



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:43 PM UTC

PDB ID : 5C70 / pdb_00005c70
Title : The structure of Aspergillus oryzae beta-glucuronidase
Authors : Sun, H.L.; Lv, B.; Huang, S.; Sun, Q.F.; Li, C.; Jiang, T.
Deposited on : 2015-06-24
Resolution : 3.10 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

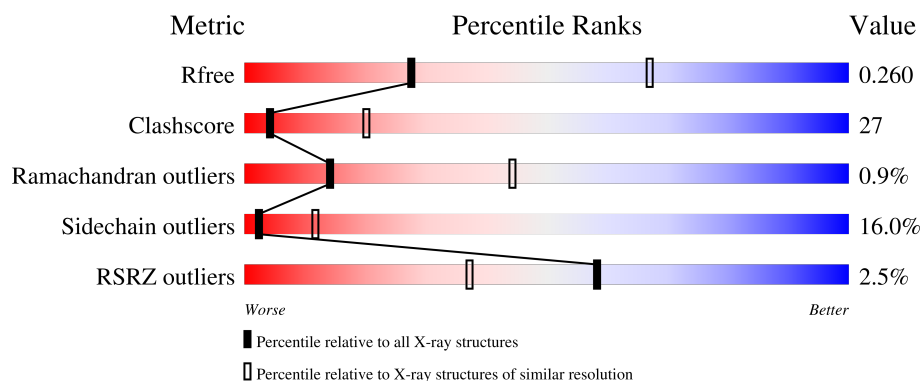
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	612	 2% 52% 35% 8% . .
1	B	612	 2% 54% 34% 6% . 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9320 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 Glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4670	2965	806	886	13			
1	B	584	Total	C	N	O	S	0	0	0
			4650	2950	801	886	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ALA	-	expression tag	UNP A7XS03
A	-6	ALA	-	expression tag	UNP A7XS03
A	-5	GLN	-	expression tag	UNP A7XS03
A	-4	GLY	-	expression tag	UNP A7XS03
A	-3	SER	-	expression tag	UNP A7XS03
A	-2	ALA	-	expression tag	UNP A7XS03
A	-1	GLY	-	expression tag	UNP A7XS03
A	0	SER	-	expression tag	UNP A7XS03
B	-7	ALA	-	expression tag	UNP A7XS03
B	-6	ALA	-	expression tag	UNP A7XS03
B	-5	GLN	-	expression tag	UNP A7XS03
B	-4	GLY	-	expression tag	UNP A7XS03
B	-3	SER	-	expression tag	UNP A7XS03
B	-2	ALA	-	expression tag	UNP A7XS03
B	-1	GLY	-	expression tag	UNP A7XS03
B	0	SER	-	expression tag	UNP A7XS03

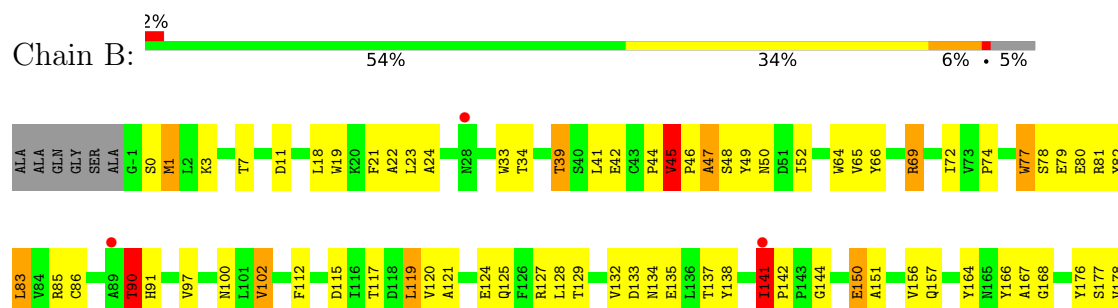
3 Residue-property plots

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: Glucuronidase



• Molecule 1: Glucuronidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	110.32Å 110.32Å 480.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.10 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.10) 98.9 (30.00-3.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.45 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.254 0.209 , 0.260	Depositor DCC
R_{free} test set	1655 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9320	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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	0.69	0/4790	1.07	28/6521 (0.4%)
1	B	0.67	0/4770	1.06	23/6496 (0.4%)
All	All	0.68	0/9560	1.06	51/13017 (0.4%)

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	2
1	B	0	4
All	All	0	6

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	141	ILE	CA-C-N	-17.24	102.62	120.38
1	B	141	ILE	C-N-CA	-17.24	102.62	120.38
1	B	474	THR	N-CA-C	15.56	130.00	111.02
1	A	141	ILE	CA-C-N	-14.56	105.39	120.38
1	A	141	ILE	C-N-CA	-14.56	105.39	120.38
1	A	380	ARG	N-CA-C	9.45	125.69	111.04
1	A	162	ASP	N-CA-C	9.27	121.15	111.14
1	B	474	THR	CB-CA-C	-9.14	96.39	110.92
1	A	162	ASP	CB-CA-C	-8.98	96.72	110.90
1	A	302	ASN	N-CA-C	8.26	119.97	110.97
1	A	429	LEU	CA-C-N	-8.14	110.56	119.19
1	A	429	LEU	C-N-CA	-8.14	110.56	119.19
1	B	468	ARG	CB-CA-C	-7.79	97.42	109.89
1	B	354	THR	CA-C-N	-7.69	112.99	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	THR	C-N-CA	-7.69	112.99	120.83
1	A	474	THR	N-CA-C	7.27	118.89	110.97
1	B	552	PHE	N-CA-C	-7.17	103.39	111.14
1	B	45	VAL	CA-C-N	-6.77	111.38	119.84
1	B	45	VAL	C-N-CA	-6.77	111.38	119.84
1	B	475	GLN	N-CA-C	-6.72	96.49	110.80
1	A	520	THR	CA-C-N	6.66	126.62	119.76
1	A	520	THR	C-N-CA	6.66	126.62	119.76
1	A	142	PRO	CA-C-N	6.56	126.48	119.85
1	A	142	PRO	C-N-CA	6.56	126.48	119.85
1	B	437	ASP	CA-C-N	6.53	126.22	119.56
1	B	437	ASP	C-N-CA	6.53	126.22	119.56
1	B	302	ASN	N-CA-C	6.50	118.25	111.03
1	A	380	ARG	CB-CA-C	-6.46	101.12	111.39
1	B	90	THR	N-CA-C	-6.19	100.14	109.79
1	B	49	TYR	N-CA-C	6.17	120.01	112.23
1	A	302	ASN	CA-C-N	-5.98	115.29	122.35
1	A	302	ASN	C-N-CA	-5.98	115.29	122.35
1	A	474	THR	CB-CA-C	-5.97	101.76	110.96
1	A	45	VAL	CA-C-N	-5.91	112.45	119.84
1	A	45	VAL	C-N-CA	-5.91	112.45	119.84
1	A	90	THR	O-C-N	5.80	128.28	122.08
1	A	296	GLY	N-CA-C	-5.79	104.67	112.14
1	A	161	HIS	CB-CA-C	5.64	122.07	110.40
1	A	381	ILE	N-CA-CB	5.63	119.31	112.10
1	B	90	THR	CB-CA-C	-5.62	100.64	113.33
1	B	357	VAL	CB-CA-C	-5.54	104.17	111.70
1	A	362	SER	N-CA-CB	-5.36	104.35	110.35
1	A	243	GLN	CA-C-N	5.33	125.04	119.82
1	A	243	GLN	C-N-CA	5.33	125.04	119.82
1	B	468	ARG	N-CA-C	5.29	117.90	109.96
1	A	-2	ALA	N-CA-C	5.21	116.82	107.80
1	B	47	ALA	N-CA-C	5.16	121.78	110.80
1	B	176	TYR	N-CA-C	5.15	117.02	109.24
1	B	302	ASN	CA-C-N	-5.02	116.16	121.84
1	B	302	ASN	C-N-CA	-5.02	116.16	121.84
1	A	331	SER	N-CA-C	5.01	116.65	108.63

