



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:45 AM GMT

PDB ID : 3FU9
Title : Melanocarpus albomyces laccase crystal soaked (20 min) with 2,6-dimethoxyphenol
Authors : Kallio, J.P.; Hakulinen, N.; Rouvinen, J.
Deposited on : 2009-01-14
Resolution : 2.00 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

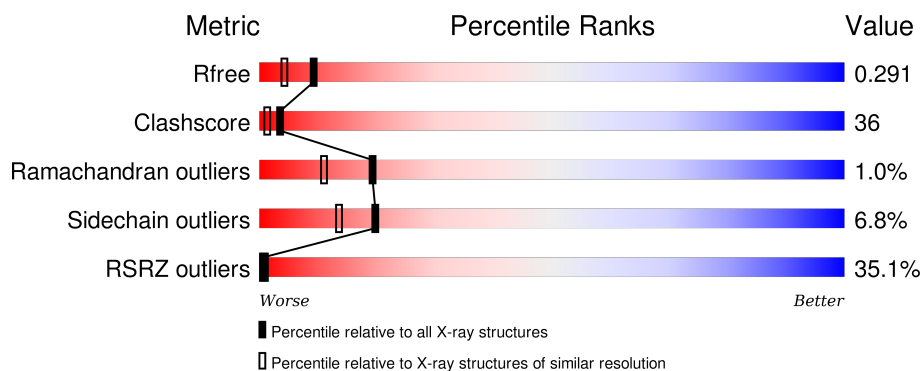
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	559	<div> <div>38%</div> <div>52%</div> <div>40%</div> <div>7%</div> </div>
1	B	559	<div> <div>32%</div> <div>48%</div> <div>42%</div> <div>9%</div> </div>

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	CL	A	610	-	-	X	X
5	NAG	A	731	-	-	-	X
7	KIB	B	2001	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9692 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 Laccase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4369	2764	759	831	15			
1	B	559	Total	C	N	O	S	0	0	0
			4369	2764	759	831	15			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Cu	0	0
			4	4		
2	A	4	Total	Cu	0	0
			4	4		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

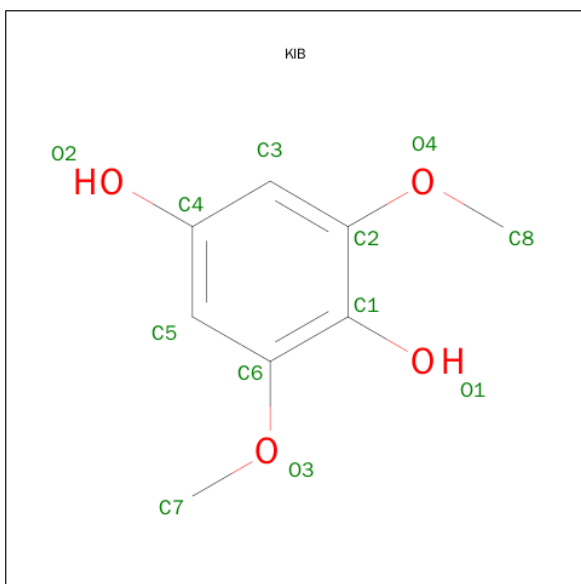
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2,6-DIMETHOXYBENZENE-1,4-DIOL (three-letter code: KIB) (formula: $C_8H_{10}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	8	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			12	8	4		

