



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:40 PM UTC

PDB ID : 8EXD / pdb_00008exd
Title : Crystal structure of Aspergillus fumigatus sterylglucosidase A
Authors : Pereira de Sa, N.; Del Poeta, M.; Airola, M.V.
Deposited on : 2022-10-25
Resolution : 3.80 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

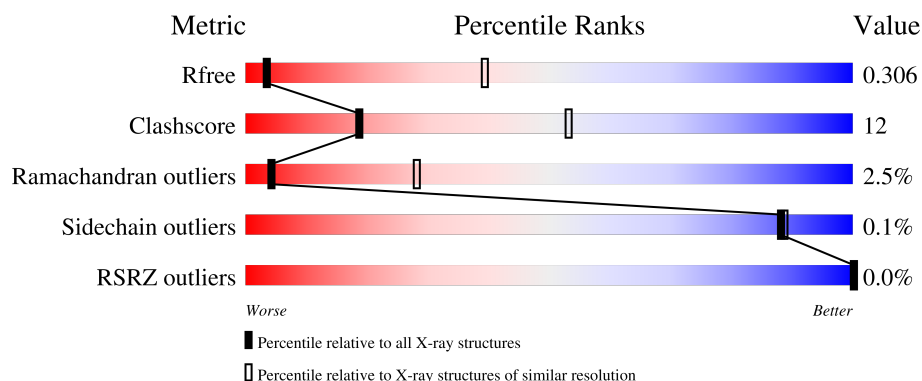
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	779	
1	B	779	
1	C	779	
1	D	779	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21118 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 Sterylglucosidase A (SglA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	670	Total	C	N	O	S	0	0	0
			5426	3486	921	1002	17			
1	B	659	Total	C	N	O	S	0	0	0
			5338	3426	908	987	17			
1	C	655	Total	C	N	O	S	0	0	0
			5309	3411	900	981	17			
1	D	623	Total	C	N	O	S	0	0	0
			5045	3248	852	929	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q4WXA7
A	-18	GLY	-	expression tag	UNP Q4WXA7
A	-17	SER	-	expression tag	UNP Q4WXA7
A	-16	SER	-	expression tag	UNP Q4WXA7
A	-15	HIS	-	expression tag	UNP Q4WXA7
A	-14	HIS	-	expression tag	UNP Q4WXA7
A	-13	HIS	-	expression tag	UNP Q4WXA7
A	-12	HIS	-	expression tag	UNP Q4WXA7
A	-11	HIS	-	expression tag	UNP Q4WXA7
A	-10	HIS	-	expression tag	UNP Q4WXA7
A	-9	SER	-	expression tag	UNP Q4WXA7
A	-8	SER	-	expression tag	UNP Q4WXA7
A	-7	GLY	-	expression tag	UNP Q4WXA7
A	-6	LEU	-	expression tag	UNP Q4WXA7
A	-5	VAL	-	expression tag	UNP Q4WXA7
A	-4	PRO	-	expression tag	UNP Q4WXA7
A	-3	ARG	-	expression tag	UNP Q4WXA7
A	-2	GLY	-	expression tag	UNP Q4WXA7
A	-1	SER	-	expression tag	UNP Q4WXA7
A	0	HIS	-	expression tag	UNP Q4WXA7
B	-19	MET	-	initiating methionine	UNP Q4WXA7

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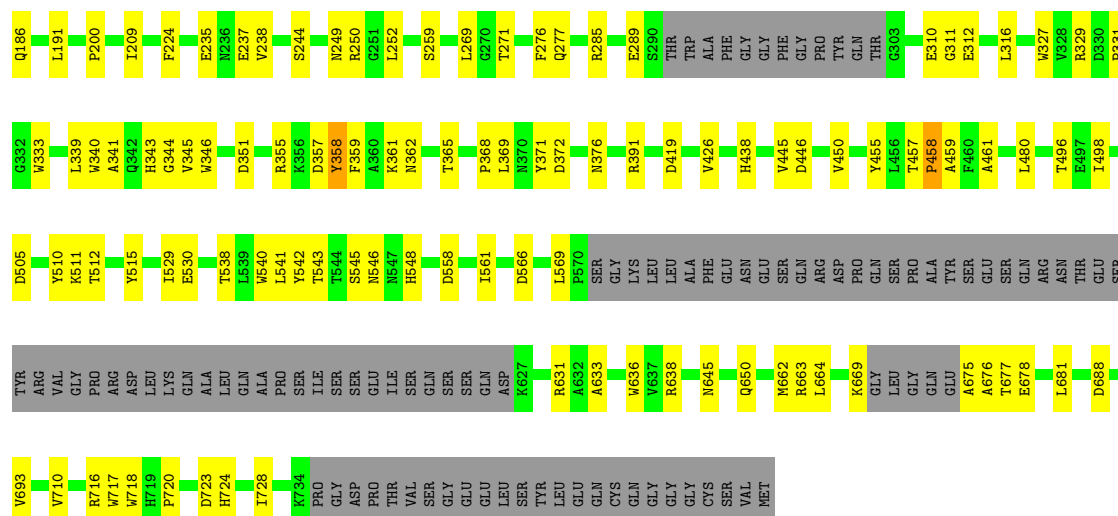
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q4WXA7
B	-17	SER	-	expression tag	UNP Q4WXA7
B	-16	SER	-	expression tag	UNP Q4WXA7
B	-15	HIS	-	expression tag	UNP Q4WXA7
B	-14	HIS	-	expression tag	UNP Q4WXA7
B	-13	HIS	-	expression tag	UNP Q4WXA7
B	-12	HIS	-	expression tag	UNP Q4WXA7
B	-11	HIS	-	expression tag	UNP Q4WXA7
B	-10	HIS	-	expression tag	UNP Q4WXA7
B	-9	SER	-	expression tag	UNP Q4WXA7
B	-8	SER	-	expression tag	UNP Q4WXA7
B	-7	GLY	-	expression tag	UNP Q4WXA7
B	-6	LEU	-	expression tag	UNP Q4WXA7
B	-5	VAL	-	expression tag	UNP Q4WXA7
B	-4	PRO	-	expression tag	UNP Q4WXA7
B	-3	ARG	-	expression tag	UNP Q4WXA7
B	-2	GLY	-	expression tag	UNP Q4WXA7
B	-1	SER	-	expression tag	UNP Q4WXA7
B	0	HIS	-	expression tag	UNP Q4WXA7
C	-19	MET	-	initiating methionine	UNP Q4WXA7
C	-18	GLY	-	expression tag	UNP Q4WXA7
C	-17	SER	-	expression tag	UNP Q4WXA7
C	-16	SER	-	expression tag	UNP Q4WXA7
C	-15	HIS	-	expression tag	UNP Q4WXA7
C	-14	HIS	-	expression tag	UNP Q4WXA7
C	-13	HIS	-	expression tag	UNP Q4WXA7
C	-12	HIS	-	expression tag	UNP Q4WXA7
