



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:23 PM UTC

PDB ID : 7BJ5 / pdb_00007bj5
Title : Inulosucrase from Halalkalicoccus jeotgali
Authors : Ghauri, K.; Pijning, T.; Munawar, N.; Ali, H.; Ghauri, M.A.; Anwar, M.A.; Wallis, R.
Deposited on : 2021-01-14
Resolution : 2.75 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

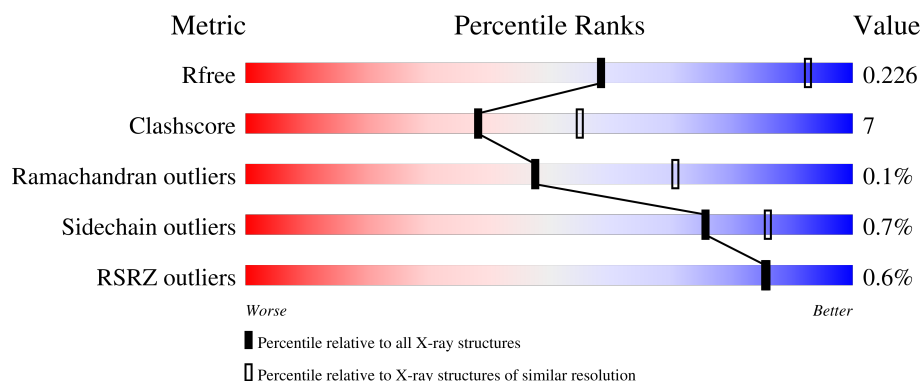
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	428	 81% 13% 5%
1	B	428	 79% 16% 5%
1	C	428	 83% 12% 5%
1	D	428	 79% 16% 5%
1	E	428	 82% 13% 5%

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Mol	Chain	Length	Quality of chain
1	F	428	83%12%5%
1	G	428	% 77%17%5%
1	H	428	2% 74%20%5%
1	I	428	% 78%16%5%
1	J	428	81%14%5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31875 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 Levansucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	B	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	C	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	D	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	E	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	F	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	G	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	H	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	I	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	J	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	6	Total	O	0	0
			6	6		
2	C	11	Total	O	0	0
			11	11		
2	D	14	Total	O	0	0
			14	14		

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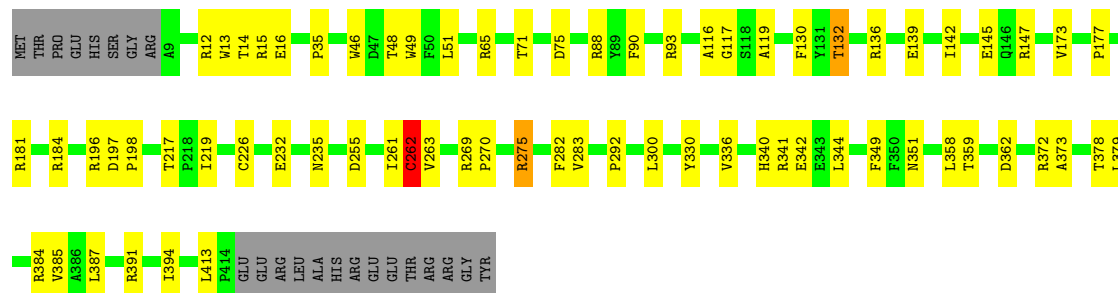
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	9	Total 9	O 9	0	0
2	F	16	Total 16	O 16	0	0
2	H	4	Total 4	O 4	0	0
2	I	8	Total 8	O 8	0	0
2	J	4	Total 4	O 4	0	0

