



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:03 AM UTC

PDB ID : 1HRD / pdb_00001hrd
Title : GLUTAMATE DEHYDROGENASE
Authors : Britton, K.L.; Baker, P.J.; Stillman, T.J.; Rice, D.W.
Deposited on : 1996-04-03
Resolution : 1.96 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

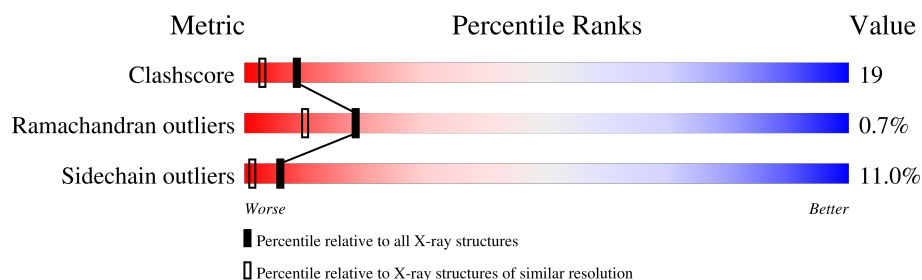
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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))
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	449	 74% 20% 5%
1	B	449	 63% 26% 11%
1	C	449	 62% 27% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10901 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	449	Total	C	N	O	S	0	0	0
			3460	2198	583	660	19			
1	B	449	Total	C	N	O	S	0	0	0
			3460	2198	583	660	19			
1	C	449	Total	C	N	O	S	0	0	0
			3460	2198	583	660	19			

- Molecule 2 is water.

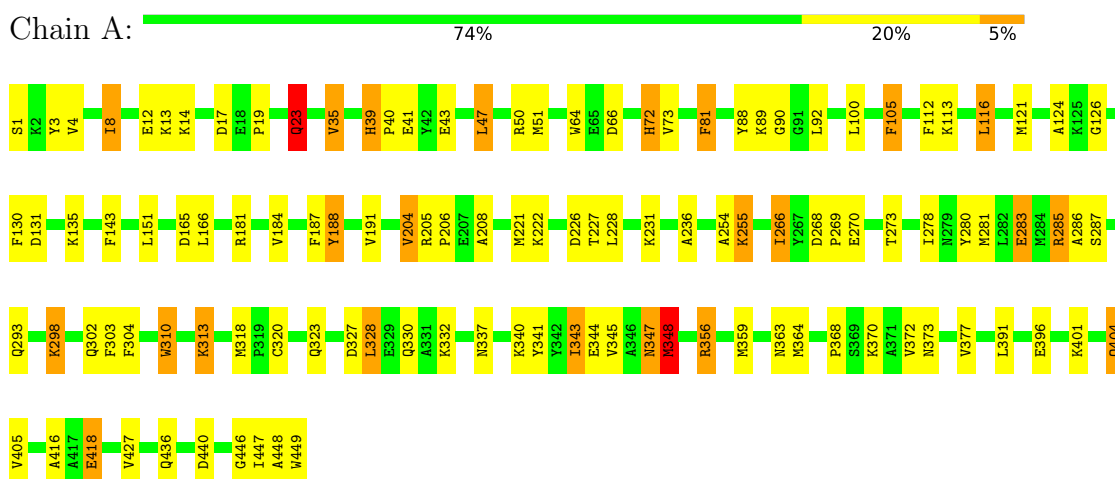
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	191	Total	O	0	0
			191	191		
2	B	152	Total	O	0	0
			152	152		
2	C	178	Total	O	0	0
			178	178		

3 Residue-property plots

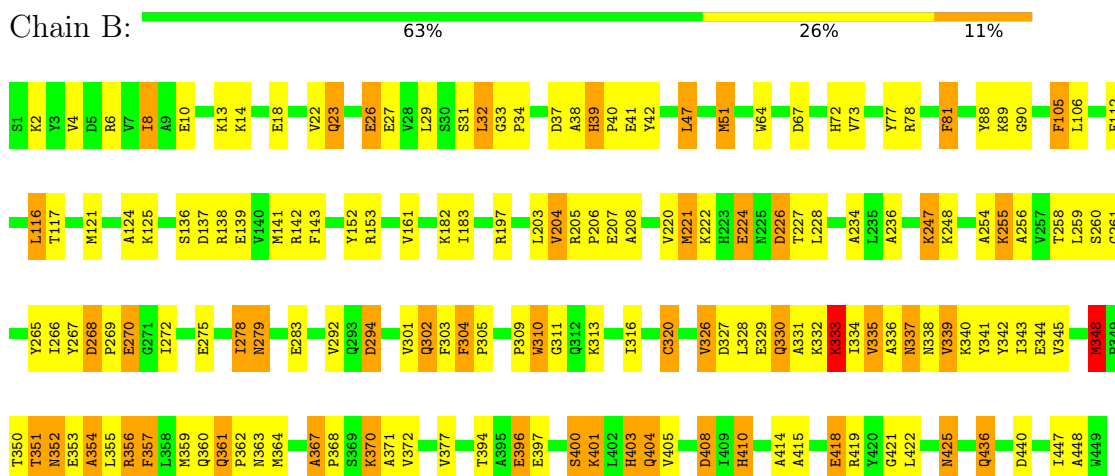
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: GLUTAMATE DEHYDROGENASE

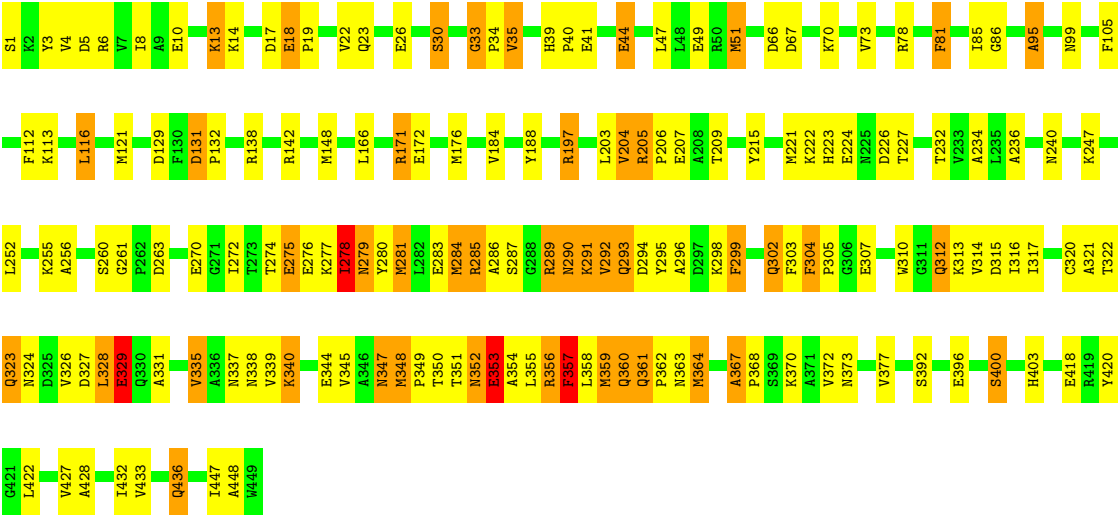


• Molecule 1: GLUTAMATE DEHYDROGENASE



• Molecule 1: GLUTAMATE DEHYDROGENASE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.10Å 151.30Å 94.60Å 90.00° 132.75° 90.00°	Depositor
Resolution (Å)	37.80 – 1.96	Depositor
% Data completeness (in resolution range)	88.0 (37.80-1.96)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10901	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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	0.80	0/3535	1.49	32/4781 (0.7%)
1	B	0.82	0/3535	1.57	50/4781 (1.0%)
1	C	0.79	0/3535	1.59	54/4781 (1.1%)
All	All	0.80	0/10605	1.55	136/14343 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	2	0

There are no bond length outliers.

