



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:31 PM UTC

PDB ID : 3EXA / pdb_00003exa
Title : Crystal structure of the full-length tRNA isopentenylpyrophosphate transferase (BH2366) from *Bacillus halodurans*, Northeast Structural Genomics Consortium target BhR41.
Authors : Forouhar, F.; Abashidze, M.; Neely, H.; Seetharaman, J.; Shastry, R.; Janjua, H.; Cunningham, K.; Ma, L.-C.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-10-16
Resolution : 2.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
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)

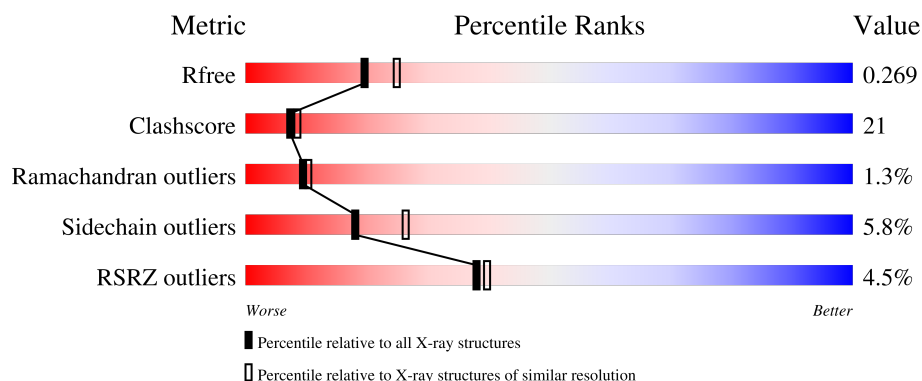
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	322	
1	B	322	
1	C	322	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	322	5% 60% 29% • • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10249 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 tRNA delta(2)-isopentenylpyrophosphate transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	Se	0	0	0
			2426	1530	428	457	1	10			
1	B	302	Total	C	N	O	S	Se	0	0	0
			2416	1524	425	456	1	10			
1	C	303	Total	C	N	O	S	Se	0	0	0
			2426	1530	428	457	1	10			
1	D	302	Total	C	N	O	S	Se	0	0	0
			2416	1524	425	456	1	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	LEU	-	expression tag	UNP Q9KAC3
A	316	GLU	-	expression tag	UNP Q9KAC3
A	317	HIS	-	expression tag	UNP Q9KAC3
A	318	HIS	-	expression tag	UNP Q9KAC3
A	319	HIS	-	expression tag	UNP Q9KAC3
A	320	HIS	-	expression tag	UNP Q9KAC3
A	321	HIS	-	expression tag	UNP Q9KAC3
A	322	HIS	-	expression tag	UNP Q9KAC3
B	315	LEU	-	expression tag	UNP Q9KAC3
B	316	GLU	-	expression tag	UNP Q9KAC3
B	317	HIS	-	expression tag	UNP Q9KAC3
B	318	HIS	-	expression tag	UNP Q9KAC3
B	319	HIS	-	expression tag	UNP Q9KAC3
B	320	HIS	-	expression tag	UNP Q9KAC3
B	321	HIS	-	expression tag	UNP Q9KAC3
B	322	HIS	-	expression tag	UNP Q9KAC3
C	315	LEU	-	expression tag	UNP Q9KAC3
C	316	GLU	-	expression tag	UNP Q9KAC3
C	317	HIS	-	expression tag	UNP Q9KAC3
C	318	HIS	-	expression tag	UNP Q9KAC3
C	319	HIS	-	expression tag	UNP Q9KAC3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	320	HIS	-	expression tag	UNP Q9KAC3
C	321	HIS	-	expression tag	UNP Q9KAC3
C	322	HIS	-	expression tag	UNP Q9KAC3
D	315	LEU	-	expression tag	UNP Q9KAC3
D	316	GLU	-	expression tag	UNP Q9KAC3
D	317	HIS	-	expression tag	UNP Q9KAC3
D	318	HIS	-	expression tag	UNP Q9KAC3
D	319	HIS	-	expression tag	UNP Q9KAC3
D	320	HIS	-	expression tag	UNP Q9KAC3
D	321	HIS	-	expression tag	UNP Q9KAC3
D	322	HIS	-	expression tag	UNP Q9KAC3

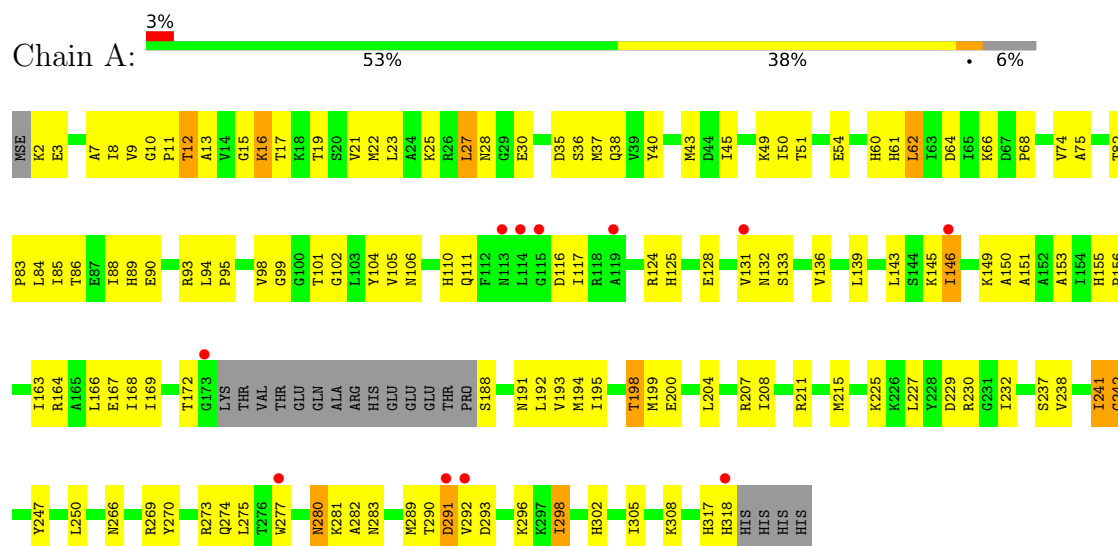
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	194	Total 194	O 194	0	0
2	B	132	Total 132	O 132	0	0
2	C	134	Total 134	O 134	0	0
2	D	105	Total 105	O 105	0	0

