



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:17 PM UTC

PDB ID : 4FCC / pdb_00004fcc
Title : Glutamate dehydrogenase from E. coli
Authors : Bilokapic, S.; Schwartz, T.U.
Deposited on : 2012-05-24
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

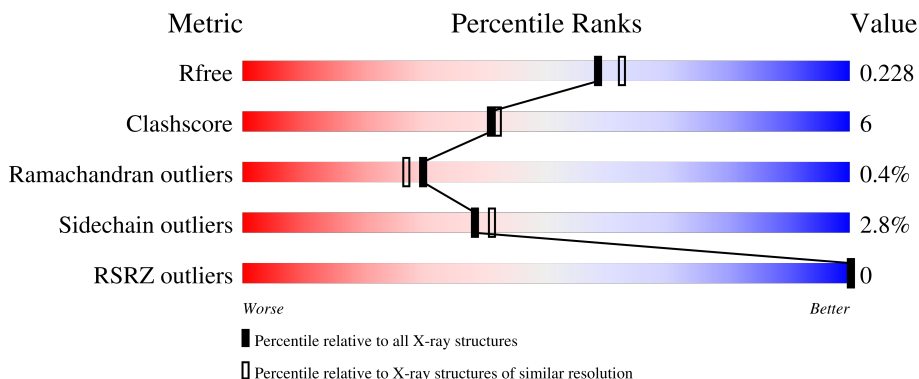
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	450	 88% 10%
1	B	450	 83% 15%
1	C	450	 80% 16%
1	D	450	 85% 13%
1	E	450	 88% 10%

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Mol	Chain	Length	Quality of chain
1	F	450	 87% 11% .
1	G	450	 86% 11% .
1	H	450	 78% 19% ..
1	I	450	 82% 14% ..
1	J	450	 85% 13% .
1	K	450	 84% 12% ..
1	L	450	 88% 9% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 44159 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
			Total	C	N	O	S			
1	A	442	3366	2119	594	632	21	0	0	0
1	B	442	3370	2122	594	633	21	0	1	0
1	C	435	3318	2094	582	621	21	0	1	0
1	D	442	3366	2119	594	632	21	0	0	0
1	E	442	3366	2119	594	632	21	0	0	0
1	F	442	3373	2124	596	632	21	0	1	0
1	G	442	3366	2119	594	632	21	0	0	0
1	H	438	3337	2104	587	625	21	0	0	0
1	I	442	3366	2119	594	632	21	0	0	0
1	J	442	3366	2119	594	632	21	0	0	0
1	K	442	3366	2119	594	632	21	0	0	0
1	L	442	3366	2119	594	632	21	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	expression tag	UNP Q8XDW9
A	-1	GLY	-	expression tag	UNP Q8XDW9
A	0	SER	-	expression tag	UNP Q8XDW9
B	-2	PRO	-	expression tag	UNP Q8XDW9
B	-1	GLY	-	expression tag	UNP Q8XDW9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP Q8XDW9
C	-2	PRO	-	expression tag	UNP Q8XDW9
C	-1	GLY	-	expression tag	UNP Q8XDW9
C	0	SER	-	expression tag	UNP Q8XDW9
D	-2	PRO	-	expression tag	UNP Q8XDW9
D	-1	GLY	-	expression tag	UNP Q8XDW9
D	0	SER	-	expression tag	UNP Q8XDW9
E	-2	PRO	-	expression tag	UNP Q8XDW9
E	-1	GLY	-	expression tag	UNP Q8XDW9
E	0	SER	-	expression tag	UNP Q8XDW9
F	-2	PRO	-	expression tag	UNP Q8XDW9
F	-1	GLY	-	expression tag	UNP Q8XDW9
F	0	SER	-	expression tag	UNP Q8XDW9
G	-2	PRO	-	expression tag	UNP Q8XDW9
G	-1	GLY	-	expression tag	UNP Q8XDW9
G	0	SER	-	expression tag	UNP Q8XDW9
H	-2	PRO	-	expression tag	UNP Q8XDW9
H	-1	GLY	-	expression tag	UNP Q8XDW9
H	0	SER	-	expression tag	UNP Q8XDW9
I	-2	PRO	-	expression tag	UNP Q8XDW9
I	-1	GLY	-	expression tag	UNP Q8XDW9
I	0	SER	-	expression tag	UNP Q8XDW9
J	-2	PRO	-	expression tag	UNP Q8XDW9
J	-1	GLY	-	expression tag	UNP Q8XDW9
J	0	SER	-	expression tag	UNP Q8XDW9
K	-2	PRO	-	expression tag	UNP Q8XDW9
K	-1	GLY	-	expression tag	UNP Q8XDW9
K	0	SER	-	expression tag	UNP Q8XDW9
L	-2	PRO	-	expression tag	UNP Q8XDW9
L	-1	GLY	-	expression tag	UNP Q8XDW9
L	0	SER	-	expression tag	UNP Q8XDW9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	409	Total O 409 409	0	0
2	B	277	Total O 277 277	0	0
2	C	300	Total O 300 300	0	0
2	D	254	Total O 254 254	0	0

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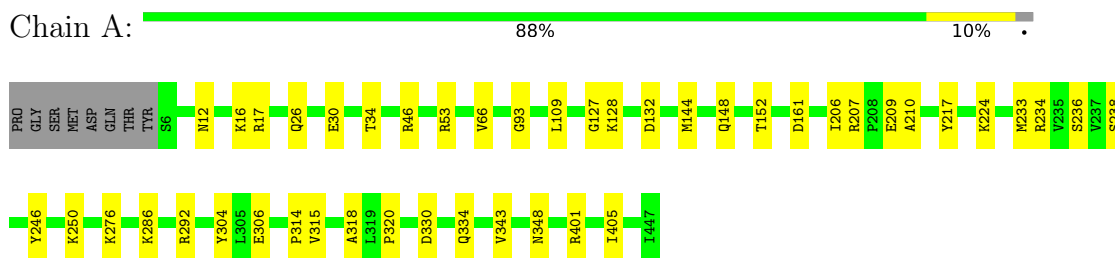
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	351	Total O 351 351	0	0
2	F	323	Total O 323 323	0	0
2	G	370	Total O 370 370	0	0
2	H	288	Total O 288 288	0	0
2	I	276	Total O 276 276	0	0
2	J	325	Total O 325 325	0	0
2	K	335	Total O 335 335	0	0
2	L	325	Total O 325 325	0	0