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	361	GLN	CA-C-N	10.47	130.13	119.56
1	C	361	GLN	C-N-CA	10.47	130.13	119.56
1	C	347	ASN	CA-CB-CG	-9.40	103.19	112.60
1	C	364	MET	N-CA-C	8.64	121.93	110.53
1	B	81	PHE	N-CA-C	8.20	119.91	110.97
1	A	285	ARG	N-CA-CB	8.16	122.11	110.12
1	A	448	ALA	N-CA-C	-8.14	99.22	111.34
1	C	357	PHE	CA-CB-CG	-7.98	105.82	113.80
1	C	112	PHE	CA-CB-CG	-7.94	105.86	113.80
1	B	39	HIS	CA-C-N	7.85	127.91	119.28
1	B	39	HIS	C-N-CA	7.85	127.91	119.28
1	C	278	ILE	N-CA-CB	7.52	120.77	110.54
1	A	112	PHE	CA-CB-CG	-7.50	106.30	113.80
1	B	112	PHE	CA-CB-CG	-7.47	106.33	113.80
1	C	278	ILE	N-CA-C	7.37	118.14	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	345	VAL	N-CA-CB	7.26	118.75	111.57
1	B	259	LEU	N-CA-C	-7.15	98.48	109.14
1	B	408	ASP	CA-CB-CG	-7.04	105.56	112.60
1	B	448	ALA	N-CA-C	-6.98	95.94	110.80
1	C	299	PHE	N-CA-C	6.97	121.95	113.38
1	C	81	PHE	N-CA-C	6.91	118.50	110.97
1	A	143	PHE	CA-CB-CG	-6.86	106.94	113.80
1	B	208	ALA	N-CA-C	6.75	122.43	111.37
1	C	347	ASN	N-CA-CB	6.70	120.79	109.87
1	A	364	MET	N-CA-C	6.69	120.51	110.14
1	B	367	ALA	CA-C-N	6.63	126.39	119.76
1	B	367	ALA	C-N-CA	6.63	126.39	119.76
1	C	367	ALA	CA-C-N	6.58	126.81	119.90
1	C	367	ALA	C-N-CA	6.58	126.81	119.90
1	C	95	ALA	CA-C-N	6.56	126.25	119.56
1	C	95	ALA	C-N-CA	6.56	126.25	119.56
1	B	78	ARG	N-CA-CB	6.55	119.94	110.37
1	B	29	LEU	CB-CA-C	-6.47	98.24	110.67
1	A	188	TYR	CB-CA-C	-6.45	102.39	111.80
1	C	85	ILE	N-CA-C	6.45	119.09	112.90
1	C	78	ARG	N-CA-CB	6.38	120.47	110.71
1	A	81	PHE	N-CA-C	6.37	117.91	110.97
1	B	326	VAL	N-CA-CB	6.34	117.63	110.72
1	B	339	VAL	N-CA-CB	6.33	120.01	110.13
1	B	403	HIS	CA-CB-CG	-6.30	107.50	113.80
1	B	27	GLU	N-CA-CB	-6.29	100.89	110.01
1	C	33	GLY	CA-C-N	6.28	127.68	119.84
1	C	33	GLY	C-N-CA	6.28	127.68	119.84
1	A	14	LYS	N-CA-C	6.27	117.78	111.07
1	C	276	GLU	N-CA-CB	-6.25	100.95	110.01
1	B	182	LYS	CA-CB-CG	-6.24	101.63	114.10
1	C	304	PHE	CA-C-N	6.22	126.25	119.90
1	C	304	PHE	C-N-CA	6.22	126.25	119.90
1	B	348	MET	N-CA-CB	-6.19	101.73	111.70
1	A	347	ASN	N-CA-CB	6.18	119.06	109.85
1	C	18	GLU	CA-C-N	6.16	125.64	119.24
1	C	18	GLU	C-N-CA	6.16	125.64	119.24
1	A	23	GLN	N-CA-CB	-6.03	101.25	110.12
1	C	23	GLN	CB-CA-C	-6.02	101.42	110.88
1	A	344	GLU	CA-C-N	-6.01	116.79	123.16
1	A	344	GLU	C-N-CA	-6.01	116.79	123.16
1	A	47	LEU	N-CA-C	6.01	117.50	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	364	MET	N-CA-C	5.99	118.94	110.50
1	B	345	VAL	N-CA-C	-5.95	106.92	111.62
1	B	410	HIS	CA-CB-CG	-5.94	107.86	113.80
1	A	72	HIS	CA-CB-CG	-5.89	107.91	113.80
1	B	268	ASP	CA-C-N	5.86	125.48	119.56
1	B	268	ASP	C-N-CA	5.86	125.48	119.56
1	C	372	VAL	N-CA-C	5.85	116.59	110.62
1	B	247	LYS	CB-CA-C	-5.81	101.51	110.81
1	B	344	GLU	CA-C-N	-5.81	117.00	123.16
1	B	344	GLU	C-N-CA	-5.81	117.00	123.16
1	C	322	THR	N-CA-C	5.80	118.39	110.55
1	C	344	GLU	CA-C-N	-5.80	117.29	122.97
1	C	344	GLU	C-N-CA	-5.80	117.29	122.97
1	B	143	PHE	CA-CB-CG	-5.77	108.03	113.80
1	C	352	ASN	CA-CB-CG	-5.77	106.83	112.60
1	C	188	TYR	CB-CA-C	-5.71	103.38	111.95
1	C	448	ALA	N-CA-C	-5.69	98.67	110.80
1	B	356	ARG	CB-CA-C	-5.68	102.20	110.96
1	C	278	ILE	CB-CA-C	5.68	119.81	112.14
1	A	446	GLY	CA-C-N	5.68	126.99	121.65
1	A	446	GLY	C-N-CA	5.68	126.99	121.65
1	A	100	LEU	N-CA-C	5.64	117.11	111.07
1	A	208	ALA	N-CA-C	5.61	120.58	111.37
1	C	240	ASN	N-CA-C	5.58	118.08	111.33
1	A	151	LEU	N-CA-C	5.57	117.35	111.28
1	C	285	ARG	CA-C-N	5.57	128.53	120.79
1	C	285	ARG	C-N-CA	5.57	128.53	120.79
1	B	316	ILE	N-CA-C	5.55	116.74	108.46
1	A	348	MET	N-CA-CB	-5.54	105.51	111.66
1	A	348	MET	CB-CA-C	-5.51	107.28	111.20
1	C	329	GLU	CB-CA-C	5.49	121.45	109.99
1	B	14	LYS	N-CA-C	5.48	117.25	111.28
1	A	310	TRP	N-CA-C	5.46	119.69	113.19
1	A	343	ILE	N-CA-C	5.46	114.60	106.85
1	B	183	ILE	N-CA-CB	5.43	116.78	110.65
1	B	330	GLN	CB-CA-C	5.41	120.95	110.46
1	C	447	ILE	CB-CA-C	-5.40	105.75	112.45
1	B	396	GLU	N-CA-CB	5.39	118.05	110.12
1	A	17	ASP	CA-CB-CG	5.39	117.99	112.60
1	C	329	GLU	N-CA-CB	5.39	119.19	110.40
1	C	321	ALA	O-C-N	5.36	124.80	120.83
1	B	320	CYS	CA-C-N	-5.35	115.16	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	CYS	C-N-CA	-5.35	115.16	121.90
1	B	77	TYR	CB-CA-C	-5.35	98.83	109.79
1	A	436	GLN	N-CA-C	5.33	117.08	111.28
1	B	333	LYS	CA-C-N	5.31	127.20	120.72
1	B	333	LYS	C-N-CA	5.31	127.20	120.72
1	B	357	PHE	CA-CB-CG	-5.30	108.50	113.80
1	B	372	VAL	N-CA-C	5.29	116.07	110.72
1	C	321	ALA	CA-C-O	5.29	122.78	119.77
1	C	291	LYS	N-CA-C	5.28	118.03	107.62
1	B	226	ASP	N-CA-C	5.26	114.98	108.19
1	B	23	GLN	CB-CA-C	-5.21	102.71	110.88
1	C	14	LYS	N-CA-C	5.20	116.95	111.28
1	C	359	MET	CA-CB-CG	-5.19	103.71	114.10
1	A	298	LYS	N-CA-C	5.19	116.75	111.14
1	B	447	ILE	CB-CA-C	-5.18	105.19	111.88
1	A	313	LYS	CB-CA-C	5.17	118.85	110.22
1	B	27	GLU	CB-CA-C	5.16	118.98	110.88
1	B	339	VAL	CB-CA-C	5.16	119.11	111.26
1	C	131	ASP	CA-C-N	5.16	124.83	119.56
1	C	131	ASP	C-N-CA	5.16	124.83	119.56
1	C	209	THR	N-CA-C	5.15	116.58	111.07
1	C	35	VAL	CB-CA-C	-5.15	105.29	111.88
1	A	304	PHE	CB-CA-C	-5.15	102.84	110.97
1	C	353	GLU	N-CA-CB	5.14	117.42	109.91
1	B	47	LEU	N-CA-C	5.14	117.28	111.11
1	C	321	ALA	N-CA-C	5.14	116.32	108.30
1	B	343	ILE	N-CA-C	5.14	114.89	106.72
1	B	425	ASN	CA-CB-CG	-5.13	107.47	112.60
1	C	310	TRP	N-CA-C	5.12	119.16	113.01
1	C	358	LEU	CA-C-O	5.08	125.89	120.20
1	A	39	HIS	N-CA-C	5.08	117.87	108.94
1	A	372	VAL	N-CA-C	5.05	115.77	110.62
1	B	354	ALA	N-CA-C	-5.05	105.90	111.71
1	A	130	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	416	ALA	N-CA-C	5.02	116.56	111.14
1	B	255	LYS	N-CA-C	5.01	117.32	108.75
1	C	313	LYS	N-CA-CB	5.01	118.17	110.21

