



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:37 PM GMT

PDB ID : 3U75
Title : Structure of E230A-fructofuranosidase from Schwanniomyces occidentalis
complexed with fructosylmaltose
Authors : Sainz-Polo, M.A.; Sanz-Aparicio, J.
Deposited on : 2011-10-13
Resolution : 2.68 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

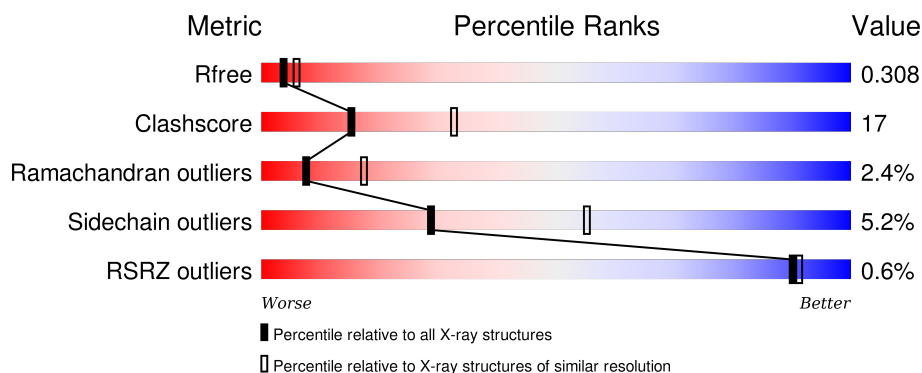
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.68 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}	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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. 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	535	 67% 26% . .
1	B	535	 70% 23% . .
1	C	535	 59% 33% . .
1	D	535	 54% 37% 5% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17209 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 Fructofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			4152	2668	680	798	6			
1	B	512	Total	C	N	O	S	0	0	0
			4152	2668	680	798	6			
1	C	512	Total	C	N	O	S	0	0	0
			4152	2668	680	798	6			
1	D	512	Total	C	N	O	S	0	0	0
			4152	2668	680	798	6			

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	5	Total	C	O	0	0
			56	30	26		
2	B	5	Total	C	O	0	0
			56	30	26		
2	C	5	Total	C	O	0	0
			56	30	26		
2	D	5	Total	C	O	0	0
			56	30	26		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

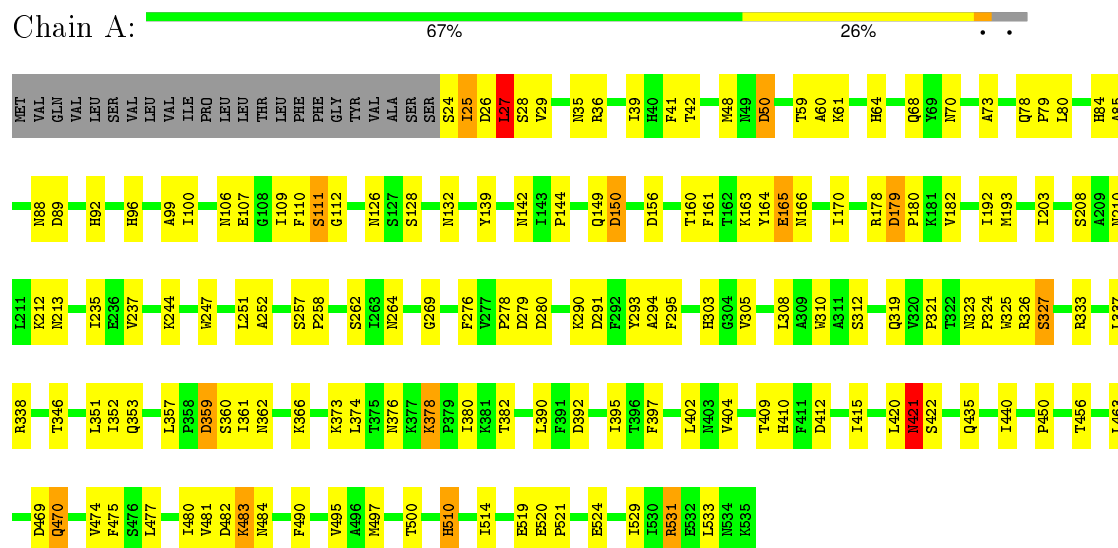
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		
4	D	57	Total	O	0	0
			57	57		
4	B	69	Total	O	0	0
			69	69		
4	C	71	Total	O	0	0
			71	71		

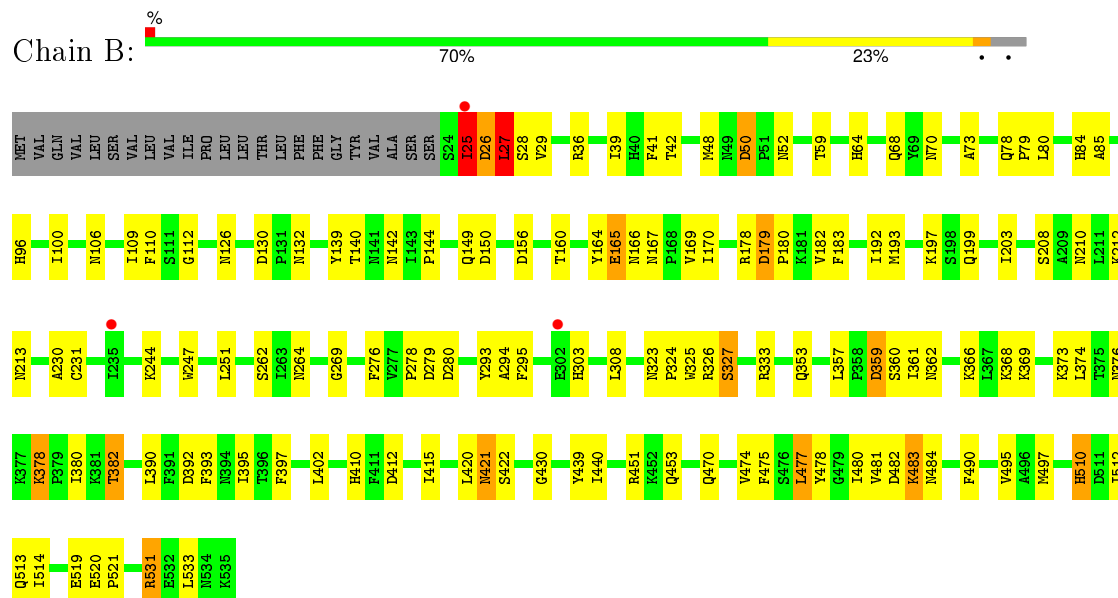
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Fructofuranosidase

