



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:11 AM GMT

PDB ID : 3DFY
Title : Crystal structure of apo dipeptide epimerase from *Thermotoga maritima*
Authors : Fedorov, A.A.; Fedorov, E.V.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2008-06-12
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

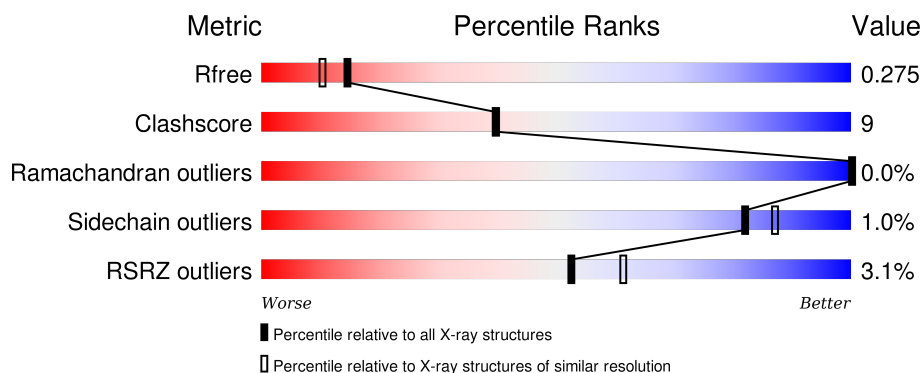
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	345	<div> <div>2%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	B	345	<div> <div>3%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>
1	C	345	<div> <div>4%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	D	345	<div> <div>5%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	E	345	<div> <div>3%</div> <div>72%</div> <div>23%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	345	<div> <div>4%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	G	345	<div> <div>2%</div> <div>71%</div> <div>24%</div> <div>..</div> </div>
1	H	345	<div> <div>%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	I	345	<div> <div>%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	J	345	<div> <div>4%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>
1	K	345	<div> <div>3%</div> <div>70%</div> <div>25%</div> <div>..</div> </div>
1	L	345	<div> <div>2%</div> <div>78%</div> <div>18%</div> <div>.</div> </div>
1	M	345	<div> <div>4%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	N	345	<div> <div>3%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>
1	O	345	<div> <div>3%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
1	P	345	<div> <div>3%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 43115 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 Muconate cycloisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2660	1689	457	504	10			
1	B	332	Total	C	N	O	S	0	0	0
			2622	1664	450	498	10			
1	C	338	Total	C	N	O	S	0	0	0
			2660	1689	457	504	10			
1	D	332	Total	C	N	O	S	0	0	0
			2622	1664	450	498	10			
1	E	330	Total	C	N	O	S	0	0	0
			2606	1653	447	496	10			
1	F	333	Total	C	N	O	S	0	0	0
			2628	1667	451	500	10			
1	G	330	Total	C	N	O	S	0	0	0
			2606	1653	447	496	10			
1	H	331	Total	C	N	O	S	0	0	0
			2615	1659	449	497	10			
1	I	338	Total	C	N	O	S	0	0	0
			2660	1689	457	504	10			
1	J	331	Total	C	N	O	S	0	0	0
			2615	1659	449	497	10			
1	K	330	Total	C	N	O	S	0	0	0
			2606	1653	447	496	10			
1	L	331	Total	C	N	O	S	0	0	0
			2612	1656	448	498	10			
1	M	338	Total	C	N	O	S	0	0	0
			2660	1689	457	504	10			
1	N	332	Total	C	N	O	S	0	0	0
			2621	1662	450	499	10			
1	O	331	Total	C	N	O	S	0	0	0
			2612	1656	448	498	10			
1	P	332	Total	C	N	O	S	0	0	0
			2622	1664	450	498	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total 1	Mg 1	0	0
2	G	1	Total 1	Mg 1	0	0
2	J	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	K	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	H	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	I	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	A	1	Total 1	Mg 1	0	0
2	N	1	Total 1	Mg 1	0	0
2	O	1	Total 1	Mg 1	0	0
2	L	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0
2	M	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	73	Total 73	O 73	0	0
3	C	67	Total 67	O 67	0	0

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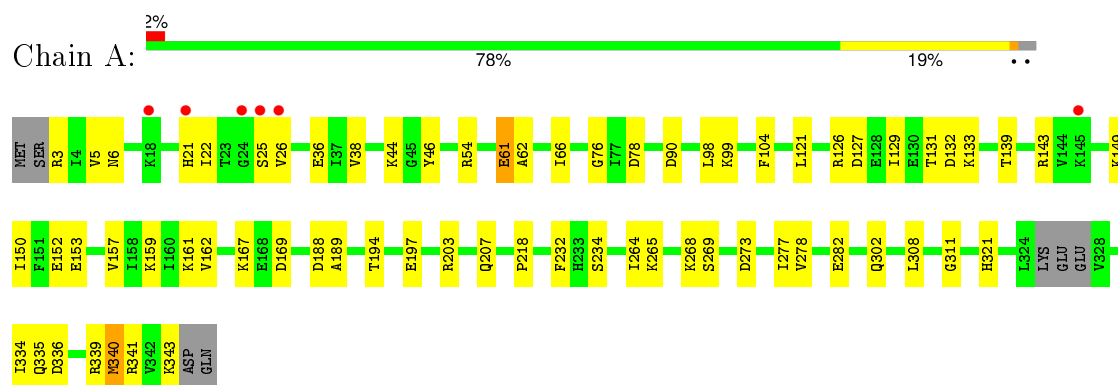
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	52	Total	O	0	0
			52	52		
3	E	63	Total	O	0	0
			63	63		
3	F	63	Total	O	0	0
			63	63		
3	G	65	Total	O	0	0
			65	65		
3	H	78	Total	O	0	0
			78	78		
3	I	77	Total	O	0	0
			77	77		
3	J	75	Total	O	0	0
			75	75		
3	K	56	Total	O	0	0
			56	56		
3	L	59	Total	O	0	0
			59	59		
3	M	67	Total	O	0	0
			67	67		
3	N	65	Total	O	0	0
			65	65		
3	O	63	Total	O	0	0
			63	63		
3	P	66	Total	O	0	0
			66	66		

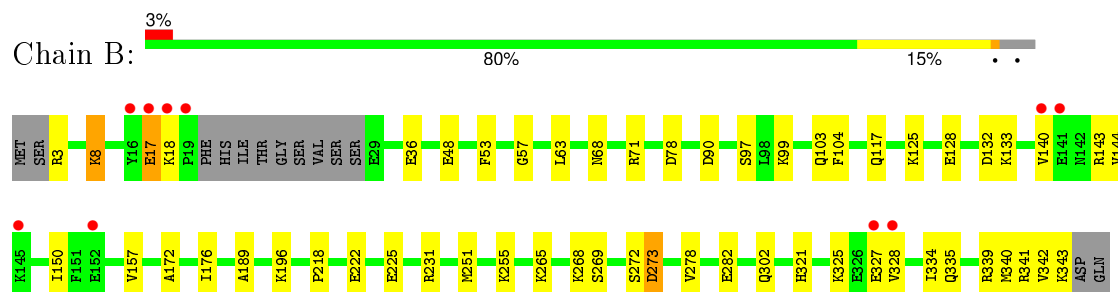
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