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	278	ILE	CA

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Mol	Chain	Res	Type	Atom
1	C	329	GLU	CA

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	3460	0	3390	79	0
1	B	3460	0	3390	155	0
1	C	3460	0	3390	153	0
2	A	191	0	0	2	0
2	B	152	0	0	5	0
2	C	178	0	0	4	0
All	All	10901	0	10170	386	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 19.

All (386) 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:A:347:ASN:HD22	1:A:348:MET:N	1.27	1.32
1:C:280:TYR:CE2	1:C:284:MET:HE3	1.71	1.25
1:B:360:GLN:O	1:B:362:PRO:HD3	1.33	1.24
1:C:280:TYR:O	1:C:283:GLU:HB2	1.44	1.17
1:B:221:MET:HA	1:B:221:MET:HE2	1.27	1.12
1:C:302:GLN:HA	1:C:302:GLN:OE1	1.46	1.10
1:C:323:GLN:OE1	1:C:348:MET:HG2	1.50	1.08
1:B:313:LYS:HG3	1:B:337:ASN:HB3	1.34	1.06
1:C:289:ARG:NH2	1:C:291:LYS:HD2	1.70	1.05
1:A:347:ASN:ND2	1:A:348:MET:N	2.05	1.03
1:B:267:TYR:CE2	1:B:269:PRO:HG3	1.95	1.01
1:C:280:TYR:HA	1:C:283:GLU:HG3	1.47	0.94
1:A:347:ASN:HD22	1:A:348:MET:H	1.09	0.94
1:C:280:TYR:CE2	1:C:284:MET:CE	2.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:THR:OG1	1:B:397:GLU:HG3	1.68	0.92
1:A:35:VAL:O	1:A:39:HIS:HD2	1.53	0.90
1:B:360:GLN:O	1:B:362:PRO:CD	2.21	0.89
1:C:347:ASN:OD1	1:C:348:MET:N	2.05	0.88
1:C:1:SER:O	1:C:5:ASP:OD2	1.91	0.87
1:C:323:GLN:CD	1:C:348:MET:HG2	1.99	0.87
1:C:352:ASN:O	1:C:356:ARG:HG2	1.75	0.85
1:B:331:ALA:O	1:B:335:VAL:HG22	1.77	0.84
1:B:138:ARG:HD2	1:B:141:MET:HE1	1.59	0.84
1:C:323:GLN:HG2	1:C:348:MET:O	1.77	0.84
1:B:116:LEU:C	1:B:116:LEU:HD23	2.02	0.83
1:B:236:ALA:HB2	1:B:310:TRP:CZ2	2.13	0.83
1:B:302:GLN:HB3	1:B:304:PHE:CE1	2.14	0.83
1:B:331:ALA:O	1:B:335:VAL:CG2	2.26	0.83
1:C:26:GLU:O	1:C:30:SER:OG	1.97	0.82
1:A:89:LYS:HE3	2:A:573:HOH:O	1.76	0.82
1:B:313:LYS:HE2	1:B:337:ASN:HB3	1.60	0.82
1:C:280:TYR:CD2	1:C:284:MET:HE3	2.14	0.82
1:C:35:VAL:O	1:C:39:HIS:HD2	1.62	0.82
1:C:323:GLN:CG	1:C:348:MET:HG2	2.11	0.80
1:A:347:ASN:HD22	1:A:347:ASN:C	1.87	0.80
1:B:313:LYS:HE2	1:B:337:ASN:CA	2.12	0.80
1:B:313:LYS:CE	1:B:337:ASN:HB3	2.12	0.80
1:B:313:LYS:HE2	1:B:337:ASN:CB	2.12	0.79
1:B:4:VAL:O	1:B:8:ILE:HG13	1.82	0.79
1:A:348:MET:CG	1:A:348:MET:O	2.26	0.79
1:B:221:MET:HA	1:B:221:MET:CE	2.10	0.79
1:B:226:ASP:OD1	1:B:227:THR:N	2.16	0.79
1:A:227:THR:O	1:A:231:LYS:HE3	1.83	0.78
1:A:116:LEU:C	1:A:116:LEU:HD23	2.08	0.78
1:B:310:TRP:HB2	1:B:330:GLN:HB3	1.64	0.78
1:C:340:LYS:O	1:C:340:LYS:HG3	1.81	0.78
1:C:323:GLN:HG2	1:C:348:MET:HG2	1.66	0.78
1:B:221:MET:HE1	1:B:341:TYR:CZ	2.19	0.77
1:C:331:ALA:O	1:C:335:VAL:HG23	1.83	0.77
1:B:340:LYS:HG2	1:B:340:LYS:O	1.83	0.77
1:C:323:GLN:OE1	1:C:348:MET:CG	2.31	0.77
1:B:330:GLN:OE1	1:B:333:LYS:HE3	1.84	0.76
1:C:355:LEU:O	1:C:359:MET:HB2	1.86	0.76
1:B:23:GLN:O	1:B:26:GLU:HB3	1.85	0.75
1:B:221:MET:HE2	1:B:221:MET:CA	2.13	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LYS:HG3	1:B:337:ASN:CB	2.14	0.74
1:B:236:ALA:HB2	1:B:310:TRP:HZ2	1.53	0.74
1:B:313:LYS:HE2	1:B:337:ASN:HA	1.70	0.74
1:B:313:LYS:CG	1:B:337:ASN:HB3	2.14	0.73
1:C:280:TYR:HD1	1:C:283:GLU:HG3	1.52	0.73
1:C:304:PHE:O	1:C:307:GLU:HB2	1.87	0.73
1:C:328:LEU:HB2	1:C:353:GLU:OE1	1.89	0.72
1:B:224:GLU:OE1	1:B:224:GLU:HA	1.90	0.71
1:B:302:GLN:HB3	1:B:304:PHE:HE1	1.55	0.71
1:A:418:GLU:HB2	2:A:602:HOH:O	1.91	0.71
1:C:355:LEU:HG	1:C:359:MET:HE2	1.72	0.71
1:A:340:LYS:HG3	1:A:363:ASN:O	1.91	0.70
1:C:420:TYR:C	1:C:422:LEU:HD12	2.17	0.70
1:B:267:TYR:CZ	1:B:269:PRO:HG3	2.25	0.70
1:C:263:ASP:O	1:C:305:PRO:HA	1.91	0.69
1:B:313:LYS:CE	1:B:337:ASN:CB	2.70	0.69
1:A:4:VAL:O	1:A:8:ILE:HD12	1.92	0.69
1:A:204:VAL:HG12	1:A:204:VAL:O	1.91	0.69
1:C:17:ASP:C	1:C:19:PRO:HD3	2.18	0.69
1:B:404:GLN:O	1:B:408:ASP:OD2	2.10	0.68
1:B:138:ARG:HD2	1:B:141:MET:CE	2.23	0.68
1:A:35:VAL:O	1:A:39:HIS:CD2	2.42	0.68
1:A:327:ASP:OD1	1:A:330:GLN:HG2	1.93	0.68
1:C:13:LYS:HD2	1:C:13:LYS:N	2.07	0.67
1:A:347:ASN:ND2	1:A:347:ASN:C	2.46	0.67
1:B:337:ASN:N	1:B:337:ASN:HD22	1.91	0.67
1:B:265:TYR:CE2	1:B:309:PRO:HA	2.30	0.66
1:B:335:VAL:HG21	1:B:357:PHE:CZ	2.31	0.66
1:C:275:GLU:O	1:C:279:ASN:ND2	2.29	0.66
1:C:289:ARG:O	1:C:291:LYS:N	2.28	0.66
1:C:280:TYR:CD1	1:C:283:GLU:HG3	2.31	0.66
1:B:267:TYR:O	1:B:301:VAL:HB	1.96	0.65
1:C:284:MET:HE1	1:C:295:TYR:CA	2.27	0.65
1:C:289:ARG:HH21	1:C:291:LYS:HD2	1.58	0.64
1:C:1:SER:HB3	1:C:4:VAL:HB	1.79	0.64
