



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:12 PM UTC

PDB ID : 1HCU / pdb_00001hcu
Title : alpha-1,2-mannosidase from Trichoderma reesei
Authors : Van Petegem, F.; Contreras, H.; Contreras, R.; Van Beeumen, J.
Deposited on : 2001-05-09
Resolution : 2.37 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

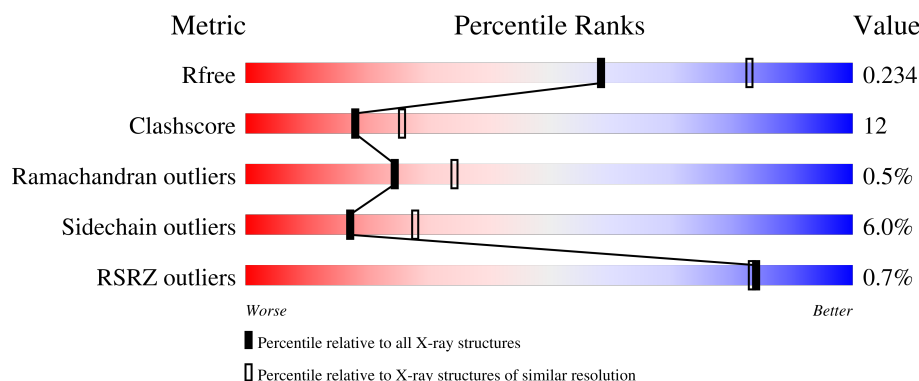
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	503	0% 71% 22% • •
1	B	503	77% 17% • •
1	C	503	71% 22% • •
1	D	503	2% 66% 26% 5% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16084 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 ALPHA-1,2-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3718	2366	612	735	5			
1	B	489	Total	C	N	O	S	0	0	0
			3730	2372	616	737	5			
1	C	485	Total	C	N	O	S	0	0	0
			3697	2353	608	731	5			
1	D	486	Total	C	N	O	S	0	0	0
			3701	2355	612	729	5			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

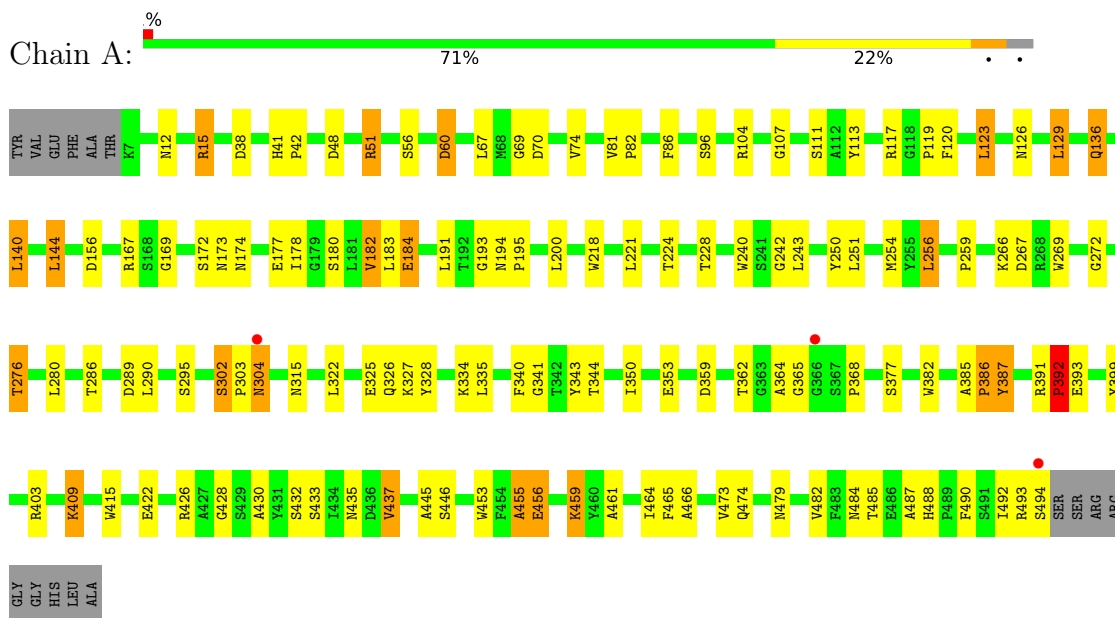
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	315	Total	O	0	0
			315	315		
4	B	311	Total	O	0	0
			311	311		
4	C	270	Total	O	0	0
			270	270		
4	D	198	Total	O	0	0
			198	198		