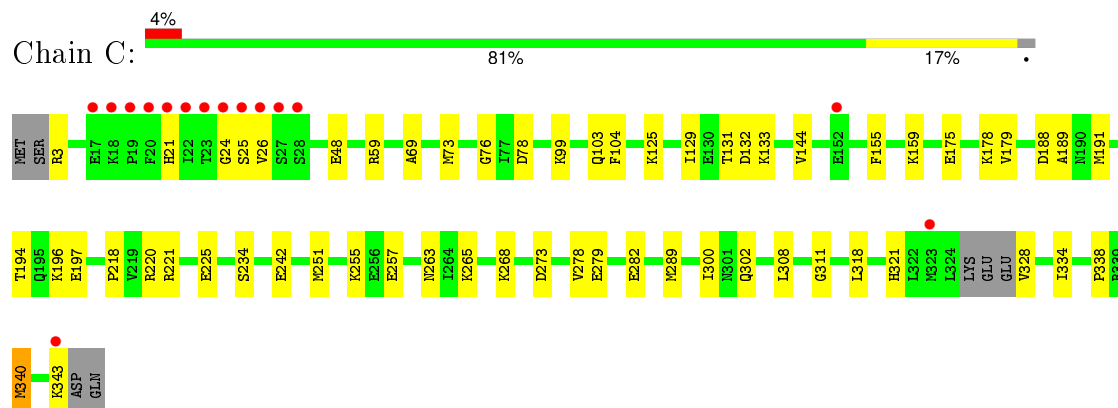
- Molecule 1: Muconate cycloisomerase



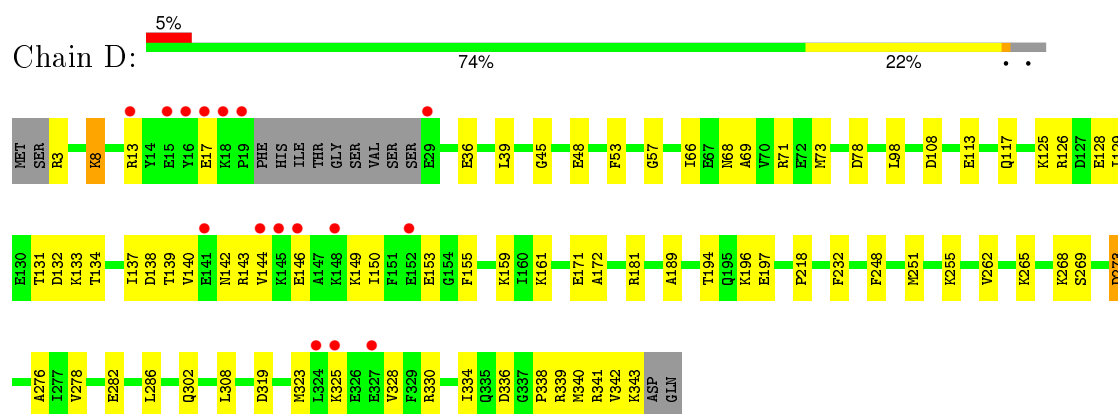
- Molecule 1: Muconate cycloisomerase



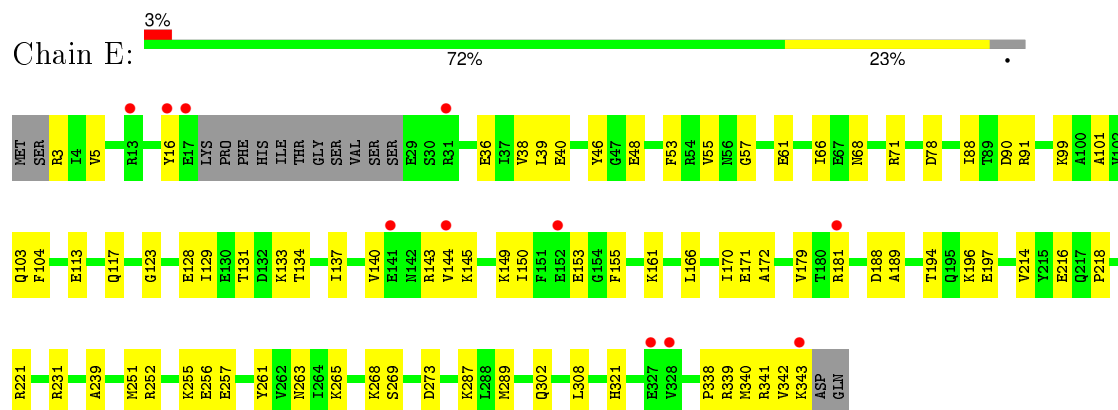
- Molecule 1: Muconate cycloisomerase



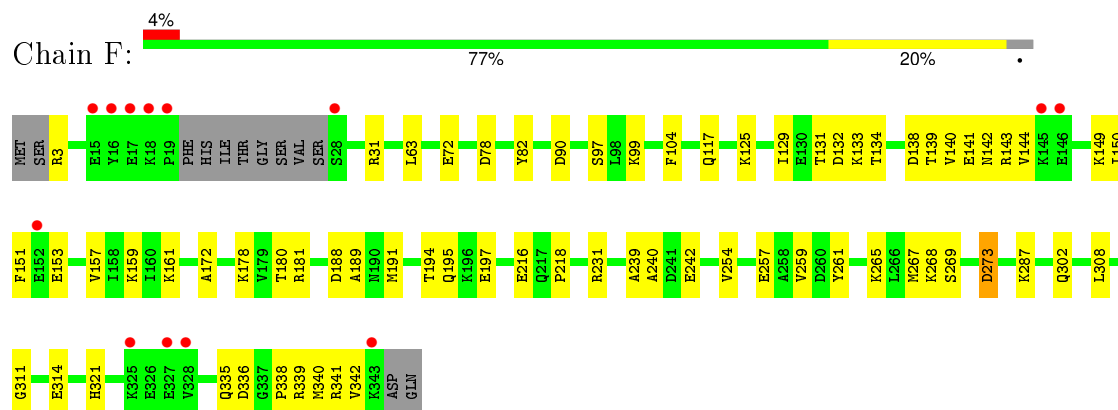
- Molecule 1: Muconate cycloisomerase



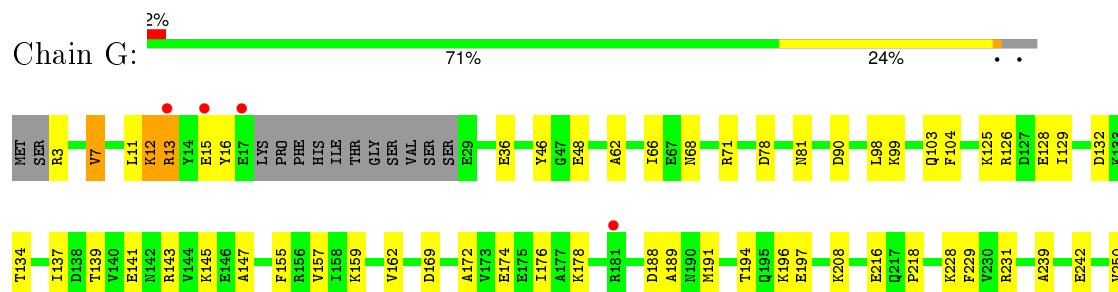
• Molecule 1: Muconate cycloisomerase



• Molecule 1: Muconate cycloisomerase

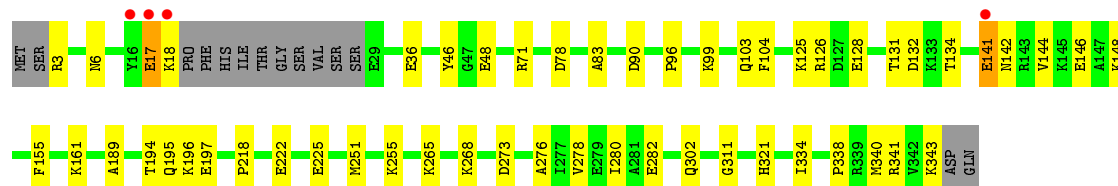
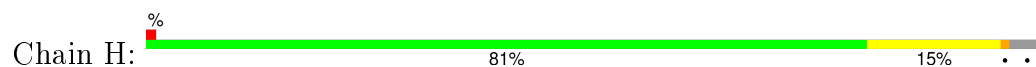


• Molecule 1: Muconate cycloisomerase

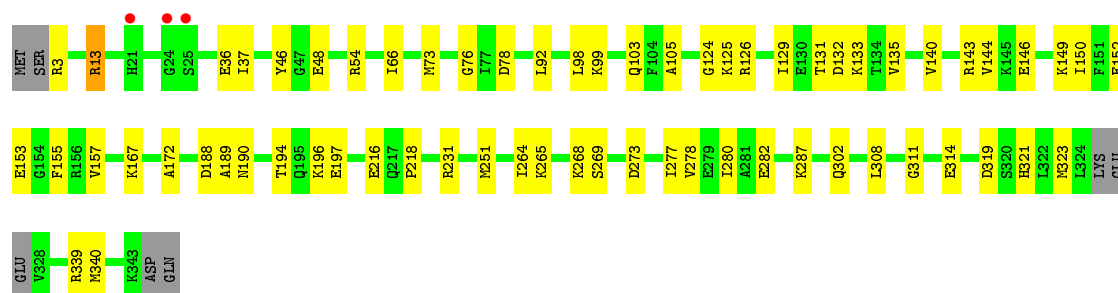




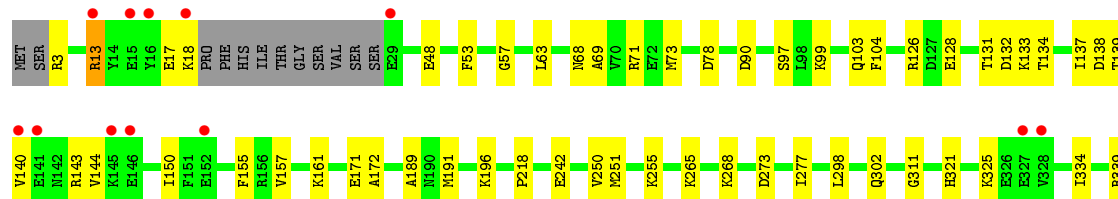
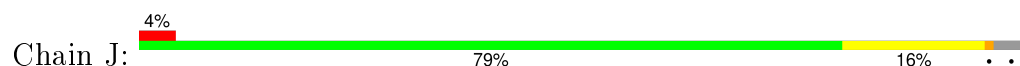
- Molecule 1: Muconate cycloisomerase



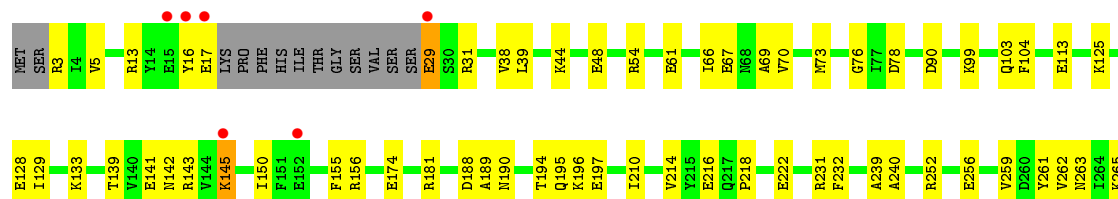
- Molecule 1: Muconate cycloisomerase



- Molecule 1: Muconate cycloisomerase

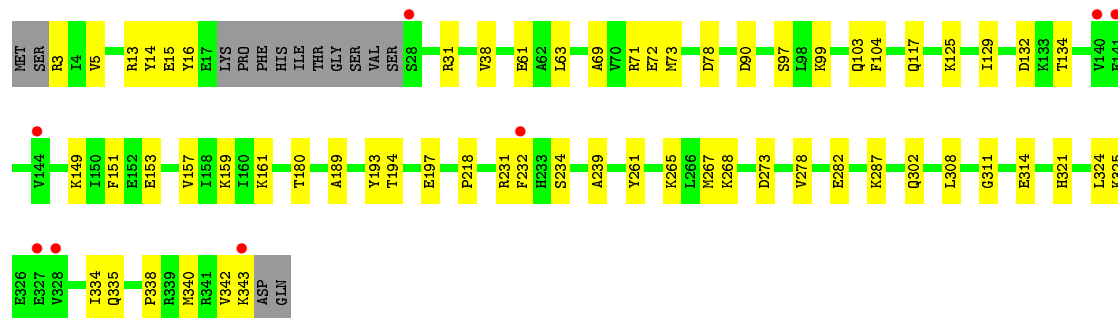
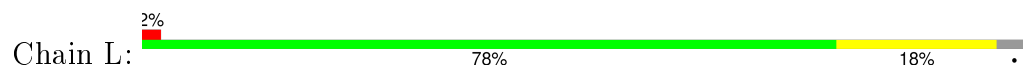


- Molecule 1: Muconate cycloisomerase

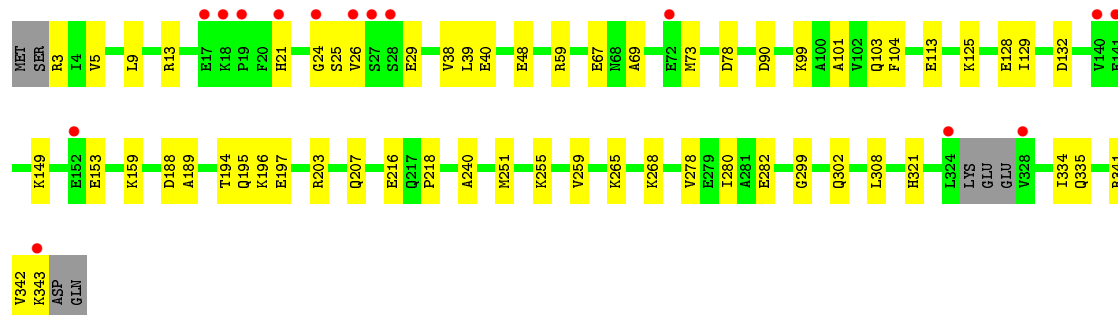
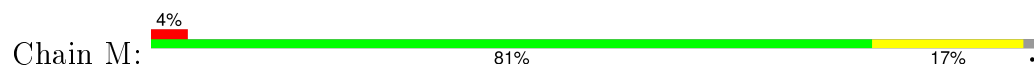




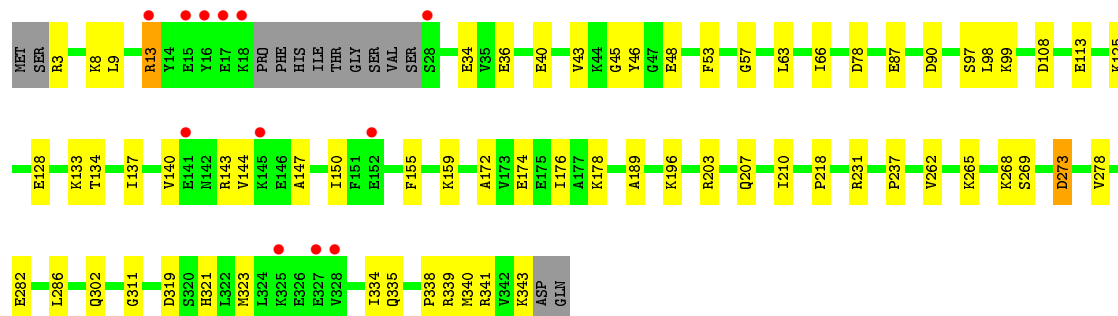
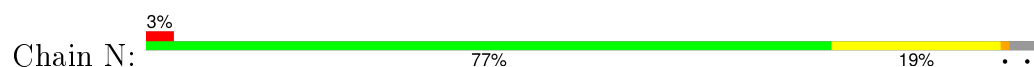
• Molecule 1: Muconate cycloisomerase



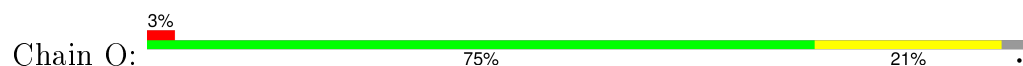
• Molecule 1: Muconate cycloisomerase

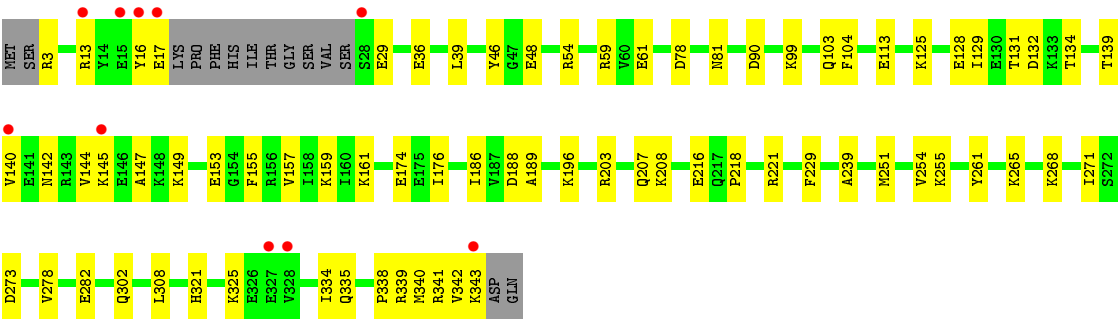


• Molecule 1: Muconate cycloisomerase

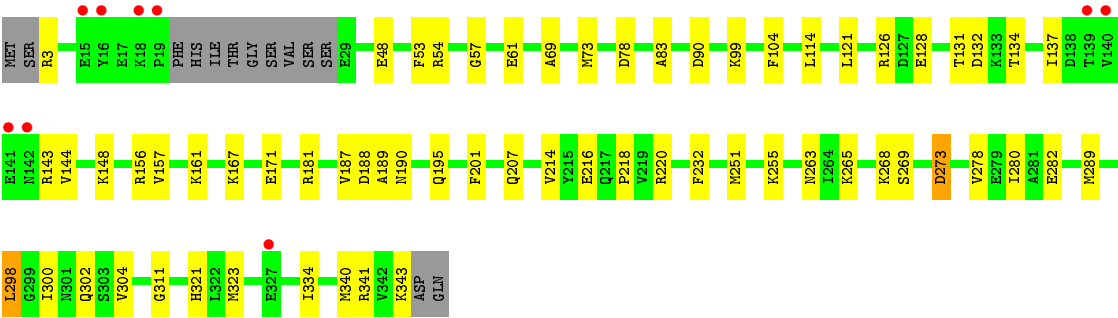
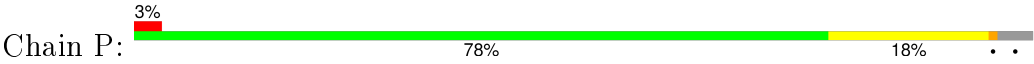