1:C:223:HIS:ND1	1:C:224:GLU:OE2	2.30	0.64
1:A:348:MET:O	1:A:348:MET:HG3	1.97	0.64
1:B:304:PHE:CD1	1:B:304:PHE:N	2.66	0.64
1:A:328:LEU:HD13	1:A:332:LYS:HE3	1.79	0.64
1:C:226:ASP:OD1	1:C:227:THR:N	2.30	0.63
1:B:348:MET:O	1:B:348:MET:CG	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:TYR:CD1	1:C:6:ARG:NH2	2.66	0.63
1:C:256:ALA:O	1:C:272:ILE:HD12	1.98	0.63
1:C:420:TYR:O	1:C:422:LEU:HD12	1.99	0.63
1:B:224:GLU:OE1	1:B:224:GLU:CA	2.44	0.63
1:C:284:MET:HE1	1:C:295:TYR:N	2.14	0.63
1:B:228:LEU:O	1:B:254:ALA:HB2	1.99	0.63
1:B:268:ASP:OD1	1:B:268:ASP:C	2.42	0.62
1:C:354:ALA:O	1:C:357:PHE:HB3	1.98	0.62
1:B:355:LEU:HG	1:B:359:MET:HE2	1.80	0.62
1:A:266:ILE:C	1:A:266:ILE:HD12	2.24	0.62
1:C:323:GLN:HG2	1:C:348:MET:CG	2.30	0.62
1:B:205:ARG:HB3	1:B:206:PRO:HD3	1.82	0.62
1:C:35:VAL:O	1:C:39:HIS:CD2	2.50	0.61
1:C:121:MET:HE1	1:C:377:VAL:HG12	1.82	0.61
1:C:348:MET:O	1:C:348:MET:HG3	2.00	0.61
1:B:275:GLU:O	1:B:279:ASN:OD1	2.18	0.61
1:A:3:TYR:CD2	1:A:43:GLU:HB2	2.36	0.61
1:C:33:GLY:N	1:C:34:PRO:HD2	2.15	0.61
1:C:348:MET:O	1:C:348:MET:CG	2.45	0.61
1:C:420:TYR:O	1:C:422:LEU:CD1	2.50	0.60
1:C:204:VAL:HG12	1:C:204:VAL:O	2.01	0.60
1:B:138:ARG:CD	1:B:141:MET:CE	2.79	0.60
1:A:404:GLN:HG2	1:A:405:VAL:N	2.15	0.60
1:C:348:MET:HA	2:C:576:HOH:O	2.02	0.59
1:C:302:GLN:HB3	1:C:304:PHE:CE1	2.37	0.59
1:C:337:ASN:O	1:C:338:ASN:HB2	2.02	0.59
1:A:3:TYR:CE2	1:A:43:GLU:HB2	2.38	0.59
1:A:368:PRO:HG3	1:A:427:VAL:HA	1.85	0.59
1:C:338:ASN:HD22	1:C:338:ASN:N	2.01	0.59
1:C:261:GLY:HA3	1:C:292:VAL:HB	1.86	0.58
1:B:414:ALA:O	1:B:418:GLU:HB2	2.05	0.57
1:C:327:ASP:OD1	1:C:329:GLU:N	2.37	0.57
1:B:32:LEU:C	1:B:34:PRO:HD2	2.29	0.57
1:C:347:ASN:OD1	1:C:347:ASN:C	2.39	0.57
1:C:280:TYR:HE2	1:C:284:MET:CE	2.16	0.57
1:B:40:PRO:HD2	1:B:41:GLU:OE1	2.05	0.56
1:B:121:MET:HE1	1:B:377:VAL:CG1	2.35	0.56
1:B:348:MET:O	1:B:348:MET:HG3	2.05	0.56
1:C:327:ASP:OD1	1:C:327:ASP:C	2.48	0.56
1:C:280:TYR:HA	1:C:283:GLU:CG	2.28	0.56
1:C:328:LEU:HD22	1:C:328:LEU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASP:CG	1:A:166:LEU:H	2.13	0.56
1:C:352:ASN:H	1:C:352:ASN:ND2	2.03	0.56
1:A:121:MET:HE1	1:A:377:VAL:HG12	1.88	0.56
1:C:121:MET:HE1	1:C:377:VAL:CG1	2.35	0.56
1:C:280:TYR:CE1	1:C:298:LYS:HD3	2.41	0.55
1:C:284:MET:HE1	1:C:295:TYR:HB2	1.88	0.55
1:C:302:GLN:OE1	1:C:302:GLN:CA	2.31	0.55
1:B:313:LYS:CE	1:B:337:ASN:HA	2.36	0.55
1:C:317:ILE:HG12	1:C:339:VAL:HG11	1.88	0.55
1:C:422:LEU:HD12	1:C:422:LEU:N	2.22	0.55
1:B:331:ALA:HB1	1:B:357:PHE:CD2	2.41	0.55
1:A:19:PRO:O	1:A:23:GLN:HB2	2.05	0.55
1:B:203:LEU:C	1:B:204:VAL:HG23	2.31	0.55
1:B:138:ARG:HD3	1:B:141:MET:HE2	1.88	0.55
1:B:38:ALA:C	1:B:40:PRO:HD3	2.31	0.55
1:C:327:ASP:HA	1:C:351:THR:CG2	2.37	0.55
1:B:236:ALA:O	1:B:320:CYS:HB2	2.07	0.54
1:B:342:TYR:HH	1:B:350:THR:HG1	1.55	0.54
1:B:415:ALA:HA	1:B:418:GLU:HB2	1.89	0.54
1:B:348:MET:HA	2:B:528:HOH:O	2.06	0.54
1:A:236:ALA:HB2	1:A:310:TRP:CZ2	2.42	0.54
1:B:335:VAL:HG21	1:B:357:PHE:CE2	2.43	0.54
1:B:335:VAL:O	1:B:338:ASN:N	2.39	0.54
1:B:138:ARG:CD	1:B:141:MET:HE1	2.34	0.54
1:B:400:SER:O	1:B:404:GLN:HG3	2.08	0.54
1:B:327:ASP:O	1:B:331:ALA:N	2.34	0.53
1:A:348:MET:O	1:A:348:MET:HG2	2.06	0.53
1:B:116:LEU:C	1:B:116:LEU:CD2	2.79	0.53
1:B:272:ILE:O	1:B:278:ILE:HD11	2.08	0.53
1:A:280:TYR:HA	1:A:283:GLU:HG3	1.89	0.53
1:A:440:ASP:HB3	2:B:505:HOH:O	2.09	0.53
1:A:280:TYR:CD1	1:A:283:GLU:HG3	2.44	0.53
1:B:138:ARG:CD	1:B:141:MET:HE2	2.39	0.53
1:C:236:ALA:O	1:C:320:CYS:HB2	2.09	0.53
1:C:293:GLN:HB2	1:C:303:PHE:CD1	2.43	0.53
1:C:280:TYR:CZ	1:C:298:LYS:HD3	2.44	0.53
1:B:396:GLU:CD	1:B:396:GLU:H	2.17	0.52
1:A:88:TYR:HB3	1:A:124:ALA:HB2	1.91	0.52
1:C:289:ARG:O	1:C:290:ASN:C	2.50	0.52
1:A:50:ARG:HD2	1:A:449:TRP:OXT	2.10	0.52
1:A:347:ASN:ND2	1:A:348:MET:CB	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:OD1	1:B:142:ARG:NH2	2.35	0.52
1:A:328:LEU:O	1:A:332:LYS:HG3	2.10	0.51
1:A:269:PRO:HD2	1:A:270:GLU:H	1.75	0.51
1:B:403:HIS:HD2	1:B:403:HIS:O	1.93	0.51
1:C:113:LYS:HE3	1:C:370:LYS:O	2.10	0.51
1:C:327:ASP:HA	1:C:351:THR:HG23	1.92	0.51
1:B:121:MET:HE1	1:B:377:VAL:HG12	1.93	0.51
1:B:261:GLY:HA3	1:B:292:VAL:HB	1.92	0.51
1:B:330:GLN:NE2	2:B:564:HOH:O	2.43	0.51
1:B:90:GLY:HA3	1:B:124:ALA:O	2.10	0.51
1:B:6:ARG:O	1:B:10:GLU:HG3	2.11	0.51
1:C:289:ARG:C	1:C:291:LYS:N	2.68	0.51
1:C:47:LEU:O	1:C:51:MET:HG3	2.11	0.51
1:C:171:ARG:HD2	1:C:172:GLU:OE2	2.10	0.51
