



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:37 PM UTC

PDB ID : 7QYF / pdb_00007qyf
Title : Structure of the transaminase PluriZyme variant (TR2E2)
Authors : Roda, S.; Fernandez-Lopez, L.; Benedens, M.; Bollinger, A.; Thies, S.; Schumacher, J.; Coscolin, C.; Kazemi, M.; Santiago, G.; Gertzen, C.G.; Gonzalez-Alfonso, J.; Plou, F.J.; Jaeger, K.E.; Smits, S.H.; Ferrer, M.; Guallar, V.
Deposited on : 2022-01-28
Resolution : 3.30 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)	:	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

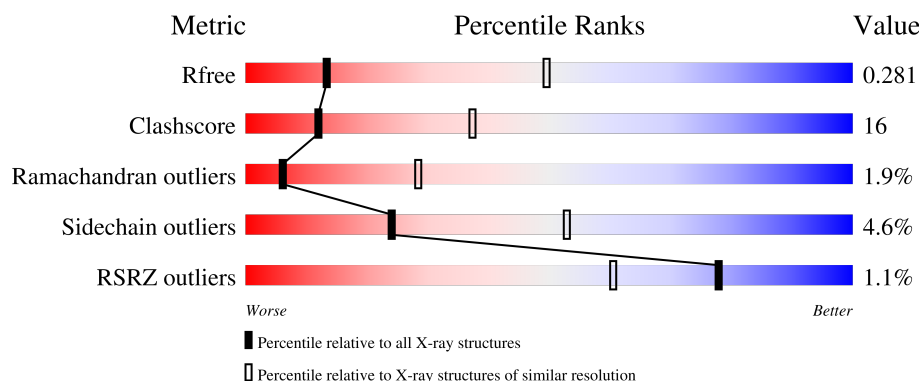
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	465	% 57% 31% 10%
1	B	465	2% 58% 31% 9%
1	C	465	% 64% 25% 10%
1	D	465	% 56% 31% 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12927 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 Aminotransferase TR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3244	2058	566	600	20			
1	B	424	Total	C	N	O	S	0	0	0
			3274	2074	572	608	20			
1	C	418	Total	C	N	O	S	0	0	0
			3229	2045	566	598	20			
1	D	412	Total	C	N	O	S	0	0	0
			3180	2017	553	591	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	SER	ALA	conflict	UNP A0A3G5BC54
A	173	HIS	GLN	conflict	UNP A0A3G5BC54
A	458	LEU	-	expression tag	UNP A0A3G5BC54
A	459	GLU	-	expression tag	UNP A0A3G5BC54
A	460	HIS	-	expression tag	UNP A0A3G5BC54
A	461	HIS	-	expression tag	UNP A0A3G5BC54
A	462	HIS	-	expression tag	UNP A0A3G5BC54
A	463	HIS	-	expression tag	UNP A0A3G5BC54
A	464	HIS	-	expression tag	UNP A0A3G5BC54
A	465	HIS	-	expression tag	UNP A0A3G5BC54
B	172	SER	ALA	conflict	UNP A0A3G5BC54
B	173	HIS	GLN	conflict	UNP A0A3G5BC54
B	458	LEU	-	expression tag	UNP A0A3G5BC54
B	459	GLU	-	expression tag	UNP A0A3G5BC54
B	460	HIS	-	expression tag	UNP A0A3G5BC54
B	461	HIS	-	expression tag	UNP A0A3G5BC54
B	462	HIS	-	expression tag	UNP A0A3G5BC54
B	463	HIS	-	expression tag	UNP A0A3G5BC54
B	464	HIS	-	expression tag	UNP A0A3G5BC54
B	465	HIS	-	expression tag	UNP A0A3G5BC54
C	172	SER	ALA	conflict	UNP A0A3G5BC54

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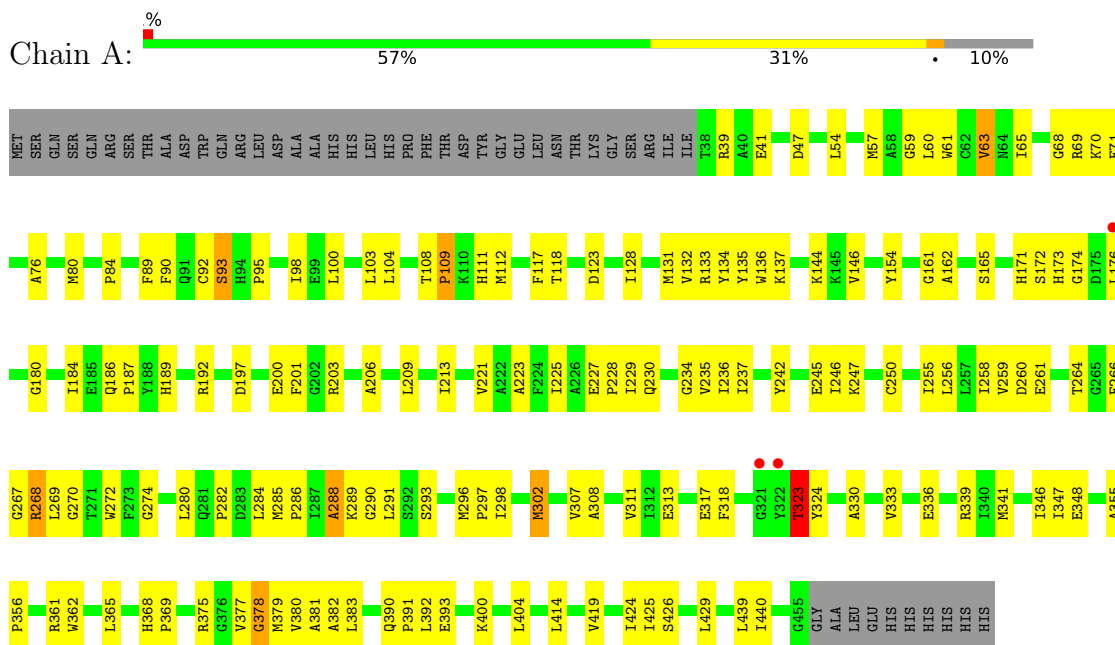
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Chain	Residue	Modelled	Actual	Comment	Reference
C	173	HIS	GLN	conflict	UNP A0A3G5BC54
C	458	LEU	-	expression tag	UNP A0A3G5BC54
C	459	GLU	-	expression tag	UNP A0A3G5BC54
C	460	HIS	-	expression tag	UNP A0A3G5BC54
C	461	HIS	-	expression tag	UNP A0A3G5BC54
C	462	HIS	-	expression tag	UNP A0A3G5BC54
C	463	HIS	-	expression tag	UNP A0A3G5BC54
C	464	HIS	-	expression tag	UNP A0A3G5BC54
C	465	HIS	-	expression tag	UNP A0A3G5BC54
D	172	SER	ALA	conflict	UNP A0A3G5BC54
D	173	HIS	GLN	conflict	UNP A0A3G5BC54
D	458	LEU	-	expression tag	UNP A0A3G5BC54
D	459	GLU	-	expression tag	UNP A0A3G5BC54
D	460	HIS	-	expression tag	UNP A0A3G5BC54
D	461	HIS	-	expression tag	UNP A0A3G5BC54
D	462	HIS	-	expression tag	UNP A0A3G5BC54
D	463	HIS	-	expression tag	UNP A0A3G5BC54
D	464	HIS	-	expression tag	UNP A0A3G5BC54
D	465	HIS	-	expression tag	UNP A0A3G5BC54

