



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AOE
Title : Crystal structure of hetero-hexameric glutamate dehydrogenase from *Thermus thermophilus* (Leu bound form)
Authors : Tomita, T.; Kuzuyama, T.; Nishiyama, M.
Deposited on : 2010-09-27
Resolution : 2.60 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

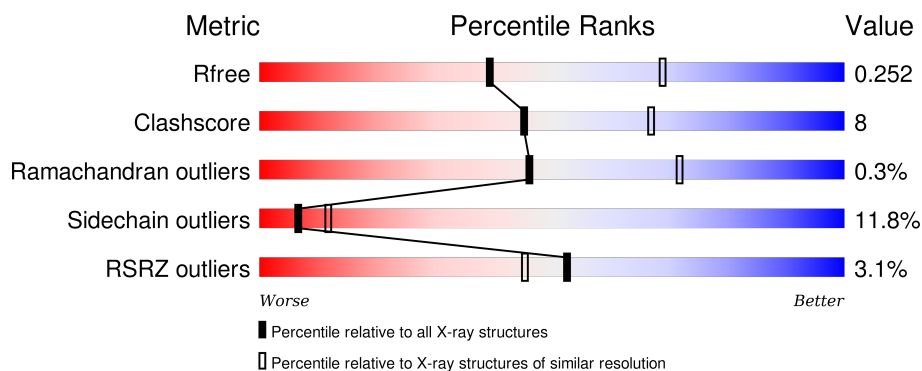
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	424	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 76%, yellow 19%, orange 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 76% 19% . </div> </div>
1	B	424	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 80%, yellow 17%, orange 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 80% 17% . </div> </div>
2	C	419	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 80%, yellow 17%, orange 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 80% 17% . </div> </div>
2	D	419	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 78%, yellow 18%, orange 2%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 78% 18% .. </div> </div>
2	E	419	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 77%, yellow 19%, orange 2%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 77% 19% .. </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	419	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment at the beginning labeled '9%', a green segment in the middle labeled '80%', and a yellow segment at the end labeled '17%'. The bar ends with two small black dots.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19355 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.

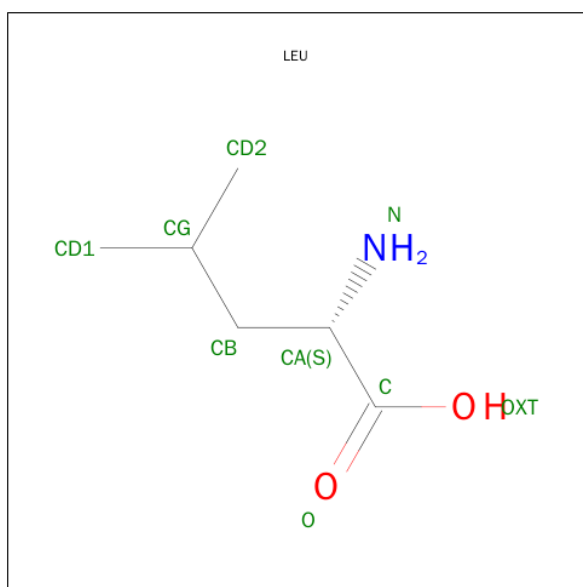
- Molecule 1 is a protein called Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	1	0
			3250	2068	583	593	6			
1	B	424	Total	C	N	O	S	0	1	0
			3267	2079	586	595	7			

- Molecule 2 is a protein called Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	416	Total	C	N	O	S	0	0	0
			3114	1972	552	579	11			
2	F	417	Total	C	N	O	S	0	0	0
			3122	1978	553	580	11			
2	C	417	Total	C	N	O	S	0	0	0
			3122	1978	553	580	11			
2	D	416	Total	C	N	O	S	0	0	0
			3114	1972	552	579	11			

- Molecule 3 is LEUCINE (three-letter code: LEU) (formula: C₆H₁₃NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	E	1	Total	C	N	O	0	0
			9	6	1	2		
3	F	1	Total	C	N	O	0	0
			9	6	1	2		
3	C	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		

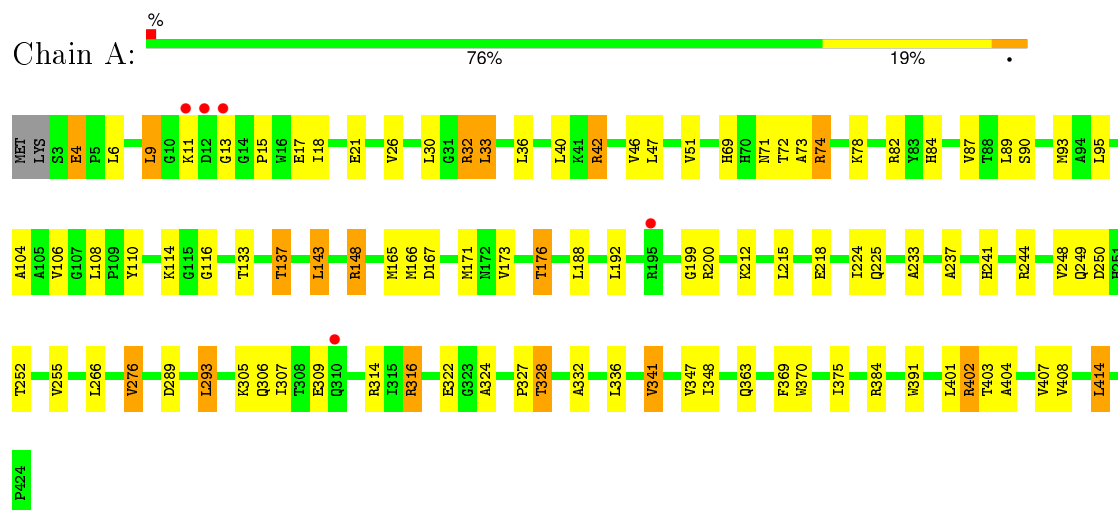
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	58	Total	O	0	0
			58	58		
4	E	55	Total	O	0	0
			55	55		
4	F	28	Total	O	0	0
			28	28		
4	C	57	Total	O	0	0
			57	57		
4	D	61	Total	O	0	0
			61	61		

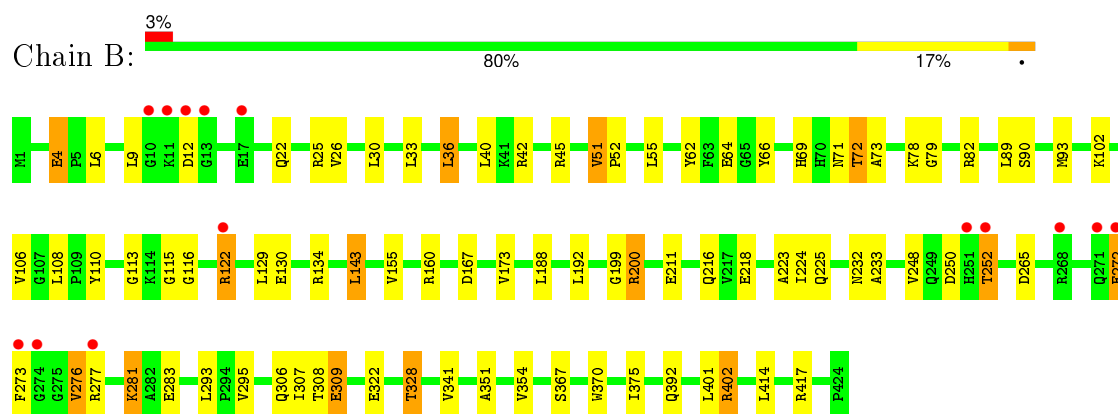
3 Residue-property plots

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.