- Molecule 1: Levansucrase



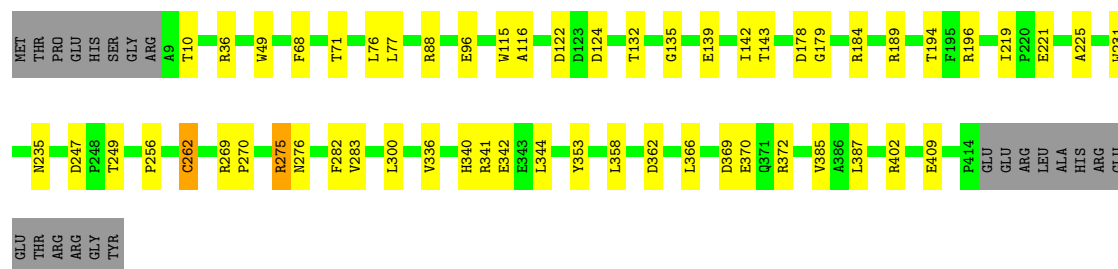
● Molecule 1: Levansucrase

Chain D:  79% 16% 5%



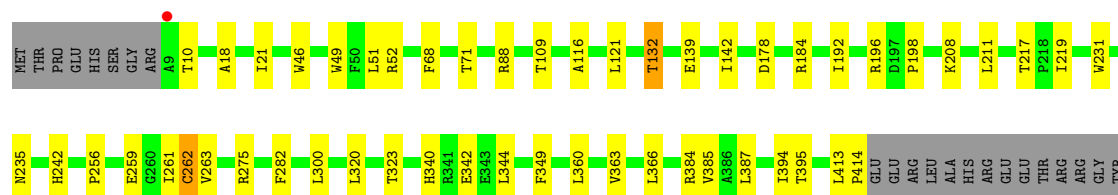
● Molecule 1: Levansucrase

Chain E:  82% 13% 5%



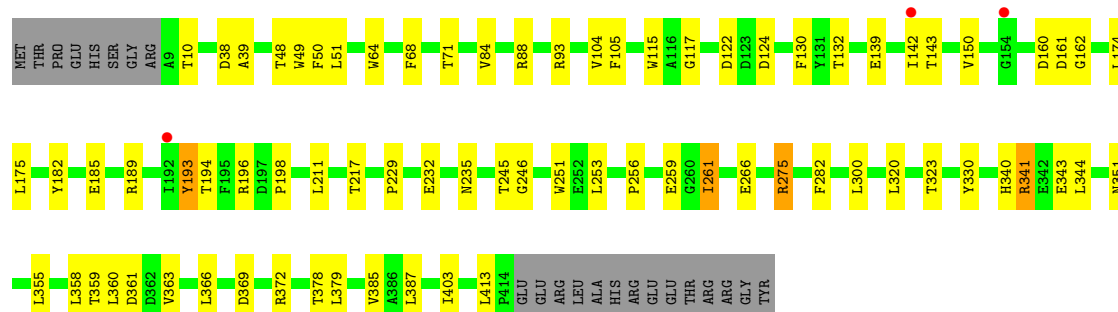
● Molecule 1: Levansucrase

Chain F:  83% 12% 5%

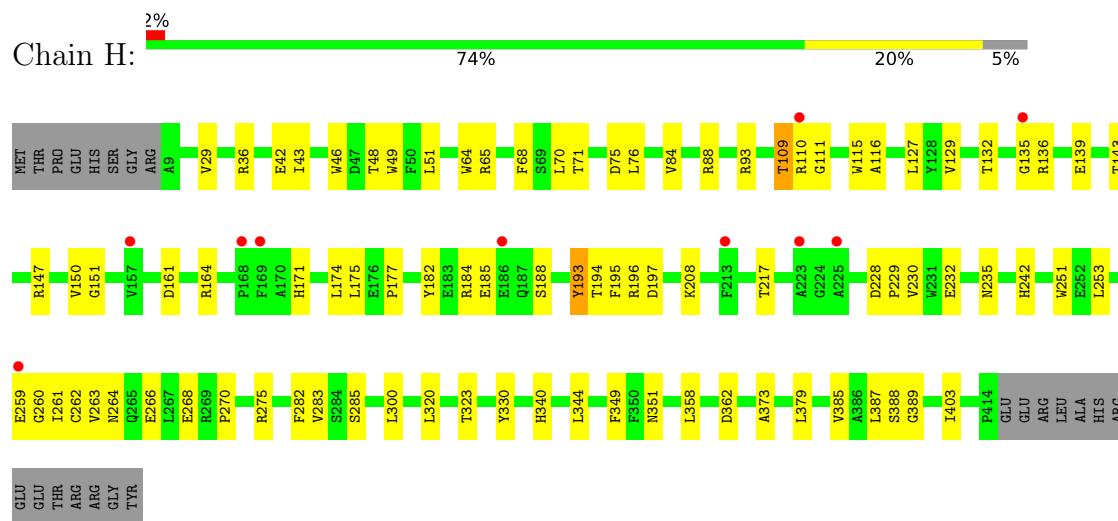


● Molecule 1: Levansucrase

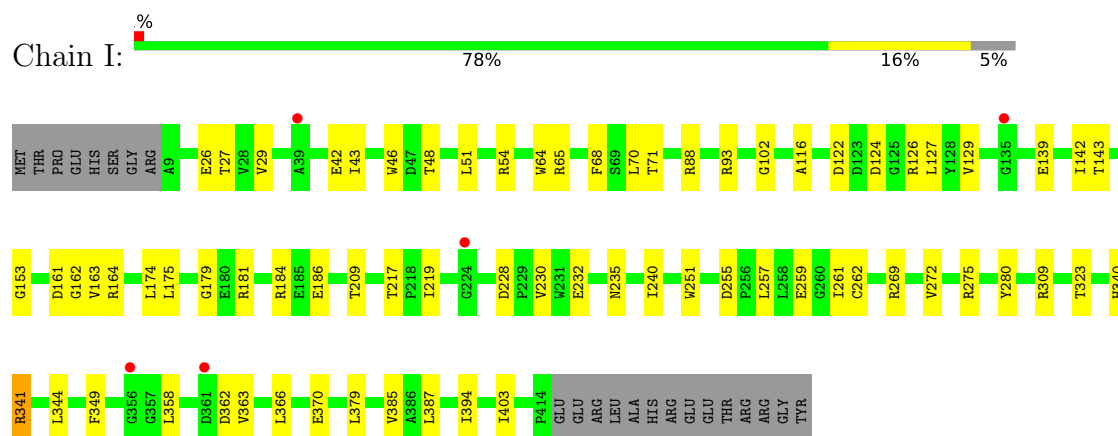
Chain G:  77% 17% 5%



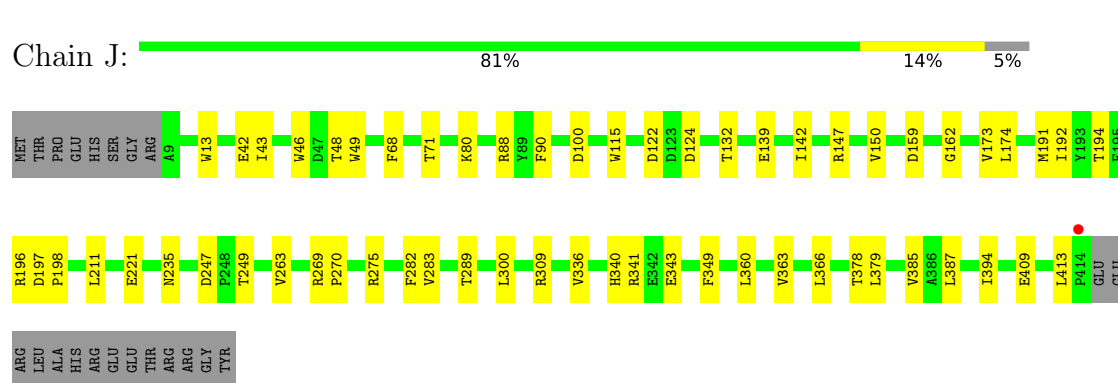
● Molecule 1: Levansucrase



● Molecule 1: Levansucrase



● Molecule 1: Levansucrase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.54Å 143.26Å 172.76Å 90.00° 98.30° 90.00°	Depositor
Resolution (Å)	105.82 – 2.75 105.82 – 2.75	Depositor EDS
% Data completeness (in resolution range)	57.9 (105.82-2.75) 58.1 (105.82-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.26	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.182 , 0.228 0.184 , 0.226	Depositor DCC
R_{free} test set	4331 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31875	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 35.61 % 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 5.6812e-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	0.23	0/3274	0.50	0/4466
1	B	0.24	0/3274	0.54	2/4466 (0.0%)
1	C	0.24	0/3274	0.52	2/4466 (0.0%)
1	D	0.26	0/3274	0.53	1/4466 (0.0%)
1	E	0.25	0/3274	0.54	2/4466 (0.0%)
1	F	0.25	0/3274	0.52	3/4466 (0.1%)
1	G	0.22	0/3274	0.51	0/4466
1	H	0.25	0/3274	0.55	2/4466 (0.0%)
1	I	0.23	0/3274	0.49	0/4466
1	J	0.23	0/3274	0.52	2/4466 (0.0%)
All	All	0.24	0/32740	0.52	14/44660 (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
1	D	0	2
1	E	0	1
1	G	0	2
1	I	0	1
All	All	0	7

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	262	CYS	CA-CB-SG	-6.66	99.09	114.40
1	D	262	CYS	CA-CB-SG	6.14	128.51	114.40
1	H	340	HIS	CA-C-N	5.64	132.31	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	340	HIS	C-N-CA	5.64	132.31	121.54
1	E	340	HIS	CA-C-N	5.58	132.20	121.54
1	E	340	HIS	C-N-CA	5.58	132.20	121.54
1	C	340	HIS	CA-C-N	5.52	132.08	121.54
1	C	340	HIS	C-N-CA	5.52	132.08	121.54
1	J	340	HIS	CA-C-N	5.47	131.99	121.54
1	J	340	HIS	C-N-CA	5.47	131.99	121.54
1	B	340	HIS	CA-C-N	5.47	131.98	121.54
1	B	340	HIS	C-N-CA	5.47	131.98	121.54
1	F	340	HIS	CA-C-N	5.46	131.97	121.54
1	F	340	HIS	C-N-CA	5.46	131.97	121.54

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	HIS	Peptide
1	D	275	ARG	Peptide
1	D	340	HIS	Peptide
1	E	275	ARG	Peptide
1	G	275	ARG	Peptide
1	G	340	HIS	Peptide
1	I	340	HIS	Peptide

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	3180	0	2977	38	0
1	B	3180	0	2977	44	0
1	C	3180	0	2977	36	0
1	D	3180	0	2977	46	0
1	E	3180	0	2977	35	0
1	F	3180	0	2977	35	0
1	G	3180	0	2977	51	0
1	H	3180	0	2977	58	0
1	I	3180	0	2977	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3180	0	2977	38	0
2	A	3	0	0	0	0
2	B	6	0	0	1	0
2	C	11	0	0	1	0
2	D	14	0	0	2	0
2	E	9	0	0	0	0
2	F	16	0	0	4	0
2	H	4	0	0	0	0
2	I	8	0	0	3	0
2	J	4	0	0	0	0
All	All	31875	0	29770	422	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 7.