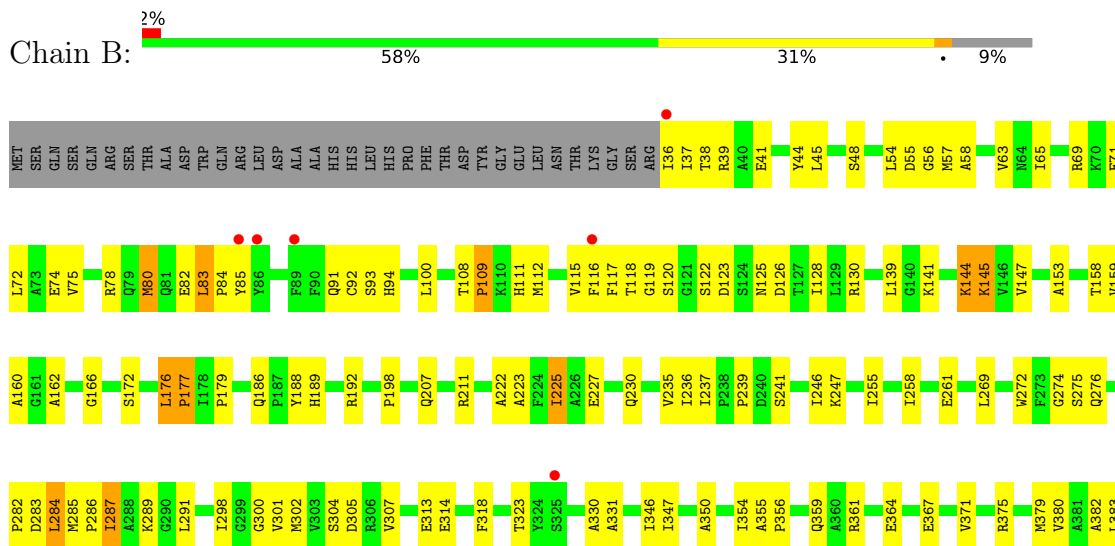
3 Residue-property plots

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: Aminotransferase TR2

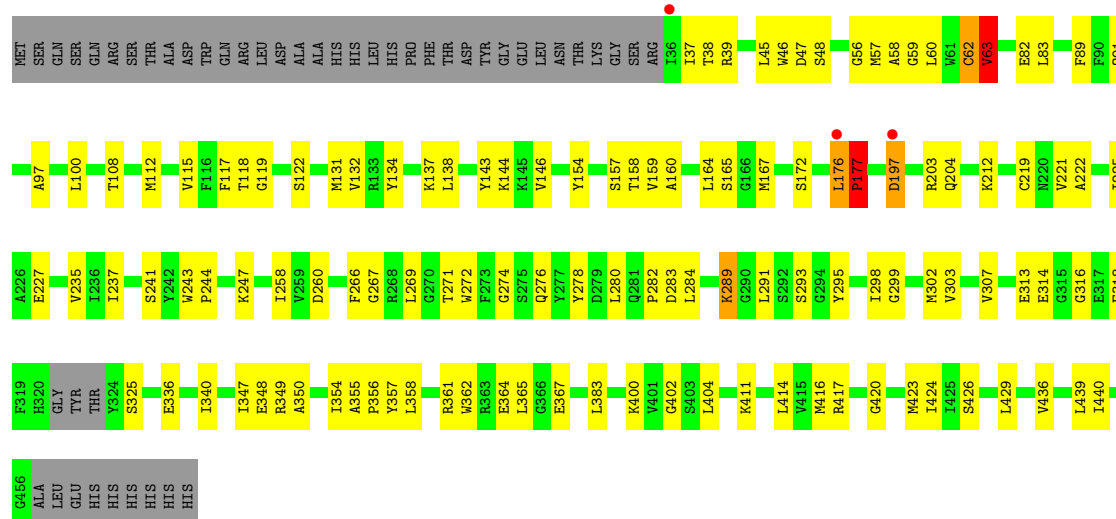


- Molecule 1: Aminotransferase TR2

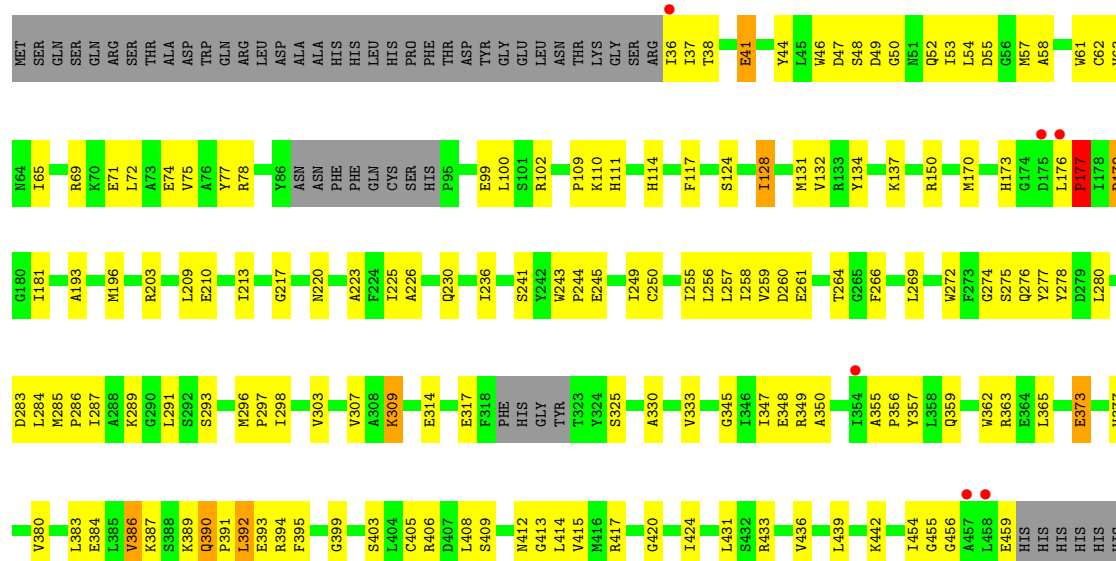




• Molecule 1: Aminotransferase TR2



• Molecule 1: Aminotransferase TR2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.36Å 108.99Å 212.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.65 – 3.30 39.65 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.65-3.30) 98.4 (39.65-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.226 , 0.280 0.227 , 0.281	Depositor DCC
R_{free} test set	1937 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å ²)	109.5	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12927	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% 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

