



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:14 AM UTC

PDB ID : 2ZR1 / pdb_00002zr1
Title : Agglutinin from Abrus Precatorius
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Deposited on : 2008-08-22
Resolution : 2.60 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

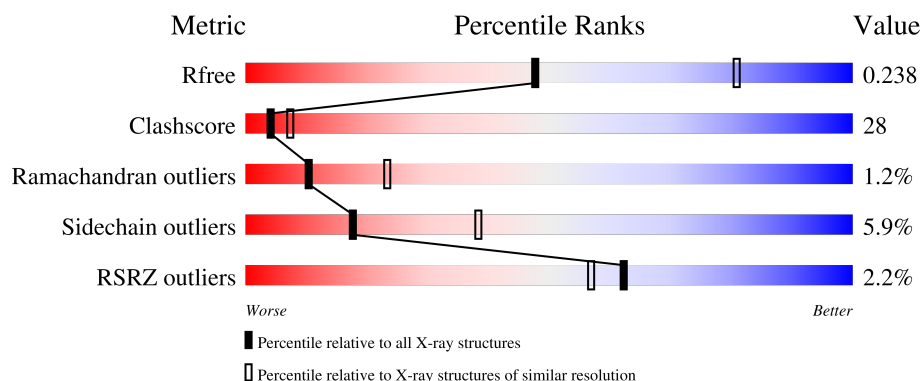
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	258	% 66% 26% • •
1	C	258	5% 45% 46% 5% •
2	B	267	58% 35% 5% •
2	D	267	2% 48% 47% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	268	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8271 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.

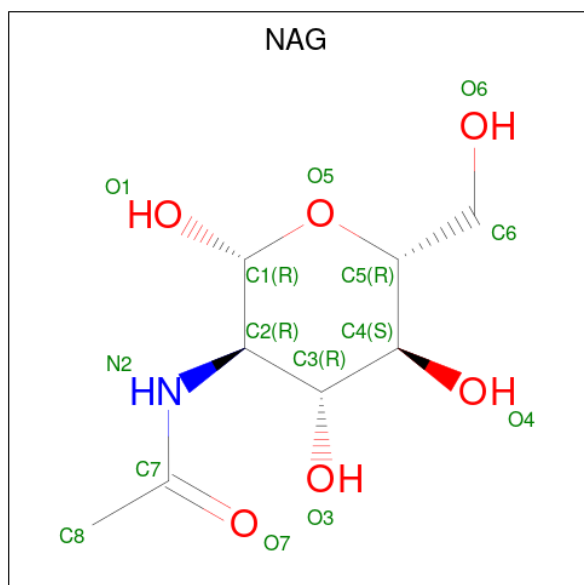
- Molecule 1 is a protein called Agglutinin-1 chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1963	1246	337	376	4			
1	C	250	Total	C	N	O	S	0	0	0
			1963	1246	337	376	4			

- Molecule 2 is a protein called Agglutinin-1 chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	263	Total	C	N	O	S	0	0	0
			2067	1298	348	401	20			
2	D	263	Total	C	N	O	S	0	0	0
			2067	1298	348	401	20			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

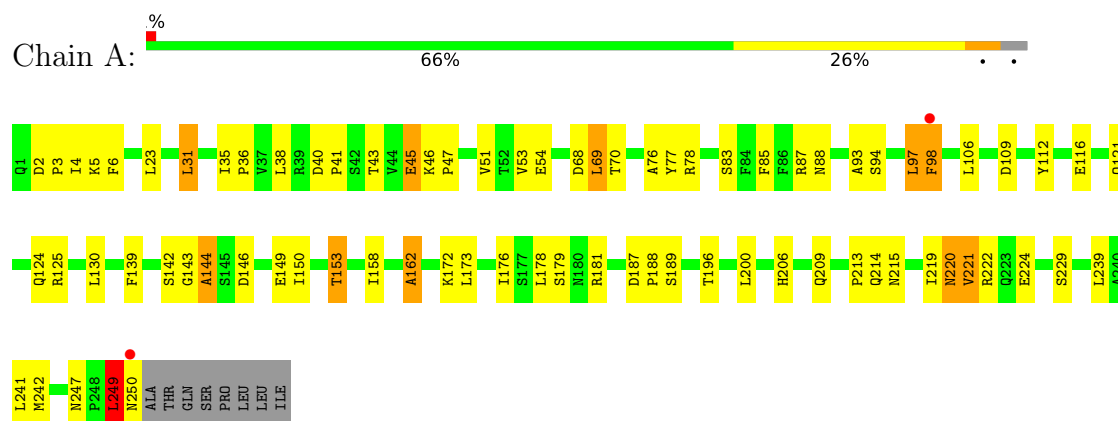
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	49	Total	O	0	0
			49	49		
4	C	50	Total	O	0	0
			50	50		
4	D	34	Total	O	0	0
			34	34		

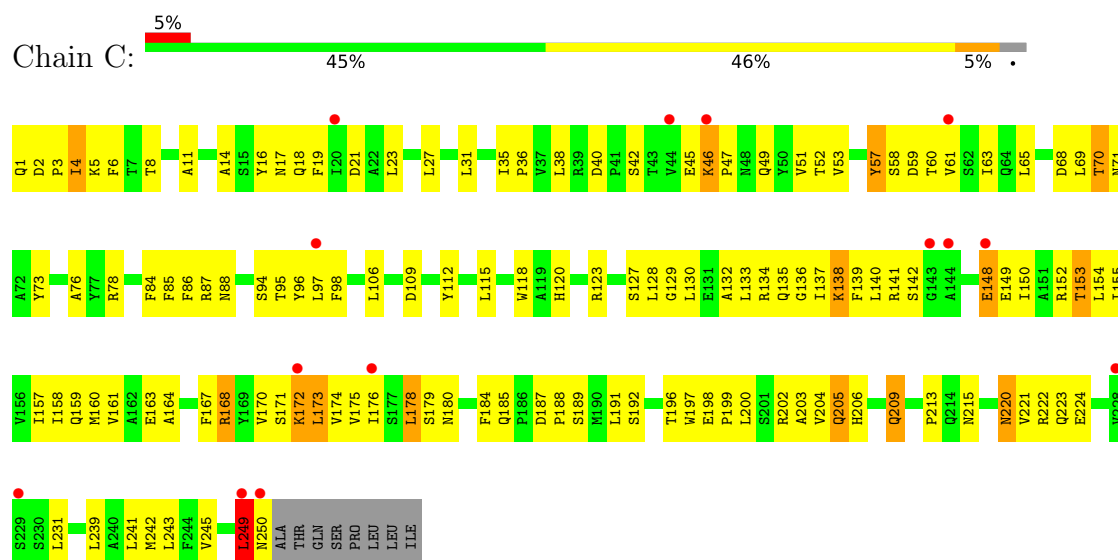
3 Residue-property plots

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.

