



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:01 AM UTC

PDB ID : 1XFH / pdb_00001xfh
Title : Structure of glutamate transporter homolog from *Pyrococcus horikoshii*
Authors : Yernool, D.; Boudker, O.; Jin, Y.; Gouaux, E.
Deposited on : 2004-09-14
Resolution : 3.50 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

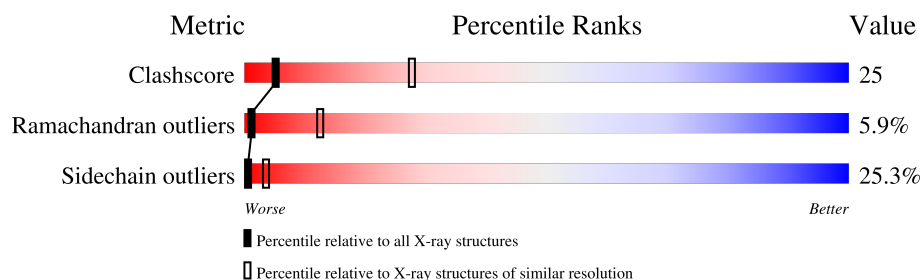
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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	422	 43% 39% 13% . .
1	B	422	 44% 40% 12% . .
1	C	422	 47% 36% 13% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8652 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 proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	1
			2884	1895	464	508	17			
1	B	406	Total	C	N	O	S	0	0	1
			2884	1895	464	508	17			
1	C	406	Total	C	N	O	S	0	0	1
			2884	1895	464	508	17			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	418	THR	-	cloning artifact	UNP O59010
A	419	LEU	-	cloning artifact	UNP O59010
A	420	VAL	-	cloning artifact	UNP O59010
A	421	PRO	-	cloning artifact	UNP O59010
A	422	ARG	-	cloning artifact	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
B	418	THR	-	cloning artifact	UNP O59010
B	419	LEU	-	cloning artifact	UNP O59010
B	420	VAL	-	cloning artifact	UNP O59010
B	421	PRO	-	cloning artifact	UNP O59010

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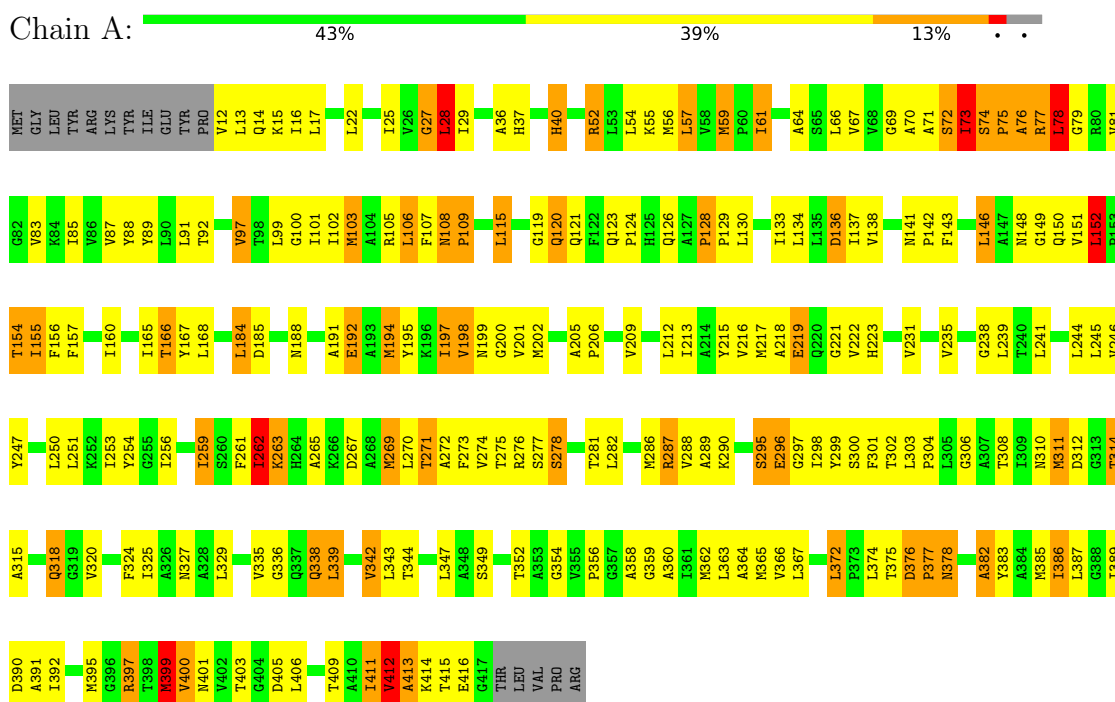
Chain	Residue	Modelled	Actual	Comment	Reference
B	422	ARG	-	cloning artifact	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	418	THR	-	cloning artifact	UNP O59010
C	419	LEU	-	cloning artifact	UNP O59010
C	420	VAL	-	cloning artifact	UNP O59010
C	421	PRO	-	cloning artifact	UNP O59010
C	422	ARG	-	cloning artifact	UNP O59010

3 Residue-property plots

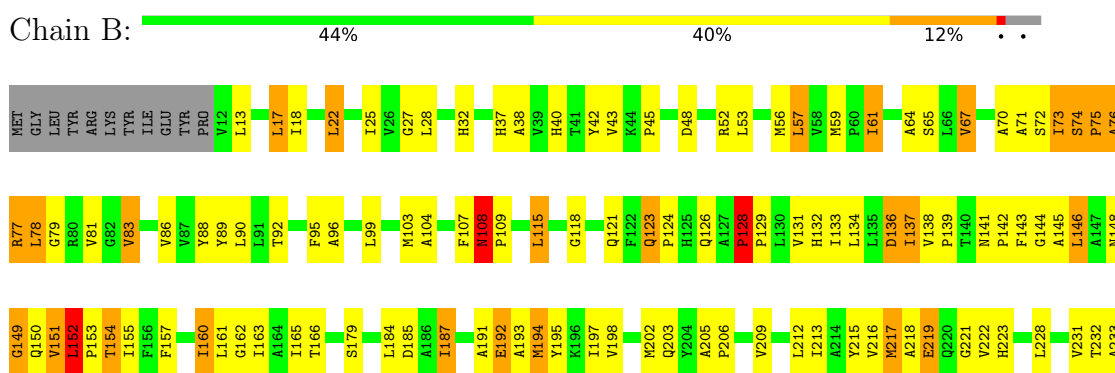
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

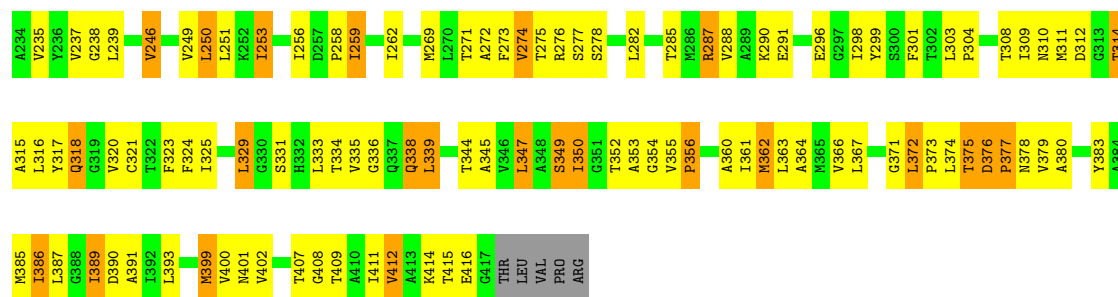
Note EDS was not executed.