• Molecule 1: Muconate cycloisomerase





• Molecule 1: Muconate cycloisomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.81Å 165.14Å 209.64Å 90.00° 96.06° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 39.73 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-2.10) 93.9 (39.73-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.88Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.277 0.246 , 0.275	Depositor DCC
R_{free} test set	20322 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.778	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.42$	Xtriage
Outliers	12 of 534042 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	43115	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.51 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.5515e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.35	0/2698	0.62	0/3624
1	B	0.34	0/2658	0.61	0/3568
1	C	0.34	0/2698	0.62	0/3624
1	D	0.33	0/2658	0.60	0/3568
1	E	0.35	0/2641	0.61	0/3545
1	F	0.34	0/2664	0.60	0/3576
1	G	0.35	0/2641	0.61	0/3545
1	H	0.35	0/2650	0.62	0/3556
1	I	0.35	0/2698	0.62	0/3624
1	J	0.35	0/2650	0.61	0/3556
1	K	0.34	0/2641	0.61	0/3545
1	L	0.32	0/2647	0.60	0/3553
1	M	0.33	0/2698	0.62	0/3624
1	N	0.34	0/2656	0.61	0/3564
1	O	0.34	0/2647	0.61	0/3553
1	P	0.34	0/2658	0.61	0/3568
All	All	0.34	0/42603	0.61	0/57193