1:B:332:LYS:C	1:B:335:VAL:HG23	2.36	0.51
1:B:332:LYS:O	1:B:335:VAL:HG23	2.11	0.51
1:C:283:GLU:O	1:C:286:ALA:HB3	2.10	0.51
1:C:274:THR:OG1	1:C:277:LYS:HB2	2.11	0.50
1:B:234:ALA:HA	1:B:258:THR:OG1	2.12	0.50
1:B:396:GLU:HB2	2:B:576:HOH:O	2.10	0.50
1:A:313:LYS:HB2	1:A:337:ASN:OD1	2.12	0.50
1:B:340:LYS:O	1:B:340:LYS:CG	2.55	0.50
1:B:221:MET:CE	1:B:221:MET:CA	2.81	0.50
1:B:440:ASP:HB3	2:C:532:HOH:O	2.11	0.50
1:C:315:ASP:C	1:C:316:ILE:HG13	2.36	0.50
1:C:348:MET:HA	2:C:578:HOH:O	2.12	0.50
1:C:280:TYR:C	1:C:283:GLU:HB2	2.30	0.49
1:C:312:GLN:OE1	1:C:312:GLN:HA	2.11	0.49
1:B:335:VAL:HG21	1:B:357:PHE:HZ	1.74	0.49
1:A:255:LYS:HB2	1:A:273:THR:CG2	2.42	0.49
1:B:403:HIS:C	1:B:403:HIS:CD2	2.89	0.49
1:C:8:ILE:HD13	1:C:26:GLU:HA	1.95	0.49
1:C:357:PHE:C	1:C:359:MET:N	2.71	0.49
1:B:266:ILE:C	1:B:266:ILE:HD12	2.38	0.49
1:B:33:GLY:O	1:B:37:ASP:N	2.30	0.49
1:B:302:GLN:HA	1:B:302:GLN:HE21	1.78	0.49
1:B:89:LYS:HD2	1:B:161:VAL:O	2.12	0.49
1:B:304:PHE:N	1:B:304:PHE:HD1	2.11	0.49
1:A:47:LEU:O	1:A:51:MET:HG3	2.13	0.48
1:B:302:GLN:HE21	1:B:302:GLN:CA	2.26	0.48
1:C:66:ASP:OD1	1:C:66:ASP:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:O	1:B:338:ASN:HA	2.13	0.48
1:A:1:SER:HB3	1:A:4:VAL:HB	1.96	0.48
1:C:116:LEU:HD23	1:C:433:VAL:HG13	1.94	0.48
1:A:90:GLY:HA3	1:A:124:ALA:O	2.13	0.48
1:A:236:ALA:O	1:A:320:CYS:HB2	2.14	0.48
1:B:333:LYS:NZ	2:B:597:HOH:O	2.47	0.48
1:C:278:ILE:HD13	1:C:278:ILE:C	2.39	0.48
1:C:280:TYR:CD2	1:C:299:PHE:HE2	2.31	0.48
1:A:205:ARG:N	1:A:206:PRO:CD	2.77	0.48
1:A:204:VAL:O	1:A:204:VAL:CG1	2.61	0.47
1:B:39:HIS:N	1:B:40:PRO:HD3	2.29	0.47
1:B:64:TRP:CE2	1:B:72:HIS:HB2	2.49	0.47
1:B:303:PHE:CD2	1:B:305:PRO:HD3	2.49	0.47
1:A:66:ASP:OD1	1:A:66:ASP:C	2.55	0.47
1:A:278:ILE:O	1:A:281:MET:HB2	2.13	0.47
1:B:47:LEU:O	1:B:51:MET:HG3	2.14	0.47
1:B:309:PRO:C	1:B:311:GLY:H	2.21	0.47
1:B:401:LYS:O	1:B:405:VAL:HG23	2.14	0.47
1:C:116:LEU:HD23	1:C:433:VAL:CG1	2.42	0.47
1:B:330:GLN:OE1	1:B:333:LYS:CE	2.59	0.47
1:B:331:ALA:O	1:B:335:VAL:HG23	2.11	0.47
1:B:224:GLU:HG3	1:B:340:LYS:NZ	2.30	0.47
1:C:347:ASN:O	1:C:348:MET:HB3	2.14	0.47
1:C:260:SER:HA	1:C:292:VAL:HG21	1.97	0.47
1:B:313:LYS:HE3	1:B:337:ASN:CG	2.40	0.47
1:B:335:VAL:CG1	1:B:361:GLN:HG3	2.45	0.47
1:C:350:THR:HG22	1:C:354:ALA:HB3	1.97	0.47
1:A:121:MET:HE1	1:A:377:VAL:CG1	2.45	0.47
1:A:187:PHE:CZ	1:C:86:GLY:HA2	2.49	0.47
1:C:263:ASP:HB2	1:C:303:PHE:HZ	1.80	0.46
1:C:368:PRO:HG3	1:C:427:VAL:HA	1.96	0.46
1:B:294:ASP:N	1:B:294:ASP:OD1	2.47	0.46
1:C:296:ALA:CB	1:C:303:PHE:HB2	2.46	0.46
1:A:347:ASN:ND2	1:A:348:MET:H	1.91	0.46
1:A:283:GLU:H	1:A:283:GLU:HG2	1.42	0.46
1:C:323:GLN:HG3	1:C:348:MET:HB3	1.98	0.46
1:C:339:VAL:O	1:C:364:MET:HE3	2.15	0.46
1:A:39:HIS:HA	1:A:40:PRO:HD2	1.82	0.46
1:A:226:ASP:OD1	1:A:231:LYS:NZ	2.37	0.46
1:A:116:LEU:C	1:A:116:LEU:CD2	2.85	0.46
1:C:428:ALA:O	1:C:432:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LYS:HA	1:B:335:VAL:CG2	2.46	0.46
1:C:348:MET:N	1:C:349:PRO:HD3	2.31	0.46
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.71	0.46
1:B:152:TYR:CD1	1:B:152:TYR:C	2.93	0.46
1:A:280:TYR:HA	1:A:283:GLU:CG	2.46	0.46
1:C:247:LYS:HD2	1:C:278:ILE:HD11	1.98	0.45
1:C:261:GLY:CA	1:C:292:VAL:HB	2.46	0.45
1:B:4:VAL:O	1:B:8:ILE:CG1	2.59	0.45
1:B:221:MET:O	1:B:222:LYS:C	2.59	0.45
1:C:354:ALA:O	1:C:357:PHE:CB	2.65	0.45
1:B:220:VAL:O	1:B:221:MET:C	2.60	0.45
1:B:355:LEU:HG	1:B:359:MET:CE	2.44	0.45
1:C:396:GLU:O	1:C:400:SER:HB2	2.17	0.45
1:C:284:MET:HE1	1:C:295:TYR:CB	2.45	0.45
1:C:420:TYR:C	1:C:422:LEU:CD1	2.90	0.45
1:A:286:ALA:O	1:A:287:SER:C	2.60	0.45
1:B:256:ALA:O	1:B:272:ILE:HD12	2.16	0.45
1:B:336:ALA:C	1:B:338:ASN:H	2.25	0.45
1:A:330:GLN:HA	1:A:330:GLN:NE2	2.32	0.45
1:C:263:ASP:OD1	1:C:263:ASP:N	2.42	0.45
1:B:39:HIS:HA	1:B:40:PRO:HD2	1.78	0.45
1:B:106:LEU:HB2	1:B:125:LYS:HG2	1.99	0.45
1:B:351:THR:O	1:B:354:ALA:N	2.50	0.45
1:C:18:GLU:N	1:C:19:PRO:HD3	2.32	0.45
1:C:280:TYR:CD2	1:C:299:PHE:CE2	3.05	0.45
1:C:292:VAL:HG12	1:C:303:PHE:HE1	1.81	0.45
1:A:43:GLU:O	1:A:43:GLU:HG2	2.16	0.45
1:A:113:LYS:HE2	1:A:377:VAL:HG21	1.98	0.45
1:B:327:ASP:OD1	1:B:330:GLN:N	2.41	0.45
1:C:148:MET:CE	1:C:176:MET:HB3	2.47	0.45
1:C:148:MET:HE2	1:C:176:MET:HB3	1.99	0.44
1:B:367:ALA:HA	1:B:368:PRO:HD3	1.84	0.44
1:C:171:ARG:NH1	1:C:172:GLU:OE2	2.45	0.44
1:C:215:TYR:CD2	1:C:403:HIS:HA	2.52	0.44
1:C:280:TYR:CD1	1:C:283:GLU:CG	2.99	0.44