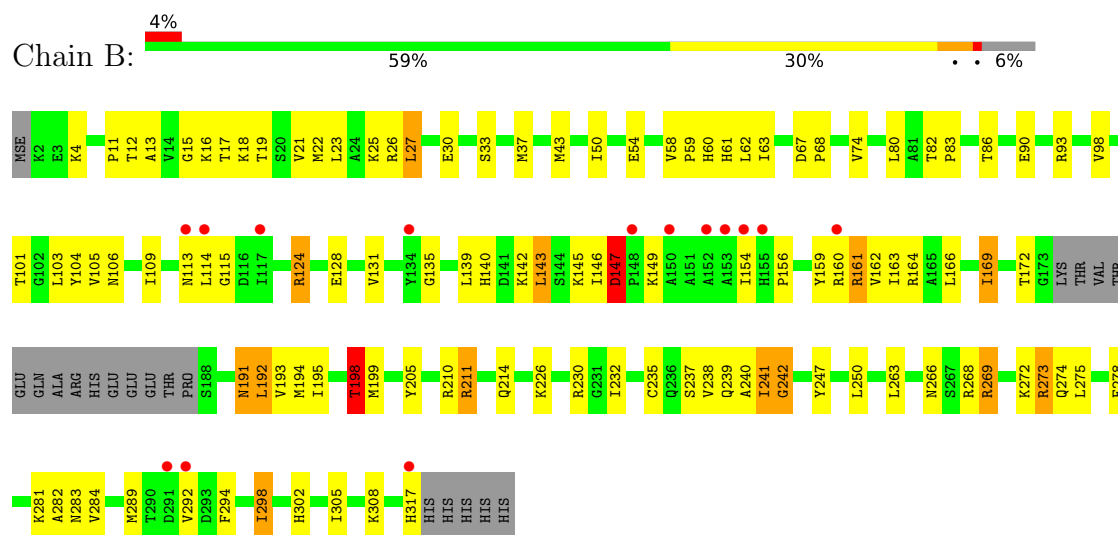
3 Residue-property plots [i](#)

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: tRNA delta(2)-isopentenylpyrophosphate transferase

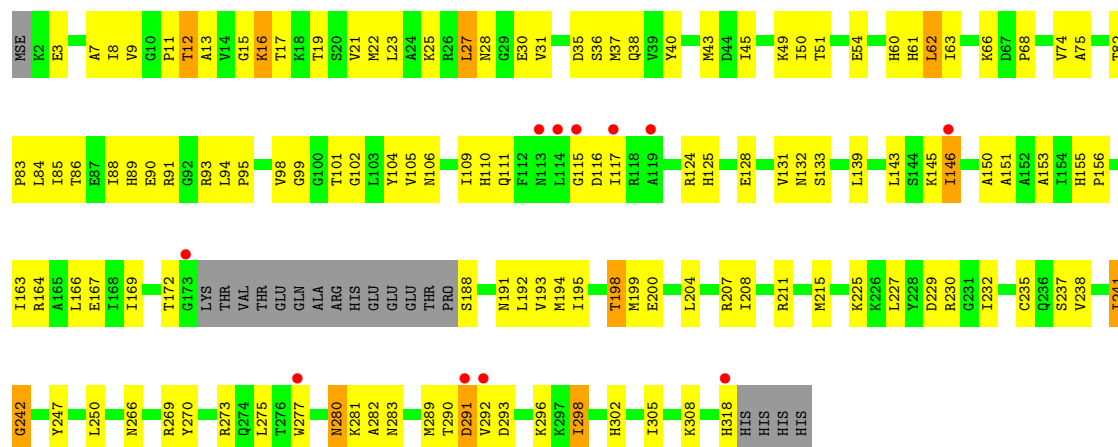


• Molecule 1: tRNA delta(2)-isopentenylpyrophosphate transferase

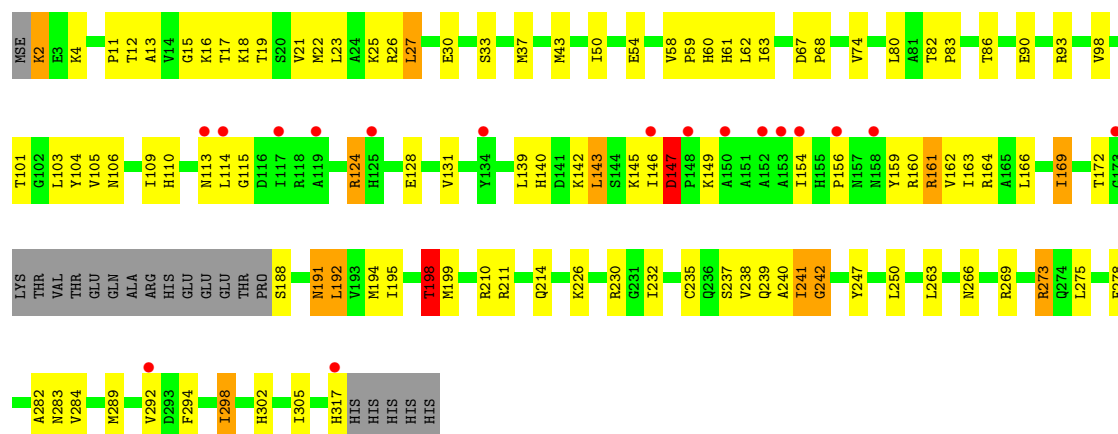


• Molecule 1: tRNA delta(2)-isopentenylpyrophosphate transferase





- Molecule 1: tRNA delta(2)-isopentenylpyrophosphate transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.80Å 73.82Å 95.56Å 89.99° 93.73° 90.02°	Depositor
Resolution (Å)	19.96 – 2.30 19.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	68.4 (19.96-2.30) 81.7 (19.96-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2, XTALVIEW	Depositor
R, R_{free}	0.220 , 0.263 0.232 , 0.269	Depositor DCC
R_{free} test set	4065 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.458 for -h,k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10249	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9084e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.44	0/2457	0.86	2/3294 (0.1%)
1	B	0.45	0/2446	0.97	14/3279 (0.4%)
1	C	0.45	0/2457	0.86	3/3294 (0.1%)
1	D	0.43	0/2446	0.94	13/3279 (0.4%)
All	All	0.44	0/9806	0.91	32/13146 (0.2%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	ARG	NE-CZ-NH2	8.54	126.89	119.20
1	B	164	ARG	NE-CZ-NH1	-8.50	113.00	121.50
1	B	161	ARG	NE-CZ-NH2	8.22	126.59	119.20
1	B	160	ARG	NE-CZ-NH2	8.03	126.43	119.20
1	B	161	ARG	NE-CZ-NH1	-7.65	113.85	121.50
1	B	160	ARG	NE-CZ-NH1	-7.61	113.89	121.50
1	C	191	ASN	N-CA-C	-6.91	96.53	108.56
1	A	191	ASN	N-CA-C	-6.89	96.56	108.56
1	D	164	ARG	CD-NE-CZ	6.60	133.63	124.40
1	D	164	ARG	NE-CZ-NH2	-6.54	113.31	119.20
1	D	161	ARG	CD-NE-CZ	6.42	133.39	124.40
1	D	161	ARG	NE-CZ-NH2	-6.26	113.57	119.20
1	B	164	ARG	CD-NE-CZ	6.21	133.09	124.40
1	B	160	ARG	CD-NE-CZ	5.96	132.75	124.40
1	D	160	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	B	191	ASN	N-CA-C	-5.83	98.41	108.56
1	C	98	VAL	N-CA-C	5.82	116.97	108.53
1	D	160	ARG	CD-NE-CZ	5.82	132.54	124.40
1	B	161	ARG	CD-NE-CZ	5.81	132.54	124.40
1	A	98	VAL	N-CA-C	5.76	116.89	108.53
1	D	191	ASN	N-CA-C	-5.66	98.71	108.56
1	D	164	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	D	161	ARG	NE-CZ-NH1	5.60	127.10	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	THR	CB-CA-C	-5.57	101.80	112.43
1	D	198	THR	CB-CA-C	-5.52	101.89	112.43
1	D	147	ASP	CA-C-N	5.35	124.99	119.05
1	D	147	ASP	C-N-CA	5.35	124.99	119.05
1	D	98	VAL	N-CA-C	5.18	115.37	108.11
1	C	31	VAL	N-CA-C	5.17	115.76	108.36
1	B	147	ASP	CA-C-N	5.14	124.76	119.05
1	B	147	ASP	C-N-CA	5.14	124.76	119.05
1	B	98	VAL	N-CA-C	5.05	115.17	108.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2426	0	2431	113	0
1	B	2416	0	2424	94	0
1	C	2426	0	2431	112	0
1	D	2416	0	2424	88	0
2	A	194	0	0	20	0
2	B	132	0	0	11	0
2	C	134	0	0	21	0
2	D	105	0	0	10	0
All	All	10249	0	9710	398	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 21.