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2660	0	2697	43	0
1	B	2622	0	2661	42	0
1	C	2660	0	2697	48	0
1	D	2622	0	2661	61	0
1	E	2606	0	2641	57	0
1	F	2628	0	2666	46	0
1	G	2606	0	2641	64	0
1	H	2615	0	2654	37	0
1	I	2660	0	2697	50	0
1	J	2615	0	2654	47	0
1	K	2606	0	2641	61	0
1	L	2612	0	2646	37	0
1	M	2660	0	2697	40	0
1	N	2621	0	2659	44	0
1	O	2612	0	2646	53	0
1	P	2622	0	2661	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	83	0	0	2	0
3	B	73	0	0	1	0
3	C	67	0	0	1	0
3	D	52	0	0	0	0
3	E	63	0	0	0	0
3	F	63	0	0	1	0
3	G	65	0	0	0	0
3	H	78	0	0	1	0
3	I	77	0	0	3	0
3	J	75	0	0	0	0
3	K	56	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	59	0	0	1	0
3	M	67	0	0	0	0
3	N	65	0	0	0	0
3	O	63	0	0	0	0
3	P	66	0	0	2	0
All	All	43115	0	42619	742	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (742) 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:O:334:ILE:HD11	1:O:343:LYS:HG2	1.50	0.92
1:C:191:MET:HE3	1:C:221:ARG:H	1.37	0.89
1:D:334:ILE:HD11	1:D:343:LYS:HE3	1.59	0.84
1:J:131:THR:HG22	1:J:340:MET:HE1	1.60	0.84
1:G:339:ARG:HB2	1:G:339:ARG:HH11	1.48	0.79
1:K:13:ARG:HD2	1:K:31:ARG:HG2	1.66	0.78
1:B:68:ASN:HD21	1:B:71:ARG:HH22	1.32	0.77
1:L:134:THR:HG21	1:L:161:LYS:HE3	1.66	0.77
1:D:339:ARG:HB2	1:D:339:ARG:HH11	1.50	0.77
1:G:339:ARG:HB2	1:G:339:ARG:NH1	2.02	0.74
1:D:334:ILE:HD11	1:D:343:LYS:HB2	1.70	0.74
1:K:222:GLU:HG2	3:K:412:HOH:O	1.86	0.73
1:I:265:LYS:HB2	1:I:268:LYS:HE2	1.70	0.73
1:E:231:ARG:HH21	1:H:195:GLN:HE22	1.38	0.71
1:H:265:LYS:HB2	1:H:268:LYS:HE2	1.71	0.71
1:O:134:THR:HG21	1:O:161:LYS:HE3	1.73	0.71
1:C:191:MET:CE	1:C:221:ARG:H	2.04	0.70
1:C:334:ILE:HD11	1:C:343:LYS:HD3	1.73	0.69
1:O:339:ARG:HH11	1:O:339:ARG:HB2	1.55	0.69
1:F:133:LYS:HB3	1:F:150:ILE:HD13	1.75	0.69
1:J:133:LYS:HD3	1:J:150:ILE:HG12	1.72	0.69
1:A:139:THR:O	1:A:143:ARG:HG3	1.92	0.69
1:B:68:ASN:ND2	1:B:71:ARG:HH22	1.89	0.69
1:B:334:ILE:HD11	1:B:343:LYS:HE3	1.74	0.68
1:P:298:LEU:HD12	1:P:298:LEU:O	1.94	0.68
1:O:334:ILE:HD11	1:O:343:LYS:CG	2.21	0.68
1:C:191:MET:HE3	1:C:221:ARG:N	2.09	0.68
1:L:265:LYS:HB2	1:L:268:LYS:HE2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:13:ARG:HH11	1:J:13:ARG:H	1.41	0.68
1:J:189:ALA:HB3	1:J:218:PRO:HA	1.76	0.67
1:F:195:GLN:HE22	1:G:231:ARG:HH22	1.39	0.67
1:F:339:ARG:HB2	1:F:339:ARG:HH11	1.60	0.67
1:D:140:VAL:HG21	1:D:171:GLU:OE1	1.95	0.66
1:C:225:GLU:OE1	1:F:257:GLU:HG2	1.96	0.66
1:K:142:ASN:HA	1:K:145:LYS:HG2	1.76	0.66
1:O:339:ARG:NH1	1:O:339:ARG:HB2	2.10	0.66
1:J:17:GLU:HA	1:J:325:LYS:HE3	1.78	0.66
1:K:265:LYS:HB2	1:K:268:LYS:HE2	1.78	0.66
1:G:251:MET:HG3	1:G:255:LYS:HE3	1.77	0.66
1:F:189:ALA:HB3	1:F:218:PRO:HA	1.78	0.65
1:K:181:ARG:HH11	1:K:181:ARG:HG2	1.61	0.65
1:I:149:LYS:O	1:I:152:GLU:HG2	1.95	0.65
1:D:265:LYS:HB2	1:D:268:LYS:HE2	1.79	0.65
1:F:134:THR:HG21	1:F:161:LYS:HE3	1.78	0.65
1:J:339:ARG:NH1	1:J:339:ARG:HB2	2.11	0.65
1:E:129:ILE:HG23	1:E:308:LEU:HD23	1.79	0.65
1:O:125:LYS:HE3	1:P:83:ALA:HB1	1.79	0.65
1:D:133:LYS:HD2	1:D:155:PHE:CE2	2.31	0.65
1:H:131:THR:HG22	1:H:340:MET:HE1	1.79	0.64
1:G:189:ALA:HB3	1:G:218:PRO:HA	1.78	0.64
1:F:139:THR:HB	1:F:142:ASN:HD22	1.63	0.64
1:D:339:ARG:HB2	1:D:339:ARG:NH1	2.12	0.64
1:F:125:LYS:HG2	1:F:311:GLY:HA3	1.80	0.64
1:O:128:GLU:HB2	1:O:341:ARG:HG2	1.79	0.63
1:A:133:LYS:HB3	1:A:150:ILE:HD13	1.79	0.63
1:K:145:LYS:NZ	1:K:145:LYS:HB2	2.13	0.63
1:G:325:LYS:NZ	1:G:325:LYS:HB3	2.13	0.63
1:C:131:THR:HG22	1:C:340:MET:HE1	1.80	0.63
1:K:231:ARG:HH21	1:P:195:GLN:HE22	1.47	0.63
1:O:149:LYS:O	1:O:153:GLU:HG3	1.98	0.63
1:L:287:LYS:HD3	1:L:314:GLU:HG3	1.81	0.63
1:I:287:LYS:HE3	1:I:314:GLU:HG3	1.81	0.62
1:K:287:LYS:HE2	1:K:314:GLU:HG3	1.79	0.62
1:F:265:LYS:HB2	1:F:268:LYS:HE2	1.81	0.62
1:J:265:LYS:HB2	1:J:268:LYS:HE2	1.80	0.62
1:K:263:ASN:HB2	1:K:289:MET:HE3	1.81	0.62
1:O:189:ALA:HB3	1:O:218:PRO:HA	1.79	0.62
1:I:143:ARG:HD3	1:I:172:ALA:HB1	1.81	0.62
1:G:265:LYS:HB2	1:G:268:LYS:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:99:LYS:O	1:L:103:GLN:HG3	1.99	0.62
1:J:137:ILE:HG12	1:J:143:ARG:HH21	1.64	0.62
1:D:134:THR:HG21	1:D:161:LYS:NZ	2.14	0.62
1:K:54:ARG:HH12	1:K:190:ASN:HB3	1.65	0.62
1:P:181:ARG:NH1	1:P:181:ARG:HB2	2.15	0.62
1:O:334:ILE:CD1	1:O:343:LYS:HG2	2.26	0.61
1:G:134:THR:OG1	1:G:159:LYS:HE2	1.99	0.61
1:E:265:LYS:HB2	1:E:268:LYS:HE2	1.82	0.61
1:C:175:GLU:HA	1:C:178:LYS:HD3	1.81	0.61
1:H:134:THR:HG21	1:H:161:LYS:HE3	1.82	0.61
1:P:134:THR:HG21	1:P:161:LYS:HE3	1.82	0.61
1:H:17:GLU:O	1:H:18:LYS:HG3	2.00	0.61
1:D:251:MET:HG3	1:D:255:LYS:HE3	1.81	0.61
1:L:334:ILE:HD11	1:L:343:LYS:HB2	1.82	0.61
1:B:265:LYS:HB2	1:B:268:LYS:HE2	1.81	0.61
1:B:339:ARG:HB2	1:B:339:ARG:NH1	2.16	0.60
1:K:252:ARG:O	1:K:256:GLU:HG2	2.00	0.60
1:J:68:ASN:ND2	1:J:71:ARG:HH22	1.98	0.60
1:M:128:GLU:OE1	1:M:341:ARG:HD2	2.02	0.60
1:F:90:ASP:HA	1:F:99:LYS:HD2	1.83	0.60
1:N:128:GLU:OE2	1:N:339:ARG:HD2	2.01	0.59
1:J:140:VAL:O	1:J:144:VAL:HG23	2.02	0.59
1:I:13:ARG:HG3	1:I:13:ARG:HH21	1.67	0.59
1:A:265:LYS:HB2	1:A:268:LYS:HE2	1.83	0.59
1:F:139:THR:HG22	1:F:141:GLU:H	1.67	0.59
1:N:140:VAL:O	1:N:144:VAL:HG23	2.03	0.59
1:P:131:THR:HG22	1:P:340:MET:HE1	1.83	0.59
1:L:194:THR:OG1	1:L:197:GLU:HG3	2.03	0.59
1:E:149:LYS:O	1:E:153:GLU:HG3	2.03	0.59
1:I:278:VAL:O	1:I:282:GLU:HG3	2.03	0.59
1:L:13:ARG:NH2	1:L:31:ARG:HH12	2.01	0.58
1:J:104:PHE:CD2	1:J:302:GLN:HG2	2.38	0.58
1:K:90:ASP:OD1	1:K:99:LYS:HE3	2.03	0.58
1:D:8:LYS:HD3	1:D:36:GLU:OE1	2.03	0.58
1:D:48:GLU:H	1:D:302:GLN:NE2	1.99	0.58
1:M:334:ILE:HD11	1:M:343:LYS:HB2	1.85	0.58
1:O:265:LYS:HB2	1:O:268:LYS:HE2	1.85	0.58
1:B:132:ASP:HB3	1:B:157:VAL:HG12	1.85	0.58
1:L:3:ARG:HA	1:L:78:ASP:HA	1.86	0.58
1:K:189:ALA:HB3	1:K:218:PRO:HA	1.86	0.58
1:O:132:ASP:HB3	1:O:157:VAL:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:ASP:OD1	1:L:99:LYS:HE3	2.04	0.57
1:H:104:PHE:CD2	1:H:302:GLN:HG2	2.39	0.57
1:H:128:GLU:HB2	1:H:341:ARG:HG2	1.86	0.57
1:J:13:ARG:N	1:J:13:ARG:HD3	2.19	0.57
1:D:134:THR:OG1	1:D:159:LYS:HE2	2.04	0.57
1:E:194:THR:OG1	1:E:197:GLU:HG3	2.04	0.57
1:C:251:MET:HG3	1:C:255:LYS:HE3	1.85	0.57
1:G:7:VAL:CG1	1:G:71:ARG:HA	2.34	0.57
1:N:265:LYS:HB2	1:N:268:LYS:HE2	1.86	0.57
1:I:3:ARG:HA	1:I:78:ASP:HA	1.85	0.57
1:P:181:ARG:HB2	1:P:181:ARG:CZ	2.35	0.57
1:K:16:TYR:O	1:K:325:LYS:HE2	2.05	0.57
1:C:194:THR:OG1	1:C:197:GLU:HG3	2.04	0.57
1:C:3:ARG:HH11	1:C:3:ARG:HG3	1.69	0.57
1:P:265:LYS:HB2	1:P:268:LYS:HE2	1.86	0.57
1:E:189:ALA:HB3	1:E:218:PRO:HA	1.86	0.57
1:P:334:ILE:HD11	1:P:343:LYS:CD	2.35	0.57
1:L:149:LYS:O	1:L:153:GLU:HG3	2.04	0.56
1:I:66:ILE:HG21	1:O:59:ARG:HG3	1.87	0.56
1:D:140:VAL:O	1:D:144:VAL:HG23	2.04	0.56
1:M:13:ARG:HD2	1:M:29:GLU:OE2	2.05	0.56
1:C:3:ARG:HA	1:C:78:ASP:HA	1.88	0.56
1:I:135:VAL:HA	1:I:146:GLU:OE1	2.06	0.56
1:J:137:ILE:HG12	1:J:143:ARG:NH2	2.21	0.56
1:G:321:HIS:NE2	1:G:335:GLN:NE2	2.54	0.56
1:G:194:THR:OG1	1:G:197:GLU:HG3	2.04	0.56
1:M:149:LYS:O	1:M:153:GLU:HG3	2.05	0.56
1:K:214:VAL:HG11	1:K:289:MET:HE1	1.86	0.56
1:E:5:VAL:HG22	1:E:38:VAL:O	2.06	0.56
1:E:90:ASP:OD1	1:E:99:LYS:HE3	2.05	0.56
1:E:144:VAL:HG23	1:E:179:VAL:HG21	1.88	0.56
1:I:48:GLU:H	1:I:302:GLN:NE2	2.03	0.56
1:K:5:VAL:HG22	1:K:38:VAL:O	2.06	0.56
1:F:151:PHE:HB2	1:F:180:THR:HG22	1.88	0.56
1:K:336:ASP:CG	1:K:339:ARG:HH12	2.10	0.56
1:M:69:ALA:O	1:M:73:MET:HG3	2.05	0.56
1:J:17:GLU:HA	1:J:325:LYS:CE	2.36	0.55
1:E:140:VAL:HG21	1:E:171:GLU:OE1	2.05	0.55
1:C:278:VAL:O	1:C:282:GLU:HG3	2.06	0.55
1:F:338:PRO:O	1:F:340:MET:HE2	2.07	0.55
1:N:66:ILE:HD11	1:N:98:LEU:HD23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:194:THR:OG1	1:K:197:GLU:HG3	2.06	0.55
1:I:133:LYS:HD2	1:I:155:PHE:CE2	2.42	0.55
1:O:131:THR:HG22	1:O:340:MET:HE1	1.89	0.55
1:L:189:ALA:HB3	1:L:218:PRO:HA	1.88	0.55
1:E:3:ARG:HA	1:E:78:ASP:HA	1.88	0.55
1:E:263:ASN:HB2	1:E:289:MET:HE3	1.87	0.55
1:E:155:PHE:CD1	1:E:338:PRO:HB3	2.42	0.55
1:B:128:GLU:HB2	1:B:341:ARG:HG2	1.89	0.55
1:G:128:GLU:HB2	1:G:341:ARG:HG2	1.89	0.55
1:N:189:ALA:HB3	1:N:218:PRO:HA	1.88	0.55
1:A:149:LYS:O	1:A:153:GLU:HG3	2.07	0.54
1:J:134:THR:HG21	1:J:161:LYS:HE2	1.89	0.54
1:I:167:LYS:NZ	1:I:167:LYS:HB2	2.22	0.54
1:L:134:THR:OG1	1:L:159:LYS:HE2	2.06	0.54
1:N:125:LYS:HG2	1:N:311:GLY:HA3	1.90	0.54
1:M:194:THR:OG1	1:M:197:GLU:HG3	2.07	0.54
1:B:140:VAL:O	1:B:144:VAL:HG23	2.07	0.54
1:K:3:ARG:HA	1:K:78:ASP:HA	1.88	0.54
1:M:3:ARG:HA	1:M:78:ASP:HA	1.89	0.54
1:N:8:LYS:HE2	1:N:36:GLU:OE1	2.08	0.54
1:A:3:ARG:HA	1:A:78:ASP:HA	1.88	0.54
1:B:103:GLN:HE22	1:B:272:SER:HB2	1.73	0.54
1:J:334:ILE:HD11	1:J:343:LYS:HG2	1.89	0.54
1:J:251:MET:HG3	1:J:255:LYS:NZ	2.22	0.54
1:C:191:MET:HE3	1:C:220:ARG:HA	1.90	0.54
1:J:133:LYS:HD2	1:J:155:PHE:CE2	2.43	0.54
1:G:336:ASP:OD2	1:G:339:ARG:NH1	2.41	0.53
1:P:189:ALA:HB3	1:P:218:PRO:HA	1.90	0.53
1:K:287:LYS:HE2	1:K:314:GLU:CG	2.39	0.53
1:G:125:LYS:HE3	1:H:83:ALA:HB1	1.89	0.53
1:M:189:ALA:HB3	1:M:218:PRO:HA	1.91	0.53
1:O:134:THR:OG1	1:O:159:LYS:HE2	2.08	0.53
1:K:339:ARG:HB2	1:K:339:ARG:NH1	2.24	0.53
1:N:134:THR:OG1	1:N:159:LYS:HE2	2.08	0.53
1:B:196:LYS:HE3	1:C:234:SER:O	2.08	0.53
1:I:189:ALA:HB3	1:I:218:PRO:HA	1.88	0.53
1:P:334:ILE:HD11	1:P:343:LYS:HD3	1.89	0.53
1:K:150:ILE:HG22	1:K:155:PHE:HB2	1.91	0.53
1:O:334:ILE:HD11	1:O:343:LYS:CD	2.38	0.53
1:P:114:LEU:HD12	1:P:121:LEU:HD11	1.89	0.53
1:F:129:ILE:HG23	1:F:308:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLU:H	1:B:302:GLN:NE2	2.06	0.53
1:O:48:GLU:H	1:O:302:GLN:NE2	2.06	0.53
1:I:196:LYS:HD3	3:P:429:HOH:O	2.07	0.53
1:J:69:ALA:O	1:J:73:MET:HG3	2.09	0.53
1:B:189:ALA:HB3	1:B:218:PRO:HA	1.89	0.53
1:H:3:ARG:HH11	1:H:3:ARG:HG3	1.73	0.53
1:H:17:GLU:HA	1:H:17:GLU:OE1	2.07	0.53
1:I:54:ARG:HH12	1:I:190:ASN:HB3	1.73	0.53
1:E:252:ARG:O	1:E:256:GLU:HG2	2.09	0.53
1:D:278:VAL:O	1:D:282:GLU:HG3	2.09	0.53
1:H:131:THR:HG22	1:H:340:MET:CE	2.38	0.53
1:E:231:ARG:NH2	1:H:195:GLN:HE22	2.05	0.53
1:M:278:VAL:O	1:M:282:GLU:HG3	2.09	0.53
1:K:39:LEU:HD23	1:K:113:GLU:CD	2.30	0.52
1:G:325:LYS:HZ3	1:G:325:LYS:HB3	1.74	0.52
1:L:69:ALA:O	1:L:73:MET:HG3	2.10	0.52
1:P:263:ASN:HB2	1:P:289:MET:HE3	1.91	0.52
1:L:129:ILE:HG23	1:L:308:LEU:HD23	1.90	0.52
1:O:321:HIS:NE2	1:O:335:GLN:NE2	2.58	0.52
1:A:203:ARG:O	1:A:207:GLN:HG2	2.09	0.52
1:G:251:MET:HE2	1:G:280:ILE:HD13	1.91	0.52
1:A:131:THR:HG22	1:A:340:MET:HE1	1.91	0.52
1:J:131:THR:CG2	1:J:340:MET:HE1	2.36	0.52
1:P:69:ALA:O	1:P:73:MET:HG3	2.10	0.52
1:E:104:PHE:CE1	1:E:302:GLN:HA	2.45	0.52
1:C:321:HIS:H	1:C:321:HIS:HD1	1.57	0.52
1:K:181:ARG:NH1	1:K:181:ARG:HG2	2.23	0.52
1:F:138:ASP:OD1	1:F:139:THR:N	2.37	0.52
1:K:48:GLU:H	1:K:302:GLN:NE2	2.08	0.52
1:D:125:LYS:HG3	1:D:126:ARG:HG3	1.92	0.52
1:A:54:ARG:HD3	3:A:422:HOH:O	2.10	0.52
1:E:214:VAL:HG11	1:E:289:MET:HE1	1.92	0.52
1:P:54:ARG:HH12	1:P:190:ASN:HB3	1.75	0.52
1:D:194:THR:OG1	1:D:197:GLU:HG3	2.09	0.52
1:P:167:LYS:O	1:P:171:GLU:HG3	2.10	0.52
1:B:104:PHE:CD2	1:B:302:GLN:HG2	2.45	0.51
1:G:155:PHE:CD1	1:G:338:PRO:HB3	2.45	0.51
1:L:125:LYS:HG2	1:L:311:GLY:HA3	1.92	0.51
1:C:133:LYS:HD2	1:C:155:PHE:CE2	2.45	0.51
1:N:203:ARG:O	1:N:207:GLN:HG2	2.09	0.51
1:I:231:ARG:O	1:N:196:LYS:NZ	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:ARG:HA	1:H:78:ASP:HA	1.91	0.51
1:G:278:VAL:O	1:G:282:GLU:HG3	2.10	0.51
1:N:143:ARG:HH11	1:N:172:ALA:CB	2.24	0.51
1:K:188:ASP:HA	1:K:216:GLU:HB3	1.92	0.51
1:F:3:ARG:HA	1:F:78:ASP:HA	1.92	0.51
1:D:17:GLU:HA	1:D:325:LYS:NZ	2.25	0.51
1:H:194:THR:OG1	1:H:197:GLU:HG3	2.09	0.51
1:G:3:ARG:HA	1:G:78:ASP:HA	1.91	0.51
1:K:67:GLU:O	1:K:70:VAL:HG22	2.11	0.51
1:C:59:ARG:HG3	1:E:66:ILE:HG21	1.93	0.51
1:B:17:GLU:HA	1:B:325:LYS:HE3	1.92	0.51
1:L:63:LEU:HD21	1:L:97:SER:OG	2.10	0.51
1:B:334:ILE:HD11	1:B:343:LYS:HB2	1.92	0.51