- Molecule 1: proton glutamate symport protein



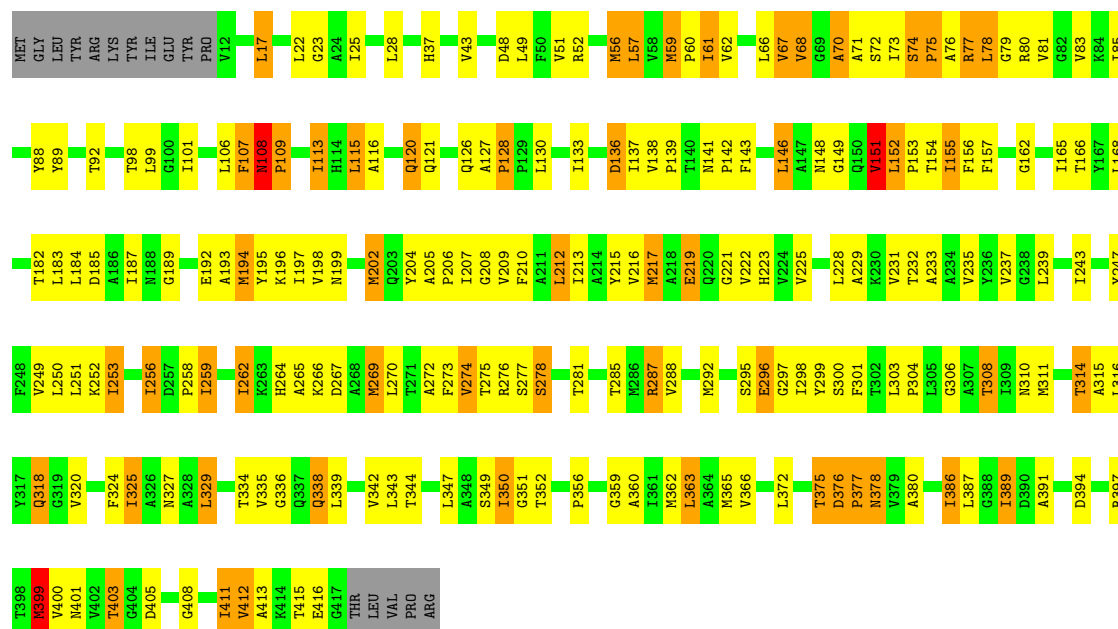
- Molecule 1: proton glutamate symport protein





- Molecule 1: proton glutamate symport protein

Chain C: 47% 36% 13% . .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	116.00Å 116.00Å 322.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.50	Depositor
% Data completeness (in resolution range)	97.1 (10.00-3.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.290 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8652	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

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	0.85	4/2937 (0.1%)	1.23	18/4019 (0.4%)
1	B	0.67	1/2937 (0.0%)	1.16	15/4019 (0.4%)
1	C	0.67	2/2937 (0.1%)	1.14	14/4019 (0.3%)
All	All	0.73	7/8811 (0.1%)	1.18	47/12057 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	GLU	C-N	-7.42	1.23	1.33
1	B	416	GLU	C-N	-7.02	1.23	1.33
1	C	416	GLU	C-N	-6.97	1.23	1.33
1	A	311	MET	SD-CE	-5.64	1.65	1.79
1	A	73	ILE	CA-CB	5.59	1.62	1.54
1	A	399	MET	CA-C	-5.21	1.49	1.52
1	C	59	MET	SD-CE	-5.03	1.67	1.79

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	VAL	N-CA-C	-12.41	98.87	110.53
1	C	67	VAL	N-CA-C	-9.70	100.43	111.00
1	B	67	VAL	N-CA-C	-8.76	101.87	110.72
1	A	339	LEU	N-CA-C	-8.52	102.87	113.18
1	B	108	ASN	N-CA-C	8.13	121.46	109.42
1	C	71	ALA	N-CA-C	-7.84	101.12	111.24
1	A	149	GLY	N-CA-C	-7.65	98.31	111.47
1	A	108	ASN	N-CA-C	7.65	121.57	109.64
1	A	338	GLN	N-CA-C	-7.63	103.04	112.88
1	C	202	MET	N-CA-C	-7.46	104.43	113.97
1	A	71	ALA	N-CA-C	-7.42	99.53	111.04
1	C	108	ASN	N-CA-C	7.17	120.21	110.31
1	C	149	GLY	N-CA-C	-7.08	98.92	110.95
1	B	71	ALA	N-CA-C	-7.01	101.94	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	399	MET	N-CA-C	-6.66	102.56	111.96
1	A	358	ALA	N-CA-C	6.57	120.00	112.57
1	B	339	LEU	N-CA-C	-6.56	104.75	112.89
1	B	128	PRO	N-CA-C	6.44	118.56	110.70
1	C	278	SER	N-CA-C	-6.39	104.23	111.07
1	B	349	SER	N-CA-C	-6.37	103.24	111.02
1	A	278	SER	N-CA-C	-6.37	104.26	111.07
1	C	339	LEU	N-CA-C	-6.25	105.62	113.18
1	A	251	LEU	N-CA-C	-6.24	103.19	111.24
1	C	338	GLN	N-CA-C	-6.19	105.31	112.92
1	C	189	GLY	N-CA-C	-6.15	105.37	112.50
1	A	382	ALA	N-CA-C	-6.00	104.37	111.03
1	B	96	ALA	N-CA-C	5.88	118.45	111.33
1	B	149	GLY	N-CA-C	-5.83	101.04	110.95
1	A	413	ALA	N-CA-C	-5.65	102.91	111.56
1	B	390	ASP	N-CA-C	5.65	118.29	111.40
1	C	68	VAL	N-CA-C	-5.63	104.87	110.62
1	A	263	LYS	N-CA-C	-5.59	106.38	113.43
1	C	182	THR	N-CA-C	-5.51	104.91	111.03
1	B	338	GLN	N-CA-C	-5.43	105.87	112.88
1	A	105	ARG	N-CA-C	-5.43	106.33	113.12
1	A	133	ILE	N-CA-C	-5.37	107.55	111.90
1	B	278	SER	N-CA-C	-5.26	105.46	111.14
1	A	120	GLN	N-CA-C	5.25	121.99	110.80
1	A	70	ALA	N-CA-C	-5.20	104.43	111.55
1	B	145	ALA	N-CA-C	-5.16	105.65	111.28
1	B	409	THR	N-CA-C	-5.16	106.14	112.90
1	C	70	ALA	N-CA-C	-5.14	104.51	111.55
1	B	376	ASP	CA-C-N	5.13	126.26	119.84
1	B	376	ASP	C-N-CA	5.13	126.26	119.84
1	C	113	ILE	N-CA-C	5.10	116.25	109.37
1	A	119	GLY	N-CA-C	5.09	121.50	113.86
1	A	390	ASP	N-CA-C	5.07	117.78	111.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2884	0	2927	165	0
1	B	2884	0	2927	150	0
1	C	2884	0	2927	136	0
All	All	8652	0	8781	429	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 25.