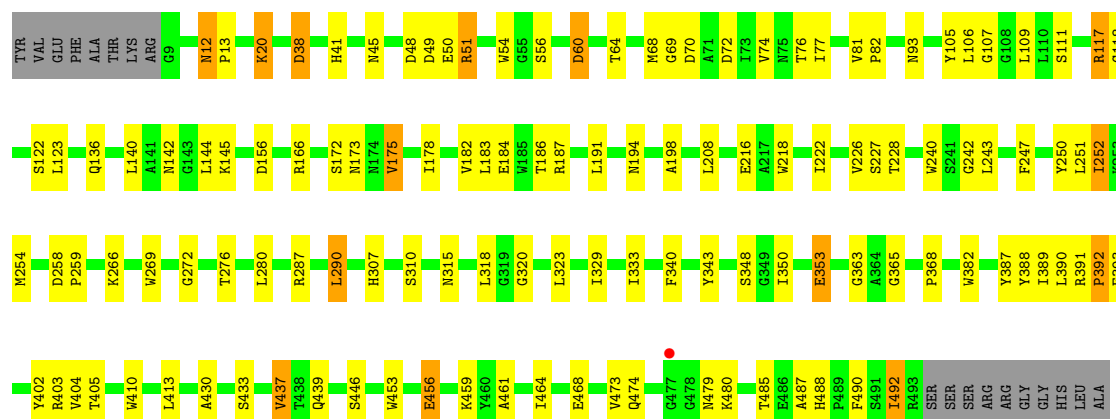
3 Residue-property plots

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: ALPHA-1,2-MANNOSIDASE

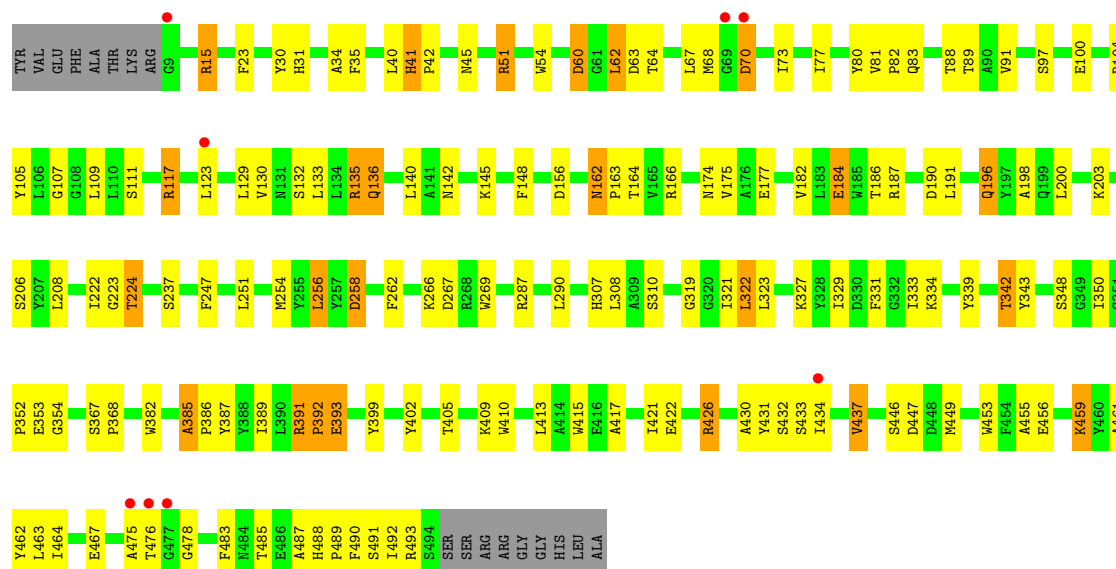


Chain C:  71% 22%



• Molecule 1: ALPHA-1,2-MANNOSIDASE

Chain D:  2% 66% 26% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.20Å 106.84Å 101.39Å 90.00° 99.42° 90.00°	Depositor
Resolution (Å)	20.00 – 2.37 20.00 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.37) 98.9 (20.00-2.37)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.35Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.177 , 0.232 0.181 , 0.234	Depositor DCC
R_{free} test set	3683 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16084	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA

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	0.45	0/3823	0.94	20/5217 (0.4%)
1	B	0.45	0/3835	0.95	18/5233 (0.3%)
1	C	0.42	0/3802	0.93	19/5190 (0.4%)
1	D	0.39	0/3806	0.92	12/5195 (0.2%)
All	All	0.43	0/15266	0.94	69/20835 (0.3%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	VAL	N-CA-C	7.85	118.60	110.36
1	A	156	ASP	N-CA-C	-7.72	99.92	109.65
1	B	385	ALA	CA-C-N	7.68	127.31	119.56
1	B	385	ALA	C-N-CA	7.68	127.31	119.56
1	D	385	ALA	CA-C-N	7.53	127.24	119.56
1	D	385	ALA	C-N-CA	7.53	127.24	119.56
1	B	156	ASP	N-CA-C	-7.53	100.17	109.65
1	A	435	ASN	N-CA-C	7.51	119.25	111.14
1	B	38	ASP	N-CA-C	7.38	119.01	110.97
1	B	41	HIS	CA-C-N	7.31	127.95	119.47
1	B	41	HIS	C-N-CA	7.31	127.95	119.47
1	A	41	HIS	CA-C-N	7.31	127.95	119.47
1	A	41	HIS	C-N-CA	7.31	127.95	119.47
1	D	156	ASP	N-CA-C	-7.30	100.45	109.65
1	C	118	GLY	CA-C-N	7.09	126.77	119.82
1	C	118	GLY	C-N-CA	7.09	126.77	119.82
1	A	385	ALA	CA-C-N	7.04	126.65	119.19
1	A	385	ALA	C-N-CA	7.04	126.65	119.19
1	D	367	SER	CA-C-N	6.75	124.59	119.66
1	D	367	SER	C-N-CA	6.75	124.59	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	HIS	CA-C-N	6.72	127.27	119.47
1	C	41	HIS	C-N-CA	6.72	127.27	119.47
1	D	41	HIS	CA-C-N	6.72	126.98	119.32
1	D	41	HIS	C-N-CA	6.72	126.98	119.32
1	A	453	TRP	N-CA-C	-6.67	103.93	111.14
1	C	258	ASP	CA-C-N	6.27	126.18	119.28
1	C	258	ASP	C-N-CA	6.27	126.18	119.28
1	C	38	ASP	N-CA-C	6.18	117.71	110.97
1	A	38	ASP	N-CA-C	6.10	117.73	111.14
1	B	118	GLY	CA-C-N	6.04	125.73	119.56
1	B	118	GLY	C-N-CA	6.04	125.73	119.56
1	B	456	GLU	N-CA-C	6.03	120.40	112.13
1	C	175	VAL	N-CA-C	5.87	117.31	110.62
1	A	386	PRO	N-CA-C	5.80	121.17	113.57
1	B	435	ASN	N-CA-C	5.78	118.80	111.69
1	A	182	VAL	N-CA-C	5.75	116.48	110.62
1	B	386	PRO	N-CA-C	5.68	120.95	113.86
1	D	258	ASP	CA-C-N	5.65	125.32	119.05
1	D	258	ASP	C-N-CA	5.65	125.32	119.05
1	A	194	ASN	CA-C-N	5.64	125.31	119.56
1	A	194	ASN	C-N-CA	5.64	125.31	119.56
1	D	386	PRO	N-CA-C	5.63	121.16	113.84
1	B	365	GLY	N-CA-C	-5.57	107.35	114.37
1	C	365	GLY	N-CA-C	-5.55	108.09	114.69
1	A	456	GLU	N-CA-C	5.54	119.71	112.13
1	D	453	TRP	N-CA-C	-5.53	105.41	111.82
1	B	391	ARG	CA-C-N	5.51	126.72	119.84
1	B	391	ARG	C-N-CA	5.51	126.72	119.84
1	C	456	GLU	N-CA-C	5.49	119.47	112.12
1	B	182	VAL	N-CA-C	5.48	116.86	110.62
1	B	214	SER	CA-C-N	5.44	125.38	119.78
1	B	214	SER	C-N-CA	5.44	125.38	119.78
1	C	156	ASP	N-CA-C	-5.42	102.83	109.65
1	A	466	ALA	N-CA-C	5.41	117.06	110.41
1	B	453	TRP	N-CA-C	-5.41	105.30	111.14
1	C	194	ASN	CA-C-N	5.38	125.05	119.56
1	C	194	ASN	C-N-CA	5.38	125.05	119.56
1	C	453	TRP	N-CA-C	-5.37	105.50	111.36
1	C	363	GLY	N-CA-C	-5.32	107.98	115.32
1	A	295	SER	N-CA-C	-5.22	103.03	110.59
1	C	12	ASN	CA-C-N	5.18	124.80	119.05
1	C	12	ASN	C-N-CA	5.18	124.80	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	SER	CA-C-N	5.16	126.29	119.84
1	A	302	SER	C-N-CA	5.16	126.29	119.84
1	D	456	GLU	N-CA-C	5.09	118.94	112.12
1	A	455	ALA	N-CA-C	5.06	117.91	111.69
1	C	122	SER	N-CA-C	5.04	118.21	111.75
1	A	484	ASN	N-CA-C	-5.01	103.43	110.35
1	A	387	TYR	N-CA-C	5.01	116.57	110.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3718	0	3485	92	0
1	B	3730	0	3501	67	0
1	C	3697	0	3464	86	0
1	D	3701	0	3473	109	0
2	A	42	0	39	0	0
2	B	42	0	39	0	0
2	C	28	0	26	1	0
2	D	28	0	26	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	315	0	0	6	0
4	B	311	0	0	1	0
4	C	270	0	0	2	1
4	D	198	0	0	6	1
All	All	16084	0	14053	355	1