1:D:133:LYS:HD3	1:D:150:ILE:HG12	1.91	0.51
1:O:155:PHE:CD1	1:O:338:PRO:HB3	2.46	0.51
1:K:66:ILE:HG21	1:M:59:ARG:HG3	1.92	0.51
1:G:231:ARG:HD2	1:G:258:ALA:O	2.11	0.51
1:M:251:MET:HG3	1:M:255:LYS:HE3	1.93	0.51
1:M:159:LYS:HE3	1:M:188:ASP:HB2	1.93	0.51
1:D:138:ASP:OD1	1:D:139:THR:N	2.33	0.51
1:F:195:GLN:HE22	1:G:231:ARG:NH2	2.09	0.50
1:M:265:LYS:HB2	1:M:268:LYS:HE2	1.91	0.50
1:B:132:ASP:HB3	1:B:157:VAL:CG1	2.41	0.50
1:J:48:GLU:H	1:J:302:GLN:NE2	2.09	0.50
1:P:128:GLU:HB2	1:P:341:ARG:HG2	1.93	0.50
1:G:137:ILE:HD13	1:G:143:ARG:HH21	1.75	0.50
1:C:225:GLU:HG3	1:F:257:GLU:OE1	2.12	0.50
1:E:36:GLU:HG3	1:E:46:TYR:CE1	2.46	0.50
1:F:139:THR:HG22	1:F:141:GLU:N	2.26	0.50
1:K:133:LYS:HD2	1:K:155:PHE:CE2	2.46	0.50
1:K:61:GLU:H	1:K:61:GLU:CD	2.14	0.50
1:E:269:SER:O	1:E:273:ASP:HB2	2.12	0.50
1:B:327:GLU:HG2	1:B:328:VAL:N	2.26	0.50
1:C:3:ARG:HD2	1:C:76:GLY:O	2.12	0.50
1:C:189:ALA:HB3	1:C:218:PRO:HA	1.94	0.50
1:D:142:ASN:O	1:D:146:GLU:HG3	2.12	0.50
1:J:339:ARG:HB2	1:J:339:ARG:HH11	1.75	0.50
1:G:191:MET:CE	1:G:242:GLU:HG2	2.42	0.50
1:B:278:VAL:O	1:B:282:GLU:HG3	2.12	0.50
1:D:128:GLU:HB2	1:D:341:ARG:HG2	1.94	0.50
1:I:133:LYS:HD3	1:I:150:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:139:THR:HG22	1:K:141:GLU:H	1.77	0.49
1:K:214:VAL:HG11	1:K:289:MET:CE	2.42	0.49
1:K:196:LYS:NZ	1:N:231:ARG:O	2.45	0.49
1:B:321:HIS:NE2	1:B:335:GLN:NE2	2.59	0.49
1:N:269:SER:O	1:N:273:ASP:HB2	2.12	0.49
1:C:263:ASN:HB2	1:C:289:MET:HE3	1.93	0.49
1:B:222:GLU:HG3	1:D:248:PHE:CE1	2.47	0.49
1:F:194:THR:OG1	1:F:197:GLU:HG3	2.13	0.49
1:H:189:ALA:HB3	1:H:218:PRO:HA	1.95	0.49
1:O:174:GLU:CD	1:O:208:LYS:HD3	2.32	0.49
1:P:3:ARG:HA	1:P:78:ASP:HA	1.94	0.49
1:H:125:LYS:HG2	1:H:311:GLY:HA3	1.95	0.49
1:D:251:MET:O	1:D:255:LYS:HG3	2.12	0.49
1:A:131:THR:HG22	1:A:340:MET:CE	2.43	0.49
1:N:334:ILE:HD11	1:N:343:LYS:HB2	1.95	0.49
1:C:196:LYS:HG2	3:C:452:HOH:O	2.13	0.49
1:C:300:ILE:HD11	1:C:318:LEU:HB3	1.95	0.49
1:H:144:VAL:O	1:H:148:LYS:HG3	2.12	0.49
1:G:174:GLU:HG2	1:G:178:LYS:HE3	1.95	0.49
1:K:342:VAL:HG22	1:K:343:LYS:N	2.27	0.49
1:E:150:ILE:HG22	1:E:155:PHE:HB2	1.94	0.49
1:O:17:GLU:OE2	1:O:325:LYS:HE2	2.13	0.49
1:I:99:LYS:O	1:I:103:GLN:HG3	2.12	0.49
1:O:132:ASP:HB3	1:O:157:VAL:CG1	2.42	0.48
1:E:188:ASP:HA	1:E:216:GLU:HB3	1.94	0.48
1:M:203:ARG:O	1:M:207:GLN:HG2	2.13	0.48
1:K:336:ASP:OD2	1:K:339:ARG:NH1	2.41	0.48
1:K:155:PHE:CD1	1:K:338:PRO:HB3	2.48	0.48
1:P:3:ARG:HG3	1:P:3:ARG:HH11	1.78	0.48
1:O:99:LYS:O	1:O:103:GLN:HG3	2.14	0.48
1:D:336:ASP:OD2	1:D:339:ARG:NH1	2.46	0.48
1:P:48:GLU:H	1:P:302:GLN:NE2	2.12	0.48
1:A:234:SER:O	1:D:196:LYS:HE3	2.14	0.48
1:D:181:ARG:HG2	1:D:181:ARG:HH11	1.78	0.48
1:N:128:GLU:HB2	1:N:341:ARG:HG2	1.95	0.48
1:B:17:GLU:O	1:B:18:LYS:HD3	2.14	0.48
1:I:131:THR:HG22	1:I:340:MET:HE2	1.96	0.48
1:C:144:VAL:HG13	1:C:179:VAL:HG21	1.93	0.48
1:B:68:ASN:ND2	1:B:71:ARG:HH12	2.11	0.48
1:A:3:ARG:HD2	1:A:76:GLY:O	2.13	0.48
1:B:133:LYS:HD3	1:B:150:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:VAL:O	1:A:282:GLU:HG3	2.14	0.48
1:H:36:GLU:HG3	1:H:46:TYR:CE1	2.48	0.48
1:L:193:TYR:HB3	1:L:197:GLU:HB2	1.95	0.48
1:A:336:ASP:CG	1:A:339:ARG:HH12	2.16	0.48
1:L:16:TYR:O	1:L:325:LYS:NZ	2.42	0.48
1:B:251:MET:HG3	1:B:255:LYS:NZ	2.29	0.48
1:N:174:GLU:O	1:N:178:LYS:HG2	2.13	0.48
1:F:134:THR:OG1	1:F:159:LYS:HE2	2.14	0.48
1:H:48:GLU:H	1:H:302:GLN:NE2	2.12	0.48
1:K:296:SER:HA	1:K:324:LEU:HD12	1.96	0.48
1:A:189:ALA:HB3	1:A:218:PRO:HA	1.95	0.48
1:G:7:VAL:HG11	1:G:71:ARG:HA	1.96	0.48
1:E:342:VAL:HG22	1:E:343:LYS:N	2.27	0.48
1:E:181:ARG:NH1	1:E:181:ARG:HB3	2.28	0.48
1:O:90:ASP:OD1	1:O:99:LYS:HE3	2.14	0.47
1:F:239:ALA:HB2	1:F:261:TYR:HB2	1.95	0.47
1:D:269:SER:O	1:D:273:ASP:HB2	2.13	0.47
1:D:143:ARG:HH11	1:D:172:ALA:CB	2.27	0.47
1:N:278:VAL:O	1:N:282:GLU:HG3	2.14	0.47
1:I:269:SER:HB3	1:I:273:ASP:HB2	1.96	0.47
1:K:240:ALA:HB2	1:K:259:VAL:HG11	1.96	0.47
1:A:149:LYS:O	1:A:152:GLU:HG2	2.14	0.47
1:E:39:LEU:HD23	1:E:113:GLU:CD	2.34	0.47
1:F:63:LEU:HD21	1:F:97:SER:OG	2.14	0.47
1:J:132:ASP:HB3	1:J:157:VAL:HG12	1.94	0.47
1:E:251:MET:O	1:E:255:LYS:HG3	2.14	0.47
1:N:143:ARG:HH11	1:N:172:ALA:HB2	1.78	0.47
1:E:255:LYS:HE2	1:F:254:VAL:HG12	1.95	0.47
1:G:48:GLU:H	1:G:302:GLN:NE2	2.11	0.47
1:E:134:THR:HG21	1:E:161:LYS:HE3	1.95	0.47
1:I:339:ARG:HB2	1:I:339:ARG:NH1	2.29	0.47
1:M:99:LYS:O	1:M:103:GLN:HG3	2.14	0.47
1:L:338:PRO:O	1:L:340:MET:HE2	2.14	0.47
1:G:16:TYR:O	1:G:325:LYS:HE2	2.14	0.47
1:E:140:VAL:O	1:E:144:VAL:HG12	2.14	0.47
1:O:131:THR:HG22	1:O:340:MET:CE	2.44	0.47
1:K:3:ARG:HD2	1:K:76:GLY:O	2.14	0.47
1:P:137:ILE:HD13	1:P:143:ARG:HH21	1.79	0.47
1:P:144:VAL:O	1:P:148:LYS:HG3	2.14	0.47
1:N:53:PHE:O	1:N:57:GLY:HA2	2.13	0.47
1:A:143:ARG:NH2	1:A:161:LYS:O	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145:LYS:HZ3	1:K:145:LYS:HB2	1.77	0.47
1:E:123:GLY:HA2	1:F:82:TYR:CE2	2.50	0.47
1:N:3:ARG:HB2	1:N:40:GLU:OE2	2.14	0.47
1:F:132:ASP:HB3	1:F:157:VAL:HG12	1.97	0.47
1:H:321:HIS:H	1:H:321:HIS:HD1	1.62	0.47
1:J:138:ASP:OD1	1:J:139:THR:N	2.43	0.47
1:M:104:PHE:CD2	1:M:302:GLN:HG2	2.49	0.47
1:H:276:ALA:O	1:H:280:ILE:HG13	2.14	0.47
1:D:134:THR:HG21	1:D:161:LYS:HZ3	1.77	0.47
1:K:195:GLN:NE2	1:N:231:ARG:NH2	2.63	0.47
1:H:222:GLU:HG2	3:H:406:HOH:O	2.13	0.47
1:D:3:ARG:HA	1:D:78:ASP:HA	1.95	0.47
1:H:6:ASN:OD1	1:H:71:ARG:HD2	2.15	0.47
1:I:321:HIS:H	1:I:321:HIS:HD1	1.63	0.47
1:E:61:GLU:CD	1:E:61:GLU:H	2.18	0.47
1:D:13:ARG:HG3	1:D:13:ARG:HH11	1.78	0.47
1:L:151:PHE:HB2	1:L:180:THR:HG22	1.96	0.47
1:G:328:VAL:O	1:G:328:VAL:HG13	2.14	0.47
1:B:90:ASP:OD1	1:B:99:LYS:HE3	2.14	0.47
1:H:142:ASN:O	1:H:146:GLU:HG3	2.15	0.47
1:G:228:LYS:HE2	1:G:256:GLU:O	2.15	0.47
1:B:269:SER:HB3	1:B:273:ASP:HB2	1.96	0.47
1:P:321:HIS:HD1	1:P:321:HIS:H	1.62	0.47
1:J:321:HIS:HD1	1:J:321:HIS:H	1.63	0.47
1:J:104:PHE:CG	1:J:302:GLN:HG2	2.50	0.47
1:B:222:GLU:HG3	1:D:248:PHE:CD1	2.50	0.47
1:E:166:LEU:O	1:E:170:ILE:HG13	2.14	0.47
1:P:90:ASP:OD1	1:P:99:LYS:HE3	2.15	0.47
1:F:140:VAL:O	1:F:144:VAL:HG23	2.15	0.47
1:B:3:ARG:HA	1:B:78:ASP:HA	1.97	0.47
1:F:321:HIS:NE2	1:F:335:GLN:NE2	2.63	0.46
1:I:3:ARG:HD2	1:I:76:GLY:O	2.16	0.46
1:G:78:ASP:HB3	1:G:81:ASN:HD22	1.79	0.46
1:G:132:ASP:HB3	1:G:157:VAL:HG12	1.98	0.46
1:C:104:PHE:CD2	1:C:302:GLN:HG2	2.50	0.46
1:D:129:ILE:HG23	1:D:308:LEU:HD23	1.96	0.46
1:F:31:ARG:NH1	1:F:31:ARG:HG3	2.31	0.46
1:I:48:GLU:H	1:I:302:GLN:HE22	1.63	0.46
1:G:143:ARG:HH11	1:G:172:ALA:HB2	1.80	0.46
1:C:129:ILE:HG23	1:C:308:LEU:HD23	1.96	0.46
1:H:251:MET:HG3	1:H:255:LYS:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:251:MET:HG3	1:O:255:LYS:HE3	1.96	0.46
1:D:319:ASP:O	1:D:323:MET:HG2	2.15	0.46
1:D:265:LYS:HB2	1:D:268:LYS:CE	2.44	0.46
1:J:298:LEU:HD23	1:J:298:LEU:O	2.15	0.46
1:B:128:GLU:OE1	1:B:341:ARG:HD3	2.14	0.46
1:L:15:GLU:O	1:L:325:LYS:HG2	2.16	0.46
1:L:15:GLU:HB2	1:L:325:LYS:HD2	1.98	0.46
1:H:155:PHE:CD1	1:H:338:PRO:HB3	2.50	0.46
1:M:21:HIS:CD2	1:M:26:VAL:HG22	2.51	0.46
1:O:254:VAL:HG12	1:P:255:LYS:HE2	1.96	0.46
1:D:45:GLY:HA2	1:D:108:ASP:OD2	2.16	0.46
1:M:342:VAL:HG22	1:M:343:LYS:N	2.30	0.46
1:A:232:PHE:HE2	1:D:232:PHE:CE2	2.33	0.46
1:C:340:MET:HE3	1:C:340:MET:N	2.30	0.46
1:D:53:PHE:O	1:D:57:GLY:HA2	2.16	0.46
1:K:262:VAL:HG23	1:K:286:LEU:HD21	1.97	0.46
1:F:269:SER:O	1:F:273:ASP:HB2	2.16	0.46
1:G:334:ILE:HD11	1:G:343:LYS:HB2	1.97	0.46
1:I:125:LYS:HE3	3:I:421:HOH:O	2.14	0.46
1:K:239:ALA:HB2	1:K:261:TYR:HB2	1.98	0.46
1:F:339:ARG:HB2	1:F:339:ARG:NH1	2.30	0.46
1:J:143:ARG:HH11	1:J:172:ALA:CB	2.29	0.46
1:D:13:ARG:HG3	1:D:13:ARG:NH1	2.31	0.46
1:F:31:ARG:HH11	1:F:31:ARG:HG3	1.81	0.46
1:M:321:HIS:HD1	1:M:321:HIS:H	1.64	0.46
1:G:13:ARG:HH11	1:G:13:ARG:HG2	1.81	0.46
1:G:13:ARG:O	1:G:13:ARG:HD3	2.16	0.46
1:E:145:LYS:HD3	1:E:145:LYS:C	2.35	0.46
1:A:61:GLU:H	1:A:61:GLU:CD	2.18	0.46
1:D:134:THR:HG21	1:D:161:LYS:HZ2	1.80	0.46
1:J:104:PHE:CE1	1:J:302:GLN:HA	2.50	0.46
1:A:339:ARG:NH1	1:A:339:ARG:HB2	2.30	0.46
1:P:104:PHE:CD2	1:P:302:GLN:HG2	2.51	0.46
1:B:225:GLU:OE2	1:C:257:GLU:HG2	2.16	0.46
1:L:321:HIS:NE2	1:L:335:GLN:NE2	2.63	0.46
1:D:66:ILE:HD11	1:D:98:LEU:HD23	1.98	0.46
1:C:3:ARG:NH1	1:C:3:ARG:HG3	2.31	0.46
1:F:117:GLN:OE1	1:F:342:VAL:CG2	2.64	0.46
1:C:21:HIS:ND1	1:C:26:VAL:HG22	2.30	0.46
1:P:188:ASP:HA	1:P:216:GLU:HB3	1.98	0.45
1:K:69:ALA:O	1:K:73:MET:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:LYS:HD2	1:F:314:GLU:HG3	1.98	0.45
1:P:214:VAL:HG11	1:P:289:MET:CE	2.46	0.45
1:H:126:ARG:HD3	1:H:311:GLY:HA2	1.98	0.45
1:K:129:ILE:HG23	1:K:308:LEU:HD23	1.97	0.45
1:G:336:ASP:O	1:G:339:ARG:NH1	2.49	0.45
1:E:3:ARG:O	1:E:40:GLU:HG3	2.17	0.45
1:L:278:VAL:O	1:L:282:GLU:HG3	2.15	0.45
1:I:140:VAL:O	1:I:144:VAL:HG23	2.17	0.45
1:P:278:VAL:O	1:P:282:GLU:HG3	2.16	0.45
1:K:99:LYS:O	1:K:103:GLN:HG3	2.17	0.45
1:C:104:PHE:CE1	1:C:302:GLN:HA	2.51	0.45
1:J:90:ASP:OD1	1:J:99:LYS:HE3	2.16	0.45
1:I:265:LYS:HB2	1:I:268:LYS:CE	2.43	0.45
1:P:131:THR:HG22	1:P:340:MET:CE	2.46	0.45
1:M:13:ARG:NH2	1:M:29:GLU:OE2	2.49	0.45
1:A:321:HIS:HD1	1:A:321:HIS:H	1.64	0.45
1:O:78:ASP:HB3	1:O:81:ASN:HD22	1.82	0.45
1:O:129:ILE:HG23	1:O:308:LEU:HD23	1.98	0.45
1:A:194:THR:OG1	1:A:197:GLU:HG3	2.16	0.45
1:K:321:HIS:CE1	1:K:322:LEU:HG	2.52	0.45
1:E:99:LYS:O	1:E:103:GLN:HG3	2.17	0.45
1:C:263:ASN:HB2	1:C:289:MET:CE	2.46	0.45
1:D:68:ASN:OD1	1:D:71:ARG:NH2	2.50	0.45
1:J:128:GLU:HB2	1:J:341:ARG:HG2	1.99	0.45
1:J:191:MET:CE	1:J:242:GLU:HG2	2.45	0.45
1:G:174:GLU:CD	1:G:208:LYS:HD3	2.37	0.45
1:C:125:LYS:HG2	1:C:311:GLY:HA3	1.99	0.45
1:M:24:GLY:O	1:M:25:SER:HB2	2.17	0.45
1:O:147:ALA:CB	1:O:176:ILE:HG23	2.47	0.45
1:D:328:VAL:O	1:D:330:ARG:HG3	2.16	0.45
1:E:214:VAL:HG11	1:E:289:MET:CE	2.47	0.45
1:J:132:ASP:HB2	1:J:157:VAL:O	2.17	0.45
1:D:117:GLN:OE1	1:D:342:VAL:CG2	2.64	0.45
1:C:99:LYS:O	1:C:103:GLN:HG3	2.17	0.45
1:C:265:LYS:HB2	1:C:268:LYS:HE2	1.99	0.45
1:N:265:LYS:HB2	1:N:268:LYS:CE	2.47	0.44
1:K:38:VAL:HG22	1:K:44:LYS:HG2	1.99	0.44
1:I:126:ARG:HD3	1:I:311:GLY:HA2	1.99	0.44
1:O:54:ARG:O	1:O:221:ARG:NH2	2.49	0.44
1:I:132:ASP:HB3	1:I:157:VAL:HG12	1.99	0.44
1:L:334:ILE:HD11	1:L:343:LYS:HE3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:104:PHE:CE1	1:K:302:GLN:HA	2.51	0.44
1:C:155:PHE:CD1	1:C:338:PRO:HB3	2.52	0.44
1:H:96:PRO:O	1:H:99:LYS:HB3	2.18	0.44
1:E:321:HIS:HD1	1:E:321:HIS:H	1.64	0.44
1:D:137:ILE:HG23	1:D:143:ARG:NH2	2.32	0.44
1:E:68:ASN:ND2	1:E:71:ARG:NH2	2.65	0.44
1:F:149:LYS:O	1:F:153:GLU:HG3	2.18	0.44
1:J:140:VAL:HG21	1:J:171:GLU:OE2	2.16	0.44
1:E:133:LYS:HD3	1:E:150:ILE:HG12	2.00	0.44
1:K:196:LYS:HG3	1:N:237:PRO:HG3	2.00	0.44
1:M:48:GLU:H	1:M:302:GLN:NE2	2.15	0.44
1:B:117:GLN:OE1	1:B:342:VAL:CG2	2.66	0.44
1:P:220:ARG:NH1	1:P:220:ARG:HG3	2.32	0.44
1:P:251:MET:HG3	1:P:255:LYS:HE3	1.99	0.44
1:D:69:ALA:O	1:D:73:MET:HG3	2.17	0.44
1:G:239:ALA:HB2	1:G:261:TYR:HB2	1.99	0.44
1:J:17:GLU:HG3	1:J:18:LYS:HG2	2.00	0.44
1:D:17:GLU:HA	1:D:325:LYS:HZ2	1.82	0.44
1:C:328:VAL:O	1:C:328:VAL:HG13	2.16	0.44
1:I:265:LYS:HE2	3:I:413:HOH:O	2.16	0.44
1:M:3:ARG:HH11	1:M:3:ARG:HG3	1.83	0.44
1:P:214:VAL:HG11	1:P:289:MET:HE1	1.99	0.44
1:I:132:ASP:HB3	1:I:157:VAL:CG1	2.48	0.44
1:J:53:PHE:O	1:J:57:GLY:HA2	2.18	0.44
1:H:334:ILE:HD11	1:H:343:LYS:HB2	1.98	0.44
1:C:159:LYS:HE3	1:C:188:ASP:HB2	2.00	0.44
1:N:48:GLU:H	1:N:302:GLN:NE2	2.16	0.44
1:G:298:LEU:O	1:G:298:LEU:HD23	2.18	0.44
1:E:257:GLU:OE2	1:H:225:GLU:HG3	2.17	0.44
1:M:188:ASP:HA	1:M:216:GLU:HB3	1.99	0.44
1:E:88:ILE:HG12	1:E:91:ARG:HH22	1.83	0.44
1:G:90:ASP:OD1	1:G:99:LYS:HE3	2.18	0.44
1:O:203:ARG:O	1:O:207:GLN:HG2	2.18	0.44
1:G:15:GLU:O	1:G:325:LYS:HG2	2.17	0.44
1:P:251:MET:HE2	1:P:280:ILE:HD13	2.00	0.44