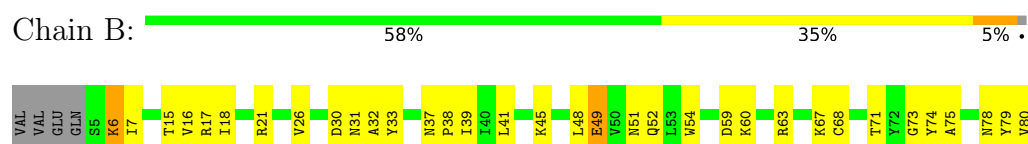
• Molecule 1: Agglutinin-1 chain A

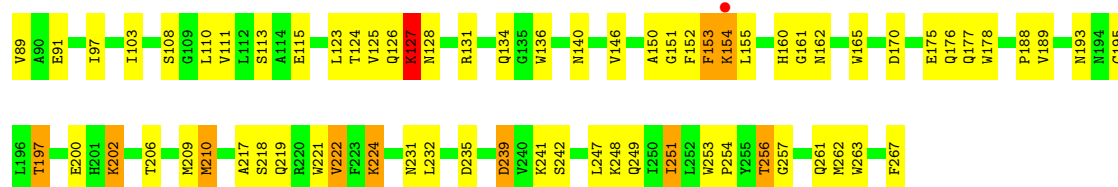


• Molecule 1: Agglutinin-1 chain A

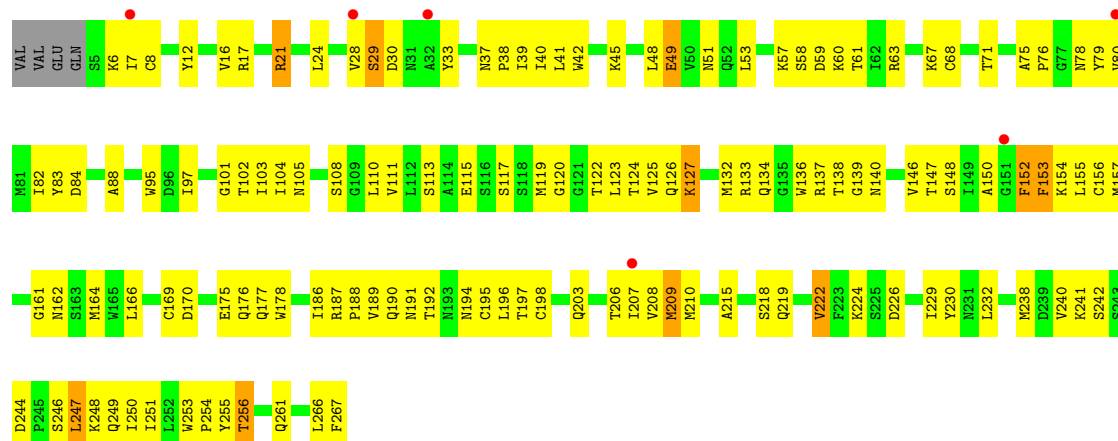


• Molecule 2: Agglutinin-1 chain B





• Molecule 2: Agglutinin-1 chain B



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.05Å 137.05Å 214.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.60 19.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.88-2.60) 99.5 (19.88-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.61Å)	Xtriage
Refinement program	CNS 2.02	Depositor
R, R_{free}	0.199 , 0.227 0.207 , 0.238	Depositor DCC
R_{free} test set	6301 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 125.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8271	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1158e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.60	0/2004	1.01	4/2730 (0.1%)
1	C	0.51	0/2004	0.90	1/2730 (0.0%)
2	B	0.54	0/2117	1.00	8/2876 (0.3%)
2	D	0.44	0/2117	0.84	2/2876 (0.1%)
All	All	0.52	0/8242	0.94	15/11212 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	256	THR	N-CA-C	-7.32	104.96	114.04
2	D	256	THR	N-CA-C	-6.35	107.38	114.62
2	B	151	GLY	N-CA-C	-6.11	103.86	112.60
2	D	101	GLY	N-CA-C	-6.09	106.30	115.32
1	A	98	PHE	CB-CA-C	-5.98	102.27	111.66
2	B	89	VAL	N-CA-C	-5.78	102.08	109.30
2	B	127	LYS	N-CA-C	-5.63	102.07	110.23
1	A	98	PHE	CA-CB-CG	5.63	119.43	113.80
2	B	68	CYS	N-CA-C	5.51	118.22	109.24
2	B	63	ARG	N-CA-C	5.37	118.82	110.17
2	B	193	ASN	N-CA-C	-5.37	106.57	113.23
2	B	251	ILE	N-CA-C	5.35	116.55	108.96
1	C	168	ARG	N-CA-C	-5.21	106.18	112.54
1	A	181	ARG	N-CA-C	-5.10	104.86	111.74
1	A	162	ALA	N-CA-C	5.01	116.43	110.97

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	1963	0	1951	87	0
1	C	1963	0	1951	139	0
2	B	2067	0	1970	98	0
2	D	2067	0	1971	142	0
3	B	28	0	26	0	0
3	D	14	0	13	0	0
4	A	36	0	0	0	0
4	B	49	0	0	1	0
4	C	50	0	0	2	0
4	D	34	0	0	2	0
All	All	8271	0	7882	440	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 28.