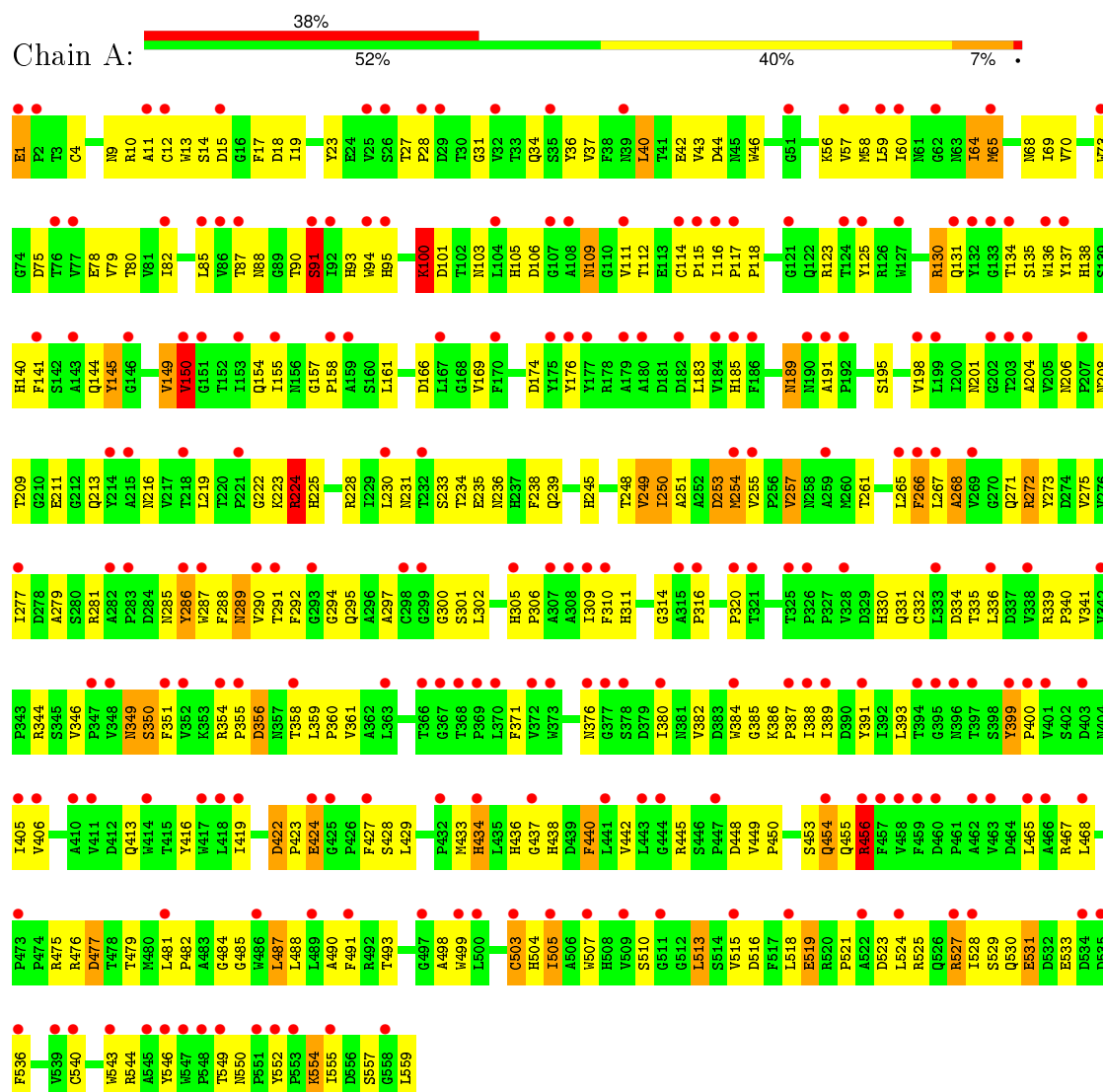
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	336	Total	O	0	0
			336	336		
8	B	364	Total	O	0	0
			364	364		