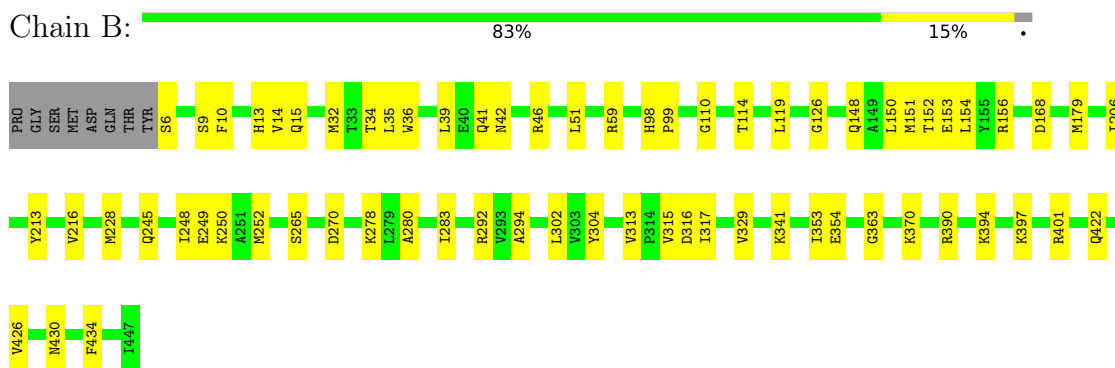
3 Residue-property plots

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

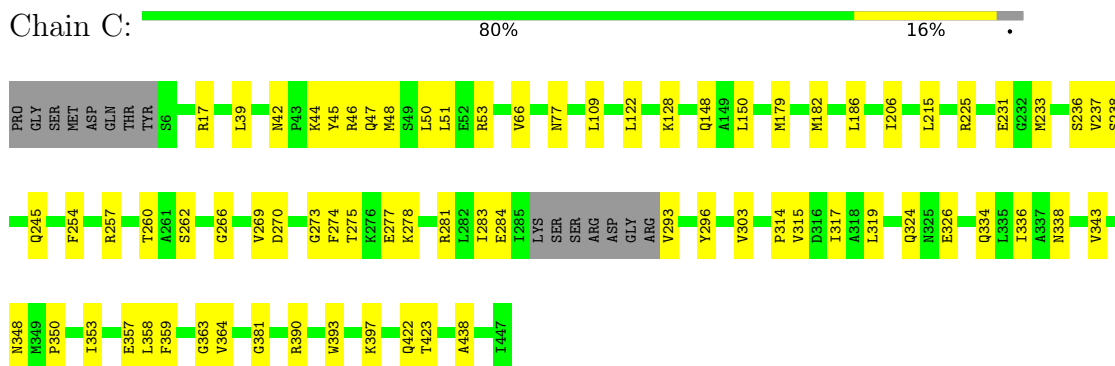
- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase

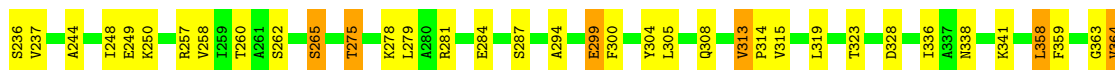


- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase

Chain I: 82% 14%



- Molecule 1: Glutamate dehydrogenase

Chain J: 85% 13%



- Molecule 1: Glutamate dehydrogenase

Chain K: 84% 12%



- Molecule 1: Glutamate dehydrogenase

Chain L: 88% 9%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.22Å 176.26Å 150.25Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	49.65 – 2.00 49.65 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.65-2.00) 98.9 (49.65-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.181 , 0.229 0.182 , 0.228	Depositor DCC
R_{free} test set	3646 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtrriage
Anisotropy	0.625	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.346 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	44159	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/3431	0.79	1/4630 (0.0%)
1	B	0.45	0/3438	0.82	3/4640 (0.1%)
1	C	0.47	0/3386	0.80	2/4571 (0.0%)
1	D	0.45	0/3431	0.81	2/4630 (0.0%)
1	E	0.48	0/3431	0.80	2/4630 (0.0%)
1	F	0.48	0/3442	0.79	0/4645
1	G	0.51	0/3431	0.80	1/4630 (0.0%)
1	H	0.45	0/3401	0.80	0/4589
1	I	0.46	0/3431	0.78	2/4630 (0.0%)
1	J	0.48	0/3431	0.79	0/4630
1	K	0.49	0/3431	0.82	1/4630 (0.0%)
1	L	0.47	0/3431	0.80	0/4630
All	All	0.47	0/41115	0.80	14/55485 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	ASN	CA-C-N	5.99	125.67	119.56
1	C	42	ASN	C-N-CA	5.99	125.67	119.56
1	G	329	VAL	N-CA-C	5.86	116.04	110.42
1	E	362	ALA	N-CA-C	-5.77	106.00	113.16
1	B	42	ASN	CA-C-N	5.41	125.49	119.32
1	B	42	ASN	C-N-CA	5.41	125.49	119.32
1	K	431	ILE	CB-CA-C	-5.38	105.08	111.97
1	A	210	ALA	N-CA-C	5.35	116.79	111.07
1	I	7	LEU	N-CA-C	-5.22	105.48	111.07
1	D	134	ASP	CA-C-N	5.13	124.75	119.56
1	D	134	ASP	C-N-CA	5.13	124.75	119.56
1	B	313	VAL	N-CA-C	5.12	113.03	108.63
1	I	262	SER	N-CA-C	5.12	116.07	108.60
1	E	360	GLN	N-CA-C	5.09	116.82	111.28

There are no chirality outliers.

There are no planarity outliers.

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	3366	0	3324	40	0
1	B	3370	0	3331	55	0
1	C	3318	0	3274	58	0
1	D	3366	0	3324	47	0
1	E	3366	0	3324	30	0
1	F	3373	0	3331	40	0
1	G	3366	0	3324	33	0
1	H	3337	0	3298	68	0
1	I	3366	0	3324	48	0
1	J	3366	0	3324	51	0
1	K	3366	0	3324	42	0
1	L	3366	0	3324	31	0
2	A	409	0	0	17	0
2	B	277	0	0	15	0
2	C	300	0	0	12	0
2	D	254	0	0	18	0
2	E	351	0	0	8	0
2	F	323	0	0	12	0
2	G	370	0	0	10	0
2	H	288	0	0	17	0
2	I	276	0	0	4	0
2	J	325	0	0	14	0
2	K	335	0	0	11	0
2	L	325	0	0	11	0
All	All	44159	0	39826	518	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 6.