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 (355) 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:C:20:LYS:HD3	1:C:68:MET:HB3	1.45	0.98
1:C:252:ILE:HD13	1:C:252:ILE:H	1.30	0.95
1:B:272:GLY:O	1:B:276:THR:HG23	1.68	0.93
1:A:256:LEU:HD13	1:A:482:VAL:HG22	1.49	0.92
1:C:474:GLN:H	1:C:479:ASN:HD21	1.14	0.92
1:C:117:ARG:HH11	1:C:117:ARG:HB3	1.39	0.87
1:D:136:GLN:HE21	1:D:136:GLN:HA	1.40	0.86
1:D:64:THR:HG22	1:D:68:MET:HE2	1.58	0.85
1:C:474:GLN:H	1:C:479:ASN:ND2	1.76	0.82
1:B:136:GLN:HA	1:B:136:GLN:HE21	1.43	0.82
1:C:240:TRP:HE1	1:C:276:THR:HG21	1.45	0.82
1:B:72:ASP:O	1:B:76:THR:HG22	1.81	0.80
1:C:353:GLU:HG3	1:C:387:TYR:CE1	2.15	0.80
1:C:272:GLY:O	1:C:276:THR:HG23	1.82	0.80
1:D:342:THR:HG23	1:D:352:PRO:HD2	1.65	0.79
1:B:353:GLU:HG3	1:B:387:TYR:CE2	2.16	0.79
1:D:163:PRO:HD2	1:D:166:ARG:HH22	1.47	0.78
1:D:353:GLU:HG3	1:D:387:TYR:CE1	2.17	0.78
1:D:142:ASN:HA	1:D:145:LYS:HE3	1.65	0.78
1:A:474:GLN:H	1:A:479:ASN:HD21	1.33	0.76
1:B:441:ASN:HB2	4:B:2273:HOH:O	1.85	0.74
1:A:174:ASN:HD21	1:A:177:GLU:HG3	1.50	0.74
1:D:67:LEU:HD12	1:D:459:LYS:HD2	1.71	0.73
1:C:252:ILE:HD12	1:C:269:TRP:NE1	2.04	0.71
1:B:240:TRP:HE1	1:B:276:THR:HG21	1.56	0.71
1:A:272:GLY:O	1:A:276:THR:HG23	1.90	0.70
1:C:142:ASN:HA	1:C:145:LYS:HE3	1.74	0.70
1:D:117:ARG:HB3	1:D:117:ARG:NH2	2.07	0.69
1:A:353:GLU:HG3	1:A:387:TYR:CE2	2.27	0.69
1:C:287:ARG:HG2	1:C:290:LEU:HD22	1.75	0.69
1:C:474:GLN:N	1:C:479:ASN:HD21	1.90	0.69
1:D:117:ARG:HB3	1:D:117:ARG:HH21	1.57	0.69
1:A:344:THR:HG21	4:A:2241:HOH:O	1.94	0.67
1:B:426:ARG:HG2	1:B:431:TYR:CE2	2.30	0.67
1:C:266:LYS:HD2	1:C:323:LEU:HD21	1.75	0.67
1:A:240:TRP:HE1	1:A:276:THR:HG21	1.60	0.67
1:B:256:LEU:HD13	1:B:482:VAL:HB	1.76	0.65
1:D:224:THR:HG22	1:D:237:SER:O	1.97	0.65
1:D:88:THR:HB	2:D:600:NAG:H62	1.79	0.64
1:C:240:TRP:NE1	1:C:276:THR:HG21	2.13	0.64
1:D:287:ARG:HG2	1:D:290:LEU:HD22	1.81	0.63
1:B:15:ARG:HG2	1:B:415:TRP:CE3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:SER:OG	1:B:393:GLU:HB2	1.99	0.63
1:D:405:THR:HG21	4:D:2170:HOH:O	1.98	0.63
1:A:12:ASN:HB2	4:A:2004:HOH:O	1.98	0.63
1:D:174:ASN:HD21	1:D:177:GLU:HG3	1.63	0.62
1:B:174:ASN:ND2	1:B:177:GLU:H	1.97	0.62
1:A:474:GLN:H	1:A:479:ASN:ND2	1.97	0.61
1:C:368:PRO:HB3	1:C:382:TRP:CE3	2.35	0.61
1:D:196:GLN:O	1:D:200:LEU:HD23	2.00	0.61
1:A:276:THR:HB	1:A:280:LEU:HD12	1.82	0.61
1:D:307:HIS:O	1:D:310:SER:HB3	1.99	0.61
1:A:399:TYR:HA	1:A:464:ILE:HD12	1.83	0.61
1:C:93:ASN:HD22	1:C:166:ARG:HH21	1.49	0.61
1:A:69:GLY:HA2	1:A:123:LEU:HD21	1.83	0.61
1:D:308:LEU:HD23	4:D:2143:HOH:O	2.01	0.60
1:B:353:GLU:OE2	1:B:391:ARG:HD2	2.02	0.60
1:C:240:TRP:HE1	1:C:276:THR:CG2	2.14	0.59
1:A:67:LEU:HD12	1:A:459:LYS:HD2	1.83	0.59
1:C:461:ALA:O	1:C:464:ILE:HG22	2.03	0.59
1:D:422:GLU:O	1:D:426:ARG:HB2	2.02	0.59
1:C:252:ILE:HD12	1:C:269:TRP:CD1	2.38	0.59
1:D:319:GLY:HA2	1:D:322:LEU:HD11	1.85	0.58
1:C:175:VAL:HG11	1:C:222:ILE:HD11	1.84	0.58
1:C:480:LYS:HA	1:C:492:ILE:HD12	1.85	0.58
1:D:89:THR:HG23	1:D:91:VAL:O	2.02	0.58
1:D:107:GLY:HA2	1:D:490:PHE:HZ	1.69	0.58
1:D:136:GLN:HA	1:D:136:GLN:NE2	2.15	0.58
1:C:252:ILE:HG23	1:C:269:TRP:CG	2.39	0.58
1:D:23:PHE:CG	1:D:68:MET:HE1	2.39	0.58
1:A:136:GLN:HE21	1:A:136:GLN:HA	1.69	0.58
1:B:240:TRP:NE1	1:B:276:THR:HG21	2.19	0.58
1:D:182:VAL:HG22	1:D:254:MET:HE2	1.86	0.58
1:B:403:ARG:HD3	1:B:473:VAL:O	2.03	0.57
1:D:307:HIS:HE1	1:D:343:TYR:OH	1.87	0.57
1:A:403:ARG:HG3	1:A:473:VAL:HG22	1.86	0.57
1:A:174:ASN:ND2	1:A:177:GLU:HG3	2.19	0.57
1:D:389:ILE:HG22	1:D:433:SER:HB3	1.86	0.57
1:A:182:VAL:HG22	1:A:254:MET:HE2	1.85	0.57
1:A:240:TRP:NE1	1:A:276:THR:HG21	2.19	0.57
1:A:341:GLY:HA2	1:A:344:THR:HG22	1.85	0.57
1:D:89:THR:HG22	1:D:162:ASN:HB3	1.87	0.56
1:B:12:ASN:ND2	1:B:15:ARG:HD3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:PRO:HB3	1:B:382:TRP:CE3	2.40	0.56
1:A:180:SER:HA	1:A:250:TYR:CD1	2.41	0.56
1:A:81:VAL:HB	1:A:82:PRO:HD3	1.88	0.56
1:D:184:GLU:H	1:D:184:GLU:CD	2.13	0.56
1:A:391:ARG:HB3	1:A:393:GLU:OE2	2.05	0.56
1:C:307:HIS:O	1:C:310:SER:HB3	2.06	0.56
1:D:81:VAL:HB	1:D:82:PRO:HD3	1.88	0.55
1:B:81:VAL:HG11	1:B:133:LEU:HD12	1.88	0.55
1:A:15:ARG:HG3	1:A:415:TRP:CE3	2.41	0.55
1:C:402:TYR:HB2	1:C:410:TRP:HB2	1.89	0.55
1:A:327:LYS:HG3	1:A:328:TYR:N	2.22	0.55
1:B:116:LEU:O	1:B:121:SER:HA	2.07	0.54
1:D:339:TYR:O	1:D:342:THR:HB	2.06	0.54
1:A:386:PRO:O	1:A:437:VAL:HB	2.08	0.54
1:C:111:SER:HB3	1:C:488:HIS:HB3	1.88	0.54
1:D:15:ARG:HG2	1:D:415:TRP:CE3	2.43	0.54
1:D:60:ASP:O	1:D:455:ALA:HB2	2.08	0.54
1:D:15:ARG:HG2	1:D:415:TRP:CD2	2.42	0.54
1:C:93:ASN:ND2	1:C:166:ARG:HH21	2.05	0.53
1:C:107:GLY:HA2	1:C:490:PHE:HZ	1.72	0.53
1:A:433:SER:HB2	1:A:446:SER:OG	2.07	0.53
1:D:391:ARG:HB3	1:D:393:GLU:OE1	2.08	0.53
1:D:42:PRO:HG3	1:D:431:TYR:O	2.09	0.53
1:A:304:ASN:HD22	1:A:304:ASN:H	1.57	0.53
1:B:276:THR:HB	1:B:280:LEU:HD12	1.91	0.53
1:B:81:VAL:HB	1:B:82:PRO:HD3	1.90	0.53
1:B:140:LEU:HD22	1:B:144:LEU:HD22	1.90	0.53
1:A:113:TYR:CZ	1:A:117:ARG:HD2	2.44	0.53
1:C:404:VAL:HG13	1:C:405:THR:HG23	1.90	0.53
1:A:362:THR:HG23	1:A:364:ALA:H	1.74	0.52
1:C:329:ILE:O	1:C:333:ILE:HG12	2.09	0.52
1:D:353:GLU:OE2	1:D:391:ARG:HD2	2.08	0.52
1:D:342:THR:HG21	4:D:2141:HOH:O	2.09	0.52
1:A:104:ARG:HG3	1:A:104:ARG:HH11	1.75	0.52