C	-11	HIS	-	expression tag	UNP Q4WXA7
C	-10	HIS	-	expression tag	UNP Q4WXA7
C	-9	SER	-	expression tag	UNP Q4WXA7
C	-8	SER	-	expression tag	UNP Q4WXA7
C	-7	GLY	-	expression tag	UNP Q4WXA7
C	-6	LEU	-	expression tag	UNP Q4WXA7
C	-5	VAL	-	expression tag	UNP Q4WXA7
C	-4	PRO	-	expression tag	UNP Q4WXA7
C	-3	ARG	-	expression tag	UNP Q4WXA7
C	-2	GLY	-	expression tag	UNP Q4WXA7
C	-1	SER	-	expression tag	UNP Q4WXA7
C	0	HIS	-	expression tag	UNP Q4WXA7
D	-19	MET	-	initiating methionine	UNP Q4WXA7
D	-18	GLY	-	expression tag	UNP Q4WXA7
D	-17	SER	-	expression tag	UNP Q4WXA7

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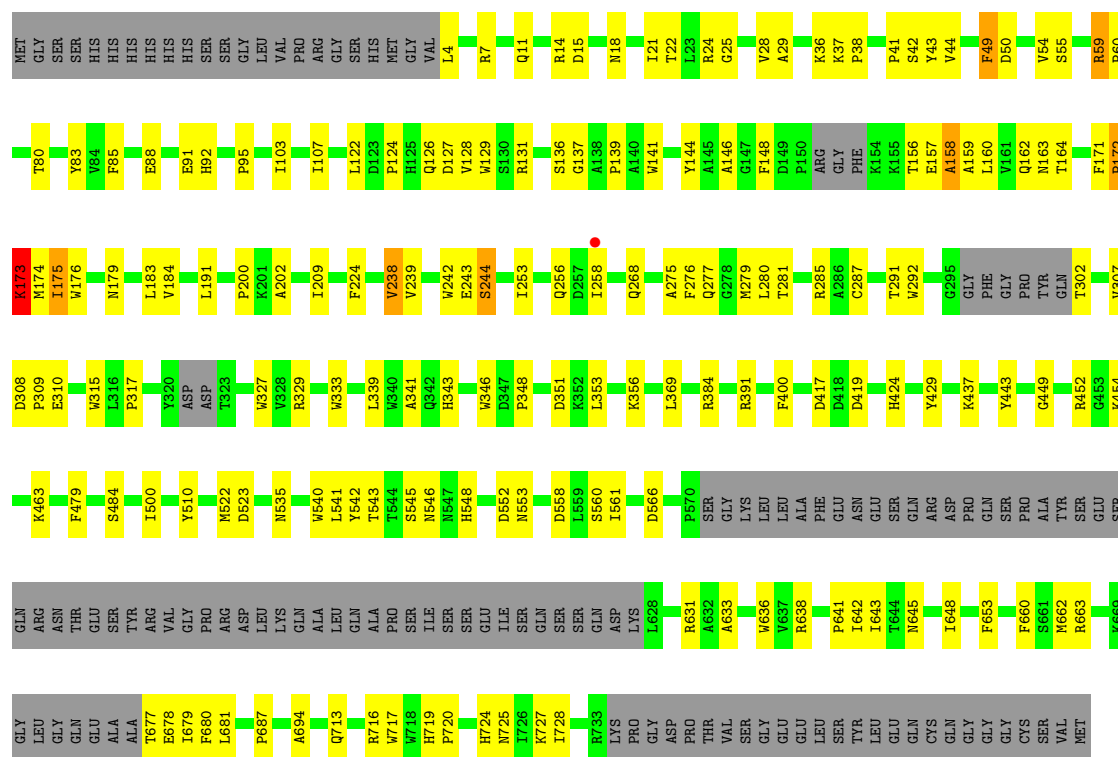
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q4WXA7
D	-15	HIS	-	expression tag	UNP Q4WXA7
D	-14	HIS	-	expression tag	UNP Q4WXA7
D	-13	HIS	-	expression tag	UNP Q4WXA7
D	-12	HIS	-	expression tag	UNP Q4WXA7
D	-11	HIS	-	expression tag	UNP Q4WXA7
D	-10	HIS	-	expression tag	UNP Q4WXA7
D	-9	SER	-	expression tag	UNP Q4WXA7
D	-8	SER	-	expression tag	UNP Q4WXA7
D	-7	GLY	-	expression tag	UNP Q4WXA7
D	-6	LEU	-	expression tag	UNP Q4WXA7
D	-5	VAL	-	expression tag	UNP Q4WXA7
D	-4	PRO	-	expression tag	UNP Q4WXA7
D	-3	ARG	-	expression tag	UNP Q4WXA7
D	-2	GLY	-	expression tag	UNP Q4WXA7
D	-1	SER	-	expression tag	UNP Q4WXA7
D	0	HIS	-	expression tag	UNP Q4WXA7



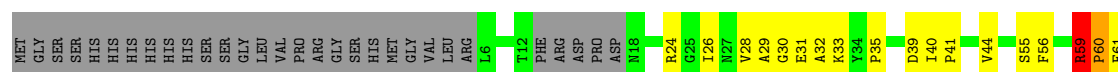
• Molecule 1: Sterylglucosidase A (SglA)

Chain C: 62% 21% 16%



• Molecule 1: Sterylglucosidase A (SglA)

Chain D: 59% 20% 20%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.73Å 112.79Å 139.10Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	58.21 – 3.80 58.21 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (58.21-3.80) 99.1 (58.21-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.279 , 0.324 0.286 , 0.306	Depositor DCC
R_{free} test set	2000 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	134.4	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 153.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21118	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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	0.13	0/5596	0.38	0/7613
1	B	0.11	0/5501	0.34	0/7481
1	C	0.17	0/5472	0.36	0/7443
1	D	0.18	0/5201	0.39	1/7076 (0.0%)
All	All	0.15	0/21770	0.37	1/29613 (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	3
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	GLY	N-CA-C	6.83	120.42	112.50

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	ALA	Peptide
1	A	301	GLN	Peptide
1	A	540	TRP	Peptide
1	B	59	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	C	59	ARG	Peptide
1	D	59	ARG	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	5426	0	5152	124	0
1	B	5338	0	5080	115	0
1	C	5309	0	5041	132	0
1	D	5045	0	4778	120	0
All	All	21118	0	20051	491	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 12.