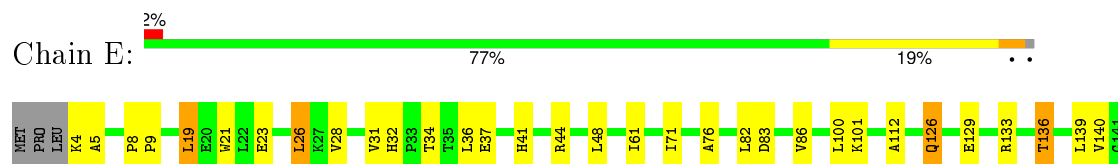
• Molecule 1: Glutamate dehydrogenase

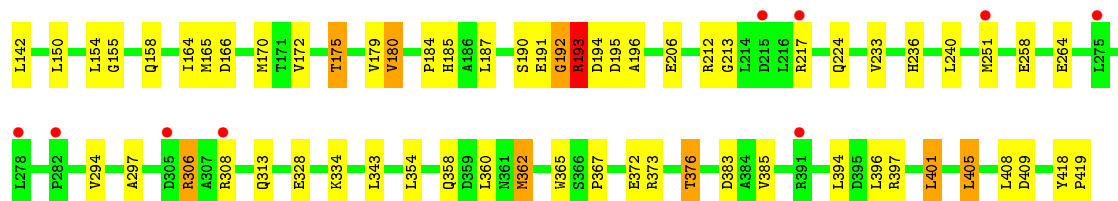


• Molecule 1: Glutamate dehydrogenase

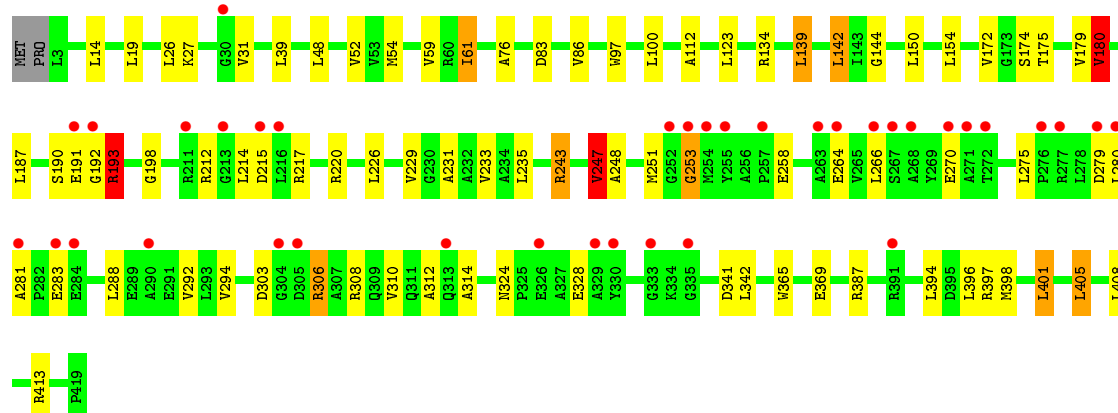
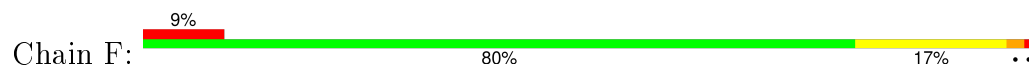


• Molecule 2: Glutamate dehydrogenase

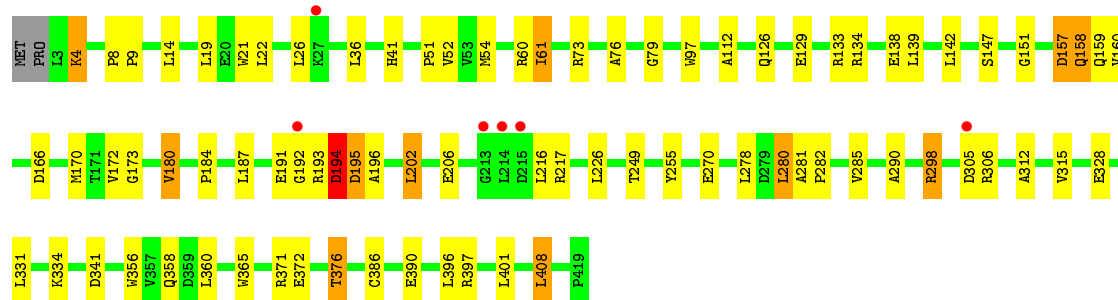




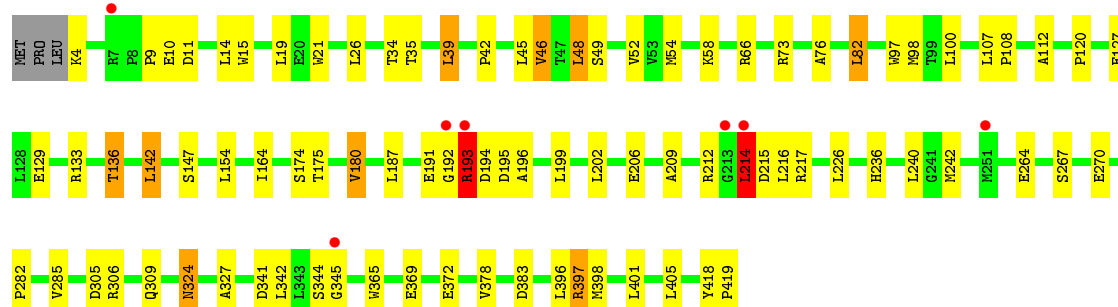
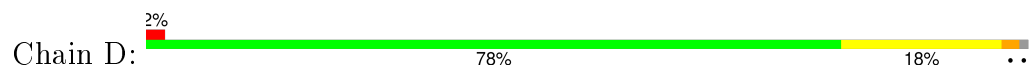
• Molecule 2: Glutamate dehydrogenase



