Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2020 – 05:29 PM BST

PDB ID	:	1HCU
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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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.
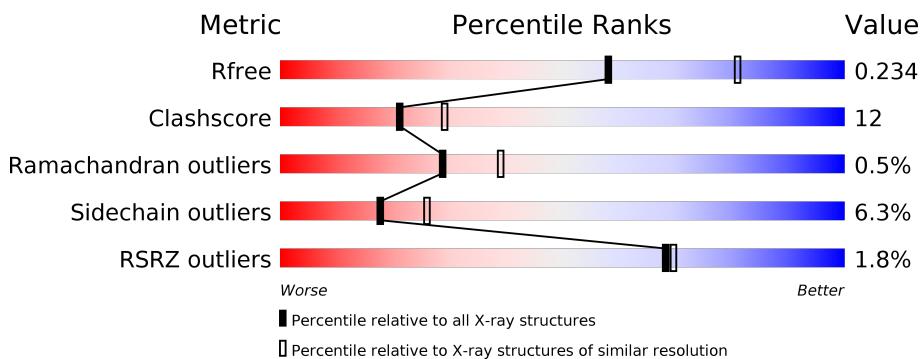
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 on 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 <=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	72% ... 22% ..
1	B	503	79% ... 16% ..
1	C	503	73% ... 21% ..
1	D	503	67% ... 26% ..
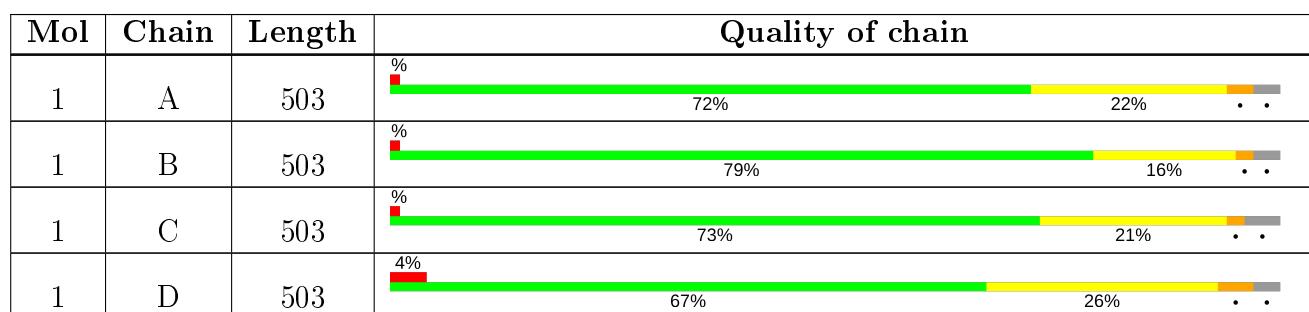
2 Entry composition (i)

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 3718	C 2366	N 612	O 735	S 5	0	0	0
1	B	489	Total 3730	C 2372	N 616	O 737	S 5	0	0	0
1	C	485	Total 3697	C 2353	N 608	O 731	S 5	0	0	0
1	D	486	Total 3701	C 2355	N 612	O 729	S 5	0	0	0

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

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

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is water.