All (491) 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:192:PHE:CZ	1:D:214:GLN:HG2	1.97	0.99
1:B:30:GLY:H	1:B:541:LEU:HD21	1.38	0.88
1:A:291:THR:H	1:A:302:THR:HG21	1.41	0.86
1:B:329:ARG:HD3	1:B:333:TRP:HD1	1.45	0.80
1:A:645:ASN:H	1:A:677:THR:HG22	1.49	0.78
1:D:330:ASP:HB2	1:D:331:PRO:HD2	1.65	0.78
1:D:93:GLU:O	1:D:325:TYR:OH	2.01	0.77
1:D:700:TRP:HB3	1:D:717:TRP:HD1	1.50	0.77
1:C:645:ASN:H	1:C:677:THR:HG22	1.51	0.76
1:A:258:ILE:HB	1:A:275:ALA:HB3	1.68	0.76
1:C:678:GLU:HG2	1:C:716:ARG:HG2	1.66	0.75
1:A:317:PRO:HG2	1:A:320:TYR:HB2	1.68	0.75
1:B:362:ASN:HD21	1:B:365:THR:HG22	1.51	0.74
1:C:329:ARG:HD3	1:C:333:TRP:HD1	1.52	0.74
1:A:322:ASP:O	1:A:327:TRP:NE1	2.21	0.74
1:D:190:THR:O	1:D:194:GLY:HA3	1.86	0.74
1:A:195:GLY:H	1:A:210:GLN:HB2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ALA:HA	1:C:183:LEU:HB3	1.71	0.71
1:C:91:GLU:O	1:C:141:TRP:NE1	2.19	0.71
1:A:329:ARG:HD3	1:A:333:TRP:HD1	1.54	0.71
1:B:150:PRO:O	1:B:152:GLY:N	2.24	0.71
1:D:32:ALA:HA	1:D:59:ARG:HG3	1.73	0.70
1:C:543:THR:HB	1:C:546:ASN:HB2	1.74	0.69
1:A:323:THR:HG22	1:A:323:THR:O	1.93	0.69
1:A:159:ALA:HB2	1:A:184:VAL:HG21	1.72	0.69
1:C:146:ALA:HB2	1:C:333:TRP:HZ2	1.57	0.69
1:A:642:ILE:HG22	1:A:643:ILE:HG13	1.74	0.69
1:D:192:PHE:CZ	1:D:214:GLN:CG	2.75	0.69
1:C:543:THR:HG22	1:C:545:SER:H	1.58	0.69
1:A:322:ASP:O	1:A:324:ARG:N	2.25	0.68
1:B:543:THR:HG22	1:B:545:SER:H	1.59	0.68
1:B:148:PHE:HA	1:B:316:LEU:H	1.58	0.68
1:C:24:ARG:NH2	1:C:636:TRP:O	2.26	0.68
1:C:38:PRO:HD2	1:C:54:VAL:HG13	1.77	0.67
1:D:110:LEU:HB3	1:D:238:VAL:HG11	1.74	0.67
1:C:36:LYS:HD3	1:C:59:ARG:HG3	1.77	0.67
1:D:543:THR:HB	1:D:546:ASN:HB2	1.77	0.67
1:B:31:GLU:OE1	1:B:59:ARG:NH1	2.28	0.66
1:C:54:VAL:HG12	1:C:55:SER:H	1.59	0.66
1:D:24:ARG:NH2	1:D:636:TRP:O	2.29	0.66
1:D:543:THR:HG22	1:D:545:SER:H	1.60	0.66
1:A:107:ILE:HA	1:A:110:LEU:HD12	1.78	0.65
1:A:52:ASP:OD1	1:A:325:TYR:OH	2.14	0.65
1:A:288:GLU:HG2	1:A:304:ARG:HE	1.62	0.65
1:B:645:ASN:H	1:B:677:THR:HG22	1.62	0.64
1:A:197:ASP:HB3	1:A:363:PRO:HG3	1.79	0.64
1:D:372:ASP:OD1	1:D:373:LYS:N	2.31	0.64
1:B:446:ASP:HB3	1:B:455:TYR:HE2	1.63	0.64
1:B:662:MET:HE3	1:B:664:LEU:HD23	1.79	0.64
1:C:95:PRO:HG3	1:C:327:TRP:HE3	1.63	0.64
1:C:11:GLN:O	1:C:535:ASN:ND2	2.29	0.63
1:C:175:ILE:HG12	1:C:175:ILE:O	1.98	0.63
1:C:540:TRP:CE2	1:C:541:LEU:HD12	2.33	0.63
1:A:11:GLN:O	1:A:535:ASN:ND2	2.27	0.63
1:C:42:SER:O	1:C:163:ASN:ND2	2.30	0.63
1:B:30:GLY:N	1:B:541:LEU:HD21	2.12	0.63
1:B:357:ASP:OD1	1:B:358:TYR:N	2.31	0.63
1:B:693:VAL:HG13	1:B:728:ILE:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:LYS:HG3	1:B:512:THR:HG23	1.81	0.62
1:D:31:GLU:HB3	1:D:59:ARG:HH11	1.64	0.62
1:A:299:PRO:HB3	1:A:302:THR:HB	1.80	0.62
1:C:162:GLN:O	1:C:171:PHE:CZ	2.52	0.62
1:D:158:ALA:HB1	1:D:183:LEU:HB3	1.80	0.62
1:D:330:ASP:O	1:D:332:GLY:N	2.29	0.62
1:B:158:ALA:HB1	1:B:184:VAL:HG13	1.82	0.62
1:B:128:VAL:HG11	1:B:179:ASN:HB2	1.82	0.61
1:B:329:ARG:HD3	1:B:333:TRP:CD1	2.30	0.61
1:C:54:VAL:O	1:C:92:HIS:NE2	2.31	0.61
1:D:238:VAL:HG12	1:D:239:VAL:HG23	1.81	0.61
1:A:24:ARG:NH2	1:A:636:TRP:O	2.33	0.61
1:C:280:LEU:HD22	1:C:285:ARG:HB2	1.80	0.61
1:B:541:LEU:HD23	1:B:542:TYR:N	2.16	0.61
1:C:159:ALA:HB2	1:C:184:VAL:HG21	1.82	0.61
1:A:662:MET:HE3	1:A:664:LEU:HD23	1.82	0.60
1:D:143:LEU:HB3	1:D:148:PHE:CD2	2.35	0.60
1:B:372:ASP:O	1:B:376:ASN:ND2	2.34	0.60
1:B:19:ARG:NH1	1:B:676:ALA:O	2.33	0.60
1:C:642:ILE:HG22	1:C:643:ILE:HG13	1.83	0.60
1:D:254:GLY:HA2	1:D:369:LEU:HG	1.82	0.60
1:A:182:ARG:NH2	1:A:271:THR:O	2.35	0.60
1:B:678:GLU:HG2	1:B:716:ARG:HG2	1.84	0.59
1:C:541:LEU:HD23	1:C:542:TYR:N	2.17	0.59
1:B:540:TRP:CE2	1:B:541:LEU:HD12	2.37	0.59
1:A:36:LYS:HD3	1:A:59:ARG:HD3	1.83	0.59
1:B:548:HIS:NE2	1:B:566:ASP:OD1	2.32	0.59
1:B:161:VAL:HG12	1:B:163:ASN:H	1.68	0.59
1:A:36:LYS:HB2	1:A:59:ARG:HG2	1.84	0.59
1:A:329:ARG:HD3	1:A:333:TRP:CD1	2.35	0.59
1:A:401:CYS:N	1:A:423:VAL:O	2.35	0.58
1:A:158:ALA:HB1	1:A:184:VAL:HG13	1.85	0.58