All (398) 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:D:273:ARG:HB2	1:D:273:ARG:HH21	1.32	0.95
1:B:273:ARG:HH21	1:B:273:ARG:HB2	1.32	0.94
1:C:102:GLY:HA3	1:C:277:TRP:CD1	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLY:HA3	1:A:277:TRP:CD1	2.17	0.79
1:C:51:THR:OG1	1:C:54:GLU:HG3	1.85	0.76
1:A:51:THR:OG1	1:A:54:GLU:HG3	1.86	0.75
1:D:128:GLU:OE2	2:D:374:HOH:O	2.05	0.74
1:B:19:THR:HG21	1:B:289:MSE:HE2	1.70	0.74
1:A:274:GLN:HG3	2:A:498:HOH:O	1.87	0.73
1:D:26:ARG:HB2	2:D:560:HOH:O	1.88	0.72
1:D:19:THR:HG21	1:D:289:MSE:HE2	1.70	0.72
1:B:86:THR:O	1:B:90:GLU:HG2	1.90	0.71
1:D:37:MSE:HG3	2:D:388:HOH:O	1.88	0.71
1:B:198:THR:HG23	1:B:275:LEU:HD21	1.71	0.71
1:D:86:THR:O	1:D:90:GLU:HG2	1.91	0.70
1:C:86:THR:O	1:C:90:GLU:HG2	1.92	0.69
1:C:19:THR:HG21	1:C:289:MSE:HE2	1.74	0.69
1:B:273:ARG:HB2	1:B:273:ARG:NH2	2.07	0.69
1:B:241:ILE:HD11	1:B:266:ASN:HB3	1.72	0.69
1:A:242:GLY:HA3	2:A:355:HOH:O	1.91	0.69
1:D:198:THR:HG23	1:D:275:LEU:HD21	1.73	0.69
1:A:19:THR:HG21	1:A:289:MSE:HE2	1.74	0.68
1:A:292:VAL:HG22	1:A:293:ASP:H	1.59	0.68
1:C:37:MSE:HG3	2:C:563:HOH:O	1.93	0.68
1:D:166:LEU:O	1:D:169:ILE:HG22	1.93	0.67
1:D:241:ILE:HD11	1:D:266:ASN:HB3	1.75	0.67
1:B:166:LEU:O	1:B:169:ILE:HG22	1.94	0.67
1:C:192:LEU:HD21	1:C:194:MSE:HB2	1.76	0.67
1:A:102:GLY:HA3	1:A:277:TRP:NE1	2.09	0.67
1:C:102:GLY:HA3	1:C:277:TRP:NE1	2.09	0.67
1:A:155:HIS:CD2	1:A:156:PRO:HD2	2.31	0.66
1:C:155:HIS:CD2	1:C:156:PRO:HD2	2.31	0.65
1:B:161:ARG:HG3	2:B:376:HOH:O	1.96	0.65
1:A:86:THR:O	1:A:90:GLU:HG2	1.95	0.65
1:D:58:VAL:O	1:D:60:HIS:HD2	1.79	0.65
1:B:226:LYS:HD3	2:B:329:HOH:O	1.96	0.65
1:A:192:LEU:HD21	1:A:194:MSE:HB2	1.78	0.65
1:C:195:ILE:HD13	1:C:305:ILE:HD11	1.78	0.65
1:C:82:THR:HB	1:C:83:PRO:HD3	1.79	0.64
1:D:273:ARG:HB2	1:D:273:ARG:NH2	2.07	0.64
1:A:37:MSE:HG3	2:A:354:HOH:O	1.96	0.64
1:B:74:VAL:HG23	1:B:104:TYR:HA	1.79	0.64
1:C:292:VAL:HG22	1:C:293:ASP:H	1.61	0.64
1:A:195:ILE:HD13	1:A:305:ILE:HD11	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:THR:HB	1:A:83:PRO:HD3	1.80	0.64
1:D:238:VAL:HG11	1:D:247:TYR:CE1	2.33	0.64
1:B:58:VAL:O	1:B:60:HIS:HD2	1.81	0.63
1:D:142:LYS:HA	1:D:145:LYS:HD3	1.81	0.63
1:A:241:ILE:HD11	1:A:266:ASN:HB3	1.81	0.63
1:D:74:VAL:HG23	1:D:104:TYR:HA	1.80	0.63
1:D:21:VAL:HG23	1:D:22:MSE:HE2	1.80	0.63
1:A:149:LYS:HD2	2:A:413:HOH:O	1.99	0.63
1:C:241:ILE:HD11	1:C:266:ASN:HB3	1.81	0.62
1:D:131:VAL:HG12	1:D:139:LEU:HB2	1.80	0.62
1:B:131:VAL:HG12	1:B:139:LEU:HB2	1.80	0.62
1:A:273:ARG:HH21	1:A:273:ARG:HG3	1.64	0.62
1:C:282:ALA:O	1:C:283:ASN:HB2	1.99	0.62
1:A:282:ALA:O	1:A:283:ASN:HB2	1.99	0.62
1:B:238:VAL:HG11	1:B:247:TYR:CE1	2.35	0.62
1:D:131:VAL:HG11	1:D:139:LEU:HD22	1.82	0.62
1:A:38:GLN:HB2	2:A:368:HOH:O	1.99	0.62
1:B:195:ILE:HD13	1:B:305:ILE:HD11	1.82	0.62
1:A:136:VAL:HG12	2:A:408:HOH:O	1.99	0.61
1:B:156:PRO:HG3	1:C:28:ASN:HB2	1.81	0.61
1:B:21:VAL:HG23	1:B:22:MSE:HE2	1.80	0.61
1:B:142:LYS:HA	1:B:145:LYS:HD3	1.81	0.61
1:A:198:THR:HG23	1:A:275:LEU:HD21	1.82	0.61
2:C:342:HOH:O	1:D:114:LEU:HD22	2.00	0.61
1:D:195:ILE:HD13	1:D:305:ILE:HD11	1.81	0.61
1:B:131:VAL:HG11	1:B:139:LEU:HD22	1.83	0.60
1:D:82:THR:HB	1:D:83:PRO:HD3	1.82	0.60
1:A:143:LEU:HD23	1:A:166:LEU:HD23	1.84	0.60
1:B:82:THR:HB	1:B:83:PRO:HD3	1.82	0.60
1:D:210:ARG:O	1:D:214:GLN:HG3	2.01	0.60
1:A:11:PRO:HD3	1:A:275:LEU:HG	1.83	0.60
1:C:273:ARG:HH21	1:C:273:ARG:HG3	1.67	0.59
1:A:242:GLY:N	2:A:355:HOH:O	2.35	0.59
1:B:210:ARG:O	1:B:214:GLN:HG3	2.02	0.59
1:A:146:ILE:HD13	1:A:146:ILE:O	2.03	0.59
1:C:143:LEU:HD23	1:C:166:LEU:HD23	1.84	0.59
1:B:80:LEU:O	1:B:83:PRO:HD2	2.03	0.59
1:C:146:ILE:HD13	1:C:146:ILE:O	2.03	0.59
1:D:23:LEU:O	1:D:27:LEU:HB2	2.02	0.59
1:C:198:THR:HG23	1:C:275:LEU:HD21	1.83	0.58
1:C:11:PRO:HD3	1:C:275:LEU:HG	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:GLU:HB3	2:C:565:HOH:O	2.03	0.58
1:D:80:LEU:O	1:D:83:PRO:HD2	2.02	0.58
1:B:23:LEU:O	1:B:27:LEU:HB2	2.02	0.58
1:C:23:LEU:O	1:C:27:LEU:HB2	2.03	0.58
1:C:198:THR:HG22	1:C:199:MSE:H	1.68	0.58
1:A:198:THR:HG22	1:A:199:MSE:H	1.67	0.58
1:A:94:LEU:HD12	1:A:95:PRO:HD2	1.86	0.58
1:A:23:LEU:O	1:A:27:LEU:HB2	2.04	0.58
1:A:128:GLU:HB3	1:B:103:LEU:HD13	1.86	0.57
1:A:273:ARG:HG3	1:A:273:ARG:NH2	2.19	0.57
1:B:235:CYS:O	1:B:239:GLN:HG3	2.03	0.57
1:D:93:ARG:HG3	1:D:93:ARG:HH11	1.70	0.57
1:C:94:LEU:HD12	1:C:95:PRO:HD2	1.87	0.57
1:B:26:ARG:HB2	2:B:369:HOH:O	2.04	0.57
1:A:7:ALA:HB3	1:A:194:MSE:HG3	1.86	0.57