1:B:389:ILE:HD11	1:B:391:ARG:NH1	2.24	0.52
1:C:320:GLY:HA3	1:C:329:ILE:HG13	1.91	0.52
1:D:321:ILE:HG23	1:D:475:ALA:O	2.10	0.52
1:D:331:PHE:HA	1:D:334:LYS:HE3	1.92	0.52
1:B:417:ALA:O	1:B:421:ILE:HG13	2.10	0.52
1:D:190:ASP:OD2	1:D:493:ARG:HD3	2.09	0.52
1:D:433:SER:HB2	1:D:446:SER:OG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:THR:HB	4:D:2194:HOH:O	2.10	0.52
1:B:160:PHE:O	1:B:165:VAL:HA	2.09	0.52
1:B:242:GLY:O	1:B:243:LEU:HB2	2.10	0.52
1:D:162:ASN:C	1:D:162:ASN:HD22	2.18	0.51
1:A:96:SER:HB2	4:A:2084:HOH:O	2.09	0.51
1:A:461:ALA:O	1:A:464:ILE:HG22	2.11	0.51
1:B:10:SER:HB2	1:B:11:PRO:HD2	1.90	0.51
1:B:359:ASP:OD2	1:B:361:VAL:HG22	2.10	0.51
1:B:104:ARG:HG3	1:B:104:ARG:HH11	1.76	0.51
1:B:174:ASN:HD22	1:B:176:ALA:H	1.59	0.51
1:D:23:PHE:CD2	1:D:68:MET:HE1	2.46	0.51
1:C:136:GLN:HA	1:C:136:GLN:HE21	1.76	0.51
1:D:329:ILE:O	1:D:333:ILE:HG13	2.11	0.51
1:B:353:GLU:HG3	1:B:387:TYR:CD2	2.46	0.50
1:C:186:THR:HA	1:C:198:ALA:HB2	1.94	0.50
1:C:287:ARG:CG	1:C:290:LEU:HD22	2.41	0.50
1:A:174:ASN:ND2	1:A:177:GLU:H	2.09	0.50
1:B:456:GLU:HG2	1:B:487:ALA:HB3	1.93	0.50
1:C:51:ARG:HA	1:C:51:ARG:NE	2.26	0.50
1:D:148:PHE:HB3	1:D:200:LEU:HD12	1.93	0.50
1:C:250:TYR:O	1:C:254:MET:HG2	2.11	0.50
1:C:252:ILE:H	1:C:252:ILE:CD1	2.12	0.50
1:A:184:GLU:CD	1:A:184:GLU:H	2.19	0.50
1:A:325:GLU:OE1	1:A:327:LYS:HE3	2.12	0.50
1:D:135:ARG:CZ	1:D:135:ARG:HA	2.42	0.50
1:B:350:ILE:HB	1:B:437:VAL:CG2	2.42	0.49
1:D:174:ASN:ND2	1:D:177:GLU:HG3	2.27	0.49
1:C:173:ASN:HB3	1:C:178:ILE:HD11	1.94	0.49
1:C:259:PRO:HG3	4:C:2134:HOH:O	2.13	0.49
1:A:60:ASP:O	1:A:455:ALA:HB2	2.13	0.49
1:D:130:VAL:HA	1:D:133:LEU:HD23	1.95	0.49
1:D:487:ALA:O	1:D:489:PRO:HD3	2.13	0.49
1:A:242:GLY:O	1:A:243:LEU:HB2	2.13	0.49
1:A:482:VAL:HG23	1:A:492:ILE:HG22	1.94	0.49
1:B:59:ILE:N	1:B:59:ILE:HD12	2.28	0.49
1:D:40:LEU:HD23	1:D:449:MET:HE2	1.92	0.49
1:C:252:ILE:HD11	1:C:315:ASN:HD21	1.77	0.49
1:C:307:HIS:HD2	1:C:393:GLU:CG	2.25	0.49
1:D:51:ARG:HA	1:D:51:ARG:NE	2.28	0.49
1:D:148:PHE:CB	1:D:200:LEU:HD12	2.43	0.49
1:D:399:TYR:HA	1:D:464:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ASN:C	1:C:12:ASN:HD22	2.21	0.48
1:B:422:GLU:HG3	1:B:431:TYR:HE2	1.79	0.48
1:D:186:THR:HA	1:D:198:ALA:HB2	1.96	0.48
1:A:409:LYS:O	1:A:409:LYS:HD3	2.13	0.48
1:C:117:ARG:HB3	1:C:117:ARG:NH1	2.18	0.48
1:C:340:PHE:CE2	1:C:413:LEU:HG	2.48	0.48
1:A:359:ASP:CG	1:A:362:THR:HG22	2.39	0.48
1:A:286:THR:HG21	1:A:377:SER:HA	1.96	0.48
1:C:72:ASP:O	1:C:76:THR:HG23	2.14	0.47
1:C:340:PHE:O	1:C:343:TYR:HB2	2.14	0.47
1:A:426:ARG:NH2	1:A:428:GLY:O	2.46	0.47
1:B:252:ILE:HG13	1:B:322:LEU:HD12	1.96	0.47
1:C:81:VAL:HB	1:C:82:PRO:HD3	1.95	0.47
1:C:172:SER:HA	1:C:228:THR:HG23	1.96	0.47
1:C:389:ILE:HD11	1:C:391:ARG:NH2	2.29	0.47
1:D:89:THR:HG21	4:D:2059:HOH:O	2.14	0.47
1:D:203:LYS:O	1:D:206:SER:HB3	2.14	0.47
1:B:107:GLY:HA2	1:B:490:PHE:HZ	1.80	0.47
1:C:276:THR:HG22	1:C:280:LEU:HD12	1.96	0.47
1:B:174:ASN:ND2	1:B:176:ALA:HB3	2.30	0.47
1:A:474:GLN:N	1:A:479:ASN:HD21	2.04	0.47
1:C:216:GLU:HG2	1:C:218:TRP:O	2.13	0.47
1:D:111:SER:HB3	1:D:488:HIS:HB3	1.96	0.47
1:A:422:GLU:O	1:A:426:ARG:HB2	2.14	0.47
1:B:456:GLU:HG2	1:B:487:ALA:CB	2.44	0.47
1:A:42:PRO:HG3	1:A:432:SER:HB2	1.97	0.47
1:B:136:GLN:HA	1:B:136:GLN:NE2	2.23	0.47
1:A:51:ARG:HA	1:A:51:ARG:NE	2.29	0.47
1:D:30:TYR:CD2	1:D:34:ALA:HB3	2.50	0.47
1:D:342:THR:CG2	1:D:352:PRO:HD2	2.42	0.47
1:A:193:GLY:O	1:A:195:PRO:HD3	2.15	0.46
1:A:173:ASN:HB3	1:A:178:ILE:HD11	1.98	0.46
1:C:106:LEU:HD23	1:C:184:GLU:HB3	1.97	0.46
1:C:69:GLY:HA2	1:C:123:LEU:HD21	1.97	0.46
1:B:51:ARG:HA	1:B:51:ARG:NE	2.31	0.46
1:B:180:SER:HA	1:B:250:TYR:CD1	2.50	0.46
1:C:403:ARG:HD3	1:C:473:VAL:O	2.15	0.46
1:A:392:PRO:HG3	1:A:456:GLU:CB	2.45	0.46
1:B:362:THR:HG22	1:B:364:ALA:H	1.79	0.46
1:D:70:ASP:HB3	1:D:73:ILE:HD12	1.98	0.46
1:B:44:SER:O	1:B:45:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ASN:HD21	1:B:177:GLU:H	1.63	0.46
1:D:208:LEU:HD23	1:D:247:PHE:CD2	2.50	0.46
1:D:483:PHE:CE2	1:D:489:PRO:HG3	2.50	0.46
1:B:362:THR:HG22	1:B:364:ALA:N	2.30	0.46
1:D:461:ALA:O	1:D:464:ILE:HG22	2.16	0.46
1:A:42:PRO:CG	1:A:432:SER:HB2	2.46	0.46
1:A:167:ARG:HH21	1:A:169:GLY:HA2	1.81	0.46
1:D:175:VAL:HG11	1:D:222:ILE:HD11	1.99	0.45
1:D:319:GLY:O	1:D:322:LEU:HD12	2.16	0.45
1:A:51:ARG:CB	1:A:56:SER:HB2	2.46	0.45
1:B:269:TRP:HE1	1:B:315:ASN:HD21	1.64	0.45
1:D:266:LYS:HE3	1:D:267:ASP:OD1	2.16	0.45
1:A:266:LYS:HE3	1:A:267:ASP:OD1	2.16	0.45
1:A:221:LEU:HD21	1:A:276:THR:HG22	1.99	0.45
1:A:353:GLU:HG3	1:A:387:TYR:CD2	2.52	0.45
1:B:64:THR:O	1:B:68:MET:HG3	2.17	0.45
1:D:164:THR:H	1:D:166:ARG:NH2	2.15	0.45
1:B:230:ASN:OD1	1:B:232:THR:HG22	2.17	0.45
1:C:252:ILE:HG23	1:C:269:TRP:CD2	2.52	0.45
1:A:392:PRO:HG3	1:A:456:GLU:HB2	1.99	0.45
1:C:389:ILE:HG22	1:C:433:SER:HB3	1.99	0.45
1:D:31:HIS:HA	1:D:35:PHE:HB2	1.98	0.45
1:D:62:LEU:HG	1:D:77:ILE:HG21	1.99	0.45
1:B:240:TRP:HE1	1:B:276:THR:CG2	2.27	0.45
1:B:174:ASN:HD22	1:B:176:ALA:N	2.15	0.45
1:B:461:ALA:O	1:B:464:ILE:HG22	2.16	0.45
1:C:388:TYR:CZ	1:C:390:LEU:HA	2.52	0.45
1:A:107:GLY:HA2	1:A:490:PHE:HZ	1.82	0.44
1:B:106:LEU:HD13	1:B:140:LEU:HD13	1.99	0.44
1:D:175:VAL:HG21	1:D:223:GLY:O	2.17	0.44
1:A:140:LEU:HD22	1:A:144:LEU:HD22	1.97	0.44