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ILE	Peptide
1	A	295	PHE	Peptide
1	B	141	ILE	Peptide
1	B	295	PHE	Peptide
1	B	48	SER	Peptide
1	B	550	TRP	Peptide

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	4670	0	4505	253	0
1	B	4650	0	4477	251	0
All	All	9320	0	8982	497	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 27.

All (497) 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:361:PHE:CZ	1:A:380:ARG:HD2	1.71	1.25
1:A:90:THR:CG2	1:A:91:HIS:H	1.50	1.23
1:B:467:ASN:HB3	1:B:505:GLU:CG	1.73	1.18
1:B:21:PHE:O	1:B:39:THR:HG21	1.43	1.16
1:A:90:THR:OG1	1:A:167:ALA:HA	1.47	1.11
1:A:90:THR:HG23	1:A:91:HIS:N	1.65	1.11
1:B:90:THR:CG2	1:B:91:HIS:N	2.11	1.10
1:B:90:THR:HG23	1:B:91:HIS:H	1.17	1.08
1:B:467:ASN:HB3	1:B:505:GLU:HG3	1.37	1.07
1:B:82:TYR:H	1:B:117:THR:HG22	1.18	1.05
1:A:251:GLN:HG2	1:A:268:LYS:HE2	1.36	1.03
1:A:297:LYS:O	1:A:331:SER:HB2	1.58	1.02
1:B:39:THR:HG23	1:B:41:LEU:H	1.18	1.01
1:A:90:THR:HB	1:A:168:GLY:H	1.25	1.00
1:B:567:ASN:HD21	1:B:569:LYS:HB2	1.26	1.00
1:A:90:THR:CG2	1:A:91:HIS:N	2.19	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:CB	1:A:168:GLY:H	1.77	0.98
1:B:470:PHE:HA	1:B:474:THR:OG1	1.63	0.97
1:A:50:ASN:HD21	1:A:167:ALA:H	1.10	0.96
1:B:467:ASN:HB3	1:B:505:GLU:HG2	1.42	0.96
1:A:357:VAL:HG12	1:A:413:ASN:HB3	1.46	0.96
1:B:323:MET:HA	1:B:586:ARG:HG3	1.49	0.95
1:B:468:ARG:HG3	1:B:470:PHE:CE2	2.02	0.94
1:B:39:THR:CG2	1:B:41:LEU:H	1.80	0.94
1:A:90:THR:HG23	1:A:91:HIS:H	1.18	0.94
1:B:505:GLU:HB2	1:B:550:TRP:HB2	1.49	0.93
1:A:332:HIS:CG	1:A:357:VAL:HG11	2.02	0.93
1:A:81:ARG:HG3	1:A:117:THR:HG21	1.49	0.92
1:A:115:ASP:OD1	1:A:117:THR:HG23	1.70	0.92
1:A:361:PHE:HZ	1:A:380:ARG:HD2	1.30	0.92
1:A:332:HIS:HB3	1:A:357:VAL:HG21	1.50	0.92
1:A:162:ASP:O	1:A:557:THR:HB	1.70	0.92
1:A:361:PHE:CZ	1:A:380:ARG:CD	2.53	0.92
1:B:90:THR:HG22	1:B:91:HIS:N	1.82	0.92
1:A:5:GLN:HE22	1:A:268:LYS:H	1.15	0.91
1:A:181:GLN:HE22	1:A:207:THR:H	1.16	0.91
1:B:474:THR:HB	1:B:475:GLN:CD	1.96	0.90
1:B:213:GLN:HG3	1:B:257:ILE:HG13	1.54	0.89
1:A:181:GLN:NE2	1:A:207:THR:H	1.71	0.89
1:B:503:MET:HG3	1:B:538:PHE:CZ	2.07	0.88
1:A:357:VAL:CG1	1:A:413:ASN:HB3	2.02	0.88
1:B:90:THR:CG2	1:B:91:HIS:H	1.79	0.88
1:B:474:THR:HB	1:B:475:GLN:NE2	1.89	0.88
1:B:326:ASN:C	1:B:326:ASN:HD22	1.82	0.88
1:B:467:ASN:CB	1:B:505:GLU:HG2	2.04	0.87
1:A:90:THR:HG22	1:A:91:HIS:H	1.37	0.86
1:B:468:ARG:H	1:B:503:MET:HE1	1.41	0.85
1:A:90:THR:OG1	1:A:167:ALA:CA	2.23	0.85
1:A:256:ILE:HG22	1:A:256:ILE:O	1.77	0.84
1:B:90:THR:HG23	1:B:91:HIS:N	1.84	0.84
1:B:474:THR:HB	1:B:475:GLN:OE1	1.78	0.84
1:B:503:MET:HG3	1:B:538:PHE:HZ	1.43	0.82
1:A:82:TYR:H	1:A:117:THR:HG22	1.45	0.82
1:B:547:GLU:OE1	1:B:588:ARG:NH1	2.12	0.81
1:B:81:ARG:HG3	1:B:117:THR:HG21	1.61	0.81
1:B:340:MET:HA	1:B:340:MET:HE2	1.61	0.81
1:B:423:ARG:HA	1:B:457:ILE:HD11	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASN:ND2	1:A:569:LYS:H	1.80	0.80
1:A:5:GLN:NE2	1:A:268:LYS:H	1.78	0.80
1:B:217:ILE:HG12	1:B:223:THR:HG22	1.63	0.80
1:B:213:GLN:HG3	1:B:257:ILE:CG1	2.12	0.80
1:A:474:THR:HB	1:A:475:GLN:CD	2.07	0.79
1:A:474:THR:HB	1:A:475:GLN:NE2	1.96	0.79
1:B:11:ASP:HB3	1:B:77:TRP:CH2	2.18	0.79
1:B:468:ARG:HG3	1:B:470:PHE:HE2	1.44	0.79
1:A:64:TRP:CD2	1:A:133:ASP:HB2	2.18	0.79
1:B:50:ASN:HD21	1:B:167:ALA:H	1.32	0.78
1:A:83:LEU:HB2	1:A:114:ALA:O	1.83	0.77
1:B:567:ASN:ND2	1:B:569:LYS:HB2	1.99	0.77
1:B:467:ASN:CG	1:B:505:GLU:HG2	2.10	0.77
1:A:470:PHE:HA	1:A:474:THR:OG1	1.83	0.77
1:B:82:TYR:H	1:B:117:THR:CG2	1.97	0.77
1:A:332:HIS:HB3	1:A:357:VAL:CG2	2.13	0.77
1:B:90:THR:HB	1:B:132:VAL:CG1	2.15	0.76
1:B:256:ILE:O	1:B:264:ILE:HG22	1.84	0.76