All (422) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:ASP:OD1	1:H:164:ARG:NH1	2.04	0.89
1:E:275:ARG:HD3	1:E:387:LEU:HD12	1.59	0.83
1:I:54:ARG:NH1	2:I:501:HOH:O	2.12	0.82
1:G:150:VAL:HG12	1:G:174:LEU:HD11	1.61	0.81
1:J:341:ARG:HH12	1:J:409:GLU:HG2	1.50	0.77
1:I:255:ASP:HB2	1:I:309:ARG:HH22	1.51	0.76
1:E:219:ILE:HD11	1:E:225:ALA:HB3	1.67	0.75
1:C:219:ILE:HD11	1:C:225:ALA:HB3	1.67	0.74
1:H:109:THR:HA	1:H:171:HIS:CE1	2.22	0.74
1:B:175:LEU:HD11	1:B:251:TRP:HB2	1.69	0.73
1:I:54:ARG:NH2	1:I:209:THR:OG1	2.20	0.73
1:A:341:ARG:HH12	1:A:409:GLU:HG2	1.53	0.72
1:J:132:THR:HG21	1:J:197:ASP:H	1.53	0.72
1:H:150:VAL:O	1:H:171:HIS:HB2	1.90	0.71
1:F:52:ARG:NH1	2:F:502:HOH:O	2.18	0.71
1:G:10:THR:HG21	1:G:256:PRO:HG2	1.73	0.71
1:C:10:THR:HG21	1:C:256:PRO:HG2	1.73	0.69
1:J:363:VAL:HA	1:J:366:LEU:HD13	1.73	0.69
1:B:372:ARG:NH2	1:J:221:GLU:OE2	2.25	0.68
1:J:159:ASP:OD1	1:J:162:GLY:N	2.25	0.68
1:D:181:ARG:NH1	1:D:255:ASP:OD1	2.28	0.67
1:F:10:THR:HG21	1:F:256:PRO:HG2	1.76	0.67
1:C:189:ARG:HH21	1:C:219:ILE:HG23	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ARG:HE	1:D:173:VAL:HG21	1.61	0.65
1:D:261:ILE:O	1:D:262:CYS:HB2	1.96	0.65
1:E:341:ARG:HH12	1:E:409:GLU:HG2	1.59	0.65
1:E:179:GLY:HA3	1:E:184:ARG:NH2	2.12	0.64
1:A:161:ASP:OD1	1:C:147:ARG:NH2	2.29	0.64
1:B:136:ARG:N	1:B:139:GLU:OE2	2.31	0.63
1:J:385:VAL:HG12	1:J:394:ILE:HD13	1.80	0.63
1:G:115:TRP:HB2	1:G:132:THR:HB	1.81	0.63
1:D:270:PRO:HB3	1:D:283:VAL:HG12	1.81	0.63
1:E:10:THR:HG21	1:E:256:PRO:HG2	1.79	0.63
1:H:174:LEU:HB3	1:H:175:LEU:HD12	1.81	0.62
1:E:96:GLU:OE2	1:E:402:ARG:NH1	2.32	0.62
1:H:175:LEU:HD11	1:H:251:TRP:HB2	1.80	0.62
1:J:115:TRP:HB2	1:J:132:THR:OG1	1.99	0.62
1:F:208:LYS:HE3	1:F:242:HIS:CE1	2.35	0.62
1:E:275:ARG:HH22	1:E:342:GLU:HA	1.65	0.62
1:G:229:PRO:O	1:G:232:GLU:HG2	2.00	0.62
1:F:385:VAL:HG12	1:F:394:ILE:HD13	1.82	0.62
1:B:275:ARG:HH22	1:B:342:GLU:HA	1.65	0.61
1:C:363:VAL:HA	1:C:366:LEU:HD13	1.82	0.61
1:H:320:LEU:HD11	1:H:323:THR:HB	1.83	0.61
1:F:414:PRO:O	2:F:501:HOH:O	2.16	0.61
1:B:184:ARG:HG2	1:B:186:GLU:OE1	2.01	0.60
1:D:132:THR:HG23	1:D:198:PRO:HD3	1.81	0.60
1:I:175:LEU:HD11	1:I:251:TRP:HB2	1.84	0.60
1:J:191:MET:HE1	1:J:289:THR:HG22	1.82	0.60
1:H:151:GLY:HA2	1:H:171:HIS:HB3	1.83	0.60
1:I:363:VAL:HA	1:I:366:LEU:HD13	1.83	0.60
1:C:132:THR:HG21	1:C:197:ASP:H	1.66	0.59
1:I:65:ARG:NH1	1:I:403:ILE:O	2.33	0.59
1:H:217:THR:HG21	1:H:259:GLU:OE2	2.02	0.59
1:A:341:ARG:NH1	1:A:409:GLU:HG2	2.18	0.59
1:C:132:THR:HG23	1:C:198:PRO:HD3	1.85	0.58
1:C:243:SER:OG	1:C:245:THR:O	2.15	0.58
1:D:385:VAL:HG12	1:D:394:ILE:HD13	1.85	0.58
1:G:182:TYR:HD2	1:G:253:LEU:HD23	1.68	0.58
1:H:229:PRO:O	1:H:232:GLU:HG2	2.02	0.58
1:G:189:ARG:NH1	1:G:232:GLU:OE2	2.36	0.58
1:G:275:ARG:HD3	1:G:387:LEU:HD12	1.86	0.58
1:G:142:ILE:H	1:G:142:ILE:HD12	1.67	0.58
1:J:147:ARG:HE	1:J:173:VAL:HG21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:27:THR:HA	1:I:394:ILE:HD13	1.86	0.57
1:J:247:ASP:OD2	1:J:249:THR:OG1	2.19	0.57
1:B:275:ARG:HD3	1:B:387:LEU:HD12	1.87	0.57
1:G:174:LEU:HD23	1:G:251:TRP:CD1	2.40	0.57
1:A:139:GLU:OE2	1:A:142:ILE:HA	2.05	0.57
1:E:189:ARG:HD2	1:E:221:GLU:HG2	1.86	0.57
1:D:359:THR:HG22	1:D:362:ASP:CG	2.30	0.56
1:A:115:TRP:HB2	1:A:132:THR:HB	1.87	0.56
1:F:282:PHE:HB3	1:F:300:LEU:HD11	1.88	0.56
1:H:185:GLU:H	1:H:185:GLU:CD	2.13	0.56
1:H:194:THR:HG21	1:H:266:GLU:HG2	1.88	0.56
1:D:275:ARG:HD3	1:D:387:LEU:HD12	1.88	0.56
1:F:275:ARG:HH22	1:F:342:GLU:HA	1.71	0.55
1:E:247:ASP:OD2	1:E:249:THR:OG1	2.20	0.55
1:A:359:THR:OG1	1:A:361:ASP:OD1	2.24	0.55
1:B:65:ARG:HH22	1:B:408:GLU:CD	2.13	0.55
1:B:235:ASN:HA	1:B:261:ILE:HD13	1.89	0.55
1:F:413:LEU:O	2:F:501:HOH:O	2.18	0.55
1:G:320:LEU:HD11	1:G:323:THR:HB	1.89	0.55
1:E:269:ARG:HH21	1:E:336:VAL:HG11	1.72	0.55
1:I:139:GLU:OE2	1:I:142:ILE:HA	2.07	0.55
1:H:136:ARG:O	1:H:139:GLU:HG3	2.06	0.55
1:B:363:VAL:HA	1:B:366:LEU:HD13	1.89	0.54
1:A:136:ARG:NH1	1:A:145:GLU:OE2	2.40	0.54
1:B:136:ARG:O	1:B:139:GLU:HG3	2.07	0.54
1:G:175:LEU:HD11	1:G:251:TRP:HB2	1.90	0.54
1:B:282:PHE:HB3	1:B:300:LEU:HD11	1.89	0.54
1:E:353:TYR:OH	1:H:36:ARG:NH2	2.41	0.54
1:B:174:LEU:HB3	1:B:175:LEU:HD12	1.90	0.54
1:B:185:GLU:HG3	1:B:193:TYR:CE1	2.43	0.54
1:H:109:THR:HA	1:H:171:HIS:HE1	1.69	0.53
1:A:269:ARG:NH1	1:A:334:SER:OG	2.37	0.53
1:I:261:ILE:HG22	1:I:262:CYS:SG	2.48	0.53
1:D:132:THR:HG21	1:D:196:ARG:HA	1.89	0.53
1:F:219:ILE:HD11	1:F:261:ILE:HD12	1.90	0.53
1:J:275:ARG:HD2	1:J:387:LEU:HD12	1.90	0.53
1:A:384:ARG:NH2	1:A:413:LEU:HD11	2.24	0.53
1:C:282:PHE:HB3	1:C:300:LEU:HD11	1.90	0.53
1:J:71:THR:HG21	1:J:88:ARG:HD3	1.90	0.53
1:J:132:THR:HG21	1:J:196:ARG:HB2	1.90	0.52
1:E:369:ASP:OD1	1:E:372:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:LEU:HB3	1:I:175:LEU:HD12	1.92	0.52
1:B:217:THR:OG1	1:B:261:ILE:HD11	2.09	0.52