1:D:322:ASP:HB3	1:D:327:TRP:CZ3	2.38	0.58
1:D:148:PHE:CZ	1:D:184:VAL:HB	2.39	0.58
1:B:69:HIS:ND1	1:B:542:TYR:OH	2.36	0.58
1:A:457:THR:O	1:A:459:ALA:N	2.37	0.58
1:C:353:LEU:HD23	1:C:356:LYS:HB3	1.86	0.58
1:B:113:ALA:HB1	1:B:118:PHE:HD2	1.68	0.57
1:A:148:PHE:HA	1:A:316:LEU:N	2.19	0.57
1:D:391:ARG:NH2	1:D:419:ASP:OD2	2.29	0.57
1:D:700:TRP:HB3	1:D:717:TRP:CD1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:LEU:HD13	1:C:7:ARG:HG3	1.86	0.57
1:C:329:ARG:HD3	1:C:333:TRP:CD1	2.36	0.57
1:D:182:ARG:NH2	1:D:271:THR:O	2.37	0.57
1:D:33:LYS:HB3	1:D:136:SER:HB3	1.87	0.57
1:B:61:PHE:HE2	1:B:66:ALA:HA	1.70	0.56
1:B:249:ASN:OD1	1:B:250:ARG:N	2.33	0.56
1:D:30:GLY:HA3	1:D:541:LEU:HD21	1.86	0.56
1:D:192:PHE:CD2	1:D:192:PHE:C	2.84	0.56
1:A:128:VAL:HG11	1:A:179:ASN:HB2	1.86	0.56
1:D:190:THR:HG23	1:D:253:ILE:HG13	1.87	0.56
1:D:201:LYS:HG2	1:D:332:GLY:HA2	1.87	0.56
1:A:92:HIS:HE1	1:A:99:ASP:HB2	1.71	0.56
1:D:94:GLY:HA3	1:D:325:TYR:CZ	2.41	0.56
1:D:277:GLN:HA	1:D:280:LEU:HD12	1.87	0.56
1:A:334:LYS:HE3	1:A:342:GLN:HB2	1.87	0.56
1:A:441:ARG:NH2	1:A:520:SER:OG	2.38	0.56
1:B:496:THR:O	1:B:538:THR:OG1	2.25	0.55
1:B:147:GLY:HA2	1:B:316:LEU:HD12	1.88	0.55
1:B:250:ARG:HD2	1:B:371:TYR:HE2	1.71	0.55
1:A:103:ILE:O	1:A:107:ILE:HG12	2.06	0.55
1:C:200:PRO:HD2	1:C:343:HIS:CD2	2.42	0.55
1:C:49:PHE:HZ	1:C:163:ASN:HB3	1.70	0.55
1:B:61:PHE:CE2	1:B:66:ALA:HA	2.42	0.55
1:C:131:ARG:HB3	1:C:136:SER:HA	1.88	0.55
1:A:463:LYS:HD2	1:A:472:CYS:HB2	1.89	0.55
1:A:537:PHE:HE2	1:A:539:LEU:HG	1.71	0.55
1:C:429:TYR:HH	1:C:540:TRP:CD1	2.26	0.54
1:A:15:ASP:HB2	1:A:16:PRO:HD2	1.88	0.54
1:C:157:GLU:O	1:C:159:ALA:N	2.39	0.54
1:B:362:ASN:HB3	1:B:369:LEU:HD21	1.90	0.54
1:B:645:ASN:N	1:B:677:THR:HG22	2.21	0.54
1:D:365:THR:OG1	1:D:366:GLY:N	2.40	0.54
1:C:346:TRP:CZ3	1:C:348:PRO:HA	2.42	0.54
1:D:55:SER:OG	1:D:92:HIS:NE2	2.40	0.54
1:B:333:TRP:CZ3	1:B:339:LEU:HD13	2.43	0.53
1:C:14:ARG:NH1	1:C:18:ASN:O	2.37	0.53
1:B:681:LEU:HD21	1:B:728:ILE:HG21	1.89	0.53
1:D:140:ALA:HB1	1:D:144:TYR:HE2	1.73	0.53
1:A:111:ARG:HG3	1:A:114:LYS:HE3	1.91	0.53
1:D:322:ASP:HB3	1:D:327:TRP:HZ3	1.73	0.53
1:D:546:ASN:ND2	1:D:552:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLN:HB3	1:A:252:LEU:HG	1.91	0.53
1:A:391:ARG:NH2	1:A:419:ASP:OD2	2.37	0.53
1:B:200:PRO:HD2	1:B:343:HIS:CD2	2.43	0.53
1:C:523:ASP:OD1	1:C:638:ARG:NH1	2.34	0.53
1:A:200:PRO:HD2	1:A:343:HIS:CD2	2.44	0.53
1:A:228:ILE:HG22	1:A:235:GLU:HG3	1.91	0.53
1:A:274:THR:H	1:A:277:GLN:HB2	1.74	0.53
1:B:310:GLU:O	1:B:312:GLU:N	2.41	0.53
1:D:83:TYR:HB3	1:D:122:LEU:HD23	1.91	0.53
1:B:391:ARG:NH2	1:B:419:ASP:OD2	2.28	0.53
1:C:41:PRO:HB3	1:C:553:ASN:HB3	1.91	0.52
1:C:541:LEU:HD23	1:C:542:TYR:C	2.34	0.52
1:A:162:GLN:OE1	1:A:555:ASN:HA	2.09	0.52
1:A:292:TRP:C	1:A:299:PRO:HB2	2.34	0.52
1:A:148:PHE:HA	1:A:316:LEU:H	1.74	0.52
1:B:28:VAL:HG13	1:B:29:ALA:HB2	1.92	0.52
1:C:162:GLN:O	1:C:171:PHE:HZ	1.92	0.52
1:C:174:MET:HB2	1:C:176:TRP:NE1	2.23	0.52
1:C:510:TYR:OH	1:C:558:ASP:OD2	2.19	0.52
1:A:148:PHE:CD1	1:A:153:PHE:HZ	2.28	0.52
1:B:457:THR:O	1:B:459:ALA:N	2.41	0.52
1:C:339:LEU:HD11	1:C:343:HIS:CE1	2.45	0.52
1:A:294:PHE:CD1	1:A:297:PHE:HB3	2.45	0.52
1:A:645:ASN:ND2	1:A:675:ALA:O	2.42	0.52
1:B:60:PRO:HD2	1:B:105:PHE:HE2	1.75	0.52
1:C:83:TYR:HB3	1:C:122:LEU:HD23	1.91	0.52
1:B:83:TYR:HB3	1:B:122:LEU:HD23	1.92	0.52
1:C:128:VAL:HG11	1:C:179:ASN:HB2	1.91	0.52
1:C:202:ALA:HA	1:C:333:TRP:CE3	2.44	0.52
1:B:344:GLY:O	1:B:355:ARG:HG3	2.10	0.52
1:A:198:PHE:HE2	1:A:253:ILE:HA	1.75	0.51
1:B:106:THR:HG21	1:B:224:PHE:HZ	1.75	0.51
1:A:132:LEU:HD13	1:A:150:PRO:HG3	1.91	0.51
1:D:510:TYR:OH	1:D:558:ASP:OD2	2.22	0.51
1:B:498:ILE:HD13	1:B:529:ILE:HD11	1.93	0.51
1:C:157:GLU:HG3	1:C:281:THR:HG21	1.92	0.51
1:A:11:GLN:HG3	1:A:490:THR:HG23	1.92	0.51
1:D:61:PHE:CD1	1:D:66:ALA:HA	2.46	0.51
1:A:178:THR:HG22	1:A:267:LEU:HD21	1.93	0.51
1:B:28:VAL:HG22	1:B:542:TYR:HB3	1.93	0.51