1:A:340:MET:HE2	1:A:340:MET:HA	1.66	0.76
1:B:457:ILE:HG23	1:B:461:PHE:HE2	1.50	0.76
1:B:467:ASN:CB	1:B:505:GLU:CG	2.59	0.75
1:A:188:VAL:HG11	1:A:271:THR:HG21	1.69	0.75
1:B:90:THR:OG1	1:B:167:ALA:HA	1.86	0.75
1:B:201:TYR:O	1:B:231:ASN:HB2	1.86	0.74
1:B:470:PHE:CA	1:B:474:THR:HG1	2.01	0.74
1:B:141:ILE:HG23	1:B:142:PRO:HD3	1.69	0.74
1:A:567:ASN:HD21	1:A:569:LYS:HB2	1.52	0.74
1:A:11:ASP:HB3	1:A:77:TRP:CH2	2.24	0.73
1:A:217:ILE:HG12	1:A:223:THR:HG22	1.71	0.73
1:A:326:ASN:HD22	1:A:327:SER:N	1.87	0.73
1:A:446:ASN:ND2	1:A:468:ARG:HH12	1.88	0.72
1:B:470:PHE:CA	1:B:474:THR:OG1	2.38	0.71
1:B:45:VAL:O	1:B:46:PRO:C	2.32	0.71
1:A:474:THR:HB	1:A:475:GLN:OE1	1.91	0.71
1:B:11:ASP:CB	1:B:77:TRP:CH2	2.73	0.71
1:B:39:THR:HG23	1:B:41:LEU:N	2.02	0.71
1:B:457:ILE:HG23	1:B:461:PHE:CE2	2.27	0.70
1:B:357:VAL:HG13	1:B:413:ASN:HB3	1.74	0.70
1:A:399:ARG:HD2	1:A:400:ASP:OD1	1.92	0.69
1:B:21:PHE:O	1:B:39:THR:CG2	2.34	0.69
1:A:256:ILE:O	1:A:264:ILE:HG22	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASN:HD22	1:A:326:ASN:C	2.00	0.69
1:A:469:TYR:OH	1:A:505:GLU:HB3	1.91	0.69
1:A:17:GLY:H	1:A:45:VAL:HG23	1.58	0.69
1:B:468:ARG:N	1:B:503:MET:HE1	2.08	0.69
1:B:188:VAL:HG11	1:B:271:THR:HG21	1.74	0.69
1:A:332:HIS:HB3	1:A:357:VAL:HG11	1.73	0.68
1:B:138:TYR:HB3	1:B:380:ARG:O	1.93	0.68
1:B:100:ASN:HD22	1:B:119:LEU:HD11	1.59	0.68
1:B:474:THR:CB	1:B:475:GLN:OE1	2.41	0.68
1:A:90:THR:HG22	1:A:132:VAL:HG12	1.76	0.68
1:B:470:PHE:HB3	1:B:475:GLN:OE1	1.94	0.68
1:B:474:THR:HB	1:B:475:GLN:HE22	1.58	0.68
1:A:90:THR:CG2	1:A:132:VAL:HG12	2.23	0.68
1:A:90:THR:HG22	1:A:132:VAL:CG1	2.24	0.68
1:B:83:LEU:HB3	1:B:115:ASP:HA	1.77	0.67
1:B:510:THR:HG21	1:B:527:GLN:HB2	1.76	0.67
1:A:332:HIS:CB	1:A:357:VAL:HG11	2.24	0.67
1:B:466:LEU:C	1:B:467:ASN:OD1	2.38	0.66
1:B:503:MET:CG	1:B:538:PHE:CZ	2.78	0.66
1:B:82:TYR:N	1:B:117:THR:HG22	2.02	0.66
1:A:446:ASN:HD22	1:A:468:ARG:HH12	1.44	0.66
1:A:102:VAL:HG12	1:A:114:ALA:HB1	1.77	0.66
1:B:256:ILE:O	1:B:264:ILE:CG2	2.43	0.66
1:A:162:ASP:O	1:A:557:THR:CB	2.45	0.65
1:A:357:VAL:CG1	1:A:413:ASN:CB	2.76	0.64
1:B:141:ILE:HG21	1:B:355:PRO:HG2	1.79	0.64
1:B:181:GLN:HG3	1:B:207:THR:HG23	1.80	0.64
1:A:258:ASP:OD1	1:A:258:ASP:C	2.40	0.64
1:B:494:THR:HG22	1:B:501:ILE:CD1	2.27	0.64
1:A:83:LEU:HB3	1:A:115:ASP:HA	1.79	0.64
1:A:386:ARG:HB2	1:A:425:TYR:CE1	2.33	0.64
1:A:467:ASN:O	1:A:468:ARG:HD3	1.98	0.64
1:A:1:MET:HE1	1:A:182:HIS:NE2	2.12	0.63
1:A:11:ASP:CB	1:A:77:TRP:CH2	2.80	0.63
1:B:567:ASN:ND2	1:B:569:LYS:H	1.95	0.63
1:B:475:GLN:HG2	1:B:482:ALA:HA	1.78	0.63
1:A:293:THR:H	1:A:326:ASN:HD21	1.44	0.63
1:A:457:ILE:HG23	1:A:461:PHE:HE2	1.62	0.63
1:A:474:THR:CB	1:A:475:GLN:OE1	2.47	0.63
1:A:39:THR:HB	1:A:41:LEU:H	1.64	0.62
1:A:469:TYR:HH	1:A:550:TRP:CD1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:TRP:O	1:B:80:GLU:CB	2.48	0.62
1:B:166:TYR:HB2	1:B:306:LYS:HG3	1.81	0.62
1:A:314:VAL:O	1:A:318:GLN:HG2	1.99	0.62
1:B:90:THR:OG1	1:B:167:ALA:CA	2.47	0.62
1:A:258:ASP:OD1	1:A:260:SER:N	2.30	0.62
1:A:468:ARG:HG3	1:A:470:PHE:CE2	2.34	0.62
1:B:503:MET:HE3	1:B:505:GLU:O	1.99	0.62
1:A:45:VAL:O	1:A:47:ALA:N	2.33	0.62
1:A:470:PHE:C	1:A:472:TRP:H	2.06	0.62
1:B:472:TRP:CE3	1:B:508:ALA:HB1	2.35	0.62
1:A:16:ASP:HA	1:A:45:VAL:HG21	1.82	0.62
1:A:82:TYR:H	1:A:117:THR:CG2	2.11	0.62
1:B:90:THR:HG1	1:B:167:ALA:HA	1.64	0.62
1:B:423:ARG:HA	1:B:457:ILE:CD1	2.29	0.62
1:B:467:ASN:HA	1:B:505:GLU:O	2.00	0.62
1:A:138:TYR:HB3	1:A:380:ARG:O	2.00	0.62
1:A:475:GLN:CD	1:A:475:GLN:N	2.58	0.62
1:A:567:ASN:C	1:A:567:ASN:HD22	2.08	0.61
1:B:317:PHE:HA	1:B:320:LEU:HD12	1.80	0.61
1:A:7:THR:HG21	1:A:266:THR:HG23	1.82	0.61
1:A:90:THR:HG1	1:A:167:ALA:HA	1.65	0.61