1:C:338:ASN:N	1:C:338:ASN:ND2	2.66	0.44
1:A:269:PRO:CD	1:A:270:GLU:H	2.31	0.44
1:B:352:ASN:O	1:B:356:ARG:HG2	2.17	0.44
1:A:293:GLN:HG3	1:A:303:PHE:CG	2.52	0.44
1:A:64:TRP:CE2	1:A:72:HIS:HB2	2.53	0.44
1:B:421:GLY:C	1:B:422:LEU:HD23	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ARG:N	1:C:206:PRO:CD	2.81	0.44
1:A:221:MET:HE1	1:A:341:TYR:CZ	2.53	0.43
1:B:33:GLY:N	1:B:34:PRO:HD2	2.33	0.43
1:B:116:LEU:HD23	1:B:117:THR:N	2.33	0.43
1:C:39:HIS:HA	1:C:40:PRO:HD2	1.74	0.43
1:C:293:GLN:HB2	1:C:303:PHE:CG	2.52	0.43
1:C:328:LEU:HD22	1:C:328:LEU:C	2.42	0.43
1:B:88:TYR:HB3	1:B:124:ALA:HB2	1.99	0.43
1:C:131:ASP:HA	1:C:132:PRO:HD3	1.78	0.43
1:B:337:ASN:N	1:B:337:ASN:ND2	2.64	0.43
1:B:410:HIS:ND1	1:B:410:HIS:C	2.75	0.43
1:C:3:TYR:OH	1:C:49:GLU:OE1	2.34	0.43
1:B:436:GLN:OE1	1:B:436:GLN:HA	2.17	0.43
1:A:228:LEU:O	1:A:254:ALA:HB2	2.18	0.43
1:C:18:GLU:N	1:C:19:PRO:CD	2.79	0.43
1:C:95:ALA:O	1:C:129:ASP:HA	2.18	0.43
1:C:203:LEU:C	1:C:204:VAL:HG23	2.42	0.43
1:C:436:GLN:O	1:C:436:GLN:HG3	2.17	0.43
1:B:33:GLY:N	1:B:34:PRO:CD	2.82	0.43
1:C:138:ARG:HG3	1:C:142:ARG:NH1	2.34	0.43
1:C:197:ARG:HD3	1:C:203:LEU:HD23	2.00	0.43
1:C:323:GLN:CG	1:C:348:MET:CG	2.89	0.43
1:C:326:VAL:O	1:C:351:THR:HG23	2.18	0.43
1:A:268:ASP:C	1:A:268:ASP:OD1	2.62	0.43
1:A:318:MET:HE2	1:A:345:VAL:HG21	2.00	0.43
1:B:203:LEU:O	1:B:204:VAL:HB	2.18	0.43
1:B:270:GLU:H	1:B:270:GLU:HG2	1.68	0.43
1:C:367:ALA:HA	1:C:368:PRO:HD3	1.80	0.43
1:B:310:TRP:CD1	1:B:326:VAL:HG22	2.53	0.42
1:B:370:LYS:HG3	1:B:371:ALA:N	2.34	0.42
1:B:425:ASN:OD1	1:B:425:ASN:C	2.61	0.42
1:B:18:GLU:O	1:B:22:VAL:HG23	2.19	0.42
1:B:265:TYR:CD2	1:B:309:PRO:HA	2.54	0.42
1:C:289:ARG:NH2	1:C:291:LYS:CD	2.61	0.42
1:B:332:LYS:CA	1:B:335:VAL:HG23	2.50	0.42
1:B:400:SER:O	1:B:404:GLN:CG	2.66	0.42
1:C:67:ASP:OD1	1:C:142:ARG:NH2	2.41	0.42
1:B:332:LYS:HA	1:B:335:VAL:HG23	2.02	0.42
1:B:334:ILE:HG22	1:B:335:VAL:N	2.34	0.42
1:C:17:ASP:C	1:C:19:PRO:CD	2.90	0.42
1:C:18:GLU:O	1:C:22:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:MET:HE3	1:C:51:MET:HB3	1.82	0.42
1:A:92:LEU:O	1:A:165:ASP:HB3	2.20	0.42
1:B:51:MET:HE2	1:B:51:MET:HB3	1.72	0.42
1:B:275:GLU:O	1:B:279:ASN:CG	2.61	0.42
1:C:323:GLN:O	1:C:324:ASN:C	2.62	0.42
1:C:350:THR:HG22	1:C:351:THR:O	2.20	0.42
1:B:41:GLU:HG2	1:B:42:TYR:N	2.34	0.42
1:B:203:LEU:HA	1:B:203:LEU:HD23	1.84	0.42
1:C:203:LEU:HD23	1:C:203:LEU:HA	1.83	0.42
1:C:323:GLN:CG	1:C:348:MET:HB3	2.50	0.42
1:C:360:GLN:HG3	2:C:609:HOH:O	2.19	0.42
1:A:51:MET:HE2	1:A:51:MET:HB3	1.78	0.42
1:B:136:SER:OG	1:B:139:GLU:HG3	2.20	0.42
1:A:105:PHE:CD1	1:A:105:PHE:C	2.98	0.41
1:A:41:GLU:OE1	1:A:41:GLU:N	2.35	0.41
1:C:361:GLN:HA	1:C:362:PRO:HD3	1.64	0.41
1:C:278:ILE:O	1:C:281:MET:HB2	2.20	0.41
1:A:236:ALA:HB2	1:A:310:TRP:CH2	2.56	0.41
1:B:331:ALA:O	1:B:334:ILE:HB	2.21	0.41
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.89	0.41
1:A:131:ASP:O	1:A:135:LYS:NZ	2.45	0.41
1:B:348:MET:C	1:B:350:THR:H	2.28	0.41
1:B:350:THR:CG2	1:B:354:ALA:HB3	2.51	0.41
1:C:323:GLN:OE1	1:C:348:MET:SD	2.78	0.41
1:A:356:ARG:HA	1:A:356:ARG:HD3	1.31	0.41
1:C:41:GLU:HA	1:C:44:GLU:CD	2.46	0.41
1:C:113:LYS:HZ2	1:C:370:LYS:HA	1.86	0.41
1:C:373:ASN:C	1:C:373:ASN:OD1	2.62	0.41
1:A:188:TYR:O	1:A:191:VAL:HG12	2.21	0.41
1:B:105:PHE:CD1	1:B:105:PHE:C	2.99	0.41
1:B:313:LYS:CD	1:B:337:ASN:HB3	2.51	0.41
1:C:284:MET:HE2	1:C:294:ASP:HB3	2.03	0.41
1:A:318:MET:HG2	1:A:343:ILE:HB	2.02	0.41
1:A:113:LYS:NZ	1:A:373:ASN:OD1	2.51	0.41
1:A:266:ILE:HD12	1:A:266:ILE:O	2.19	0.41
1:B:152:TYR:CG	1:B:153:ARG:N	2.88	0.41
1:B:228:LEU:HA	1:B:228:LEU:HD23	1.78	0.40
1:A:92:LEU:HA	1:A:126:GLY:O	2.22	0.40
1:A:340:LYS:O	1:A:340:LYS:HG2	2.21	0.40
1:C:99:ASN:C	1:C:99:ASN:OD1	2.64	0.40
1:C:234:ALA:HB2	1:C:314:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLU:OE1	1:B:207:GLU:N	2.47	0.40
1:B:267:TYR:HB3	1:B:302:GLN:HB2	2.04	0.40
1:B:396:GLU:CD	1:B:396:GLU:N	2.78	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	447/449 (100%)	432 (97%)	14 (3%)	1 (0%)	43	36
1	B	447/449 (100%)	424 (95%)	18 (4%)	5 (1%)	11	4
1	C	447/449 (100%)	420 (94%)	23 (5%)	4 (1%)	14	6
All	All	1341/1347 (100%)	1276 (95%)	55 (4%)	10 (1%)	18	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	290	ASN
1	B	204	VAL
1	B	310	TRP
1	B	361	GLN
1	C	289	ARG
1	A	204	VAL
1	B	329	GLU
1	B	352	ASN
1	C	204	VAL
1	C	357	PHE