All (440) 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)
2:B:153:PHE:O	2:B:154:LYS:HG3	1.49	1.12
1:C:61:VAL:HG13	1:C:141:ARG:HG2	1.42	1.01
1:C:167:PHE:HB2	1:C:170:VAL:HG23	1.43	1.00
2:B:256:THR:H	2:B:261:GLN:HE22	1.06	0.98
1:A:78:ARG:HB2	1:A:98:PHE:CE1	1.99	0.98
1:A:149:GLU:O	1:A:153:THR:HG22	1.64	0.97
2:D:157:MET:HE3	2:D:164:MET:HE2	1.45	0.96
2:B:71:THR:HG21	2:B:125:VAL:HG11	1.49	0.94
2:D:41:LEU:HG	2:D:123:LEU:HD21	1.51	0.92
1:A:249:LEU:C	1:A:249:LEU:HD23	1.95	0.92
1:A:85:PHE:CZ	1:A:98:PHE:HD2	1.90	0.89
2:D:229:ILE:HG21	2:D:238:MET:HE2	1.54	0.89
1:A:78:ARG:HB2	1:A:98:PHE:HE1	1.36	0.87
2:D:169:CYS:HA	2:D:176:GLN:HE22	1.40	0.87
1:C:118:TRP:O	1:C:148:GLU:HG3	1.75	0.86
2:B:170:ASP:H	2:B:176:GLN:HE22	1.23	0.85
1:A:85:PHE:CE1	1:A:98:PHE:HD2	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:THR:H	2:B:261:GLN:NE2	1.74	0.84
2:B:197:THR:HB	2:B:219:GLN:HG2	1.58	0.84
1:C:220:ASN:ND2	1:C:224:GLU:H	1.77	0.82
1:A:249:LEU:HD23	1:A:250:ASN:N	1.94	0.82
1:C:209:GLN:HE21	1:C:209:GLN:HA	1.45	0.82
1:C:27:LEU:HD23	1:C:69:LEU:HD12	1.60	0.81
1:A:220:ASN:ND2	1:A:224:GLU:H	1.77	0.81
2:B:153:PHE:C	2:B:154:LYS:HG3	2.06	0.80
1:C:221:VAL:HG23	1:C:222:ARG:HD3	1.63	0.80
2:D:197:THR:HB	2:D:219:GLN:HG2	1.62	0.80
1:A:41:PRO:HG3	1:A:70:THR:HG23	1.62	0.80
1:A:85:PHE:CE1	1:A:98:PHE:CD2	2.71	0.79
1:C:149:GLU:O	1:C:153:THR:HG22	1.81	0.78
2:B:197:THR:HG21	2:B:210:MET:HB2	1.66	0.78
2:D:79:TYR:HA	2:D:124:THR:HG22	1.65	0.77
1:C:187:ASP:HB2	1:C:188:PRO:HD2	1.67	0.77
1:A:220:ASN:HD21	1:A:224:GLU:H	1.32	0.77
1:A:85:PHE:CZ	1:A:98:PHE:CD2	2.73	0.76
1:C:52:THR:HG22	1:C:97:LEU:HD11	1.66	0.76
1:C:170:VAL:O	1:C:174:VAL:HG23	1.85	0.76
1:C:51:VAL:CG2	1:C:69:LEU:HD13	2.16	0.76
2:D:229:ILE:HB	2:D:238:MET:HG3	1.69	0.74
2:B:177:GLN:HB3	2:B:189:VAL:HG21	1.69	0.74
2:D:256:THR:H	2:D:261:GLN:HE22	1.35	0.74
2:D:39:ILE:HB	2:D:80:VAL:HG23	1.69	0.73
2:D:207:ILE:HD12	2:D:250:ILE:HG22	1.69	0.73
2:B:108:SER:HB2	2:B:110:LEU:HD13	1.68	0.72
2:D:75:ALA:H	2:D:78:ASN:ND2	1.87	0.72
1:C:120:HIS:CE1	1:C:148:GLU:OE1	2.42	0.72
1:C:168:ARG:O	1:C:172:LYS:HD2	1.89	0.72
1:C:171:SER:O	1:C:175:VAL:HG23	1.89	0.72
2:D:83:TYR:CD1	2:D:88:ALA:HB2	2.24	0.72
1:A:209:GLN:HE21	1:A:209:GLN:HA	1.55	0.72
1:A:239:LEU:HD21	1:A:242:MET:HG2	1.73	0.71
1:C:220:ASN:HD21	1:C:224:GLU:H	1.36	0.71
1:A:83:SER:HB2	1:A:98:PHE:CG	2.26	0.71
1:A:179:SER:HB3	2:B:154:LYS:HG2	1.71	0.71
1:C:205:GLN:HE21	1:C:245:VAL:HB	1.54	0.71
2:B:73:GLY:C	2:B:78:ASN:HD22	1.98	0.70
2:B:188:PRO:HG3	2:B:209:MET:HE1	1.74	0.69
1:C:120:HIS:CE1	1:C:148:GLU:CD	2.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:VAL:HA	2:B:178:TRP:O	1.94	0.68
1:A:83:SER:HB2	1:A:98:PHE:CD1	2.28	0.68
2:D:75:ALA:H	2:D:78:ASN:HD22	1.42	0.68
2:B:195:CYS:O	2:B:197:THR:HG22	1.93	0.68
1:A:78:ARG:HB2	1:A:98:PHE:CD1	2.29	0.67
1:A:78:ARG:CB	1:A:98:PHE:HE1	2.07	0.67
1:A:250:ASN:H	2:B:7:ILE:HD11	1.59	0.67
2:B:71:THR:HG22	2:B:80:VAL:HG12	1.76	0.67
1:C:35:ILE:CG2	1:C:242:MET:HE2	2.25	0.67
1:C:136:GLY:O	1:C:140:LEU:HG	1.94	0.67
1:C:57:TYR:C	1:C:57:TYR:CD2	2.72	0.67
1:C:51:VAL:HG21	1:C:69:LEU:HD13	1.77	0.67
2:B:256:THR:N	2:B:261:GLN:HE22	1.85	0.66
1:C:239:LEU:HD21	1:C:242:MET:HG2	1.77	0.66
1:A:5:LYS:HG2	1:A:6:PHE:N	2.11	0.66
1:A:35:ILE:HB	1:A:242:MET:HE2	1.78	0.66
2:B:67:LYS:HB2	2:B:82:ILE:HD11	1.77	0.66
1:C:173:LEU:HD13	1:C:176:ILE:HD11	1.77	0.66
1:C:120:HIS:ND1	1:C:148:GLU:CD	2.54	0.66
1:C:138:LYS:HD3	1:C:138:LYS:C	2.21	0.66
1:A:68:ASP:OD1	1:A:70:THR:HB	1.96	0.65
1:C:196:THR:C	1:C:199:PRO:HD2	2.22	0.65
1:A:83:SER:CB	1:A:98:PHE:CG	2.80	0.65
1:C:128:LEU:HB2	1:C:184:PHE:CE1	2.32	0.65
1:A:51:VAL:HG13	1:A:69:LEU:HD13	1.79	0.64
2:D:17:ARG:HG3	2:D:140:ASN:HA	1.78	0.64
2:B:91:GLU:HG2	4:B:288:HOH:O	1.98	0.64
2:D:115:GLU:OE1	2:D:126:GLN:HG3	1.98	0.64
1:A:83:SER:HB2	1:A:98:PHE:CD2	2.31	0.64
1:A:249:LEU:C	1:A:249:LEU:CD2	2.68	0.64
2:B:41:LEU:HG	2:B:123:LEU:HD21	1.80	0.64
1:A:222:ARG:HH22	2:B:177:GLN:HE22	1.43	0.64
1:C:205:GLN:NE2	1:C:245:VAL:HB	2.12	0.64
1:A:249:LEU:CD2	1:A:250:ASN:N	2.61	0.63
1:A:45:GLU:HB3	1:A:47:PRO:HD2	1.79	0.63
1:A:76:ALA:HB1	1:A:98:PHE:HE2	1.63	0.63
1:C:139:PHE:CD2	1:C:149:GLU:OE1	2.52	0.63
2:D:152:PHE:HD1	2:D:152:PHE:H	1.47	0.63
1:A:220:ASN:HD22	1:A:220:ASN:C	2.06	0.62
1:C:65:LEU:HD11	1:C:157:ILE:CG2	2.29	0.62
2:D:40:ILE:HG22	2:D:122:THR:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LYS:H	1:C:47:PRO:HD2	1.63	0.62
1:C:57:TYR:C	1:C:57:TYR:HD2	2.07	0.62
2:D:256:THR:H	2:D:261:GLN:NE2	1.97	0.62
2:D:97:ILE:HD12	2:D:103:ILE:HD12	1.82	0.62
2:B:83:TYR:CD1	2:B:88:ALA:HB2	2.34	0.62
2:B:71:THR:HG21	2:B:125:VAL:CG1	2.25	0.62
1:A:77:TYR:C	1:A:98:PHE:CZ	2.79	0.61
1:A:83:SER:CB	1:A:98:PHE:CD1	2.84	0.61
2:D:71:THR:HG21	2:D:125:VAL:HG11	1.83	0.61
2:D:41:LEU:HD21	2:D:136:TRP:HZ3	1.65	0.60
2:B:175:GLU:CD	2:B:175:GLU:H	2.09	0.60