1:B:297:LYS:O	1:B:331:SER:HB2	2.01	0.61
1:B:375:THR:HG23	1:B:419:GLU:OE1	2.01	0.61
1:A:319:LEU:O	1:A:323:MET:HG2	2.01	0.61
1:A:50:ASN:HD21	1:A:167:ALA:N	1.92	0.60
1:B:475:GLN:CD	1:B:475:GLN:N	2.59	0.60
1:B:64:TRP:CD2	1:B:133:ASP:HB2	2.37	0.60
1:B:359:LEU:HD23	1:B:381:ILE:HG12	1.83	0.60
1:A:19:TRP:CD1	1:A:45:VAL:HG22	2.37	0.60
1:A:90:THR:HB	1:A:132:VAL:HG11	1.83	0.60
1:A:521:PRO:O	1:A:522:TRP:HB2	2.00	0.60
1:B:472:TRP:CZ3	1:B:508:ALA:HB1	2.35	0.60
1:A:78:SER:O	1:A:79:GLU:HB2	2.00	0.60
1:A:309:ASP:CG	1:B:304:ARG:HH21	2.09	0.60
1:B:470:PHE:CB	1:B:474:THR:HG1	2.15	0.60
1:A:45:VAL:HB	1:A:46:PRO:HD3	1.84	0.60
1:A:332:HIS:HB3	1:A:357:VAL:CG1	2.31	0.60
1:B:45:VAL:O	1:B:47:ALA:N	2.35	0.60
1:A:5:GLN:HE22	1:A:268:LYS:N	1.95	0.59
1:B:476:THR:O	1:B:477:ALA:HB3	2.01	0.59
1:A:139:GLN:NE2	1:A:382:ASN:HD21	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLY:O	1:A:551:ASN:OD1	2.21	0.59
1:A:474:THR:HB	1:A:475:GLN:HE22	1.63	0.59
1:B:39:THR:CG2	1:B:41:LEU:N	2.60	0.59
1:B:567:ASN:HD22	1:B:569:LYS:H	1.50	0.59
1:B:547:GLU:CD	1:B:588:ARG:NH1	2.61	0.59
1:A:470:PHE:HA	1:A:474:THR:HG1	1.67	0.59
1:A:256:ILE:O	1:A:256:ILE:CG2	2.50	0.59
1:A:90:THR:HB	1:A:168:GLY:N	2.06	0.59
1:B:100:ASN:O	1:B:102:VAL:HG23	2.03	0.59
1:B:361:PHE:H	1:B:375:THR:HG21	1.68	0.58
1:B:274:ARG:HA	1:B:286:ASN:OD1	2.03	0.58
1:A:50:ASN:ND2	1:A:167:ALA:H	1.92	0.58
1:A:379:ASP:OD1	1:A:379:ASP:N	2.30	0.58
1:B:256:ILE:O	1:B:256:ILE:HG22	2.02	0.58
1:B:475:GLN:HG2	1:B:482:ALA:CA	2.33	0.58
1:B:470:PHE:O	1:B:472:TRP:N	2.37	0.57
1:A:2:LEU:HD11	1:A:186:ILE:HG13	1.84	0.57
1:A:12:LEU:HD12	1:A:13:ILE:H	1.70	0.57
1:B:326:ASN:HD22	1:B:327:SER:N	2.02	0.57
1:B:521:PRO:O	1:B:522:TRP:HB2	2.04	0.57
1:A:334:PRO:HG3	1:A:396:LEU:HD12	1.86	0.57
1:A:64:TRP:CE2	1:A:133:ASP:HB2	2.40	0.57
1:A:90:THR:CG2	1:A:132:VAL:CG1	2.83	0.56
1:A:293:THR:H	1:A:326:ASN:ND2	2.03	0.56
1:A:483:GLU:O	1:A:487:GLU:HG2	2.05	0.56
1:B:475:GLN:HB2	1:B:482:ALA:HB2	1.88	0.56
1:A:452:TYR:CE1	1:A:492:GLY:HA3	2.41	0.56
1:B:357:VAL:CG1	1:B:413:ASN:HB3	2.35	0.56
1:A:358:GLY:C	1:A:360:ALA:H	2.13	0.56
1:B:81:ARG:CG	1:B:117:THR:HG21	2.35	0.56
1:A:399:ARG:CD	1:A:400:ASP:OD1	2.53	0.56
1:B:166:TYR:CB	1:B:306:LYS:HG3	2.36	0.56
1:A:45:VAL:HB	1:A:46:PRO:CD	2.37	0.55
1:B:475:GLN:HG3	1:B:481:GLU:HG3	1.86	0.55
1:A:452:TYR:CD1	1:A:492:GLY:HA3	2.40	0.55
1:B:470:PHE:C	1:B:472:TRP:H	2.14	0.55
1:A:12:LEU:HD13	1:A:176:TYR:HB3	1.89	0.55
1:B:551:ASN:ND2	1:B:555:PHE:CD2	2.73	0.55
1:A:164:TYR:N	1:A:557:THR:HA	2.21	0.55
1:B:417:SER:HB2	1:B:455:ASP:OD1	2.07	0.55
1:A:357:VAL:HG13	1:A:413:ASN:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ASP:OD1	1:A:456:ARG:NH1	2.39	0.55
1:B:260:SER:OG	1:B:261:LYS:N	2.40	0.54
1:B:490:LEU:O	1:B:494:THR:HG23	2.07	0.54
1:A:475:GLN:OE1	1:A:475:GLN:N	2.40	0.54
1:A:33:TRP:O	1:A:127:ARG:NH1	2.40	0.54
1:A:251:GLN:HG2	1:A:268:LYS:CE	2.25	0.54
1:B:470:PHE:HB3	1:B:474:THR:HG1	1.73	0.54
1:A:469:TYR:HB2	1:A:473:TYR:HD2	1.73	0.54
1:A:199:ILE:HG12	1:A:199:ILE:O	2.06	0.54
1:B:77:TRP:O	1:B:80:GLU:HB3	2.08	0.53
1:B:446:ASN:HD21	1:B:468:ARG:HH22	1.56	0.53
1:A:31:GLN:N	1:A:32:PRO:HD3	2.23	0.53
1:B:141:ILE:CG2	1:B:142:PRO:HD3	2.37	0.53
1:B:470:PHE:C	1:B:472:TRP:N	2.65	0.53
1:B:423:ARG:NH2	1:B:460:LEU:HD21	2.23	0.53
1:A:11:ASP:HB3	1:A:77:TRP:HH2	1.72	0.53
1:A:134:ASN:HB3	1:A:167:ALA:CB	2.39	0.53
1:A:141:ILE:HD13	1:A:141:ILE:O	2.09	0.53
1:A:568:LYS:C	1:A:570:GLY:H	2.15	0.53
1:B:202:ASN:HA	1:B:231:ASN:HB3	1.90	0.53
1:A:96:TYR:HB2	1:A:129:THR:HG23	1.91	0.52
1:B:377:SER:HB2	1:B:378:PRO:HD2	1.91	0.52
1:A:519:VAL:HG12	1:A:519:VAL:O	2.09	0.52
1:B:137:THR:HA	1:B:144:GLY:O	2.09	0.52
1:B:78:SER:C	1:B:80:GLU:H	2.16	0.52