1:B:60:PRO:HD2	1:B:105:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:VAL:HG11	1:D:179:ASN:HB2	1.92	0.51
1:C:43:TYR:HE1	1:C:164:THR:HA	1.76	0.51
1:C:88:GLU:HG3	1:C:139:PRO:HA	1.91	0.51
1:C:642:ILE:HD11	1:C:680:PHE:HB2	1.93	0.51
1:A:226:GLN:HA	1:A:393:VAL:HG11	1.93	0.51
1:C:28:VAL:HG13	1:C:29:ALA:HB2	1.92	0.51
1:C:540:TRP:CZ2	1:C:541:LEU:HD12	2.46	0.51
1:C:694:ALA:HB3	1:C:727:LYS:HB3	1.93	0.51
1:A:205:ASP:H	1:A:328:VAL:HG23	1.76	0.50
1:B:146:ALA:HB3	1:B:148:PHE:HE2	1.75	0.50
1:C:449:GLY:HA2	1:C:454:LYS:HD3	1.92	0.50
1:D:540:TRP:CE2	1:D:541:LEU:HD12	2.46	0.50
1:D:633:ALA:HA	1:D:636:TRP:CE2	2.46	0.50
1:A:678:GLU:HG2	1:A:716:ARG:HG2	1.93	0.50
1:B:14:ARG:NH1	1:B:18:ASN:O	2.41	0.50
1:B:541:LEU:HD23	1:B:542:TYR:C	2.37	0.50
1:C:384:ARG:NE	1:C:417:ASP:OD2	2.41	0.50
1:B:134:GLY:N	1:B:161:VAL:HG22	2.26	0.50
1:D:62:SER:OG	1:D:65:ASP:OD2	2.29	0.50
1:A:61:PHE:HD2	1:A:544:THR:HG21	1.75	0.50
1:C:500:ILE:HG13	1:C:522:MET:HE3	1.93	0.50
1:A:113:ALA:HB1	1:A:118:PHE:HD2	1.77	0.50
1:C:268:GLN:O	1:C:292:TRP:NE1	2.40	0.50
1:B:141:TRP:HB2	1:B:327:TRP:HZ2	1.77	0.50
1:B:510:TYR:OH	1:B:558:ASP:OD2	2.28	0.50
1:A:543:THR:HB	1:A:546:ASN:HB2	1.93	0.50
1:B:677:THR:OG1	1:B:717:TRP:HB3	2.12	0.50
1:B:543:THR:HB	1:B:546:ASN:HB2	1.94	0.50
1:D:147:GLY:HA2	1:D:316:LEU:HD12	1.94	0.50
1:C:156:THR:HG22	1:C:309:PRO:HB3	1.94	0.49
1:D:88:GLU:OE2	1:D:131:ARG:NE	2.44	0.49
1:B:645:ASN:ND2	1:B:675:ALA:O	2.45	0.49
1:C:174:MET:HB2	1:C:176:TRP:CD1	2.48	0.49
1:A:165:PHE:HD1	1:A:166:ASP:H	1.60	0.49
1:C:173:LYS:HE2	1:C:437:LYS:HD2	1.93	0.49
1:C:256:GLN:NE2	1:C:369:LEU:O	2.46	0.49
1:D:61:PHE:CZ	1:D:109:VAL:HG13	2.48	0.49
1:B:24:ARG:NH2	1:B:636:TRP:O	2.46	0.49
1:B:141:TRP:HB2	1:B:327:TRP:CZ2	2.47	0.49
1:D:541:LEU:HD23	1:D:542:TYR:N	2.26	0.49
1:B:131:ARG:HB3	1:B:136:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ALA:O	1:C:209:ILE:N	2.46	0.49
1:C:633:ALA:HA	1:C:636:TRP:CE2	2.47	0.49
1:D:129:TRP:CD1	1:D:143:LEU:HD21	2.48	0.49
1:D:130:SER:HB3	1:D:143:LEU:HD11	1.95	0.49
1:D:143:LEU:HD22	1:D:148:PHE:CE2	2.47	0.49
1:D:558:ASP:OD1	1:D:631:ARG:NH2	2.46	0.49
1:B:179:ASN:HA	1:B:182:ARG:HB2	1.94	0.49
1:B:271:THR:HB	1:B:289:GLU:OE1	2.12	0.49
1:D:65:ASP:HB3	1:D:69:HIS:CE1	2.47	0.49
1:D:115:GLN:HB3	1:D:708:HIS:NE2	2.28	0.49
1:A:633:ALA:HA	1:A:636:TRP:CE2	2.48	0.49
1:C:160:LEU:CD2	1:C:175:ILE:HD13	2.43	0.49
1:B:277:GLN:HE22	1:B:289:GLU:HA	1.77	0.49
1:C:36:LYS:HG3	1:C:37:LYS:HG3	1.94	0.49
1:A:162:GLN:C	1:A:164:THR:H	2.20	0.48
1:C:141:TRP:HA	1:C:144:TYR:CE1	2.48	0.48
1:C:276:PHE:CG	1:C:353:LEU:HD11	2.48	0.48
1:A:51:ALA:O	1:A:53:ASN:N	2.46	0.48
1:A:238:VAL:HG13	1:A:239:VAL:HG23	1.95	0.48
1:C:49:PHE:CZ	1:C:163:ASN:HB3	2.49	0.48
1:C:172:PRO:O	1:C:172:PRO:HG2	2.12	0.48
1:A:88:GLU:OE2	1:A:131:ARG:NE	2.42	0.48
1:B:333:TRP:HZ3	1:B:339:LEU:HD13	1.78	0.48
1:C:546:ASN:ND2	1:C:552:ASP:OD1	2.47	0.48
1:D:444:ASN:OD1	1:D:445:VAL:N	2.42	0.48
1:C:103:ILE:O	1:C:107:ILE:HG12	2.12	0.48
1:D:394:TRP:HE1	1:D:396:GLU:HB2	1.79	0.48
1:A:31:GLU:OE2	1:A:545:SER:N	2.46	0.48
1:B:285:ARG:NH2	1:B:351:ASP:OD2	2.45	0.48
1:C:95:PRO:HG3	1:C:327:TRP:CE3	2.45	0.48
1:C:339:LEU:HD11	1:C:343:HIS:HE1	1.78	0.48
1:A:258:ILE:HG21	1:A:359:PHE:HD2	1.79	0.48
1:C:243:GLU:HA	1:C:400:PHE:HB2	1.94	0.48
1:A:723:ASP:O	1:A:724:HIS:ND1	2.47	0.48
1:B:633:ALA:HA	1:B:636:TRP:CE2	2.49	0.48
1:C:238:VAL:HG13	1:C:239:VAL:HG23	1.96	0.48
1:C:307:VAL:HG12	1:C:309:PRO:HD2	1.96	0.48
1:D:695:VAL:HG21	1:D:717:TRP:HE1	1.78	0.48
1:C:663:ARG:HG3	1:C:725:ASN:HB3	1.96	0.47
1:A:148:PHE:HD1	1:A:153:PHE:HZ	1.61	0.47
1:B:37:LYS:HB2	1:B:55:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ARG:NH2	1:C:348:PRO:O	2.46	0.47
1:D:367:GLU:N	1:D:368:PRO:HD2	2.29	0.47
1:D:543:THR:HG22	1:D:545:SER:N	2.29	0.47
1:B:561:ILE:HD12	1:B:636:TRP:CZ3	2.49	0.47
1:C:308:ASP:N	1:C:309:PRO:HD2	2.28	0.47
1:D:192:PHE:HE2	1:D:214:GLN:HE21	1.56	0.47
1:A:92:HIS:CE1	1:A:99:ASP:HB2	2.49	0.47
1:B:498:ILE:HG21	1:B:529:ILE:HD11	1.96	0.47