1:H:275:ARG:HD3	1:H:387:LEU:HD12	1.92	0.52
1:G:182:TYR:CD2	1:G:253:LEU:HD23	2.44	0.52
1:C:275:ARG:HH22	1:C:342:GLU:HA	1.74	0.52
1:J:275:ARG:NH2	1:J:343:GLU:O	2.43	0.52
1:F:363:VAL:HA	1:F:366:LEU:HD13	1.92	0.52
1:J:132:THR:CG2	1:J:197:ASP:H	2.22	0.52
1:B:161:ASP:OD1	1:B:162:GLY:N	2.43	0.51
1:C:64:TRP:CZ3	1:C:93:ARG:HG3	2.45	0.51
1:G:363:VAL:HA	1:G:366:LEU:HD13	1.93	0.51
1:E:282:PHE:HB3	1:E:300:LEU:HD11	1.93	0.51
1:I:344:LEU:HB3	1:I:385:VAL:HG22	1.93	0.51
1:D:391:ARG:NH2	2:D:502:HOH:O	2.44	0.51
1:E:358:LEU:HD22	1:E:362:ASP:HB3	1.93	0.51
1:I:240:ILE:HD12	1:I:257:LEU:HD11	1.92	0.51
1:E:344:LEU:HD22	1:E:387:LEU:HD11	1.93	0.51
1:D:358:LEU:HD22	1:D:362:ASP:HB3	1.93	0.51
1:E:116:ALA:HB1	1:E:269:ARG:NH1	2.26	0.50
1:H:136:ARG:HG2	1:H:147:ARG:HH22	1.76	0.50
1:D:14:THR:OG1	1:D:16:GLU:HG2	2.11	0.50
1:H:193:TYR:CD1	1:H:193:TYR:C	2.89	0.50
1:D:71:THR:HG21	1:D:88:ARG:HD3	1.93	0.50
1:H:196:ARG:NH1	1:H:197:ASP:OD1	2.45	0.50
1:D:269:ARG:HH21	1:D:336:VAL:HG11	1.76	0.50
1:E:71:THR:HG21	1:E:88:ARG:HD2	1.93	0.50
1:J:270:PRO:HB3	1:J:283:VAL:HG12	1.92	0.50
1:C:275:ARG:HD3	1:C:387:LEU:HD12	1.94	0.50
1:G:369:ASP:OD1	1:G:372:ARG:NH1	2.45	0.50
1:H:151:GLY:HA2	1:H:171:HIS:CB	2.41	0.50
1:I:344:LEU:HD22	1:I:387:LEU:HD11	1.93	0.50
1:A:194:THR:HG22	1:A:196:ARG:HH12	1.76	0.50
1:D:12:ARG:NH2	2:D:501:HOH:O	2.28	0.50
1:G:359:THR:OG1	1:G:361:ASP:OD1	2.26	0.50
1:H:185:GLU:HA	1:H:188:SER:HB2	1.94	0.50
1:A:385:VAL:HG12	1:A:394:ILE:HD13	1.93	0.49
1:B:36:ARG:HH12	1:D:373:ALA:HB2	1.77	0.49
1:B:71:THR:HG21	1:B:88:ARG:HD3	1.94	0.49
1:A:13:TRP:O	1:A:263:VAL:HG21	2.12	0.49
1:D:136:ARG:NH1	1:D:145:GLU:OE2	2.44	0.49
1:F:132:THR:HG23	1:F:198:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:THR:HG21	1:D:196:ARG:CA	2.42	0.49
1:E:231:TRP:HB3	1:E:262:CYS:HB3	1.94	0.49
1:G:64:TRP:CZ3	1:G:93:ARG:HG3	2.48	0.49
1:D:219:ILE:HD11	1:D:261:ILE:HG12	1.94	0.49
1:D:275:ARG:HH22	1:D:342:GLU:HA	1.77	0.49
1:I:275:ARG:HD3	1:I:387:LEU:HD12	1.94	0.49
1:F:275:ARG:HD3	1:F:387:LEU:HD12	1.94	0.49
1:B:115:TRP:HB2	1:B:132:THR:HB	1.94	0.49
1:D:282:PHE:HB3	1:D:300:LEU:HD11	1.95	0.49
1:F:139:GLU:OE2	1:F:142:ILE:HA	2.13	0.49
1:F:71:THR:HG21	1:F:88:ARG:HD3	1.94	0.48
1:F:320:LEU:HD11	1:F:323:THR:HB	1.96	0.48
1:A:76:LEU:HD23	1:A:77:LEU:O	2.13	0.48
1:A:282:PHE:HB3	1:A:300:LEU:HD11	1.95	0.48
1:A:358:LEU:HD22	1:A:362:ASP:HB3	1.94	0.48
1:C:132:THR:HG21	1:C:196:ARG:HA	1.94	0.48
1:F:46:TRP:HB2	1:F:349:PHE:CE1	2.49	0.48
1:D:217:THR:OG1	1:D:261:ILE:HD11	2.13	0.48
1:G:282:PHE:HB3	1:G:300:LEU:HD11	1.96	0.48
1:I:142:ILE:HD12	1:I:142:ILE:H	1.78	0.48
1:C:189:ARG:NH1	2:C:504:HOH:O	2.45	0.48
1:J:343:GLU:OE1	1:J:413:LEU:HD11	2.14	0.48
1:F:132:THR:HG21	1:F:196:ARG:HA	1.94	0.48
1:C:132:THR:HG21	1:C:196:ARG:CA	2.44	0.48
1:E:235:ASN:OD1	1:E:235:ASN:N	2.47	0.48
1:B:42:GLU:OE1	1:B:42:GLU:N	2.40	0.48
1:G:38:ASP:OD1	1:G:39:ALA:N	2.47	0.48
1:H:282:PHE:HB3	1:H:300:LEU:HD11	1.95	0.48
1:F:18:ALA:HA	1:F:21:ILE:HG13	1.95	0.48
1:J:42:GLU:HG3	1:J:43:ILE:HG23	1.96	0.48
1:G:139:GLU:OE2	1:G:142:ILE:HA	2.14	0.47
1:H:29:VAL:HG22	1:H:323:THR:O	2.14	0.47
1:H:177:PRO:HG2	1:H:184:ARG:HD3	1.96	0.47
1:H:65:ARG:NH1	1:H:403:ILE:O	2.47	0.47
1:H:270:PRO:HB3	1:H:283:VAL:HG12	1.96	0.47
1:I:366:LEU:HD23	1:I:370:GLU:HB3	1.95	0.47
1:A:71:THR:HG21	1:A:88:ARG:HD2	1.96	0.47
1:A:341:ARG:H	1:A:341:ARG:HG3	1.39	0.47
1:D:139:GLU:OE2	1:D:142:ILE:HA	2.15	0.47
1:E:122:ASP:HB3	1:E:124:ASP:OD1	2.14	0.47
1:H:70:LEU:HD11	1:H:116:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ASP:HB3	1:B:124:ASP:OD1	2.14	0.47
1:B:235:ASN:OD1	1:B:235:ASN:N	2.47	0.47
1:G:93:ARG:NH2	1:G:160:ASP:OD1	2.47	0.47
1:I:64:TRP:CZ3	1:I:93:ARG:HG3	2.49	0.47
1:I:358:LEU:HD22	1:I:362:ASP:HB3	1.95	0.47
1:A:217:THR:OG1	1:A:261:ILE:HD11	2.15	0.47
1:H:136:ARG:HG2	1:H:147:ARG:NH2	2.29	0.47
1:H:110:ARG:H	1:H:171:HIS:HE1	1.62	0.47
1:J:341:ARG:NH1	1:J:409:GLU:HG2	2.23	0.47
1:C:47:ASP:HB2	1:C:70:LEU:HD23	1.97	0.47
1:D:139:GLU:CD	1:D:142:ILE:HA	2.39	0.47
1:G:71:THR:HG21	1:G:88:ARG:HD2	1.97	0.47
1:G:194:THR:HG21	1:G:266:GLU:HG2	1.96	0.47
1:G:245:THR:OG1	1:G:246:GLY:N	2.46	0.47
1:H:51:LEU:HB2	1:H:68:PHE:HE1	1.80	0.47
1:B:18:ALA:HA	1:B:21:ILE:HG13	1.97	0.47
1:G:122:ASP:HB3	1:G:124:ASP:OD1	2.15	0.47
1:G:139:GLU:OE1	1:G:143:THR:HG22	2.15	0.47
1:H:111:GLY:HA2	1:H:135:GLY:C	2.40	0.47
1:I:161:ASP:OD1	1:I:162:GLY:N	2.47	0.47
1:C:117:GLY:HA2	1:C:198:PRO:HD2	1.96	0.46
1:D:48:THR:HG21	1:D:379:LEU:HD21	1.97	0.46
1:G:174:LEU:HB3	1:G:175:LEU:HD12	1.97	0.46
1:H:182:TYR:HD2	1:H:253:LEU:HD23	1.80	0.46
1:H:344:LEU:HD22	1:H:387:LEU:HD11	1.97	0.46
1:J:269:ARG:HH21	1:J:336:VAL:HG11	1.80	0.46
1:F:217:THR:HG21	1:F:259:GLU:OE2	2.16	0.46
1:G:49:TRP:CE2	1:G:68:PHE:HB2	2.50	0.46
1:G:51:LEU:HB2	1:G:68:PHE:HE2	1.81	0.46
1:G:150:VAL:CG1	1:G:174:LEU:HD11	2.38	0.46