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

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

• Molecule 1: ALPHA-1,2-MANNOSIDASE

• Molecule 1: ALPHA-1,2-MANNOSIDASE

• Molecule 1: ALPHA-1,2-MANNOSIDASE

Chain D:
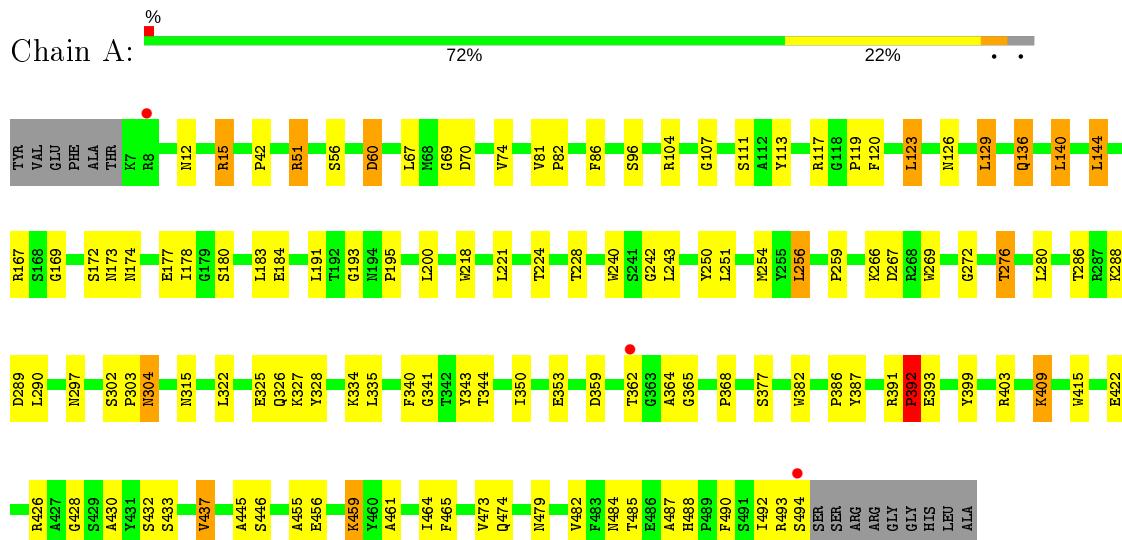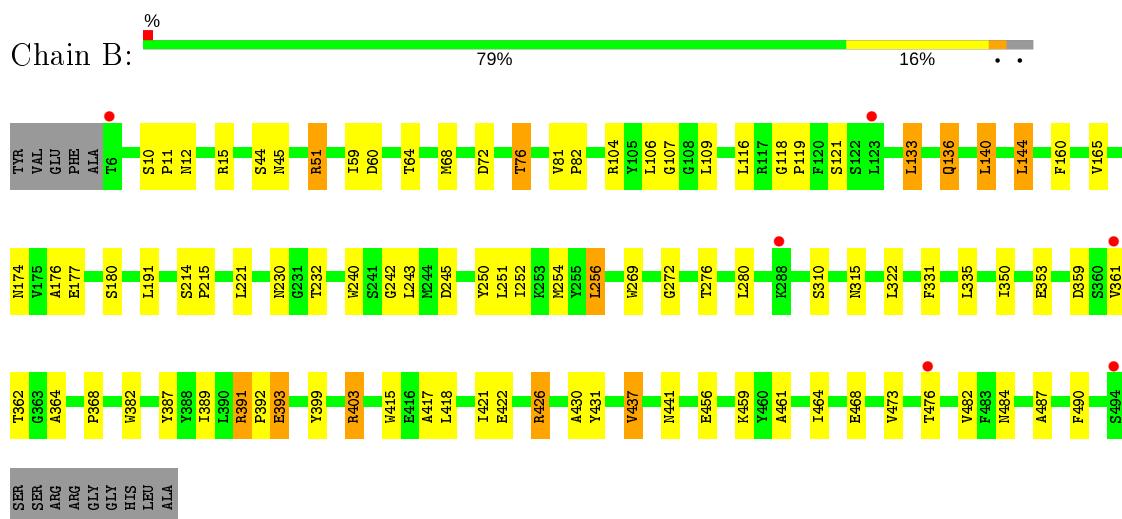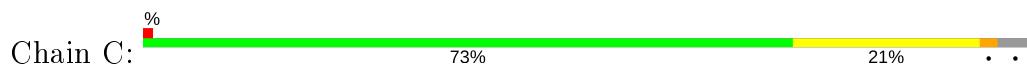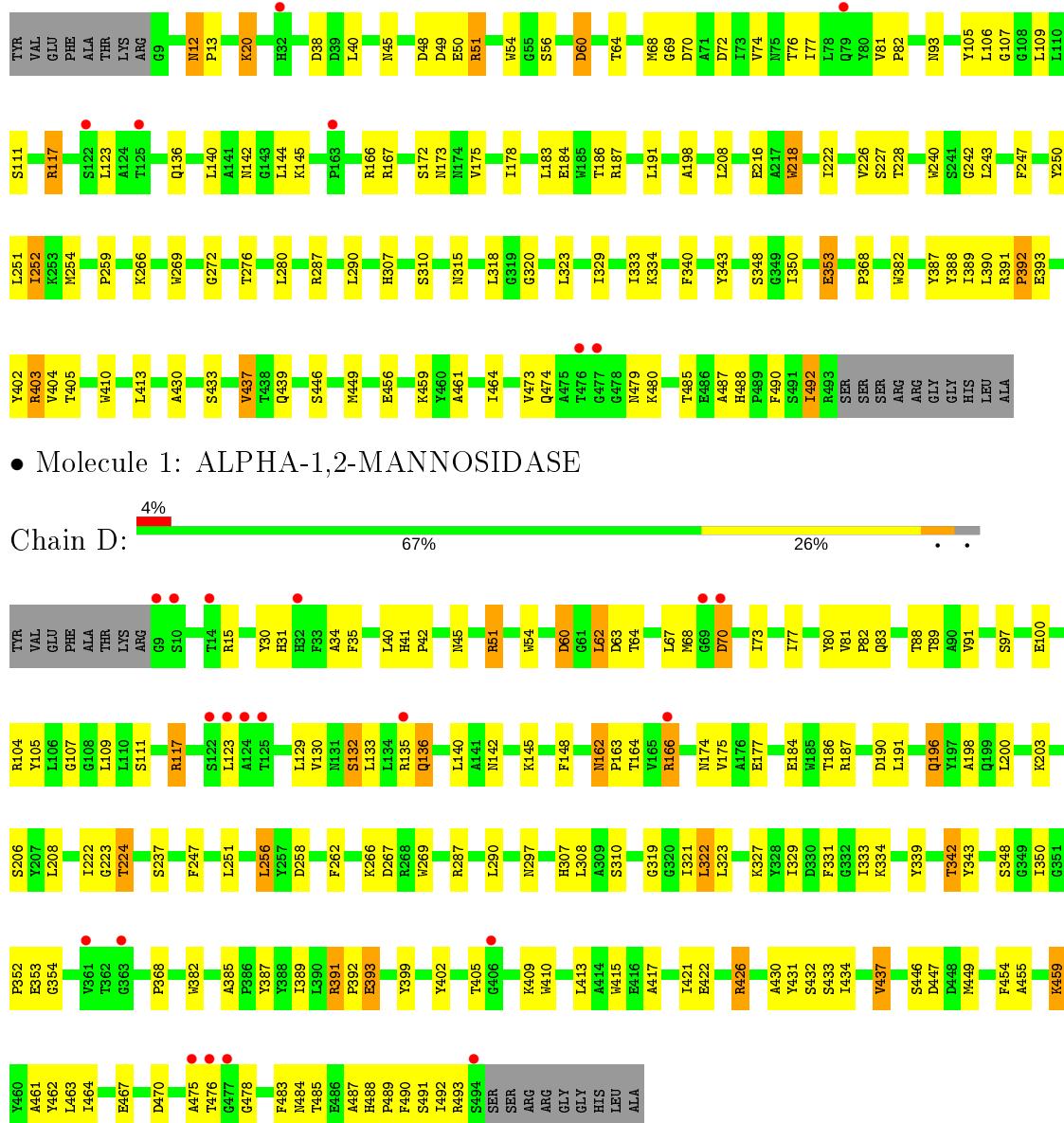
4 Data and refinement statistics (i)