1:C:70:ASP:O	1:C:74:VAL:HG23	2.16	0.44
1:D:162:ASN:HD22	1:D:163:PRO:N	2.15	0.44
1:D:258:ASP:HB3	1:D:262:PHE:CD1	2.52	0.44
1:A:256:LEU:HB2	1:A:322:LEU:HD21	1.98	0.44
1:B:221:LEU:HD21	1:B:276:THR:HG22	2.00	0.44
1:D:67:LEU:HD12	1:D:459:LYS:CD	2.46	0.44
1:A:269:TRP:HE1	1:A:315:ASN:HD21	1.66	0.44
1:C:348:SER:HB3	1:C:439:GLN:O	2.17	0.44
1:C:54:TRP:HB2	1:C:105:TYR:CZ	2.53	0.44
1:A:126:ASN:ND2	1:A:129:LEU:HD22	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PRO:HG3	4:A:2184:HOH:O	2.16	0.44
1:C:350:ILE:HB	1:C:437:VAL:HG22	1.98	0.44
1:C:473:VAL:HA	1:C:479:ASN:ND2	2.33	0.44
1:A:269:TRP:HE1	1:A:315:ASN:ND2	2.15	0.44
1:C:242:GLY:O	1:C:243:LEU:HB2	2.18	0.44
1:C:403:ARG:HH22	1:C:468:GLU:CD	2.26	0.44
1:D:350:ILE:HB	1:D:437:VAL:CG2	2.48	0.44
1:A:473:VAL:HA	1:A:479:ASN:HD21	1.83	0.44
1:A:350:ILE:HB	1:A:437:VAL:HG22	2.00	0.43
1:C:388:TYR:CE1	1:C:390:LEU:HA	2.52	0.43
1:C:433:SER:HB2	1:C:446:SER:OG	2.18	0.43
1:A:174:ASN:HA	1:A:224:THR:O	2.19	0.43
1:D:175:VAL:HG12	1:D:247:PHE:HB2	2.00	0.43
1:C:77:ILE:O	1:C:81:VAL:HG23	2.19	0.43
1:D:175:VAL:HG23	1:D:224:THR:O	2.18	0.43
1:A:218:TRP:HB2	1:A:221:LEU:HD12	2.01	0.43
1:A:302:SER:HA	1:A:303:PRO:HD3	1.77	0.43
1:B:15:ARG:HG2	1:B:415:TRP:CD2	2.54	0.43
1:D:51:ARG:HD3	1:D:104:ARG:HD2	2.00	0.43
1:D:402:TYR:HB2	1:D:410:TRP:HB2	2.00	0.43
1:D:41:HIS:HB3	1:D:447:ASP:OD2	2.19	0.43
1:D:368:PRO:HG3	1:D:382:TRP:CE3	2.53	0.43
1:A:303:PRO:HG2	1:A:365:GLY:CA	2.48	0.43
1:A:473:VAL:HA	1:A:479:ASN:ND2	2.34	0.43
1:C:175:VAL:HG12	1:C:247:PHE:HB2	2.00	0.43
1:C:459:LYS:HD2	1:C:487:ALA:HB1	2.00	0.43
1:D:30:TYR:HA	1:D:40:LEU:HD22	2.01	0.43
1:A:15:ARG:HG3	1:A:415:TRP:CZ3	2.54	0.42
1:A:240:TRP:HE1	1:A:276:THR:CG2	2.29	0.42
1:A:326:GLN:HG3	4:A:2232:HOH:O	2.18	0.42
1:B:269:TRP:HE1	1:B:315:ASN:ND2	2.17	0.42
1:C:392:PRO:HG3	1:C:456:GLU:CB	2.49	0.42
1:A:250:TYR:O	1:A:254:MET:HG2	2.19	0.42
1:C:12:ASN:HA	1:C:13:PRO:HD2	1.87	0.42
1:C:64:THR:OG1	1:C:459:LYS:HE2	2.18	0.42
1:C:117:ARG:HH11	1:C:117:ARG:CB	2.20	0.42
1:C:389:ILE:HD11	1:C:391:ARG:CZ	2.50	0.42
1:D:392:PRO:O	1:D:393:GLU:C	2.62	0.42
1:C:187:ARG:NH2	1:C:191:LEU:HD21	2.34	0.42
1:C:252:ILE:HD11	1:C:315:ASN:ND2	2.34	0.42
2:C:601:NAG:H83	2:C:601:NAG:H3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:PRO:HG2	1:D:432:SER:HB2	2.01	0.42
1:A:172:SER:HA	1:A:228:THR:HG23	2.01	0.42
1:A:368:PRO:HG3	1:A:382:TRP:CE3	2.54	0.42
1:A:493:ARG:O	1:A:494:SER:HB2	2.19	0.42
1:B:104:ARG:HG3	1:B:104:ARG:NH1	2.35	0.42
1:C:56:SER:O	1:C:60:ASP:HB2	2.20	0.42
1:A:445:ALA:HB2	4:A:2279:HOH:O	2.19	0.42
1:D:417:ALA:O	1:D:421:ILE:HG13	2.19	0.42
1:A:15:ARG:HB3	1:A:465:PHE:CG	2.55	0.42
1:A:86:PHE:CD1	1:A:140:LEU:HG	2.54	0.42
1:B:176:ALA:HB2	1:B:243:LEU:C	2.45	0.42
1:C:492:ILE:N	1:C:492:ILE:HD13	2.35	0.42
1:D:97:SER:HB3	1:D:100:GLU:HB2	2.02	0.42
1:A:111:SER:HB3	1:A:488:HIS:HB3	2.02	0.42
1:B:45:ASN:HD22	1:B:45:ASN:HA	1.60	0.42
1:D:41:HIS:HA	1:D:42:PRO:HD2	1.85	0.42
1:B:399:TYR:HA	1:B:464:ILE:HD12	2.02	0.41
1:C:276:THR:HA	1:C:280:LEU:HG	2.01	0.41
1:D:409:LYS:O	1:D:413:LEU:HD13	2.20	0.41
1:A:456:GLU:HG2	1:A:487:ALA:HB3	2.01	0.41
1:C:51:ARG:HG2	1:C:56:SER:HB3	2.02	0.41
1:C:269:TRP:HE1	1:C:315:ASN:ND2	2.18	0.41
1:D:54:TRP:HB2	1:D:105:TYR:CZ	2.56	0.41
1:D:162:ASN:C	1:D:162:ASN:ND2	2.77	0.41
1:D:224:THR:HG21	4:D:2031:HOH:O	2.20	0.41
1:D:269:TRP:CH2	1:D:319:GLY:HA3	2.55	0.41
1:A:70:ASP:O	1:A:74:VAL:HG23	2.19	0.41
1:C:172:SER:HB2	1:C:226:VAL:O	2.20	0.41
1:C:252:ILE:HD13	1:C:252:ILE:N	2.13	0.41
1:B:214:SER:HA	1:B:215:PRO:HD3	1.91	0.41
1:D:129:LEU:O	1:D:132:SER:HB2	2.20	0.41
1:D:462:TYR:HD1	1:D:463:LEU:HD12	1.85	0.41
1:A:289:ASP:O	1:A:334:LYS:HE3	2.21	0.41
1:B:331:PHE:CE1	1:B:335:LEU:HD11	2.56	0.41
1:D:266:LYS:HD2	1:D:323:LEU:HD21	2.02	0.41
1:D:256:LEU:HD22	1:D:492:ILE:CD1	2.50	0.41
1:D:354:GLY:N	1:D:385:ALA:HB3	2.35	0.41
1:C:48:ASP:OD2	1:C:50:GLU:HG2	2.20	0.41
1:D:63:ASP:O	1:D:67:LEU:HG	2.20	0.41
1:A:104:ARG:HG3	1:A:104:ARG:NH1	2.34	0.41
1:A:403:ARG:HG3	1:A:473:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASP:OD2	1:B:48:ASP:C	2.64	0.41
1:B:256:LEU:HG	1:B:322:LEU:HD21	2.03	0.41
1:D:45:ASN:HD22	1:D:45:ASN:HA	1.65	0.41
1:D:187:ARG:NH2	1:D:491:SER:OG	2.54	0.41
1:D:348:SER:OG	1:D:437:VAL:HG22	2.21	0.41
1:A:48:ASP:OD2	1:A:48:ASP:C	2.63	0.41
1:A:304:ASN:HD22	1:A:304:ASN:N	2.16	0.41
1:B:250:TYR:O	1:B:254:MET:HG2	2.20	0.41
1:D:42:PRO:CG	1:D:432:SER:HB2	2.50	0.41
1:A:340:PHE:O	1:A:343:TYR:HB2	2.20	0.40
1:A:482:VAL:CG2	1:A:492:ILE:HG22	2.51	0.40
1:B:242:GLY:O	1:B:243:LEU:CB	2.69	0.40
1:C:38:ASP:HB2	1:C:49:ASP:HA	2.03	0.40
1:D:174:ASN:ND2	1:D:177:GLU:H	2.18	0.40
1:D:393:GLU:H	1:D:393:GLU:CD	2.29	0.40
1:A:67:LEU:HD12	1:A:459:LYS:CD	2.50	0.40
1:C:251:LEU:HB3	1:C:269:TRP:HB2	2.04	0.40
1:C:323:LEU:HD22	4:C:2143:HOH:O	2.22	0.40
1:B:476:THR:HG22	1:B:476:THR:O	2.21	0.40
1:D:80:TYR:HA	1:D:83:GLN:OE1	2.21	0.40
1:D:104:ARG:HH11	1:D:104:ARG:HG3	1.85	0.40
1:D:175:VAL:HG12	1:D:247:PHE:CB	2.52	0.40
1:D:368:PRO:HG3	1:D:382:TRP:CZ3	2.57	0.40
1:A:119:PRO:HG2	1:A:120:PHE:HD1	1.86	0.40
1:B:118:GLY:HA3	1:B:119:PRO:HD2	1.93	0.40
1:D:331:PHE:HA	1:D:334:LYS:CE	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2146:HOH:O	4:D:2109:HOH:O[1_554]	2.16	0.04