1:H:111:GLY:HA2	1:H:135:GLY:O	2.16	0.46
1:H:235:ASN:N	1:H:235:ASN:OD1	2.47	0.46
1:F:235:ASN:OD1	1:F:235:ASN:N	2.49	0.46
1:D:132:THR:HG21	1:D:196:ARG:HB2	1.97	0.46
1:D:270:PRO:HA	1:D:282:PHE:O	2.16	0.46
1:E:341:ARG:NH1	1:E:409:GLU:HG2	2.28	0.46
1:I:181:ARG:NH1	1:I:255:ASP:HA	2.31	0.46
1:D:330:TYR:O	1:D:351:ASN:HB3	2.16	0.46
1:G:217:THR:HG21	1:G:259:GLU:OE2	2.16	0.46
1:G:235:ASN:OD1	1:G:235:ASN:N	2.49	0.46
1:H:193:TYR:CE2	1:H:195:PHE:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:26:GLU:CD	2:I:502:HOH:O	2.58	0.46
1:A:90:PHE:CD1	1:A:100:ASP:HA	2.51	0.46
1:F:231:TRP:HB3	1:F:262:CYS:SG	2.55	0.46
1:H:344:LEU:HB3	1:H:385:VAL:HG22	1.97	0.46
1:B:372:ARG:HH22	1:J:221:GLU:CD	2.23	0.46
1:I:122:ASP:HB3	1:I:124:ASP:OD1	2.15	0.46
1:I:139:GLU:OE1	1:I:143:THR:HG22	2.16	0.46
1:A:235:ASN:OD1	1:A:235:ASN:N	2.49	0.45
1:C:217:THR:HG21	1:C:259:GLU:OE2	2.16	0.45
1:H:264:ASN:ND2	1:H:285:SER:OG	2.49	0.45
1:J:13:TRP:O	1:J:263:VAL:HG21	2.16	0.45
1:J:192:ILE:HD12	1:J:192:ILE:H	1.81	0.45
1:J:282:PHE:HB3	1:J:300:LEU:HD11	1.98	0.45
1:H:208:LYS:HE2	1:H:242:HIS:NE2	2.31	0.45
1:J:360:LEU:HD23	1:J:360:LEU:HA	1.73	0.45
1:B:185:GLU:HG3	1:B:193:TYR:CZ	2.52	0.45
1:J:378:THR:OG1	1:J:379:LEU:N	2.50	0.45
1:D:117:GLY:HA3	1:D:130:PHE:O	2.16	0.45
1:D:235:ASN:OD1	1:D:235:ASN:N	2.48	0.45
1:I:344:LEU:HB3	1:I:385:VAL:CG2	2.46	0.45
1:C:330:TYR:O	1:C:351:ASN:HB3	2.16	0.45
1:E:115:TRP:HB2	1:E:132:THR:HB	1.99	0.45
1:E:139:GLU:OE1	1:E:142:ILE:HA	2.16	0.45
1:G:378:THR:OG1	1:G:379:LEU:N	2.49	0.45
1:H:46:TRP:HB2	1:H:349:PHE:CE1	2.52	0.45
1:I:179:GLY:HA2	1:I:184:ARG:HG3	1.97	0.45
1:C:115:TRP:HB2	1:C:132:THR:OG1	2.17	0.45
1:E:344:LEU:HB3	1:E:385:VAL:HG22	1.99	0.45
1:G:84:VAL:HG12	1:G:84:VAL:O	2.16	0.45
1:J:139:GLU:OE2	1:J:142:ILE:HD13	2.17	0.45
1:C:47:ASP:CB	1:C:70:LEU:HD23	2.47	0.45
1:C:122:ASP:HB3	1:C:124:ASP:OD1	2.17	0.45
1:C:360:LEU:HD23	1:C:360:LEU:HA	1.77	0.44
1:A:157:VAL:HG22	1:A:164:ARG:HB2	1.99	0.44
1:C:51:LEU:HB2	1:C:68:PHE:HE1	1.82	0.44
1:D:116:ALA:HB1	1:D:269:ARG:NH1	2.31	0.44
1:H:139:GLU:OE1	1:H:143:THR:HG22	2.18	0.44
1:J:49:TRP:CE2	1:J:68:PHE:HB2	2.52	0.44
1:F:360:LEU:HD23	1:F:360:LEU:HA	1.79	0.44
1:H:64:TRP:CZ3	1:H:93:ARG:HG3	2.52	0.44
1:H:84:VAL:HG12	1:H:84:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:ASP:HB3	1:J:124:ASP:OD1	2.16	0.44
1:E:270:PRO:HB3	1:E:283:VAL:HG12	2.00	0.44
1:F:344:LEU:HD22	1:F:387:LEU:HD11	1.99	0.44
1:F:384:ARG:O	1:F:395:THR:HG22	2.18	0.44
1:H:261:ILE:HG22	1:H:262:CYS:SG	2.58	0.44
1:F:49:TRP:CZ3	1:F:116:ALA:HA	2.53	0.44
1:H:48:THR:HG21	1:H:379:LEU:HD21	1.99	0.44
1:I:71:THR:HG21	1:I:88:ARG:HD3	1.99	0.44
1:A:90:PHE:HD1	1:A:100:ASP:HA	1.81	0.44
1:A:161:ASP:HA	1:C:136:ARG:HH11	1.82	0.44
1:H:115:TRP:HB2	1:H:132:THR:HB	1.98	0.44
1:I:70:LEU:HD11	1:I:116:ALA:HA	2.00	0.44
1:I:235:ASN:OD1	1:I:235:ASN:N	2.51	0.44
1:J:235:ASN:N	1:J:235:ASN:OD1	2.51	0.44
1:H:330:TYR:O	1:H:351:ASN:HB3	2.18	0.44
1:J:269:ARG:HH21	1:J:336:VAL:CG1	2.31	0.44
1:J:198:PRO:HB2	1:J:211:LEU:HD11	2.00	0.44
1:A:29:VAL:HG22	1:A:323:THR:O	2.18	0.43
1:B:231:TRP:HB3	1:B:262:CYS:HB3	2.00	0.43
1:F:198:PRO:HB2	1:F:211:LEU:HD11	1.98	0.43
1:G:104:VAL:HG13	1:G:105:PHE:CD1	2.53	0.43
1:G:360:LEU:HA	1:G:360:LEU:HD23	1.75	0.43
1:A:48:THR:HG21	1:A:379:LEU:HD21	1.99	0.43
1:B:225:ALA:N	1:B:232:GLU:OE2	2.51	0.43
1:D:226:CYS:HB2	1:D:232:GLU:HG3	2.00	0.43
1:E:366:LEU:HB3	1:E:370:GLU:HB2	2.00	0.43
1:G:50:PHE:CE1	1:G:403:ILE:HG12	2.53	0.43
1:G:330:TYR:O	1:G:351:ASN:HB3	2.19	0.43
1:A:64:TRP:CZ3	1:A:93:ARG:HG3	2.53	0.43
1:A:344:LEU:HB3	1:A:385:VAL:CG2	2.48	0.43
1:B:159:ASP:HB2	1:B:161:ASP:OD1	2.18	0.43
1:D:49:TRP:CZ3	1:D:116:ALA:HA	2.53	0.43
1:G:355:LEU:O	1:G:358:LEU:HD13	2.17	0.43
1:I:219:ILE:HG21	1:I:232:GLU:HB3	1.99	0.43
1:F:132:THR:HG21	1:F:196:ARG:HB2	2.00	0.43
1:I:255:ASP:HB2	1:I:309:ARG:NH2	2.27	0.43
1:D:132:THR:HG21	1:D:197:ASP:H	1.83	0.43
1:E:36:ARG:NH2	1:H:373:ALA:O	2.52	0.43
1:G:185:GLU:H	1:G:185:GLU:CD	2.22	0.43
1:G:198:PRO:HB2	1:G:211:LEU:HD11	2.01	0.43
1:G:344:LEU:HB3	1:G:385:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:THR:HG21	1:I:379:LEU:HD21	2.00	0.43
1:C:132:THR:HG21	1:C:196:ARG:HB2	2.00	0.43
1:I:42:GLU:HG3	1:I:43:ILE:HG13	2.00	0.43
1:I:126:ARG:HE	1:I:153:GLY:HA2	1.84	0.43
1:D:35:PRO:HG3	1:D:378:THR:HG21	1.99	0.43
1:D:269:ARG:HH21	1:D:336:VAL:CG1	2.32	0.43
1:D:344:LEU:HB3	1:D:385:VAL:HG22	2.01	0.43
1:D:384:ARG:NH2	1:D:413:LEU:HD11	2.33	0.43
1:G:193:TYR:CD1	1:G:193:TYR:C	2.96	0.43
1:A:49:TRP:CZ3	1:A:116:ALA:HA	2.53	0.43
1:D:46:TRP:HB2	1:D:349:PHE:CE1	2.54	0.43
1:H:49:TRP:CZ3	1:H:116:ALA:HA	2.54	0.43
1:I:26:GLU:OE1	2:I:502:HOH:O	2.21	0.43
1:J:150:VAL:HB	1:J:174:LEU:HD11	2.01	0.43
1:B:29:VAL:HG22	1:B:323:THR:O	2.19	0.42
1:C:13:TRP:O	1:C:263:VAL:HG21	2.18	0.42
1:C:235:ASN:N	1:C:235:ASN:OD1	2.50	0.42