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	358/358 (100%)	328 (92%)	30 (8%)	10	3
1	B	358/358 (100%)	316 (88%)	42 (12%)	5	1
1	C	358/358 (100%)	312 (87%)	46 (13%)	4	1
All	All	1074/1074 (100%)	956 (89%)	118 (11%)	6	1

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	12	GLU
1	A	13	LYS
1	A	23	GLN
1	A	35	VAL
1	A	73	VAL
1	A	81	PHE
1	A	105	PHE
1	A	116	LEU
1	A	181	ARG
1	A	184	VAL
1	A	222	LYS
1	A	255	LYS
1	A	266	ILE
1	A	283	GLU
1	A	285	ARG
1	A	298	LYS
1	A	302	GLN
1	A	323	GLN
1	A	328	LEU
1	A	348	MET
1	A	356	ARG
1	A	359	MET
1	A	370	LYS
1	A	391	LEU
1	A	396	GLU

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Mol	Chain	Res	Type
1	A	401	LYS
1	A	404	GLN
1	A	418	GLU
1	A	447	ILE
1	B	2	LYS
1	B	8	ILE
1	B	13	LYS
1	B	26	GLU
1	B	31	SER
1	B	32	LEU
1	B	51	MET
1	B	73	VAL
1	B	81	PHE
1	B	105	PHE
1	B	116	LEU
1	B	137	ASP
1	B	197	ARG
1	B	221	MET
1	B	224	GLU
1	B	247	LYS
1	B	248	LYS
1	B	255	LYS
1	B	260	SER
1	B	270	GLU
1	B	278	ILE
1	B	279	ASN
1	B	283	GLU
1	B	294	ASP
1	B	302	GLN
1	B	304	PHE
1	B	328	LEU
1	B	333	LYS
1	B	335	VAL
1	B	337	ASN
1	B	339	VAL
1	B	348	MET
1	B	351	THR
1	B	353	GLU
1	B	363	ASN
1	B	370	LYS
1	B	400	SER
1	B	401	LYS