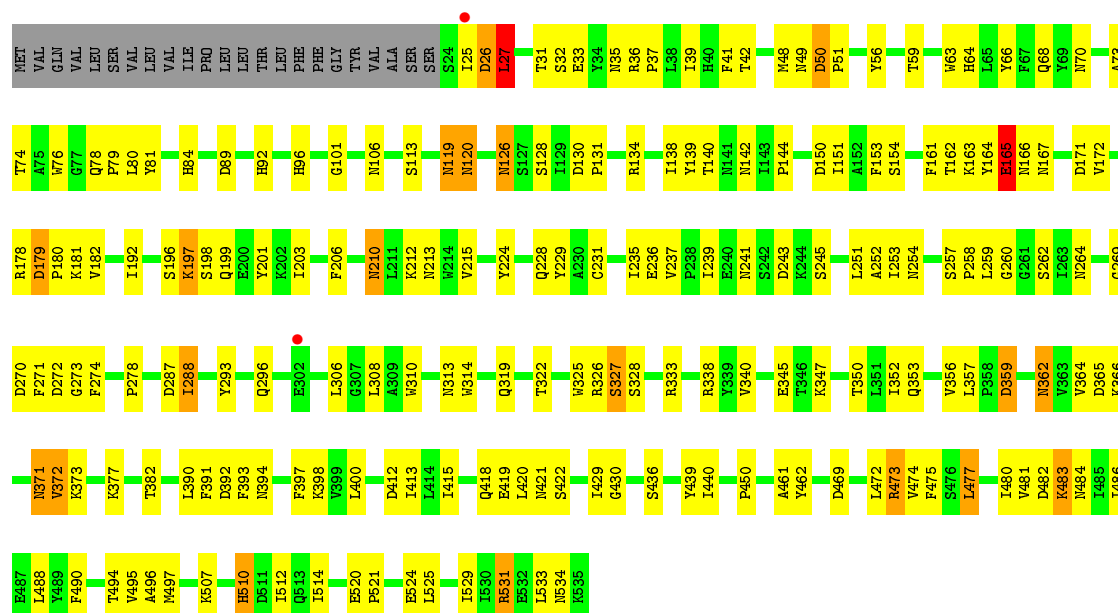


• Molecule 1: Fructofuranosidase



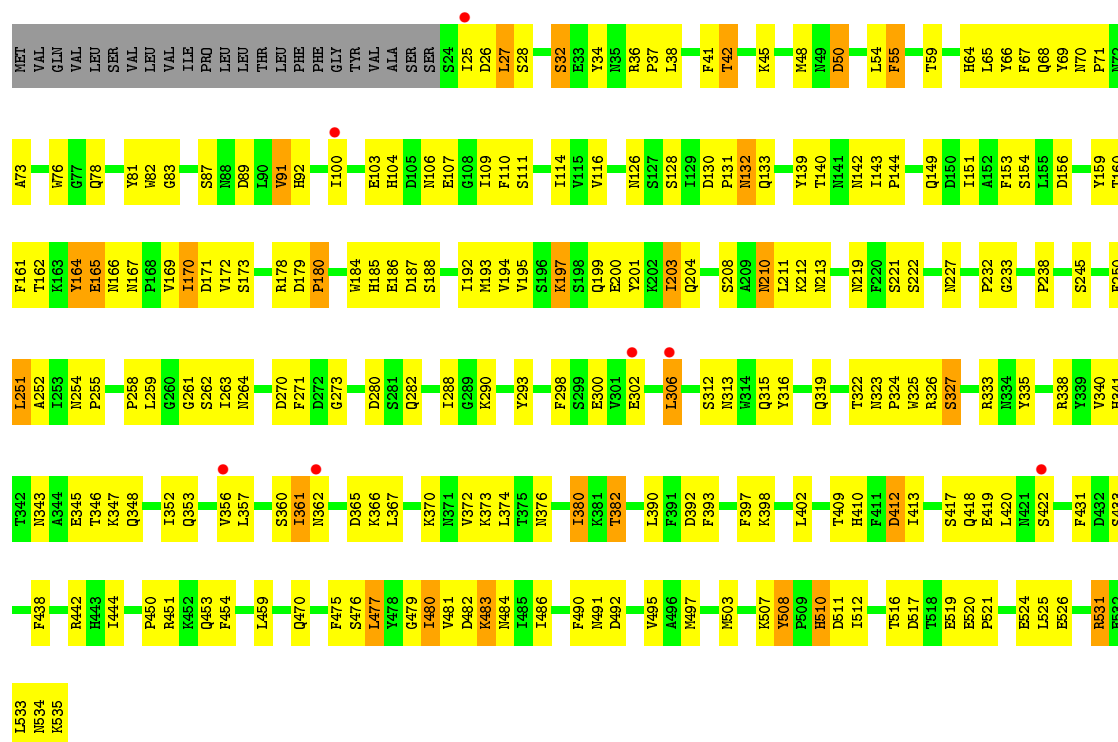
• Molecule 1: Fructofuranosidase

Chain C:  59% 33%



• Molecule 1: Fructofuranosidase

Chain D:  54% 37% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.21Å 92.66Å 117.75Å 89.91° 82.96° 85.82°	Depositor
Resolution (Å)	50.00 – 2.68 58.43 – 2.68	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-2.68) 79.2 (58.43-2.68)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.241 , 0.308 0.241 , 0.308	Depositor DCC
R_{free} test set	3720 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 13.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 73956 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17209	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GLC, NAG, FRU

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	0.66	0/4273	0.74	1/5820 (0.0%)
1	B	0.64	0/4273	0.73	1/5820 (0.0%)
1	C	0.73	0/4273	0.80	2/5820 (0.0%)
1	D	0.66	0/4273	0.76	1/5820 (0.0%)
All	All	0.67	0/17092	0.76	5/23280 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	LEU	CA-CB-CG	6.60	130.49	115.30
1	A	27	LEU	CA-CB-CG	5.92	128.92	115.30
1	C	27	LEU	CA-CB-CG	5.34	127.58	115.30
1	D	251	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	27	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	197	LYS	Peptide
1	D	197	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4152	0	3940	115	0
1	B	4152	0	3939	108	0
1	C	4152	0	3939	161	0
1	D	4152	0	3939	187	0
2	A	56	0	52	5	0
2	B	56	0	52	3	0
2	C	56	0	52	4	0
2	D	56	0	52	5	0
3	A	14	0	13	0	0
3	B	28	0	26	1	0
3	C	28	0	26	0	0
3	D	28	0	26	1	0
4	A	82	0	0	4	0
4	B	69	0	0	3	0
4	C	71	0	0	6	0
4	D	57	0	0	5	0
All	All	17209	0	16056	573	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 17.