1:A:45:ILE:O	1:A:215:MSE:HE2	2.04	0.57
1:A:238:VAL:HG11	1:A:247:TYR:CE1	2.40	0.56
1:C:9:VAL:HG11	1:C:194:MSE:HE3	1.87	0.56
1:C:28:ASN:ND2	1:C:93:ARG:HD3	2.20	0.56
1:C:45:ILE:O	1:C:215:MSE:HE2	2.05	0.56
1:B:93:ARG:HG3	1:B:93:ARG:HH11	1.70	0.56
1:C:238:VAL:HG11	1:C:247:TYR:CE1	2.40	0.56
1:D:235:CYS:O	1:D:239:GLN:HG3	2.05	0.56
1:C:8:ILE:HG12	1:C:195:ILE:HD11	1.88	0.56
1:C:116:ASP:C	1:C:117:ILE:HD12	2.31	0.56
1:D:58:VAL:O	1:D:60:HIS:CD2	2.58	0.56
1:C:7:ALA:HB3	1:C:194:MSE:HG3	1.87	0.56
1:A:116:ASP:C	1:A:117:ILE:HD12	2.31	0.56
1:A:9:VAL:HG11	1:A:194:MSE:HE3	1.87	0.56
1:D:61:HIS:O	1:D:62:LEU:HB2	2.06	0.56
1:A:82:THR:HG21	1:A:111:GLN:HE22	1.71	0.55
1:C:82:THR:HG21	1:C:111:GLN:HE22	1.71	0.55
1:C:128:GLU:HB3	1:D:103:LEU:HD13	1.88	0.55
1:A:102:GLY:HA3	1:A:277:TRP:HE1	1.71	0.55
1:B:194:MSE:HE2	1:B:284:VAL:HG22	1.89	0.55
1:D:194:MSE:HE2	1:D:284:VAL:HG22	1.89	0.55
1:A:242:GLY:CA	2:A:355:HOH:O	2.50	0.55
1:D:43:MSE:SE	1:D:68:PRO:HB3	2.57	0.55
1:C:273:ARG:HG3	1:C:273:ARG:NH2	2.21	0.55
1:D:21:VAL:HG21	2:D:390:HOH:O	2.06	0.55
1:A:28:ASN:ND2	1:A:93:ARG:HD3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ILE:CD1	1:B:266:ASN:HB3	2.37	0.54
1:C:131:VAL:HB	1:C:139:LEU:HD22	1.88	0.54
1:B:43:MSE:SE	1:B:68:PRO:HB3	2.57	0.54
1:B:273:ARG:HH21	1:B:273:ARG:CB	2.15	0.54
1:D:19:THR:HG21	1:D:289:MSE:CE	2.38	0.54
1:A:131:VAL:HB	1:A:139:LEU:HD22	1.90	0.54
1:C:85:ILE:HB	2:C:388:HOH:O	2.06	0.54
1:D:230:ARG:HG3	1:D:232:ILE:HG12	1.90	0.54
1:C:241:ILE:HG12	1:C:241:ILE:O	2.08	0.53
1:A:21:VAL:HG23	1:A:22:MSE:HE2	1.91	0.53
1:B:298:ILE:HD13	1:B:298:ILE:O	2.09	0.53
1:D:37:MSE:SE	1:D:240:ALA:HB2	2.59	0.53
1:B:19:THR:HG21	1:B:289:MSE:CE	2.38	0.53
1:B:58:VAL:O	1:B:60:HIS:CD2	2.60	0.53
1:C:242:GLY:HA3	2:C:430:HOH:O	2.08	0.53
1:C:102:GLY:HA3	1:C:277:TRP:HE1	1.71	0.53
1:A:74:VAL:HG13	1:A:75:ALA:N	2.24	0.53
1:D:188:SER:N	2:D:362:HOH:O	2.42	0.53
1:A:128:GLU:O	1:A:131:VAL:HG12	2.09	0.53
1:A:241:ILE:HG12	1:A:241:ILE:O	2.08	0.53
1:B:146:ILE:O	1:B:147:ASP:HB2	2.09	0.53
1:C:21:VAL:HG23	1:C:22:MSE:HE2	1.91	0.53
1:A:21:VAL:O	1:A:25:LYS:HG3	2.09	0.52
1:D:4:LYS:HA	1:D:191:ASN:HB3	1.91	0.52
1:D:273:ARG:HH21	1:D:273:ARG:CB	2.15	0.52
1:A:8:ILE:HG12	1:A:195:ILE:HD11	1.90	0.52
1:C:298:ILE:HD13	1:C:298:ILE:O	2.09	0.52
1:B:4:LYS:HA	1:B:191:ASN:HB3	1.92	0.52
1:D:298:ILE:HD13	1:D:298:ILE:O	2.09	0.52
1:B:61:HIS:O	1:B:62:LEU:HB2	2.08	0.52
1:C:21:VAL:O	1:C:25:LYS:HG3	2.09	0.52
1:C:230:ARG:HG3	1:C:232:ILE:HG12	1.92	0.52
1:D:19:THR:HG22	1:D:294:PHE:HE1	1.75	0.52
1:D:146:ILE:O	1:D:147:ASP:HB2	2.08	0.52
1:B:230:ARG:HG3	1:B:232:ILE:HG12	1.92	0.52
1:A:101:THR:HG22	1:A:270:TYR:OH	2.10	0.51
1:D:140:HIS:CD2	1:D:156:PRO:HA	2.45	0.51
1:A:61:HIS:O	1:A:62:LEU:HB2	2.10	0.51
1:B:140:HIS:CD2	1:B:156:PRO:HA	2.46	0.51
1:B:241:ILE:CG1	1:B:266:ASN:HB3	2.40	0.51
1:D:241:ILE:CG1	1:D:266:ASN:HB3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:HIS:HE1	1:C:281:LYS:NZ	2.09	0.51
1:D:67:ASP:HB2	2:D:356:HOH:O	2.09	0.51
1:A:143:LEU:HB2	1:A:166:LEU:HD21	1.91	0.51
1:C:101:THR:HG22	1:C:270:TYR:OH	2.10	0.51
1:A:110:HIS:HE1	1:A:281:LYS:NZ	2.08	0.51
1:D:198:THR:HG22	1:D:199:MSE:H	1.76	0.51
1:C:128:GLU:O	1:C:131:VAL:HG12	2.11	0.50
1:D:169:ILE:HD13	1:D:169:ILE:O	2.11	0.50
1:A:89:HIS:CE1	2:A:379:HOH:O	2.65	0.50
1:B:105:VAL:HG23	1:B:106:ASN:N	2.27	0.50
1:D:80:LEU:C	1:D:83:PRO:HD2	2.37	0.50
1:D:105:VAL:HG23	1:D:106:ASN:N	2.27	0.50
1:A:298:ILE:HD13	1:A:298:ILE:O	2.10	0.50
1:C:74:VAL:HG13	1:C:75:ALA:N	2.26	0.50
1:B:19:THR:HG22	1:B:294:PHE:HE1	1.76	0.50
1:A:230:ARG:HG3	1:A:232:ILE:HG12	1.92	0.50
1:A:280:ASN:ND2	1:C:91:ARG:HD2	2.27	0.50
1:C:143:LEU:HB2	1:C:166:LEU:HD21	1.93	0.50
1:A:168:ILE:HD12	2:A:421:HOH:O	2.12	0.50
1:B:37:MSE:SE	1:B:240:ALA:HB2	2.62	0.50
1:D:241:ILE:CD1	1:D:266:ASN:HB3	2.39	0.50
1:B:194:MSE:HE2	1:B:284:VAL:CG2	2.41	0.50
1:B:274:GLN:HG3	2:B:364:HOH:O	2.12	0.50
1:D:194:MSE:HE2	1:D:284:VAL:CG2	2.42	0.50
1:B:50:ILE:HG13	1:B:54:GLU:HB2	1.94	0.49
1:C:207:ARG:HD2	2:C:499:HOH:O	2.12	0.49
1:C:188:SER:N	2:C:360:HOH:O	2.45	0.49
1:B:80:LEU:C	1:B:83:PRO:HD2	2.37	0.49
1:B:106:ASN:HA	1:B:109:ILE:HG12	1.94	0.49
1:B:273:ARG:NH1	2:B:399:HOH:O	2.46	0.49
1:C:61:HIS:O	1:C:62:LEU:HB2	2.12	0.49
1:C:63:ILE:HB	2:C:539:HOH:O	2.13	0.49
1:D:143:LEU:HD12	1:D:162:VAL:HG13	1.94	0.49
1:B:169:ILE:HD13	1:B:169:ILE:O	2.12	0.49
1:D:30:GLU:OE2	1:D:93:ARG:NH1	2.46	0.49
1:A:90:GLU:HB2	2:A:397:HOH:O	2.13	0.49