All (518) 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:H:151:MET:SD	2:H:508:HOH:O	2.07	1.10
1:C:179:MET:SD	2:C:639:HOH:O	2.17	1.01
1:H:153:GLU:O	1:H:156:ARG:NH1	1.93	1.00
1:J:375:GLY:HA2	1:J:406:MET:HE1	1.41	0.97
1:J:153:GLU:O	1:J:156:ARG:NH1	1.98	0.96
1:J:406:MET:SD	2:J:542:HOH:O	2.23	0.95
1:I:46:ARG:NH2	2:I:715:HOH:O	2.01	0.93
1:B:153:GLU:O	1:B:156:ARG:NH1	2.06	0.89
1:B:34:THR:O	2:B:646:HOH:O	1.92	0.88
1:C:48:MET:SD	2:F:691:HOH:O	2.32	0.86
1:G:6:SER:N	2:G:815:HOH:O	2.09	0.83
1:C:274:PHE:O	2:C:727:HOH:O	1.97	0.83
1:H:156:ARG:NE	2:H:700:HOH:O	2.05	0.82
1:C:257:ARG:NH2	2:C:725:HOH:O	2.13	0.82
1:H:324:GLN:HG3	1:H:349:MET:HG3	1.63	0.81
1:B:153:GLU:HA	1:B:156:ARG:HH12	1.46	0.81
1:L:347:ALA:HB3	1:L:350:PRO:HG3	1.63	0.80
1:J:153:GLU:HA	1:J:156:ARG:HH12	1.46	0.79
1:A:207:ARG:NH2	2:A:801:HOH:O	2.08	0.79
1:F:299:GLU:OE1	2:F:649:HOH:O	2.01	0.79
1:D:168:ASP:OD1	1:D:169:ILE:N	2.16	0.78
1:H:270:ASP:OD2	1:H:278:LYS:NZ	2.16	0.78
1:J:156:ARG:NE	2:J:775:HOH:O	2.08	0.78
1:A:144:MET:SD	2:A:719:HOH:O	2.42	0.77
1:I:248:ILE:HG13	1:I:258:VAL:HG11	1.66	0.77
1:H:254:PHE:O	2:H:722:HOH:O	2.01	0.76
1:L:12:ASN:ND2	2:L:748:HOH:O	2.08	0.76
1:A:292:ARG:NH2	2:A:651:HOH:O	2.17	0.76
1:F:23:GLU:OE2	2:F:525:HOH:O	2.02	0.76
1:D:134:ASP:OD2	2:D:744:HOH:O	2.03	0.76
1:A:401:ARG:NH1	2:A:858:HOH:O	2.18	0.76
1:D:199:LEU:O	2:D:555:HOH:O	2.03	0.76
1:H:153:GLU:HA	1:H:156:ARG:HH12	1.51	0.76
1:B:114[A]:THR:HG22	1:B:126:GLY:HA3	1.67	0.75
1:G:255:GLY:O	2:G:754:HOH:O	2.03	0.75
1:L:360:GLN:O	2:L:795:HOH:O	2.03	0.75
1:I:228:MET:SD	1:I:341:LYS:NZ	2.59	0.75
1:A:224:LYS:NZ	2:A:774:HOH:O	2.19	0.75
1:G:47:GLN:HG3	1:G:48:MET:HG2	1.69	0.75
1:D:116:LYS:NZ	2:D:728:HOH:O	2.18	0.75
1:B:302:LEU:O	2:B:753:HOH:O	2.05	0.75
1:E:401:ARG:NH1	2:E:759:HOH:O	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:184:LYS:NZ	2:J:656:HOH:O	2.14	0.74
1:B:156:ARG:NE	2:B:767:HOH:O	2.07	0.74
1:K:317:ILE:HG22	1:K:342:ALA:HB3	1.69	0.73
1:C:270:ASP:OD2	1:C:278:LYS:NZ	2.22	0.73
1:I:109:LEU:HB3	1:I:128:LYS:HE3	1.69	0.72
1:C:314:PRO:HA	1:C:338:ASN:HB3	1.72	0.71
1:K:347:ALA:HB3	1:K:350:PRO:HG3	1.72	0.71
1:L:288:SER:O	2:L:805:HOH:O	2.08	0.71
1:I:47:GLN:HG3	1:I:48:MET:HG2	1.72	0.71
1:J:375:GLY:CA	1:J:406:MET:HE1	2.20	0.71
1:H:156:ARG:NH2	2:H:700:HOH:O	2.24	0.70
1:A:66:VAL:HG11	1:C:53:ARG:HD3	1.72	0.70
1:B:245:GLN:OE1	2:B:718:HOH:O	2.08	0.70
1:C:46:ARG:NH1	2:C:660:HOH:O	2.20	0.70
1:J:156:ARG:NH2	2:J:775:HOH:O	2.24	0.70
1:F:8:GLU:OE2	1:F:29:ARG:NH2	2.23	0.70
1:J:214:GLY:HA3	1:J:406:MET:HE3	1.73	0.70
1:L:292:ARG:NH1	2:L:772:HOH:O	2.25	0.70
1:K:345:GLU:OE1	2:K:780:HOH:O	2.09	0.70
1:J:390:ARG:NH1	2:J:579:HOH:O	2.20	0.69
1:D:46:ARG:O	2:D:622:HOH:O	2.10	0.69
1:D:231:GLU:OE1	2:D:732:HOH:O	2.09	0.69
1:J:233:MET:SD	2:J:759:HOH:O	2.50	0.69
1:K:419:GLU:OE2	2:K:705:HOH:O	2.11	0.68
1:L:325:ASN:OD1	2:L:824:HOH:O	2.11	0.68
1:G:66:VAL:HG11	1:I:53:ARG:HD3	1.75	0.68
1:I:150:LEU:HD22	1:I:179:MET:HE2	1.73	0.68
1:I:394:LYS:HG3	2:I:771:HOH:O	1.92	0.68
1:J:370:LYS:HD3	2:J:551:HOH:O	1.93	0.67
1:J:375:GLY:HA2	1:J:406:MET:CE	2.23	0.67
1:D:46:ARG:NH1	2:D:702:HOH:O	2.28	0.67
1:I:47:GLN:NE2	2:I:721:HOH:O	2.27	0.67
1:H:34:THR:O	2:H:579:HOH:O	2.12	0.67
1:C:50:LEU:HD21	1:C:438:ALA:HB1	1.77	0.67
1:J:199:LEU:O	2:J:670:HOH:O	2.12	0.67
1:C:254:PHE:O	2:C:577:HOH:O	2.13	0.66
1:C:363:GLY:HA2	1:C:422:GLN:HE22	1.59	0.66
1:C:47:GLN:HG3	1:C:48:MET:HG2	1.78	0.66
1:D:333:HIS:NE2	2:D:667:HOH:O	2.28	0.66
1:L:47:GLN:HG3	1:L:48:MET:HG2	1.77	0.66
1:D:328:ASP:OD1	2:D:625:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:312:SER:HA	1:F:334:GLN:HG2	1.78	0.66
1:B:6:SER:N	2:B:738:HOH:O	2.28	0.66
1:J:324:GLN:NE2	2:J:773:HOH:O	2.28	0.66
1:E:225:ARG:NH2	1:E:423:THR:OG1	2.29	0.65
1:K:13:HIS:HA	1:K:16:LYS:HE2	1.76	0.65
1:E:324:GLN:N	1:E:324:GLN:OE1	2.28	0.65
1:D:408:ASP:OD2	2:D:718:HOH:O	2.15	0.65
1:H:233:MET:HE1	1:H:341:LYS:HD2	1.79	0.65
1:H:156:ARG:CZ	2:H:700:HOH:O	2.43	0.65
1:F:328:ASP:HB2	2:F:820:HOH:O	1.95	0.65
1:K:47:GLN:HG2	1:K:48:MET:HG2	1.77	0.65
1:B:280:ALA:HA	1:B:283:ILE:HD12	1.79	0.65
1:L:271:GLU:OE2	2:L:822:HOH:O	2.12	0.65
1:B:316:ASP:HB3	1:B:341:LYS:HE3	1.79	0.65
1:F:348:ASN:ND2	2:F:779:HOH:O	2.30	0.65
1:E:234:ARG:NH1	2:E:760:HOH:O	2.30	0.65
1:H:265:SER:O	1:H:304:TYR:OH	2.16	0.64
1:J:69:ASP:OD2	1:J:71:ARG:NH2	2.31	0.64
1:A:306:GLU:OE2	2:A:870:HOH:O	2.15	0.64
1:J:156:ARG:CZ	2:J:775:HOH:O	2.45	0.64
1:J:153:GLU:CA	1:J:156:ARG:HH12	2.10	0.64
1:H:259:ILE:HG13	1:H:260:THR:HG23	1.79	0.64
1:H:284:GLU:OE1	2:H:785:HOH:O	2.15	0.63
1:K:12:ASN:ND2	2:K:662:HOH:O	2.30	0.63
1:H:281:ARG:NH2	2:H:635:HOH:O	2.31	0.63
1:J:119:LEU:HD22	1:J:370:LYS:HE2	1.81	0.63
1:F:40:GLU:OE2	1:F:46:ARG:NH2	2.32	0.63
1:D:329:VAL:HG23	1:D:358:LEU:HD22	1.81	0.62
1:D:276:LYS:NZ	1:D:277:GLU:OE2	2.32	0.62
1:E:47:GLN:HG3	1:E:48:MET:HG2	1.80	0.62
1:I:236:SER:HB3	1:I:315:VAL:HG11	1.80	0.62
1:L:345:GLU:OE2	1:L:351:THR:HG22	1.98	0.62
1:G:132:ASP:OD2	1:I:17:ARG:HD3	1.99	0.62
1:C:293:VAL:N	2:C:757:HOH:O	2.32	0.62
1:H:59:ARG:HD3	1:K:153:GLU:OE2	2.00	0.62
1:K:6:SER:N	2:K:797:HOH:O	2.32	0.62
1:B:216:VAL:HG21	1:B:250:LYS:HG3	1.80	0.62
1:H:153:GLU:CA	1:H:156:ARG:HH12	2.13	0.62
1:A:53:ARG:HD3	1:C:66:VAL:HG11	1.82	0.62
1:D:29:ARG:NE	2:D:703:HOH:O	2.31	0.61
1:I:265:SER:OG	1:I:304:TYR:OH	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:TRP:O	1:F:40:GLU:HG2	2.00	0.61
1:B:156:ARG:NH2	2:B:767:HOH:O	2.30	0.61
1:G:334:GLN:NE2	2:G:837:HOH:O	2.34	0.61
1:J:53:ARG:HD3	1:L:66:VAL:HG11	1.81	0.61
1:E:117:ASN:O	1:E:120:THR:OG1	2.18	0.61
1:G:289:ARG:NH2	2:G:818:HOH:O	2.20	0.61
1:J:281:ARG:NH2	1:J:284:GLU:OE1	2.33	0.61
1:B:41:GLN:NE2	2:B:642:HOH:O	2.21	0.60
1:B:363:GLY:O	1:B:422:GLN:NE2	2.34	0.60
1:A:46:ARG:NH2	2:A:610:HOH:O	2.34	0.60