1:B:180:TYR:HA	1:B:185:SER:HB2	1.97	0.47
1:B:530:GLU:OE2	1:B:638:ARG:NE	2.38	0.47
1:C:280:LEU:HD11	1:C:351:ASP:HB3	1.97	0.47
1:C:720:PRO:HG2	1:C:724:HIS:NE2	2.30	0.47
1:D:26:ILE:HA	1:D:539:LEU:H	1.79	0.47
1:D:35:PRO:C	1:D:59:ARG:HH21	2.22	0.47
1:D:65:ASP:HB3	1:D:69:HIS:HE1	1.80	0.47
1:D:167:ASP:OD1	1:D:170:GLU:N	2.48	0.47
1:D:678:GLU:HG2	1:D:716:ARG:HG2	1.97	0.47
1:A:143:LEU:O	1:A:147:GLY:N	2.45	0.47
1:D:190:THR:O	1:D:194:GLY:CA	2.60	0.47
1:A:322:ASP:HB3	1:A:327:TRP:CZ2	2.50	0.47
1:B:676:ALA:HB2	1:B:718:TRP:NE1	2.30	0.47
1:A:156:THR:HA	1:A:309:PRO:HG3	1.96	0.47
1:C:391:ARG:NH2	1:C:419:ASP:OD2	2.48	0.47
1:D:375:THR:HA	1:D:379:PHE:HB3	1.97	0.47
1:A:521:ALA:O	1:A:525:ASN:ND2	2.35	0.46
1:C:268:GLN:C	1:C:292:TRP:HE1	2.23	0.46
1:C:648:ILE:HG23	1:C:662:MET:HE3	1.96	0.46
1:A:362:ASN:HB3	1:A:366:GLY:H	1.79	0.46
1:C:277:GLN:HE21	1:C:287:CYS:HB3	1.80	0.46
1:B:693:VAL:HG22	1:B:728:ILE:HG23	1.98	0.46
1:B:723:ASP:O	1:B:724:HIS:ND1	2.48	0.46
1:D:439:TRP:HB2	1:D:521:ALA:HB2	1.98	0.46
1:A:63:LEU:HG	1:A:105:PHE:CE2	2.51	0.46
1:A:391:ARG:NH2	1:A:421:ASN:HB3	2.31	0.46
1:D:94:GLY:HA2	1:D:141:TRP:CD1	2.51	0.46
1:C:291:THR:O	1:C:302:THR:N	2.49	0.46
1:A:6:LEU:HD21	1:A:13:PHE:CD1	2.51	0.46
1:B:650:GLN:HG2	1:B:663:ARG:HB3	1.98	0.46
1:D:31:GLU:HB3	1:D:59:ARG:NH1	2.30	0.46
1:C:391:ARG:HH22	1:C:419:ASP:CG	2.24	0.46
1:B:445:VAL:HG13	1:B:461:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ARG:HA	1:D:59:ARG:HD3	1.66	0.46
1:D:540:TRP:CZ2	1:D:541:LEU:HD12	2.51	0.46
1:A:362:ASN:HB3	1:A:367:GLU:H	1.81	0.46
1:A:720:PRO:HG2	1:A:724:HIS:NE2	2.31	0.46
1:C:677:THR:OG1	1:C:717:TRP:HB3	2.16	0.46
1:A:91:GLU:O	1:A:141:TRP:NE1	2.45	0.45
1:A:139:PRO:HG2	1:A:142:THR:HG23	1.98	0.45
1:B:128:VAL:O	1:B:133:SER:OG	2.31	0.45
1:C:25:GLY:HA3	1:C:80:THR:HB	1.99	0.45
1:D:40:ILE:HA	1:D:44:VAL:HG11	1.98	0.45
1:D:159:ALA:HB2	1:D:184:VAL:HG22	1.98	0.45
1:D:645:ASN:HB3	1:D:719:HIS:NE2	2.31	0.45
1:C:452:ARG:HG3	1:C:479:PHE:CE2	2.50	0.45
1:D:28:VAL:HA	1:D:29:ALA:HA	1.72	0.45
1:A:54:VAL:HG22	1:A:92:HIS:CG	2.52	0.45
1:A:294:PHE:HB3	1:A:297:PHE:O	2.16	0.45
1:C:333:TRP:CZ3	1:C:339:LEU:HD13	2.52	0.45
1:D:645:ASN:H	1:D:677:THR:HG22	1.81	0.45
1:D:687:PRO:O	1:D:691:THR:OG1	2.20	0.45
1:B:340:TRP:HB3	1:B:345:VAL:HG21	1.99	0.45
1:C:22:THR:HB	1:C:641:PRO:O	2.16	0.45
1:D:457:THR:C	1:D:459:ALA:H	2.25	0.45
1:A:540:TRP:CD1	1:A:559:LEU:HD13	2.51	0.45
1:C:85:PHE:HE1	1:C:122:LEU:HB3	1.81	0.45
1:C:160:LEU:HD12	1:C:160:LEU:HA	1.81	0.45
1:A:57:VAL:HG22	1:A:102:TRP:HA	1.99	0.45
1:C:148:PHE:HB2	1:C:315:TRP:C	2.42	0.45
1:C:341:ALA:HB1	1:C:348:PRO:HD3	1.99	0.45
1:C:424:HIS:HD1	1:C:484:SER:HB2	1.81	0.45
1:D:471:ASN:OD1	1:D:474:ARG:NH1	2.50	0.45
1:D:153:PHE:CZ	1:D:184:VAL:HG11	2.52	0.45
1:D:330:ASP:CB	1:D:331:PRO:HD2	2.39	0.45
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.80	0.44
1:B:250:ARG:HD2	1:B:371:TYR:CE2	2.51	0.44
1:B:446:ASP:HB3	1:B:455:TYR:CE2	2.47	0.44
1:A:418:ASP:OD1	1:A:491:HIS:NE2	2.48	0.44
1:B:175:ILE:O	1:B:178:THR:HG22	2.16	0.44
1:C:258:ILE:HG12	1:C:356:LYS:O	2.18	0.44
1:C:333:TRP:CH2	1:C:339:LEU:HD22	2.52	0.44
1:D:250:ARG:HD2	1:D:253:ILE:O	2.17	0.44
1:C:540:TRP:HA	1:C:541:LEU:HA	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HA	1:A:292:TRP:O	2.17	0.44
1:A:285:ARG:O	1:A:309:PRO:HD2	2.17	0.44
1:B:15:ASP:HB3	1:B:21:ILE:HD11	1.98	0.44
1:C:15:ASP:HB3	1:C:21:ILE:HD11	2.00	0.44
1:A:235:GLU:C	1:A:237:GLU:H	2.25	0.44
1:A:561:ILE:HD12	1:A:636:TRP:CZ3	2.52	0.44
1:B:341:ALA:HB2	1:B:346:TRP:NE1	2.32	0.44
1:A:300:TYR:CG	1:A:300:TYR:O	2.70	0.44
1:D:540:TRP:HA	1:D:541:LEU:HA	1.77	0.44
1:A:228:ILE:HG23	1:A:234:ILE:HG13	2.00	0.44
1:A:327:TRP:HH2	1:A:329:ARG:NH2	2.15	0.44
1:C:191:LEU:HD22	1:C:209:ILE:HG21	2.00	0.44
1:C:443:TYR:HA	1:C:463:LYS:O	2.18	0.44
1:D:148:PHE:CD2	1:D:153:PHE:HZ	2.36	0.44
1:B:153:PHE:HB3	1:B:159:ALA:O	2.17	0.44
1:B:540:TRP:CZ2	1:B:541:LEU:HD12	2.53	0.44
1:C:148:PHE:CE2	1:C:317:PRO:HD3	2.53	0.44
1:D:192:PHE:O	1:D:210:GLN:HG3	2.17	0.44