All (573) 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:B:36:ARG:O	1:B:483:LYS:HD3	1.56	1.06
2:C:1003:FRU:H61	4:C:582:HOH:O	1.55	1.04
1:D:333:ARG:HH11	1:D:353:GLN:NE2	1.56	1.02
1:C:164:TYR:O	1:C:165:GLU:HB2	1.60	1.00
1:A:170:ILE:HD12	1:A:193:MET:HE1	1.45	0.97
1:B:510:HIS:HB3	4:B:544:HOH:O	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:GLN:HE22	1:C:142:ASN:ND2	1.62	0.95
1:A:420:LEU:O	1:A:422:SER:N	2.00	0.95
1:D:481:VAL:HG22	1:D:486:ILE:HD12	1.47	0.94
1:D:50:ASP:OD2	2:D:1000:FRU:H11	1.68	0.94
1:C:59:THR:HG21	1:C:130:ASP:OD1	1.69	0.92
1:C:78:GLN:HE22	1:C:142:ASN:HD22	1.00	0.92
1:C:74:THR:HG23	1:C:326:ARG:HH12	1.34	0.92
1:B:170:ILE:HD12	1:B:193:MET:HE1	1.50	0.92
1:A:36:ARG:O	1:A:483:LYS:HD3	1.70	0.91
1:C:50:ASP:OD2	2:C:1000:FRU:H11	1.71	0.90
1:D:70:ASN:HD21	1:D:73:ALA:HB3	1.34	0.90
1:C:481:VAL:HG22	1:C:486:ILE:HG13	1.53	0.89
1:B:420:LEU:O	1:B:422:SER:N	2.06	0.88
1:D:333:ARG:HH11	1:D:353:GLN:HE21	1.22	0.86
1:D:201:TYR:O	1:D:221:SER:OG	1.96	0.83
1:D:290:LYS:HG3	1:D:316:TYR:OH	1.78	0.83
1:C:36:ARG:NH1	1:C:42:THR:HG21	1.94	0.83
1:A:397:PHE:CZ	1:A:475:PHE:HB2	2.13	0.83
1:B:490:PHE:HD1	1:B:495:VAL:CG2	1.93	0.82
1:B:357:LEU:HD22	1:B:361:ILE:CD1	2.08	0.82
1:C:36:ARG:O	1:C:483:LYS:HD3	1.79	0.82
1:B:333:ARG:HH11	1:B:353:GLN:NE2	1.78	0.81
1:C:338:ARG:HB3	1:C:352:ILE:HD13	1.61	0.81
1:B:26:ASP:O	1:B:27:LEU:HG	1.78	0.80
1:C:78:GLN:NE2	1:C:142:ASN:HD22	1.79	0.80
1:B:490:PHE:HD1	1:B:495:VAL:HG23	1.48	0.79
1:B:78:GLN:HE22	1:B:142:ASN:HD22	1.29	0.79
1:C:224:TYR:CE2	1:C:258:PRO:HD3	2.17	0.79
1:C:481:VAL:CG2	1:C:486:ILE:HG13	2.13	0.79
1:A:164:TYR:O	1:A:165:GLU:HB2	1.81	0.79
1:B:357:LEU:HD22	1:B:361:ILE:HD13	1.63	0.78
1:D:333:ARG:NH1	1:D:353:GLN:NE2	2.32	0.78
1:C:373:LYS:HD3	1:C:524:GLU:HG3	1.66	0.77
1:D:36:ARG:O	1:D:483:LYS:HD3	1.83	0.77
1:D:170:ILE:HD12	1:D:193:MET:HE1	1.66	0.77
1:A:333:ARG:HH11	1:A:353:GLN:HE21	1.32	0.77
1:D:418:GLN:HB3	1:D:510:HIS:CD2	2.18	0.77
1:A:106:ASN:ND2	1:A:144:PRO:HG3	2.00	0.77
1:C:262:SER:H	1:C:313:ASN:HD21	1.31	0.77
1:A:208:SER:HB2	1:A:213:ASN:O	1.85	0.76
1:D:261:GLY:HA3	1:D:313:ASN:OD1	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:HIS:HB3	4:A:541:HOH:O	1.85	0.76
1:B:106:ASN:ND2	1:B:144:PRO:HG3	2.01	0.75
1:C:36:ARG:NH1	1:C:42:THR:CG2	2.49	0.75
1:D:59:THR:HG21	1:D:130:ASP:OD1	1.86	0.75
1:D:323:ASN:OD1	1:D:324:PRO:HA	1.87	0.74
1:C:345:GLU:HB2	1:D:199:GLN:HE21	1.53	0.74
1:A:333:ARG:HH11	1:A:353:GLN:NE2	1.84	0.73
1:A:357:LEU:HD22	1:A:361:ILE:HD13	1.68	0.73
1:D:68:GLN:HE22	1:D:110:PHE:HA	1.53	0.73
1:B:333:ARG:HH11	1:B:353:GLN:HE21	1.35	0.72
1:A:490:PHE:HD1	1:A:495:VAL:CG2	2.03	0.72
1:A:106:ASN:HD22	1:A:144:PRO:HG3	1.54	0.72
1:D:48:MET:HG3	1:D:67:PHE:HB2	1.71	0.72
1:B:397:PHE:CZ	1:B:475:PHE:HB2	2.24	0.72
1:A:68:GLN:HE22	1:A:110:PHE:HA	1.54	0.72
1:C:74:THR:HG23	1:C:326:ARG:NH1	2.05	0.71
1:C:113:SER:HB3	1:C:181:LYS:HD2	1.72	0.71
1:D:210:ASN:OD1	1:D:213:ASN:ND2	2.24	0.71
1:C:397:PHE:CZ	1:C:475:PHE:HB2	2.25	0.71
1:C:64:HIS:HD2	1:C:84:HIS:NE2	1.88	0.71
1:C:333:ARG:HH11	1:C:353:GLN:NE2	1.88	0.71
1:D:227:ASN:CB	1:D:255:PRO:HD2	2.21	0.71
1:D:402:LEU:HD21	1:D:520:GLU:HB2	1.71	0.71
1:C:490:PHE:HD1	1:C:495:VAL:CG2	2.04	0.70
1:B:164:TYR:O	1:B:165:GLU:HB2	1.90	0.70
1:D:476:SER:O	1:D:491:ASN:N	2.25	0.70
1:D:282:GLN:HE22	1:D:348:GLN:HE22	1.40	0.70
1:C:150:ASP:HB3	1:C:167:ASN:ND2	2.07	0.70
1:B:68:GLN:HE22	1:B:110:PHE:HA	1.57	0.70
1:B:440:ILE:HG21	1:B:497:MET:HE3	1.74	0.70
1:A:357:LEU:HD22	1:A:361:ILE:CD1	2.21	0.70
1:C:106:ASN:ND2	1:C:144:PRO:HG3	2.07	0.70
1:A:490:PHE:HD1	1:A:495:VAL:HG23	1.57	0.69
1:C:394:ASN:HB3	1:C:529:ILE:HD12	1.74	0.69
1:C:68:GLN:NE2	1:C:80:LEU:HD21	2.07	0.69
1:B:208:SER:HB2	1:B:213:ASN:O	1.93	0.69
1:D:290:LYS:HG2	1:D:442:ARG:NH2	2.08	0.68
1:C:210:ASN:HB3	1:C:212:LYS:H	1.59	0.68
1:B:415:ILE:HD13	1:B:481:VAL:HG21	1.75	0.68
1:D:36:ARG:HH11	1:D:42:THR:CG2	2.06	0.68
1:C:490:PHE:HD1	1:C:495:VAL:HG23	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLN:OE1	1:B:180:PRO:HG3	1.94	0.68
1:C:199:GLN:NE2	1:D:345:GLU:HB2	2.08	0.68
1:A:440:ILE:HG21	1:A:497:MET:HE3	1.75	0.68
1:D:185:HIS:HD2	1:D:188:SER:H	1.42	0.68
1:D:91:VAL:HG11	1:D:361:ILE:HD11	1.76	0.68
1:B:26:ASP:O	1:B:27:LEU:CG	2.42	0.67
1:C:106:ASN:HD22	1:C:144:PRO:HG3	1.58	0.67
1:D:70:ASN:ND2	1:D:73:ALA:HB3	2.09	0.67
1:D:338:ARG:HB3	1:D:352:ILE:CD1	2.24	0.66
1:D:262:SER:HB2	1:D:293:TYR:CD1	2.30	0.66
2:B:1003:FRU:H62	4:B:556:HOH:O	1.96	0.66
1:C:119:ASN:O	1:C:120:ASN:C	2.35	0.65
1:D:170:ILE:HD12	1:D:193:MET:CE	2.25	0.65
1:D:193:MET:HE3	1:D:195:VAL:HB	1.78	0.65
1:B:164:TYR:O	1:B:165:GLU:CB	2.45	0.65
1:B:149:GLN:O	1:B:169:VAL:HG22	1.96	0.65
1:D:142:ASN:OD1	4:D:572:HOH:O	2.14	0.64
1:C:440:ILE:HG21	1:C:497:MET:HE3	1.78	0.64
1:B:410:HIS:HD2	1:B:412:ASP:OD1	1.80	0.64
1:C:239:ILE:HG13	1:C:245:SER:HA	1.79	0.64
2:D:1002:FRU:O6	2:D:1003:FRU:O5	2.16	0.64
1:D:280:ASP:OD2	1:D:282:GLN:HG2	1.97	0.63
1:C:262:SER:H	1:C:313:ASN:ND2	1.96	0.63
1:C:203:ILE:HD11	1:C:251:LEU:HD13	1.80	0.63
1:D:210:ASN:HB3	1:D:212:LYS:H	1.64	0.63
1:C:199:GLN:HE21	1:D:345:GLU:HB2	1.63	0.62
1:A:164:TYR:O	1:A:165:GLU:CB	2.47	0.62
1:A:156:ASP:OD2	1:A:160:THR:OG1	2.17	0.62
1:D:481:VAL:CG2	1:D:486:ILE:HD12	2.24	0.62
1:D:508:TYR:N	1:D:508:TYR:HD2	1.97	0.62
1:D:497:MET:HG2	1:D:497:MET:O	2.00	0.61
1:A:410:HIS:HD2	1:A:412:ASP:OD1	1.84	0.61
1:C:36:ARG:HH12	1:C:42:THR:CG2	2.13	0.61
1:B:390:LEU:HG	1:B:533:LEU:HB2	1.82	0.61
1:D:335:TYR:CE2	1:D:353:GLN:HB3	2.36	0.61
1:A:149:GLN:OE1	1:A:180:PRO:HG3	2.01	0.61
1:B:210:ASN:HD21	1:B:212:LYS:HD2	1.64	0.61
1:C:254:ASN:OD1	4:C:583:HOH:O	2.16	0.61
1:A:50:ASP:OD2	2:A:1000:FRU:H11	2.01	0.61
1:A:390:LEU:HG	1:A:533:LEU:HB2	1.82	0.61
1:D:376:ASN:HD21	1:D:519:GLU:HG3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ILE:HD13	1:A:481:VAL:HG21	1.83	0.60
1:A:78:GLN:HE22	1:A:142:ASN:HD22	1.49	0.60
1:D:36:ARG:HD3	1:D:42:THR:HG21	1.84	0.60
1:B:164:TYR:CE2	1:B:166:ASN:HB2	2.35	0.60
1:C:338:ARG:CB	1:C:352:ILE:HD13	2.30	0.60
2:D:1003:FRU:H61	2:D:1004:GLC:H3	1.83	0.60
1:C:235:ILE:HG12	1:C:236:GLU:H	1.65	0.60
1:D:413:ILE:HD11	1:D:477:LEU:HD21	1.82	0.60
1:B:78:GLN:HE22	1:B:142:ASN:ND2	1.99	0.60
1:D:357:LEU:HD23	1:D:361:ILE:HD13	1.82	0.60
1:B:269:GLY:HA2	1:B:279:ASP:OD1	2.01	0.60
1:C:42:THR:HG23	1:C:325:TRP:CD1	2.37	0.59
1:C:372:VAL:HG23	1:C:525:LEU:HB2	1.83	0.59
1:D:490:PHE:HD1	1:D:495:VAL:HG23	1.67	0.59
1:B:59:THR:HG23	1:B:132:ASN:HB2	1.83	0.59
1:B:156:ASP:OD2	1:B:160:THR:OG1	2.19	0.59
1:B:106:ASN:HD22	1:B:144:PRO:HG3	1.67	0.59
1:C:440:ILE:HG22	1:C:497:MET:HE1	1.85	0.59
1:C:64:HIS:CD2	1:C:84:HIS:NE2	2.69	0.59
1:D:393:PHE:HE1	1:D:477:LEU:HD11	1.68	0.59
1:B:278:PRO:HB2	1:B:280:ASP:O	2.03	0.59
1:D:508:TYR:N	1:D:508:TYR:CD2	2.69	0.58
1:A:64:HIS:HD2	1:A:84:HIS:NE2	2.01	0.58
1:D:333:ARG:NH1	1:D:353:GLN:HE21	1.95	0.58
1:A:333:ARG:NH1	1:A:353:GLN:NE2	2.51	0.58
1:B:78:GLN:NE2	1:B:142:ASN:HD22	2.00	0.58
1:B:440:ILE:CG2	1:B:497:MET:HE3	2.34	0.58
1:C:138:ILE:HD13	1:C:182:VAL:HG21	1.85	0.58
1:C:36:ARG:HH12	1:C:42:THR:HG22	1.67	0.58
1:B:482:ASP:O	1:B:484:ASN:N	2.31	0.58
1:D:130:ASP:HB3	1:D:133:GLN:HB2	1.85	0.58
1:D:204:GLN:NE2	1:D:219:ASN:OD1	2.36	0.58
1:A:392:ASP:OD1	1:A:531:ARG:HB2	2.03	0.58
1:A:402:LEU:HD21	1:A:520:GLU:HB2	1.85	0.58
1:A:29:VAL:HB	1:A:323:ASN:HD22	1.69	0.57
1:C:164:TYR:CE2	1:C:166:ASN:HB2	2.39	0.57
1:B:490:PHE:CD1	1:B:495:VAL:CG2	2.82	0.57
1:A:42:THR:HG23	1:A:325:TRP:CD1	2.40	0.57
1:D:69:TYR:CE2	1:D:71:PRO:HB3	2.40	0.57
1:C:288:ILE:CD1	1:C:461:ALA:HB2	2.34	0.57
1:C:224:TYR:CD2	1:C:258:PRO:HD3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ASN:HB3	1:D:255:PRO:HD2	1.85	0.56
1:A:244:LYS:NZ	4:A:563:HOH:O	2.37	0.56
1:B:333:ARG:HD3	1:B:353:GLN:HE21	1.70	0.56
1:D:338:ARG:HB3	1:D:352:ILE:HD13	1.85	0.56
1:D:508:TYR:HD2	1:D:508:TYR:H	1.52	0.56
1:A:290:LYS:HE2	1:A:456:THR:OG1	2.05	0.56
1:C:68:GLN:NE2	2:C:1000:FRU:O6	2.33	0.56
1:C:235:ILE:HG12	1:C:236:GLU:N	2.21	0.56
1:C:113:SER:CB	1:C:181:LYS:HD2	2.35	0.56
1:D:497:MET:CG	1:D:497:MET:O	2.54	0.56
1:C:228:GLN:O	1:C:253:ILE:HA	2.06	0.56
1:D:397:PHE:HB3	1:D:525:LEU:HD23	1.87	0.56
1:D:333:ARG:HD3	1:D:353:GLN:HE21	1.71	0.55
1:C:206:PHE:HA	1:C:215:VAL:O	2.06	0.55
1:A:376:ASN:HD21	1:A:519:GLU:HG2	1.70	0.55
1:A:323:ASN:OD1	1:A:324:PRO:HA	2.06	0.55
1:A:107:GLU:HB3	1:A:142:ASN:O	2.07	0.55
1:D:238:PRO:HA	1:D:245:SER:CB	2.37	0.55
1:B:36:ARG:HH11	1:B:42:THR:HG22	1.72	0.55
1:C:78:GLN:HA	1:C:79:PRO:C	2.27	0.55