All (429) 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:155:ILE:HD11	1:A:304:PRO:HB2	1.40	1.02
1:C:81:VAL:HG21	1:C:298:ILE:HD12	1.42	1.01
1:A:311:MET:HE1	1:A:352:THR:O	1.64	0.98
1:A:81:VAL:HG21	1:A:298:ILE:HD12	1.46	0.96
1:A:109:PRO:HB3	1:A:324:PHE:HA	1.48	0.92
1:A:138:VAL:O	1:C:52:ARG:NH1	2.03	0.92
1:A:235:VAL:HG22	1:A:320:VAL:HG11	1.53	0.91
1:B:311:MET:HE1	1:B:352:THR:O	1.72	0.90
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.53	0.88
1:B:194:MET:HE3	1:B:197:ILE:HD12	1.57	0.85
1:A:376:ASP:O	1:A:378:ASN:N	2.10	0.84
1:A:375:THR:O	1:A:377:PRO:HD3	1.77	0.83
1:A:197:ILE:HD13	1:B:160:ILE:HG22	1.62	0.82
1:B:142:PRO:O	1:B:146:LEU:HB2	1.81	0.81
1:B:362:MET:HE3	1:B:362:MET:HA	1.61	0.81
1:C:109:PRO:HB3	1:C:324:PHE:HA	1.62	0.81
1:A:56:MET:HE2	1:B:157:PHE:HD1	1.48	0.79
1:B:311:MET:HG2	1:B:401:ASN:ND2	1.97	0.78
1:A:115:LEU:HD12	1:A:115:LEU:H	1.49	0.77
1:B:52:ARG:NH1	1:C:138:VAL:O	2.18	0.77
1:B:249:VAL:O	1:B:253:ILE:HG22	1.85	0.77
1:A:198:VAL:O	1:A:202:MET:HB2	1.84	0.76
1:C:311:MET:HG2	1:C:401:ASN:ND2	2.00	0.74
1:A:265:ALA:O	1:A:269:MET:HB2	1.88	0.74
1:C:267:ASP:OD2	1:C:287:ARG:NH2	2.21	0.73
1:B:285:THR:HG22	1:B:303:LEU:HD13	1.71	0.73
1:C:273:PHE:HB2	1:C:399:MET:HG3	1.69	0.72
1:B:155:ILE:HD11	1:B:304:PRO:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:PHE:HB2	1:B:399:MET:HG3	1.71	0.72
1:A:76:ALA:O	1:A:77:ARG:C	2.32	0.72
1:C:256:ILE:O	1:C:258:PRO:HD3	1.89	0.71
1:B:235:VAL:HG22	1:B:320:VAL:HG11	1.71	0.71
1:C:262:ILE:HG22	1:C:262:ILE:O	1.88	0.71
1:A:81:VAL:HG23	1:A:412:VAL:HG12	1.71	0.71
1:C:310:ASN:HB3	1:C:405:ASP:OD1	1.91	0.70
1:A:61:ILE:HG13	1:A:194:MET:HB3	1.72	0.70
1:A:12:VAL:O	1:A:14:GLN:N	2.25	0.70
1:A:239:LEU:HB3	1:A:400:VAL:HG21	1.73	0.69
1:A:296:GLU:HA	1:A:299:TYR:CE1	2.27	0.69
1:A:83:VAL:O	1:A:87:VAL:HG23	1.93	0.69
1:C:142:PRO:O	1:C:146:LEU:HB2	1.93	0.68
1:B:325:ILE:O	1:B:329:LEU:HB2	1.93	0.68
1:C:205:ALA:O	1:C:209:VAL:HG23	1.94	0.68
1:B:317:TYR:HE1	1:B:393:LEU:HD13	1.58	0.68
1:A:136:ASP:HA	1:C:52:ARG:HH22	1.59	0.67
1:B:296:GLU:HA	1:B:299:TYR:CE1	2.28	0.67
1:C:194:MET:HE3	1:C:197:ILE:HD12	1.77	0.66
1:A:311:MET:HG2	1:A:401:ASN:ND2	2.09	0.66
1:A:363:LEU:O	1:A:366:VAL:HG12	1.95	0.66
1:C:215:TYR:CE1	1:C:219:GLU:HG3	2.30	0.66
1:A:157:PHE:HD1	1:C:56:MET:HE2	1.60	0.66
1:A:199:ASN:OD1	1:A:287:ARG:NH1	2.28	0.66
1:B:76:ALA:O	1:B:77:ARG:C	2.37	0.66
1:B:81:VAL:HG21	1:B:298:ILE:HD12	1.77	0.66
1:B:212:LEU:HB3	1:B:274:VAL:HG12	1.78	0.66
1:B:56:MET:HE2	1:C:157:PHE:HD1	1.61	0.66
1:C:76:ALA:O	1:C:77:ARG:C	2.38	0.66
1:B:256:ILE:O	1:B:258:PRO:HD3	1.96	0.66
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.30	0.65
1:C:311:MET:HE1	1:C:352:THR:O	1.96	0.65
1:A:399:MET:C	1:A:401:ASN:H	2.04	0.65
1:A:160:ILE:HG22	1:C:197:ILE:HD13	1.79	0.64
1:B:272:ALA:CB	1:B:402:VAL:HG21	2.28	0.64
1:B:61:ILE:HG13	1:B:194:MET:HB3	1.80	0.64
1:A:197:ILE:HD13	1:B:160:ILE:CG2	2.28	0.64
1:C:233:ALA:O	1:C:237:VAL:HG12	1.98	0.63
1:A:246:VAL:O	1:A:250:LEU:HB2	1.98	0.63
1:B:88:TYR:CE2	1:B:408:GLY:HA3	2.34	0.63
1:C:325:ILE:O	1:C:329:LEU:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ILE:CG2	1:A:262:ILE:O	2.47	0.62
1:A:315:ALA:HB2	1:A:349:SER:OG	1.98	0.62
1:A:78:LEU:O	1:A:81:VAL:HG12	1.99	0.62
1:A:399:MET:C	1:A:401:ASN:N	2.57	0.62
1:A:12:VAL:O	1:A:15:LYS:N	2.32	0.62
1:B:198:VAL:O	1:B:202:MET:HB2	2.00	0.62
1:B:344:THR:HB	1:B:366:VAL:HG23	1.80	0.62
1:A:52:ARG:NH1	1:B:138:VAL:O	2.32	0.62
1:A:74:SER:HB3	1:A:75:PRO:HD3	1.82	0.62
1:A:136:ASP:HA	1:C:52:ARG:NH2	2.14	0.62
1:B:362:MET:HA	1:B:362:MET:CE	2.30	0.61
1:B:195:TYR:O	1:B:198:VAL:HG12	2.00	0.61
1:C:139:PRO:HG3	1:C:153:PRO:HB3	1.82	0.61
1:C:296:GLU:HA	1:C:299:TYR:CE1	2.35	0.61
1:B:363:LEU:O	1:B:366:VAL:HG12	2.01	0.61
1:A:304:PRO:C	1:A:306:GLY:H	2.07	0.61
1:C:89:TYR:CD2	1:C:310:ASN:HB2	2.34	0.61
1:C:265:ALA:O	1:C:269:MET:HB2	2.00	0.61
1:B:81:VAL:HG21	1:B:298:ILE:HG23	1.83	0.61
1:C:295:SER:C	1:C:297:GLY:H	2.08	0.60
1:C:198:VAL:O	1:C:202:MET:HB2	2.01	0.60
1:C:336:GLY:H	1:C:338:GLN:HE21	1.46	0.60
1:B:205:ALA:O	1:B:209:VAL:HG23	2.02	0.60
1:C:249:VAL:O	1:C:253:ILE:HG22	2.02	0.60
1:A:362:MET:HE3	1:A:362:MET:HA	1.83	0.60
1:A:399:MET:O	1:A:401:ASN:N	2.35	0.60
1:B:104:ALA:O	1:B:109:PRO:HD3	2.01	0.60
1:A:221:GLY:C	1:A:223:HIS:H	2.10	0.59
1:B:325:ILE:HG21	1:B:379:VAL:HG13	1.84	0.59
1:C:221:GLY:C	1:C:223:HIS:H	2.10	0.59
1:A:275:THR:HG22	1:A:277:SER:H	1.66	0.59
1:A:352:THR:CG2	1:A:359:GLY:HA2	2.33	0.59
1:A:336:GLY:H	1:A:338:GLN:HE21	1.50	0.59
1:B:52:ARG:NH2	1:C:136:ASP:HA	2.17	0.59
1:C:376:ASP:O	1:C:378:ASN:N	2.33	0.59
1:C:141:ASN:OD1	1:C:143:PHE:HB2	2.03	0.59
1:A:102:ILE:HG22	1:A:106:LEU:HD11	1.85	0.58