1:C:51:VAL:HG23	1:C:69:LEU:HD13	1.83	0.60
2:D:30:ASP:HB2	4:D:287:HOH:O	2.00	0.60
1:A:85:PHE:CZ	1:A:94:SER:HA	2.37	0.60
1:C:2:ASP:CG	1:C:3:PRO:HD2	2.26	0.60
1:C:61:VAL:HG13	1:C:141:ARG:CG	2.26	0.60
2:D:177:GLN:HB3	2:D:189:VAL:HG21	1.83	0.60
1:A:215:ASN:OD1	1:A:229:SER:HB2	2.02	0.60
1:C:222:ARG:NH1	2:D:177:GLN:HE22	1.99	0.60
2:D:191:ASN:HD22	2:D:194:ASN:HD22	1.48	0.60
1:A:83:SER:HB2	1:A:98:PHE:CE1	2.37	0.60
1:C:180:ASN:OD1	2:D:154:LYS:HD2	2.02	0.59
2:D:175:GLU:HG3	2:D:190:GLN:NE2	2.17	0.59
1:C:49:GLN:O	1:C:49:GLN:HG2	2.01	0.59
2:D:16:VAL:HB	2:D:139:GLY:HA2	1.84	0.59
1:C:139:PHE:HE2	1:C:150:ILE:HG13	1.67	0.59
1:C:191:LEU:HD12	1:C:192:SER:N	2.18	0.59
2:B:6:LYS:HE2	2:B:7:ILE:HG22	1.84	0.59
1:C:155:ILE:HG22	1:C:159:GLN:HE21	1.67	0.59
2:D:57:LYS:HE2	2:D:63:ARG:NH1	2.17	0.59
2:D:157:MET:HE3	2:D:164:MET:CE	2.26	0.59
2:D:148:SER:HB2	2:D:266:LEU:HB2	1.84	0.59
2:D:146:VAL:HA	2:D:178:TRP:O	2.02	0.58
2:D:40:ILE:HD12	2:D:120:GLY:HA2	1.85	0.58
1:C:35:ILE:HB	1:C:242:MET:HE2	1.85	0.58
1:A:4:ILE:HD13	1:A:23:LEU:HA	1.86	0.58
1:C:196:THR:O	1:C:199:PRO:HD2	2.04	0.58
2:B:59:ASP:O	2:B:60:LYS:HB2	2.04	0.58
1:C:204:VAL:HG13	1:C:231:LEU:HD11	1.86	0.58
1:A:31:LEU:HD12	1:A:36:PRO:HA	1.86	0.57
2:D:175:GLU:HG3	2:D:190:GLN:HE22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:ILE:HD13	2:D:238:MET:SD	2.44	0.57
1:A:76:ALA:CB	1:A:98:PHE:HE2	2.17	0.57
1:A:247:ASN:O	2:B:7:ILE:HD12	2.03	0.57
1:C:58:SER:C	1:C:60:THR:H	2.12	0.57
1:C:8:THR:OG1	1:C:134:ARG:HG2	2.04	0.57
2:D:222:VAL:HG13	2:D:230:TYR:HB3	1.86	0.57
2:B:39:ILE:HB	2:B:80:VAL:HG23	1.86	0.57
2:B:33:TYR:OH	2:B:51:ASN:HA	2.05	0.57
2:D:97:ILE:HG23	2:D:103:ILE:HD13	1.87	0.57
2:D:177:GLN:O	2:D:189:VAL:HG23	2.04	0.57
2:B:222:VAL:HG22	2:B:224:LYS:HG2	1.86	0.57
1:A:222:ARG:NH2	2:B:177:GLN:HE22	2.03	0.56
1:A:76:ALA:HB1	1:A:98:PHE:CE2	2.40	0.56
1:C:198:GLU:HB3	1:C:199:PRO:HD3	1.86	0.56
1:C:173:LEU:O	1:C:176:ILE:HG12	2.05	0.56
1:C:209:GLN:HA	1:C:209:GLN:NE2	2.19	0.56
2:B:79:TYR:HA	2:B:124:THR:HG22	1.87	0.56
2:B:153:PHE:C	2:B:154:LYS:CG	2.77	0.56
1:A:77:TYR:O	1:A:98:PHE:CZ	2.59	0.56
1:A:93:ALA:O	1:A:97:LEU:HB2	2.06	0.56
1:C:63:ILE:HD13	1:C:140:LEU:HD12	1.87	0.56
2:D:33:TYR:OH	2:D:51:ASN:HA	2.05	0.56
1:C:14:ALA:O	1:C:18:GLN:HG3	2.06	0.56
2:D:71:THR:HG23	2:D:95:TRP:CZ2	2.41	0.56
2:D:97:ILE:HG23	2:D:103:ILE:CD1	2.36	0.56
2:B:202:LYS:HB2	2:B:202:LYS:NZ	2.21	0.55
1:C:222:ARG:HH12	2:D:177:GLN:HE22	1.53	0.55
2:D:147:THR:HB	2:D:267:PHE:HB3	1.87	0.55
2:B:75:ALA:H	2:B:78:ASN:ND2	2.05	0.55
1:C:46:LYS:HB2	1:C:47:PRO:HD3	1.88	0.55
1:A:125:ARG:HG3	1:A:125:ARG:HH11	1.71	0.55
1:A:209:GLN:HE22	2:B:97:ILE:H	1.55	0.55
2:B:17:ARG:HG3	2:B:140:ASN:HA	1.88	0.55
1:C:23:LEU:HD13	1:C:53:VAL:HG21	1.88	0.55
1:A:87:ARG:HB2	1:A:106:LEU:O	2.08	0.54
1:A:196:THR:O	1:A:196:THR:HG22	2.07	0.54
1:C:130:LEU:HD22	1:C:178:LEU:HD21	1.89	0.54
1:A:172:LYS:O	1:A:172:LYS:HD3	2.07	0.54
1:C:17:ASN:O	1:C:21:ASP:CG	2.51	0.54
2:D:155:LEU:HD13	2:D:166:LEU:HD13	1.90	0.54
2:B:175:GLU:CD	2:B:175:GLU:N	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ILE:HG23	2:B:103:ILE:HD13	1.90	0.54
2:D:79:TYR:CA	2:D:124:THR:HG22	2.35	0.54
1:A:83:SER:HB2	1:A:98:PHE:CE2	2.43	0.53
2:B:71:THR:CG2	2:B:125:VAL:CG1	2.86	0.53
2:D:48:LEU:HD12	2:D:53:LEU:HD21	1.91	0.53
2:D:137:ARG:HG2	2:D:138:THR:N	2.23	0.53
1:C:38:LEU:HD13	1:C:242:MET:O	2.09	0.53
1:C:133:LEU:O	1:C:137:ILE:HG13	2.09	0.53
2:B:239:ASP:C	2:B:239:ASP:OD2	2.50	0.53
1:C:159:GLN:HA	1:C:163:GLU:CG	2.38	0.53
2:D:153:PHE:O	2:D:155:LEU:HG	2.08	0.53
2:D:178:TRP:CE3	2:D:186:ILE:HG22	2.44	0.53
2:D:191:ASN:HD22	2:D:194:ASN:ND2	2.06	0.52
1:A:220:ASN:ND2	1:A:220:ASN:C	2.66	0.52
2:B:131:ARG:HA	2:B:217:ALA:HA	1.91	0.52
1:C:138:LYS:HD3	1:C:138:LYS:O	2.09	0.52
2:B:241:LYS:HD2	2:B:249:GLN:OE1	2.09	0.52
1:C:68:ASP:HB3	1:C:71:ASN:OD1	2.09	0.52
2:D:246:SER:O	2:D:248:LYS:HG3	2.10	0.52
2:B:262:MET:HE2	2:B:262:MET:HA	1.91	0.52
1:C:46:LYS:HB3	1:C:96:TYR:CE2	2.44	0.52
1:A:139:PHE:CE1	1:A:144:ALA:HB3	2.45	0.52
1:A:206:HIS:HB3	1:A:213:PRO:HG2	1.91	0.52
1:A:5:LYS:HE2	1:A:54:GLU:OE2	2.10	0.52
1:C:36:PRO:HB2	1:C:241:LEU:HD23	1.92	0.52
1:C:209:GLN:NE2	2:D:97:ILE:H	2.07	0.52
1:C:249:LEU:HD13	1:C:250:ASN:ND2	2.25	0.52
1:C:249:LEU:H	2:D:7:ILE:HD11	1.75	0.51
1:A:83:SER:HB2	1:A:98:PHE:CZ	2.45	0.51
2:D:45:LYS:HE3	2:D:49:GLU:HG3	1.92	0.51
2:D:67:LYS:HD2	2:D:84:ASP:HA	1.93	0.51
2:D:206:THR:HA	2:D:251:ILE:HA	1.93	0.51
2:D:67:LYS:HB2	2:D:82:ILE:HD11	1.92	0.51
2:B:257:GLY:H	2:B:261:GLN:NE2	2.08	0.51
2:D:206:THR:HG21	2:D:249:GLN:HE21	1.75	0.51
2:D:71:THR:HG22	2:D:80:VAL:HG12	1.92	0.51
2:D:48:LEU:HD11	2:D:140:ASN:HB3	1.91	0.51
2:D:197:THR:HG21	2:D:210:MET:HB2	1.92	0.51
2:D:224:LYS:HE2	2:D:230:TYR:HB2	1.94	0.50
1:A:46:LYS:N	1:A:47:PRO:HD2	2.27	0.50
2:B:6:LYS:NZ	2:B:6:LYS:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:LEU:HD21	2:B:136:TRP:HZ3	1.76	0.50