1:B:469:TYR:OH	1:B:550:TRP:CB	2.58	0.52
1:B:81:ARG:HA	1:B:117:THR:HG21	1.91	0.52
1:A:68:GLN:HE21	1:A:129:THR:HB	1.74	0.52
1:B:466:LEU:O	1:B:504:THR:N	2.42	0.52
1:A:274:ARG:NH1	1:A:404:PRO:HA	2.25	0.52
1:A:309:ASP:OD2	1:B:304:ARG:NH2	2.38	0.52
1:A:396:LEU:CD2	1:A:409:TRP:CZ3	2.92	0.52
1:A:470:PHE:C	1:A:472:TRP:N	2.67	0.52
1:B:293:THR:O	1:B:327:SER:OG	2.25	0.52
1:A:188:VAL:CG1	1:A:271:THR:HG21	2.39	0.52
1:A:357:VAL:HG13	1:A:413:ASN:HB3	1.88	0.52
1:A:483:GLU:OE1	1:A:536:ARG:NH2	2.41	0.52
1:A:567:ASN:HD22	1:A:569:LYS:H	1.57	0.51
1:B:491:ARG:O	1:B:495:GLU:HB2	2.10	0.51
1:A:434:ARG:HG3	1:A:434:ARG:HH11	1.75	0.51
1:A:470:PHE:O	1:A:472:TRP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASN:HD21	1:A:569:LYS:CB	2.21	0.51
1:A:136:LEU:HD22	1:A:142:PRO:O	2.11	0.51
1:A:377:SER:HB2	1:A:378:PRO:CD	2.41	0.51
1:B:329:ARG:HH21	1:B:413:ASN:ND2	2.08	0.51
1:B:549:VAL:HG21	1:B:585:LEU:HD11	1.93	0.51
1:A:36:GLN:HE21	1:A:127:ARG:HD3	1.76	0.51
1:B:100:ASN:ND2	1:B:119:LEU:HD11	2.25	0.51
1:B:496:LYS:HG2	1:B:497:TYR:CD2	2.46	0.51
1:B:19:TRP:CZ2	1:B:69:ARG:HD3	2.46	0.51
1:B:551:ASN:ND2	1:B:555:PHE:CE2	2.79	0.51
1:A:542:GLU:O	1:A:542:GLU:HG2	2.10	0.51
1:B:550:TRP:O	1:B:550:TRP:CG	2.62	0.51
1:B:33:TRP:CD1	1:B:34:THR:HG23	2.45	0.51
1:B:494:THR:HG22	1:B:501:ILE:HD12	1.91	0.51
1:A:134:ASN:HB3	1:A:167:ALA:HB2	1.93	0.50
1:A:309:ASP:CG	1:B:304:ARG:NH2	2.70	0.50
1:B:472:TRP:CZ2	1:B:509:ASP:HB2	2.47	0.50
1:B:510:THR:CG2	1:B:527:GLN:HB2	2.42	0.50
1:B:11:ASP:HB3	1:B:77:TRP:CZ2	2.46	0.50
1:A:509:ASP:O	1:A:522:TRP:HA	2.12	0.50
1:B:448:GLY:HA2	1:B:468:ARG:NH1	2.26	0.50
1:B:463:VAL:HG22	1:B:500:PRO:HG2	1.93	0.50
1:A:44:PRO:HB3	1:B:310:ASP:HB3	1.94	0.50
1:B:475:GLN:HG2	1:B:482:ALA:N	2.26	0.50
1:B:230:SER:O	1:B:231:ASN:HB3	2.11	0.49
1:A:90:THR:OG1	1:A:168:GLY:N	2.44	0.49
1:A:434:ARG:NH2	1:A:460:LEU:O	2.43	0.49
1:B:72:ILE:CG1	1:B:125:GLN:HG3	2.41	0.49
1:B:201:TYR:CE1	1:B:231:ASN:HA	2.47	0.49
1:A:95:ILE:HG13	1:A:103:ALA:HB3	1.94	0.49
1:A:469:TYR:HB2	1:A:473:TYR:CD2	2.46	0.49
1:B:90:THR:HB	1:B:132:VAL:HG11	1.90	0.49
1:B:291:TYR:HA	1:B:545:ALA:O	2.13	0.49
1:A:0:SER:O	1:A:398:HIS:HE1	1.94	0.49
1:A:258:ASP:O	1:A:259:SER:C	2.56	0.49
1:B:361:PHE:HD2	1:B:375:THR:HB	1.77	0.49
1:B:427:ALA:HB3	1:B:428:PRO:HD3	1.94	0.49
1:B:446:ASN:HB3	1:B:466:LEU:HD23	1.95	0.49
1:B:1:MET:O	1:B:85:ARG:NH2	2.43	0.49
1:A:475:GLN:HG2	1:A:482:ALA:HA	1.94	0.49
1:B:135:GLU:HA	1:B:157:GLN:HE22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ILE:HG23	1:A:461:PHE:CE2	2.47	0.48
1:A:210:GLY:HA3	1:A:257:ILE:O	2.14	0.48
1:A:389:HIS:O	1:A:393:ILE:HG13	2.13	0.48
1:A:12:LEU:HD12	1:A:13:ILE:N	2.27	0.48
1:A:120:VAL:HG12	1:A:121:ALA:N	2.28	0.48
1:A:19:TRP:CH2	1:A:128:LEU:HD13	2.48	0.48
1:B:514:LEU:HD23	1:B:515:HIS:N	2.29	0.48
1:B:50:ASN:H	1:B:50:ASN:ND2	2.12	0.48
1:B:503:MET:CE	1:B:505:GLU:O	2.62	0.48
1:A:380:ARG:C	1:A:381:ILE:HD12	2.38	0.48
1:B:466:LEU:O	1:B:467:ASN:OD1	2.30	0.48
1:A:45:VAL:O	1:A:46:PRO:C	2.55	0.48
1:B:213:GLN:HG3	1:B:257:ILE:HG12	1.94	0.48
1:B:509:ASP:O	1:B:510:THR:HG23	2.14	0.48
1:B:575:ASP:O	1:B:576:ARG:HB2	2.12	0.48
1:A:432:LEU:HD22	1:A:436:LEU:CD1	2.44	0.47
1:A:137:THR:C	1:A:144:GLY:O	2.56	0.47
1:A:377:SER:CB	1:A:378:PRO:CD	2.92	0.47
1:B:213:GLN:CG	1:B:257:ILE:CG1	2.90	0.47
1:B:90:THR:HG21	1:B:134:ASN:HA	1.97	0.47
1:B:475:GLN:OE1	1:B:475:GLN:N	2.48	0.47
1:B:503:MET:HE2	1:B:506:TYR:HB3	1.96	0.47
1:A:467:ASN:CB	1:A:505:GLU:HB2	2.45	0.47
1:A:475:GLN:HB2	1:A:482:ALA:HB2	1.96	0.47
1:B:83:LEU:HD23	1:B:83:LEU:N	2.29	0.47
1:A:575:ASP:O	1:A:576:ARG:HB2	2.13	0.47
1:A:198:LEU:HA	1:A:234:ILE:O	2.14	0.47
1:A:434:ARG:HG3	1:A:434:ARG:NH1	2.29	0.47