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 19.97 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.37) 98.9 (19.97-2.37)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [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)	0.34 , 53.6	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.39	0/3823	0.60	0/5217
1	B	0.39	0/3835	0.60	0/5233
1	C	0.36	0/3802	0.57	0/5190
1	D	0.34	0/3806	0.56	0/5195
All	All	0.37	0/15266	0.58	0/20835

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3718	0	3485	90	0
1	B	3730	0	3501	66	0
1	C	3697	0	3464	88	0
1	D	3701	0	3473	105	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	350	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 (350) 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:H	1:C:252:ILE:HD13	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: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:64:THR:HG22	1:D:68:MET:HE1	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:117:ARG:HB3	1:D:117:ARG:HH21	1.57	0.69
1:C:474:GLN:N	1:C:479:ASN:HD21	1.90	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
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:107:GLY:HA2	1:D:490:PHE:HZ	1.69	0.58
1:D:136:GLN:NE2	1:D:136:GLN:HA	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:THR:HG23	1:D:91:VAL:O	2.02	0.58
1:C:252:ILE:HG23	1:C:269:TRP:CG	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: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: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
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: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:C:334:LYS:HZ3	1:C:334:LYS:HB3	1.71	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:C:334:LYS:CB	1:C:334:LYS:HZ3	2.19	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:64:THR:O	1:D:68:MET:HE2	2.07	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:107:GLY:HA2	1:C:490:PHE:HZ	1.72	0.53
1:C:93:ASN:ND2	1:C:166:ARG:HH21	2.05	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:H	1:A:304:ASN:HD22	1.57	0.53
1:B:276:THR:HB	1:B:280:LEU:HD12	1.91	0.53
1:B:140:LEU:HD22	1:B:144:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:VAL:HB	1:B:82:PRO:HD3	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:C:40:LEU:HD23	1:C:449:MET:HE2	1.91	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:HH11	1:A:104:ARG:HG3	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:331:PHE:HA	1:D:334:LYS:HE3	1.92	0.52
1:D:321:ILE:HG23	1:D:475:ALA:O	2.10	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
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: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:D:184:GLU:CD	1:D:184:GLU:H	2.13	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:C:136:GLN:HE21	1:C:136:GLN:HA	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:NE	1:C:51:ARG:HA	2.26	0.50
1:D:148:PHE:HB3	1:D:200:LEU:HD12	1.93	0.50
1:C:252:ILE:H	1:C:252:ILE:CD1	2.12	0.50
1:C:250:TYR:O	1:C:254:MET:HG2	2.11	0.50
1:A:325:GLU:OE1	1:A:327:LYS:HE3	2.12	0.50
1:D:135:ARG:HA	1:D:135:ARG:CZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:D:51:ARG:HA	1:D:51:ARG:NE	2.28	0.49
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:HD3	1:A:409:LYS:O	2.13	0.48
1:C:117:ARG:NH1	1:C:117:ARG:HB3	2.18	0.48
1:C:340:PHE:CE2	1:C:413:LEU:HG	2.48	0.48
1:A:286:THR:HG21	1:A:377:SER:HA	1.96	0.48
1:C:340:PHE:O	1:C:343:TYR:HB2	2.14	0.47
1:C:72:ASP:O	1:C:76:THR:HG23	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: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:C:81:VAL:HB	1:C:82:PRO:HD3	1.95	0.47
1:D:203:LYS:O	1:D:206:SER:HB3	2.14	0.47
1:D:89:THR:HG21	4:D:2059:HOH:O	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:D:64:THR:HG22	1:D:68:MET:CE	2.41	0.47
1:D:162:ASN:HD22	1:D:162:ASN:C	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:SER:HA	1:B:250:TYR:CD1	2.50	0.46
1:B:51:ARG:HA	1:B:51:ARG:NE	2.31	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:174:ASN:HD21	1:B:177:GLU:H	1.63	0.46
1:B:44:SER:O	1:B:45:ASN:HB2	2.15	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:167:ARG:HH21	1:A:169:GLY:HA2	1.81	0.46
1:A:42:PRO:CG	1:A:432:SER:HB2	2.46	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:184:GLU:H	1:A:184:GLU:CD	2.19	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:D:449:MET:HE3	1:D:454:PHE:CZ	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:12:ASN:C	1:C:12:ASN:HD22	2.21	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:A:359:ASP:CG	1:A:362:THR:HG22	2.39	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:368:PRO:HG3	1:D:382:TRP:CE3	2.53	0.43
1:D:41:HIS:HB3	1:D:447:ASP:OD2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:117:ARG:HH11	1:C:117:ARG:CB	2.20	0.42
1:C:12:ASN:HA	1:C:13:PRO:HD2	1.87	0.42
1:C:389:ILE:HD11	1:C:391:ARG:CZ	2.50	0.42
1:C:64:THR:OG1	1:C:459:LYS:HE2	2.18	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:H3	2:C:601:NAG:H83	2.01	0.42
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:C:492:ILE:HD13	1:C:492:ILE:N	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:HA	1:B:45:ASN:HD22	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:269:TRP:HE1	1:C:315:ASN:ND2	2.18	0.41
1:C:51:ARG:HG2	1:C:56:SER:HB3	2.02	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:D:54:TRP:HB2	1:D:105:TYR:CZ	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:310:SER:HG	1:B:393:GLU:HB2	1.86	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:403:ARG:HG3	1:A:473:VAL:CG2	2.51	0.41
1:B:256:LEU:HG	1:B:322:LEU:HD21	2.03	0.41
1:D:348:SER:OG	1:D:437:VAL:HG22	2.21	0.41
1:D:45:ASN:HA	1:D:45:ASN:HD22	1.65	0.41
1:A:104:ARG:HG3	1:A:104:ARG:NH1	2.34	0.41
1:D:187:ARG:NH2	1:D:491:SER:OG	2.54	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: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:O	1:B:476:THR:HG22	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:D:80:TYR:HA	1:D:83:GLN:OE1	2.21	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%)	34	46
1	B	487/503 (97%)	460 (94%)	25 (5%)	2 (0%)	34	46
1	C	483/503 (96%)	454 (94%)	28 (6%)	1 (0%)	47	61
1	D	484/503 (96%)	448 (93%)	32 (7%)	4 (1%)	19	27
All	All	1940/2012 (96%)	1816 (94%)	115 (6%)	9 (0%)	29	39