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	0.57	0/3320	0.84	0/4494
1	B	0.67	1/3348 (0.0%)	0.95	3/4533 (0.1%)
1	C	0.63	0/3301	0.92	0/4467
1	D	0.60	0/3248	0.86	2/4393 (0.0%)
All	All	0.62	1/13217 (0.0%)	0.89	5/17887 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	LYS	C-O	-5.23	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	HIS	CB-CA-C	7.12	117.59	110.33
1	D	38	THR	N-CA-C	-5.51	108.34	114.62
1	B	145	LYS	N-CA-C	5.16	118.35	111.75
1	B	284	LEU	CA-CB-CG	-5.11	98.43	116.30
1	D	177	PRO	N-CA-C	-5.03	102.11	112.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	ARG	Sidechain

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	3244	0	3204	117	2
1	B	3274	0	3237	105	0
1	C	3229	0	3195	87	2
1	D	3180	0	3167	108	0
All	All	12927	0	12803	403	2

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 16.

All (403) 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:225:ILE:HG22	1:A:258:ILE:HB	1.34	1.05
1:A:69:ARG:NH1	1:A:71:GLU:OE2	1.99	0.95
1:D:359:GLN:HB3	1:D:363:ARG:HH21	1.35	0.90
1:C:132:VAL:HG21	1:C:258:ILE:HD11	1.53	0.89
1:C:37:ILE:HG13	1:C:48:SER:H	1.37	0.86
1:B:39:ARG:NH2	1:B:41:GLU:OE1	2.09	0.86
1:D:431:LEU:HD21	1:D:436:VAL:HG12	1.56	0.85
1:D:110:LYS:HG3	1:D:111:HIS:H	1.42	0.85
1:B:160:ALA:HB2	1:C:159:VAL:HG11	1.61	0.82
1:B:438:GLU:O	1:B:442:LYS:HG3	1.79	0.81
1:D:257:LEU:HD21	1:D:280:LEU:HD23	1.63	0.81
1:A:65:ILE:HD12	1:A:69:ARG:HG3	1.62	0.80
1:B:69:ARG:NH1	1:B:71:GLU:OE2	2.16	0.78
1:B:159:VAL:HG11	1:C:160:ALA:HB2	1.67	0.76
1:C:347:ILE:HD12	1:C:348:GLU:H	1.50	0.75
1:C:400:LYS:O	1:C:404:LEU:HG	1.86	0.74
1:A:272:TRP:CE2	1:A:347:ILE:HG12	2.22	0.74
1:C:39:ARG:HG3	1:C:47:ASP:OD2	1.85	0.74
1:C:108:THR:HG21	1:C:302:MET:HE2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:ARG:HB2	1:C:424:ILE:HD11	1.70	0.74
1:D:431:LEU:HD21	1:D:436:VAL:CG1	2.17	0.74
1:B:413:GLY:O	1:B:442:LYS:NZ	2.19	0.74
1:A:296:MET:HG2	1:A:330:ALA:HA	1.69	0.73
1:A:128:ILE:HG23	1:A:284:LEU:HD22	1.71	0.73
1:C:347:ILE:HD12	1:C:348:GLU:N	2.05	0.72
1:B:111:HIS:CD2	1:B:304:SER:HB2	2.25	0.71
1:A:65:ILE:HG23	1:A:341:MET:HE2	1.72	0.70
1:C:241:SER:C	1:C:244:PRO:HD2	2.15	0.70
1:A:414:LEU:HD11	1:A:439:LEU:HD22	1.73	0.70
1:C:267:GLY:HA3	1:C:429:LEU:HD11	1.73	0.70
1:C:272:TRP:HB2	1:C:276:GLN:HE22	1.56	0.69
1:C:146:VAL:HB	1:C:221:VAL:HA	1.75	0.68
1:D:347:ILE:HD12	1:D:348:GLU:H	1.57	0.68
1:D:117:PHE:HD2	1:D:325:SER:HA	1.59	0.67
1:D:357:TYR:HD2	1:D:436:VAL:HG21	1.60	0.67
1:D:403:SER:OG	1:D:406:ARG:NH2	2.27	0.67
1:B:38:THR:HG23	1:B:39:ARG:H	1.59	0.67
1:C:37:ILE:HG13	1:C:47:ASP:HB3	1.75	0.67
1:A:132:VAL:HG23	1:A:256:LEU:HD22	1.76	0.67
1:C:271:THR:HB	1:C:276:GLN:HE21	1.59	0.67
1:D:347:ILE:HD12	1:D:348:GLU:N	2.10	0.66
1:C:362:TRP:CZ2	1:C:383:LEU:HG	2.31	0.66
1:A:109:PRO:HB2	1:A:112:MET:HE3	1.77	0.66
1:D:357:TYR:CD2	1:D:436:VAL:HG21	2.31	0.66
1:A:235:VAL:HG22	1:A:382:ALA:HB2	1.78	0.66
1:A:242:TYR:CZ	1:A:246:ILE:HD11	2.31	0.65
1:B:36:ILE:HA	1:B:48:SER:OG	1.97	0.65
1:A:230:GLN:HB2	1:A:236:ILE:HB	1.79	0.65
1:B:272:TRP:CE2	1:B:347:ILE:HG12	2.32	0.65
1:B:230:GLN:HB2	1:B:236:ILE:HB	1.77	0.65
1:B:350:ALA:HA	1:B:354:ILE:HG12	1.79	0.64
1:B:272:TRP:HB2	1:B:276:GLN:HE22	1.62	0.64
1:A:76:ALA:O	1:A:80:MET:HB2	1.97	0.64
1:D:69:ARG:NH1	1:D:71:GLU:OE2	2.30	0.64
1:B:57:MET:SD	1:B:417:ARG:HG3	2.38	0.64
1:A:234:GLY:H	1:A:419:VAL:HG21	1.63	0.63
1:D:62:CYS:HB3	1:D:289:LYS:HB3	1.81	0.63
1:B:361:ARG:HB3	1:B:440:ILE:HG21	1.79	0.63
1:C:365:LEU:HD13	1:C:383:LEU:HD11	1.81	0.62
1:A:213:ILE:HD13	1:A:221:VAL:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:NH1	1:A:426:SER:OG	2.33	0.62
1:B:160:ALA:CB	1:C:159:VAL:HG11	2.28	0.62
1:A:135:TYR:CD2	1:A:256:LEU:HD11	2.34	0.61
1:A:379:MET:HG3	1:A:429:LEU:HD22	1.83	0.61
1:D:433:ARG:O	1:D:436:VAL:HG22	2.00	0.61
1:C:358:LEU:HA	1:C:436:VAL:HG21	1.81	0.61
1:B:390:GLN:HB3	1:B:391:PRO:HD3	1.83	0.61
1:B:433:ARG:O	1:B:436:VAL:HG22	2.01	0.61
1:B:414:LEU:HD11	1:B:439:LEU:HD12	1.81	0.60
1:B:118:THR:OG1	1:B:123:ASP:HB3	2.01	0.60
1:A:203:ARG:HG3	1:A:245:GLU:HG3	1.83	0.60
1:A:362:TRP:CZ2	1:A:383:LEU:HG	2.37	0.60
1:A:390:GLN:HB3	1:A:391:PRO:HD3	1.84	0.60
1:B:57:MET:HB2	1:B:415:VAL:HG12	1.83	0.60
1:D:61:TRP:CH2	1:D:424:ILE:HD12	2.37	0.60
1:D:225:ILE:HG22	1:D:258:ILE:HD12	1.84	0.60
1:A:361:ARG:HB3	1:A:440:ILE:HG13	1.84	0.60
1:B:186:GLN:H	1:B:192:ARG:HH21	1.49	0.59
1:B:355:ALA:HB3	1:B:356:PRO:HD3	1.84	0.59
1:B:261:GLU:OE2	1:B:275:SER:N	2.36	0.59
1:B:172:SER:O	1:C:137:LYS:NZ	2.29	0.59
1:D:261:GLU:HA	1:D:264:THR:OG1	2.02	0.59
1:A:57:MET:HE1	1:A:425:ILE:HA	1.85	0.59
1:C:57:MET:HG2	1:C:417:ARG:HG3	1.85	0.59
1:D:128:ILE:HG23	1:D:284:LEU:HD22	1.84	0.59