1:C:350:THR:O	1:C:352:ILE:HD12	2.07	0.55
1:B:36:ARG:HH11	1:B:42:THR:CG2	2.19	0.55
1:D:185:HIS:NE2	1:D:187:ASP:HB2	2.21	0.55
1:C:340:VAL:O	1:C:347:LYS:HA	2.06	0.55
1:D:87:SER:CB	1:D:92:HIS:O	2.54	0.54
1:D:87:SER:HB2	1:D:92:HIS:O	2.08	0.54
1:C:288:ILE:HD11	1:C:461:ALA:HB2	1.89	0.54
1:B:402:LEU:HD21	1:B:520:GLU:HB2	1.89	0.54
1:D:91:VAL:HG23	1:D:92:HIS:HD1	1.72	0.54
1:D:338:ARG:HB3	1:D:352:ILE:HD11	1.88	0.54
1:C:138:ILE:HG23	1:C:151:ILE:HG22	1.89	0.54
1:D:164:TYR:CE2	1:D:166:ASN:HB2	2.42	0.54
1:C:398:LYS:HG3	1:C:474:VAL:HG22	1.90	0.54
1:D:390:LEU:HG	1:D:533:LEU:HB2	1.88	0.54
1:D:259:LEU:O	1:D:290:LYS:NZ	2.40	0.54
1:D:36:ARG:HH11	1:D:42:THR:HG21	1.72	0.54
1:D:26:ASP:HB3	4:D:548:HOH:O	2.06	0.54
1:D:197:LYS:NZ	1:D:200:GLU:OE2	2.40	0.54
1:D:372:VAL:HA	4:D:587:HOH:O	2.08	0.54
1:A:278:PRO:HB2	1:A:280:ASP:O	2.07	0.54
1:B:326:ARG:O	1:B:327:SER:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:PHE:CD1	1:B:495:VAL:HG23	2.36	0.54
1:C:153:PHE:O	1:C:161:PHE:HA	2.08	0.54
1:C:269:GLY:HA3	1:C:278:PRO:HA	1.89	0.54
1:D:315:GLN:O	1:D:451:ARG:HD2	2.09	0.53
1:B:36:ARG:NH1	1:B:42:THR:HG22	2.23	0.53
1:C:373:LYS:HB3	1:C:521:PRO:HB3	1.90	0.53
1:A:440:ILE:CG2	1:A:497:MET:HE3	2.38	0.53
1:B:323:ASN:OD1	1:B:324:PRO:HA	2.09	0.53
1:C:36:ARG:HH11	1:C:42:THR:HG21	1.69	0.53
1:D:534:ASN:OD1	1:D:535:LYS:N	2.33	0.53
1:D:32:SER:O	1:D:483:LYS:NZ	2.40	0.53
1:A:50:ASP:CG	2:A:1000:FRU:H11	2.28	0.53
1:C:81:TYR:HD2	1:C:101:GLY:HA2	1.73	0.53
1:D:252:ALA:HB1	1:D:293:TYR:CE1	2.43	0.53
1:D:210:ASN:O	1:D:211:LEU:HB2	2.06	0.53
1:D:76:TRP:HB3	2:D:1004:GLC:H1	1.90	0.53
1:D:203:ILE:HD11	1:D:251:LEU:HD13	1.90	0.53
1:D:319:GLN:OE1	1:D:450:PRO:HG2	2.09	0.53
1:B:183:PHE:CE2	1:B:192:ILE:HB	2.44	0.53
1:C:35:ASN:ND2	1:C:322:THR:HG22	2.23	0.53
1:B:100:ILE:HG22	1:B:109:ILE:HG13	1.90	0.53
1:D:390:LEU:HD12	1:D:481:VAL:O	2.08	0.53
1:A:333:ARG:NH1	1:A:353:GLN:HE21	2.04	0.53
1:C:66:TYR:CE2	1:C:84:HIS:CD2	2.97	0.53
1:D:417:SER:HB2	1:D:507:LYS:HB3	1.89	0.52
1:A:440:ILE:HB	1:A:497:MET:HE1	1.91	0.52
1:A:269:GLY:HA2	1:A:279:ASP:OD1	2.09	0.52
1:C:362:ASN:HB3	1:C:534:ASN:HB3	1.92	0.52
1:C:78:GLN:NE2	1:C:142:ASN:ND2	2.44	0.52
1:D:107:GLU:HG2	1:D:143:ILE:HA	1.91	0.52
1:A:490:PHE:CD1	1:A:495:VAL:CG2	2.91	0.52
1:D:164:TYR:CZ	1:D:166:ASN:HB2	2.45	0.52
1:D:333:ARG:HB2	1:D:335:TYR:CE1	2.45	0.52
1:A:346:THR:OG1	1:B:199:GLN:O	2.27	0.52
1:C:440:ILE:CG2	1:C:497:MET:CE	2.87	0.52
1:C:31:THR:O	1:C:35:ASN:HB2	2.09	0.52
1:C:440:ILE:CG2	1:C:497:MET:HE1	2.40	0.52
1:C:413:ILE:CD1	1:C:477:LEU:HD21	2.40	0.52
1:C:39:ILE:HD11	1:C:480:ILE:HD11	1.91	0.52
1:A:59:THR:HG23	1:A:132:ASN:HB2	1.90	0.52
1:D:48:MET:HA	1:D:68:GLN:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:TRP:HB2	1:D:100:ILE:HB	1.92	0.52
1:C:430:GLY:HA3	1:C:439:TYR:CZ	2.45	0.52
1:B:373:LYS:HB2	1:B:378:LYS:NZ	2.25	0.51
1:B:262:SER:HB2	1:B:293:TYR:CD1	2.45	0.51
1:A:50:ASP:OD1	2:A:1000:FRU:H11	2.10	0.51
1:C:392:ASP:OD1	1:C:392:ASP:C	2.49	0.51
1:D:55:PHE:HE2	1:D:64:HIS:CG	2.28	0.51
1:C:482:ASP:O	1:C:484:ASN:N	2.41	0.51
1:B:70:ASN:ND2	1:B:73:ALA:HB3	2.25	0.51
1:C:139:TYR:CE1	1:C:150:ASP:HB2	2.45	0.51
1:B:140:THR:HG21	1:B:178:ARG:HB3	1.93	0.51
1:C:237:VAL:O	1:C:245:SER:HB2	2.11	0.51
1:D:130:ASP:HB3	1:D:133:GLN:HE21	1.76	0.51
1:C:126:ASN:HB3	1:C:128:SER:H	1.76	0.51
1:D:290:LYS:CG	1:D:316:TYR:OH	2.57	0.51
1:D:89:ASP:OD2	1:D:92:HIS:ND1	2.44	0.50
1:A:78:GLN:NE2	1:A:142:ASN:HD22	2.10	0.50
1:D:393:PHE:CZ	1:D:479:GLY:HA3	2.46	0.50
1:A:395:ILE:HD11	1:A:514:ILE:HD11	1.93	0.50
1:D:380:ILE:O	1:D:380:ILE:HG22	2.11	0.50
1:A:164:TYR:CE2	1:A:166:ASN:HB2	2.46	0.50
1:C:398:LYS:HA	1:C:473:ARG:O	2.11	0.50
1:C:41:PHE:CG	1:C:42:THR:N	2.79	0.50
1:D:164:TYR:O	1:D:165:GLU:CB	2.59	0.50
1:C:382:THR:HB	1:C:512:ILE:H	1.77	0.50
1:D:233:GLY:O	1:D:250:PHE:N	2.32	0.50
1:D:373:LYS:HD3	1:D:524:GLU:HG3	1.93	0.50
1:B:203:ILE:HD11	1:B:251:LEU:HD13	1.93	0.50
1:D:290:LYS:HG2	1:D:442:ARG:HH22	1.73	0.50
1:D:42:THR:O	1:D:42:THR:HG22	2.12	0.50
1:C:436:SER:HB3	1:C:462:TYR:CE1	2.46	0.50
1:C:74:THR:CG2	1:C:326:ARG:HH12	2.16	0.50
1:C:326:ARG:O	1:C:327:SER:HB2	2.12	0.50
1:B:78:GLN:HA	1:B:79:PRO:C	2.32	0.50
1:B:50:ASP:OD2	1:B:231:CYS:SG	2.70	0.50
1:B:27:LEU:HD12	1:B:28:SER:H	1.77	0.50
1:D:365:ASP:OD2	1:D:366:LYS:N	2.45	0.50
1:D:271:PHE:CE2	1:D:273:GLY:HA2	2.47	0.50
1:A:78:GLN:HA	1:A:79:PRO:C	2.33	0.50
1:A:50:ASP:HB2	1:A:68:GLN:HG3	1.94	0.49
1:C:287:ASP:OD1	1:C:287:ASP:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:ILE:HG21	1:C:497:MET:CE	2.42	0.49
1:B:150:ASP:HB3	1:B:167:ASN:ND2	2.27	0.49
1:D:159:TYR:O	1:D:160:THR:HG23	2.13	0.49
1:C:319:GLN:HG3	1:C:450:PRO:HB2	1.93	0.49
3:D:1394:NAG:O7	3:D:1394:NAG:H3	2.12	0.49
1:C:68:GLN:NE2	1:C:80:LEU:CD2	2.74	0.49
1:C:338:ARG:HB3	1:C:352:ILE:CD1	2.39	0.49
1:A:203:ILE:HD11	1:A:251:LEU:HD13	1.93	0.49
1:D:398:LYS:HE2	1:D:526:GLU:OE2	2.12	0.49
1:D:367:LEU:HD23	1:D:367:LEU:C	2.33	0.49
1:C:171:ASP:C	1:C:171:ASP:OD2	2.51	0.49
1:A:337:LEU:HD23	1:A:351:LEU:HA	1.95	0.49
1:C:140:THR:HG21	1:C:178:ARG:CB	2.43	0.49
1:D:184:TRP:HE1	1:D:186:GLU:HG2	1.77	0.49
1:B:247:TRP:O	1:B:276:PHE:HE1	1.96	0.49
1:A:89:ASP:OD2	1:A:92:HIS:ND1	2.40	0.49
1:D:370:LYS:O	1:D:372:VAL:HG13	2.13	0.49
1:B:29:VAL:HB	1:B:323:ASN:HD22	1.77	0.48
1:C:415:ILE:HD12	1:C:429:ILE:CD1	2.43	0.48
1:D:54:LEU:HB3	1:D:298:PHE:CD2	2.47	0.48
1:D:338:ARG:CB	1:D:352:ILE:HD13	2.43	0.48
1:D:326:ARG:O	1:D:327:SER:CB	2.61	0.48
1:C:179:ASP:HB3	1:C:231:CYS:HA	1.95	0.48
1:D:149:GLN:OE1	1:D:180:PRO:HG3	2.13	0.48
1:C:488:LEU:O	1:C:496:ALA:HA	2.13	0.48
1:D:70:ASN:HD21	1:D:73:ALA:CB	2.16	0.48
1:D:130:ASP:OD2	1:D:131:PRO:HD2	2.13	0.48
1:A:490:PHE:CD1	1:A:495:VAL:HG23	2.43	0.48
1:D:59:THR:HG23	1:D:132:ASN:HB2	1.95	0.48
1:C:130:ASP:O	1:C:134:ARG:HG3	2.14	0.48
1:C:36:ARG:NH1	1:C:42:THR:HG22	2.24	0.48
1:A:257:SER:OG	1:A:258:PRO:HD2	2.13	0.48
1:C:153:PHE:CE2	1:C:162:THR:HB	2.49	0.48
1:D:149:GLN:HE22	1:D:178:ARG:HA	1.79	0.48
1:C:420:LEU:O	1:C:422:SER:N	2.42	0.48
1:C:252:ALA:HB1	1:C:293:TYR:CE1	2.49	0.48
1:D:67:PHE:CE1	1:D:83:GLY:HA3	2.48	0.48
1:A:111:SER:HB2	2:A:1000:FRU:O4	2.12	0.48
1:D:156:ASP:OD2	1:D:160:THR:OG1	2.32	0.48
1:A:100:ILE:HG22	1:A:109:ILE:HG13	1.95	0.48
1:A:85:ALA:HA	1:A:96:HIS:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ASP:OD1	1:C:50:ASP:N	2.42	0.48
1:C:481:VAL:HG22	1:C:486:ILE:CG1	2.37	0.48
1:D:418:GLN:HG2	1:D:419:GLU:O	2.13	0.48
1:A:48:MET:HA	1:A:68:GLN:O	2.13	0.48
1:B:376:ASN:HD21	1:B:519:GLU:HG2	1.78	0.48
1:C:271:PHE:CZ	1:C:273:GLY:HA2	2.49	0.48
1:B:36:ARG:NH1	1:B:42:THR:CG2	2.76	0.47
1:D:306:LEU:HA	1:D:333:ARG:O	2.13	0.47
1:C:76:TRP:HE1	2:C:1000:FRU:HO6	1.61	0.47
1:D:357:LEU:HD11	1:D:480:ILE:HD13	1.96	0.47
1:B:440:ILE:HB	1:B:497:MET:HE1	1.96	0.47
1:A:373:LYS:HB2	1:A:378:LYS:NZ	2.29	0.47
1:B:230:ALA:O	1:B:231:CYS:C	2.51	0.47
1:A:435:GLN:HG2	1:B:451:ARG:HD3	1.95	0.47
1:D:109:ILE:HG23	1:D:139:TYR:CD1	2.49	0.47
1:C:310:TRP:HE1	1:C:327:SER:CB	2.28	0.47
1:B:333:ARG:NH1	1:B:353:GLN:NE2	2.57	0.47
1:C:151:ILE:O	1:C:151:ILE:HG13	2.12	0.47
1:D:397:PHE:CB	1:D:525:LEU:HD23	2.45	0.47
1:C:364:VAL:HG23	1:C:534:ASN:HB2	1.96	0.47
1:A:326:ARG:O	1:A:327:SER:HB2	2.15	0.47
1:B:85:ALA:HA	1:B:96:HIS:HD2	1.80	0.47
1:C:182:VAL:HG13	1:C:192:ILE:O	2.14	0.47
1:C:413:ILE:HG12	1:C:514:ILE:HG12	1.96	0.47
2:A:1001:FRU:O6	2:A:1002:FRU:H12	2.15	0.47
1:C:356:VAL:O	1:C:357:LEU:HD23	2.15	0.47
1:C:172:VAL:HG21	1:C:197:LYS:HE3	1.96	0.47
1:D:37:PRO:HA	1:D:482:ASP:OD1	2.15	0.47
1:C:345:GLU:HB2	1:D:199:GLN:NE2	2.27	0.47
1:D:392:ASP:HA	1:D:479:GLY:O	2.15	0.47
1:D:322:THR:OG1	1:D:326:ARG:HG2	2.14	0.47
1:C:400:LEU:HD23	1:C:472:LEU:HD13	1.97	0.47
1:D:107:GLU:HB3	1:D:142:ASN:O	2.15	0.47
1:C:271:PHE:CE2	1:C:273:GLY:HA2	2.49	0.47
1:B:264:ASN:HD21	1:B:295:PHE:H	1.63	0.46
1:C:310:TRP:HE1	1:C:327:SER:HB3	1.80	0.46
1:D:238:PRO:HA	1:D:245:SER:HB2	1.97	0.46
1:D:154:SER:HB2	1:D:161:PHE:CE2	2.50	0.46
1:D:417:SER:CB	1:D:507:LYS:HB3	2.46	0.46
1:D:210:ASN:HB3	1:D:213:ASN:H	1.80	0.46
1:A:109:ILE:HG23	1:A:139:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:PHE:HD1	1:B:495:VAL:HG22	1.79	0.46
1:B:41:PHE:CG	1:B:42:THR:N	2.84	0.46
1:B:359:ASP:C	1:B:361:ILE:H	2.18	0.46
1:C:56:TYR:HB2	1:C:63:TRP:CE3	2.51	0.46
1:D:282:GLN:HE22	1:D:348:GLN:NE2	2.10	0.46
1:C:352:ILE:HG13	1:C:494:THR:HA	1.98	0.46
1:A:376:ASN:HD21	1:A:519:GLU:CG	2.28	0.46
1:C:89:ASP:OD2	1:C:92:HIS:ND1	2.48	0.46
1:D:193:MET:HE3	1:D:195:VAL:CB	2.45	0.46