• Molecule 2: Glutamate dehydrogenase



• Molecule 2: Glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.99Å 146.09Å 158.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.22 – 2.60 30.22 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.22-2.60) 100.0 (30.22-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.193 , 0.260 0.188 , 0.252	Depositor DCC
R_{free} test set	4383 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 87436 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19355	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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	0.65	0/3330	0.73	2/4532 (0.0%)
1	B	0.62	0/3347	0.72	2/4553 (0.0%)
2	C	0.62	0/3179	0.77	3/4320 (0.1%)
2	D	0.62	0/3171	0.77	3/4309 (0.1%)
2	E	0.58	0/3171	0.71	0/4309
2	F	0.58	0/3179	0.71	2/4320 (0.0%)
All	All	0.61	0/19377	0.73	12/26343 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	D	0	1
2	E	0	1
2	F	0	1
All	All	0	4

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	ARG	NE-CZ-NH2	6.89	123.74	120.30
2	C	180	VAL	CB-CA-C	-6.74	98.60	111.40
1	A	74	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	402	ARG	NE-CZ-NH1	-5.90	117.35	120.30
2	D	48	LEU	CA-CB-CG	5.90	128.88	115.30
2	C	202	LEU	CA-CB-CG	-5.83	101.89	115.30
2	F	180	VAL	CB-CA-C	-5.81	100.36	111.40
2	C	26	LEU	CA-CB-CG	5.63	128.25	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	214	LEU	CA-CB-CG	5.61	128.20	115.30
1	B	402	ARG	NE-CZ-NH1	-5.60	117.50	120.30
2	D	180	VAL	CB-CA-C	-5.11	101.69	111.40
2	F	123	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	194	ASP	Peptide
2	D	345	GLY	Peptide
2	E	192	GLY	Peptide
2	F	193	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3250	0	3243	59	0
1	B	3267	0	3268	52	0
2	C	3122	0	3164	44	0
2	D	3114	0	3153	44	0
2	E	3114	0	3153	63	0
2	F	3122	0	3164	50	0
3	A	9	0	10	0	0
3	B	9	0	10	2	0
3	C	9	0	10	0	0
3	D	9	0	10	1	0
3	E	9	0	10	0	0
3	F	9	0	10	0	0
4	A	53	0	0	1	0
4	B	58	0	0	3	0
4	C	57	0	0	0	0
4	D	61	0	0	2	0
4	E	55	0	0	1	0
4	F	28	0	0	0	0
All	All	19355	0	19205	297	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 8.