1:D:44:TYR:CE1	1:D:54:LEU:HD12	2.38	0.58
1:A:65:ILE:HG22	1:A:346:ILE:HD12	1.84	0.58
1:C:143:TYR:HE2	1:C:219:CYS:HB2	1.68	0.58
1:B:109:PRO:HD3	1:B:276:GLN:OE1	2.04	0.58
1:D:230:GLN:HB2	1:D:236:ILE:HB	1.85	0.58
1:A:235:VAL:O	1:A:375:ARG:NE	2.33	0.58
1:B:144:LYS:O	1:B:222:ALA:HB2	2.04	0.58
1:C:243:TRP:CE3	1:C:280:LEU:HD21	2.40	0.57
1:A:250:CYS:SG	1:A:255:ILE:HD11	2.45	0.57
1:B:83:LEU:HD11	1:B:92:CYS:HB2	1.87	0.57
1:D:47:ASP:OD1	1:D:48:SER:N	2.38	0.57
1:D:278:TYR:HB2	1:D:280:LEU:HD12	1.87	0.57
1:B:55:ASP:HA	1:B:415:VAL:HB	1.87	0.57
1:B:153:ALA:O	1:B:166:GLY:N	2.36	0.57
1:D:269:LEU:HD12	1:D:274:GLY:HA2	1.87	0.57
1:A:347:ILE:HD12	1:A:348:GLU:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLU:HG3	1:B:285:MET:SD	2.44	0.56
1:D:74:GLU:HB2	1:D:78:ARG:NH2	2.20	0.56
1:C:272:TRP:HB2	1:C:276:GLN:NE2	2.20	0.56
1:A:135:TYR:CE2	1:A:256:LEU:HD11	2.40	0.56
1:A:391:PRO:O	1:A:393:GLU:N	2.38	0.56
1:C:361:ARG:HD2	1:C:440:ILE:HG13	1.88	0.56
1:D:359:GLN:HB3	1:D:363:ARG:NH2	2.14	0.56
1:A:95:PRO:HB2	1:A:98:ILE:HG13	1.87	0.56
1:D:63:VAL:HA	1:D:293:SER:O	2.05	0.56
1:A:128:ILE:CD1	1:A:286:PRO:HD3	2.36	0.55
1:A:266:PHE:CZ	1:A:291:LEU:HD13	2.42	0.55
1:B:125:ASN:HA	1:B:128:ILE:HD12	1.87	0.55
1:D:99:GLU:HA	1:D:102:ARG:HE	1.71	0.55
1:C:225:ILE:HG22	1:C:258:ILE:HB	1.87	0.55
1:D:412:ASN:O	1:D:442:LYS:HD3	2.06	0.55
1:D:225:ILE:HG22	1:D:258:ILE:HB	1.88	0.55
1:C:115:VAL:HG12	1:C:302:MET:SD	2.47	0.55
1:B:130:ARG:HG2	1:C:176:LEU:HD21	1.89	0.55
1:D:355:ALA:HB3	1:D:356:PRO:HD3	1.88	0.55
1:B:44:TYR:CE1	1:B:54:LEU:HD12	2.41	0.55
1:D:55:ASP:HA	1:D:415:VAL:HB	1.89	0.55
1:A:235:VAL:HG22	1:A:382:ALA:CB	2.37	0.54
1:B:437:ASP:HA	1:B:440:ILE:HG13	1.89	0.54
1:C:272:TRP:CE2	1:C:347:ILE:HG12	2.42	0.54
1:B:116:PHE:HB3	1:B:301:VAL:CG2	2.37	0.54
1:D:296:MET:HE3	1:D:297:PRO:HD2	1.90	0.54
1:C:154:TYR:HA	1:C:165:SER:HB2	1.90	0.54
1:D:272:TRP:HB2	1:D:276:GLN:OE1	2.07	0.54
1:C:38:THR:HA	1:C:47:ASP:HB2	1.89	0.54
1:A:235:VAL:HG11	1:A:380:VAL:HG22	1.90	0.54
1:B:100:LEU:HD12	1:B:331:ALA:HA	1.90	0.54
1:A:336:GLU:HA	1:A:339:ARG:HD2	1.88	0.54
1:A:365:LEU:HD13	1:A:383:LEU:HD11	1.88	0.54
1:B:44:TYR:HE1	1:B:54:LEU:HD12	1.73	0.54
1:D:241:SER:C	1:D:244:PRO:HD2	2.32	0.54
1:D:243:TRP:CZ3	1:D:280:LEU:HD21	2.43	0.53
1:A:171:HIS:HA	1:A:176:LEU:HB2	1.90	0.53
1:D:269:LEU:HD22	1:D:377:VAL:HG12	1.90	0.53
1:D:347:ILE:O	1:D:350:ALA:HB3	2.09	0.53
1:D:72:LEU:O	1:D:75:VAL:HG22	2.07	0.53
1:C:118:THR:OG1	1:C:119:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:HA	1:A:293:SER:O	2.09	0.53
1:D:176:LEU:N	1:D:177:PRO:HD3	2.25	0.53
1:D:283:ASP:C	1:D:284:LEU:HD12	2.34	0.52
1:D:223:ALA:HB2	1:D:256:LEU:HB2	1.90	0.52
1:A:261:GLU:HG3	1:A:285:MET:SD	2.49	0.52
1:B:189:HIS:CD2	1:B:198:PRO:HA	2.44	0.52
1:A:134:TYR:CD2	1:D:173:HIS:HB3	2.45	0.52
1:B:37:ILE:HG23	1:B:45:LEU:HB3	1.91	0.52
1:B:112:MET:HE1	1:B:282:PRO:HB2	1.92	0.52
1:C:269:LEU:HD12	1:C:274:GLY:HA2	1.92	0.52
1:A:225:ILE:HA	1:A:258:ILE:O	2.10	0.52
1:A:225:ILE:CG2	1:A:258:ILE:HB	2.23	0.51
1:A:296:MET:SD	1:D:296:MET:HE1	2.50	0.51
1:B:405:CYS:O	1:B:409:SER:N	2.43	0.51
1:D:53:ILE:HD12	1:D:413:GLY:HA2	1.92	0.51
1:B:120:SER:OG	1:B:122:SER:OG	2.24	0.51
1:B:235:VAL:HB	1:B:382:ALA:HB2	1.91	0.51
1:A:213:ILE:CD1	1:A:221:VAL:HG21	2.41	0.51
1:B:431:LEU:HD21	1:B:436:VAL:HG12	1.92	0.51
1:D:260:ASP:HA	1:D:286:PRO:HD2	1.93	0.51
1:D:266:PHE:HE2	1:D:287:ILE:HB	1.74	0.51
1:A:228:PRO:O	1:A:229:ILE:HG13	2.10	0.51
1:B:71:GLU:O	1:B:74:GLU:HG2	2.11	0.51
1:D:57:MET:HG3	1:D:417:ARG:HG3	1.93	0.51
1:A:68:GLY:O	1:A:70:LYS:NZ	2.43	0.51
1:A:192:ARG:HG3	1:A:192:ARG:HH11	1.76	0.50
1:B:386:VAL:HG12	1:B:394:ARG:HG3	1.94	0.50
1:D:243:TRP:CE3	1:D:280:LEU:HD21	2.47	0.50
1:C:134:TYR:CE2	1:C:138:LEU:HD11	2.46	0.50
1:D:46:TRP:CE2	1:D:52:GLN:HG3	2.47	0.50
1:D:390:GLN:HB3	1:D:391:PRO:HD3	1.92	0.50
1:B:36:ILE:HG12	1:C:91:GLN:OE1	2.12	0.50
1:A:100:LEU:HD22	1:A:117:PHE:CZ	2.46	0.50
1:D:272:TRP:CZ2	1:D:347:ILE:HG12	2.47	0.50
1:A:269:LEU:HD12	1:A:274:GLY:HA2	1.94	0.49
1:C:176:LEU:O	1:C:177:PRO:C	2.55	0.49
1:C:411:LYS:O	1:C:411:LYS:HD3	2.12	0.49
1:D:100:LEU:HD22	1:D:117:PHE:CE1	2.48	0.49
1:D:454:ILE:HD12	1:D:455:GLY:N	2.26	0.49
1:A:362:TRP:CD1	1:A:381:ALA:HB1	2.47	0.49
1:C:316:GLY:C	1:C:318:PHE:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:LEU:HD11	1:C:439:LEU:HD22	1.94	0.49
1:D:150:ARG:CZ	1:D:226:ALA:HB1	2.43	0.49
1:C:336:GLU:O	1:C:340:ILE:HG12	2.12	0.49
1:B:65:ILE:HD11	1:B:72:LEU:HD11	1.94	0.49
1:D:405:CYS:O	1:D:409:SER:HB2	2.13	0.49
1:A:112:MET:SD	1:A:285:MET:HE3	2.53	0.49
1:D:349:ARG:HB2	1:D:349:ARG:CZ	2.42	0.49
1:A:172:SER:O	1:D:137:LYS:HE3	2.12	0.48
1:A:368:HIS:CG	1:A:369:PRO:HD2	2.48	0.48