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	486/503 (97%)	454 (93%)	30 (6%)	2 (0%)	30	40
1	B	487/503 (97%)	460 (94%)	25 (5%)	2 (0%)	30	40
1	C	483/503 (96%)	454 (94%)	28 (6%)	1 (0%)	43	56
1	D	484/503 (96%)	448 (93%)	32 (7%)	4 (1%)	16	23
All	All	1940/2012 (96%)	1816 (94%)	115 (6%)	9 (0%)	24	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	245	ASP
1	D	478	GLY
1	C	430	ALA
1	A	392	PRO
1	B	430	ALA
1	D	393	GLU
1	D	430	ALA
1	A	430	ALA
1	D	392	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	390/404 (96%)	367 (94%)	23 (6%)	18	28
1	B	392/404 (97%)	369 (94%)	23 (6%)	18	28
1	C	388/404 (96%)	369 (95%)	19 (5%)	22	36
1	D	388/404 (96%)	360 (93%)	28 (7%)	13	20
All	All	1558/1616 (96%)	1465 (94%)	93 (6%)	17	28

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	51	ARG
1	A	60	ASP
1	A	123	LEU
1	A	129	LEU
1	A	136	GLN
1	A	140	LEU
1	A	144	LEU
1	A	183	LEU
1	A	184	GLU
1	A	191	LEU
1	A	200	LEU
1	A	251	LEU
1	A	256	LEU
1	A	276	THR
1	A	290	LEU
1	A	304	ASN
1	A	335	LEU
1	A	392	PRO
1	A	409	LYS
1	A	437	VAL
1	A	459	LYS
1	A	485	THR
1	B	15	ARG
1	B	45	ASN
1	B	51	ARG
1	B	60	ASP
1	B	76	THR
1	B	106	LEU
1	B	109	LEU
1	B	133	LEU
1	B	136	GLN
1	B	140	LEU
1	B	144	LEU
1	B	175	VAL
1	B	191	LEU
1	B	251	LEU
1	B	256	LEU
1	B	391	ARG
1	B	392	PRO
1	B	393	GLU
1	B	418	LEU
1	B	426	ARG