1:B:422:GLN:O	2:B:689:HOH:O	2.15	0.60
1:D:390:ARG:NH1	2:D:561:HOH:O	2.33	0.60
1:B:394:LYS:NZ	2:B:750:HOH:O	2.34	0.60
1:K:40:GLU:HA	2:K:732:HOH:O	2.01	0.60
1:D:265:SER:OG	1:D:292:ARG:NH1	2.35	0.59
1:E:17:ARG:NH2	2:E:693:HOH:O	2.33	0.59
1:K:23:GLU:O	1:K:26:GLN:HG2	2.02	0.59
1:B:426:VAL:O	1:B:430:ASN:ND2	2.33	0.59
1:C:215:LEU:HD21	1:C:319:LEU:HD22	1.84	0.59
1:H:151:MET:HE3	1:H:179:MET:SD	2.43	0.59
1:B:153:GLU:CA	1:B:156:ARG:HH12	2.14	0.59
1:C:236:SER:HB3	1:C:315:VAL:HG21	1.83	0.59
1:I:234:ARG:NH1	1:I:314:PRO:O	2.27	0.59
1:H:132:ASP:OD2	1:K:17:ARG:HD3	2.02	0.59
1:E:361:GLN:OE1	1:E:361:GLN:N	2.35	0.58
1:J:17:ARG:HD3	1:L:132:ASP:OD2	2.03	0.58
1:B:265:SER:OG	1:B:292:ARG:NH2	2.36	0.58
1:I:305:LEU:HB3	1:I:308:GLN:HB2	1.85	0.58
1:F:370:LYS:NZ	2:F:655:HOH:O	2.35	0.58
1:A:405:ILE:HG13	2:A:850:HOH:O	2.03	0.58
1:F:233:MET:HE1	1:F:341:LYS:HD2	1.85	0.58
1:G:359:PHE:O	1:G:364:VAL:HG12	2.04	0.57
1:I:419:GLU:H	1:I:419:GLU:CD	2.12	0.57
1:C:269:VAL:HB	1:C:303:VAL:HB	1.86	0.57
1:C:334:GLN:O	1:C:338:ASN:ND2	2.26	0.57
1:G:316:ASP:OD1	1:G:341:LYS:NZ	2.31	0.57
1:C:281:ARG:NH2	1:C:284:GLU:OE1	2.34	0.56
1:D:390:ARG:HH11	1:E:388:ALA:HB2	1.68	0.56
1:K:50:LEU:HD21	1:K:438:ALA:HB1	1.87	0.56
1:A:234:ARG:NH1	1:A:314:PRO:O	2.38	0.56
1:C:109:LEU:HD13	1:C:128:LYS:NZ	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LEU:O	1:E:156:ARG:NH2	2.37	0.56
1:D:390:ARG:NE	2:D:721:HOH:O	2.16	0.56
1:G:292:ARG:NH1	2:G:750:HOH:O	2.37	0.56
1:I:148:GLN:HG2	1:I:182:MET:HE3	1.86	0.56
1:K:422:GLN:NE2	2:K:710:HOH:O	2.38	0.56
1:H:153:GLU:C	1:H:156:ARG:HH12	2.13	0.56
1:I:328:ASP:HB3	2:I:776:HOH:O	2.06	0.56
1:B:156:ARG:CZ	2:B:767:HOH:O	2.48	0.56
1:I:148:GLN:CG	1:I:182:MET:HE3	2.36	0.56
1:H:81:ARG:HD3	1:H:95:MET:HE1	1.89	0.55
1:I:213:TYR:OH	1:I:249:GLU:OE2	2.20	0.55
1:J:436:LYS:HE3	2:J:730:HOH:O	2.06	0.55
1:C:390:ARG:NH2	2:C:685:HOH:O	2.31	0.55
1:H:164:VAL:HG21	1:H:384:MET:HE3	1.88	0.55
1:D:134:ASP:OD1	2:D:700:HOH:O	2.18	0.55
1:K:30:GLU:O	1:K:34:THR:HG22	2.07	0.55
1:K:235:VAL:HG22	1:K:317:ILE:HG13	1.89	0.55
1:F:8:GLU:CD	1:F:29:ARG:HH22	2.15	0.55
1:G:357:GLU:OE2	1:G:361:GLN:NE2	2.40	0.55
1:H:150:LEU:HD22	1:H:151:MET:HE2	1.87	0.55
1:I:27:ALA:O	1:I:30:GLU:HG3	2.07	0.55
1:G:54:LEU:HD12	2:G:648:HOH:O	2.05	0.55
1:B:119:LEU:HD12	1:B:370:LYS:HE2	1.90	0.54
1:C:122:LEU:HD13	1:C:381:GLY:HA3	1.89	0.54
1:F:290:ASP:N	2:F:583:HOH:O	2.09	0.54
1:K:35:LEU:HD23	1:K:431:ILE:HD13	1.89	0.54
1:J:25:ALA:HB2	2:J:601:HOH:O	2.06	0.54
1:A:234:ARG:HH12	1:A:314:PRO:HB2	1.72	0.54
1:J:49:SER:O	1:J:53:ARG:HG3	2.07	0.54
1:D:7:LEU:HD11	1:D:33:THR:HA	1.90	0.54
1:B:110:GLY:O	1:B:114[A]:THR:HG23	2.07	0.54
1:G:207:ARG:NH1	2:G:697:HOH:O	2.40	0.54
1:C:275:THR:HG23	1:C:278:LYS:HE3	1.88	0.54
1:J:402:LEU:CD1	1:J:406:MET:HE2	2.38	0.54
1:A:209:GLU:HG3	1:A:246:TYR:CD1	2.42	0.54
1:F:363:GLY:HA2	1:F:422:GLN:HE22	1.73	0.54
1:J:153:GLU:C	1:J:156:ARG:HH12	2.16	0.54
1:D:353:ILE:HD12	1:D:354:GLU:H	1.73	0.54
1:B:39:LEU:HD13	1:B:51:LEU:HD21	1.90	0.53
1:A:132:ASP:OD2	1:C:17:ARG:HD3	2.09	0.53
1:E:50:LEU:HD21	1:E:438:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:348:ASN:HB2	2:E:781:HOH:O	2.07	0.53
1:H:299:GLU:HB3	2:H:786:HOH:O	2.08	0.53
1:H:236:SER:HB2	1:H:315:VAL:HG11	1.91	0.53
1:I:217:TYR:OH	1:I:250:LYS:HE3	2.07	0.53
1:K:366:PHE:O	2:K:625:HOH:O	2.19	0.53
1:K:234:ARG:HH12	1:K:271:GLU:HG2	1.73	0.53
1:C:150:LEU:HD22	1:C:179:MET:HE2	1.91	0.53
1:B:397:LYS:NZ	2:B:598:HOH:O	2.36	0.52
1:K:396:GLU:OE2	2:K:805:HOH:O	2.18	0.52
1:A:304:TYR:CE2	1:A:306:GLU:HG2	2.43	0.52
1:D:361:GLN:NE2	2:D:689:HOH:O	2.37	0.52
1:H:151:MET:HE1	1:H:154:LEU:HD23	1.91	0.52
1:I:314:PRO:HA	1:I:338:ASN:HB3	1.91	0.52
1:L:329:VAL:HG12	1:L:333:HIS:CD2	2.44	0.52
1:D:53:ARG:HD3	1:F:66:VAL:HG11	1.92	0.52
1:L:329:VAL:HG13	1:L:358:LEU:HD22	1.92	0.52
1:H:213:TYR:OH	1:H:249:GLU:OE2	2.17	0.52
1:D:393:TRP:CG	1:D:397:LYS:HD2	2.45	0.52
1:J:320:PRO:HD2	1:J:344:ALA:O	2.09	0.52
1:F:259:ILE:HG13	1:F:260:THR:HG23	1.92	0.52
1:B:250:LYS:NZ	2:B:567:HOH:O	2.43	0.52
1:H:281:ARG:HD2	1:H:300:PHE:CE2	2.45	0.51
1:A:304:TYR:HE2	1:A:306:GLU:HG2	1.74	0.51
1:B:151:MET:HE3	1:B:179:MET:HB3	1.91	0.51
1:C:225:ARG:HE	1:C:423:THR:CG2	2.22	0.51
1:G:259:ILE:HD11	1:G:315:VAL:HG12	1.93	0.51
1:B:270:ASP:OD2	1:B:278:LYS:NZ	2.38	0.51
1:H:151:MET:HE3	1:H:179:MET:HB3	1.92	0.51
1:F:35:LEU:HD21	1:F:434:PHE:CG	2.46	0.51
1:J:402:LEU:HD11	1:J:406:MET:HE2	1.93	0.51
1:J:286:LYS:NZ	2:J:583:HOH:O	2.44	0.51
1:A:46:ARG:HG3	2:A:852:HOH:O	2.11	0.51
1:A:234:ARG:HD3	2:A:853:HOH:O	2.10	0.51
1:A:236:SER:HB3	1:A:315:VAL:HG11	1.92	0.51
1:H:248:ILE:HG12	1:H:258:VAL:HG11	1.91	0.51
1:H:390:ARG:NH2	2:H:518:HOH:O	2.44	0.50
1:K:427:GLN:O	1:K:431:ILE:HG12	2.11	0.50
1:G:148:GLN:O	1:G:152:THR:HG23	2.11	0.50
1:G:401:ARG:NH1	2:G:665:HOH:O	2.43	0.50
1:B:59:ARG:HD3	1:E:153:GLU:OE2	2.10	0.50
1:J:283:ILE:HG13	1:J:284:GLU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ASN:ND2	2:A:724:HOH:O	2.21	0.50
1:B:32:MET:HE2	1:B:36:TRP:HZ3	1.77	0.50
1:D:231:GLU:OE1	2:D:698:HOH:O	2.20	0.50
1:K:345:GLU:CD	1:K:350:PRO:HD2	2.36	0.50
1:L:345:GLU:OE2	1:L:350:PRO:HD2	2.11	0.50
1:A:217:TYR:CE1	1:A:250:LYS:HD3	2.46	0.50
1:D:420:GLY:O	2:D:688:HOH:O	2.19	0.50
1:F:290:ASP:HB3	2:F:791:HOH:O	2.12	0.50
1:K:338:ASN:OD1	2:K:796:HOH:O	2.19	0.49
1:C:275:THR:H	1:C:278:LYS:HG2	1.76	0.49
1:K:411:HIS:O	1:K:415:GLU:HG2	2.11	0.49
1:J:397:LYS:O	1:J:401:ARG:HG2	2.12	0.49
1:C:422:GLN:NE2	2:C:785:HOH:O	2.46	0.49
1:H:304:TYR:CE2	1:H:306:GLU:HB3	2.47	0.49
1:C:275:THR:OG1	2:C:735:HOH:O	2.20	0.49
1:L:401:ARG:NH2	2:L:692:HOH:O	2.44	0.49
1:A:148:GLN:O	1:A:152:THR:HG23	2.12	0.49
1:F:22:THR:HG22	2:F:567:HOH:O	2.12	0.49
1:B:35:LEU:HD21	1:B:434:PHE:CD1	2.48	0.49
1:C:148:GLN:CG	1:C:182:MET:HE3	2.43	0.48
1:L:207:ARG:NH1	2:L:768:HOH:O	2.45	0.48