1:C:362:TRP:O	1:C:365:LEU:HB2	2.12	0.48
1:D:77:TYR:HD2	1:D:78:ARG:HD3	1.78	0.48
1:A:132:VAL:O	1:A:135:TYR:HB3	2.13	0.48
1:A:361:ARG:HD2	1:A:440:ILE:HG13	1.94	0.48
1:B:409:SER:O	1:B:414:LEU:N	2.31	0.48
1:B:347:ILE:C	1:B:347:ILE:HD12	2.38	0.48
1:B:414:LEU:HD21	1:B:439:LEU:HD12	1.95	0.48
1:D:259:VAL:HG21	1:D:280:LEU:HD22	1.95	0.48
1:B:116:PHE:HB3	1:B:301:VAL:HG22	1.95	0.48
1:A:57:MET:HE1	1:A:424:ILE:O	2.13	0.48
1:C:357:TYR:CD2	1:C:436:VAL:HG11	2.48	0.48
1:D:296:MET:HE2	1:D:330:ALA:HB2	1.95	0.48
1:B:225:ILE:HG22	1:B:258:ILE:HB	1.95	0.48
1:A:154:TYR:HA	1:A:165:SER:HB2	1.94	0.48
1:A:161:GLY:O	1:A:165:SER:HB3	2.14	0.48
1:C:298:ILE:HG12	1:C:299:GLY:H	1.79	0.48
1:C:303:VAL:HG13	1:C:307:VAL:HG13	1.94	0.48
1:D:291:LEU:HD23	1:D:298:ILE:HG23	1.95	0.48
1:D:408:LEU:O	1:D:412:ASN:ND2	2.46	0.48
1:A:132:VAL:HG21	1:A:223:ALA:HB2	1.96	0.47
1:A:308:ALA:HA	1:A:311:VAL:HG22	1.95	0.47
1:B:283:ASP:C	1:B:284:LEU:HG	2.38	0.47
1:A:209:LEU:O	1:A:213:ILE:HG12	2.14	0.47
1:C:349:ARG:O	1:C:354:ILE:HG12	2.15	0.47
1:D:132:VAL:HG21	1:D:258:ILE:HD11	1.96	0.47
1:A:92:CYS:SG	1:A:93:SER:N	2.88	0.47
1:A:186:GLN:O	1:A:192:ARG:NH1	2.48	0.47
1:C:241:SER:O	1:C:244:PRO:HD2	2.13	0.47
1:B:239:PRO:C	1:B:241:SER:H	2.23	0.47
1:D:405:CYS:O	1:D:409:SER:N	2.48	0.47
1:C:402:GLY:HA3	1:C:420:GLY:O	2.15	0.47
1:D:49:ASP:OD1	1:D:50:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:THR:HG21	1:A:302:MET:SD	2.55	0.47
1:A:174:GLY:H	1:D:137:LYS:HD3	1.80	0.47
1:D:41:GLU:HG3	1:D:46:TRP:HZ3	1.80	0.47
1:D:373:GLU:H	1:D:384:GLU:HB2	1.79	0.47
1:D:209:LEU:O	1:D:213:ILE:HG12	2.15	0.46
1:A:69:ARG:HD2	1:A:71:GLU:OE2	2.15	0.46
1:D:345:GLY:O	1:D:348:GLU:N	2.48	0.46
1:A:272:TRP:CZ2	1:A:347:ILE:HG12	2.50	0.46
1:B:207:GLN:O	1:B:211:ARG:HG3	2.15	0.46
1:D:414:LEU:HD21	1:D:439:LEU:CD1	2.46	0.46
1:B:80:MET:HE3	1:C:295:TYR:HB3	1.97	0.46
1:C:272:TRP:CZ2	1:C:347:ILE:HG12	2.51	0.46
1:C:417:ARG:HB2	1:C:424:ILE:CD1	2.42	0.46
1:D:277:TYR:O	1:D:277:TYR:CG	2.68	0.46
1:C:37:ILE:CG1	1:C:48:SER:H	2.19	0.46
1:D:57:MET:SD	1:D:417:ARG:HG3	2.56	0.46
1:B:71:GLU:HA	1:B:74:GLU:HG2	1.97	0.46
1:A:197:ASP:OD2	1:A:200:GLU:HB2	2.15	0.46
1:C:225:ILE:HA	1:C:258:ILE:O	2.16	0.46
1:A:247:LYS:HA	1:A:247:LYS:HD2	1.65	0.46
1:A:269:LEU:HD12	1:A:274:GLY:CA	2.45	0.46
1:A:400:LYS:O	1:A:404:LEU:HG	2.16	0.46
1:B:189:HIS:O	1:B:189:HIS:ND1	2.49	0.46
1:B:371:VAL:HG11	1:B:383:LEU:HD22	1.97	0.46
1:B:188:TYR:CD1	1:B:236:ILE:HD12	2.50	0.45
1:B:414:LEU:HD11	1:B:439:LEU:CD1	2.45	0.45
1:D:124:SER:HB3	1:D:286:PRO:HB3	1.97	0.45
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.69	0.45
1:D:309:LYS:HA	1:D:309:LYS:HD3	1.56	0.45
1:A:112:MET:HE1	1:A:282:PRO:HD2	1.99	0.45
1:B:92:CYS:O	1:B:93:SER:C	2.58	0.45
1:B:100:LEU:HD23	1:B:100:LEU:O	2.17	0.45
1:C:46:TRP:HB3	1:C:47:ASP:H	1.55	0.45
1:C:436:VAL:O	1:C:440:ILE:HG12	2.16	0.45
1:B:56:GLY:O	1:B:426:SER:N	2.32	0.45
1:B:269:LEU:HD12	1:B:274:GLY:HA2	1.97	0.45
1:C:283:ASP:C	1:C:284:LEU:HD12	2.42	0.45
1:A:362:TRP:NE1	1:A:381:ALA:HB1	2.31	0.45
1:A:189:HIS:HA	1:A:201:PHE:CE2	2.52	0.45
1:A:291:LEU:HB3	1:A:298:ILE:HG21	1.98	0.45
1:D:170:MET:O	1:D:176:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:MET:HG3	1:B:429:LEU:HD22	1.99	0.45
1:D:131:MET:HA	1:D:134:TYR:HB3	1.99	0.45
1:A:39:ARG:HH22	1:A:41:GLU:HB2	1.82	0.45
1:A:229:ILE:HG21	1:A:237:ILE:HD13	1.97	0.45
1:B:258:ILE:HG12	1:B:284:LEU:HB2	1.98	0.45
1:A:317:GLU:HB3	1:D:173:HIS:CE1	2.52	0.44
1:C:58:ALA:O	1:C:60:LEU:N	2.50	0.44
1:C:60:LEU:HD11	1:C:417:ARG:HD2	1.99	0.44
1:A:228:PRO:HD2	1:A:264:THR:HG21	1.98	0.44
1:B:108:THR:HG21	1:B:302:MET:HE2	2.00	0.44
1:B:223:ALA:HA	1:B:255:ILE:HB	1.98	0.44
1:B:443:ALA:O	1:B:444:ARG:C	2.60	0.44
1:D:203:ARG:HG3	1:D:245:GLU:HG3	1.99	0.44
1:B:443:ALA:O	1:B:446:THR:N	2.50	0.44
1:B:448:ASP:O	1:B:452:LYS:HG2	2.17	0.44
1:C:56:GLY:O	1:C:426:SER:N	2.50	0.44
1:C:83:LEU:HD23	1:C:83:LEU:HA	1.72	0.44
1:C:278:TYR:HB2	1:C:280:LEU:CD1	2.48	0.44
1:C:361:ARG:O	1:C:364:GLU:HB3	2.18	0.44
1:A:137:LYS:HE2	1:A:137:LYS:HB3	1.61	0.44
1:B:158:THR:O	1:B:162:ALA:N	2.45	0.44
1:C:416:MET:HE3	1:C:423:MET:HE2	2.00	0.44
1:B:409:SER:O	1:B:413:GLY:N	2.51	0.44
1:D:459:GLU:H	1:D:459:GLU:HG2	1.62	0.44
1:A:323:THR:HB	1:A:324:TYR:H	1.72	0.44
1:B:111:HIS:NE2	1:B:304:SER:HB2	2.33	0.44
1:B:176:LEU:O	1:B:177:PRO:C	2.60	0.43
1:C:144:LYS:O	1:C:222:ALA:HB2	2.18	0.43
1:D:261:GLU:OE2	1:D:275:SER:N	2.50	0.43
1:B:126:ASP:OD2	1:C:158:THR:HB	2.18	0.43
1:B:298:ILE:HB	1:B:330:ALA:HB1	2.00	0.43
1:A:54:LEU:HB3	1:A:414:LEU:HD12	1.99	0.43
1:A:187:PRO:HG3	1:A:242:TYR:CZ	2.53	0.43
1:A:267:GLY:O	1:A:270:GLY:N	2.40	0.43
1:C:122:SER:HB2	1:C:157:SER:H	1.82	0.43