1:A:415:ILE:HD13	1:A:481:VAL:CG2	2.45	0.46
1:C:365:ASP:OD2	1:C:366:LYS:N	2.48	0.46
1:C:391:PHE:N	1:C:391:PHE:CD1	2.84	0.46
1:D:315:GLN:CD	1:D:454:PHE:HB3	2.37	0.46
1:C:418:GLN:HB3	1:C:510:HIS:CD2	2.50	0.46
1:A:469:ASP:O	1:A:470:GLN:HB2	2.15	0.46
1:A:262:SER:HB2	1:A:293:TYR:CD1	2.51	0.46
1:A:150:ASP:N	1:A:150:ASP:OD1	2.49	0.46
1:C:333:ARG:HD2	1:C:353:GLN:HE21	1.81	0.45
1:C:529:ILE:HG22	1:C:531:ARG:HD3	1.98	0.45
1:C:362:ASN:CB	1:C:534:ASN:HB3	2.46	0.45
1:C:70:ASN:OD1	4:C:563:HOH:O	2.20	0.45
1:D:343:ASN:OD1	1:D:346:THR:N	2.46	0.45
1:D:164:TYR:HB3	1:D:167:ASN:OD1	2.15	0.45
1:B:48:MET:HA	1:B:68:GLN:O	2.16	0.45
1:D:140:THR:HG21	1:D:178:ARG:HB3	1.98	0.45
1:C:420:LEU:HD12	1:C:507:LYS:HG3	1.98	0.45
1:D:417:SER:HA	1:D:508:TYR:O	2.16	0.45
1:C:490:PHE:CD1	1:C:495:VAL:HG23	2.46	0.45
1:B:42:THR:HG23	1:B:325:TRP:CD1	2.52	0.45
1:D:258:PRO:HG2	1:D:259:LEU:HD12	1.98	0.45
1:A:326:ARG:O	1:A:327:SER:CB	2.65	0.45
1:A:210:ASN:HD21	1:A:212:LYS:HD2	1.81	0.45
1:A:264:ASN:HD21	1:A:295:PHE:H	1.63	0.45
1:A:247:TRP:O	1:A:276:PHE:HE1	1.99	0.45
1:D:516:THR:OG1	1:D:517:ASP:N	2.49	0.45
1:A:36:ARG:NH1	1:A:42:THR:HG22	2.31	0.45
1:B:410:HIS:CD2	1:B:412:ASP:OD1	2.66	0.45
1:D:149:GLN:O	1:D:169:VAL:HG22	2.16	0.45
1:D:116:VAL:HB	1:D:300:GLU:OE2	2.16	0.45
1:C:96:HIS:O	4:C:580:HOH:O	2.21	0.45
1:B:366:LYS:HB3	1:B:531:ARG:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:GLN:HA	4:C:547:HOH:O	2.17	0.45
1:D:104:HIS:C	1:D:106:ASN:H	2.20	0.45
1:B:59:THR:HG21	1:B:130:ASP:OD1	2.16	0.45
1:A:402:LEU:CD2	1:A:520:GLU:HB2	2.47	0.45
1:A:29:VAL:HB	1:A:323:ASN:ND2	2.32	0.45
1:D:322:THR:OG1	1:D:326:ARG:HA	2.17	0.45
1:A:404:VAL:CG2	4:A:612:HOH:O	2.64	0.45
1:A:397:PHE:CZ	1:A:475:PHE:CB	2.94	0.45
1:A:366:LYS:HB3	1:A:531:ARG:HG3	1.99	0.45
1:A:482:ASP:O	1:A:484:ASN:N	2.39	0.45
1:A:60:ALA:O	1:A:61:LYS:C	2.55	0.45
1:C:164:TYR:O	1:C:165:GLU:CB	2.43	0.45
1:C:74:THR:O	1:C:326:ARG:NH1	2.48	0.45
1:B:382:THR:HB	1:B:512:ILE:H	1.82	0.45
1:B:112:GLY:HA2	1:B:180:PRO:HD2	1.99	0.44
1:A:41:PHE:CG	1:A:42:THR:N	2.85	0.44
1:D:41:PHE:CD2	1:D:42:THR:N	2.86	0.44
1:A:78:GLN:HE22	1:A:142:ASN:ND2	2.12	0.44
1:D:451:ARG:C	1:D:453:GLN:H	2.19	0.44
1:A:252:ALA:HB1	1:A:293:TYR:CE1	2.52	0.44
1:D:431:PHE:CE2	1:D:433:SER:HA	2.53	0.44
1:B:27:LEU:O	4:B:573:HOH:O	2.21	0.44
1:A:374:LEU:O	1:A:521:PRO:HA	2.18	0.44
1:D:66:TYR:CE1	1:D:114:ILE:HD12	2.52	0.44
1:A:397:PHE:CE1	1:A:475:PHE:HB2	2.53	0.44
1:D:38:LEU:O	1:D:535:LYS:HD3	2.17	0.44
1:D:534:ASN:ND2	4:D:554:HOH:O	2.50	0.44
1:D:335:TYR:OH	1:D:353:GLN:NE2	2.50	0.44
1:A:36:ARG:HH11	1:A:42:THR:HG22	1.83	0.44
1:D:338:ARG:HH12	1:D:492:ASP:HB3	1.82	0.44
1:C:272:ASP:OD1	1:C:274:PHE:HB2	2.17	0.44
1:D:302:GLU:HA	1:D:302:GLU:OE1	2.18	0.44
1:A:70:ASN:ND2	1:A:73:ALA:HB3	2.32	0.44
1:B:64:HIS:HD2	1:B:84:HIS:NE2	2.16	0.44
1:B:109:ILE:HG23	1:B:139:TYR:CD1	2.53	0.44
1:B:373:LYS:HB3	1:B:521:PRO:HB3	2.00	0.44
1:D:340:VAL:O	1:D:347:LYS:HA	2.18	0.44
1:C:32:SER:HA	1:C:36:ARG:HB2	1.99	0.44
1:B:430:GLY:HA3	1:B:439:TYR:CZ	2.53	0.44
1:A:338:ARG:NH2	1:A:352:ILE:HG21	2.33	0.44
1:B:25:ILE:O	1:B:26:ASP:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1002:FRU:O3	4:D:591:HOH:O	2.11	0.44
1:B:395:ILE:HD11	1:B:514:ILE:HD11	2.00	0.44
1:A:170:ILE:CD1	1:A:193:MET:HE1	2.33	0.43
1:C:140:THR:OG1	1:C:178:ARG:HA	2.18	0.43
1:D:149:GLN:NE2	1:D:178:ARG:HA	2.33	0.43
1:B:326:ARG:O	1:B:327:SER:CB	2.66	0.43
1:C:154:SER:HB2	1:C:161:PHE:CE2	2.53	0.43
1:D:259:LEU:HD13	1:D:263:ILE:HD12	2.00	0.43
1:D:392:ASP:OD1	1:D:531:ARG:HB2	2.19	0.43
1:D:397:PHE:CZ	1:D:475:PHE:HB2	2.54	0.43
1:C:420:LEU:C	1:C:422:SER:N	2.71	0.43
1:C:70:ASN:HD21	1:C:73:ALA:HB3	1.82	0.43
1:D:444:ILE:HG21	1:D:503:MET:HA	1.99	0.43
1:B:368:LYS:O	1:B:369:LYS:HG2	2.18	0.43
1:C:49:ASN:HD22	1:C:50:ASP:H	1.66	0.43
1:B:39:ILE:HD11	1:B:480:ILE:HD11	2.00	0.43
1:D:382:THR:HB	1:D:512:ILE:O	2.18	0.43
1:A:374:LEU:HD11	1:A:514:ILE:HG22	2.01	0.43
1:B:393:PHE:HE1	1:B:477:LEU:HD11	1.84	0.43
1:C:257:SER:O	1:C:260:GLY:N	2.49	0.43
1:A:319:GLN:HG3	1:A:450:PRO:HB2	2.00	0.43
1:C:201:TYR:O	1:C:229:TYR:CE2	2.72	0.43
1:C:520:GLU:HB3	1:C:521:PRO:CD	2.49	0.43
1:D:55:PHE:CE2	1:D:64:HIS:CG	3.06	0.43
1:C:270:ASP:OD1	1:C:271:PHE:N	2.52	0.43
1:B:478:TYR:CE1	3:B:1394:NAG:H83	2.54	0.43
1:C:36:ARG:HA	1:C:37:PRO:HD3	1.93	0.43
1:D:459:LEU:HB2	1:D:497:MET:CE	2.49	0.43
1:A:182:VAL:HA	1:A:192:ILE:O	2.19	0.43
1:B:50:ASP:HB2	1:B:68:GLN:HG3	2.00	0.42
1:D:398:LYS:HB2	1:D:524:GLU:HB3	2.01	0.42
1:D:126:ASN:HB3	1:D:128:SER:H	1.84	0.42
1:C:130:ASP:OD2	1:C:131:PRO:HD2	2.19	0.42
1:C:48:MET:HA	1:C:68:GLN:O	2.18	0.42
1:D:32:SER:HA	1:D:36:ARG:HB2	2.00	0.42
1:D:78:GLN:NE2	1:D:142:ASN:HD22	2.17	0.42
1:D:106:ASN:ND2	1:D:144:PRO:HG3	2.33	0.42
1:A:88:ASN:OD1	1:A:88:ASN:N	2.50	0.42
1:D:390:LEU:HG	1:D:533:LEU:HD12	2.01	0.42
1:B:402:LEU:CD2	1:B:520:GLU:HB2	2.50	0.42
1:B:264:ASN:HD21	1:B:294:ALA:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ASP:C	1:B:392:ASP:OD1	2.58	0.42
1:A:112:GLY:HA2	1:A:180:PRO:HD2	2.00	0.42
1:D:410:HIS:HD2	1:D:412:ASP:OD1	2.02	0.42
1:B:244:LYS:HA	1:B:244:LYS:HD3	1.90	0.42
1:D:208:SER:OG	1:D:213:ASN:O	2.27	0.42
1:A:244:LYS:HA	1:A:244:LYS:HD3	1.91	0.42
1:B:182:VAL:HG13	1:B:192:ILE:O	2.20	0.42
1:A:126:ASN:HB3	1:A:128:SER:H	1.84	0.42
1:D:306:LEU:HD21	1:D:356:VAL:HG21	2.01	0.42
1:D:263:ILE:HG12	1:D:264:ASN:H	1.85	0.42
1:D:374:LEU:O	1:D:521:PRO:HA	2.20	0.42
1:A:178:ARG:HB2	1:A:179:ASP:OD1	2.19	0.42
1:C:390:LEU:HG	1:C:533:LEU:HB2	2.01	0.42
1:A:463:LEU:HD11	1:A:495:VAL:CG2	2.49	0.42
1:C:413:ILE:HD11	1:C:477:LEU:HD21	2.01	0.42
1:B:178:ARG:HB2	1:B:179:ASP:OD1	2.20	0.42
1:A:68:GLN:NE2	1:A:80:LEU:HD21	2.35	0.42
1:B:210:ASN:ND2	1:B:212:LYS:HD2	2.31	0.42
1:D:41:PHE:C	1:D:41:PHE:CD2	2.92	0.41
1:C:397:PHE:CE1	1:C:475:PHE:HB2	2.55	0.41
1:C:398:LYS:HD3	1:C:469:ASP:HB3	2.02	0.41
1:A:39:ILE:HD11	1:A:480:ILE:HD11	2.02	0.41
1:B:397:PHE:O	1:B:474:VAL:HA	2.20	0.41
1:B:68:GLN:NE2	1:B:80:LEU:HD21	2.35	0.41
1:D:393:PHE:CE1	1:D:477:LEU:HD11	2.50	0.41
1:D:482:ASP:O	1:D:484:ASN:N	2.44	0.41
1:D:490:PHE:CD1	1:D:495:VAL:HG23	2.50	0.41
1:D:81:TYR:HB3	1:D:100:ILE:O	2.20	0.41
1:C:50:ASP:HA	1:C:51:PRO:HD2	1.92	0.41
1:B:52:ASN:ND2	1:B:68:GLN:OE1	2.52	0.41
1:A:392:ASP:OD1	1:A:392:ASP:C	2.58	0.41
1:A:99:ALA:HB1	1:A:161:PHE:CE1	2.55	0.41
1:A:421:ASN:OD1	1:A:421:ASN:N	2.51	0.41
2:B:1003:FRU:H61	2:B:1004:GLC:H5	2.02	0.41
1:D:373:LYS:HB3	1:D:521:PRO:HB3	2.02	0.41
1:D:171:ASP:C	1:D:171:ASP:OD2	2.58	0.41
1:A:397:PHE:CE2	1:A:475:PHE:HB2	2.55	0.41
1:C:210:ASN:HB3	1:C:213:ASN:H	1.85	0.41
1:D:333:ARG:HH11	1:D:353:GLN:HE22	1.56	0.41
1:C:393:PHE:HA	1:C:529:ILE:O	2.20	0.41
1:C:419:GLU:HG2	1:C:422:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:TRP:HE1	1:A:327:SER:HB3	1.86	0.41
1:B:374:LEU:HD11	1:B:514:ILE:HG22	2.03	0.41
1:A:237:VAL:HG22	1:A:305:VAL:HG21	2.03	0.41
1:A:397:PHE:O	1:A:474:VAL:HA	2.20	0.41
1:A:359:ASP:C	1:A:361:ILE:H	2.24	0.41
1:C:140:THR:HG21	1:C:178:ARG:HB3	2.02	0.41
1:B:392:ASP:OD1	1:B:531:ARG:HB2	2.21	0.41
1:A:24:SER:N	4:A:608:HOH:O	2.53	0.41
1:D:343:ASN:C	1:D:345:GLU:H	2.24	0.41
1:B:451:ARG:HA	1:B:453:GLN:OE1	2.21	0.41
1:C:391:PHE:HD1	1:C:391:PHE:N	2.19	0.41
1:A:264:ASN:HD21	1:A:294:ALA:N	2.19	0.41
1:B:50:ASP:OD2	2:B:1000:FRU:H11	2.21	0.41
1:D:390:LEU:CD1	1:D:481:VAL:O	2.68	0.40
1:B:50:ASP:HB2	1:B:68:GLN:CG	2.50	0.40
1:D:180:PRO:HA	1:D:194:VAL:O	2.21	0.40
1:B:380:ILE:O	1:B:513:GLN:HA	2.21	0.40
1:D:254:ASN:HA	1:D:255:PRO:HA	1.81	0.40
1:C:314:TRP:HB2	4:C:583:HOH:O	2.21	0.40
1:C:253:ILE:HG13	1:C:253:ILE:O	2.20	0.40
1:D:55:PHE:CE2	1:D:64:HIS:ND1	2.89	0.40
1:C:179:ASP:H	1:C:180:PRO:HD3	1.86	0.40
1:A:373:LYS:HD3	1:A:524:GLU:HG3	2.02	0.40
1:A:291:ASP:OD2	1:A:500:THR:N	2.40	0.40
1:D:418:GLN:NE2	1:D:507:LYS:HA	2.36	0.40
1:B:397:PHE:CE1	1:B:475:PHE:HB2	2.57	0.40
1:C:35:ASN:O	1:C:484:ASN:ND2	2.54	0.40
1:A:99:ALA:C	1:A:100:ILE:HG13	2.41	0.40
1:B:376:ASN:HD21	1:B:519:GLU:CG	2.35	0.40
1:A:35:ASN:ND2	1:A:321:PRO:O	2.54	0.40
1:D:192:ILE:HG22	1:D:193:MET:N	2.36	0.40
1:D:438:PHE:CD1	1:D:490:PHE:CD2	3.10	0.40
1:D:153:PHE:CE2	1:D:162:THR:HB	2.56	0.40
1:D:172:VAL:O	1:D:173:SER:HB2	2.22	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	510/535 (95%)	463 (91%)	35 (7%)	12 (2%)	7	17
1	B	510/535 (95%)	462 (91%)	36 (7%)	12 (2%)	7	17
1	C	510/535 (95%)	448 (88%)	51 (10%)	11 (2%)	8	20
1	D	510/535 (95%)	438 (86%)	58 (11%)	14 (3%)	6	14
All	All	2040/2140 (95%)	1811 (89%)	180 (9%)	49 (2%)	7	17