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Mol	Chain	Res	Type
1	B	437	VAL
1	B	468	GLU
1	B	485	THR
1	C	20	LYS
1	C	45	ASN
1	C	51	ARG
1	C	60	ASP
1	C	109	LEU
1	C	117	ARG
1	C	140	LEU
1	C	144	LEU
1	C	183	LEU
1	C	208	LEU
1	C	227	SER
1	C	252	ILE
1	C	290	LEU
1	C	318	LEU
1	C	353	GLU
1	C	392	PRO
1	C	437	VAL
1	C	485	THR
1	C	492	ILE
1	D	15	ARG
1	D	51	ARG
1	D	60	ASP
1	D	62	LEU
1	D	70	ASP
1	D	109	LEU
1	D	117	ARG
1	D	123	LEU
1	D	135	ARG
1	D	136	GLN
1	D	140	LEU
1	D	162	ASN
1	D	184	GLU
1	D	191	LEU
1	D	196	GLN
1	D	224	THR
1	D	251	LEU
1	D	256	LEU
1	D	322	LEU
1	D	327	LYS

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Mol	Chain	Res	Type
1	D	342	THR
1	D	391	ARG
1	D	426	ARG
1	D	434	ILE
1	D	437	VAL
1	D	459	LYS
1	D	467	GLU
1	D	485	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	28	ASN
1	A	45	ASN
1	A	52	ASN
1	A	75	ASN
1	A	136	GLN
1	A	138	GLN
1	A	174	ASN
1	A	199	GLN
1	A	202	GLN
1	A	297	ASN
1	A	304	ASN
1	A	315	ASN
1	A	439	GLN
1	A	472	GLN
1	A	479	ASN
1	B	24	GLN
1	B	28	ASN
1	B	45	ASN
1	B	83	GLN
1	B	136	GLN
1	B	174	ASN
1	B	199	GLN
1	B	202	GLN
1	B	315	ASN
1	B	324	ASN
1	B	441	ASN
1	C	24	GLN
1	C	28	ASN
1	C	45	ASN