1:D:362:TRP:O	1:D:365:LEU:HB2	2.18	0.43
1:B:417:ARG:HB2	1:B:424:ILE:HG13	2.00	0.43
1:C:367:GLU:N	1:C:367:GLU:OE1	2.51	0.43
1:D:412:ASN:HB3	1:D:442:LYS:HG2	2.00	0.43
1:D:414:LEU:HD12	1:D:414:LEU:HA	1.87	0.43
1:C:100:LEU:HD22	1:C:117:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PHE:O	1:A:90:PHE:HB2	2.19	0.43
1:C:112:MET:HE1	1:C:282:PRO:HD2	2.01	0.43
1:C:243:TRP:CZ3	1:C:280:LEU:HD21	2.54	0.43
1:A:61:TRP:CH2	1:A:424:ILE:HD12	2.53	0.43
1:A:111:HIS:NE2	1:A:112:MET:HE2	2.34	0.43
1:A:146:VAL:HB	1:A:221:VAL:HA	2.01	0.43
1:A:291:LEU:HB3	1:A:298:ILE:CG2	2.49	0.43
1:D:193:ALA:HB1	1:D:196:MET:HE3	1.99	0.43
1:D:266:PHE:HZ	1:D:287:ILE:HD12	1.84	0.43
1:A:136:TRP:CE3	1:A:144:LYS:HD3	2.54	0.43
1:B:225:ILE:HA	1:B:258:ILE:O	2.19	0.43
1:A:225:ILE:HG22	1:A:258:ILE:CB	2.25	0.43
1:C:131:MET:HG2	1:C:318:PHE:HE2	1.83	0.43
1:C:38:THR:CA	1:C:47:ASP:HB2	2.49	0.42
1:C:62:CYS:O	1:C:63:VAL:C	2.61	0.42
1:A:162:ALA:HB3	1:A:176:LEU:HD12	2.01	0.42
1:B:112:MET:HE1	1:B:282:PRO:HD2	2.02	0.42
1:D:210:GLU:HB2	1:D:249:ILE:HG12	2.01	0.42
1:C:227:GLU:H	1:C:227:GLU:HG3	1.66	0.42
1:A:203:ARG:HG3	1:A:245:GLU:CG	2.49	0.42
1:B:111:HIS:HD2	1:B:305:ASP:H	1.66	0.42
1:B:235:VAL:HG12	1:B:237:ILE:HG13	2.01	0.42
1:B:287:ILE:HG12	1:B:302:MET:HG2	2.00	0.42
1:B:443:ALA:O	1:B:447:LEU:N	2.42	0.42
1:C:225:ILE:HG22	1:C:258:ILE:HD12	2.01	0.42
1:D:65:ILE:HG12	1:D:293:SER:OG	2.19	0.42
1:A:184:ILE:HG21	1:A:184:ILE:HD13	1.75	0.42
1:B:72:LEU:O	1:B:75:VAL:HG22	2.19	0.42
1:D:386:VAL:HG12	1:D:394:ARG:HA	2.02	0.42
1:A:118:THR:OG1	1:A:123:ASP:HB3	2.19	0.42
1:A:173:HIS:HB2	1:A:176:LEU:HD23	2.01	0.42
1:B:57:MET:CG	1:B:417:ARG:HG3	2.49	0.42
1:A:288:ALA:O	1:A:290:GLY:N	2.53	0.42
1:A:296:MET:CE	1:A:333:VAL:HG21	2.50	0.42
1:A:355:ALA:HB3	1:A:356:PRO:HD3	2.02	0.42
1:D:58:ALA:C	1:D:63:VAL:HG22	2.45	0.42
1:D:150:ARG:HE	1:D:150:ARG:HB2	1.53	0.42
1:A:440:ILE:HD13	1:A:440:ILE:HA	1.86	0.42
1:B:58:ALA:HB1	1:B:63:VAL:O	2.19	0.42
1:B:246:ILE:O	1:B:247:LYS:C	2.62	0.42
1:B:272:TRP:NE1	1:B:347:ILE:HD11	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ILE:HG21	1:B:430:VAL:HG22	2.01	0.42
1:A:131:MET:HE3	1:A:284:LEU:HD21	2.01	0.41
1:A:377:VAL:O	1:A:378:GLY:C	2.63	0.41
1:B:63:VAL:O	1:B:63:VAL:HG23	2.20	0.41
1:B:115:VAL:HG12	1:B:302:MET:SD	2.60	0.41
1:D:193:ALA:CB	1:D:196:MET:HE3	2.50	0.41
1:A:133:ARG:NH2	1:A:180:GLY:HA3	2.34	0.41
1:A:288:ALA:O	1:A:291:LEU:N	2.53	0.41
1:B:112:MET:HG2	1:B:302:MET:HB3	2.03	0.41
1:C:350:ALA:HA	1:C:354:ILE:HG13	2.02	0.41
1:D:392:LEU:HD23	1:D:392:LEU:HA	1.78	0.41
1:B:58:ALA:HB1	1:B:63:VAL:HG22	2.03	0.41
1:C:266:PHE:CZ	1:C:291:LEU:HD13	2.55	0.41
1:A:227:GLU:HG3	1:A:260:ASP:HB3	2.01	0.41
1:B:118:THR:OG1	1:B:123:ASP:CB	2.68	0.41
1:D:362:TRP:CZ2	1:D:383:LEU:HG	2.56	0.41
1:A:103:LEU:HA	1:A:103:LEU:HD23	1.82	0.41
1:D:217:GLY:O	1:D:220:ASN:N	2.41	0.41
1:D:261:GLU:HG3	1:D:285:MET:SD	2.61	0.41
1:A:104:LEU:HD21	1:A:291:LEU:HD11	2.02	0.41
1:A:206:ALA:HB2	1:A:242:TYR:CD1	2.56	0.41
1:B:239:PRO:C	1:B:241:SER:N	2.78	0.41
1:B:286:PRO:HA	1:B:300:GLY:O	2.21	0.41
1:C:100:LEU:C	1:C:100:LEU:HD23	2.46	0.41
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.88	0.41
1:C:350:ALA:HA	1:C:354:ILE:CG1	2.51	0.41
1:D:53:ILE:CD1	1:D:413:GLY:HA2	2.51	0.41
1:A:137:LYS:NZ	1:D:173:HIS:HA	2.36	0.41
1:C:39:ARG:O	1:C:45:LEU:HA	2.21	0.41
1:D:250:CYS:SG	1:D:255:ILE:HD11	2.61	0.41
1:A:302:MET:HB2	1:A:302:MET:HE2	1.53	0.40
1:C:247:LYS:HD2	1:C:247:LYS:HA	1.93	0.40
1:C:355:ALA:HB3	1:C:356:PRO:HD3	2.02	0.40
1:D:417:ARG:HB2	1:D:424:ILE:HG13	2.02	0.40
1:A:259:VAL:HG12	1:A:261:GLU:HG2	2.02	0.40
1:A:280:LEU:C	1:A:282:PRO:HD3	2.46	0.40
1:B:37:ILE:CG2	1:B:45:LEU:HB3	2.51	0.40
1:B:379:MET:HE3	1:B:379:MET:HB3	1.92	0.40
1:C:97:ALA:HB2	1:C:325:SER:HB2	2.03	0.40
1:C:227:GLU:HG2	1:C:260:ASP:HB3	2.04	0.40
1:C:383:LEU:HA	1:C:383:LEU:HD23	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:LEU:HD22	1:D:333:VAL:HG13	2.02	0.40
1:D:269:LEU:HD23	1:D:269:LEU:HA	1.78	0.40
1:D:296:MET:HG3	1:D:333:VAL:HG21	2.03	0.40
1:A:57:MET:CA	1:A:57:MET:HE2	2.50	0.40
1:A:187:PRO:HG3	1:A:242:TYR:CE2	2.56	0.40
1:A:272:TRP:NE1	1:A:347:ILE:HG12	2.36	0.40
1:C:414:LEU:HD11	1:C:439:LEU:CD2	2.51	0.40
1:D:128:ILE:HG21	1:D:258:ILE:HG21	2.02	0.40
1:D:266:PHE:CE2	1:D:287:ILE:HB	2.54	0.40
1:D:417:ARG:HB2	1:D:424:ILE:CG1	2.51	0.40
1:B:100:LEU:HD22	1:B:117:PHE:CZ	2.56	0.40
1:B:285:MET:HB3	1:B:302:MET:HB2	2.04	0.40
1:B:304:SER:OG	1:B:307:VAL:HG12	2.21	0.40
1:D:46:TRP:CZ2	1:D:52:GLN:HG3	2.57	0.40
1:D:399:GLY:HA2	1:D:420:GLY:HA2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASP:OD1	1:C:197:ASP:OD1[4_445]	1.69	0.51
1:A:313:GLU:OE2	1:C:313:GLU:OE2[4_545]	2.05	0.15