1:L:345:GLU:CD	1:L:350:PRO:HD2	2.37	0.48
1:F:363:GLY:HA2	1:F:422:GLN:NE2	2.28	0.48
1:J:235:VAL:HG22	1:J:317:ILE:HB	1.94	0.48
1:G:209:GLU:HG3	1:G:246:TYR:CD1	2.48	0.48
1:H:280:ALA:HA	1:H:283:ILE:HD12	1.95	0.48
1:D:48:MET:CB	1:D:53:ARG:HH21	2.27	0.48
1:K:148:GLN:O	1:K:152:THR:HG23	2.13	0.48
1:A:330:ASP:O	1:A:334:GLN:HG3	2.14	0.48
1:B:216:VAL:HG21	1:B:250:LYS:CG	2.44	0.48
1:D:17:ARG:NH2	1:F:77:ASN:HA	2.29	0.48
1:D:324:GLN:HG3	1:D:349:MET:HB2	1.96	0.48
1:G:341:LYS:C	1:G:364:VAL:HG23	2.39	0.48
1:H:310:PRO:O	2:H:569:HOH:O	2.19	0.48
1:I:248:ILE:HG22	1:I:279:LEU:HD22	1.95	0.48
1:F:275:THR:CG2	1:F:278:LYS:H	2.27	0.48
1:F:275:THR:HG23	1:F:278:LYS:H	1.78	0.48
1:H:285:ILE:HD12	1:H:296:TYR:HB2	1.95	0.48
1:I:275:THR:H	1:I:278:LYS:HG3	1.78	0.48
1:C:274:PHE:HA	1:C:278:LYS:HD2	1.95	0.47
1:D:48:MET:HB2	1:D:53:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:GLY:HA3	1:E:127:GLY:O	2.14	0.47
1:E:168:ASP:OD1	1:E:169:ILE:N	2.42	0.47
1:J:122:LEU:HD13	1:J:381:GLY:HA3	1.96	0.47
1:L:401:ARG:HG2	2:L:749:HOH:O	2.14	0.47
1:C:273:GLY:O	1:C:278:LYS:NZ	2.37	0.47
1:F:50:LEU:HD21	1:F:438:ALA:HB1	1.96	0.47
1:L:236:SER:HB3	1:L:315:VAL:HG11	1.96	0.47
1:C:353:ILE:O	1:C:357:GLU:HG2	2.14	0.47
1:H:41:GLN:NE2	2:H:775:HOH:O	2.45	0.47
1:I:237:VAL:HG22	1:I:319:LEU:HB2	1.96	0.47
1:I:359:PHE:HB3	1:I:364:VAL:HG22	1.95	0.47
1:H:148:GLN:CG	1:H:182:MET:HE3	2.44	0.47
1:J:214:GLY:CA	1:J:406:MET:HE3	2.42	0.47
1:E:363:GLY:O	1:E:422:GLN:NE2	2.48	0.47
1:G:248:ILE:HG12	1:G:258:VAL:HG11	1.95	0.47
1:I:237:VAL:H	1:I:260:THR:HG23	1.79	0.47
1:L:22:THR:O	1:L:26:GLN:NE2	2.47	0.47
1:A:161:ASP:OD1	1:E:390:ARG:NH2	2.46	0.47
1:D:259:ILE:HG13	1:D:260:THR:HG23	1.96	0.47
1:D:391:LEU:HD11	1:E:393:TRP:HH2	1.79	0.47
1:H:39:LEU:HD13	1:H:51:LEU:HD21	1.96	0.47
1:H:98:HIS:CG	1:H:99:PRO:HD2	2.49	0.47
1:I:250:LYS:HD2	1:I:250:LYS:HA	1.70	0.47
1:K:112:GLU:OE1	2:K:621:HOH:O	2.20	0.47
1:E:46:ARG:NH1	2:E:799:HOH:O	2.49	0.46
1:H:410:HIS:O	1:H:414:VAL:HG23	2.15	0.46
1:B:228:MET:HE3	1:B:228:MET:HB2	1.85	0.46
1:B:397:LYS:O	1:B:401:ARG:HG2	2.16	0.46
1:E:92:LYS:HD2	1:E:164:VAL:O	2.15	0.46
1:C:148:GLN:HG2	1:C:182:MET:HE3	1.96	0.46
1:C:359:PHE:O	1:C:364:VAL:HG13	2.16	0.46
1:D:29:ARG:NH1	2:D:674:HOH:O	2.05	0.46
1:E:109:LEU:HD13	1:E:128:LYS:HE2	1.97	0.46
1:G:313:VAL:HG12	1:G:315:VAL:HG13	1.97	0.46
1:B:10:PHE:O	1:B:14:VAL:HG23	2.14	0.46
1:E:26:GLN:OE1	2:E:605:HOH:O	2.20	0.46
1:K:98:HIS:CG	1:K:99:PRO:HD2	2.51	0.46
1:D:148:GLN:O	1:D:152:THR:HG23	2.16	0.46
1:A:34:THR:HG21	2:A:906:HOH:O	2.15	0.46
1:F:363:GLY:CA	1:F:422:GLN:HE22	2.29	0.46
1:H:445:GLY:HA2	2:H:591:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:351:THR:HG21	1:L:366:PHE:CZ	2.51	0.46
1:B:294:ALA:HB2	1:B:304:TYR:CZ	2.51	0.46
1:L:349:MET:HG3	2:L:824:HOH:O	2.16	0.46
1:G:53:ARG:HD3	1:I:66:VAL:HG11	1.99	0.45
1:H:229:GLY:O	1:H:233:MET:HG3	2.16	0.45
1:A:30:GLU:HG3	2:A:840:HOH:O	2.16	0.45
1:C:324:GLN:HG3	1:C:348:ASN:O	2.16	0.45
1:F:361:GLN:NE2	2:F:806:HOH:O	2.45	0.45
1:K:308:GLN:CD	1:K:309:GLN:H	2.24	0.45
1:L:349:MET:N	1:L:350:PRO:HD3	2.31	0.45
1:A:217:TYR:CZ	1:A:250:LYS:HD3	2.51	0.45
1:B:153:GLU:CD	1:B:156:ARG:NH1	2.75	0.45
1:G:66:VAL:HG12	1:I:446:VAL:HG13	1.99	0.45
1:H:353:ILE:HD12	1:H:353:ILE:H	1.81	0.45
1:J:236:SER:HB3	1:J:315:VAL:HG11	1.99	0.45
1:B:46:ARG:HD2	2:B:770:HOH:O	2.16	0.45
1:H:148:GLN:HG2	1:H:182:MET:HE3	1.99	0.45
1:I:313:VAL:HG22	1:I:314:PRO:HD2	1.99	0.45
1:A:93:GLY:HA3	1:A:127:GLY:O	2.17	0.45
1:B:315:VAL:HG13	1:B:317:ILE:N	2.32	0.45
1:B:353:ILE:HD12	1:B:354:GLU:N	2.32	0.45
1:C:326:GLU:N	1:C:350:PRO:O	2.50	0.45
1:D:279:LEU:O	1:D:283:ILE:HG13	2.17	0.45
1:A:238:SER:OG	1:A:320:PRO:HA	2.17	0.45
1:C:262:SER:HB2	1:C:266:GLY:O	2.17	0.45
1:C:44:LYS:HE3	1:C:45:TYR:CE2	2.52	0.45
1:C:277:GLU:N	2:C:735:HOH:O	2.27	0.45
1:C:53:ARG:HD2	2:C:521:HOH:O	2.16	0.45
1:E:236:SER:HB3	1:E:315:VAL:HG11	1.99	0.45
1:G:309:GLN:NE2	1:G:326:GLU:O	2.49	0.45
1:L:353:ILE:HG22	2:L:767:HOH:O	2.17	0.45
1:D:285:ILE:O	1:D:291:GLY:HA3	2.16	0.45
1:G:236:SER:HB3	1:G:315:VAL:HG11	1.99	0.45
1:H:275:THR:HG23	1:H:278:LYS:HD3	1.99	0.45
1:B:148:GLN:O	1:B:152:THR:HG23	2.16	0.44
1:E:285:ILE:O	1:E:291:GLY:HA3	2.17	0.44
1:I:7:LEU:HD23	1:I:36:TRP:CE3	2.52	0.44
1:I:244:ALA:O	1:I:248:ILE:HD13	2.16	0.44
1:F:26:GLN:OE1	2:F:770:HOH:O	2.20	0.44
1:J:324:GLN:HG3	1:J:348:ASN:O	2.17	0.44
1:E:289:ARG:HA	1:E:289:ARG:HD3	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:313:VAL:HG23	1:F:315:VAL:HG13	1.99	0.44
1:G:92:LYS:HD3	1:G:124:MET:HE2	1.99	0.44
1:K:93:GLY:HA3	1:K:127:GLY:O	2.18	0.44
1:K:416:HIS:ND1	2:K:686:HOH:O	2.36	0.44
1:D:417:GLY:HA3	1:D:423:THR:HG23	1.98	0.44
1:F:363:GLY:C	1:F:422:GLN:HE22	2.26	0.44
1:H:281:ARG:HD2	1:H:300:PHE:CZ	2.53	0.44
1:C:45:TYR:O	1:C:50:LEU:HD23	2.18	0.44
1:C:262:SER:OG	2:C:630:HOH:O	2.21	0.44
1:J:66:VAL:HG12	1:L:446:VAL:HG13	1.99	0.44
1:K:235:VAL:HG22	1:K:317:ILE:CG1	2.47	0.44
1:I:363:GLY:HA2	1:I:422:GLN:OE1	2.17	0.44
1:D:236:SER:HB3	1:D:315:VAL:HG11	1.99	0.44
1:D:421:GLU:CD	1:D:421:GLU:N	2.76	0.44
1:E:421:GLU:N	2:E:643:HOH:O	2.51	0.44
1:I:336:ILE:HD12	1:I:358:LEU:HD13	1.99	0.44
1:B:153:GLU:C	1:B:156:ARG:HH12	2.26	0.43
1:C:39:LEU:HD13	1:C:51:LEU:HD11	1.99	0.43
1:C:343:VAL:HG21	1:C:359:PHE:CE2	2.53	0.43
1:H:48:MET:HE3	1:H:48:MET:HB3	1.82	0.43
1:H:184:LYS:NZ	2:H:670:HOH:O	2.30	0.43
1:B:397:LYS:HE3	1:B:401:ARG:NH2	2.33	0.43
1:G:25:ALA:HB2	2:G:556:HOH:O	2.17	0.43
1:B:150:LEU:CD2	1:B:151:MET:HE2	2.47	0.43
1:H:323:THR:OG1	1:H:324:GLN:N	2.52	0.43
1:J:290:ASP:OD1	1:J:290:ASP:N	2.52	0.43
1:F:265:SER:CB	1:F:292:ARG:HH21	2.30	0.43
1:I:299:GLU:HB3	1:I:300:PHE:CD1	2.54	0.43
1:A:318:ALA:HB3	1:A:343:VAL:HG22	2.00	0.43
1:B:150:LEU:HD22	1:B:151:MET:HE2	1.99	0.43
1:B:390:ARG:NH2	1:F:161:ASP:OD1	2.51	0.43
1:L:216:VAL:HG13	1:L:230:PHE:CE2	2.53	0.43