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Mol	Chain	Res	Type
1	C	79	GLN
1	C	93	ASN
1	C	136	GLN
1	C	196	GLN
1	C	264	HIS
1	C	297	ASN
1	C	299	GLN
1	C	307	HIS
1	C	315	ASN
1	C	326	GLN
1	C	474	GLN
1	C	479	ASN
1	D	24	GLN
1	D	28	ASN
1	D	45	ASN
1	D	75	ASN
1	D	136	GLN
1	D	162	ASN
1	D	174	ASN
1	D	202	GLN
1	D	297	ASN
1	D	307	HIS
1	D	324	ASN
1	D	326	GLN
1	D	411	GLN
1	D	439	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	600	1	14,14,15	0.50	0	17,19,21	0.64	0
2	NAG	D	600	1	14,14,15	0.55	0	17,19,21	0.60	0
2	NAG	B	601	1	14,14,15	0.49	0	17,19,21	0.72	1 (5%)
2	NAG	C	601	1	14,14,15	0.62	0	17,19,21	0.86	1 (5%)
2	NAG	B	602	1	14,14,15	0.52	0	17,19,21	0.78	1 (5%)
2	NAG	B	600	1	14,14,15	0.49	0	17,19,21	0.67	0
2	NAG	A	601	1	14,14,15	0.48	0	17,19,21	0.63	0
2	NAG	A	602	1	14,14,15	0.50	0	17,19,21	0.66	0
2	NAG	C	600	1	14,14,15	0.46	0	17,19,21	0.79	1 (5%)
2	NAG	D	602	1	14,14,15	0.47	0	17,19,21	0.76	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	600	1	-	3/6/23/26	0/1/1/1
2	NAG	D	600	1	-	2/6/23/26	0/1/1/1
2	NAG	B	601	1	-	2/6/23/26	0/1/1/1
2	NAG	C	601	1	-	3/6/23/26	0/1/1/1
2	NAG	B	602	1	-	4/6/23/26	0/1/1/1
2	NAG	B	600	1	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	5/6/23/26	0/1/1/1
2	NAG	C	600	1	-	4/6/23/26	0/1/1/1
2	NAG	D	602	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	NAG	C2-N2-C7	-2.56	119.47	122.90
2	C	600	NAG	C2-N2-C7	-2.53	119.51	122.90
2	C	601	NAG	C2-N2-C7	-2.41	119.67	122.90
2	B	602	NAG	C2-N2-C7	-2.35	119.75	122.90
2	B	601	NAG	C2-N2-C7	-2.16	120.00	122.90

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	NAG	O7-C7-N2-C2
2	A	602	NAG	C8-C7-N2-C2
2	A	602	NAG	O7-C7-N2-C2
2	B	602	NAG	C8-C7-N2-C2
2	B	602	NAG	O7-C7-N2-C2
2	C	601	NAG	C8-C7-N2-C2
2	C	601	NAG	O7-C7-N2-C2
2	D	602	NAG	C8-C7-N2-C2
2	D	602	NAG	O7-C7-N2-C2
2	A	600	NAG	C8-C7-N2-C2
2	A	602	NAG	O5-C5-C6-O6
2	B	602	NAG	O5-C5-C6-O6
2	C	600	NAG	O5-C5-C6-O6
2	B	602	NAG	C4-C5-C6-O6
2	A	602	NAG	C4-C5-C6-O6
2	C	600	NAG	C8-C7-N2-C2
2	B	601	NAG	C8-C7-N2-C2
2	C	600	NAG	C4-C5-C6-O6
2	B	601	NAG	O7-C7-N2-C2
2	C	600	NAG	O7-C7-N2-C2
2	D	600	NAG	C8-C7-N2-C2
2	D	600	NAG	O7-C7-N2-C2
2	A	600	NAG	C4-C5-C6-O6
2	A	602	NAG	C3-C2-N2-C7
2	C	601	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	NAG	1	0

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	488/503 (97%)	-0.45	3 (0%) 85 85	7, 15, 30, 45	0
1	B	489/503 (97%)	-0.52	1 (0%) 91 90	6, 14, 26, 47	0
1	C	485/503 (96%)	-0.29	1 (0%) 91 90	9, 20, 34, 56	0
1	D	486/503 (96%)	-0.02	8 (1%) 70 69	12, 25, 44, 61	0
All	All	1948/2012 (96%)	-0.32	13 (0%) 84 83	6, 18, 36, 61	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	476	THR	3.6
1	D	9	GLY	3.0
1	B	123	LEU	2.8
1	A	366	GLY	2.6
1	D	70	ASP	2.5
1	D	123	LEU	2.5
1	D	69	GLY	2.4
1	D	434	ILE	2.3
1	C	477	GLY	2.3
1	A	494	SER	2.3
1	A	304	ASN	2.2
1	D	475	ALA	2.2
1	D	477	GLY	2.1

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

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	601	14/15	0.59	0.17	64,69,72,73	0
2	NAG	A	602	14/15	0.69	0.14	52,54,56,57	0
2	NAG	B	602	14/15	0.72	0.14	51,55,58,58	0
2	NAG	D	602	14/15	0.75	0.11	63,66,68,68	0
2	NAG	A	600	14/15	0.81	0.12	45,50,52,52	0
2	NAG	D	600	14/15	0.87	0.09	40,41,42,43	0
2	NAG	B	601	14/15	0.88	0.08	28,31,35,38	0
2	NAG	C	600	14/15	0.91	0.09	24,27,33,33	0
2	NAG	A	601	14/15	0.94	0.06	18,22,24,28	0
2	NAG	B	600	14/15	0.94	0.07	18,22,29,31	0
3	CA	D	1495	1/1	0.97	0.06	36,36,36,36	0
3	CA	B	1495	1/1	0.98	0.06	30,30,30,30	0
3	CA	C	1494	1/1	0.98	0.07	33,33,33,33	0
3	CA	A	1495	1/1	0.98	0.03	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.