All (297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:193:ARG:HB3	2:E:195:ASP:HB3	1.25	1.13
2:D:192:GLY:HA2	2:D:193:ARG:HB3	1.30	1.12
1:A:9:LEU:HD11	1:A:93:MET:HE1	1.32	1.11
2:F:192:GLY:HA2	2:F:193:ARG:HB2	1.12	1.11
2:C:298:ARG:HG2	2:C:298:ARG:HH11	1.21	1.02
2:C:193:ARG:HB3	2:C:196:ALA:HB2	1.43	1.00
2:E:26:LEU:HD11	2:E:36:LEU:HD11	1.45	0.96
1:A:225:GLN:HE22	1:A:306:GLN:HE21	1.01	0.95
2:C:193:ARG:HA	2:C:195:ASP:H	1.35	0.92
1:A:9:LEU:HD11	1:A:93:MET:CE	2.01	0.91
2:D:192:GLY:HA2	2:D:193:ARG:CB	2.04	0.87
1:B:89:LEU:HG	1:B:93:MET:CE	2.05	0.85
1:A:225:GLN:NE2	1:A:306:GLN:HE21	1.74	0.85
2:E:193:ARG:HB3	2:E:195:ASP:CB	2.09	0.83
2:E:136:THR:HG21	2:E:164:ILE:HA	1.62	0.81
2:E:358:GLN:HE21	2:E:365:TRP:H	1.29	0.81
2:F:233:VAL:HG11	2:F:294:VAL:HG11	1.62	0.80
2:E:193:ARG:CB	2:E:195:ASP:H	1.95	0.80
2:F:192:GLY:CA	2:F:193:ARG:HB2	2.05	0.80
1:A:250:ASP:HB3	1:A:252:THR:H	1.48	0.79
2:F:192:GLY:HA2	2:F:193:ARG:CB	1.94	0.78
2:E:193:ARG:HA	2:E:194:ASP:HB2	1.65	0.77
2:F:31:VAL:HG21	2:F:405:LEU:HD12	1.65	0.77
1:A:95:LEU:HB3	1:A:114:LYS:HD2	1.64	0.77
2:D:136:THR:HG21	2:D:164:ILE:HA	1.67	0.77
2:E:193:ARG:HB2	2:E:195:ASP:H	1.49	0.76
1:B:106:VAL:HG23	1:B:108:LEU:HG	1.67	0.75
1:B:200:ARG:HD2	4:B:471:HOH:O	1.85	0.75
1:A:176:THR:HG22	4:A:444:HOH:O	1.86	0.75
2:E:175:THR:HG22	4:E:432:HOH:O	1.86	0.74
1:B:225:GLN:HE22	1:B:306:GLN:HG3	1.52	0.73
1:A:316:ARG:HH11	1:A:316:ARG:HB3	1.53	0.72
2:F:248:ALA:HB3	2:F:253:GLY:HA2	1.73	0.70
2:E:26:LEU:HD11	2:E:36:LEU:CD1	2.20	0.70
1:A:225:GLN:HE22	1:A:306:GLN:NE2	1.84	0.70
2:D:193:ARG:HH11	2:D:193:ARG:HG3	1.56	0.70
2:E:190:SER:HB3	2:E:191:GLU:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:OE1	1:A:328:THR:HG23	1.92	0.69
1:A:71:ASN:ND2	1:A:73:ALA:H	1.91	0.69
1:B:122:ARG:HA	1:B:122:ARG:HE	1.58	0.69
2:F:97:TRP:HZ3	2:F:341:ASP:CG	1.96	0.68
1:A:74:ARG:NH2	1:A:108:LEU:O	2.27	0.68
2:C:193:ARG:HA	2:C:195:ASP:N	2.09	0.67
1:B:79:GLY:HA3	1:B:113:GLY:O	1.96	0.66
2:E:190:SER:HB3	2:E:191:GLU:CA	2.26	0.66
2:E:76:ALA:HB1	2:E:112:ALA:HB2	1.78	0.66
2:E:4:LYS:HE3	2:E:23:GLU:OE2	1.94	0.66
1:A:106:VAL:HG13	1:A:108:LEU:HG	1.77	0.65
1:A:137:THR:HG21	1:A:165:MET:HG2	1.77	0.65
2:E:372:GLU:O	2:E:376:THR:HG22	1.96	0.65
2:C:298:ARG:HG2	2:C:298:ARG:NH1	1.97	0.65
2:D:54:MET:HE2	2:D:127:GLU:HG2	1.79	0.64
1:B:322:GLU:OE1	1:B:328:THR:HG23	1.98	0.64
2:E:190:SER:CB	2:E:191:GLU:HA	2.29	0.63
2:E:26:LEU:CD1	2:E:36:LEU:HD11	2.26	0.63
2:C:341:ASP:OD2	2:C:397:ARG:NH1	2.32	0.62
2:D:46:VAL:HG13	2:D:66:ARG:O	2.00	0.62
2:E:150:LEU:HB2	2:E:180:VAL:HG13	1.81	0.62
2:E:224:GLN:NE2	2:E:297:ALA:HB3	2.14	0.62
1:A:266:LEU:HD11	1:A:276:VAL:HG22	1.81	0.61
2:C:51:PRO:HB3	2:C:61:ILE:HD13	1.82	0.61
1:B:9:LEU:HD22	1:B:90:SER:HB3	1.83	0.61
2:C:191:GLU:O	2:C:193:ARG:N	2.33	0.61
1:B:281:LYS:O	1:B:281:LYS:HD3	2.01	0.61
2:E:126:GLN:H	2:E:126:GLN:NE2	1.97	0.61
1:B:307:ILE:HB	1:B:328:THR:HB	1.83	0.61
2:E:179:VAL:HG13	2:E:180:VAL:HG22	1.81	0.61
2:E:328:GLU:OE1	2:E:397:ARG:NH2	2.33	0.61
2:F:190:SER:C	2:F:192:GLY:H	2.05	0.60
1:A:336:LEU:HB3	1:A:341:VAL:HG22	1.83	0.60
2:C:193:ARG:NH1	2:C:371:ARG:HE	2.00	0.60
2:E:358:GLN:NE2	2:E:365:TRP:H	1.97	0.60
2:E:193:ARG:HD3	2:E:196:ALA:HB2	1.82	0.60
2:E:37:GLU:HG3	2:F:61:ILE:HD13	1.84	0.59
2:C:76:ALA:HB1	2:C:112:ALA:HB2	1.84	0.59
2:E:372:GLU:O	2:E:376:THR:CG2	2.51	0.59
2:F:280:LEU:HD11	2:F:288:LEU:HD21	1.84	0.59
1:A:225:GLN:HE21	1:A:249:GLN:HE21	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:ARG:CD	2:D:196:ALA:HB2	2.33	0.58
2:F:142:LEU:HD12	2:F:142:LEU:N	2.18	0.58
2:F:179:VAL:HG13	2:F:180:VAL:HG22	1.86	0.58
1:A:322:GLU:CD	1:A:402:ARG:HH12	2.06	0.58
1:A:363:GLN:NE2	1:A:370:TRP:H	2.02	0.58
2:C:372:GLU:O	2:C:376:THR:HG23	2.04	0.58
2:F:97:TRP:CZ3	2:F:341:ASP:OD1	2.57	0.57
2:E:184:PRO:HG2	2:E:187:LEU:HD22	1.86	0.57
2:C:73:ARG:HD3	2:C:408:LEU:HD13	1.87	0.56
2:F:97:TRP:HZ3	2:F:341:ASP:OD1	1.87	0.56
1:B:216:GLN:HE21	1:B:218:GLU:HB2	1.71	0.56
2:E:418:TYR:CD1	2:E:419:PRO:HA	2.41	0.55
2:F:220:ARG:HA	2:F:243:ARG:O	2.07	0.55
1:A:84:HIS:HB3	1:A:87:VAL:HG23	1.87	0.55
1:A:9:LEU:CD1	1:A:93:MET:HE1	2.21	0.55
1:A:42:ARG:HD2	1:B:62:TYR:HB3	1.87	0.55
1:B:252:THR:HG22	1:B:277:ARG:HB2	1.88	0.55
1:A:237:ALA:O	1:A:241:HIS:HD2	1.90	0.55
2:C:193:ARG:HH12	2:C:371:ARG:HE	1.53	0.55
2:E:193:ARG:CB	2:E:195:ASP:N	2.68	0.55
1:A:404:ALA:O	1:A:408:VAL:HG23	2.08	0.54
1:A:90:SER:HA	1:A:93:MET:HE2	1.89	0.54
1:B:22:GLN:NE2	1:B:25:ARG:HH21	2.05	0.54
2:E:190:SER:HB3	2:E:191:GLU:HB2	1.90	0.54