1:B:113:ASN:CG	1:B:115:GLY:H	2.20	0.49
1:B:198:THR:HG22	1:B:199:MSE:H	1.77	0.49
1:D:50:ILE:HG13	1:D:54:GLU:HB2	1.93	0.49
1:B:282:ALA:O	1:B:283:ASN:HB2	2.12	0.49
1:C:12:THR:O	1:C:13:ALA:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:O	1:B:13:ALA:HB3	2.13	0.48
1:A:290:THR:O	1:A:291:ASP:C	2.56	0.48
1:A:292:VAL:HG22	1:A:293:ASP:N	2.27	0.48
1:A:292:VAL:HG12	2:A:515:HOH:O	2.13	0.48
1:B:30:GLU:OE2	1:B:93:ARG:NH1	2.46	0.48
1:D:106:ASN:HA	1:D:109:ILE:HG12	1.94	0.48
1:A:280:ASN:HD22	1:C:91:ARG:HD2	1.79	0.48
2:A:332:HOH:O	1:B:114:LEU:HD22	2.12	0.48
1:C:89:HIS:CE1	2:C:449:HOH:O	2.65	0.48
1:B:67:ASP:HB2	2:B:351:HOH:O	2.13	0.48
1:D:113:ASN:CG	1:D:115:GLY:H	2.20	0.48
1:A:12:THR:O	1:A:13:ALA:HB3	2.13	0.48
1:C:163:ILE:O	1:C:167:GLU:HG3	2.14	0.48
1:B:143:LEU:HD12	1:B:162:VAL:HG13	1.96	0.48
1:B:33:SER:HB2	1:B:63:ILE:HD11	1.96	0.48
1:B:194:MSE:SE	2:B:482:HOH:O	2.82	0.47
1:C:38:GLN:HB2	2:C:391:HOH:O	2.14	0.47
1:C:290:THR:O	1:C:291:ASP:C	2.56	0.47
1:D:93:ARG:HG3	1:D:93:ARG:NH1	2.28	0.47
1:B:109:ILE:HB	1:B:192:LEU:HD11	1.96	0.47
1:C:145:LYS:O	1:C:145:LYS:HG2	2.13	0.47
1:D:109:ILE:HB	1:D:192:LEU:HD11	1.97	0.47
1:D:226:LYS:HD3	2:D:469:HOH:O	2.13	0.47
1:D:241:ILE:HD11	1:D:266:ASN:O	2.14	0.47
1:B:27:LEU:HD13	1:B:302:HIS:CD2	2.50	0.47
1:B:241:ILE:HD11	1:B:266:ASN:O	2.14	0.47
1:C:241:ILE:HD11	1:C:266:ASN:O	2.14	0.47
1:C:15:GLY:O	1:C:19:THR:HG23	2.15	0.47
1:A:145:LYS:O	1:A:145:LYS:HG2	2.14	0.46
1:C:90:GLU:HB2	2:C:413:HOH:O	2.13	0.46
1:D:110:HIS:HD2	2:D:362:HOH:O	1.98	0.46
1:D:241:ILE:O	1:D:241:ILE:HG23	2.15	0.46
1:D:282:ALA:O	1:D:283:ASN:HB2	2.14	0.46
1:C:102:GLY:HA2	1:C:105:VAL:HG22	1.96	0.46
1:B:93:ARG:HG3	1:B:93:ARG:NH1	2.29	0.46
1:D:27:LEU:HD13	1:D:302:HIS:CD2	2.50	0.46
1:C:292:VAL:HG22	1:C:293:ASP:N	2.28	0.46
1:D:241:ILE:HG22	2:D:562:HOH:O	2.14	0.46
1:A:102:GLY:HA2	1:A:105:VAL:HG22	1.96	0.46
1:A:125:HIS:HD2	2:A:479:HOH:O	1.99	0.46
1:A:241:ILE:HD11	1:A:266:ASN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ARG:HG2	2:B:355:HOH:O	2.15	0.46
1:C:293:ASP:OD2	1:C:296:LYS:HB2	2.16	0.46
1:B:19:THR:HG22	1:B:294:PHE:CE1	2.51	0.46
1:D:124:ARG:O	1:D:128:GLU:HG3	2.16	0.46
1:D:159:TYR:O	1:D:163:ILE:HG13	2.15	0.46
1:A:15:GLY:O	1:A:19:THR:HG23	2.16	0.46
1:A:308:LYS:HB2	2:A:467:HOH:O	2.15	0.46
1:B:11:PRO:HD3	1:B:275:LEU:HG	1.98	0.46
1:D:17:THR:O	1:D:21:VAL:HG13	2.15	0.46
1:A:225:LYS:O	1:A:229:ASP:HB2	2.16	0.45
1:B:156:PRO:CG	1:C:28:ASN:HB2	2.45	0.45
1:C:125:HIS:HD2	2:C:370:HOH:O	1.98	0.45
1:C:282:ALA:O	1:C:283:ASN:CB	2.64	0.45
1:C:242:GLY:N	2:C:430:HOH:O	2.48	0.45
1:A:280:ASN:HD22	1:A:280:ASN:HA	1.59	0.45
1:B:17:THR:O	1:B:21:VAL:HG13	2.16	0.45
1:C:40:TYR:HA	1:C:66:LYS:O	2.17	0.45
1:D:19:THR:HG22	1:D:294:PHE:CE1	2.51	0.45
1:D:131:VAL:CG1	1:D:139:LEU:HD22	2.45	0.45
1:B:43:MSE:HE1	1:B:237:SER:HB2	1.97	0.45
1:A:207:ARG:NH2	2:A:350:HOH:O	2.45	0.45
1:A:282:ALA:O	1:A:283:ASN:CB	2.64	0.45
1:D:21:VAL:O	1:D:25:LYS:HG3	2.17	0.45
1:D:33:SER:HB2	1:D:63:ILE:HD11	1.97	0.45
1:A:280:ASN:HD21	1:C:93:ARG:CZ	2.29	0.45
1:C:115:GLY:N	2:C:448:HOH:O	2.49	0.45
1:A:163:ILE:O	1:A:167:GLU:HG3	2.16	0.44
1:A:293:ASP:OD2	1:A:296:LYS:HB2	2.17	0.44
1:B:131:VAL:CG1	1:B:139:LEU:HD22	2.46	0.44
1:D:11:PRO:HD3	1:D:275:LEU:HG	1.99	0.44
1:A:2:LYS:N	2:A:426:HOH:O	2.50	0.44
1:B:241:ILE:HG23	1:B:241:ILE:O	2.16	0.44
1:C:225:LYS:O	1:C:229:ASP:HB2	2.17	0.44
1:A:188:SER:N	2:A:439:HOH:O	2.50	0.44
1:C:235:CYS:HB3	2:C:367:HOH:O	2.17	0.44
1:C:17:THR:O	1:C:21:VAL:HG13	2.17	0.44
1:D:12:THR:O	1:D:13:ALA:HB3	2.16	0.44
1:C:318:HIS:HB3	2:C:366:HOH:O	2.16	0.44
1:C:19:THR:HG21	1:C:289:MSE:CE	2.47	0.44
1:D:43:MSE:HE1	1:D:237:SER:HB2	1.99	0.44
1:A:74:VAL:CG1	1:A:75:ALA:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:GLY:O	1:B:19:THR:HG23	2.18	0.44
1:B:159:TYR:O	1:B:163:ILE:HG13	2.18	0.44
1:B:198:THR:HG23	1:B:275:LEU:CD2	2.43	0.44
1:C:280:ASN:HD22	1:C:280:ASN:HA	1.59	0.44
1:D:18:LYS:O	1:D:21:VAL:HG22	2.18	0.44
1:B:33:SER:CB	1:B:63:ILE:HD11	2.48	0.44
1:A:85:ILE:HB	2:A:493:HOH:O	2.18	0.43
1:A:238:VAL:O	1:A:238:VAL:CG1	2.66	0.43
1:B:124:ARG:O	1:B:128:GLU:HG3	2.17	0.43
1:A:40:TYR:HA	1:A:66:LYS:O	2.18	0.43
1:C:22:MSE:SE	2:C:385:HOH:O	2.86	0.43
1:C:105:VAL:HG23	1:C:106:ASN:N	2.33	0.43
1:A:117:ILE:HD12	1:A:117:ILE:N	2.33	0.43
1:A:317:HIS:O	1:A:318:HIS:C	2.61	0.43
1:C:30:GLU:OE1	1:C:88:ILE:HG12	2.19	0.43
1:C:169:ILE:O	1:C:172:THR:HG22	2.17	0.43
1:A:204:LEU:O	1:A:208:ILE:HG13	2.18	0.43
1:B:230:ARG:NH1	2:B:412:HOH:O	2.51	0.43