1:P:220:ARG:HH11	1:P:220:ARG:HG3	1.83	0.44
1:N:155:PHE:CD1	1:N:338:PRO:HB3	2.53	0.43
1:A:5:VAL:HG22	1:A:38:VAL:O	2.18	0.43
1:B:8:LYS:HD3	1:B:36:GLU:OE1	2.17	0.43
1:I:143:ARG:HG2	1:I:143:ARG:HH11	1.83	0.43
1:C:48:GLU:H	1:C:302:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14:TYR:HB2	1:L:324:LEU:HD13	2.00	0.43
1:B:231:ARG:NH1	3:B:456:HOH:O	2.51	0.43
1:F:104:PHE:CD2	1:F:302:GLN:HG2	2.53	0.43
1:C:24:GLY:O	1:C:25:SER:HB3	2.18	0.43
1:H:141:GLU:H	1:H:141:GLU:CD	2.20	0.43
1:I:251:MET:HE2	1:I:280:ILE:HD13	2.00	0.43
1:F:131:THR:HG22	1:F:340:MET:HE2	1.99	0.43
1:N:137:ILE:HA	1:N:143:ARG:HH21	1.82	0.43
1:O:3:ARG:HA	1:O:78:ASP:HA	1.99	0.43
1:N:90:ASP:OD1	1:N:99:LYS:HE3	2.19	0.43
1:N:319:ASP:O	1:N:323:MET:HG2	2.18	0.43
1:G:188:ASP:HA	1:G:216:GLU:HB3	2.00	0.43
1:D:39:LEU:HD23	1:D:113:GLU:CD	2.39	0.43
1:P:126:ARG:HD3	1:P:311:GLY:HA2	2.00	0.43
1:E:128:GLU:HB2	1:E:341:ARG:HG2	2.00	0.43
1:O:13:ARG:NE	1:O:29:GLU:OE2	2.51	0.43
1:P:61:GLU:H	1:P:61:GLU:CD	2.20	0.43
1:K:156:ARG:HD3	1:K:156:ARG:HA	1.89	0.43
1:H:99:LYS:O	1:H:103:GLN:HG3	2.18	0.43
1:N:133:LYS:HB3	1:N:150:ILE:HG21	1.99	0.43
1:O:188:ASP:HA	1:O:216:GLU:HB3	2.00	0.43
1:N:43:VAL:HG21	1:N:113:GLU:HG2	1.99	0.43
1:O:145:LYS:C	1:O:145:LYS:HD3	2.38	0.43
1:M:3:ARG:O	1:M:40:GLU:HG2	2.18	0.43
1:N:36:GLU:HG3	1:N:46:TYR:CE1	2.52	0.43
1:E:48:GLU:H	1:E:302:GLN:NE2	2.17	0.43
1:I:131:THR:HG22	1:I:340:MET:CE	2.48	0.43
1:I:124:GLY:HA2	3:I:440:HOH:O	2.18	0.43
1:K:125:LYS:HG2	1:K:311:GLY:HA3	2.01	0.43
1:C:196:LYS:NZ	1:F:231:ARG:O	2.51	0.43
1:L:117:GLN:OE1	1:L:342:VAL:CG2	2.67	0.43
1:D:128:GLU:OE1	1:D:341:ARG:HD3	2.19	0.43
1:A:334:ILE:HD11	1:A:343:LYS:HD2	2.00	0.43
1:G:129:ILE:HG23	1:G:308:LEU:HD23	2.00	0.43
1:A:90:ASP:OD1	1:A:99:LYS:HE3	2.18	0.43
1:E:88:ILE:HG23	1:E:91:ARG:NH2	2.33	0.43
1:P:53:PHE:O	1:P:57:GLY:HA2	2.19	0.43
1:J:3:ARG:HA	1:J:78:ASP:HA	2.00	0.43
1:D:189:ALA:HB3	1:D:218:PRO:HA	2.01	0.43
1:I:37:ILE:HD12	1:I:105:ALA:HB3	2.01	0.43
1:E:143:ARG:HH11	1:E:172:ALA:CB	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:LYS:O	1:G:145:LYS:HD2	2.18	0.43
1:M:129:ILE:HG23	1:M:308:LEU:HD23	2.01	0.43
1:F:336:ASP:OD1	1:F:341:ARG:NH2	2.51	0.43
1:J:251:MET:HG3	1:J:255:LYS:HZ2	1.83	0.42
1:A:264:ILE:HD11	1:A:277:ILE:HG22	2.00	0.42
1:E:131:THR:HG22	1:E:340:MET:CE	2.49	0.42
1:M:251:MET:HE2	1:M:280:ILE:HD13	2.01	0.42
1:B:222:GLU:CD	1:B:222:GLU:H	2.22	0.42
1:I:125:LYS:HG2	1:I:311:GLY:HA3	2.00	0.42
1:A:21:HIS:ND1	1:A:26:VAL:HG22	2.34	0.42
1:A:126:ARG:HD3	1:A:311:GLY:HA2	2.02	0.42
1:I:13:ARG:NH2	1:I:13:ARG:HG3	2.33	0.42
1:O:78:ASP:HB3	1:O:81:ASN:ND2	2.35	0.42
1:G:99:LYS:O	1:G:103:GLN:HG3	2.19	0.42
1:A:132:ASP:HB3	1:A:157:VAL:HG12	2.01	0.42
1:N:321:HIS:NE2	1:N:335:GLN:NE2	2.67	0.42
1:G:126:ARG:HD3	1:G:311:GLY:HA2	2.01	0.42
1:N:147:ALA:HB1	1:N:176:ILE:HG23	2.02	0.42
1:M:5:VAL:HG22	1:M:38:VAL:O	2.19	0.42
1:A:129:ILE:HG23	1:A:308:LEU:HD23	2.01	0.42
1:M:132:ASP:C	1:M:132:ASP:OD1	2.58	0.42
1:H:132:ASP:C	1:H:132:ASP:OD1	2.57	0.42
1:O:36:GLU:HG3	1:O:46:TYR:CE1	2.53	0.42
1:M:48:GLU:OE1	1:M:299:GLY:HA3	2.19	0.42
1:P:300:ILE:O	1:P:304:VAL:HG23	2.20	0.42
1:G:250:VAL:HG21	1:G:277:ILE:HG12	2.00	0.42
1:O:239:ALA:HB2	1:O:261:TYR:HB2	2.01	0.42
1:O:196:LYS:HE2	1:O:229:PHE:CZ	2.54	0.42
1:O:104:PHE:HD1	1:O:271:ILE:HD11	1.84	0.42
1:O:147:ALA:HB1	1:O:176:ILE:HG23	2.01	0.42
1:D:132:ASP:OD1	1:D:132:ASP:C	2.57	0.42
1:J:131:THR:HG22	1:J:340:MET:CE	2.42	0.42
1:O:13:ARG:NH2	1:O:29:GLU:OE1	2.53	0.42
1:A:321:HIS:NE2	1:A:335:GLN:NE2	2.67	0.42
1:H:90:ASP:OD1	1:H:99:LYS:HE3	2.19	0.42
1:N:63:LEU:HD21	1:N:97:SER:OG	2.20	0.42
1:A:22:ILE:HG13	1:A:25:SER:HB3	2.02	0.42
1:A:62:ALA:HB1	1:G:62:ALA:HB1	2.01	0.42
1:P:269:SER:O	1:P:273:ASP:HB2	2.19	0.42
1:L:265:LYS:HB2	1:L:268:LYS:CE	2.46	0.42
1:G:78:ASP:HB3	1:G:81:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:132:ASP:HB3	1:J:157:VAL:CG1	2.50	0.42
1:C:268:LYS:HB2	1:C:268:LYS:HE3	1.91	0.42
1:J:126:ARG:HD3	1:J:311:GLY:HA2	2.01	0.42
1:L:234:SER:O	1:M:196:LYS:HE3	2.20	0.42
1:P:132:ASP:HB3	1:P:157:VAL:HG12	2.00	0.42
1:F:188:ASP:HA	1:F:216:GLU:HB3	2.01	0.42
1:L:71:ARG:HG3	1:L:71:ARG:HH11	1.84	0.42
1:G:139:THR:OG1	1:G:141:GLU:HG3	2.19	0.42
1:B:68:ASN:ND2	1:B:71:ARG:NH2	2.63	0.42
1:G:328:VAL:O	1:G:330:ARG:HG3	2.20	0.42
1:A:159:LYS:HE3	1:A:188:ASP:HB2	2.02	0.42
1:K:128:GLU:OE1	1:K:341:ARG:HD3	2.20	0.42
1:L:132:ASP:HB3	1:L:157:VAL:HG12	2.02	0.42
1:M:104:PHE:CE1	1:M:302:GLN:HA	2.55	0.42
1:J:298:LEU:HD23	1:J:298:LEU:C	2.40	0.42
1:C:69:ALA:O	1:C:73:MET:HG3	2.20	0.42
1:A:6:ASN:ND2	3:A:477:HOH:O	2.52	0.42
1:L:61:GLU:H	1:L:61:GLU:CD	2.23	0.42
1:A:339:ARG:C	1:A:340:MET:HE2	2.40	0.42
1:O:16:TYR:O	1:O:325:LYS:HE3	2.20	0.42
1:M:90:ASP:OD1	1:M:99:LYS:HE3	2.19	0.42
1:D:117:GLN:OE1	1:D:342:VAL:HG21	2.19	0.42
1:L:5:VAL:HG22	1:L:38:VAL:O	2.20	0.42
1:N:9:LEU:HA	1:N:34:GLU:O	2.20	0.42
1:K:29:GLU:HA	1:K:29:GLU:OE1	2.19	0.42
1:H:196:LYS:HD3	1:H:196:LYS:HA	1.88	0.42
1:E:261:TYR:CE2	1:E:287:LYS:HB3	2.55	0.42
1:I:194:THR:OG1	1:I:197:GLU:HG3	2.20	0.41
1:C:132:ASP:C	1:C:132:ASP:OD1	2.57	0.41
1:C:191:MET:SD	1:C:242:GLU:HG2	2.60	0.41
1:I:132:ASP:C	1:I:132:ASP:OD1	2.59	0.41
1:K:273:ASP:O	1:K:277:ILE:HG13	2.20	0.41
1:E:53:PHE:O	1:E:57:GLY:HA2	2.19	0.41
1:G:269:SER:O	1:G:273:ASP:HB2	2.20	0.41
1:D:131:THR:HG22	1:D:340:MET:CE	2.49	0.41
1:D:149:LYS:O	1:D:153:GLU:HG3	2.20	0.41
1:N:45:GLY:HA2	1:N:108:ASP:OD2	2.19	0.41
1:K:278:VAL:O	1:K:282:GLU:HG3	2.20	0.41
1:I:36:GLU:HG3	1:I:46:TYR:CE1	2.56	0.41
1:L:231:ARG:NH2	1:M:195:GLN:OE1	2.52	0.41
1:O:39:LEU:HD23	1:O:113:GLU:CD	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:264:ILE:HD11	1:I:277:ILE:HG22	2.02	0.41
1:M:125:LYS:HE3	1:N:87:GLU:OE1	2.20	0.41
1:O:159:LYS:HA	1:O:186:ILE:O	2.21	0.41
1:I:149:LYS:O	1:I:153:GLU:HG3	2.21	0.41
1:I:188:ASP:HA	1:I:216:GLU:HB3	2.03	0.41
1:K:232:PHE:HE2	1:P:232:PHE:CE2	2.38	0.41
1:G:334:ILE:O	1:G:340:MET:HA	2.20	0.41
1:L:267:MET:HG2	3:L:413:HOH:O	2.20	0.41
1:B:53:PHE:O	1:B:57:GLY:HA2	2.20	0.41
1:E:339:ARG:HB2	1:E:339:ARG:NH1	2.35	0.41
1:G:196:LYS:HE2	1:G:229:PHE:CZ	2.55	0.41
1:A:139:THR:O	1:A:143:ARG:CG	2.66	0.41
1:H:3:ARG:HG3	1:H:3:ARG:NH1	2.34	0.41
1:E:123:GLY:HA2	1:F:82:TYR:CZ	2.55	0.41
1:N:133:LYS:HB3	1:N:150:ILE:CG2	2.50	0.41
1:O:139:THR:OG1	1:O:142:ASN:ND2	2.54	0.41
1:A:104:PHE:CD2	1:A:302:GLN:HG2	2.55	0.41
1:G:36:GLU:HG3	1:G:46:TYR:CE1	2.56	0.41
1:O:278:VAL:O	1:O:282:GLU:HG3	2.20	0.41
1:A:66:ILE:HD11	1:A:98:LEU:HD23	2.02	0.41
1:O:334:ILE:HD11	1:O:343:LYS:HD3	2.03	0.41
1:K:339:ARG:HB2	1:K:339:ARG:HH11	1.85	0.41
1:B:321:HIS:H	1:B:321:HIS:HD1	1.68	0.41
1:D:181:ARG:HG2	1:D:181:ARG:NH1	2.36	0.41
1:G:104:PHE:CD2	1:G:302:GLN:HG2	2.55	0.41
1:K:269:SER:O	1:K:273:ASP:HB2	2.21	0.41
1:A:162:VAL:HB	1:A:169:ASP:CG	2.41	0.41
1:H:278:VAL:O	1:H:282:GLU:HG3	2.21	0.41
1:P:156:ARG:HD3	1:P:156:ARG:HA	1.90	0.41
1:F:191:MET:CE	1:F:242:GLU:HG2	2.51	0.41
1:O:342:VAL:HG22	1:O:343:LYS:N	2.36	0.41
1:I:66:ILE:HD11	1:I:98:LEU:HD23	2.03	0.41
1:O:16:TYR:HD2	1:O:29:GLU:N	2.19	0.41
1:N:174:GLU:HA	1:N:210:ILE:CD1	2.50	0.41
1:M:321:HIS:NE2	1:M:335:GLN:NE2	2.69	0.41
1:O:61:GLU:H	1:O:61:GLU:CD	2.24	0.41
1:N:174:GLU:HG2	1:N:178:LYS:NZ	2.36	0.41
1:G:13:ARG:NH1	1:G:13:ARG:HG2	2.36	0.41
1:C:21:HIS:ND1	1:C:26:VAL:CG2	2.84	0.41
1:B:117:GLN:OE1	1:B:342:VAL:HG21	2.21	0.41
1:F:143:ARG:HD3	1:F:172:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:ALA:HB2	1:F:259:VAL:HG11	2.02	0.41
1:G:143:ARG:HH11	1:G:172:ALA:CB	2.33	0.41
1:G:172:ALA:O	1:G:176:ILE:HG13	2.21	0.41
1:I:73:MET:CE	1:I:92:LEU:HD21	2.51	0.41
1:A:269:SER:HB3	1:A:273:ASP:HB2	2.02	0.41
1:M:39:LEU:HD23	1:M:113:GLU:CD	2.42	0.41
1:A:36:GLU:HG3	1:A:46:TYR:CE1	2.56	0.41
1:P:187:VAL:HG11	1:P:201:PHE:CZ	2.56	0.41
1:J:196:LYS:HA	1:J:196:LYS:HD3	1.89	0.41
1:D:262:VAL:HG23	1:D:286:LEU:HD21	2.03	0.41
1:D:262:VAL:CG2	1:D:286:LEU:HD21	2.51	0.41
1:G:336:ASP:CG	1:G:339:ARG:HH12	2.24	0.40
1:D:155:PHE:CD1	1:D:338:PRO:HB3	2.56	0.40
1:J:265:LYS:HB2	1:J:268:LYS:CE	2.49	0.40
1:I:143:ARG:NH1	1:I:143:ARG:HG2	2.36	0.40
1:E:117:GLN:OE1	1:E:342:VAL:HG23	2.21	0.40
1:P:137:ILE:HD13	1:P:143:ARG:NH2	2.36	0.40
1:N:3:ARG:HA	1:N:78:ASP:HA	2.01	0.40
1:E:239:ALA:HB2	1:E:261:TYR:HB2	2.03	0.40
1:F:267:MET:HG2	3:F:418:HOH:O	2.21	0.40
1:J:63:LEU:HD21	1:J:97:SER:OG	2.21	0.40
1:M:9:LEU:HD22	1:M:67:GLU:HB2	2.03	0.40
1:I:196:LYS:CD	3:P:429:HOH:O	2.68	0.40
1:N:174:GLU:HA	1:N:210:ILE:HD11	2.02	0.40
1:G:162:VAL:HB	1:G:169:ASP:CG	2.42	0.40
1:G:11:LEU:O	1:G:12:LYS:HD2	2.20	0.40
1:A:127:ASP:O	1:A:341:ARG:HG3	2.20	0.40
1:I:319:ASP:O	1:I:323:MET:HG2	2.21	0.40
1:B:172:ALA:O	1:B:176:ILE:HG13	2.21	0.40
1:E:55:VAL:HA	1:E:221:ARG:HH22	1.85	0.40
1:C:279:GLU:OE1	1:D:276:ALA:HB2	2.21	0.40
1:B:132:ASP:C	1:B:132:ASP:OD1	2.60	0.40
1:K:104:PHE:CD2	1:K:302:GLN:HG2	2.56	0.40
1:G:147:ALA:CB	1:G:176:ILE:HG23	2.51	0.40
1:D:137:ILE:HA	1:D:143:ARG:HH21	1.87	0.40
1:I:129:ILE:HG23	1:I:308:LEU:HD23	2.03	0.40
1:O:140:VAL:O	1:O:144:VAL:HG23	2.22	0.40
1:N:262:VAL:CG2	1:N:286:LEU:HD21	2.51	0.40
1:B:104:PHE:CE1	1:B:302:GLN:HA	2.56	0.40
1:D:143:ARG:HH11	1:D:172:ALA:HB2	1.85	0.40
1:M:101:ALA:HA	1:M:302:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:99:LYS:O	1:J:103:GLN:HG3	2.22	0.40
1:A:38:VAL:HG22	1:A:44:LYS:HG2	2.03	0.40
1:P:269:SER:HB3	1:P:273:ASP:HB2	2.03	0.40
1:M:240:ALA:HB2	1:M:259:VAL:HG11	2.03	0.40
1:F:178:LYS:O	1:F:181:ARG:NH1	2.54	0.40
1:L:239:ALA:HB2	1:L:261:TYR:HB2	2.04	0.40
1:K:174:GLU:HA	1:K:210:ILE:HD11	2.04	0.40
1:C:131:THR:CG2	1:C:340:MET:HE1	2.49	0.40
1:E:3:ARG:HB2	1:E:40:GLU:CD	2.42	0.40
1:E:101:ALA:HA	1:E:302:GLN:HE22	1.87	0.40
1:E:68:ASN:ND2	1:E:71:ARG:HH21	2.19	0.40
1:E:137:ILE:HG12	1:E:143:ARG:HH21	1.86	0.40
1:L:104:PHE:CD2	1:L:302:GLN:HG2	2.56	0.40
1:J:250:VAL:HG21	1:J:277:ILE:HG12	2.03	0.40
1:G:66:ILE:HD11	1:G:98:LEU:HD23	2.02	0.40
1:N:13:ARG:NH1	1:N:13:ARG:HG2	2.37	0.40
1:B:63:LEU:HD21	1:B:97:SER:OG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	334/345 (97%)	320 (96%)	14 (4%)	0	100	100
1	B	328/345 (95%)	316 (96%)	12 (4%)	0	100	100
1	C	334/345 (97%)	320 (96%)	14 (4%)	0	100	100
1	D	328/345 (95%)	314 (96%)	14 (4%)	0	100	100
1	E	326/345 (94%)	312 (96%)	13 (4%)	1 (0%)	46	45
1	F	329/345 (95%)	315 (96%)	14 (4%)	0	100	100
1	G	326/345 (94%)	316 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	327/345 (95%)	315 (96%)	12 (4%)	0	100	100
1	I	334/345 (97%)	320 (96%)	14 (4%)	0	100	100
1	J	327/345 (95%)	314 (96%)	13 (4%)	0	100	100
1	K	326/345 (94%)	310 (95%)	16 (5%)	0	100	100
1	L	327/345 (95%)	315 (96%)	12 (4%)	0	100	100
1	M	334/345 (97%)	321 (96%)	13 (4%)	0	100	100
1	N	328/345 (95%)	312 (95%)	16 (5%)	0	100	100
1	O	327/345 (95%)	315 (96%)	12 (4%)	0	100	100
1	P	328/345 (95%)	316 (96%)	12 (4%)	0	100	100
All	All	5263/5520 (95%)	5051 (96%)	211 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	16	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	285/292 (98%)	281 (99%)	4 (1%)	74	80
1	B	280/292 (96%)	274 (98%)	6 (2%)	61	66
1	C	285/292 (98%)	283 (99%)	2 (1%)	88	92
1	D	280/292 (96%)	278 (99%)	2 (1%)	88	92
1	E	278/292 (95%)	277 (100%)	1 (0%)	93	96
1	F	281/292 (96%)	279 (99%)	2 (1%)	88	92
1	G	278/292 (95%)	273 (98%)	5 (2%)	66	72
1	H	279/292 (96%)	276 (99%)	3 (1%)	80	85
1	I	285/292 (98%)	284 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	279/292 (96%)	276 (99%)	3 (1%)	80	85
1	K	278/292 (95%)	273 (98%)	5 (2%)	66	72
1	L	279/292 (96%)	276 (99%)	3 (1%)	80	85
1	M	285/292 (98%)	285 (100%)	0	100	100
1	N	280/292 (96%)	277 (99%)	3 (1%)	80	85
1	O	279/292 (96%)	278 (100%)	1 (0%)	93	96
1	P	280/292 (96%)	276 (99%)	4 (1%)	74	80
All	All	4491/4672 (96%)	4446 (99%)	45 (1%)	82	87