1:A:143:LEU:HB3	1:A:148:PHE:CE1	2.52	0.43
1:B:150:PRO:HB2	1:B:151:ARG:H	1.58	0.43
1:C:28:VAL:HA	1:C:29:ALA:HA	1.77	0.43
1:D:94:GLY:HA3	1:D:325:TYR:OH	2.18	0.43
1:A:407:GLU:HA	1:A:452:ARG:HH12	1.83	0.43
1:D:147:GLY:O	1:D:315:TRP:HA	2.18	0.43
1:A:284:GLY:HA2	1:A:309:PRO:HB2	2.01	0.43
1:A:243:GLU:HA	1:A:400:PHE:HB2	2.00	0.43
1:A:250:ARG:HD2	1:A:253:ILE:O	2.19	0.43
1:B:688:ASP:N	1:B:688:ASP:OD1	2.49	0.43
1:C:146:ALA:HB2	1:C:333:TRP:CZ2	2.45	0.43
1:A:63:LEU:HD22	1:A:112:ILE:HD12	1.99	0.43
1:A:279:MET:SD	1:A:340:TRP:HD1	2.42	0.43
1:B:186:GLN:HB3	1:B:252:LEU:HG	2.00	0.43
1:D:31:GLU:OE2	1:D:544:THR:OG1	2.21	0.43
1:C:561:ILE:HD12	1:C:636:TRP:CZ3	2.54	0.43
1:A:419:ASP:HB3	1:A:422:MET:HB3	2.01	0.43
1:C:548:HIS:HE2	1:C:566:ASP:CG	2.27	0.43
1:B:172:PRO:HB2	1:B:175:ILE:HB	2.01	0.43
1:B:89:ALA:HB1	1:B:102:TRP:CE2	2.54	0.43
1:B:541:LEU:HD22	1:B:543:THR:OG1	2.18	0.43
1:C:162:GLN:O	1:C:171:PHE:CE1	2.71	0.43
1:D:264:GLU:HG3	1:D:371:TYR:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:HIS:CE1	1:A:544:THR:HB	2.53	0.42
1:C:681:LEU:O	1:C:713:GLN:HB3	2.19	0.42
1:D:496:THR:O	1:D:538:THR:OG1	2.31	0.42
1:A:38:PRO:HG2	1:A:40:ILE:HD11	2.00	0.42
1:B:259:SER:HA	1:B:276:PHE:HB2	2.00	0.42
1:D:106:THR:HG21	1:D:224:PHE:HZ	1.83	0.42
1:B:48:PHE:CZ	1:B:161:VAL:HG11	2.54	0.42
1:B:59:ARG:HA	1:B:59:ARG:HD3	1.76	0.42
1:D:82:ARG:NE	1:D:243:GLU:OE1	2.46	0.42
1:D:326:GLY:O	1:D:328:VAL:HG23	2.19	0.42
1:A:114:LYS:HG3	1:A:238:VAL:HB	2.01	0.42
1:A:543:THR:HG22	1:A:545:SER:H	1.84	0.42
1:A:195:GLY:C	1:A:197:ASP:H	2.26	0.42
1:A:274:THR:N	1:A:277:GLN:HB2	2.34	0.42
1:C:49:PHE:HZ	1:C:163:ASN:CB	2.33	0.42
1:D:186:GLN:HB3	1:D:252:LEU:HG	2.02	0.42
1:D:201:LYS:HB3	1:D:343:HIS:CE1	2.55	0.42
1:C:307:VAL:CG1	1:C:309:PRO:HD2	2.50	0.42
1:C:310:GLU:N	1:C:310:GLU:OE1	2.53	0.42
1:D:28:VAL:HG13	1:D:29:ALA:HB2	2.02	0.42
1:B:515:TYR:CE2	1:B:631:ARG:HA	2.55	0.42
1:A:69:HIS:CE1	1:A:72:ARG:HH12	2.38	0.42
1:B:56:PHE:HD2	1:B:89:ALA:HB2	1.85	0.42
1:C:158:ALA:HB1	1:C:184:VAL:HG13	2.01	0.42
1:A:241:GLY:HA3	1:A:398:ILE:O	2.19	0.42
1:A:380:MET:O	1:A:384:ARG:HG3	2.20	0.42
1:D:41:PRO:O	1:D:163:ASN:ND2	2.48	0.42
1:D:405:VAL:HG12	1:D:406:MET:HG3	2.02	0.42
1:D:449:GLY:O	1:D:454:LYS:N	2.52	0.42
1:A:40:ILE:HG23	1:A:44:VAL:HG13	2.00	0.42
1:B:191:LEU:HD22	1:B:209:ILE:HG21	2.02	0.42
1:C:127:ASP:OD2	1:C:136:SER:OG	2.38	0.42
1:D:56:PHE:CD1	1:D:89:ALA:HA	2.55	0.42
1:D:330:ASP:HB2	1:D:331:PRO:CD	2.43	0.42
1:D:394:TRP:NE1	1:D:396:GLU:HB2	2.34	0.42
1:A:272:SER:HB3	1:A:290:SER:O	2.20	0.41
1:B:146:ALA:HB3	1:B:148:PHE:CE2	2.55	0.41
1:B:540:TRP:HA	1:B:541:LEU:HA	1.78	0.41
1:C:717:TRP:CE2	1:C:719:HIS:HB3	2.55	0.41
1:D:60:PRO:HG2	1:D:109:VAL:HG11	2.01	0.41
1:A:37:LYS:HA	1:A:38:PRO:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:LYS:HA	1:B:368:PRO:HA	2.02	0.41
1:C:275:ALA:O	1:C:276:PHE:HB3	2.19	0.41
1:A:498:ILE:HG21	1:A:529:ILE:HD11	2.02	0.41
1:B:235:GLU:C	1:B:237:GLU:H	2.28	0.41
1:C:638:ARG:HH21	1:C:653:PHE:HB3	1.84	0.41
1:D:258:ILE:HG13	1:D:276:PHE:HD2	1.84	0.41
1:A:362:ASN:HB3	1:A:366:GLY:N	2.35	0.41
1:A:515:TYR:CE1	1:A:631:ARG:HA	2.56	0.41
1:B:357:ASP:O	1:B:359:PHE:N	2.54	0.41
1:B:438:HIS:ND1	1:B:505:ASP:OD1	2.54	0.41
1:B:543:THR:HG22	1:B:545:SER:N	2.32	0.41
1:D:361:LYS:HG2	1:D:367:GLU:HA	2.03	0.41
1:A:15:ASP:OD1	1:A:19:ARG:N	2.49	0.41
1:C:160:LEU:HD22	1:C:175:ILE:HD13	2.03	0.41
1:C:560:SER:O	1:C:631:ARG:NH2	2.54	0.41
1:D:60:PRO:HB2	1:D:61:PHE:H	1.70	0.41
1:D:161:VAL:HG12	1:D:163:ASN:H	1.85	0.41
1:D:316:LEU:HD13	1:D:320:TYR:CE2	2.55	0.41
1:A:275:ALA:O	1:A:279:MET:HB2	2.21	0.41
1:C:126:GLN:HA	1:C:137:GLY:HA3	2.03	0.41
1:C:172:PRO:O	1:C:174:MET:N	2.53	0.41
1:C:333:TRP:HH2	1:C:339:LEU:HD22	1.84	0.41
1:D:561:ILE:HD12	1:D:636:TRP:CZ3	2.56	0.41
1:A:663:ARG:HG3	1:A:725:ASN:HB3	2.02	0.41
1:B:329:ARG:HH11	1:B:333:TRP:CD1	2.38	0.41
1:A:307:VAL:HG12	1:A:309:PRO:HD3	2.03	0.41
1:B:310:GLU:O	1:B:312:GLU:HG2	2.20	0.41