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	421	ASN
1	B	26	ASP
1	B	27	LEU
1	B	421	ASN
1	C	27	LEU
1	C	126	ASN
1	C	179	ASP
1	A	26	ASP
1	A	27	LEU
1	A	165	GLU
1	A	327	SER
1	B	165	GLU
1	B	360	SER
1	B	483	LYS
1	C	26	ASP
1	C	165	GLU
1	C	483	LYS
1	D	165	GLU
1	D	288	ILE
1	D	327	SER
1	D	409	THR

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Mol	Chain	Res	Type
1	A	470	GLN
1	A	483	LYS
1	B	126	ASN
1	C	120	ASN
1	C	371	ASN
1	D	32	SER
1	D	103	GLU
1	D	483	LYS
1	A	303	HIS
1	A	409	THR
1	B	303	HIS
1	B	327	SER
1	B	470	GLN
1	C	327	SER
1	D	27	LEU
1	D	132	ASN
1	D	360	SER
1	D	470	GLN
1	C	359	ASP
1	C	421	ASN
1	D	232	PRO
1	A	360	SER
1	A	378	LYS
1	B	25	ILE
1	D	380	ILE
1	B	378	LYS
1	D	180	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	463/484 (96%)	443 (96%)	20 (4%)	35 64
1	B	463/484 (96%)	451 (97%)	12 (3%)	54 81
1	C	463/484 (96%)	434 (94%)	29 (6%)	22 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	463/484 (96%)	428 (92%)	35 (8%)	16	35
All	All	1852/1936 (96%)	1756 (95%)	96 (5%)	29	55