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLU
1	A	121	LEU
1	A	167	LYS
1	A	340	MET
1	B	8	LYS
1	B	17	GLU
1	B	125	LYS
1	B	143	ARG
1	B	273	ASP
1	B	340	MET
1	C	273	ASP
1	C	340	MET
1	D	8	LYS
1	D	273	ASP
1	E	196	LYS
1	F	72	GLU
1	F	273	ASP
1	G	7	VAL
1	G	12	LYS
1	G	13	ARG
1	G	68	ASN
1	G	325	LYS
1	H	17	GLU
1	H	141	GLU
1	H	273	ASP
1	I	13	ARG
1	J	13	ARG
1	J	273	ASP

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Mol	Chain	Res	Type
1	J	340	MET
1	K	17	GLU
1	K	29	GLU
1	K	143	ARG
1	K	145	LYS
1	K	340	MET
1	L	72	GLU
1	L	232	PHE
1	L	273	ASP
1	N	13	ARG
1	N	273	ASP
1	N	340	MET
1	O	273	ASP
1	P	207	GLN
1	P	273	ASP
1	P	298	LEU
1	P	323	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	81	ASN
1	A	142	ASN
1	A	302	GLN
1	A	335	GLN
1	B	68	ASN
1	B	81	ASN
1	B	302	GLN
1	B	335	GLN
1	C	68	ASN
1	C	81	ASN
1	C	302	GLN
1	C	335	GLN
1	D	81	ASN
1	D	142	ASN
1	D	190	ASN
1	D	195	GLN
1	D	302	GLN
1	D	335	GLN
1	E	68	ASN
1	E	81	ASN