1:B:13:TRP:O	1:B:263:VAL:HG21	2.19	0.42
1:D:13:TRP:O	1:D:263:VAL:HG21	2.18	0.42
1:E:194:THR:HG22	1:E:196:ARG:HH12	1.83	0.42
1:F:192:ILE:HD12	1:F:192:ILE:H	1.84	0.42
1:G:48:THR:HG21	1:G:379:LEU:HD21	2.01	0.42
1:I:29:VAL:HG22	1:I:323:THR:O	2.20	0.42
1:H:42:GLU:HG3	1:H:43:ILE:HG23	2.01	0.42
1:I:163:VAL:C	1:I:164:ARG:HD2	2.44	0.42
1:F:132:THR:HG21	1:F:196:ARG:CA	2.49	0.42
1:G:343:GLU:OE2	1:G:413:LEU:HD11	2.19	0.42
1:J:46:TRP:HB2	1:J:349:PHE:CE1	2.55	0.42
1:B:60:THR:HG21	1:B:405:LEU:HD11	2.02	0.42
1:B:343:GLU:OE1	1:B:413:LEU:HD11	2.20	0.42
1:B:360:LEU:HA	1:B:360:LEU:HD23	1.71	0.42
1:B:385:VAL:HG12	1:B:394:ILE:HD13	2.00	0.42
1:D:75:ASP:O	1:D:372:ARG:NE	2.46	0.42
1:F:178:ASP:O	1:F:184:ARG:NH2	2.49	0.42
1:G:341:ARG:H	1:G:341:ARG:HG3	1.47	0.42
1:A:217:THR:HG21	1:A:259:GLU:OE2	2.20	0.42
1:A:343:GLU:CD	1:A:384:ARG:HH21	2.26	0.42
1:C:188:SER:HB2	1:C:193:TYR:HB3	2.02	0.42
1:E:76:LEU:HD23	1:E:77:LEU:O	2.19	0.42
1:I:116:ALA:HB1	1:I:269:ARG:NH1	2.35	0.42
1:A:122:ASP:HB3	1:A:124:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ARG:NH1	2:B:501:HOH:O	2.52	0.42
1:D:177:PRO:O	1:D:184:ARG:HD3	2.19	0.42
1:I:181:ARG:O	1:I:217:THR:HG22	2.20	0.42
1:B:46:TRP:HB2	1:B:349:PHE:CE1	2.55	0.42
1:D:359:THR:HG23	1:D:362:ASP:H	1.84	0.42
1:H:196:ARG:NH2	1:H:268:GLU:OE2	2.53	0.42
1:I:181:ARG:NH2	1:I:255:ASP:OD1	2.52	0.42
1:J:194:THR:HG22	1:J:196:ARG:HH12	1.85	0.42
1:B:208:LYS:HE3	1:B:242:HIS:NE2	2.35	0.42
1:E:344:LEU:HB3	1:E:385:VAL:CG2	2.50	0.42
1:H:344:LEU:HB3	1:H:385:VAL:CG2	2.50	0.42
1:H:358:LEU:HD22	1:H:362:ASP:HB3	2.00	0.42
1:C:275:ARG:NH2	1:C:342:GLU:HA	2.35	0.41
1:G:161:ASP:OD1	1:G:162:GLY:N	2.53	0.41
1:I:46:TRP:HB2	1:I:349:PHE:CE1	2.55	0.41
1:I:51:LEU:HB2	1:I:68:PHE:HE1	1.85	0.41
1:F:413:LEU:N	1:F:413:LEU:HD12	2.35	0.41
1:J:48:THR:HG21	1:J:379:LEU:HD21	2.01	0.41
1:B:174:LEU:C	1:B:175:LEU:HD12	2.45	0.41
1:D:15:ARG:NH2	1:D:292:PRO:O	2.53	0.41
1:E:135:GLY:HA2	1:E:143:THR:HG23	2.01	0.41
1:F:51:LEU:HD11	1:F:121:LEU:HB2	2.02	0.41
1:G:259:GLU:HB3	1:G:261:ILE:HD13	2.02	0.41
1:A:259:GLU:HB3	1:A:261:ILE:HD13	2.02	0.41
1:E:270:PRO:HA	1:E:282:PHE:O	2.21	0.41
1:E:49:TRP:CE2	1:E:68:PHE:HB2	2.55	0.41
1:E:116:ALA:HB1	1:E:269:ARG:HH11	1.85	0.41
1:H:71:THR:HG21	1:H:88:ARG:HD2	2.00	0.41
1:I:186:GLU:H	1:I:186:GLU:CD	2.27	0.41
1:C:31:ILE:HD13	1:C:325:PRO:HG3	2.01	0.41
1:D:65:ARG:NH1	1:D:93:ARG:O	2.52	0.41
1:J:90:PHE:CD2	1:J:100:ASP:HA	2.55	0.41
1:A:344:LEU:HB3	1:A:385:VAL:HG22	2.01	0.41
1:G:194:THR:HG22	1:G:196:ARG:HH12	1.86	0.41
1:H:75:ASP:OD1	1:H:76:LEU:N	2.54	0.41
1:H:388:SER:OG	1:H:389:GLY:N	2.54	0.41
1:I:127:LEU:HD21	1:I:129:VAL:HG23	2.02	0.41
1:B:216:ASN:ND2	1:B:265:GLN:OE1	2.51	0.41
1:A:65:ARG:NH2	1:A:405:LEU:HG	2.35	0.41
1:A:275:ARG:HH22	1:A:342:GLU:HA	1.86	0.41
1:B:330:TYR:O	1:B:351:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:THR:HG21	1:C:88:ARG:HD2	2.03	0.41
1:F:139:GLU:OE2	1:F:142:ILE:HD13	2.20	0.41
1:H:260:GLY:O	1:H:263:VAL:HG22	2.20	0.41
1:I:259:GLU:HB2	1:I:261:ILE:CD1	2.50	0.41
1:B:49:TRP:CE2	1:B:68:PHE:HB2	2.55	0.41
1:B:117:GLY:HA3	1:B:130:PHE:O	2.21	0.41
1:D:51:LEU:HA	1:D:119:ALA:HB3	2.03	0.41
1:F:49:TRP:CE2	1:F:68:PHE:HB2	2.56	0.41
1:G:344:LEU:HB3	1:G:385:VAL:HG22	2.03	0.41
1:I:88:ARG:NH2	1:I:102:GLY:HA2	2.36	0.41
1:I:228:ASP:OD1	1:I:230:VAL:HG12	2.21	0.41
1:I:272:VAL:HA	1:I:280:TYR:O	2.21	0.41
1:I:341:ARG:H	1:I:341:ARG:HG3	1.48	0.41
1:B:51:LEU:HB2	1:B:68:PHE:HE1	1.86	0.40
1:B:344:LEU:HB3	1:B:385:VAL:CG2	2.52	0.40
1:C:90:PHE:CD1	1:C:90:PHE:N	2.90	0.40
1:C:335:TRP:HB3	1:C:346:VAL:HG12	2.03	0.40
1:C:335:TRP:HB3	1:C:346:VAL:CG1	2.52	0.40
1:F:414:PRO:C	2:F:501:HOH:O	2.63	0.40
1:G:117:GLY:HA3	1:G:130:PHE:O	2.21	0.40
1:G:379:LEU:HD23	1:G:379:LEU:HA	1.93	0.40
1:J:309:ARG:HH11	1:J:309:ARG:HD2	1.75	0.40
1:B:270:PRO:HB3	1:B:283:VAL:HG12	2.02	0.40
1:E:178:ASP:OD1	1:E:179:GLY:N	2.55	0.40
1:H:127:LEU:HD21	1:H:129:VAL:HG23	2.03	0.40
1:H:228:ASP:OD1	1:H:230:VAL:HG12	2.21	0.40
1:A:23:ARG:HG2	1:A:323:THR:HG21	2.04	0.40
1:A:49:TRP:CE2	1:A:68:PHE:HB2	2.56	0.40
1:A:404:PRO:HG3	1:A:410:LEU:HD21	2.04	0.40
1:C:178:ASP:O	1:C:184:ARG:NH1	2.53	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	404/428 (94%)	381 (94%)	22 (5%)	1 (0%)	43	64
1	B	404/428 (94%)	382 (95%)	22 (5%)	0	100	100
1	C	404/428 (94%)	380 (94%)	24 (6%)	0	100	100
1	D	404/428 (94%)	382 (95%)	21 (5%)	1 (0%)	43	64
1	E	404/428 (94%)	379 (94%)	24 (6%)	1 (0%)	43	64
1	F	404/428 (94%)	377 (93%)	27 (7%)	0	100	100
1	G	404/428 (94%)	383 (95%)	20 (5%)	1 (0%)	43	64
1	H	404/428 (94%)	379 (94%)	25 (6%)	0	100	100
1	I	404/428 (94%)	384 (95%)	19 (5%)	1 (0%)	43	64
1	J	404/428 (94%)	382 (95%)	22 (5%)	0	100	100
All	All	4040/4280 (94%)	3809 (94%)	226 (6%)	5 (0%)	48	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	341	ARG
1	G	341	ARG
1	A	341	ARG
1	E	276	ASN
1	I	341	ARG