1:C:109:LEU:HD13	1:C:128:LYS:HZ2	1.83	0.43
1:H:150:LEU:CD2	1:H:151:MET:HE2	2.47	0.43
1:D:328:ASP:OD1	1:D:330:ASP:HB3	2.18	0.43
1:F:236:SER:HB3	1:F:315:VAL:HG11	2.01	0.43
1:H:122:LEU:HD13	1:H:381:GLY:HA3	2.00	0.43
1:B:98:HIS:CG	1:B:99:PRO:HD2	2.54	0.43
1:B:329:VAL:HG22	1:B:354:GLU:OE2	2.18	0.43
1:H:29:ARG:NH1	2:H:757:HOH:O	2.52	0.43
1:H:209:GLU:HG3	1:H:246:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:401:ARG:HD3	1:I:401:ARG:HA	1.83	0.43
1:E:432:ALA:O	1:E:436:LYS:HG3	2.19	0.43
1:F:353:ILE:HG22	2:F:801:HOH:O	2.19	0.43
1:K:314:PRO:HB3	1:K:338:ASN:HB2	2.00	0.43
1:A:233:MET:HE2	1:A:233:MET:HA	2.00	0.42
1:B:213:TYR:OH	1:B:249:GLU:OE2	2.30	0.42
1:K:358:LEU:HD23	1:K:359:PHE:N	2.34	0.42
1:F:213:TYR:OH	1:F:249:GLU:OE2	2.33	0.42
1:B:15:GLN:NE2	2:B:675:HOH:O	2.48	0.42
1:L:148:GLN:O	1:L:152:THR:HG23	2.18	0.42
1:F:31:VAL:HG12	1:F:32:MET:HE2	2.01	0.42
1:H:10:PHE:O	1:H:14:VAL:HG23	2.19	0.42
1:H:266:GLY:HA3	1:H:304:TYR:OH	2.20	0.42
1:I:236:SER:HA	1:I:260:THR:HG22	2.01	0.42
1:G:17:ARG:NH2	1:I:77:ASN:HA	2.34	0.42
1:I:294:ALA:HB2	1:I:304:TYR:CZ	2.53	0.42
1:J:269:VAL:HB	1:J:303:VAL:HB	2.02	0.42
1:J:391:LEU:HD11	1:K:393:TRP:HH2	1.85	0.42
1:K:39:LEU:HD13	1:K:51:LEU:HD11	2.02	0.42
1:L:289:ARG:NH2	1:L:290:ASP:OD2	2.53	0.42
1:C:315:VAL:HG12	1:C:317:ILE:H	1.85	0.42
1:A:286:LYS:HD2	1:A:286:LYS:HA	1.83	0.42
1:B:370:LYS:HD3	2:B:706:HOH:O	2.20	0.42
1:C:275:THR:H	1:C:278:LYS:CG	2.33	0.42
1:H:95:MET:HE2	1:H:165:PRO:HB3	2.02	0.42
1:K:119:LEU:HG	1:K:409:ILE:HG23	2.02	0.42
1:L:426:VAL:O	1:L:430:ASN:ND2	2.53	0.42
1:C:363:GLY:CA	1:C:422:GLN:HE22	2.27	0.42
1:J:151:MET:HE2	1:J:183:MET:HB2	2.02	0.42
1:J:353:ILE:O	1:J:357:GLU:HG3	2.20	0.42
1:A:144:MET:HE2	1:D:445:GLY:HA2	2.01	0.41
1:B:9:SER:O	1:B:13:HIS:ND1	2.43	0.41
1:K:349:MET:N	1:K:350:PRO:HD3	2.34	0.41
1:D:323:THR:OG1	1:D:324:GLN:N	2.53	0.41
1:H:238:SER:HB3	1:H:311:TRP:CH2	2.55	0.41
1:H:354:GLU:CD	1:H:354:GLU:H	2.27	0.41
1:H:417:GLY:HA3	1:H:423:THR:HG23	2.02	0.41
1:J:148:GLN:CG	1:J:182:MET:HE3	2.49	0.41
1:K:401:ARG:HA	1:K:401:ARG:HD2	1.74	0.41
1:C:278:LYS:HD3	1:C:296:TYR:OH	2.20	0.41
1:E:50:LEU:HD22	1:E:442:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:310:PRO:HD3	2:J:734:HOH:O	2.19	0.41
1:C:336:ILE:HD12	1:C:358:LEU:HG	2.02	0.41
1:H:250:LYS:HA	1:H:250:LYS:HD3	1.89	0.41
1:J:134:ASP:OD1	1:J:136:LYS:HG2	2.20	0.41
1:C:245:GLN:CD	1:C:283:ILE:HG12	2.44	0.41
1:G:313:VAL:HA	1:G:314:PRO:HD3	1.93	0.41
1:I:148:GLN:CD	1:I:182:MET:HE3	2.45	0.41
1:A:17:ARG:NH2	1:C:77:ASN:HA	2.36	0.41
1:A:26:GLN:NE2	2:A:611:HOH:O	2.52	0.41
1:A:53:ARG:HD2	2:A:701:HOH:O	2.21	0.41
1:F:98:HIS:CG	1:F:99:PRO:HD2	2.56	0.41
1:H:248:ILE:O	1:H:252:MET:HG3	2.20	0.41
1:I:88:ILE:HD11	1:I:436:LYS:HG2	2.03	0.41
1:I:281:ARG:HA	1:I:281:ARG:HD2	1.88	0.41
1:J:153:GLU:CD	1:J:156:ARG:NH1	2.79	0.41
1:B:151:MET:HE1	1:B:154:LEU:HD23	2.03	0.41
1:D:281:ARG:NE	1:D:299:GLU:OE2	2.54	0.41
1:G:98:HIS:CG	1:G:99:PRO:HD2	2.56	0.41
1:L:122:LEU:HD13	1:L:381:GLY:HA3	2.02	0.41
1:B:151:MET:HE3	1:B:179:MET:SD	2.61	0.41
1:B:248:ILE:O	1:B:252:MET:HG3	2.21	0.41
1:C:393:TRP:HB3	1:C:397:LYS:HG2	2.03	0.41
1:F:88:ILE:CD1	1:F:436:LYS:HD2	2.51	0.41
1:F:148:GLN:O	1:F:152:THR:HG23	2.21	0.41
1:F:417:GLY:HA3	1:F:423:THR:HG23	2.03	0.41
1:H:273:GLY:O	1:H:278:LYS:NZ	2.54	0.41
1:H:282:LEU:O	1:H:286:LYS:HG2	2.21	0.41
1:H:370:LYS:HE3	2:H:537:HOH:O	2.19	0.41
1:J:370:LYS:HD2	1:J:370:LYS:O	2.21	0.41
1:K:45:TYR:O	1:K:50:LEU:HD23	2.21	0.41
1:K:108:PHE:CD1	1:K:108:PHE:C	2.98	0.41
1:K:363:GLY:HA2	1:K:422:GLN:OE1	2.21	0.41
1:L:205:LEU:O	1:L:206:ILE:HB	2.21	0.41
1:A:401:ARG:NE	2:A:850:HOH:O	2.13	0.41
1:C:231:GLU:C	1:C:233:MET:H	2.29	0.41
1:D:119:LEU:HG	1:D:409:ILE:HG23	2.03	0.41
1:D:122:LEU:HB2	1:D:124:MET:HE2	2.03	0.41
1:H:36:TRP:NE1	2:H:691:HOH:O	2.54	0.41
1:H:313:VAL:HA	1:H:314:PRO:HD3	1.97	0.41
1:C:237:VAL:H	1:C:260:THR:HG23	1.86	0.40
1:C:238:SER:OG	1:C:326:GLU:OE1	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:GLY:HA2	2:D:738:HOH:O	2.21	0.40
1:G:330:ASP:O	1:G:334:GLN:HG3	2.22	0.40
1:A:109:LEU:HD13	1:A:128:LYS:HE2	2.03	0.40
1:E:411:HIS:O	1:E:415:GLU:HG2	2.21	0.40
1:H:36:TRP:O	1:H:40:GLU:HG3	2.22	0.40
1:I:382:LEU:HD21	1:I:405:ILE:HD11	2.03	0.40
1:D:438:ALA:O	1:D:442:LEU:HG	2.22	0.40
1:G:59:ARG:HD3	1:I:153:GLU:OE2	2.22	0.40
1:I:88:ILE:CD1	1:I:436:LYS:HG2	2.51	0.40
1:I:419:GLU:CD	1:I:419:GLU:N	2.80	0.40
1:J:144:MET:O	1:J:148:GLN:HG3	2.22	0.40
1:J:148:GLN:O	1:J:152:THR:HG23	2.21	0.40
1:K:323:THR:OG1	1:K:324:GLN:N	2.55	0.40
1:A:12:ASN:OD1	1:A:16:LYS:NZ	2.54	0.40
1:A:276:LYS:NZ	2:A:802:HOH:O	2.52	0.40
1:B:250:LYS:HD3	1:B:250:LYS:HA	1.80	0.40
1:F:35:LEU:HD21	1:F:434:PHE:CD1	2.56	0.40
1:F:95:MET:O	1:F:168:ASP:HB3	2.20	0.40
1:H:238:SER:OG	1:H:326:GLU:OE1	2.38	0.40
1:I:284:GLU:O	1:I:287:SER:HB3	2.22	0.40
1:D:421:GLU:CD	1:D:421:GLU:H	2.29	0.40
1:E:25:ALA:HB2	2:E:812:HOH:O	2.22	0.40
1:G:69:ASP:HB2	1:G:142:GLU:OE2	2.21	0.40
1:G:397:LYS:NZ	2:G:869:HOH:O	2.54	0.40
1:J:98:HIS:HB3	1:J:101:VAL:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	440/450 (98%)	433 (98%)	6 (1%)	1 (0%)	43 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	441/450 (98%)	427 (97%)	12 (3%)	2 (0%)	24	21
1	C	432/450 (96%)	420 (97%)	11 (2%)	1 (0%)	43	42
1	D	440/450 (98%)	421 (96%)	15 (3%)	4 (1%)	14	9
1	E	440/450 (98%)	431 (98%)	8 (2%)	1 (0%)	43	42
1	F	441/450 (98%)	429 (97%)	10 (2%)	2 (0%)	24	21
1	G	440/450 (98%)	430 (98%)	8 (2%)	2 (0%)	24	21
1	H	434/450 (96%)	418 (96%)	15 (4%)	1 (0%)	43	42
1	I	440/450 (98%)	429 (98%)	9 (2%)	2 (0%)	24	21
1	J	440/450 (98%)	428 (97%)	10 (2%)	2 (0%)	24	21
1	K	440/450 (98%)	430 (98%)	8 (2%)	2 (0%)	24	21
1	L	440/450 (98%)	431 (98%)	8 (2%)	1 (0%)	43	42
All	All	5268/5400 (98%)	5127 (97%)	120 (2%)	21 (0%)	30	27