1:B:281:LYS:HG2	2:B:454:HOH:O	2.18	0.43
1:A:169:ILE:O	1:A:172:THR:HG22	2.18	0.43
1:C:16:LYS:HE2	1:C:99:GLY:HA2	2.00	0.43
1:C:38:GLN:HE22	1:C:49:LYS:HA	1.82	0.43
1:D:2:LYS:NZ	1:D:2:LYS:HB2	2.33	0.43
1:D:154:ILE:HD12	1:D:162:VAL:HG22	2.00	0.43
1:D:198:THR:HG23	1:D:275:LEU:CD2	2.45	0.43
1:A:36:SER:HB3	1:A:104:TYR:CE2	2.54	0.43
1:B:241:ILE:O	1:B:241:ILE:HG12	2.18	0.43
1:A:192:LEU:C	1:A:192:LEU:HD23	2.44	0.43
1:B:18:LYS:O	1:B:21:VAL:HG22	2.19	0.43
1:A:150:ALA:O	1:A:153:ALA:HB3	2.18	0.43
1:C:238:VAL:O	1:C:238:VAL:CG1	2.67	0.43
1:A:38:GLN:HE22	1:A:49:LYS:HA	1.83	0.43
1:A:132:ASN:ND2	1:B:101:THR:HB	2.34	0.43
1:B:154:ILE:HD12	1:B:162:VAL:HG22	2.00	0.43
1:C:50:ILE:HG13	1:C:54:GLU:HB2	2.01	0.43
1:C:277:TRP:NE1	2:C:392:HOH:O	2.51	0.43
1:C:117:ILE:HD12	1:C:117:ILE:N	2.33	0.42
1:C:242:GLY:CA	2:C:430:HOH:O	2.66	0.42
2:C:351:HOH:O	1:D:74:VAL:HG12	2.19	0.42
1:A:3:GLU:OE1	1:A:85:ILE:HG22	2.18	0.42
1:A:17:THR:O	1:A:21:VAL:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HG13	1:A:54:GLU:HB2	2.02	0.42
1:A:241:ILE:CD1	1:A:266:ASN:HB3	2.48	0.42
1:C:150:ALA:O	1:C:153:ALA:HB3	2.19	0.42
1:A:40:TYR:CD1	1:A:68:PRO:HA	2.54	0.42
1:A:105:VAL:HG23	1:A:106:ASN:N	2.33	0.42
1:B:242:GLY:HA2	1:B:263:LEU:HD13	2.01	0.42
1:C:204:LEU:O	1:C:208:ILE:HG13	2.19	0.42
1:C:241:ILE:CD1	1:C:266:ASN:HB3	2.49	0.42
1:A:16:LYS:HE2	1:A:99:GLY:HA2	2.01	0.42
1:A:155:HIS:HD2	1:A:156:PRO:HD2	1.83	0.42
1:C:35:ASP:OD2	1:C:35:ASP:C	2.62	0.42
1:C:110:HIS:HE1	1:C:281:LYS:HZ1	1.67	0.42
1:C:193:VAL:HG22	1:C:308:LYS:HD3	2.01	0.42
1:D:15:GLY:O	1:D:19:THR:HG23	2.18	0.42
1:A:30:GLU:OE1	1:A:88:ILE:HG12	2.19	0.42
1:A:151:ALA:C	1:A:153:ALA:H	2.27	0.42
1:C:43:MSE:SE	1:C:237:SER:HB2	2.70	0.42
1:D:33:SER:CB	1:D:63:ILE:HD11	2.49	0.42
1:A:43:MSE:SE	1:A:237:SER:HB2	2.70	0.42
1:C:40:TYR:CD1	1:C:68:PRO:HA	2.55	0.42
1:C:27:LEU:HD13	1:C:302:HIS:CD2	2.54	0.42
1:C:132:ASN:ND2	1:D:101:THR:HB	2.35	0.42
1:C:151:ALA:C	1:C:153:ALA:H	2.28	0.42
1:A:35:ASP:C	1:A:35:ASP:OD2	2.61	0.42
1:C:3:GLU:OE1	1:C:85:ILE:HG22	2.20	0.42
1:C:30:GLU:OE2	1:C:93:ARG:NH1	2.53	0.42
1:A:27:LEU:HD13	1:A:302:HIS:CD2	2.55	0.41
1:A:110:HIS:HE1	1:A:281:LYS:HZ1	1.66	0.41
1:C:43:MSE:HG2	1:C:227:LEU:HD11	2.02	0.41
1:C:50:ILE:HD13	1:C:60:HIS:CE1	2.55	0.41
1:C:106:ASN:HA	1:C:109:ILE:HG12	2.02	0.41
1:D:241:ILE:O	1:D:241:ILE:HG12	2.20	0.41
1:B:26:ARG:HG3	1:B:302:HIS:CD2	2.55	0.41
1:C:36:SER:HB3	1:C:104:TYR:CE2	2.55	0.41
1:C:155:HIS:HD2	1:C:156:PRO:HD2	1.84	0.41
1:A:193:VAL:HG22	1:A:308:LYS:HD3	2.02	0.41
1:D:131:VAL:HG13	1:D:139:LEU:HD13	2.01	0.41
1:C:74:VAL:CG1	1:C:75:ALA:N	2.82	0.41
1:B:21:VAL:O	1:B:25:LYS:HG3	2.19	0.41
1:B:105:VAL:HG21	1:B:278:PHE:HE2	1.85	0.41
1:A:241:ILE:HD13	1:A:270:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LYS:HE2	1:B:272:LYS:HB3	1.87	0.41
1:D:162:VAL:HG21	2:D:361:HOH:O	2.20	0.41
1:A:30:GLU:OE2	1:A:93:ARG:NH1	2.54	0.41
1:A:50:ILE:HD13	1:A:60:HIS:CE1	2.56	0.41
1:A:200:GLU:CD	1:A:290:THR:HG21	2.45	0.41
1:B:135:GLY:N	2:B:340:HOH:O	2.51	0.41
1:C:200:GLU:CD	1:C:290:THR:HG21	2.46	0.41
1:A:143:LEU:HD22	1:A:146:ILE:HG22	2.02	0.41
1:B:21:VAL:HG11	1:B:54:GLU:O	2.21	0.41
1:B:193:VAL:HG22	1:B:308:LYS:HD3	2.03	0.41
1:B:269:ARG:NH2	1:B:269:ARG:HG2	2.36	0.41
1:C:74:VAL:HG12	2:C:376:HOH:O	2.21	0.41
1:C:241:ILE:HD13	1:C:270:TYR:HB2	2.01	0.41
1:D:242:GLY:HA2	1:D:263:LEU:HD13	2.02	0.41
1:A:241:ILE:C	2:A:355:HOH:O	2.64	0.40
1:D:105:VAL:HG21	1:D:278:PHE:HE2	1.86	0.40
1:A:10:GLY:O	1:A:16:LYS:HE3	2.21	0.40
1:A:43:MSE:HG2	1:A:227:LEU:HD11	2.03	0.40
1:B:205:TYR:CG	1:B:268:ARG:HD2	2.56	0.40
1:D:26:ARG:HG3	1:D:302:HIS:CD2	2.56	0.40
1:B:30:GLU:HB3	1:B:59:PRO:HG2	2.03	0.40
1:B:131:VAL:HG13	1:B:139:LEU:HD13	2.03	0.40
1:D:30:GLU:HB3	1:D:59:PRO:HG2	2.03	0.40
1:A:19:THR:HG21	1:A:289:MSE:CE	2.46	0.40
1:A:49:LYS:NZ	1:A:64:ASP:OD2	2.53	0.40
1:C:151:ALA:C	1:C:153:ALA:N	2.79	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	299/322 (93%)	280 (94%)	16 (5%)	3 (1%)	12	15
1	B	298/322 (92%)	279 (94%)	14 (5%)	5 (2%)	7	7
1	C	299/322 (93%)	279 (93%)	17 (6%)	3 (1%)	12	15
1	D	298/322 (92%)	280 (94%)	13 (4%)	5 (2%)	7	7
All	All	1194/1288 (93%)	1118 (94%)	60 (5%)	16 (1%)	9	10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	ILE
1	B	241	ILE
1	C	241	ILE
1	D	241	ILE
1	A	291	ASP
1	A	242	GLY
1	B	242	GLY
1	C	242	GLY
1	C	291	ASP
1	D	242	GLY
1	B	292	VAL
1	D	147	ASP
1	D	292	VAL
1	B	147	ASP
1	B	172	THR
1	D	172	THR

