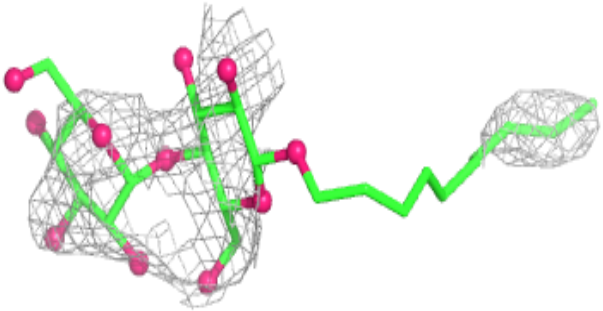


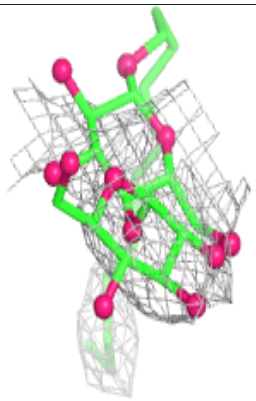


Electron density around UMQ D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

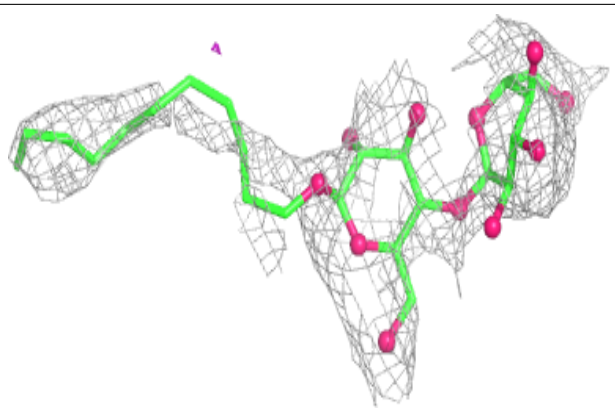


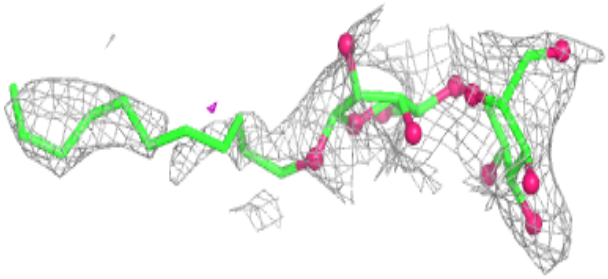


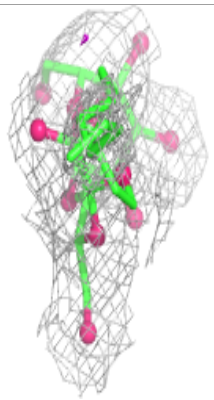


Electron density around UMQ A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

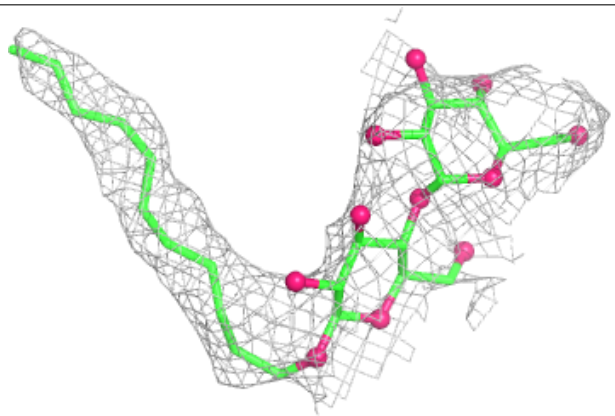


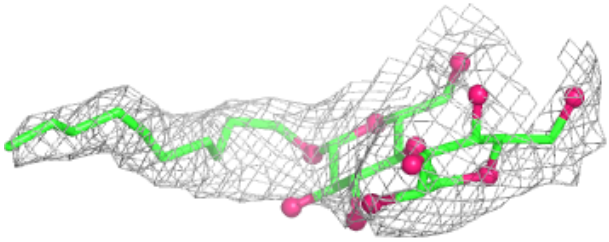


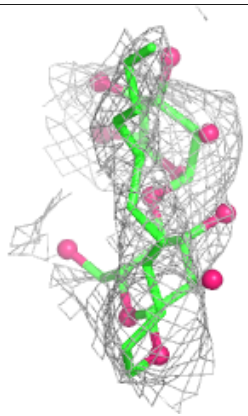


Electron density around UMQ E 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