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	416/465 (90%)	357 (86%)	48 (12%)	11 (3%)	4	23
1	B	422/465 (91%)	362 (86%)	53 (13%)	7 (2%)	7	30
1	C	414/465 (89%)	370 (89%)	34 (8%)	10 (2%)	4	24
1	D	406/465 (87%)	350 (86%)	52 (13%)	4 (1%)	12	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1658/1860 (89%)	1439 (87%)	187 (11%)	32 (2%)	6	28

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	ALA
1	A	392	LEU
1	B	458	LEU
1	C	63	VAL
1	C	177	PRO
1	C	235	VAL
1	D	177	PRO
1	A	289	LYS
1	B	119	GLY
1	C	59	GLY
1	C	89	PHE
1	C	293	SER
1	A	93	SER
1	B	289	LYS
1	C	82	GLU
1	C	289	LYS
1	A	59	GLY
1	B	177	PRO
1	A	84	PRO
1	A	323	THR
1	B	82	GLU
1	C	176	LEU
1	C	314	GLU
1	D	109	PRO
1	A	63	VAL
1	A	109	PRO
1	D	456	GLY
1	B	84	PRO
1	B	109	PRO
1	D	179	PRO
1	A	378	GLY
1	A	297	PRO

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	338/378 (89%)	333 (98%)	5 (2%)	57	72
1	B	340/378 (90%)	315 (93%)	25 (7%)	13	38
1	C	336/378 (89%)	325 (97%)	11 (3%)	33	59
1	D	331/378 (88%)	310 (94%)	21 (6%)	16	44
All	All	1345/1512 (89%)	1283 (95%)	62 (5%)	24	53