1:B:74:SER:HB3	1:B:75:PRO:HD3	1.84	0.58
1:B:233:ALA:O	1:B:237:VAL:HG12	2.04	0.58
1:A:56:MET:HE2	1:B:157:PHE:CD1	2.35	0.58
1:A:198:VAL:HG13	1:A:287:ARG:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PRO:O	1:A:146:LEU:HB2	2.04	0.58
1:B:407:THR:O	1:B:411:ILE:HG12	2.03	0.58
1:C:318:GLN:HG2	1:C:366:VAL:HG11	1.85	0.57
1:B:192:GLU:HB3	1:C:168:LEU:HD11	1.86	0.57
1:A:89:TYR:CG	1:A:310:ASN:HB2	2.39	0.57
1:C:231:VAL:HG21	1:C:324:PHE:CD1	2.38	0.57
1:B:209:VAL:HG13	1:B:274:VAL:HG21	1.87	0.57
1:A:195:TYR:O	1:A:198:VAL:HG12	2.04	0.57
1:A:352:THR:HG23	1:A:359:GLY:HA2	1.87	0.57
1:B:231:VAL:O	1:B:235:VAL:HG23	2.05	0.56
1:A:235:VAL:HG22	1:A:320:VAL:CG1	2.33	0.56
1:B:273:PHE:HB2	1:B:399:MET:CG	2.35	0.56
1:C:139:PRO:HG3	1:C:153:PRO:CB	2.35	0.56
1:C:195:TYR:O	1:C:198:VAL:HG12	2.06	0.56
1:C:61:ILE:HG13	1:C:194:MET:HB3	1.85	0.56
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.41	0.56
1:B:162:GLY:O	1:B:165:ILE:N	2.39	0.56
1:B:317:TYR:CE1	1:B:393:LEU:HD13	2.38	0.56
1:C:221:GLY:O	1:C:223:HIS:N	2.32	0.56
1:B:52:ARG:HH22	1:C:136:ASP:HA	1.71	0.55
1:A:52:ARG:NH2	1:B:136:ASP:HA	2.21	0.55
1:A:318:GLN:HG2	1:A:366:VAL:HG11	1.86	0.55
1:C:78:LEU:O	1:C:81:VAL:HG12	2.06	0.55
1:B:251:LEU:O	1:B:256:ILE:HG22	2.05	0.55
1:B:408:GLY:O	1:B:412:VAL:HG23	2.06	0.55
1:B:272:ALA:HB2	1:B:402:VAL:HG21	1.89	0.55
1:B:275:THR:O	1:B:276:ARG:HB2	2.07	0.55
1:B:221:GLY:C	1:B:223:HIS:H	2.16	0.54
1:B:139:PRO:HG3	1:B:153:PRO:HB3	1.90	0.54
1:C:262:ILE:O	1:C:262:ILE:CG2	2.56	0.54
1:C:107:PHE:HD1	1:C:237:VAL:HG11	1.73	0.54
1:C:199:ASN:OD1	1:C:287:ARG:NH1	2.41	0.54
1:B:139:PRO:HG3	1:B:153:PRO:CB	2.38	0.54
1:B:134:LEU:O	1:B:137:ILE:HB	2.07	0.54
1:C:81:VAL:HG23	1:C:412:VAL:HG12	1.90	0.54
1:A:363:LEU:O	1:A:366:VAL:CG1	2.55	0.54
1:C:155:ILE:HG22	1:C:156:PHE:N	2.23	0.54
1:A:310:ASN:HB3	1:A:405:ASP:OD1	2.08	0.54
1:A:301:PHE:CG	1:A:301:PHE:O	2.61	0.53
1:A:336:GLY:H	1:A:338:GLN:NE2	2.05	0.53
1:C:311:MET:HB3	1:C:314:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:PHE:HZ	1:B:338:GLN:OE1	1.91	0.53
1:A:200:GLY:C	1:A:202:MET:H	2.16	0.53
1:A:81:VAL:HG23	1:A:412:VAL:CG1	2.38	0.53
1:B:141:ASN:OD1	1:B:143:PHE:HB2	2.09	0.53
1:A:267:ASP:OD2	1:A:287:ARG:NH2	2.38	0.53
1:B:272:ALA:HB1	1:B:402:VAL:HG21	1.91	0.53
1:B:275:THR:HG22	1:B:277:SER:H	1.74	0.53
1:C:275:THR:O	1:C:276:ARG:HB2	2.08	0.52
1:C:205:ALA:N	1:C:206:PRO:HD2	2.24	0.52
1:C:228:LEU:HD22	1:C:389:ILE:HG12	1.91	0.52
1:A:360:ALA:O	1:A:363:LEU:HB3	2.09	0.52
1:B:92:THR:HB	1:B:312:ASP:OD2	2.09	0.52
1:A:205:ALA:O	1:A:209:VAL:HG23	2.10	0.52
1:B:74:SER:CB	1:B:75:PRO:HD3	2.39	0.52
1:B:76:ALA:O	1:B:79:GLY:N	2.42	0.52
1:C:76:ALA:O	1:C:80:ARG:N	2.36	0.52
1:C:109:PRO:HB3	1:C:324:PHE:CA	2.36	0.52
1:C:231:VAL:O	1:C:235:VAL:HG23	2.09	0.52
1:C:73:ILE:O	1:C:77:ARG:HB2	2.10	0.51
1:C:235:VAL:HG22	1:C:320:VAL:HG11	1.91	0.51
1:A:235:VAL:O	1:A:239:LEU:HG	2.10	0.51
1:A:76:ALA:O	1:A:78:LEU:N	2.43	0.51
1:C:23:GLY:HA2	1:C:210:PHE:CD2	2.45	0.51
1:A:74:SER:CB	1:A:75:PRO:HD3	2.40	0.51
1:B:275:THR:HG22	1:B:277:SER:HB3	1.93	0.51
1:C:165:ILE:HG21	1:C:184:LEU:HB2	1.93	0.51
1:B:103:MET:HE3	1:B:238:GLY:HA2	1.92	0.51
1:B:309:ILE:HG23	1:B:350:ILE:HG23	1.93	0.51
1:C:247:TYR:O	1:C:251:LEU:HG	2.11	0.51
1:A:40:HIS:ND1	1:A:40:HIS:O	2.44	0.51
1:B:79:GLY:O	1:B:83:VAL:HG23	2.10	0.51
1:B:77:ARG:O	1:B:81:VAL:HG12	2.11	0.51
1:C:225:VAL:HA	1:C:229:ALA:HB2	1.92	0.50
1:A:295:SER:C	1:A:297:GLY:H	2.19	0.50
1:B:88:TYR:O	1:B:92:THR:HG23	2.10	0.50
1:A:231:VAL:O	1:A:235:VAL:HG23	2.11	0.50
1:B:275:THR:CG2	1:B:277:SER:HB3	2.42	0.50
1:B:345:ALA:O	1:B:349:SER:OG	2.26	0.50
1:A:89:TYR:CD2	1:A:310:ASN:HB2	2.46	0.50
1:A:194:MET:HE1	1:B:157:PHE:HE1	1.75	0.50
1:B:371:GLY:O	1:B:373:PRO:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:O	1:A:103:MET:HB2	2.11	0.50
1:A:36:ALA:HB1	1:A:219:GLU:HG2	1.93	0.50
1:A:109:PRO:CB	1:A:324:PHE:HA	2.31	0.50
1:A:28:LEU:HD13	1:A:217:MET:HG3	1.94	0.49
1:B:131:VAL:C	1:B:133:ILE:H	2.20	0.49
1:C:360:ALA:O	1:C:363:LEU:HB3	2.12	0.49
1:A:194:MET:HE3	1:A:197:ILE:HD12	1.94	0.49
1:C:109:PRO:HA	1:C:231:VAL:HG22	1.93	0.49
1:C:193:ALA:O	1:C:197:ILE:HG13	2.13	0.49
1:A:271:THR:HG22	1:A:281:THR:HG23	1.93	0.49
1:A:271:THR:CG2	1:A:281:THR:HG23	2.43	0.49
1:A:254:TYR:CD2	1:A:411:ILE:HG23	2.48	0.49
1:B:165:ILE:HG21	1:B:184:LEU:HB2	1.93	0.48
1:B:361:ILE:C	1:B:363:LEU:H	2.20	0.48
1:C:209:VAL:HG22	1:C:274:VAL:HG21	1.94	0.48
1:C:79:GLY:O	1:C:83:VAL:HG23	2.13	0.48
1:A:59:MET:HE3	1:A:154:THR:HG21	1.94	0.48
1:A:191:ALA:O	1:A:195:TYR:HD1	1.96	0.48
1:C:61:ILE:CG2	1:C:62:VAL:N	2.76	0.48
1:B:149:GLY:O	1:B:150:GLN:HB2	2.12	0.48
1:B:360:ALA:O	1:B:363:LEU:HB3	2.14	0.48
1:C:239:LEU:HD22	1:C:400:VAL:HG21	1.95	0.48