3 Residue-property plots

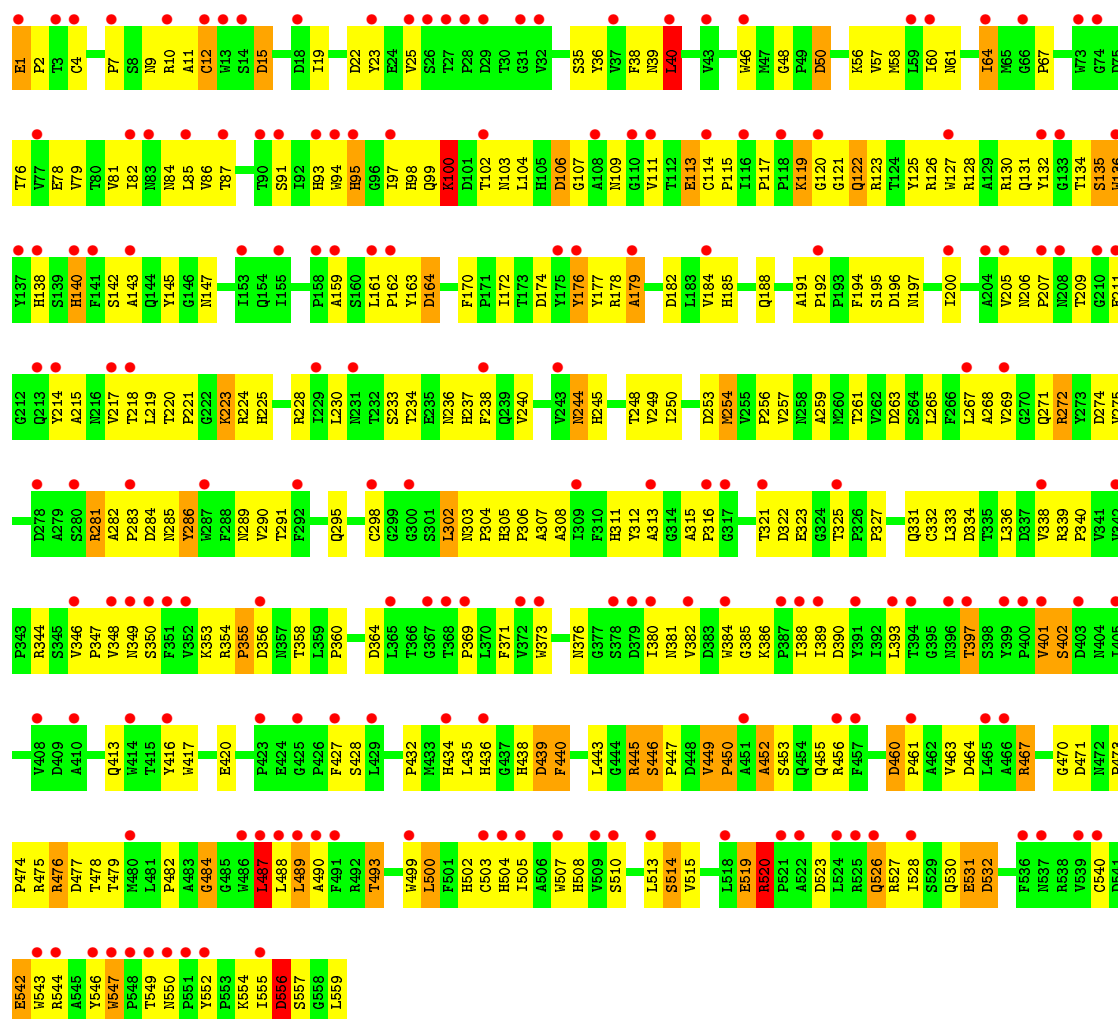
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: Laccase-1



• Molecule 1: Laccase-1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.12Å 60.23Å 117.13Å 90.00° 98.36° 90.00°	Depositor
Resolution (Å)	19.61 – 2.00 19.06 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.61-2.00) 96.4 (19.06-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.330 0.291 , 0.291	Depositor DCC
R_{free} test set	3958 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	1.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 91900 reflections	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	9692	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: KIB, SO4, NAG, CU, CL

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	1.44	29/4506 (0.6%)	1.26	22/6191 (0.4%)
1	B	1.40	20/4506 (0.4%)	1.33	37/6191 (0.6%)
All	All	1.42	49/9012 (0.5%)	1.30	59/12382 (0.5%)