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ILE
1	B	206	ILE
1	C	206	ILE
1	D	206	ILE
1	E	206	ILE
1	F	206	ILE
1	G	206	ILE
1	H	206	ILE
1	I	206	ILE
1	J	206	ILE
1	K	206	ILE
1	L	206	ILE
1	D	264	SER
1	D	289	ARG
1	K	291	GLY
1	B	168	ASP
1	F	168	ASP
1	G	168	ASP
1	I	168	ASP
1	J	168	ASP
1	D	231	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	328/354 (93%)	319 (97%)	9 (3%)	39	42
1	H	344/354 (97%)	334 (97%)	10 (3%)	37	40
1	I	347/354 (98%)	332 (96%)	15 (4%)	26	25
1	J	347/354 (98%)	342 (99%)	5 (1%)	59	66
1	K	347/354 (98%)	338 (97%)	9 (3%)	40	44
1	L	347/354 (98%)	338 (97%)	9 (3%)	40	44
All	All	2060/2124 (97%)	2003 (97%)	57 (3%)	38	41

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	34	THR
1	G	50	LEU
1	G	108	PHE
1	G	156	ARG
1	G	289	ARG
1	G	323	THR
1	G	327	LEU
1	G	358	LEU
1	G	401	ARG
1	H	29	ARG
1	H	48	MET
1	H	71	ARG
1	H	108	PHE
1	H	216	VAL
1	H	224	LYS
1	H	305	LEU
1	H	354	GLU
1	H	390	ARG
1	H	394	LYS
1	I	30	GLU
1	I	61	ILE
1	I	108	PHE