1:B:78:SER:O	1:B:79:GLU:HB2	2.15	0.47
1:B:309:ASP:C	1:B:309:ASP:OD1	2.57	0.47
1:B:396:LEU:C	1:B:396:LEU:HD23	2.40	0.47
1:B:473:TYR:O	1:B:476:THR:OG1	2.32	0.47
1:B:547:GLU:OE2	1:B:588:ARG:NH1	2.48	0.47
1:B:550:TRP:O	1:B:551:ASN:HB2	2.14	0.47
1:A:16:ASP:HA	1:A:45:VAL:CG2	2.44	0.47
1:A:361:PHE:CE2	1:A:380:ARG:HD2	2.38	0.47
1:B:236:ILE:HA	1:B:237:PRO:HD2	1.75	0.47
1:A:72:ILE:HG12	1:A:125:GLN:HE21	1.80	0.47
1:A:219:GLU:HG3	1:A:248:TYR:CE1	2.50	0.47
1:A:377:SER:HB2	1:A:378:PRO:HD2	1.96	0.47
1:B:77:TRP:O	1:B:80:GLU:HB2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:H	1:A:157:GLN:NE2	2.11	0.46
1:A:181:GLN:HA	1:A:206:SER:OG	2.15	0.46
1:A:391:GLN:O	1:A:395:GLU:HG3	2.15	0.46
1:A:474:THR:OG1	1:A:475:GLN:OE1	2.30	0.46
1:B:11:ASP:CB	1:B:77:TRP:CZ2	2.99	0.46
1:B:18:LEU:HB3	1:B:42:GLU:HB3	1.97	0.46
1:B:64:TRP:CE3	1:B:133:ASP:HB2	2.50	0.46
1:B:253:HIS:CE1	1:B:268:LYS:HG3	2.51	0.46
1:B:377:SER:HB2	1:B:378:PRO:CD	2.44	0.46
1:B:396:LEU:CD2	1:B:409:TRP:CZ3	2.98	0.46
1:B:509:ASP:HA	1:B:569:LYS:HA	1.98	0.46
1:B:518:MET:HE3	1:B:518:MET:HB3	1.65	0.46
1:A:46:PRO:O	1:A:47:ALA:HB2	2.15	0.46
1:B:164:TYR:N	1:B:557:THR:HA	2.31	0.46
1:B:437:ASP:HA	1:B:438:PRO:HD2	1.77	0.46
1:A:97:VAL:HG23	1:A:102:VAL:HG21	1.97	0.46
1:B:554:ASP:OD1	1:B:568:LYS:HA	2.16	0.46
1:A:390:ALA:O	1:A:394:ARG:HG3	2.16	0.45
1:A:256:ILE:O	1:A:264:ILE:CG2	2.64	0.45
1:B:141:ILE:CG2	1:B:355:PRO:HG2	2.45	0.45
1:A:191:ASP:OD2	1:A:192:VAL:N	2.44	0.45
1:A:218:ASP:HB2	1:A:248:TYR:OH	2.15	0.45
1:B:150:GLU:HG3	1:B:151:ALA:N	2.27	0.45
1:B:503:MET:CE	1:B:506:TYR:HB3	2.47	0.45
1:B:192:VAL:HG23	1:B:275:THR:HG23	1.98	0.45
1:B:445:ALA:HB1	1:B:467:ASN:HD21	1.80	0.45
1:B:326:ASN:C	1:B:326:ASN:ND2	2.55	0.45
1:B:72:ILE:HG13	1:B:125:GLN:HG3	1.99	0.45
1:A:19:TRP:NE1	1:A:45:VAL:HG22	2.32	0.45
1:A:330:THR:HA	1:A:335:TYR:CZ	2.52	0.45
1:A:361:PHE:HE2	1:A:380:ARG:HB3	1.82	0.45
1:A:567:ASN:ND2	1:A:567:ASN:C	2.74	0.45
1:B:11:ASP:HB3	1:B:77:TRP:HH2	1.77	0.45
1:B:257:ILE:HG22	1:B:258:ASP:N	2.32	0.45
1:A:37:LEU:HD12	1:A:38:LYS:H	1.81	0.44
1:A:141:ILE:HG13	1:A:389:HIS:HA	1.99	0.44
1:B:505:GLU:O	1:B:506:TYR:HB3	2.16	0.44
1:A:251:GLN:OE1	1:A:270:ALA:HB2	2.17	0.44
1:A:503:MET:HG3	1:A:538:PHE:CZ	2.52	0.44
1:B:97:VAL:HB	1:B:102:VAL:HG21	1.99	0.44
1:B:533:MET:C	1:B:533:MET:SD	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HD23	1:A:65:VAL:HG12	1.99	0.44
1:A:90:THR:CB	1:A:168:GLY:N	2.61	0.44
1:A:306:LYS:CE	1:A:333:TYR:CZ	3.00	0.44
1:B:258:ASP:OD1	1:B:258:ASP:C	2.60	0.44
1:A:236:ILE:HA	1:A:237:PRO:HD2	1.75	0.44
1:A:306:LYS:HE2	1:A:333:TYR:CZ	2.53	0.44
1:A:467:ASN:HB3	1:A:505:GLU:HB2	1.98	0.44
1:A:292:PHE:HB2	1:A:546:GLY:HA3	2.00	0.44
1:A:294:GLY:HA3	1:A:327:SER:O	2.18	0.44
1:A:377:SER:HB2	1:A:379:ASP:OD1	2.17	0.44
1:B:45:VAL:C	1:B:47:ALA:N	2.76	0.44
1:A:521:PRO:O	1:A:522:TRP:CB	2.65	0.44
1:B:564:VAL:O	1:B:564:VAL:HG12	2.18	0.44
1:A:503:MET:HE2	1:A:506:TYR:HB3	1.99	0.43
1:B:141:ILE:HD12	1:B:141:ILE:HA	1.60	0.43
1:B:381:ILE:HG13	1:B:385:THR:HG21	2.00	0.43
1:A:267:TYR:HE1	1:A:269:LEU:HB2	1.83	0.43
1:B:353:GLU:OE2	1:B:413:ASN:HB2	2.18	0.43
1:B:381:ILE:O	1:B:381:ILE:HG22	2.17	0.43
1:B:399:ARG:HD3	1:B:400:ASP:OD1	2.17	0.43
1:B:78:SER:C	1:B:80:GLU:N	2.77	0.43
1:B:247:ALA:HB2	1:B:347:GLY:N	2.32	0.43
1:A:82:TYR:O	1:A:117:THR:HG22	2.18	0.43
1:B:528:VAL:HG13	1:B:584:LEU:HD13	1.99	0.43
1:A:377:SER:CB	1:A:379:ASP:OD1	2.66	0.43
1:A:568:LYS:C	1:A:570:GLY:N	2.76	0.43
1:B:121:ALA:O	1:B:124:GLU:HB2	2.18	0.43
1:B:411:ILE:HG12	1:B:443:THR:O	2.18	0.43
1:A:295:PHE:O	1:A:328:PHE:HA	2.19	0.43
1:B:81:ARG:HG3	1:B:81:ARG:NH1	2.33	0.43
1:A:47:ALA:HA	1:A:307:GLY:HA3	2.01	0.43