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	302	MET
1	A	307	VAL
1	A	318	PHE
1	A	323	THR
1	B	78	ARG
1	B	80	MET
1	B	83	LEU
1	B	85	TYR
1	B	91	GLN
1	B	139	LEU
1	B	141	LYS
1	B	145	LYS
1	B	147	VAL
1	B	176	LEU
1	B	179	PRO
1	B	225	ILE
1	B	227	GLU
1	B	287	ILE
1	B	291	LEU
1	B	313	GLU
1	B	314	GLU
1	B	318	PHE
1	B	323	THR
1	B	359	GLN
1	B	364	GLU
1	B	367	GLU
1	B	375	ARG

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Mol	Chain	Res	Type
1	B	380	VAL
1	B	392	LEU
1	C	62	CYS
1	C	63	VAL
1	C	167	MET
1	C	172	SER
1	C	177	PRO
1	C	197	ASP
1	C	203	ARG
1	C	204	GLN
1	C	212	LYS
1	C	237	ILE
1	C	289	LYS
1	D	36	ILE
1	D	37	ILE
1	D	41	GLU
1	D	114	HIS
1	D	128	ILE
1	D	179	PRO
1	D	181	ILE
1	D	303	VAL
1	D	307	VAL
1	D	309	LYS
1	D	314	GLU
1	D	317	GLU
1	D	373	GLU
1	D	380	VAL
1	D	386	VAL
1	D	387	LYS
1	D	389	LYS
1	D	390	GLN
1	D	392	LEU
1	D	393	GLU
1	D	395	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	113	ASN
1	A	114	HIS
1	A	173	HIS

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Mol	Chain	Res	Type
1	A	337	ASN
1	A	368	HIS
1	A	451	HIS
1	B	111	HIS
1	B	451	HIS
1	C	88	ASN
1	C	113	ASN
1	C	220	ASN
1	C	276	GLN
1	C	412	ASN
1	D	111	HIS
1	D	183	HIS
1	D	359	GLN

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 ⓘ

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	418/465 (89%)	-0.23	3 (0%) 84 70	30, 87, 128, 151	0
1	B	424/465 (91%)	-0.07	7 (1%) 69 50	65, 94, 134, 160	0
1	C	418/465 (89%)	-0.19	3 (0%) 84 70	66, 88, 127, 153	0
1	D	412/465 (88%)	-0.13	6 (1%) 72 53	71, 100, 138, 163	0
All	All	1672/1860 (89%)	-0.16	19 (1%) 78 60	30, 92, 133, 163	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	GLY	6.0
1	D	176	LEU	3.0
1	C	36	ILE	2.9
1	A	322	TYR	2.7
1	D	458	LEU	2.6
1	D	36	ILE	2.4
1	C	197	ASP	2.4
1	B	116	PHE	2.4
1	C	176	LEU	2.4
1	D	175	ASP	2.4
1	B	85	TYR	2.4
1	B	457	ALA	2.2
1	B	36	ILE	2.2
1	D	354	ILE	2.1
1	D	457	ALA	2.1
1	B	86	TYR	2.1
1	B	325	SER	2.1
1	A	176	LEU	2.0
1	B	89	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.