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	329/348 (94%)	322 (98%)	7 (2%)	47	67
1	B	329/348 (94%)	327 (99%)	2 (1%)	78	88
1	C	329/348 (94%)	326 (99%)	3 (1%)	70	82
1	D	329/348 (94%)	326 (99%)	3 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	329/348 (94%)	328 (100%)	1 (0%)	86	93
1	F	329/348 (94%)	326 (99%)	3 (1%)	70	82
1	G	329/348 (94%)	327 (99%)	2 (1%)	78	88
1	H	329/348 (94%)	327 (99%)	2 (1%)	78	88
1	I	329/348 (94%)	329 (100%)	0	100	100
1	J	329/348 (94%)	328 (100%)	1 (0%)	86	93
All	All	3290/3480 (94%)	3266 (99%)	24 (1%)	76	86

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	THR
1	A	109	THR
1	A	156	VAL
1	A	157	VAL
1	A	226	CYS
1	A	261	ILE
1	A	343	GLU
1	B	90	PHE
1	B	262	CYS
1	C	90	PHE
1	C	104	VAL
1	C	109	THR
1	D	90	PHE
1	D	132	THR
1	D	262	CYS
1	E	262	CYS
1	F	109	THR
1	F	132	THR
1	F	263	VAL
1	G	193	TYR
1	G	261	ILE
1	H	109	THR
1	H	193	TYR
1	J	80	LYS