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	261/268 (97%)	246 (94%)	15 (6%)	18	27
1	B	260/268 (97%)	246 (95%)	14 (5%)	20	29
1	C	261/268 (97%)	246 (94%)	15 (6%)	18	27
1	D	260/268 (97%)	244 (94%)	16 (6%)	16	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1042/1072 (97%)	982 (94%)	60 (6%)	18	26

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	16	LYS
1	A	27	LEU
1	A	62	LEU
1	A	84	LEU
1	A	124	ARG
1	A	133	SER
1	A	146	ILE
1	A	164	ARG
1	A	198	THR
1	A	211	ARG
1	A	250	LEU
1	A	269	ARG
1	A	280	ASN
1	A	298	ILE
1	B	16	LYS
1	B	27	LEU
1	B	124	ARG
1	B	143	LEU
1	B	149	LYS
1	B	169	ILE
1	B	192	LEU
1	B	198	THR
1	B	211	ARG
1	B	250	LEU
1	B	269	ARG
1	B	273	ARG
1	B	298	ILE
1	B	317	HIS
1	C	12	THR
1	C	16	LYS
1	C	27	LEU
1	C	62	LEU
1	C	84	LEU
1	C	124	ARG
1	C	133	SER
1	C	146	ILE

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Mol	Chain	Res	Type
1	C	164	ARG
1	C	198	THR
1	C	211	ARG
1	C	250	LEU
1	C	269	ARG
1	C	280	ASN
1	C	298	ILE
1	D	2	LYS
1	D	16	LYS
1	D	27	LEU
1	D	124	ARG
1	D	143	LEU
1	D	149	LYS
1	D	161	ARG
1	D	169	ILE
1	D	192	LEU
1	D	198	THR
1	D	211	ARG
1	D	250	LEU
1	D	269	ARG
1	D	273	ARG
1	D	298	ILE
1	D	317	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	38	GLN
1	A	60	HIS
1	A	110	HIS
1	A	111	GLN
1	A	113	ASN
1	A	125	HIS
1	A	132	ASN
1	A	137	GLN
1	A	155	HIS
1	A	157	ASN
1	A	253	ASN
1	A	280	ASN
1	A	283	ASN
1	A	302	HIS