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Mol	Chain	Res	Type
1	I	228	MET
1	I	257	ARG
1	I	265	SER
1	I	275	THR
1	I	299	GLU
1	I	313	VAL
1	I	323	THR
1	I	358	LEU
1	I	364	VAL
1	I	394	LYS
1	I	419	GLU
1	I	423	THR
1	J	39	LEU
1	J	50	LEU
1	J	108	PHE
1	J	286	LYS
1	J	329	VAL
1	K	30	GLU
1	K	34	THR
1	K	108	PHE
1	K	317	ILE
1	K	338	ASN
1	K	354	GLU
1	K	358	LEU
1	K	361	GLN
1	K	364	VAL
1	L	26	GLN
1	L	35	LEU
1	L	48	MET
1	L	108	PHE
1	L	353	ILE
1	L	361	GLN
1	L	394	LYS
1	L	401	ARG
1	L	421	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	41	GLN
1	G	360	GLN
1	H	20	ASN

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Mol	Chain	Res	Type
1	H	42	ASN
1	H	242	ASN
1	H	334	GLN
1	H	416	HIS
1	H	430	ASN
1	I	12	ASN
1	I	113	GLN
1	I	404	HIS
1	J	20	ASN
1	J	334	GLN
1	J	416	HIS
1	K	15	GLN
1	K	73	GLN
1	K	333	HIS
1	K	334	GLN
1	K	416	HIS
1	L	15	GLN
1	L	242	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/450 (98%)	-1.55	0 100 100	15, 26, 45, 79	0
1	B	442/450 (98%)	-1.43	0 100 100	14, 32, 68, 129	1 (0%)
1	C	435/450 (96%)	-1.32	0 100 100	14, 31, 78, 104	1 (0%)
1	D	442/450 (98%)	-1.42	0 100 100	17, 33, 59, 108	0
1	E	442/450 (98%)	-1.56	0 100 100	15, 28, 49, 80	0
1	F	442/450 (98%)	-1.54	0 100 100	15, 28, 47, 69	1 (0%)
1	G	442/450 (98%)	-1.52	0 100 100	14, 26, 48, 69	0
1	H	438/450 (97%)	-1.40	0 100 100	17, 32, 75, 111	0
1	I	442/450 (98%)	-1.33	0 100 100	14, 33, 81, 132	0
1	J	442/450 (98%)	-1.57	0 100 100	15, 26, 48, 86	0
1	K	442/450 (98%)	-1.52	0 100 100	15, 28, 50, 68	0
1	L	442/450 (98%)	-1.51	0 100 100	14, 29, 54, 77	0
All	All	5293/5400 (98%)	-1.47	0 100 100	14, 29, 62, 132	3 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.