1:A:322:GLU:OE2	1:A:402:ARG:NH1	2.41	0.54
1:A:32:ARG:HH11	1:A:32:ARG:HB3	1.73	0.54
2:C:9:PRO:HB2	2:D:9:PRO:HB2	1.90	0.53
2:F:191:GLU:OE1	2:F:191:GLU:HA	2.08	0.53
2:F:226:LEU:HD11	2:F:247:VAL:HB	1.91	0.53
1:A:307:ILE:HB	1:A:328:THR:HB	1.90	0.53
2:E:19:LEU:O	2:E:23:GLU:HG3	2.09	0.53
1:A:255:VAL:HG13	1:A:276:VAL:HG13	1.91	0.53
2:C:386:CYS:O	2:C:390:GLU:HG2	2.09	0.53
2:E:28:VAL:HG11	2:E:394:LEU:HD21	1.90	0.53
2:E:362:MET:HG2	2:C:356:TRP:CH2	2.44	0.53
2:E:41:HIS:CG	2:F:61:ILE:HG21	2.44	0.53
2:F:328:GLU:OE1	2:F:397:ARG:NH2	2.41	0.52
2:E:126:GLN:H	2:E:126:GLN:HE21	1.57	0.52
2:D:76:ALA:HB1	2:D:112:ALA:HB2	1.90	0.52
1:B:89:LEU:HG	1:B:93:MET:HE1	1.89	0.52
2:F:97:TRP:CZ3	2:F:341:ASP:OD2	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:358:GLN:HE21	2:C:365:TRP:H	1.58	0.52
2:F:97:TRP:HZ3	2:F:341:ASP:OD2	1.92	0.51
2:E:193:ARG:HA	2:E:194:ASP:CB	2.33	0.51
2:F:76:ALA:HB1	2:F:112:ALA:HB2	1.91	0.51
2:D:21:TRP:HZ3	2:D:398:MET:HE2	1.76	0.51
2:D:191:GLU:O	2:D:193:ARG:HA	2.10	0.51
1:A:74:ARG:NH2	1:A:104:ALA:HA	2.26	0.51
1:B:89:LEU:HG	1:B:93:MET:HE2	1.91	0.51
2:E:192:GLY:N	2:E:193:ARG:HG3	2.25	0.51
1:A:133:THR:O	1:A:137:THR:HG23	2.11	0.51
2:D:192:GLY:CA	2:D:193:ARG:CB	2.86	0.50
1:A:363:GLN:HE21	1:A:370:TRP:H	1.59	0.50
1:B:160:ARG:HG3	4:D:469:HOH:O	2.10	0.50
2:C:52:VAL:HG12	2:C:54:MET:HE2	1.93	0.50
2:E:41:HIS:CD2	2:F:61:ILE:HG21	2.46	0.50
2:D:42:PRO:HG2	2:D:45:LEU:HD11	1.94	0.50
1:A:167:ASP:O	1:A:171:MET:HG2	2.11	0.50
2:D:418:TYR:CD1	2:D:419:PRO:HA	2.47	0.50
2:D:206:GLU:OE2	2:D:240:LEU:HD13	2.12	0.50
2:F:190:SER:C	2:F:192:GLY:N	2.65	0.50
2:C:157:ASP:HB3	2:C:159:GLN:H	1.77	0.50
2:D:54:MET:CE	2:D:54:MET:HA	2.41	0.49
1:B:322:GLU:CD	1:B:402:ARG:HH12	2.15	0.49
1:B:370:TRP:HE3	1:B:375:ILE:HD13	1.77	0.49
2:E:258:GLU:OE1	2:E:258:GLU:N	2.43	0.49
2:C:193:ARG:CB	2:C:196:ALA:HB2	2.29	0.49
2:E:365:TRP:CE2	2:E:373:ARG:NH1	2.80	0.49
1:B:367:SER:HB3	2:D:108:PRO:HG3	1.94	0.49
1:A:46:VAL:HG11	1:A:89:LEU:HD11	1.94	0.49
2:D:341:ASP:OD1	2:D:397:ARG:NH1	2.46	0.49
1:B:417:ARG:CD	3:B:500:LEU:HD23	2.42	0.49
2:F:229:VAL:O	2:F:233:VAL:HG23	2.13	0.49
2:E:44:ARG:HB3	2:F:48:LEU:HD23	1.94	0.49
2:E:343:LEU:HD13	2:E:385:VAL:HG21	1.95	0.49
1:B:322:GLU:OE2	1:B:402:ARG:NH1	2.44	0.48
2:C:54:MET:HE3	2:C:60:ARG:HB3	1.96	0.48
2:F:52:VAL:HG12	2:F:54:MET:CE	2.43	0.48
1:A:199:GLY:HA3	1:A:233:ALA:HB3	1.95	0.48
1:B:199:GLY:HA3	1:B:233:ALA:HB3	1.95	0.48
2:E:236:HIS:O	2:E:240:LEU:HG	2.13	0.48
1:B:417:ARG:HD2	3:B:500:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:129:GLU:O	2:E:133:ARG:HG3	2.13	0.48
1:B:392:GLN:NE2	4:B:467:HOH:O	2.46	0.48
1:A:82:ARG:O	1:A:116:GLY:HA2	2.12	0.48
1:B:308:THR:HG22	1:B:309:GLU:N	2.29	0.48
1:A:42:ARG:HD2	1:B:62:TYR:CB	2.43	0.48
1:A:33:LEU:HG	1:A:414:LEU:HB3	1.96	0.48
2:E:32:HIS:HD2	2:E:409:ASP:OD1	1.95	0.47
1:B:102:LYS:HZ3	1:B:351:ALA:HA	1.79	0.47
2:E:21:TRP:HB3	2:E:401:LEU:HD21	1.95	0.47
1:B:122:ARG:CA	1:B:122:ARG:HE	2.26	0.47
2:C:315:VAL:HG21	2:C:331:LEU:HD13	1.95	0.47
1:B:22:GLN:HE22	1:B:25:ARG:HH21	1.62	0.46
1:A:347:VAL:HG23	1:A:348:ILE:HG23	1.97	0.46
2:F:253:GLY:O	2:F:280:LEU:HB2	2.15	0.46
1:A:363:GLN:HE21	1:A:369:PHE:HA	1.80	0.46
2:C:41:HIS:HB3	2:D:49:SER:OG	2.15	0.46
2:C:158:GLN:HG3	2:C:184:PRO:HG3	1.98	0.46
1:B:4:GLU:O	1:B:42:ARG:NH2	2.49	0.46
2:E:192:GLY:C	2:E:193:ARG:HG3	2.36	0.46
2:E:4:LYS:HA	2:E:5:ALA:HB2	1.98	0.46
2:C:328:GLU:OE1	2:C:397:ARG:NH2	2.39	0.46
1:A:212:LYS:HE3	1:A:391:TRP:CD1	2.51	0.46
2:F:342:LEU:HD11	2:F:401:LEU:HD13	1.97	0.46
2:C:8:PRO:HA	2:C:9:PRO:HD3	1.77	0.46
2:C:129:GLU:O	2:C:133:ARG:HG3	2.16	0.46
1:A:69:HIS:CE1	1:A:143:LEU:HG	2.50	0.46
2:E:224:GLN:HE22	2:E:297:ALA:HB3	1.79	0.46
2:D:15:TRP:CH2	2:D:42:PRO:HD3	2.50	0.46
2:D:73:ARG:NH2	2:D:107:LEU:O	2.49	0.46
2:D:21:TRP:CZ3	2:D:398:MET:HE2	2.50	0.45
2:D:54:MET:HA	2:D:54:MET:HE2	1.96	0.45
1:B:167:ASP:OD1	3:D:500:LEU:N	2.49	0.45
2:C:290:ALA:O	2:C:312:ALA:HA	2.16	0.45
1:B:82:ARG:HG3	1:B:155:VAL:HB	1.97	0.45
1:A:370:TRP:HE3	1:A:375:ILE:HD13	1.81	0.45
2:E:190:SER:HB3	2:E:191:GLU:CB	2.46	0.45
2:C:134:ARG:O	2:C:138:GLU:HG2	2.16	0.45
1:A:225:GLN:HE21	1:A:249:GLN:NE2	2.12	0.45
2:F:342:LEU:CD1	2:F:401:LEU:HD13	2.45	0.45
2:C:281:ALA:HB1	2:C:282:PRO:HD2	1.99	0.45
2:F:150:LEU:HB2	2:F:180:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:292:VAL:HG22	2:F:314:ALA:HB3	1.98	0.45
2:F:394:LEU:HB3	2:F:398:MET:HB3	1.98	0.45
2:D:142:LEU:N	2:D:142:LEU:HD12	2.31	0.45
2:C:255:TYR:HB2	2:C:280:LEU:HD11	1.98	0.45