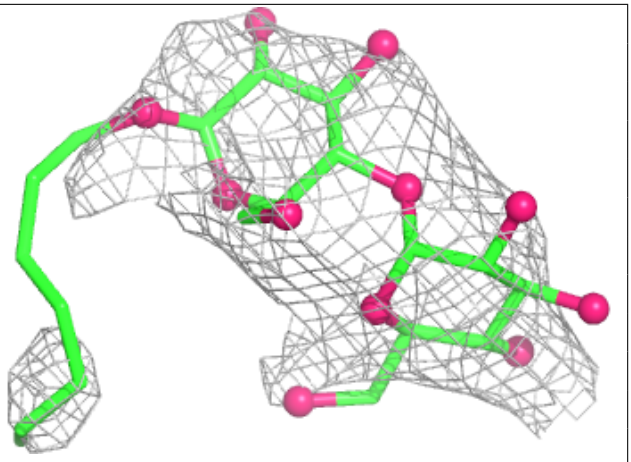


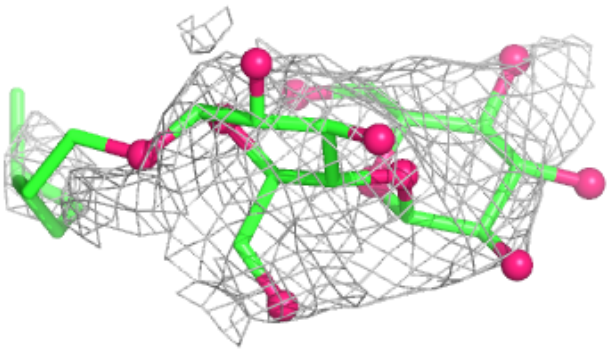




Electron density around UMQ B 401:

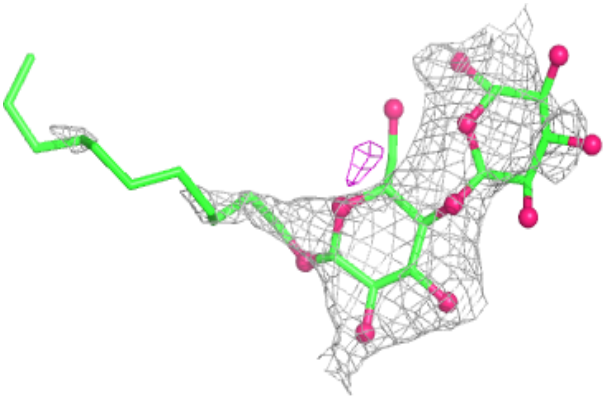
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

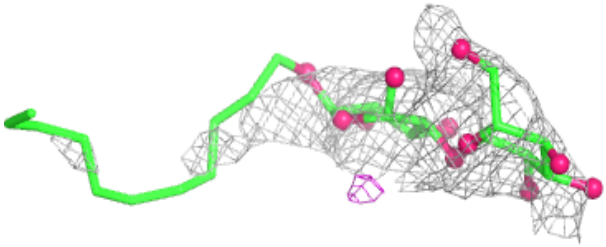


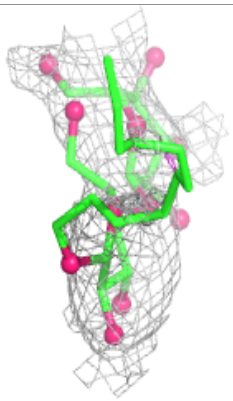


Electron density around UMQ C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

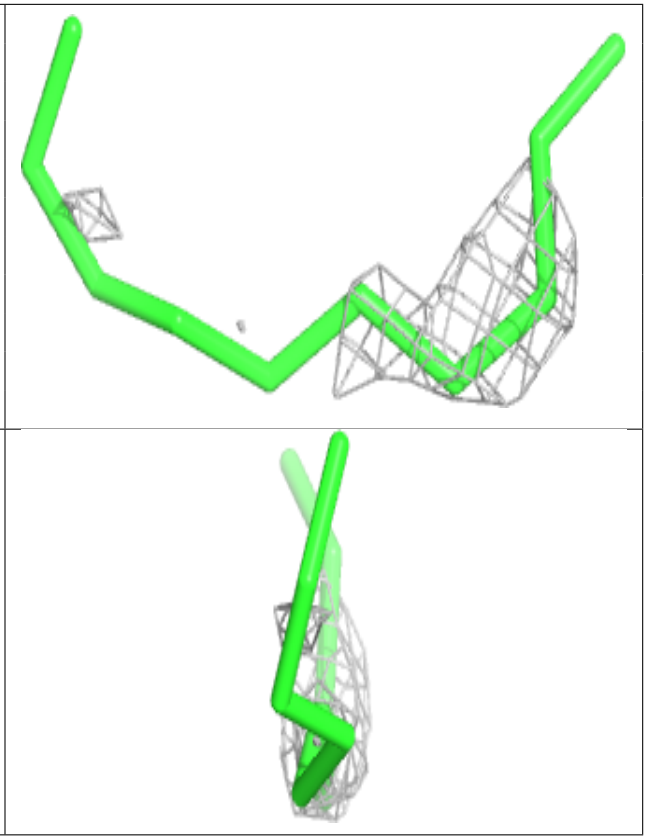






Electron density around UMQ B 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.