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 (i)

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%)	365 (94%)	25 (6%)	17	25
1	B	392/404 (97%)	371 (95%)	21 (5%)	22	33
1	C	388/404 (96%)	366 (94%)	22 (6%)	20	30
1	D	388/404 (96%)	358 (92%)	30 (8%)	13	18
All	All	1558/1616 (96%)	1460 (94%)	98 (6%)	18	26

All (98) 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	191	LEU
1	A	200	LEU
1	A	251	LEU
1	A	256	LEU
1	A	276	THR
1	A	288	LYS
1	A	290	LEU
1	A	297	ASN
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	484	ASN
1	A	485	THR
1	B	51	ARG
1	B	60	ASP
1	B	76	THR
1	B	109	LEU
1	B	133	LEU
1	B	136	GLN
1	B	140	LEU
1	B	144	LEU

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Mol	Chain	Res	Type
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	403	ARG
1	B	418	LEU
1	B	426	ARG
1	B	437	VAL
1	B	459	LYS
1	B	468	GLU
1	B	484	ASN
1	C	12	ASN
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	167	ARG
1	C	183	LEU
1	C	208	LEU
1	C	218	TRP
1	C	227	SER
1	C	252	ILE
1	C	318	LEU
1	C	353	GLU
1	C	392	PRO
1	C	403	ARG
1	C	437	VAL
1	C	485	THR
1	C	492	ILE
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

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Mol	Chain	Res	Type
1	D	132	SER
1	D	136	GLN
1	D	140	LEU
1	D	162	ASN
1	D	166	ARG
1	D	191	LEU
1	D	196	GLN
1	D	224	THR
1	D	251	LEU
1	D	256	LEU
1	D	297	ASN
1	D	322	LEU
1	D	327	LYS
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	470	ASP
1	D	484	ASN
1	D	485	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) 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	136	GLN
1	A	174	ASN
1	A	199	GLN
1	A	202	GLN
1	A	234	GLN
1	A	297	ASN
1	A	299	GLN
1	A	304	ASN
1	A	315	ASN
1	A	472	GLN
1	A	479	ASN

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Mol	Chain	Res	Type
1	B	24	GLN
1	B	28	ASN
1	B	45	ASN
1	B	52	ASN
1	B	136	GLN
1	B	174	ASN
1	B	199	GLN
1	B	202	GLN
1	B	264	HIS
1	B	315	ASN
1	B	324	ASN
1	B	441	ASN
1	B	474	GLN
1	C	12	ASN
1	C	24	GLN
1	C	28	ASN
1	C	45	ASN
1	C	52	ASN
1	C	79	GLN
1	C	93	ASN
1	C	136	GLN
1	C	196	GLN
1	C	202	GLN
1	C	264	HIS
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	28	ASN
1	D	45	ASN
1	D	52	ASN
1	D	75	ASN
1	D	136	GLN
1	D	162	ASN
1	D	174	ASN
1	D	196	GLN
1	D	202	GLN
1	D	264	HIS
1	D	297	ASN
1	D	307	HIS