1:C:660:PHE:HE2	1:C:679:ILE:HD13	1.86	0.41
1:D:403:PRO:HB3	1:D:410:PRO:HD3	2.03	0.41
1:A:113:ALA:HB1	1:A:118:PHE:CD2	2.56	0.41
1:B:71:SER:HB2	1:B:710:VAL:HG22	2.03	0.41
1:B:720:PRO:HG2	1:B:724:HIS:NE2	2.35	0.41
1:C:141:TRP:HA	1:C:144:TYR:CD1	2.56	0.41
1:C:173:LYS:HE2	1:C:437:LYS:CD	2.50	0.41
1:C:681:LEU:HD21	1:C:728:ILE:HG21	2.03	0.41
1:D:81:ILE:HB	1:D:120:VAL:HG22	2.02	0.41
1:A:438:HIS:ND1	1:A:505:ASP:OD1	2.53	0.41
1:B:450:VAL:HG11	1:B:458:PRO:HG3	2.03	0.41
1:B:569:LEU:HD23	1:B:569:LEU:HA	1.94	0.41
1:D:156:THR:HG21	1:D:314:ALA:N	2.36	0.41
1:B:91:GLU:HG2	1:B:94:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:VAL:HG11	1:B:480:LEU:HD13	2.04	0.40
1:B:541:LEU:HD23	1:B:542:TYR:H	1.86	0.40
1:C:224:PHE:HD2	1:C:242:TRP:HH2	1.69	0.40
1:D:194:GLY:CA	1:D:253:ILE:HD11	2.51	0.40
1:D:695:VAL:HG11	1:D:717:TRP:NE1	2.36	0.40
1:A:191:LEU:HD22	1:A:209:ILE:HG21	2.03	0.40
1:C:124:PRO:HG2	1:C:244:SER:O	2.22	0.40
1:C:329:ARG:HH11	1:C:333:TRP:CD1	2.38	0.40
1:D:186:GLN:O	1:D:190:THR:OG1	2.30	0.40
1:D:418:ASP:OD1	1:D:491:HIS:NE2	2.53	0.40
1:B:74:ARG:HD2	1:B:74:ARG:HA	1.96	0.40
1:D:540:TRP:CD1	1:D:559:LEU:HD13	2.56	0.40
1:A:444:ASN:OD1	1:A:445:VAL:N	2.53	0.40
1:B:669:LYS:HA	1:B:669:LYS:HD2	1.88	0.40
1:C:172:PRO:HG2	1:C:175:ILE:HG22	2.04	0.40
1:C:175:ILE:O	1:C:175:ILE:CG1	2.68	0.40
1:C:276:PHE:HA	1:C:279:MET:HB2	2.03	0.40
1:C:353:LEU:HD23	1:C:356:LYS:CB	2.49	0.40
1:D:413:LYS:HD2	1:D:489:GLY:HA2	2.02	0.40
1:C:160:LEU:HD23	1:C:175:ILE:HD13	2.04	0.40
1:D:26:ILE:HA	1:D:539:LEU:N	2.36	0.40
1:D:70:PHE:HE2	1:D:113:ALA:HB2	1.87	0.40
1:D:172:PRO:HB2	1:D:175:ILE:HB	2.03	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	664/779 (85%)	597 (90%)	47 (7%)	20 (3%)	3	25
1	B	651/779 (84%)	593 (91%)	41 (6%)	17 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	643/779 (82%)	588 (91%)	44 (7%)	11 (2%)	7	34
1	D	607/779 (78%)	550 (91%)	41 (7%)	16 (3%)	4	27
All	All	2565/3116 (82%)	2328 (91%)	173 (7%)	64 (2%)	4	28

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	149	ASP
1	A	294	PHE
1	A	300	TYR
1	A	323	THR
1	B	51	ALA
1	B	149	ASP
1	B	150	PRO
1	B	151	ARG
1	B	358	TYR
1	C	44	VAL
1	C	173	LYS
1	D	60	PRO
1	D	330	ASP
1	A	244	SER
1	A	541	LEU
1	B	161	VAL
1	D	120	VAL
1	D	195	GLY
1	D	372	ASP
1	A	238	VAL
1	A	285	ARG
1	B	52	ASP
1	B	60	PRO
1	B	244	SER
1	C	50	ASP
1	C	238	VAL
1	D	159	ALA
1	D	196	ARG
1	D	331	PRO
1	A	292	TRP
1	A	301	GLN
1	B	183	LEU
1	C	129	TRP

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Mol	Chain	Res	Type
1	C	158	ALA
1	D	39	ASP
1	D	203	ILE
1	D	244	SER
1	A	129	TRP
1	A	147	GLY
1	A	148	PHE
1	A	159	ALA
1	A	163	ASN
1	A	458	PRO
1	B	129	TRP
1	B	238	VAL
1	B	269	LEU
1	B	311	GLY
1	B	458	PRO
1	C	49	PHE
1	C	244	SER
1	C	687	PRO
1	D	239	VAL
1	A	154	LYS
1	C	60	PRO
1	D	59	ARG
1	D	129	TRP
1	B	59	ARG
1	D	204	ILE
1	A	194	GLY
1	B	331	PRO
1	D	458	PRO
1	C	253	ILE
1	A	60	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	569/661 (86%)	569 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	562/661 (85%)	562 (100%)	0	100	100
1	C	559/661 (85%)	556 (100%)	3 (0%)	81	81
1	D	530/661 (80%)	530 (100%)	0	100	100
All	All	2220/2644 (84%)	2217 (100%)	3 (0%)	88	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	172	PRO
1	C	173	LYS
1	C	175	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	125	HIS
1	A	229	HIS
1	A	256	GLN
1	A	265	GLN
1	A	268	GLN
1	A	277	GLN
1	A	508	HIS
1	B	11	GLN
1	B	268	GLN
1	B	362	ASN
1	C	69	HIS
1	C	125	HIS
1	C	277	GLN
1	C	427	HIS
1	D	402	GLN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	670/779 (86%)	-0.47	0 100 100	89, 179, 220, 239	0
1	B	659/779 (84%)	-0.48	0 100 100	86, 179, 223, 238	0
1	C	655/779 (84%)	-0.33	1 (0%) 91 81	30, 180, 218, 249	0
1	D	623/779 (79%)	-0.45	0 100 100	93, 190, 224, 243	0
All	All	2607/3116 (83%)	-0.43	1 (0%) 100 100	30, 182, 223, 249	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	258	ILE	2.2

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.