1:C:68:ASP:OD1	1:C:70:THR:HG22	2.11	0.50
2:D:78:ASN:O	2:D:125:VAL:HG22	2.12	0.50
1:A:209:GLN:HA	1:A:209:GLN:NE2	2.23	0.50
2:D:132:MET:HE2	2:D:215:ALA:HB2	1.93	0.50
2:B:37:ASN:ND2	2:B:38:PRO:HD2	2.26	0.50
2:D:115:GLU:OE2	2:D:133:ARG:HD2	2.12	0.50
2:B:206:THR:HA	2:B:251:ILE:HG22	1.92	0.50
2:B:153:PHE:O	2:B:155:LEU:HG	2.12	0.50
1:C:35:ILE:CB	1:C:242:MET:HE2	2.42	0.50
1:C:52:THR:CG2	1:C:97:LEU:HD11	2.38	0.49
1:C:187:ASP:OD2	1:C:189:SER:OG	2.30	0.49
2:B:247:LEU:O	2:B:248:LYS:C	2.56	0.49
2:D:17:ARG:HB2	2:D:139:GLY:O	2.13	0.49
1:C:88:ASN:HB2	1:C:109:ASP:HB3	1.94	0.49
1:C:172:LYS:HE3	1:C:172:LYS:CA	2.42	0.49
2:D:152:PHE:N	2:D:152:PHE:CD1	2.80	0.49
2:D:157:MET:HE1	2:D:196:LEU:CD1	2.42	0.49
1:A:143:GLY:O	1:A:144:ALA:C	2.54	0.49
2:D:28:VAL:O	2:D:29:SER:C	2.56	0.49
1:A:88:ASN:HB2	1:A:109:ASP:HB3	1.94	0.49
1:A:130:LEU:HD13	1:A:178:LEU:HD21	1.93	0.49
2:B:45:LYS:HD2	2:B:49:GLU:HG3	1.95	0.49
2:B:80:VAL:HG22	2:B:123:LEU:HB2	1.95	0.49
1:C:206:HIS:CE1	2:D:8:CYS:HB3	2.48	0.49
1:C:1:GLN:HG3	4:C:290:HOH:O	2.12	0.49
2:D:155:LEU:CD1	2:D:166:LEU:HD13	2.43	0.49
1:A:2:ASP:HB2	1:A:3:PRO:HD2	1.94	0.49
1:A:187:ASP:OD1	1:A:187:ASP:N	2.37	0.49
1:A:77:TYR:C	1:A:98:PHE:HZ	2.21	0.49
2:B:31:ASN:HD22	2:B:51:ASN:HB3	1.78	0.49
2:D:197:THR:HA	2:D:218:SER:O	2.11	0.49
2:B:15:THR:HA	2:B:54:TRP:O	2.12	0.48
1:C:249:LEU:N	2:D:7:ILE:HD11	2.28	0.48
1:C:45:GLU:HG2	1:C:46:LYS:HG3	1.95	0.48
1:C:213:PRO:HB3	2:D:12:TYR:CD2	2.48	0.48
2:D:187:ARG:HD3	2:D:192:THR:O	2.12	0.48
2:B:161:GLY:C	2:B:162:ASN:HD22	2.20	0.48
1:C:172:LYS:HE3	1:C:172:LYS:HA	1.95	0.48
2:D:16:VAL:HB	2:D:139:GLY:CA	2.43	0.48
2:B:18:ILE:O	2:B:26:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LYS:CE	1:C:142:SER:HB3	2.43	0.48
1:A:146:ASP:O	1:A:150:ILE:HG13	2.14	0.48
1:C:46:LYS:H	1:C:47:PRO:CD	2.27	0.48
1:C:187:ASP:OD1	1:C:187:ASP:N	2.45	0.48
1:C:16:TYR:CE2	1:C:174:VAL:HB	2.48	0.48
1:A:209:GLN:NE2	2:B:97:ILE:H	2.12	0.48
2:B:39:ILE:HG12	2:B:81:MET:HA	1.95	0.48
2:B:71:THR:CG2	2:B:125:VAL:HG11	2.31	0.48
1:C:78:ARG:HD2	1:C:98:PHE:CD1	2.49	0.48
1:A:78:ARG:CB	1:A:98:PHE:CE1	2.82	0.48
2:D:224:LYS:HB2	2:D:226:ASP:OD1	2.14	0.48
1:A:77:TYR:C	1:A:98:PHE:CE1	2.92	0.48
1:A:221:VAL:HG22	2:B:267:PHE:O	2.14	0.48
2:D:104:ILE:HB	2:D:111:VAL:HG12	1.96	0.48
2:D:108:SER:HB2	2:D:110:LEU:HD13	1.94	0.48
2:B:32:ALA:HB3	2:B:37:ASN:OD1	2.14	0.47
2:B:113:SER:OG	2:B:134:GLN:HG2	2.13	0.47
1:C:172:LYS:HE3	1:C:172:LYS:N	2.29	0.47
2:B:177:GLN:O	2:B:189:VAL:HG23	2.14	0.47
1:C:132:ALA:O	1:C:135:GLN:HB3	2.13	0.47
2:D:71:THR:HG23	2:D:95:TRP:HZ2	1.78	0.47
2:D:154:LYS:HG3	2:D:154:LYS:O	2.15	0.47
1:A:76:ALA:CB	1:A:98:PHE:CE2	2.97	0.47
2:B:251:ILE:C	2:B:251:ILE:HD12	2.39	0.47
2:B:111:VAL:CG1	2:B:128:ASN:HB2	2.45	0.47
1:C:58:SER:C	1:C:60:THR:N	2.72	0.47
1:C:112:TYR:CE1	1:C:123:ARG:HD3	2.49	0.47
1:C:222:ARG:O	1:C:223:GLN:HB2	2.15	0.47
2:D:127:LYS:NZ	2:D:127:LYS:HB3	2.29	0.47
2:D:150:ALA:HA	2:D:156:CYS:HA	1.96	0.47
1:A:172:LYS:HD3	1:A:172:LYS:C	2.39	0.47
2:B:165:TRP:CD2	2:B:248:LYS:HB3	2.50	0.47
1:C:161:VAL:O	1:C:164:ALA:HB3	2.14	0.47
2:B:73:GLY:CA	2:B:78:ASN:HD22	2.27	0.47
2:B:170:ASP:H	2:B:176:GLN:NE2	2.02	0.47
1:C:17:ASN:O	1:C:21:ASP:OD2	2.33	0.47
1:C:206:HIS:HB3	1:C:213:PRO:HG2	1.97	0.47
2:D:253:TRP:CG	2:D:254:PRO:HD2	2.49	0.47
1:A:40:ASP:O	1:A:43:THR:HB	2.15	0.46
1:A:189:SER:HA	1:A:219:ILE:O	2.15	0.46
2:B:67:LYS:HB2	2:B:82:ILE:CD1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:GLN:CG	4:C:290:HOH:O	2.62	0.46
1:C:204:VAL:HG13	1:C:231:LEU:CD1	2.44	0.46
2:D:161:GLY:C	2:D:162:ASN:HD22	2.24	0.46
1:C:87:ARG:HB2	1:C:106:LEU:O	2.15	0.46
1:C:205:GLN:NE2	1:C:245:VAL:H	2.13	0.46
1:C:127:SER:HA	1:C:185:GLN:HG2	1.97	0.46
1:C:129:GLY:C	1:C:160:MET:HE1	2.40	0.46
2:D:42:TRP:CE3	2:D:119:MET:HG2	2.49	0.46
2:D:206:THR:HG21	2:D:249:GLN:NE2	2.30	0.46
2:B:127:LYS:NZ	2:B:127:LYS:HB3	2.31	0.46
1:C:154:LEU:O	1:C:158:ILE:HG13	2.15	0.46
2:B:253:TRP:CG	2:B:254:PRO:HD2	2.50	0.46
2:D:246:SER:C	2:D:248:LYS:H	2.23	0.46
1:C:209:GLN:HE22	2:D:97:ILE:H	1.63	0.46
2:D:24:LEU:HD21	2:D:119:MET:HE2	1.98	0.46
1:A:249:LEU:HB3	2:B:7:ILE:CD1	2.46	0.46
2:D:152:PHE:HD1	2:D:152:PHE:N	2.12	0.46
1:A:249:LEU:HD23	1:A:250:ASN:CA	2.45	0.45
2:B:16:VAL:HA	2:B:140:ASN:OD1	2.16	0.45
1:C:31:LEU:HD12	1:C:35:ILE:C	2.41	0.45
1:A:77:TYR:N	1:A:98:PHE:HZ	2.15	0.45
1:C:8:THR:HA	1:C:11:ALA:HB2	1.97	0.45
2:D:63:ARG:HG2	2:D:68:CYS:SG	2.56	0.45
1:A:88:ASN:HB2	1:A:109:ASP:CB	2.46	0.45
2:B:150:ALA:O	2:B:263:TRP:HA	2.16	0.45
1:C:71:ASN:OD1	1:C:73:TYR:HB2	2.17	0.45
1:A:78:ARG:CA	1:A:98:PHE:HE1	2.29	0.45
2:D:97:ILE:HD12	2:D:103:ILE:CD1	2.46	0.45
2:B:153:PHE:O	2:B:154:LYS:C	2.58	0.45
2:D:104:ILE:HA	2:D:111:VAL:HA	1.99	0.45
2:D:247:LEU:O	2:D:248:LYS:C	2.59	0.45
1:A:83:SER:HB3	1:A:98:PHE:CD1	2.52	0.45