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	27	LEU
1	A	28	SER
1	A	50	ASP
1	A	111	SER
1	A	150	ASP
1	A	163	LYS
1	A	179	ASP
1	A	235	ILE
1	A	308	LEU
1	A	312	SER
1	A	359	ASP
1	A	362	ASN
1	A	380	ILE
1	A	382	THR
1	A	421	ASN
1	A	477	LEU
1	A	510	HIS
1	A	529	ILE
1	A	531	ARG
1	B	25	ILE
1	B	27	LEU
1	B	50	ASP
1	B	179	ASP
1	B	308	LEU
1	B	359	ASP
1	B	362	ASN
1	B	382	THR
1	B	421	ASN
1	B	477	LEU
1	B	510	HIS
1	B	531	ARG
1	C	25	ILE
1	C	26	ASP
1	C	27	LEU
1	C	33	GLU

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Mol	Chain	Res	Type
1	C	50	ASP
1	C	119	ASN
1	C	163	LYS
1	C	165	GLU
1	C	196	SER
1	C	197	LYS
1	C	198	SER
1	C	210	ASN
1	C	241	ASN
1	C	243	ASP
1	C	264	ASN
1	C	288	ILE
1	C	306	LEU
1	C	308	LEU
1	C	328	SER
1	C	359	ASP
1	C	362	ASN
1	C	371	ASN
1	C	372	VAL
1	C	377	LYS
1	C	412	ASP
1	C	473	ARG
1	C	477	LEU
1	C	510	HIS
1	C	531	ARG
1	D	25	ILE
1	D	27	LEU
1	D	28	SER
1	D	34	TYR
1	D	42	THR
1	D	45	LYS
1	D	50	ASP
1	D	55	PHE
1	D	65	LEU
1	D	91	VAL
1	D	111	SER
1	D	151	ILE
1	D	164	TYR
1	D	170	ILE
1	D	179	ASP
1	D	203	ILE
1	D	210	ASN

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Mol	Chain	Res	Type
1	D	222	SER
1	D	270	ASP
1	D	306	LEU
1	D	312	SER
1	D	325	TRP
1	D	341	HIS
1	D	361	ILE
1	D	362	ASN
1	D	382	THR
1	D	412	ASP
1	D	420	LEU
1	D	422	SER
1	D	477	LEU
1	D	480	ILE
1	D	508	TYR
1	D	510	HIS
1	D	511	ASP
1	D	531	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	64	HIS
1	A	68	GLN
1	A	78	GLN
1	A	106	ASN
1	A	118	HIS
1	A	133	GLN
1	A	185	HIS
1	A	199	GLN
1	A	210	ASN
1	A	213	ASN
1	A	264	ASN
1	A	296	GLN
1	A	323	ASN
1	A	348	GLN
1	A	353	GLN
1	A	410	HIS
1	A	435	GLN
1	B	52	ASN
1	B	64	HIS

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Mol	Chain	Res	Type
1	B	68	GLN
1	B	78	GLN
1	B	106	ASN
1	B	118	HIS
1	B	185	HIS
1	B	199	GLN
1	B	210	ASN
1	B	213	ASN
1	B	241	ASN
1	B	264	ASN
1	B	296	GLN
1	B	348	GLN
1	B	353	GLN
1	B	362	ASN
1	B	410	HIS
1	C	52	ASN
1	C	64	HIS
1	C	68	GLN
1	C	78	GLN
1	C	106	ASN
1	C	185	HIS
1	C	199	GLN
1	C	228	GLN
1	C	264	ASN
1	C	296	GLN
1	C	313	ASN
1	C	348	GLN
1	C	353	GLN
1	C	410	HIS
1	C	513	GLN
1	D	52	ASN
1	D	64	HIS
1	D	68	GLN
1	D	70	ASN
1	D	72	ASN
1	D	133	GLN
1	D	142	ASN
1	D	185	HIS
1	D	199	GLN
1	D	213	ASN
1	D	264	ASN
1	D	341	HIS

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Mol	Chain	Res	Type
1	D	348	GLN
1	D	353	GLN
1	D	362	ASN
1	D	371	ASN
1	D	376	ASN
1	D	410	HIS
1	D	510	HIS

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 ⓘ

20 carbohydrates 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	$\# Z > 2$
2	FRU	A	1000	2	11,11,12	0.51	0	15,15,18	1.44	3 (20%)
2	FRU	A	1001	2	11,11,12	0.69	0	15,15,18	1.09	1 (6%)
2	FRU	A	1002	2	11,11,12	0.49	0	15,15,18	1.09	1 (6%)
2	FRU	A	1003	2	11,11,12	0.32	0	15,15,18	0.71	0
2	GLC	A	1004	2	12,12,12	0.43	0	17,17,17	1.77	3 (17%)
2	FRU	B	1000	2	11,11,12	0.49	0	15,15,18	1.45	2 (13%)
2	FRU	B	1001	2	11,11,12	0.50	0	15,15,18	1.39	3 (20%)
2	FRU	B	1002	2	11,11,12	0.54	0	15,15,18	1.07	0
2	FRU	B	1003	2	11,11,12	0.41	0	15,15,18	0.77	0
2	GLC	B	1004	2	12,12,12	0.66	0	17,17,17	1.41	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FRU	C	1000	2	11,11,12	0.34	0	15,15,18	1.33	2 (13%)
2	FRU	C	1001	2	11,11,12	0.51	0	15,15,18	1.28	2 (13%)
2	FRU	C	1002	2	11,11,12	0.63	0	15,15,18	0.95	0
2	FRU	C	1003	2	11,11,12	0.41	0	15,15,18	1.23	1 (6%)
2	GLC	C	1004	2	12,12,12	0.87	0	17,17,17	1.92	4 (23%)
2	FRU	D	1000	2	11,11,12	0.32	0	15,15,18	1.30	2 (13%)
2	FRU	D	1001	2	11,11,12	0.74	0	15,15,18	1.23	3 (20%)
2	FRU	D	1002	2	11,11,12	0.44	0	15,15,18	1.10	0
2	FRU	D	1003	2	11,11,12	0.38	0	15,15,18	1.27	1 (6%)
2	GLC	D	1004	2	12,12,12	0.56	0	17,17,17	1.69	4 (23%)