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

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

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	TYR	CD2-CE2	11.69	1.56	1.39
1	B	286	TYR	CD1-CE1	9.74	1.53	1.39
1	B	286	TYR	CD2-CE2	8.73	1.52	1.39
1	A	531	GLU	CG-CD	8.67	1.65	1.51
1	A	255	VAL	CB-CG2	8.35	1.70	1.52
1	A	503	CYS	CB-SG	-8.08	1.68	1.82
1	A	150	VAL	CB-CG2	7.15	1.67	1.52
1	A	154	GLN	C-O	-7.14	1.09	1.23
1	A	286	TYR	CD1-CE1	6.99	1.49	1.39
1	A	233	SER	CB-OG	6.76	1.51	1.42
1	B	257	VAL	CB-CG1	6.55	1.66	1.52
1	A	361	VAL	CA-CB	6.43	1.68	1.54
1	A	1	GLU	CG-CD	6.33	1.61	1.51
1	B	113	GLU	CG-CD	6.32	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	VAL	CB-CG1	6.16	1.65	1.52
1	B	519	GLU	CG-CD	6.06	1.61	1.51
1	A	145	TYR	CD1-CE1	6.04	1.48	1.39
1	A	356	ASP	CB-CG	6.03	1.64	1.51
1	A	257	VAL	CB-CG2	-5.98	1.40	1.52
1	B	531	GLU	CB-CG	5.94	1.63	1.52
1	B	452	ALA	CA-CB	5.86	1.64	1.52
1	A	250	ILE	CB-CG2	5.83	1.71	1.52
1	A	249	VAL	CB-CG1	5.75	1.65	1.52
1	B	445	ARG	CZ-NH2	5.70	1.40	1.33
1	A	399	TYR	CD2-CE2	5.68	1.47	1.39
1	A	266	PHE	CE1-CZ	5.64	1.48	1.37
1	A	136	TRP	CB-CG	5.63	1.60	1.50
1	B	499	TRP	CB-CG	5.61	1.60	1.50
1	A	288	PHE	CE2-CZ	5.51	1.47	1.37
1	A	505	ILE	C-O	5.50	1.33	1.23
1	A	78	GLU	CB-CG	5.47	1.62	1.52
1	B	446	SER	CB-OG	-5.43	1.35	1.42
1	A	339	ARG	CG-CD	5.40	1.65	1.51
1	B	136	TRP	CB-CG	5.38	1.59	1.50
1	A	519	GLU	CG-CD	5.30	1.59	1.51
1	A	191	ALA	CA-CB	5.28	1.63	1.52
1	B	257	VAL	CB-CG2	-5.26	1.41	1.52
1	A	440	PHE	CE2-CZ	5.26	1.47	1.37
1	B	179	ALA	CA-CB	5.25	1.63	1.52
1	B	531	GLU	CG-CD	5.24	1.59	1.51
1	B	542	GLU	CD-OE2	5.17	1.31	1.25
1	A	513	LEU	C-O	5.12	1.33	1.23
1	B	449	VAL	CB-CG2	5.10	1.63	1.52
1	A	482	PRO	C-O	5.09	1.33	1.23
1	B	176	TYR	CD2-CE2	-5.08	1.31	1.39
1	B	275	VAL	CA-CB	5.04	1.65	1.54
1	A	289	ASN	CG-ND2	5.03	1.45	1.32
1	B	547	TRP	CB-CG	-5.02	1.41	1.50
1	B	358	THR	CA-CB	5.01	1.66	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	40	LEU	CA-CB-CG	10.27	138.93	115.30
1	B	130	ARG	NE-CZ-NH1	9.37	124.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	520	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	A	554	LYS	CD-CE-NZ	-8.64	91.82	111.70
1	B	489	LEU	CA-CB-CG	7.78	133.19	115.30
1	A	527	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	439	ASP	CB-CG-OD1	7.59	125.13	118.30
1	B	520	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	75	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	B	350	SER	N-CA-C	7.01	129.93	111.00
1	A	101	ASP	CB-CG-OD1	-6.92	112.07	118.30
1	A	467	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	B	10	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	467	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	B	50	ASP	CB-CG-OD1	-6.63	112.33	118.30
1	B	500	LEU	CA-CB-CG	6.54	130.35	115.30
1	B	50	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	302	LEU	CB-CG-CD1	-6.40	100.12	111.00
1	B	446	SER	C-N-CD	6.38	141.79	128.40
1	B	532	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	161	LEU	CB-CG-CD1	6.23	121.58	111.00
1	B	467	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	460	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	166	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	155	ILE	N-CA-C	-5.85	95.22	111.00
1	B	334	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	253	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	284	ASP	CB-CG-OD1	5.78	123.51	118.30
1	A	130	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	128	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	488	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	B	119	LYS	CD-CE-NZ	5.75	124.92	111.70
1	A	448	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	44	ASP	CB-CG-OD1	5.68	123.42	118.30
1	B	257	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	A	350	SER	N-CA-C	5.66	126.28	111.00
1	B	284	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	525	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	40	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	B	556	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	164	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	344	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	476	ARG	CA-CB-CG	5.43	125.34	113.40
1	A	70	VAL	N-CA-C	-5.40	96.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	364	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	106	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	249	VAL	CB-CA-C	-5.33	101.28	111.40
1	A	64	ILE	CG1-CB-CG2	5.30	123.06	111.40
1	B	298	CYS	CA-CB-SG	-5.27	104.51	114.00
1	A	253	ASP	CB-CA-C	5.27	120.93	110.40
1	B	120	GLY	N-CA-C	5.26	126.24	113.10
1	B	40	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	556	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	487	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	198	VAL	CG1-CB-CG2	-5.06	102.80	110.90
1	B	487	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	224	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	A	456	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	GLY	Peptide
1	B	514	SER	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	4369	0	4114	252	0
1	B	4369	0	4114	365	1
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	1	0	0	3	0
3	B	1	0	0	0	0
4	A	42	0	39	5	1
4	B	56	0	52	0	0
5	A	56	0	48	8	0
5	B	56	0	50	12	0
6	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	5	0	0	0	0
7	A	12	0	8	1	0
7	B	12	0	8	7	0
8	A	336	0	0	108	0
8	B	364	0	0	182	0
All	All	9692	0	8433	630	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 36.