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Mol	Chain	Res	Type
1	D	326	GLN
1	D	411	GLN
1	D	439	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	0.48	0	17,19,21	0.61	0
2	NAG	B	600	1	14,14,15	0.47	0	17,19,21	0.64	0
2	NAG	A	602	1	14,14,15	0.49	0	17,19,21	0.63	0
2	NAG	D	600	1	14,14,15	0.53	0	17,19,21	0.58	0
2	NAG	C	601	1	14,14,15	0.62	0	17,19,21	0.83	1 (5%)
2	NAG	A	601	1	14,14,15	0.47	0	17,19,21	0.60	0
2	NAG	B	601	1	14,14,15	0.48	0	17,19,21	0.69	1 (5%)
2	NAG	B	602	1	14,14,15	0.51	0	17,19,21	0.75	1 (5%)
2	NAG	C	600	1	14,14,15	0.45	0	17,19,21	0.76	1 (5%)
2	NAG	D	602	1	14,14,15	0.46	0	17,19,21	0.73	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	B	600	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	6/6/23/26	0/1/1/1
2	NAG	D	600	1	-	2/6/23/26	0/1/1/1
2	NAG	C	601	1	-	4/6/23/26	0/1/1/1
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1	-	2/6/23/26	0/1/1/1
2	NAG	B	602	1	-	4/6/23/26	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(^{o})	Ideal(^{o})
2	D	602	NAG	C2-N2-C7	-2.41	119.47	122.90
2	C	600	NAG	C2-N2-C7	-2.38	119.51	122.90
2	C	601	NAG	C2-N2-C7	-2.27	119.67	122.90
2	B	602	NAG	C2-N2-C7	-2.21	119.75	122.90
2	B	601	NAG	C2-N2-C7	-2.04	120.00	122.90

There are no chirality outliers.

All (27) 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	C	601	NAG	C8-C7-N2-C2
2	C	601	NAG	O7-C7-N2-C2
2	B	602	NAG	C8-C7-N2-C2
2	B	602	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

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Mol	Chain	Res	Type	Atoms
2	C	600	NAG	C8-C7-N2-C2
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	B	601	NAG	C8-C7-N2-C2
2	A	602	NAG	C1-C2-N2-C7
2	C	601	NAG	C1-C2-N2-C7
2	B	601	NAG	O7-C7-N2-C2
2	C	600	NAG	O7-C7-N2-C2
2	C	600	NAG	C4-C5-C6-O6
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
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 (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	488/503 (97%)	-0.23	3 (0%)	89	89	7, 15, 30, 45	0
1	B	489/503 (97%)	-0.32	6 (1%)	79	80	6, 14, 26, 47	0
1	C	485/503 (96%)	-0.08	7 (1%)	75	77	9, 20, 34, 56	0
1	D	486/503 (96%)	0.23	19 (3%)	39	42	12, 25, 44, 61	0
All	All	1948/2012 (96%)	-0.10	35 (1%)	68	70	6, 18, 36, 61	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	123	LEU	5.0
1	D	476	THR	4.6
1	D	9	GLY	4.3
1	B	476	THR	3.9
1	B	6	THR	3.7
1	B	494	SER	3.7
1	D	69	GLY	3.7
1	D	125	THR	3.6
1	A	8	ARG	3.4
1	D	122	SER	3.4
1	D	494	SER	3.1
1	D	361	VAL	3.0
1	C	476	THR	3.0
1	C	477	GLY	3.0
1	A	494	SER	2.9
1	C	125	THR	2.9
1	C	79	GLN	2.9
1	D	124	ALA	2.8
1	D	135	ARG	2.8
1	C	163	PRO	2.8
1	D	477	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	123	LEU	2.6
1	C	122	SER	2.6
1	D	363	GLY	2.6
1	D	406	GLY	2.5
1	D	70	ASP	2.5
1	C	32	HIS	2.5
1	D	475	ALA	2.3
1	D	14	THR	2.3
1	D	32	HIS	2.3
1	D	166	ARG	2.2
1	B	361	VAL	2.2
1	D	10	SER	2.1
1	A	362	THR	2.0
1	B	288	LYS	2.0

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 ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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($Å^2$)	Q<0.9
2	NAG	C	601	14/15	0.68	0.34	64,69,72,73	0
2	NAG	A	600	14/15	0.79	0.29	45,50,52,52	0
2	NAG	D	602	14/15	0.81	0.39	63,66,68,68	0
2	NAG	A	602	14/15	0.82	0.30	52,54,56,57	0
2	NAG	B	602	14/15	0.85	0.28	51,55,58,58	0
2	NAG	D	600	14/15	0.88	0.34	40,41,42,43	0
2	NAG	B	601	14/15	0.91	0.22	28,31,35,38	0
2	NAG	C	600	14/15	0.92	0.15	24,27,33,33	0
2	NAG	B	600	14/15	0.94	0.16	18,22,29,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	NAG	A	601	14/15	0.96	0.17	18,22,24,28	0
3	CA	A	1495	1/1	0.97	0.04	23,23,23,23	0
3	CA	B	1495	1/1	0.97	0.07	30,30,30,30	0
3	CA	D	1495	1/1	0.98	0.07	36,36,36,36	0
3	CA	C	1494	1/1	0.98	0.07	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.