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Mol	Chain	Res	Type
1	E	190	ASN
1	E	302	GLN
1	E	335	GLN
1	F	81	ASN
1	F	142	ASN
1	F	195	GLN
1	F	302	GLN
1	F	335	GLN
1	G	68	ASN
1	G	81	ASN
1	G	142	ASN
1	G	195	GLN
1	G	302	GLN
1	G	335	GLN
1	H	81	ASN
1	H	142	ASN
1	H	190	ASN
1	H	195	GLN
1	H	302	GLN
1	H	335	GLN
1	I	81	ASN
1	I	142	ASN
1	I	302	GLN
1	I	335	GLN
1	J	68	ASN
1	J	81	ASN
1	J	142	ASN
1	J	302	GLN
1	J	335	GLN
1	K	81	ASN
1	K	195	GLN
1	K	302	GLN
1	K	335	GLN
1	L	81	ASN
1	L	142	ASN
1	L	302	GLN
1	L	335	GLN
1	M	21	HIS
1	M	68	ASN
1	M	81	ASN
1	M	302	GLN
1	M	335	GLN

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Mol	Chain	Res	Type
1	N	81	ASN
1	N	142	ASN
1	N	302	GLN
1	N	335	GLN
1	O	81	ASN
1	O	142	ASN
1	O	195	GLN
1	O	302	GLN
1	O	335	GLN
1	P	81	ASN
1	P	142	ASN
1	P	190	ASN
1	P	195	GLN
1	P	302	GLN
1	P	335	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	338/345 (97%)	-0.17	6 (1%) 71 76	18, 28, 47, 58	0
1	B	332/345 (96%)	-0.13	10 (3%) 54 62	20, 29, 51, 66	0
1	C	338/345 (97%)	-0.09	15 (4%) 38 47	19, 30, 52, 62	0
1	D	332/345 (96%)	0.05	16 (4%) 34 43	22, 33, 54, 67	0
1	E	330/345 (95%)	-0.05	11 (3%) 50 59	21, 31, 51, 65	0
1	F	333/345 (96%)	0.01	13 (3%) 43 52	20, 32, 52, 66	0
1	G	330/345 (95%)	-0.06	8 (2%) 62 68	19, 30, 49, 65	0
1	H	331/345 (95%)	-0.20	4 (1%) 81 85	18, 28, 47, 65	0
1	I	338/345 (97%)	-0.10	3 (0%) 85 88	18, 27, 48, 58	0
1	J	331/345 (95%)	-0.08	13 (3%) 43 52	19, 29, 50, 64	0
1	K	330/345 (95%)	-0.00	11 (3%) 50 59	22, 32, 51, 65	0
1	L	331/345 (95%)	-0.08	8 (2%) 62 68	22, 33, 52, 64	0
1	M	338/345 (97%)	-0.07	15 (4%) 38 47	20, 30, 53, 64	0
1	N	332/345 (96%)	-0.00	12 (3%) 46 55	21, 31, 53, 66	0
1	O	331/345 (95%)	-0.10	10 (3%) 54 62	18, 30, 49, 63	0
1	P	332/345 (96%)	-0.10	9 (2%) 58 65	18, 30, 49, 65	0
All	All	5327/5520 (96%)	-0.07	164 (3%) 52 61	18, 30, 51, 67	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	19	PRO	8.8
1	F	19	PRO	7.3
1	O	28	SER	7.0
1	F	18	LYS	6.3
1	E	327	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	328	VAL	5.1
1	K	327	GLU	5.1
1	D	18	LYS	5.1
1	D	19	PRO	5.0
1	C	24	GLY	4.9
1	N	327	GLU	4.9
1	F	328	VAL	4.8
1	B	18	LYS	4.8
1	G	327	GLU	4.7
1	D	327	GLU	4.6
1	K	328	VAL	4.6
1	G	13	ARG	4.5
1	C	26	VAL	4.5
1	B	327	GLU	4.5
1	P	18	LYS	4.4
1	F	17	GLU	4.3
1	O	327	GLU	4.2
1	N	28	SER	4.2
1	H	18	LYS	4.1
1	N	325	LYS	4.0
1	L	327	GLU	4.0
1	C	18	LYS	4.0
1	C	19	PRO	4.0
1	J	140	VAL	3.9
1	N	17	GLU	3.9
1	B	19	PRO	3.8
1	D	16	TYR	3.8
1	K	17	GLU	3.8
1	C	20	PHE	3.8
1	J	18	LYS	3.8
1	C	28	SER	3.7
1	D	17	GLU	3.7
1	C	17	GLU	3.6
1	J	328	VAL	3.6
1	N	16	TYR	3.5
1	D	152	GLU	3.5
1	M	343	LYS	3.5
1	A	24	GLY	3.4
1	G	328	VAL	3.4
1	P	140	VAL	3.4
1	F	28	SER	3.4
1	J	327	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	152	GLU	3.4
1	L	328	VAL	3.3
1	N	15	GLU	3.3
1	O	13	ARG	3.3
1	M	26	VAL	3.3
1	P	141	GLU	3.2
1	N	13	ARG	3.2
1	B	17	GLU	3.2
1	M	24	GLY	3.1
1	J	145	LYS	3.1
1	E	343	LYS	3.1
1	F	325	LYS	3.1
1	A	21	HIS	3.0
1	O	16	TYR	3.0
1	C	27	SER	3.0
1	B	145	LYS	3.0
1	C	21	HIS	3.0
1	D	15	GLU	3.0
1	L	28	SER	3.0
1	N	152	GLU	3.0
1	K	145	LYS	3.0
1	E	17	GLU	2.9
1	M	18	LYS	2.9
1	E	16	TYR	2.9
1	K	29	GLU	2.9
1	C	343	LYS	2.9
1	K	343	LYS	2.9
1	O	328	VAL	2.9
1	F	327	GLU	2.9
1	K	15	GLU	2.9
1	F	15	GLU	2.9
1	I	24	GLY	2.8
1	D	145	LYS	2.8
1	M	17	GLU	2.8
1	M	328	VAL	2.8
1	M	19	PRO	2.7
1	M	27	SER	2.7
1	E	152	GLU	2.7
1	B	16	TYR	2.7
1	K	16	TYR	2.7
1	G	343	LYS	2.7
1	J	13	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	21	HIS	2.6
1	J	16	TYR	2.6
1	C	152	GLU	2.6
1	C	25	SER	2.6
1	D	141	GLU	2.6
1	J	152	GLU	2.6
1	H	16	TYR	2.6
1	D	325	LYS	2.6
1	E	144	VAL	2.6
1	F	343	LYS	2.5
1	D	29	GLU	2.5
1	J	29	GLU	2.5
1	E	31	ARG	2.5
1	L	141	GLU	2.5
1	I	25	SER	2.5
1	P	327	GLU	2.5
1	B	328	VAL	2.5
1	E	141	GLU	2.4
1	O	17	GLU	2.4
1	K	152	GLU	2.4
1	F	16	TYR	2.4
1	A	18	LYS	2.4
1	F	152	GLU	2.4
1	N	141	GLU	2.4
1	N	145	LYS	2.4
1	C	323	MET	2.4
1	D	144	VAL	2.4
1	K	324	LEU	2.4
1	P	16	TYR	2.4
1	E	13	ARG	2.4
1	G	342	VAL	2.3
1	C	22	ILE	2.3
1	P	142	ASN	2.3
1	B	140	VAL	2.3
1	O	140	VAL	2.3
1	O	343	LYS	2.3
1	D	13	ARG	2.3
1	G	181	ARG	2.3
1	H	17	GLU	2.3
1	L	140	VAL	2.3
1	D	146	GLU	2.3
1	N	328	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	325	LYS	2.3
1	M	152	GLU	2.2
1	D	148	LYS	2.2
1	D	324	LEU	2.2
1	M	324	LEU	2.2
1	M	72	GLU	2.2
1	O	15	GLU	2.2
1	M	28	SER	2.2
1	H	141	GLU	2.2
1	L	144	VAL	2.2
1	M	140	VAL	2.2
1	J	15	GLU	2.1
1	L	232	PHE	2.1
1	J	343	LYS	2.1
1	B	141	GLU	2.1
1	F	146	GLU	2.1
1	O	145	LYS	2.1
1	G	15	GLU	2.1
1	J	141	GLU	2.1
1	A	145	LYS	2.1
1	C	23	THR	2.1
1	G	17	GLU	2.1
1	P	139	THR	2.0
1	P	15	GLU	2.0
1	M	21	HIS	2.0
1	L	343	LYS	2.0
1	M	141	GLU	2.0
1	A	26	VAL	2.0
1	E	181	ARG	2.0
1	F	145	LYS	2.0
1	N	18	LYS	2.0
1	J	146	GLU	2.0
1	A	25	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	MG	C	401	1/1	0.93	0.13	0.96	24,24,24,24	0
2	MG	A	401	1/1	0.81	0.12	0.29	26,26,26,26	0
2	MG	O	401	1/1	0.89	0.10	-0.39	27,27,27,27	0
2	MG	I	401	1/1	0.88	0.10	-0.50	26,26,26,26	0
2	MG	M	401	1/1	0.88	0.11	-0.56	27,27,27,27	0
2	MG	J	401	1/1	0.79	0.10	-0.71	27,27,27,27	0
2	MG	L	401	1/1	0.82	0.09	-0.81	29,29,29,29	0
2	MG	P	401	1/1	0.87	0.09	-0.82	25,25,25,25	0
2	MG	H	401	1/1	0.91	0.08	-1.06	25,25,25,25	0
2	MG	F	401	1/1	0.86	0.09	-1.26	29,29,29,29	0
2	MG	N	401	1/1	0.87	0.07	-1.32	29,29,29,29	0
2	MG	D	401	1/1	0.85	0.07	-1.78	28,28,28,28	0
2	MG	G	401	1/1	0.96	0.08	-1.92	26,26,26,26	0
2	MG	B	401	1/1	0.92	0.07	-2.08	27,27,27,27	0
2	MG	E	401	1/1	0.97	0.06	-2.56	29,29,29,29	0
2	MG	K	401	1/1	0.96	0.06	-3.33	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.