1:A:303:ILE:HD13	1:B:315:HIS:CG	2.53	0.43
1:B:82:TYR:N	1:B:117:THR:CG2	2.71	0.43
1:A:83:LEU:N	1:A:83:LEU:HD23	2.34	0.43
1:A:89:ALA:O	1:A:90:THR:C	2.61	0.43
1:A:120:VAL:CG1	1:A:124:GLU:HB3	2.49	0.43
1:A:530:MET:O	1:A:531:LEU:C	2.61	0.43
1:B:24:ALA:HB2	1:B:66:TYR:HE2	1.84	0.43
1:A:326:ASN:C	1:A:326:ASN:ND2	2.71	0.43
1:B:292:PHE:HB2	1:B:546:GLY:HA3	1.99	0.43
1:B:426:PHE:O	1:B:427:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HG13	1:A:124:GLU:CD	2.44	0.42
1:B:112:PHE:N	1:B:112:PHE:CD1	2.86	0.42
1:A:361:PHE:CE2	1:A:380:ARG:HB3	2.54	0.42
1:A:447:VAL:HG22	1:A:448:GLY:N	2.34	0.42
1:B:341:GLU:O	1:B:344:ASP:HB2	2.19	0.42
1:A:386:ARG:HD3	1:A:425:TYR:O	2.19	0.42
1:A:39:THR:HB	1:A:41:LEU:HB2	2.02	0.42
1:A:120:VAL:CG1	1:A:121:ALA:N	2.82	0.42
1:A:160:GLN:HG3	1:A:358:GLY:O	2.19	0.42
1:A:396:LEU:CD2	1:A:409:TRP:HZ3	2.30	0.42
1:A:557:THR:OG1	1:A:566:GLY:HA2	2.19	0.42
1:A:581:ALA:O	1:A:582:ALA:C	2.63	0.42
1:B:475:GLN:HG3	1:B:481:GLU:CG	2.50	0.42
1:A:509:ASP:HB3	1:A:522:TRP:CZ3	2.55	0.42
1:B:294:GLY:O	1:B:548:GLN:HA	2.20	0.42
1:A:310:ASP:HB3	1:B:44:PRO:HB3	2.02	0.42
1:A:78:SER:O	1:A:79:GLU:CB	2.66	0.42
1:A:219:GLU:HG3	1:A:248:TYR:CZ	2.55	0.42
1:A:503:MET:HE1	1:A:505:GLU:O	2.20	0.42
1:A:68:GLN:HG3	1:A:129:THR:HB	2.01	0.41
1:B:213:GLN:CG	1:B:257:ILE:HG12	2.50	0.41
1:B:295:PHE:O	1:B:328:PHE:HB2	2.20	0.41
1:B:299:GLU:HG3	1:B:335:TYR:CD1	2.55	0.41
1:B:496:LYS:HG2	1:B:497:TYR:CE2	2.55	0.41
1:A:141:ILE:HD11	1:A:356:ALA:HB2	2.01	0.41
1:A:503:MET:HE3	1:A:503:MET:HB3	1.82	0.41
1:B:550:TRP:O	1:B:550:TRP:CD1	2.73	0.41
1:A:358:GLY:C	1:A:360:ALA:N	2.77	0.41
1:B:11:ASP:HB2	1:B:77:TRP:CH2	2.55	0.41
1:B:22:ALA:HB2	1:B:39:THR:HB	2.03	0.41
1:A:120:VAL:HG13	1:A:124:GLU:HB3	2.02	0.41
1:A:267:TYR:CE1	1:A:269:LEU:HB2	2.56	0.41
1:B:90:THR:OG1	1:B:168:GLY:N	2.50	0.41
1:A:50:ASN:ND2	1:A:50:ASN:H	2.19	0.41
1:A:260:SER:O	1:A:262:LYS:N	2.48	0.41
1:A:567:ASN:ND2	1:A:569:LYS:N	2.58	0.41
1:B:361:PHE:HB2	1:B:375:THR:HG22	2.02	0.41
1:B:258:ASP:O	1:B:259:SER:C	2.63	0.41
1:B:476:THR:O	1:B:477:ALA:CB	2.66	0.41
1:A:243:GLN:HB2	1:A:246:ALA:HB3	2.03	0.41
1:A:257:ILE:N	1:A:257:ILE:HD13	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ASP:OD2	1:A:262:LYS:HD2	2.20	0.41
1:B:377:SER:C	1:B:379:ASP:H	2.29	0.41
1:B:413:ASN:HD22	1:B:445:ALA:HB3	1.86	0.41
1:A:181:GLN:HA	1:A:181:GLN:HE21	1.86	0.41
1:A:361:PHE:HD2	1:A:375:THR:HB	1.86	0.41
1:A:422:ALA:C	1:A:457:ILE:HD11	2.46	0.41
1:B:0:SER:HB3	1:B:1:MET:H	1.65	0.41
1:B:74:PRO:HG2	1:B:77:TRP:CE2	2.56	0.41
1:B:90:THR:OG1	1:B:167:ALA:CB	2.69	0.41
1:B:509:ASP:OD2	1:B:569:LYS:NZ	2.37	0.41
1:B:542:GLU:O	1:B:542:GLU:HG2	2.21	0.41
1:A:503:MET:CE	1:A:505:GLU:O	2.69	0.41
1:B:85:ARG:HG2	1:B:86:CYS:N	2.36	0.41
1:B:468:ARG:HA	1:B:468:ARG:HD3	1.70	0.41
1:B:19:TRP:CE2	1:B:45:VAL:HG21	2.56	0.40
1:B:274:ARG:HG2	1:B:275:THR:N	2.36	0.40
1:B:361:PHE:H	1:B:375:THR:CG2	2.34	0.40
1:A:82:TYR:N	1:A:117:THR:HG22	2.23	0.40
1:A:475:GLN:HB3	1:A:478:GLU:HB2	2.03	0.40
1:A:551:ASN:CG	1:A:552:PHE:N	2.79	0.40
1:B:81:ARG:CG	1:B:81:ARG:HH11	2.34	0.40
1:B:264:ILE:O	1:B:264:ILE:HG13	2.20	0.40
1:A:193:GLN:HB2	1:A:198:LEU:HD21	2.04	0.40
1:B:23:LEU:HA	1:B:65:VAL:HA	2.02	0.40
1:B:330:THR:HA	1:B:335:TYR:CZ	2.56	0.40
1:A:44:PRO:HD3	1:B:314:VAL:HG21	2.04	0.40
1:A:134:ASN:CB	1:A:167:ALA:HB2	2.51	0.40
1:A:253:HIS:CE1	1:A:268:LYS:HG3	2.56	0.40
1:B:316:ASP:OD1	1:B:552:PHE:HE2	2.04	0.40
1:B:452:TYR:CE1	1:B:492:GLY:HA3	2.56	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	582/612 (95%)	527 (90%)	46 (8%)	9 (2%)	8	32
1	B	580/612 (95%)	514 (89%)	64 (11%)	2 (0%)	36	67
All	All	1162/1224 (95%)	1041 (90%)	110 (10%)	11 (1%)	14	44