2:B:162:ASN:HD22	2:B:162:ASN:N	2.15	0.45
2:D:58:SER:C	2:D:60:LYS:H	2.25	0.45
2:D:147:THR:OG1	2:D:148:SER:N	2.50	0.45
1:C:86:PHE:CE2	1:C:115:LEU:HD21	2.51	0.45
1:A:158:ILE:O	1:A:162:ALA:HB3	2.17	0.44
1:A:179:SER:CB	2:B:154:LYS:HG2	2.44	0.44
1:C:57:TYR:CD2	1:C:57:TYR:O	2.70	0.44
1:C:58:SER:O	1:C:60:THR:N	2.49	0.44
2:D:240:VAL:O	2:D:241:LYS:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:256:THR:N	2:D:261:GLN:HE22	2.08	0.44
2:B:221:TRP:CZ3	2:B:231:ASN:HB2	2.52	0.44
1:C:76:ALA:HB2	1:C:85:PHE:HA	1.99	0.44
2:D:157:MET:HE1	2:D:196:LEU:HD13	2.00	0.44
2:D:178:TRP:HE3	2:D:186:ILE:HG22	1.82	0.44
2:D:196:LEU:HA	2:D:208:VAL:O	2.18	0.44
1:C:222:ARG:HH22	2:D:146:VAL:HG12	1.82	0.44
2:B:41:LEU:HD21	2:B:136:TRP:CZ3	2.52	0.44
1:C:176:ILE:HG22	2:D:154:LYS:HA	2.00	0.44
1:C:179:SER:HB3	2:D:154:LYS:HD3	1.98	0.44
1:C:202:ARG:HG3	1:C:245:VAL:HG11	1.99	0.44
2:D:155:LEU:HD13	2:D:166:LEU:HB3	1.98	0.44
2:B:6:LYS:HB3	2:B:6:LYS:HZ3	1.83	0.44
1:C:205:GLN:HE22	1:C:245:VAL:H	1.64	0.44
2:D:150:ALA:HB2	2:D:156:CYS:SG	2.58	0.44
2:B:111:VAL:HG13	2:B:128:ASN:HB2	2.00	0.44
1:C:200:LEU:O	1:C:204:VAL:HG23	2.17	0.44
2:D:49:GLU:HB2	2:D:51:ASN:OD1	2.18	0.44
2:B:83:TYR:HD1	2:B:88:ALA:HB2	1.80	0.43
1:C:4:ILE:HG22	1:C:4:ILE:O	2.17	0.43
1:C:6:PHE:HB2	1:C:19:PHE:CE1	2.53	0.43
2:B:160:HIS:CD2	2:B:165:TRP:CE2	3.05	0.43
2:D:195:CYS:O	2:D:197:THR:HG22	2.18	0.43
2:D:232:LEU:H	2:D:232:LEU:HD22	1.84	0.43
1:C:5:LYS:HG2	1:C:6:PHE:N	2.34	0.43
2:D:57:LYS:HE2	2:D:63:ARG:HH11	1.83	0.43
1:A:112:TYR:O	1:A:116:GLU:HG3	2.18	0.43
1:C:138:LYS:HE2	1:C:142:SER:HB3	2.01	0.43
1:C:164:ALA:HA	1:C:170:VAL:HB	2.00	0.43
2:D:188:PRO:HG2	2:D:209:MET:HE1	1.99	0.43
2:D:6:LYS:HG2	2:D:7:ILE:N	2.34	0.43
2:D:255:TYR:HA	2:D:261:GLN:HE22	1.83	0.43
1:A:78:ARG:N	1:A:98:PHE:HE1	2.17	0.43
1:A:51:VAL:CG1	1:A:69:LEU:HD13	2.47	0.42
1:C:40:ASP:C	1:C:42:SER:N	2.77	0.42
1:C:196:THR:O	1:C:196:THR:HG22	2.19	0.42
2:D:57:LYS:HG3	2:D:63:ARG:HD2	2.01	0.42
2:D:169:CYS:HA	2:D:176:GLN:NE2	2.21	0.42
1:C:155:ILE:CG2	1:C:159:GLN:HE21	2.32	0.42
2:D:207:ILE:CD1	2:D:250:ILE:HG22	2.45	0.42
2:B:235:ASP:O	2:B:235:ASP:CG	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:TRP:CH2	1:C:243:LEU:HD23	2.54	0.42
2:D:244:ASP:HB3	2:D:247:LEU:HD12	2.01	0.42
2:D:115:GLU:HG2	4:D:271:HOH:O	2.19	0.42
2:D:175:GLU:CD	2:D:175:GLU:H	2.26	0.42
1:A:179:SER:HB2	2:B:154:LYS:HB3	2.01	0.42
1:C:6:PHE:HB2	1:C:19:PHE:CD1	2.55	0.42
2:D:17:ARG:HG2	2:D:53:LEU:HD23	2.02	0.42
1:C:78:ARG:HB2	1:C:98:PHE:CZ	2.55	0.42
1:C:220:ASN:C	1:C:220:ASN:HD22	2.27	0.42
2:D:41:LEU:HD23	2:D:41:LEU:HA	1.94	0.42
2:D:123:LEU:HD22	2:D:136:TRP:HH2	1.84	0.42
2:B:241:LYS:O	2:B:242:SER:C	2.63	0.41
2:B:241:LYS:HD3	2:B:247:LEU:HD13	2.01	0.41
1:C:130:LEU:HB2	1:C:178:LEU:HG	2.02	0.41
1:C:95:THR:O	1:C:95:THR:HG22	2.19	0.41
1:C:220:ASN:ND2	1:C:220:ASN:C	2.78	0.41
2:D:45:LYS:NZ	2:D:51:ASN:HD21	2.19	0.41
2:D:113:SER:OG	2:D:134:GLN:HG2	2.20	0.41
2:B:115:GLU:OE1	2:B:126:GLN:HG3	2.20	0.41
2:D:37:ASN:OD1	2:D:38:PRO:HD2	2.20	0.41
1:C:152:ARG:HH11	1:C:152:ARG:HG2	1.85	0.41
1:C:173:LEU:HD13	1:C:176:ILE:CD1	2.47	0.41
2:D:246:SER:C	2:D:248:LYS:N	2.78	0.41
2:D:6:LYS:HG2	2:D:7:ILE:H	1.86	0.41
2:B:197:THR:HA	2:B:218:SER:O	2.21	0.41
2:D:79:TYR:HA	2:D:124:THR:HA	2.03	0.41
2:B:91:GLU:HA	2:B:91:GLU:OE2	2.21	0.41
1:C:139:PHE:CE2	1:C:150:ILE:HG13	2.52	0.41
1:C:172:LYS:O	1:C:176:ILE:HG23	2.21	0.41
2:B:200:GLU:OE1	2:B:202:LYS:HD3	2.21	0.41
2:D:170:ASP:H	2:D:176:GLN:NE2	2.18	0.41
2:B:45:LYS:HE3	2:B:52:GLN:CD	2.46	0.41
2:B:73:GLY:HA3	2:B:78:ASN:ND2	2.36	0.41
2:B:74:TYR:OH	2:B:91:GLU:HB2	2.20	0.41
2:B:202:LYS:HB2	2:B:202:LYS:HZ3	1.86	0.41
1:C:249:LEU:N	2:D:7:ILE:CD1	2.84	0.41
2:D:59:ASP:CG	2:D:61:THR:HG23	2.46	0.41
2:D:104:ILE:HG12	2:D:105:ASN:N	2.35	0.41
2:B:209:MET:O	2:B:210:MET:HG2	2.21	0.41
1:C:84:PHE:CD1	1:C:84:PHE:N	2.89	0.41
1:C:176:ILE:HA	2:D:154:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ARG:O	1:C:203:ALA:C	2.64	0.41
1:A:187:ASP:HB2	1:A:188:PRO:HD2	2.03	0.40
2:D:24:LEU:CD2	2:D:119:MET:HE2	2.52	0.40
1:A:124:GLN:HG3	1:A:125:ARG:HG2	2.02	0.40
1:C:206:HIS:ND1	2:D:8:CYS:HB3	2.37	0.40
2:D:162:ASN:HA	2:D:209:MET:HB2	2.03	0.40
1:C:85:PHE:CZ	1:C:94:SER:HA	2.55	0.40
2:D:21:ARG:NH1	2:D:117:SER:HA	2.37	0.40
2:D:162:ASN:HD22	2:D:162:ASN:N	2.18	0.40
2:D:203:GLN:HG2	2:D:253:TRP:CZ3	2.57	0.40
1:C:202:ARG:HG2	1:C:206:HIS:CD2	2.56	0.40
2:D:75:ALA:HA	2:D:76:PRO:HD3	1.98	0.40
2:D:187:ARG:HA	2:D:188:PRO:HD3	1.94	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	248/258 (96%)	235 (95%)	10 (4%)	3 (1%)	10	23
1	C	248/258 (96%)	208 (84%)	35 (14%)	5 (2%)	6	12
2	B	261/267 (98%)	241 (92%)	19 (7%)	1 (0%)	30	51
2	D	261/267 (98%)	230 (88%)	28 (11%)	3 (1%)	11	25
All	All	1018/1050 (97%)	914 (90%)	92 (9%)	12 (1%)	10	23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	215	ASN
1	A	249	LEU