1:B:81:VAL:HG23	1:B:412:VAL:CG1	2.43	0.48
1:B:269:MET:HG2	1:B:399:MET:SD	2.54	0.48
1:A:184:LEU:O	1:A:184:LEU:HG	2.12	0.48
1:C:109:PRO:CB	1:C:324:PHE:HA	2.37	0.48
1:C:301:PHE:CG	1:C:301:PHE:O	2.67	0.48
1:B:318:GLN:HG2	1:B:366:VAL:HG11	1.94	0.47
1:B:18:ILE:O	1:B:22:LEU:HB3	2.14	0.47
1:A:61:ILE:HG23	1:A:286:MET:HE1	1.96	0.47
1:A:97:VAL:O	1:A:100:GLY:N	2.43	0.47
1:B:108:ASN:HA	1:B:109:PRO:HD3	1.79	0.47
1:C:295:SER:C	1:C:297:GLY:N	2.73	0.47
1:A:200:GLY:O	1:A:202:MET:N	2.48	0.47
1:A:259:ILE:H	1:A:259:ILE:HG13	1.39	0.47
1:A:275:THR:O	1:A:276:ARG:HB2	2.15	0.47
1:B:70:ALA:HB3	1:B:162:GLY:HA3	1.97	0.47
1:B:228:LEU:O	1:B:232:THR:N	2.30	0.47
1:C:216:VAL:HG13	1:C:391:ALA:HB1	1.97	0.47
1:C:362:MET:HE2	1:C:365:MET:SD	2.55	0.47
1:C:377:PRO:HA	1:C:380:ALA:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:VAL:HG13	1:B:287:ARG:HD3	1.97	0.47
1:A:54:LEU:C	1:A:56:MET:N	2.73	0.47
1:B:331:SER:C	1:B:333:LEU:H	2.23	0.47
1:B:205:ALA:N	1:B:206:PRO:HD2	2.30	0.47
1:B:376:ASP:O	1:B:378:ASN:N	2.48	0.47
1:B:217:MET:C	1:B:219:GLU:H	2.23	0.46
1:C:74:SER:HB3	1:C:75:PRO:HD3	1.97	0.46
1:C:315:ALA:HB2	1:C:349:SER:OG	2.15	0.46
1:A:150:GLN:C	1:A:152:LEU:H	2.23	0.46
1:B:141:ASN:O	1:B:142:PRO:C	2.58	0.46
1:B:78:LEU:HD22	1:B:78:LEU:HA	1.71	0.46
1:C:259:ILE:H	1:C:259:ILE:HG13	1.53	0.46
1:C:151:VAL:HA	1:C:154:THR:HG22	1.96	0.46
1:A:61:ILE:HG23	1:A:286:MET:CE	2.45	0.46
1:A:272:ALA:HB2	1:A:281:THR:HG21	1.97	0.46
1:B:78:LEU:HA	1:B:81:VAL:HG12	1.96	0.46
1:C:231:VAL:O	1:C:232:THR:C	2.59	0.46
1:C:275:THR:HG22	1:C:277:SER:H	1.79	0.46
1:B:27:GLY:O	1:B:218:ALA:HB2	2.15	0.46
1:B:95:PHE:HE2	1:B:99:LEU:HD22	1.80	0.46
1:C:351:GLY:O	1:C:352:THR:C	2.59	0.46
1:C:386:ILE:HD13	1:C:386:ILE:HA	1.82	0.46
1:A:156:PHE:HE2	1:C:56:MET:HE1	1.81	0.46
1:A:197:ILE:O	1:A:199:ASN:N	2.49	0.46
1:A:406:LEU:O	1:A:409:THR:N	2.49	0.46
1:B:315:ALA:HB2	1:B:349:SER:OG	2.16	0.46
1:C:127:ALA:HA	1:C:128:PRO:HD2	1.84	0.46
1:B:386:ILE:O	1:B:389:ILE:HG13	2.15	0.46
1:C:151:VAL:HA	1:C:154:THR:CG2	2.46	0.46
1:A:194:MET:HE1	1:B:157:PHE:CE1	2.51	0.46
1:C:76:ALA:O	1:C:79:GLY:N	2.49	0.46
1:B:56:MET:HE1	1:C:156:PHE:CE2	2.51	0.45
1:B:128:PRO:HA	1:B:129:PRO:HD3	1.83	0.45
1:C:217:MET:C	1:C:219:GLU:H	2.23	0.45
1:A:197:ILE:O	1:A:200:GLY:N	2.49	0.45
1:C:81:VAL:HG23	1:C:412:VAL:CG1	2.47	0.45
1:C:221:GLY:C	1:C:223:HIS:N	2.74	0.45
1:A:262:ILE:O	1:A:262:ILE:HG22	2.14	0.45
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.81	0.45
1:C:23:GLY:CA	1:C:210:PHE:HD2	2.30	0.45
1:B:314:THR:O	1:B:318:GLN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:SER:CB	1:C:75:PRO:HD3	2.46	0.45
1:A:273:PHE:HB2	1:A:399:MET:HG3	1.98	0.45
1:A:73:ILE:O	1:A:77:ARG:HB2	2.17	0.45
1:A:130:LEU:O	1:A:134:LEU:HG	2.17	0.45
1:A:298:ILE:C	1:A:300:SER:H	2.25	0.45
1:A:205:ALA:N	1:A:206:PRO:HD2	2.31	0.45
1:C:17:LEU:HD22	1:C:270:LEU:HD11	1.99	0.45
1:C:194:MET:CE	1:C:197:ILE:HD12	2.45	0.45
1:A:195:TYR:O	1:A:199:ASN:ND2	2.50	0.45
1:B:246:VAL:O	1:B:250:LEU:HB2	2.16	0.45
1:B:239:LEU:HD23	1:B:316:LEU:HD22	1.98	0.44
1:B:336:GLY:H	1:B:338:GLN:HE21	1.65	0.44
1:C:85:ILE:HA	1:C:88:TYR:HB3	1.98	0.44
1:A:141:ASN:OD1	1:A:143:PHE:HB2	2.16	0.44
1:A:166:THR:HG22	1:A:167:TYR:HD1	1.82	0.44
1:A:304:PRO:C	1:A:306:GLY:N	2.74	0.44
1:B:375:THR:O	1:B:377:PRO:HD3	2.17	0.44
1:A:88:TYR:O	1:A:92:THR:HG23	2.16	0.44
1:A:188:ASN:O	1:A:192:GLU:HB2	2.17	0.44
1:A:391:ALA:O	1:A:395:MET:HG3	2.18	0.44
1:C:295:SER:O	1:C:297:GLY:N	2.50	0.44
1:B:40:HIS:HB2	1:B:215:TYR:HE1	1.81	0.44
1:B:67:VAL:HB	1:B:187:ILE:HG21	1.99	0.44
1:C:394:ASP:O	1:C:397:ARG:HG3	2.17	0.44
1:C:285:THR:HG22	1:C:303:LEU:HD13	1.98	0.44
1:A:156:PHE:CE2	1:C:56:MET:HE1	2.52	0.44
1:A:261:PHE:C	1:A:263:LYS:H	2.25	0.44
1:B:27:GLY:C	1:B:218:ALA:HB2	2.42	0.44
1:A:197:ILE:O	1:A:198:VAL:C	2.61	0.44
1:A:311:MET:HB3	1:A:314:THR:HB	2.00	0.44
1:B:377:PRO:HA	1:B:380:ALA:HB3	2.00	0.44
1:C:85:ILE:HB	1:C:412:VAL:HG21	2.00	0.44
1:B:152:LEU:CB	1:B:153:PRO:HD3	2.48	0.44
1:C:264:HIS:C	1:C:266:LYS:H	2.25	0.44
1:A:40:HIS:ND1	1:A:40:HIS:C	2.75	0.43
1:A:363:LEU:HD12	1:A:366:VAL:CG1	2.48	0.43
1:A:411:ILE:C	1:A:413:ALA:H	2.25	0.43
1:A:217:MET:C	1:A:219:GLU:H	2.26	0.43
1:A:314:THR:HG22	1:A:315:ALA:N	2.33	0.43
1:B:57:LEU:O	1:B:61:ILE:HB	2.18	0.43
1:C:59:MET:CE	1:C:154:THR:HG21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LEU:HD13	1:C:300:SER:CB	2.48	0.43
1:A:78:LEU:HD22	1:A:78:LEU:HA	1.82	0.43
1:B:88:TYR:CZ	1:B:92:THR:HG21	2.53	0.43
1:B:152:LEU:HB3	1:B:153:PRO:HD3	2.00	0.43
1:C:108:ASN:HA	1:C:109:PRO:HD3	1.85	0.43
1:C:89:TYR:CD2	1:C:310:ASN:CB	3.02	0.43
1:C:349:SER:O	1:C:350:ILE:C	2.62	0.43
1:A:40:HIS:C	1:A:40:HIS:HD1	2.26	0.43
1:A:103:MET:HE1	1:A:241:LEU:HD22	2.00	0.43