2:C:202:LEU:O	2:C:206:GLU:HG2	2.17	0.45
2:D:324:ASN:HD22	2:D:324:ASN:C	2.19	0.45
1:B:72:THR:HG23	1:B:72:THR:O	2.17	0.45
1:A:224:ILE:O	1:A:248:VAL:HA	2.17	0.45
2:C:21:TRP:CZ2	2:C:397:ARG:HD3	2.53	0.44
1:B:252:THR:CG2	1:B:277:ARG:HB2	2.46	0.44
2:D:21:TRP:CH2	2:D:397:ARG:HD3	2.52	0.44
1:B:69:HIS:CE1	1:B:143:LEU:HG	2.52	0.44
2:E:8:PRO:HA	2:E:9:PRO:HD3	1.78	0.44
1:A:90:SER:HA	1:A:93:MET:CE	2.47	0.44
1:A:15:PRO:HA	1:A:18:ILE:HD12	1.98	0.44
2:F:280:LEU:HB3	2:F:281:ALA:H	1.60	0.44
2:F:52:VAL:CG1	2:F:54:MET:CE	2.96	0.44
2:D:82:LEU:HB3	2:D:120:PRO:HG3	1.99	0.44
1:A:89:LEU:O	1:A:93:MET:HG3	2.17	0.44
1:A:403:THR:O	1:A:407:VAL:HG23	2.18	0.44
1:B:71:ASN:ND2	1:B:73:ALA:H	2.15	0.44
2:F:365:TRP:HB3	2:F:369:GLU:HB3	1.99	0.44
2:C:166:ASP:O	2:C:170:MET:HG2	2.18	0.43
2:F:310:VAL:HG12	2:F:312:ALA:H	1.83	0.43
2:F:247:VAL:HB	2:F:248:ALA:H	1.60	0.43
1:B:51:VAL:HA	1:B:52:PRO:HD2	1.82	0.43
2:D:209:ALA:HB1	2:D:214:LEU:HB3	2.01	0.43
2:E:185:HIS:HD2	2:E:190:SER:HB2	1.83	0.43
1:A:289:ASP:O	1:A:293:LEU:HD13	2.19	0.43
2:F:97:TRP:CZ3	2:F:341:ASP:CG	2.84	0.43
2:F:48:LEU:HD11	2:F:139:LEU:HD13	2.01	0.43
2:F:283:GLU:HB3	2:F:306:ARG:NH1	2.33	0.43
2:D:365:TRP:HB3	2:D:369:GLU:HB2	2.00	0.43
2:E:34:THR:HG23	2:F:59:VAL:HG21	2.01	0.43
2:F:303:ASP:HA	2:F:324:ASN:HB2	2.00	0.43
1:A:250:ASP:OD2	1:A:276:VAL:HB	2.19	0.43
2:C:9:PRO:HB3	2:D:10:GLU:HG2	2.01	0.43
2:C:157:ASP:HB2	2:C:160:VAL:HG23	2.01	0.43
2:E:191:GLU:HA	2:E:192:GLY:HA2	1.61	0.42
1:B:36:LEU:HB3	1:B:414:LEU:HG	2.00	0.42
2:D:129:GLU:O	2:D:133:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:LEU:HD13	2:D:236:HIS:CE1	2.54	0.42
2:D:282:PRO:O	2:D:285:VAL:HG12	2.19	0.42
1:A:133:THR:O	1:A:137:THR:CG2	2.68	0.42
2:D:306:ARG:O	2:D:309:GLN:HB2	2.19	0.42
1:A:4:GLU:H	1:A:4:GLU:HG3	1.62	0.42
2:F:144:GLY:HA2	2:F:179:VAL:HG23	2.01	0.42
2:C:52:VAL:CG1	2:C:54:MET:CE	2.98	0.42
1:A:148:ARG:HD3	2:C:173:GLY:O	2.18	0.42
2:C:206:GLU:OE1	2:C:216:LEU:HD12	2.19	0.42
1:B:40:LEU:HG	1:B:414:LEU:HD11	2.02	0.42
1:B:224:ILE:O	1:B:248:VAL:HA	2.19	0.42
1:B:82:ARG:O	1:B:116:GLY:HA2	2.19	0.42
1:B:66:TYR:O	1:B:115:GLY:HA2	2.20	0.42
2:D:52:VAL:HG12	2:D:54:MET:HE3	2.00	0.42
2:C:52:VAL:CG1	2:C:54:MET:HE1	2.50	0.42
2:F:83:ASP:HB3	2:F:86:VAL:HG23	2.00	0.42
2:D:216:LEU:HD13	2:D:242:MET:CE	2.49	0.42
2:F:52:VAL:HB	2:F:54:MET:HE1	2.01	0.42
2:E:405:LEU:HA	2:E:405:LEU:HD12	1.89	0.42
2:F:231:ALA:HB1	2:F:266:LEU:HD11	2.02	0.42
1:A:332:ALA:O	1:A:336:LEU:HG	2.19	0.41
2:E:82:LEU:HD12	2:E:155:GLY:O	2.20	0.41
2:E:83:ASP:HB3	2:E:86:VAL:HG23	2.01	0.41
2:F:198:GLY:HA2	2:F:233:VAL:HG22	2.01	0.41
2:E:166:ASP:O	2:E:170:MET:HG2	2.20	0.41
1:B:216:GLN:HE21	1:B:218:GLU:CB	2.33	0.41
2:D:324:ASN:ND2	2:D:327:ALA:H	2.18	0.41
2:D:21:TRP:HZ3	2:D:398:MET:CE	2.33	0.41
1:A:78:LYS:HD3	1:A:110:TYR:CZ	2.55	0.41
1:A:324:ALA:O	1:A:327:PRO:HD3	2.19	0.41
1:B:250:ASP:OD2	1:B:276:VAL:HB	2.21	0.41
2:F:134:ARG:HA	2:F:134:ARG:HD2	1.84	0.41
1:B:130:GLU:O	1:B:134:ARG:HG3	2.20	0.41
2:C:194:ASP:HA	2:C:196:ALA:H	1.85	0.41
2:E:358:GLN:O	2:E:362:MET:N	2.52	0.41
2:F:397:ARG:O	2:F:401:LEU:HB2	2.20	0.41
2:E:191:GLU:HG2	2:E:367:PRO:HG3	2.02	0.41
1:A:15:PRO:HD2	1:A:90:SER:OG	2.21	0.41
1:B:223:ALA:HB2	1:B:295:VAL:HG11	2.03	0.41
2:C:4:LYS:HD3	2:C:4:LYS:HA	2.00	0.41
1:B:200:ARG:CD	4:B:471:HOH:O	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LYS:HD3	1:B:110:TYR:CZ	2.55	0.41
2:D:405:LEU:HA	2:D:405:LEU:HD13	1.64	0.41
1:A:47:LEU:HD11	1:B:45:ARG:HG3	2.02	0.41
2:D:35:THR:HG22	2:D:39:LEU:HD22	2.03	0.41
2:D:397:ARG:NH1	4:D:439:HOH:O	2.54	0.40
2:D:73:ARG:HD3	2:D:73:ARG:HH21	1.75	0.40
2:E:306:ARG:HA	2:E:306:ARG:HD2	1.82	0.40
2:D:192:GLY:CA	2:D:193:ARG:NE	2.84	0.40
1:B:64:GLU:OE1	1:B:66:TYR:OH	2.34	0.40
1:B:272:GLU:HB3	1:B:273:PHE:CD1	2.56	0.40
2:E:362:MET:HG2	2:C:356:TRP:HH2	1.85	0.40
2:E:233:VAL:HG11	2:E:294:VAL:HG11	2.04	0.40
2:D:193:ARG:HH11	2:D:193:ARG:CG	2.28	0.40
2:C:79:GLY:HA2	2:C:151:GLY:O	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	421/424 (99%)	407 (97%)	13 (3%)	1 (0%)	52	77
1	B	423/424 (100%)	409 (97%)	14 (3%)	0	100	100
2	C	415/419 (99%)	400 (96%)	14 (3%)	1 (0%)	52	77
2	D	414/419 (99%)	399 (96%)	14 (3%)	1 (0%)	52	77
2	E	414/419 (99%)	392 (95%)	20 (5%)	2 (0%)	34	60
2	F	415/419 (99%)	375 (90%)	38 (9%)	2 (0%)	34	60
All	All	2502/2524 (99%)	2382 (95%)	113 (4%)	7 (0%)	46	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	193	ARG
2	F	253	GLY
2	F	247	VAL
2	C	192	GLY
2	D	193	ARG
1	A	13	GLY
2	E	213	GLY