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Mol	Chain	Res	Type
1	C	249	LEU
2	B	153	PHE
1	C	4	ILE
1	C	46	LYS
1	C	59	ASP
2	D	29	SER
1	A	142	SER
1	A	144	ALA
2	D	153	PHE
2	D	247	LEU

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	218/225 (97%)	202 (93%)	16 (7%)	13	29
1	C	218/225 (97%)	206 (94%)	12 (6%)	19	41
2	B	229/233 (98%)	213 (93%)	16 (7%)	14	31
2	D	229/233 (98%)	220 (96%)	9 (4%)	28	55
All	All	894/916 (98%)	841 (94%)	53 (6%)	18	38

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	38	LEU
1	A	45	GLU
1	A	53	VAL
1	A	69	LEU
1	A	97	LEU
1	A	121	GLN
1	A	153	THR
1	A	173	LEU
1	A	176	ILE
1	A	200	LEU

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Mol	Chain	Res	Type
1	A	214	GLN
1	A	220	ASN
1	A	221	VAL
1	A	241	LEU
1	A	249	LEU
2	B	6	LYS
2	B	21	ARG
2	B	30	ASP
2	B	48	LEU
2	B	49	GLU
2	B	81	MET
2	B	127	LYS
2	B	152	PHE
2	B	154	LYS
2	B	197	THR
2	B	202	LYS
2	B	210	MET
2	B	222	VAL
2	B	224	LYS
2	B	232	LEU
2	B	239	ASP
1	C	57	TYR
1	C	70	THR
1	C	138	LYS
1	C	148	GLU
1	C	153	THR
1	C	172	LYS
1	C	173	LEU
1	C	178	LEU
1	C	205	GLN
1	C	209	GLN
1	C	220	ASN
1	C	249	LEU
2	D	21	ARG
2	D	49	GLU
2	D	102	THR
2	D	127	LYS
2	D	152	PHE
2	D	198	CYS
2	D	209	MET
2	D	222	VAL
2	D	242	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	102	GLN
1	A	185	GLN
1	A	209	GLN
1	A	214	GLN
1	A	220	ASN
1	A	223	GLN
2	B	31	ASN
2	B	35	ASN
2	B	37	ASN
2	B	78	ASN
2	B	162	ASN
2	B	176	GLN
2	B	177	GLN
2	B	190	GLN
2	B	203	GLN
2	B	214	ASN
2	B	261	GLN
1	C	17	ASN
1	C	18	GLN
1	C	49	GLN
1	C	88	ASN
1	C	124	GLN
1	C	159	GLN
1	C	185	GLN
1	C	205	GLN
1	C	206	HIS
1	C	209	GLN
1	C	214	GLN
1	C	215	ASN
1	C	220	ASN
1	C	250	ASN
2	D	35	ASN
2	D	51	ASN
2	D	78	ASN
2	D	162	ASN
2	D	176	GLN
2	D	177	GLN
2	D	190	GLN
2	D	194	ASN
2	D	203	GLN