1:A:200:GLY:C	1:A:202:MET:N	2.77	0.43
1:A:221:GLY:C	1:A:223:HIS:N	2.75	0.43
1:B:45:PRO:HA	1:B:48:ASP:HB2	2.00	0.43
1:A:374:LEU:HD11	1:A:383:TYR:CG	2.53	0.43
1:B:301:PHE:O	1:B:301:PHE:CG	2.72	0.43
1:A:215:TYR:O	1:A:216:VAL:C	2.61	0.43
1:B:161:LEU:O	1:B:165:ILE:HG13	2.19	0.43
1:B:231:VAL:HG21	1:B:324:PHE:CD1	2.53	0.43
1:B:57:LEU:H	1:B:57:LEU:HG	1.58	0.43
1:B:77:ARG:O	1:B:81:VAL:N	2.41	0.43
1:C:411:ILE:C	1:C:413:ALA:N	2.77	0.43
1:B:38:ALA:O	1:B:42:TYR:HB2	2.19	0.43
1:C:99:LEU:HD12	1:C:99:LEU:O	2.19	0.43
1:A:289:ALA:HB2	1:A:303:LEU:HD11	2.01	0.42
1:A:314:THR:HA	1:A:397:ARG:HD3	2.01	0.42
1:A:325:ILE:C	1:A:327:ASN:H	2.27	0.42
1:A:325:ILE:HG12	1:A:382:ALA:HB3	2.01	0.42
1:B:399:MET:C	1:B:401:ASN:N	2.77	0.42
1:A:85:ILE:HD13	1:A:302:THR:HB	2.01	0.42
1:A:265:ALA:O	1:A:269:MET:HE3	2.19	0.42
1:A:386:ILE:HD13	1:A:386:ILE:HA	1.72	0.42
1:C:81:VAL:CG2	1:C:298:ILE:HD12	2.30	0.42
1:A:352:THR:HG21	1:A:359:GLY:HA2	2.01	0.42
1:A:298:ILE:C	1:A:300:SER:N	2.76	0.42
1:A:325:ILE:C	1:A:327:ASN:N	2.78	0.42
1:B:355:VAL:O	1:B:356:PRO:C	2.63	0.42
1:C:23:GLY:HA2	1:C:210:PHE:HD2	1.84	0.42
1:C:59:MET:HE3	1:C:154:THR:HG21	2.02	0.42
1:C:306:GLY:C	1:C:308:THR:H	2.26	0.42
1:A:270:LEU:O	1:A:271:THR:C	2.63	0.42
1:A:311:MET:CE	1:A:352:THR:O	2.50	0.42
1:B:89:TYR:CD2	1:B:310:ASN:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LEU:HA	1:B:373:PRO:HD3	1.82	0.42
1:A:78:LEU:O	1:A:79:GLY:C	2.63	0.42
1:B:141:ASN:O	1:B:144:GLY:N	2.52	0.42
1:B:154:THR:CG2	1:B:155:ILE:N	2.82	0.42
1:B:275:THR:C	1:B:277:SER:H	2.27	0.42
1:C:399:MET:C	1:C:401:ASN:H	2.28	0.42
1:B:64:ALA:HB1	1:B:191:ALA:HB2	2.02	0.42
1:B:73:ILE:O	1:B:74:SER:C	2.62	0.42
1:B:349:SER:O	1:B:350:ILE:C	2.63	0.42
1:A:108:ASN:HA	1:A:109:PRO:HD3	1.88	0.42
1:B:374:LEU:HD11	1:B:383:TYR:CG	2.55	0.42
1:A:57:LEU:H	1:A:57:LEU:HG	1.61	0.41
1:B:40:HIS:HB2	1:B:215:TYR:CE1	2.55	0.41
1:B:216:VAL:HG13	1:B:391:ALA:HB1	2.01	0.41
1:A:73:ILE:O	1:A:74:SER:C	2.63	0.41
1:A:74:SER:CB	1:A:75:PRO:CD	2.97	0.41
1:B:152:LEU:O	1:B:155:ILE:HB	2.21	0.41
1:B:193:ALA:O	1:B:197:ILE:HG13	2.19	0.41
1:A:64:ALA:C	1:A:66:LEU:H	2.28	0.41
1:A:76:ALA:O	1:A:79:GLY:N	2.53	0.41
1:A:191:ALA:O	1:A:195:TYR:CD1	2.73	0.41
1:A:197:ILE:C	1:A:199:ASN:N	2.77	0.41
1:A:339:LEU:HA	1:A:342:VAL:HB	2.03	0.41
1:B:353:ALA:O	1:B:355:VAL:N	2.49	0.41
1:C:51:VAL:HG13	1:C:275:THR:HG23	2.02	0.41
1:C:375:THR:O	1:C:377:PRO:HD3	2.20	0.41
1:A:344:THR:HG21	1:A:366:VAL:HA	2.03	0.41
1:A:364:ALA:O	1:A:367:LEU:HB2	2.20	0.41
1:B:138:VAL:HA	1:B:139:PRO:HD3	1.90	0.41
1:C:67:VAL:HB	1:C:187:ILE:HG21	2.01	0.41
1:A:52:ARG:HH22	1:B:136:ASP:HA	1.85	0.41
1:A:123:GLN:HA	1:A:124:PRO:HD3	1.81	0.41
1:A:128:PRO:HA	1:A:129:PRO:HD3	1.70	0.41
1:A:247:TYR:OH	1:A:312:ASP:OD2	2.35	0.41
1:A:296:GLU:HG3	1:A:299:TYR:OH	2.21	0.41
1:A:304:PRO:O	1:A:306:GLY:N	2.53	0.41
1:B:123:GLN:HA	1:B:124:PRO:HD3	1.74	0.41
1:C:269:MET:HE2	1:C:403:THR:OG1	2.21	0.41
1:A:103:MET:HG2	1:A:238:GLY:CA	2.50	0.41
1:A:165:ILE:O	1:A:168:LEU:HB2	2.21	0.41
1:B:70:ALA:CB	1:B:162:GLY:HA3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:LEU:HA	1:B:350:ILE:HD12	2.01	0.41
1:C:66:LEU:HD13	1:C:300:SER:C	2.46	0.41
1:B:53:LEU:HD23	1:B:53:LEU:HA	1.88	0.41
1:B:259:ILE:H	1:B:259:ILE:HG13	1.54	0.41
1:C:48:ASP:O	1:C:49:LEU:C	2.62	0.41
1:C:130:LEU:HA	1:C:133:ILE:HD12	2.02	0.41
1:A:221:GLY:O	1:A:223:HIS:N	2.48	0.41
1:C:195:TYR:O	1:C:196:LYS:C	2.62	0.41
1:C:272:ALA:HB2	1:C:281:THR:HG21	2.01	0.41
1:C:316:LEU:O	1:C:320:VAL:HG12	2.21	0.41
1:C:327:ASN:C	1:C:329:LEU:H	2.29	0.41
1:A:66:LEU:HD13	1:A:300:SER:CB	2.50	0.41
1:A:295:SER:C	1:A:297:GLY:N	2.79	0.41
1:A:372:LEU:H	1:A:372:LEU:HG	1.72	0.41
1:B:40:HIS:ND1	1:B:40:HIS:C	2.79	0.41
1:B:364:ALA:HA	1:B:367:LEU:HB2	2.03	0.41
1:C:204:TYR:C	1:C:206:PRO:HD2	2.46	0.41
1:C:208:GLY:O	1:C:212:LEU:HB2	2.21	0.41
1:A:27:GLY:O	1:A:29:ILE:N	2.54	0.41
1:A:57:LEU:O	1:A:61:ILE:HB	2.21	0.40
1:B:239:LEU:HD22	1:B:400:VAL:HG21	2.02	0.40
1:C:70:ALA:HB3	1:C:162:GLY:HA3	2.04	0.40
1:C:197:ILE:C	1:C:199:ASN:N	2.78	0.40
1:B:13:LEU:O	1:B:17:LEU:HB2	2.21	0.40
1:B:162:GLY:O	1:B:163:ILE:C	2.63	0.40
1:C:352:THR:HG23	1:C:359:GLY:HA2	2.02	0.40
1:C:399:MET:C	1:C:401:ASN:N	2.76	0.40
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.81	0.40
1:B:81:VAL:HG23	1:B:412:VAL:HG12	2.04	0.40
1:C:57:LEU:O	1:C:60:PRO:HD2	2.20	0.40
1:C:88:TYR:CE2	1:C:408:GLY:HA3	2.57	0.40
1:C:411:ILE:C	1:C:413:ALA:H	2.29	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	404/422 (96%)	301 (74%)	69 (17%)	34 (8%)	0	7
1	B	404/422 (96%)	316 (78%)	70 (17%)	18 (4%)	2	17
1	C	404/422 (96%)	311 (77%)	74 (18%)	19 (5%)	2	17
All	All	1212/1266 (96%)	928 (77%)	213 (18%)	71 (6%)	1	12