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

Mol	Chain	Res	Type
1	A	242	HIS
1	B	114	GLN
1	C	114	GLN
1	C	242	HIS
1	D	114	GLN
1	D	242	HIS
1	D	400	HIS
1	E	114	GLN
1	E	265	GLN
1	E	400	HIS
1	F	114	GLN
1	F	242	HIS
1	G	242	HIS
1	H	114	GLN
1	H	171	HIS
1	H	351	ASN
1	I	114	GLN
1	I	242	HIS
1	J	114	GLN
1	J	171	HIS
1	J	286	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	406/428 (94%)	-0.53	1 (0%) 91 92	20, 45, 78, 99	0
1	B	406/428 (94%)	-0.13	4 (0%) 79 79	19, 66, 106, 133	0
1	C	406/428 (94%)	-0.50	0 100 100	23, 48, 83, 94	0
1	D	406/428 (94%)	-0.57	0 100 100	18, 42, 75, 94	0
1	E	406/428 (94%)	-0.46	0 100 100	25, 46, 85, 114	0
1	F	406/428 (94%)	-0.34	1 (0%) 91 92	26, 50, 89, 114	0
1	G	406/428 (94%)	-0.12	3 (0%) 84 84	27, 67, 108, 140	0
1	H	406/428 (94%)	0.07	10 (2%) 58 56	22, 75, 131, 161	0
1	I	406/428 (94%)	-0.15	5 (1%) 76 76	28, 66, 107, 126	0
1	J	406/428 (94%)	-0.45	1 (0%) 91 92	27, 50, 81, 97	0
All	All	4060/4280 (94%)	-0.32	25 (0%) 85 86	18, 54, 102, 161	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	259	GLU	3.8
1	H	168	PRO	3.4
1	H	213	PHE	3.0
1	F	9	ALA	2.8
1	B	167	GLY	2.8
1	B	184	ARG	2.8
1	I	361	ASP	2.7
1	A	414	PRO	2.7
1	I	135	GLY	2.7
1	H	157	VAL	2.7
1	H	225	ALA	2.6
1	B	173	VAL	2.6
1	G	192	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	356	GLY	2.5
1	H	223	ALA	2.4
1	H	135	GLY	2.2
1	B	168	PRO	2.2
1	I	39	ALA	2.1
1	G	154	GLY	2.1
1	I	224	GLY	2.1
1	H	169	PHE	2.1
1	H	110	ARG	2.1
1	J	414	PRO	2.1
1	H	186	GLU	2.0
1	G	142	ILE	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.