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Mol	Chain	Res	Type
1	B	404	GLN
1	B	418	GLU
1	B	419	ARG
1	B	436	GLN
1	C	10	GLU
1	C	13	LYS
1	C	30	SER
1	C	44	GLU
1	C	51	MET
1	C	70	LYS
1	C	73	VAL
1	C	81	PHE
1	C	105	PHE
1	C	116	LEU
1	C	166	LEU
1	C	171	ARG
1	C	184	VAL
1	C	197	ARG
1	C	205	ARG
1	C	207	GLU
1	C	221	MET
1	C	222	LYS
1	C	232	THR
1	C	255	LYS
1	C	270	GLU
1	C	275	GLU
1	C	278	ILE
1	C	279	ASN
1	C	281	MET
1	C	284	MET
1	C	285	ARG
1	C	287	SER
1	C	292	VAL
1	C	293	GLN
1	C	302	GLN
1	C	312	GLN
1	C	323	GLN
1	C	328	LEU
1	C	329	GLU
1	C	335	VAL
1	C	340	LYS
1	C	348	MET

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Mol	Chain	Res	Type
1	C	353	GLU
1	C	356	ARG
1	C	360	GLN
1	C	363	ASN
1	C	392	SER
1	C	400	SER
1	C	418	GLU
1	C	436	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	68	ASN
1	A	312	GLN
1	A	330	GLN
1	A	347	ASN
1	A	360	GLN
1	B	23	GLN
1	B	240	ASN
1	B	302	GLN
1	B	337	ASN
1	B	363	ASN
1	B	403	HIS
1	B	404	GLN
1	C	23	GLN
1	C	133	ASN
1	C	279	ASN
1	C	324	ASN
1	C	330	GLN
1	C	338	ASN
1	C	352	ASN
1	C	360	GLN
1	C	361	GLN
1	C	436	GLN

5.3.3 RNA ⓘ

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.