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	75	PRO
1	A	76	ALA
1	A	77	ARG
1	A	356	PRO
1	A	377	PRO
1	B	77	ARG
1	C	77	ARG
1	C	116	ALA
1	C	222	VAL
1	C	296	GLU
1	C	377	PRO
1	A	28	LEU
1	A	151	VAL
1	A	201	VAL
1	A	218	ALA
1	A	222	VAL
1	A	354	GLY
1	A	415	THR
1	B	76	ALA
1	B	115	LEU
1	B	118	GLY
1	B	151	VAL
1	B	222	VAL
1	B	377	PRO
1	B	415	THR
1	C	109	PRO
1	C	115	LEU
1	C	262	ILE
1	C	356	PRO

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Mol	Chain	Res	Type
1	C	415	THR
1	A	72	SER
1	A	73	ILE
1	A	109	PRO
1	A	128	PRO
1	A	152	LEU
1	A	245	LEU
1	B	75	PRO
1	B	132	HIS
1	B	152	LEU
1	B	356	PRO
1	C	151	VAL
1	A	55	LYS
1	A	74	SER
1	A	78	LEU
1	A	244	LEU
1	B	128	PRO
1	B	335	VAL
1	B	350	ILE
1	C	74	SER
1	C	120	GLN
1	C	152	LEU
1	A	198	VAL
1	A	296	GLU
1	A	400	VAL
1	B	73	ILE
1	B	74	SER
1	B	354	GLY
1	C	75	PRO
1	C	128	PRO
1	C	376	ASP
1	A	120	GLN
1	A	335	VAL
1	C	350	ILE
1	A	69	GLY
1	A	262	ILE
1	A	376	ASP
1	A	412	VAL
1	A	389	ILE
1	A	27	GLY
1	C	335	VAL