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Mol	Chain	Res	Type
2	D	258	ASN
2	D	261	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 ⓘ

3 ligands are modelled in this entry.

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	$\# Z > 2$
3	NAG	B	269	2	14,14,15	0.62	0	17,19,21	0.82	0
3	NAG	B	268	2	14,14,15	0.66	0	17,19,21	1.08	1 (5%)
3	NAG	D	268	2	14,14,15	0.69	0	17,19,21	0.79	0

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
3	NAG	B	269	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	268	2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	D	268	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	268	NAG	C1-O5-C5	2.68	115.78	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	268	NAG	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	268	NAG	C8-C7-N2-C2
3	B	268	NAG	O7-C7-N2-C2
3	B	269	NAG	C8-C7-N2-C2
3	D	268	NAG	C8-C7-N2-C2
3	D	268	NAG	O7-C7-N2-C2
3	B	269	NAG	O7-C7-N2-C2
3	B	268	NAG	C4-C5-C6-O6
3	B	268	NAG	O5-C5-C6-O6
3	B	269	NAG	C4-C5-C6-O6
3	B	269	NAG	O5-C5-C6-O6
3	D	268	NAG	C4-C5-C6-O6
3	D	268	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	250/258 (96%)	-0.73	2 (0%) 82 80	25, 30, 49, 91	0
1	C	250/258 (96%)	0.48	14 (5%) 30 24	40, 59, 77, 99	0
2	B	263/267 (98%)	-0.73	1 (0%) 88 86	25, 35, 53, 83	0
2	D	263/267 (98%)	0.24	6 (2%) 61 55	49, 64, 78, 85	0
All	All	1026/1050 (97%)	-0.19	23 (2%) 62 57	25, 49, 75, 99	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	PHE	7.2
2	D	207	ILE	4.4
1	C	148	GLU	4.3
1	C	20	ILE	3.7
2	D	80	VAL	3.4
1	C	172	LYS	3.2
1	C	143	GLY	3.1
1	A	250	ASN	3.0
1	C	46	LYS	2.9
2	D	7	ILE	2.9
1	C	144	ALA	2.7
1	C	249	LEU	2.6
1	C	176	ILE	2.5
1	C	250	ASN	2.4
2	D	28	VAL	2.3
1	C	97	LEU	2.3
1	C	61	VAL	2.2
1	C	229	SER	2.1
2	D	151	GLY	2.1
1	C	44	VAL	2.1
1	C	228	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	154	LYS	2.1
2	D	32	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](#)

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
3	NAG	D	268	14/15	0.88	0.10	64,67,73,74	0
3	NAG	B	268	14/15	0.95	0.07	37,43,48,62	0
3	NAG	B	269	14/15	0.96	0.06	35,38,48,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.