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	GLY
1	A	471	GLY
1	B	471	GLY
1	A	47	ALA
1	A	359	LEU
1	A	401	LYS
1	A	45	VAL
1	A	261	LYS
1	A	569	LYS
1	B	506	TYR
1	A	46	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	493/509 (97%)	405 (82%)	88 (18%)	2	9
1	B	493/509 (97%)	423 (86%)	70 (14%)	3	14
All	All	986/1018 (97%)	828 (84%)	158 (16%)	2	12

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	12	LEU

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Mol	Chain	Res	Type
1	A	13	ILE
1	A	25	SER
1	A	30	THR
1	A	38	LYS
1	A	39	THR
1	A	40	SER
1	A	45	VAL
1	A	52	ILE
1	A	56	SER
1	A	75	LYS
1	A	77	TRP
1	A	79	GLU
1	A	80	GLU
1	A	95	ILE
1	A	119	LEU
1	A	128	LEU
1	A	129	THR
1	A	141	ILE
1	A	147	GLU
1	A	149	LEU
1	A	156	VAL
1	A	160	GLN
1	A	162	ASP
1	A	175	LEU
1	A	177	SER
1	A	178	VAL
1	A	180	GLN
1	A	181	GLN
1	A	196	THR
1	A	198	LEU
1	A	199	ILE
1	A	209	GLN
1	A	227	SER
1	A	233	THR
1	A	239	VAL
1	A	251	GLN
1	A	252	LEU
1	A	255	SER
1	A	259	SER
1	A	260	SER
1	A	262	LYS
1	A	263	THR

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Mol	Chain	Res	Type
1	A	269	LEU
1	A	271	THR
1	A	274	ARG
1	A	281	THR
1	A	306	LYS
1	A	326	ASN
1	A	329	ARG
1	A	340	MET
1	A	357	VAL
1	A	362	SER
1	A	363	ILE
1	A	375	THR
1	A	377	SER
1	A	379	ASP
1	A	384	LYS
1	A	399	ARG
1	A	407	VAL
1	A	432	LEU
1	A	435	GLN
1	A	439	THR
1	A	446	ASN
1	A	468	ARG
1	A	474	THR
1	A	475	GLN
1	A	488	GLU
1	A	490	LEU
1	A	495	GLU
1	A	496	LYS
1	A	499	LYS
1	A	510	THR
1	A	511	VAL
1	A	517	VAL
1	A	519	VAL
1	A	531	LEU
1	A	533	MET
1	A	542	GLU
1	A	559	VAL
1	A	567	ASN
1	A	568	LYS
1	A	571	VAL
1	A	577	LYS
1	A	584	LEU

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Mol	Chain	Res	Type
1	A	587	LYS
1	A	593	HIS
1	B	1	MET
1	B	3	LYS
1	B	7	THR
1	B	39	THR
1	B	45	VAL
1	B	52	ILE
1	B	69	ARG
1	B	77	TRP
1	B	83	LEU
1	B	90	THR
1	B	102	VAL
1	B	119	LEU
1	B	120	VAL
1	B	127	ARG
1	B	128	LEU
1	B	129	THR
1	B	141	ILE
1	B	150	GLU
1	B	156	VAL
1	B	177	SER
1	B	178	VAL
1	B	180	GLN
1	B	196	THR
1	B	198	LEU
1	B	199	ILE
1	B	207	THR
1	B	209	GLN
1	B	212	ILE
1	B	227	SER
1	B	251	GLN
1	B	255	SER
1	B	264	ILE
1	B	269	LEU
1	B	274	ARG
1	B	284	LEU
1	B	288	LYS
1	B	303	ILE
1	B	326	ASN
1	B	329	ARG
1	B	332	HIS

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Mol	Chain	Res	Type
1	B	340	MET
1	B	357	VAL
1	B	375	THR
1	B	384	LYS
1	B	399	ARG
1	B	407	VAL
1	B	432	LEU
1	B	447	VAL
1	B	449	LEU
1	B	457	ILE
1	B	466	LEU
1	B	467	ASN
1	B	468	ARG
1	B	474	THR
1	B	475	GLN
1	B	488	GLU
1	B	490	LEU
1	B	495	GLU
1	B	496	LYS
1	B	499	LYS
1	B	504	THR
1	B	510	THR
1	B	517	VAL
1	B	518	MET
1	B	531	LEU
1	B	533	MET
1	B	542	GLU
1	B	567	ASN
1	B	568	LYS
1	B	588	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	36	GLN
1	A	50	ASN
1	A	68	GLN
1	A	125	GLN
1	A	139	GLN
1	A	157	GLN
1	A	160	GLN

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Mol	Chain	Res	Type
1	A	181	GLN
1	A	213	GLN
1	A	279	GLN
1	A	302	ASN
1	A	308	HIS
1	A	315	HIS
1	A	326	ASN
1	A	332	HIS
1	A	389	HIS
1	A	391	GLN
1	A	398	HIS
1	A	413	ASN
1	A	446	ASN
1	A	567	ASN
1	A	583	HIS
1	B	50	ASN
1	B	100	ASN
1	B	157	GLN
1	B	165	ASN
1	B	184	GLN
1	B	193	GLN
1	B	235	HIS
1	B	251	GLN
1	B	326	ASN
1	B	389	HIS
1	B	413	ASN
1	B	446	ASN
1	B	548	GLN
1	B	556	GLN
1	B	567	ASN

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	588/612 (96%)	-0.31	15 (2%)	57 36	30, 45, 63, 96	0
1	B	584/612 (95%)	-0.30	14 (2%)	59 38	29, 47, 64, 79	0
All	All	1172/1224 (95%)	-0.30	29 (2%)	58 37	29, 46, 64, 96	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	473	TYR	4.6
1	B	473	TYR	3.8
1	A	361	PHE	3.6
1	A	380	ARG	3.5
1	A	474	THR	3.4
1	B	592	LEU	3.2
1	B	362	SER	3.2
1	B	467	ASN	3.1
1	B	470	PHE	3.1
1	B	474	THR	3.1
1	A	592	LEU	2.8
1	A	363	ILE	2.8
1	B	469	TYR	2.8
1	A	358	GLY	2.7
1	A	471	GLY	2.7
1	B	141	ILE	2.6
1	A	-7	ALA	2.6
1	A	377	SER	2.5
1	A	359	LEU	2.5
1	A	141	ILE	2.5
1	B	471	GLY	2.3
1	A	360	ALA	2.3
1	B	28	ASN	2.3
1	B	373	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	261	LYS	2.3
1	B	200	ASP	2.2
1	B	264	ILE	2.2
1	A	357	VAL	2.2
1	B	89	ALA	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.