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	279/330 (84%)	209 (75%)	70 (25%)	0	4
1	B	279/330 (84%)	209 (75%)	70 (25%)	0	4
1	C	279/330 (84%)	207 (74%)	72 (26%)	0	3
All	All	837/990 (84%)	625 (75%)	212 (25%)	0	3

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	17	LEU
1	A	22	LEU
1	A	25	ILE
1	A	28	LEU
1	A	37	HIS
1	A	40	HIS
1	A	52	ARG
1	A	57	LEU
1	A	59	MET
1	A	61	ILE
1	A	72	SER
1	A	78	LEU
1	A	91	LEU
1	A	97	VAL
1	A	101	ILE
1	A	103	MET
1	A	106	LEU
1	A	107	PHE
1	A	115	LEU
1	A	121	GLN
1	A	126	GLN
1	A	136	ASP
1	A	137	ILE
1	A	146	LEU
1	A	148	ASN

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Mol	Chain	Res	Type
1	A	152	LEU
1	A	154	THR
1	A	155	ILE
1	A	166	THR
1	A	184	LEU
1	A	185	ASP
1	A	192	GLU
1	A	194	MET
1	A	197	ILE
1	A	212	LEU
1	A	213	ILE
1	A	219	GLU
1	A	253	ILE
1	A	256	ILE
1	A	259	ILE
1	A	262	ILE
1	A	269	MET
1	A	271	THR
1	A	274	VAL
1	A	278	SER
1	A	287	ARG
1	A	288	VAL
1	A	290	LYS
1	A	295	SER
1	A	308	THR
1	A	314	THR
1	A	318	GLN
1	A	329	LEU
1	A	342	VAL
1	A	343	LEU
1	A	347	LEU
1	A	365	MET
1	A	372	LEU
1	A	378	ASN
1	A	385	MET
1	A	386	ILE
1	A	387	LEU
1	A	392	ILE
1	A	397	ARG
1	A	399	MET
1	A	403	THR
1	A	411	ILE

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Mol	Chain	Res	Type
1	A	412	VAL
1	A	414	LYS
1	B	17	LEU
1	B	22	LEU
1	B	25	ILE
1	B	28	LEU
1	B	32	HIS
1	B	37	HIS
1	B	43	VAL
1	B	57	LEU
1	B	59	MET
1	B	61	ILE
1	B	65	SER
1	B	72	SER
1	B	78	LEU
1	B	83	VAL
1	B	86	VAL
1	B	90	LEU
1	B	107	PHE
1	B	108	ASN
1	B	115	LEU
1	B	121	GLN
1	B	123	GLN
1	B	126	GLN
1	B	136	ASP
1	B	137	ILE
1	B	146	LEU
1	B	148	ASN
1	B	151	VAL
1	B	152	LEU
1	B	154	THR
1	B	160	ILE
1	B	166	THR
1	B	179	SER
1	B	185	ASP
1	B	187	ILE
1	B	192	GLU
1	B	194	MET
1	B	203	GLN
1	B	213	ILE
1	B	217	MET
1	B	219	GLU

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Mol	Chain	Res	Type
1	B	246	VAL
1	B	250	LEU
1	B	253	ILE
1	B	259	ILE
1	B	262	ILE
1	B	271	THR
1	B	274	VAL
1	B	282	LEU
1	B	287	ARG
1	B	288	VAL
1	B	290	LYS
1	B	291	GLU
1	B	308	THR
1	B	314	THR
1	B	318	GLN
1	B	321	CYS
1	B	329	LEU
1	B	334	THR
1	B	339	LEU
1	B	347	LEU
1	B	362	MET
1	B	372	LEU
1	B	375	THR
1	B	385	MET
1	B	386	ILE
1	B	387	LEU
1	B	389	ILE
1	B	399	MET
1	B	412	VAL
1	B	414	LYS
1	C	17	LEU
1	C	22	LEU
1	C	25	ILE
1	C	28	LEU
1	C	37	HIS
1	C	43	VAL
1	C	56	MET
1	C	57	LEU
1	C	61	ILE
1	C	68	VAL
1	C	72	SER
1	C	78	LEU

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Mol	Chain	Res	Type
1	C	98	THR
1	C	101	ILE
1	C	106	LEU
1	C	107	PHE
1	C	108	ASN
1	C	113	ILE
1	C	115	LEU
1	C	120	GLN
1	C	121	GLN
1	C	126	GLN
1	C	136	ASP
1	C	137	ILE
1	C	146	LEU
1	C	148	ASN
1	C	151	VAL
1	C	152	LEU
1	C	155	ILE
1	C	166	THR
1	C	183	LEU
1	C	185	ASP
1	C	192	GLU
1	C	194	MET
1	C	207	ILE
1	C	212	LEU
1	C	213	ILE
1	C	217	MET
1	C	219	GLU
1	C	243	ILE
1	C	250	LEU
1	C	252	LYS
1	C	253	ILE
1	C	256	ILE
1	C	259	ILE
1	C	269	MET
1	C	274	VAL
1	C	278	SER
1	C	287	ARG
1	C	288	VAL
1	C	292	MET
1	C	308	THR
1	C	314	THR
1	C	318	GLN

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Mol	Chain	Res	Type
1	C	325	ILE
1	C	329	LEU
1	C	334	THR
1	C	342	VAL
1	C	343	LEU
1	C	344	THR
1	C	347	LEU
1	C	363	LEU
1	C	372	LEU
1	C	375	THR
1	C	378	ASN
1	C	386	ILE
1	C	387	LEU
1	C	389	ILE
1	C	399	MET
1	C	403	THR
1	C	411	ILE
1	C	412	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	223	HIS
1	A	327	ASN
1	A	338	GLN
1	A	378	ASN
1	B	40	HIS
1	B	108	ASN
1	B	123	GLN
1	B	148	ASN
1	B	310	ASN
1	B	318	GLN
1	B	327	ASN
1	B	338	GLN
1	B	378	ASN
1	C	32	HIS
1	C	126	GLN
1	C	148	ASN
1	C	223	HIS
1	C	264	HIS
1	C	310	ASN

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Mol	Chain	Res	Type
1	C	327	ASN
1	C	378	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 [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.