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	327/328 (100%)	289 (88%)	38 (12%)	7	12
1	B	329/328 (100%)	298 (91%)	31 (9%)	11	20
2	C	312/314 (99%)	278 (89%)	34 (11%)	8	14
2	D	311/314 (99%)	267 (86%)	44 (14%)	4	7
2	E	311/314 (99%)	273 (88%)	38 (12%)	6	11
2	F	312/314 (99%)	275 (88%)	37 (12%)	6	11
All	All	1902/1912 (100%)	1680 (88%)	222 (12%)	6	12

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	6	LEU
1	A	9	LEU
1	A	11	LYS
1	A	17	GLU
1	A	21	GLU
1	A	26	VAL
1	A	30	LEU
1	A	32	ARG
1	A	33	LEU
1	A	36	LEU
1	A	40	LEU

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Mol	Chain	Res	Type
1	A	42	ARG
1	A	51	VAL
1	A	72	THR
1	A	137	THR
1	A	143	LEU
1	A	148	ARG
1	A	166	MET
1	A	173	VAL
1	A	176	THR
1	A	188	LEU
1	A	192	LEU
1	A	200	ARG
1	A	215	LEU
1	A	218	GLU
1	A	244	ARG
1	A	276	VAL
1	A	293	LEU
1	A	305	LYS
1	A	309	GLU
1	A	314	ARG
1	A	316	ARG
1	A	328	THR
1	A	341	VAL
1	A	384	ARG
1	A	401	LEU
1	A	414	LEU
1	B	4	GLU
1	B	6	LEU
1	B	12	ASP
1	B	26	VAL
1	B	30	LEU
1	B	33	LEU
1	B	36	LEU
1	B	51	VAL
1	B	55	LEU
1	B	72	THR
1	B	122	ARG
1	B	129	LEU
1	B	143	LEU
1	B	173	VAL
1	B	188	LEU
1	B	192	LEU

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Mol	Chain	Res	Type
1	B	200	ARG
1	B	211	GLU
1	B	232	ASN
1	B	252	THR
1	B	265	ASP
1	B	272	GLU
1	B	276	VAL
1	B	281	LYS
1	B	283	GLU
1	B	293	LEU
1	B	309	GLU
1	B	328	THR
1	B	341	VAL
1	B	354	VAL
1	B	401	LEU
2	E	19	LEU
2	E	26	LEU
2	E	31	VAL
2	E	48	LEU
2	E	61	ILE
2	E	71	ILE
2	E	100	LEU
2	E	101	LYS
2	E	126	GLN
2	E	136	THR
2	E	139	LEU
2	E	140	VAL
2	E	142	LEU
2	E	154	LEU
2	E	158	GLN
2	E	165	MET
2	E	172	VAL
2	E	175	THR
2	E	180	VAL
2	E	193	ARG
2	E	206	GLU
2	E	212	ARG
2	E	217	ARG
2	E	251	MET
2	E	264	GLU
2	E	306	ARG
2	E	308	ARG

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Mol	Chain	Res	Type
2	E	313	GLN
2	E	334	LYS
2	E	354	LEU
2	E	360	LEU
2	E	362	MET
2	E	376	THR
2	E	383	ASP
2	E	396	LEU
2	E	401	LEU
2	E	405	LEU
2	E	408	LEU
2	F	14	LEU
2	F	19	LEU
2	F	26	LEU
2	F	27	LYS
2	F	39	LEU
2	F	61	ILE
2	F	100	LEU
2	F	139	LEU
2	F	142	LEU
2	F	154	LEU
2	F	172	VAL
2	F	174	SER
2	F	175	THR
2	F	180	VAL
2	F	187	LEU
2	F	193	ARG
2	F	212	ARG
2	F	214	LEU
2	F	215	ASP
2	F	217	ARG
2	F	235	LEU
2	F	243	ARG
2	F	247	VAL
2	F	251	MET
2	F	258	GLU
2	F	264	GLU
2	F	270	GLU
2	F	275	LEU
2	F	279	ASP
2	F	306	ARG
2	F	308	ARG

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Mol	Chain	Res	Type
2	F	387	ARG
2	F	396	LEU
2	F	401	LEU
2	F	405	LEU
2	F	408	LEU
2	F	413	ARG
2	C	4	LYS
2	C	14	LEU
2	C	19	LEU
2	C	22	LEU
2	C	36	LEU
2	C	61	ILE
2	C	97	TRP
2	C	126	GLN
2	C	139	LEU
2	C	142	LEU
2	C	147	SER
2	C	157	ASP
2	C	158	GLN
2	C	172	VAL
2	C	180	VAL
2	C	187	LEU
2	C	194	ASP
2	C	195	ASP
2	C	217	ARG
2	C	226	LEU
2	C	249	THR
2	C	270	GLU
2	C	278	LEU
2	C	280	LEU
2	C	285	VAL
2	C	298	ARG
2	C	305	ASP
2	C	306	ARG
2	C	334	LYS
2	C	360	LEU
2	C	376	THR
2	C	396	LEU
2	C	401	LEU
2	C	408	LEU
2	D	4	LYS
2	D	11	ASP