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Mol	Chain	Res	Type
1	B	28	ASN
1	B	60	HIS
1	B	61	HIS
1	B	110	HIS
1	B	113	ASN
1	B	137	GLN
1	B	140	HIS
1	B	157	ASN
1	B	253	ASN
1	B	280	ASN
1	B	283	ASN
1	C	60	HIS
1	C	110	HIS
1	C	111	GLN
1	C	113	ASN
1	C	125	HIS
1	C	132	ASN
1	C	137	GLN
1	C	155	HIS
1	C	253	ASN
1	C	280	ASN
1	C	283	ASN
1	C	302	HIS
1	D	28	ASN
1	D	60	HIS
1	D	61	HIS
1	D	110	HIS
1	D	140	HIS
1	D	157	ASN
1	D	253	ASN
1	D	280	ASN
1	D	283	ASN
1	D	302	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [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	293/322 (90%)	0.28	11 (3%) 44 46	9, 27, 52, 80	0
1	B	292/322 (90%)	0.32	14 (4%) 35 37	8, 26, 62, 75	0
1	C	293/322 (90%)	0.24	11 (3%) 44 46	10, 27, 53, 74	0
1	D	292/322 (90%)	0.36	17 (5%) 29 31	10, 27, 61, 74	0
All	All	1170/1288 (90%)	0.30	53 (4%) 38 40	8, 27, 58, 80	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	VAL	4.0
1	B	150	ALA	3.9
1	B	154	ILE	3.8
1	A	318	HIS	3.7
1	C	113	ASN	3.4
1	D	152	ALA	3.4
1	D	154	ILE	3.3
1	C	146	ILE	3.3
1	C	318	HIS	3.3
1	A	114	LEU	3.2
1	A	292	VAL	3.1
1	B	152	ALA	3.1
1	D	113	ASN	3.1
1	D	150	ALA	3.1
1	C	277	TRP	3.1
1	C	291	ASP	3.1
1	D	134	TYR	3.0
1	D	153	ALA	2.9
1	C	292	VAL	2.9
1	B	113	ASN	2.9
1	D	292	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	153	ALA	2.8
1	B	134	TYR	2.8
1	A	277	TRP	2.8
1	B	155	HIS	2.8
1	D	158	ASN	2.8
1	A	113	ASN	2.8
1	B	291	ASP	2.7
1	C	114	LEU	2.7
1	A	115	GLY	2.6
1	A	146	ILE	2.6
1	D	148	PRO	2.6
1	D	125	HIS	2.6
1	D	146	ILE	2.6
1	D	173	GLY	2.6
1	C	117	ILE	2.6
1	D	156	PRO	2.5
1	B	148	PRO	2.5
1	D	119	ALA	2.5
1	B	114	LEU	2.4
1	A	291	ASP	2.4
1	C	173	GLY	2.4
1	D	114	LEU	2.4
1	C	119	ALA	2.3
1	B	160	ARG	2.2
1	D	317	HIS	2.1
1	A	173	GLY	2.1
1	C	115	GLY	2.1
1	B	117	ILE	2.1
1	A	119	ALA	2.1
1	D	117	ILE	2.1
1	A	131	VAL	2.1
1	B	317	HIS	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.