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	FRU	A	1000	2	-	0/4/20/24	0/1/1/1
2	FRU	A	1001	2	-	0/4/20/24	0/1/1/1
2	FRU	A	1002	2	-	0/4/20/24	0/1/1/1
2	FRU	A	1003	2	-	0/4/20/24	0/1/1/1
2	GLC	A	1004	2	-	0/2/22/22	0/1/1/1
2	FRU	B	1000	2	-	0/4/20/24	0/1/1/1
2	FRU	B	1001	2	-	0/4/20/24	0/1/1/1
2	FRU	B	1002	2	-	0/4/20/24	0/1/1/1
2	FRU	B	1003	2	-	0/4/20/24	0/1/1/1
2	GLC	B	1004	2	-	0/2/22/22	0/1/1/1
2	FRU	C	1000	2	-	0/4/20/24	0/1/1/1
2	FRU	C	1001	2	-	0/4/20/24	0/1/1/1
2	FRU	C	1002	2	-	0/4/20/24	0/1/1/1
2	FRU	C	1003	2	-	0/4/20/24	0/1/1/1
2	GLC	C	1004	2	-	0/2/22/22	0/1/1/1
2	FRU	D	1000	2	-	0/4/20/24	0/1/1/1
2	FRU	D	1001	2	-	0/4/20/24	0/1/1/1
2	FRU	D	1002	2	-	0/4/20/24	0/1/1/1
2	FRU	D	1003	2	-	0/4/20/24	0/1/1/1
2	GLC	D	1004	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1004	GLC	C1-C2-C3	-3.85	104.70	110.43
2	A	1000	FRU	C1-C2-C3	-3.27	107.36	115.08
2	B	1000	FRU	C1-C2-C3	-3.19	107.54	115.08
2	C	1000	FRU	C1-C2-C3	-3.00	107.97	115.08
2	B	1000	FRU	O4-C4-C3	-2.99	102.10	111.83
2	D	1003	FRU	C6-C5-C4	-2.86	108.31	115.08
2	D	1004	GLC	C4-C3-C2	-2.80	105.56	110.79
2	B	1001	FRU	C1-C2-C3	-2.65	108.82	115.08
2	C	1003	FRU	C1-C2-C3	-2.57	109.00	115.08
2	B	1004	GLC	C1-C2-C3	-2.46	106.77	110.43
2	D	1000	FRU	C1-C2-C3	-2.42	109.35	115.08
2	A	1000	FRU	O5-C2-C3	-2.39	100.33	105.15
2	D	1004	GLC	C1-C2-C3	-2.36	106.91	110.43
2	C	1000	FRU	O6-C6-C5	-2.33	103.65	111.33
2	C	1001	FRU	C6-C5-C4	-2.20	109.88	115.08
2	B	1001	FRU	O6-C6-C5	-2.20	104.08	111.33
2	D	1001	FRU	O5-C2-C3	-2.14	100.83	105.15
2	C	1001	FRU	O1-C1-C2	2.15	118.44	111.33
2	A	1002	FRU	O5-C5-C6	2.19	113.92	109.17
2	D	1001	FRU	O1-C1-C2	2.20	118.60	111.33
2	C	1004	GLC	C3-C4-C5	2.23	114.08	110.20
2	A	1000	FRU	O5-C2-C1	2.31	114.18	109.17
2	C	1004	GLC	O5-C1-C2	2.32	113.49	109.80
2	D	1004	GLC	O5-C1-C2	2.40	113.62	109.80
2	D	1001	FRU	O3-C3-C2	2.67	119.07	111.05
2	D	1000	FRU	O5-C2-C1	2.69	115.00	109.17
2	A	1001	FRU	O1-C1-C2	2.92	120.99	111.33
2	A	1004	GLC	C1-O5-C5	3.04	119.10	113.47
2	B	1001	FRU	O1-C1-C2	3.06	121.45	111.33
2	C	1004	GLC	O5-C5-C4	3.34	115.94	109.68
2	D	1004	GLC	C1-O5-C5	3.46	119.87	113.47
2	A	1004	GLC	O5-C5-C4	3.56	116.36	109.68
2	B	1004	GLC	C1-O5-C5	3.80	120.51	113.47
2	C	1004	GLC	C1-O5-C5	5.21	123.11	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	FRU	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	FRU	1	0
2	A	1002	FRU	1	0
2	B	1000	FRU	1	0
2	B	1003	FRU	2	0
2	B	1004	GLC	1	0
2	C	1000	FRU	3	0
2	C	1003	FRU	1	0
2	D	1000	FRU	1	0
2	D	1002	FRU	2	0
2	D	1003	FRU	2	0
2	D	1004	GLC	2	0

5.6 Ligand geometry

7 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	A	1219	1	14,14,15	0.52	0	15,19,21	1.51	2 (13%)
3	NAG	B	1219	1	14,14,15	0.74	0	15,19,21	1.38	2 (13%)
3	NAG	B	1394	1	14,14,15	0.51	0	15,19,21	1.77	1 (6%)
3	NAG	C	1219	1	14,14,15	0.94	0	15,19,21	1.72	4 (26%)
3	NAG	C	1394	1	14,14,15	0.58	0	15,19,21	2.04	5 (33%)
3	NAG	D	1219	1	14,14,15	0.72	0	15,19,21	1.32	3 (20%)
3	NAG	D	1394	1	14,14,15	0.90	0	15,19,21	2.47	5 (33%)

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	A	1219	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1219	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1394	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1219	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1394	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1219	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1394	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1219	NAG	C3-C2-N2	-4.35	100.14	110.56
3	C	1394	NAG	C4-C3-C2	-3.29	106.11	111.23
3	D	1394	NAG	C3-C4-C5	-3.17	104.67	110.20
3	B	1219	NAG	O3-C3-C4	-2.86	103.89	110.34
3	A	1219	NAG	O4-C4-C3	-2.83	103.96	110.34
3	C	1219	NAG	O7-C7-C8	-2.72	117.07	122.06
3	B	1219	NAG	C2-N2-C7	-2.40	119.95	123.04
3	D	1219	NAG	O4-C4-C3	-2.12	105.57	110.34
3	D	1394	NAG	O5-C5-C6	2.07	111.83	107.35
3	C	1219	NAG	C4-C3-C2	2.21	114.66	111.23
3	C	1394	NAG	O3-C3-C2	2.28	113.62	109.11
3	C	1219	NAG	O7-C7-N2	2.30	126.56	121.86
3	D	1219	NAG	C3-C4-C5	2.37	114.33	110.20
3	D	1394	NAG	O7-C7-N2	2.55	127.06	121.86
3	C	1394	NAG	C2-N2-C7	2.60	126.37	123.04
3	C	1394	NAG	C3-C2-N2	2.73	117.10	110.56
3	D	1394	NAG	C4-C3-C2	2.88	115.71	111.23
3	D	1219	NAG	C3-C2-N2	3.07	117.91	110.56
3	C	1219	NAG	C2-N2-C7	3.79	127.91	123.04
3	C	1394	NAG	C1-O5-C5	4.93	118.50	112.25
3	B	1394	NAG	C1-O5-C5	5.97	119.83	112.25
3	D	1394	NAG	C2-N2-C7	7.06	132.11	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1394	NAG	1	0
3	D	1394	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	512/535 (95%)	-0.12	0 100 100	21, 31, 40, 51	0
1	B	512/535 (95%)	-0.05	3 (0%) 90 91	20, 31, 40, 56	0
1	C	512/535 (95%)	-0.18	2 (0%) 93 94	13, 30, 44, 59	0
1	D	512/535 (95%)	0.05	7 (1%) 78 77	18, 38, 52, 63	0
All	All	2048/2140 (95%)	-0.08	12 (0%) 90 91	13, 32, 47, 63	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	25	ILE	3.9
1	D	100	ILE	3.3
1	C	25	ILE	2.9
1	B	25	ILE	2.7
1	D	356	VAL	2.6
1	D	362	ASN	2.4
1	D	306	LEU	2.3
1	B	302	GLU	2.2
1	C	302	GLU	2.2
1	D	302	GLU	2.2
1	D	422	SER	2.1
1	B	235	ILE	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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	FRU	D	1002	11/12	0.90	0.19	0.82	31,32,35,37	0
2	FRU	C	1000	11/12	0.94	0.16	0.61	24,27,28,28	0
2	FRU	D	1001	11/12	0.92	0.16	0.28	31,35,39,40	0
2	FRU	C	1003	11/12	0.93	0.13	-0.31	27,32,33,34	0
2	FRU	B	1000	11/12	0.95	0.13	-0.75	17,20,21,23	0
2	FRU	B	1003	11/12	0.95	0.13	-0.81	33,39,40,41	0
2	FRU	D	1003	11/12	0.93	0.14	-1.09	26,33,35,37	0
2	FRU	C	1001	11/12	0.95	0.12	-1.26	26,31,33,36	0
2	FRU	D	1000	11/12	0.95	0.13	-1.37	25,29,31,33	0
2	FRU	A	1003	11/12	0.93	0.15	-1.39	28,35,37,37	0
2	FRU	A	1000	11/12	0.97	0.12	-1.86	22,23,24,25	0
2	FRU	A	1001	11/12	0.96	0.13	-2.25	26,31,36,38	0
2	FRU	B	1001	11/12	0.96	0.13	-2.45	22,29,33,37	0
2	FRU	A	1002	11/12	0.94	0.14	-	23,27,30,30	0
2	GLC	C	1004	12/12	0.93	0.11	-	33,38,40,41	0
2	GLC	D	1004	12/12	0.92	0.12	-	40,42,42,43	0
2	GLC	B	1004	12/12	0.84	0.21	-	44,47,48,49	0
2	FRU	C	1002	11/12	0.92	0.17	-	26,29,30,31	0
2	GLC	A	1004	12/12	0.92	0.16	-	40,48,50,53	0
2	FRU	B	1002	11/12	0.93	0.17	-	26,29,30,31	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	C	1219	14/15	0.89	0.14	-0.23	37,41,47,48	0
3	NAG	A	1219	14/15	0.88	0.17	-0.38	43,46,48,48	0
3	NAG	B	1219	14/15	0.88	0.16	-0.54	39,42,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	D	1219	14/15	0.89	0.16	-0.94	41,44,47,47	0
3	NAG	D	1394	14/15	0.80	0.26	-	44,46,53,54	0
3	NAG	C	1394	14/15	0.90	0.13	-	45,50,53,53	0
3	NAG	B	1394	14/15	0.85	0.16	-	48,53,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.