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Mol	Chain	Res	Type
2	D	14	LEU
2	D	19	LEU
2	D	26	LEU
2	D	34	THR
2	D	39	LEU
2	D	46	VAL
2	D	48	LEU
2	D	58	LYS
2	D	82	LEU
2	D	97	TRP
2	D	98	MET
2	D	100	LEU
2	D	136	THR
2	D	142	LEU
2	D	147	SER
2	D	154	LEU
2	D	174	SER
2	D	175	THR
2	D	180	VAL
2	D	187	LEU
2	D	193	ARG
2	D	194	ASP
2	D	195	ASP
2	D	202	LEU
2	D	212	ARG
2	D	214	LEU
2	D	215	ASP
2	D	217	ARG
2	D	226	LEU
2	D	264	GLU
2	D	267	SER
2	D	270	GLU
2	D	305	ASP
2	D	324	ASN
2	D	342	LEU
2	D	344	SER
2	D	372	GLU
2	D	378	VAL
2	D	383	ASP
2	D	396	LEU
2	D	397	ARG
2	D	401	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	71	ASN
1	A	241	HIS
1	A	249	GLN
1	A	251	HIS
1	A	269	HIS
1	A	306	GLN
1	A	363	GLN
1	B	22	GLN
1	B	71	ASN
1	B	216	GLN
1	B	225	GLN
1	B	306	GLN
1	B	376	ASN
1	B	392	GLN
2	E	32	HIS
2	E	63	GLN
2	E	90	GLN
2	E	126	GLN
2	E	159	GLN
2	E	185	HIS
2	E	311	GLN
2	E	358	GLN
2	E	361	ASN
2	F	159	GLN
2	F	228	GLN
2	C	90	GLN
2	C	126	GLN
2	C	358	GLN
2	D	159	GLN
2	D	228	GLN
2	D	309	GLN
2	D	324	ASN

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 ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	LEU	A	500	-	5,8,8	0.38	0	5,10,10	1.03	0
3	LEU	B	500	-	5,8,8	0.26	0	5,10,10	1.25	1 (20%)
3	LEU	C	500	-	5,8,8	0.32	0	5,10,10	1.21	1 (20%)
3	LEU	D	500	-	5,8,8	0.42	0	5,10,10	0.97	0
3	LEU	E	500	-	5,8,8	0.32	0	5,10,10	1.37	1 (20%)
3	LEU	F	500	-	5,8,8	0.27	0	5,10,10	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LEU	A	500	-	-	0/4/8/8	0/0/0/0
3	LEU	B	500	-	-	0/4/8/8	0/0/0/0
3	LEU	C	500	-	-	0/4/8/8	0/0/0/0
3	LEU	D	500	-	-	0/4/8/8	0/0/0/0
3	LEU	E	500	-	-	0/4/8/8	0/0/0/0
3	LEU	F	500	-	-	0/4/8/8	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	500	LEU	CG-CB-CA	2.34	119.79	114.80
3	C	500	LEU	CG-CB-CA	2.64	120.43	114.80
3	E	500	LEU	CG-CB-CA	2.92	121.02	114.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	500	LEU	2	0
3	D	500	LEU	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	422/424 (99%)	-0.40	5 (1%) 81 77	24, 38, 57, 71	1 (0%)
1	B	424/424 (100%)	-0.34	14 (3%) 50 43	25, 39, 70, 85	0
2	C	417/419 (99%)	-0.30	6 (1%) 78 74	25, 39, 61, 75	0
2	D	416/419 (99%)	-0.27	7 (1%) 73 68	25, 40, 62, 75	0
2	E	416/419 (99%)	-0.18	9 (2%) 65 59	25, 43, 76, 83	1 (0%)
2	F	417/419 (99%)	0.08	37 (8%) 12 8	26, 45, 117, 125	1 (0%)
All	All	2512/2524 (99%)	-0.24	78 (3%) 52 45	24, 40, 77, 125	3 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	252	GLY	5.3
2	D	192	GLY	5.2
2	F	280	LEU	5.1
2	D	213	GLY	5.1
1	B	272	GLU	4.7
2	F	257	PRO	4.5
1	B	13	GLY	4.3
2	F	264	GLU	4.1
1	B	273	PHE	4.0
2	F	254	MET	3.9
2	F	192	GLY	3.9
1	B	122	ARG	3.8
1	B	274	GLY	3.8
2	F	330	TYR	3.8
2	F	267	SER	3.8
2	C	192	GLY	3.7
1	A	12	ASP	3.7
2	F	304	GLY	3.6
1	B	12	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	11	LYS	3.5
2	F	271	ALA	3.5
1	B	10	GLY	3.4
2	F	335	GLY	3.4
1	B	17	GLU	3.3
2	E	391	ARG	3.3
2	D	7	ARG	3.3
2	F	391	ARG	3.2
2	F	326	GLU	3.1
2	C	215	ASP	3.1
2	C	213	GLY	3.0
2	F	255	TYR	2.9
2	F	305	ASP	2.9
2	F	270	GLU	2.9
2	F	213	GLY	2.9
2	F	268	ALA	2.8
2	F	276	PRO	2.8
2	F	215	ASP	2.8
2	F	253	GLY	2.8
2	C	214	LEU	2.7
2	F	283	GLU	2.7
2	E	217	ARG	2.7
2	F	277	ARG	2.7
2	F	263	ALA	2.7
2	F	30	GLY	2.6
2	F	281	ALA	2.6
2	F	290	ALA	2.5
1	B	271	GLN	2.5
1	B	268	ARG	2.4
2	E	282	PRO	2.4
2	F	272	THR	2.4
2	E	305	ASP	2.4
2	E	275	LEU	2.3
2	E	251	MET	2.3
1	A	310	GLN	2.3
2	E	215	ASP	2.3
2	D	251	MET	2.3
2	D	193	ARG	2.3
2	F	279	ASP	2.2
2	F	191	GLU	2.2
2	F	216	LEU	2.2
2	F	313	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	345	GLY	2.2
2	E	278	LEU	2.2
2	C	305	ASP	2.2
2	F	284	GLU	2.2
1	A	195	ARG	2.2
2	F	211	ARG	2.2
1	B	11	LYS	2.2
2	E	308	ARG	2.1
2	F	333	GLY	2.1
1	A	13	GLY	2.1
1	B	251	HIS	2.1
2	F	329	ALA	2.0
2	F	266	LEU	2.0
2	C	27	LYS	2.0
2	D	214	LEU	2.0
1	B	277	ARG	2.0
1	B	252	THR	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 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
3	LEU	B	500	9/9	0.95	0.17	1.91	40,40,41,43	0
3	LEU	D	500	9/9	0.96	0.18	1.58	25,29,29,30	0
3	LEU	F	500	9/9	0.97	0.17	1.49	33,33,34,36	0
3	LEU	C	500	9/9	0.98	0.18	1.48	31,33,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	LEU	E	500	9/9	0.98	0.17	1.20	29,30,30,31	0
3	LEU	A	500	9/9	0.98	0.12	0.45	28,31,31,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.