All (630) 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:261:THR:HG22	8:B:812:HOH:O	1.28	1.28
1:B:211:GLU:HB2	8:B:727:HOH:O	1.26	1.28
1:B:143:ALA:HA	8:B:868:HOH:O	1.29	1.27
1:B:230:LEU:HB3	8:B:907:HOH:O	1.34	1.27
1:A:510:SER:HB2	8:A:626:HOH:O	1.29	1.25
1:B:505:ILE:HD13	8:B:684:HOH:O	1.37	1.23
1:B:369:PRO:HB3	8:B:708:HOH:O	1.36	1.23
1:A:12:CYS:HB3	8:A:628:HOH:O	1.10	1.22
1:A:528:ILE:HD12	8:A:890:HOH:O	1.36	1.22
1:B:478:THR:HG22	8:B:916:HOH:O	1.36	1.21
1:B:134:THR:HG22	8:B:636:HOH:O	1.05	1.20
1:B:97:ILE:HD13	8:B:917:HOH:O	1.41	1.18
1:B:388:ILE:HG23	8:B:641:HOH:O	1.46	1.15
1:B:449:VAL:HG21	8:B:932:HOH:O	1.46	1.14
1:B:214:TYR:HA	8:B:723:HOH:O	1.44	1.13
1:B:140:HIS:CE1	8:B:623:HOH:O	1.99	1.12
1:B:217:VAL:HA	8:B:744:HOH:O	1.48	1.11
1:B:23:TYR:HB3	8:B:627:HOH:O	1.50	1.10
1:A:485:GLY:HA3	8:A:876:HOH:O	1.49	1.09
1:A:388:ILE:HD13	1:A:405:ILE:HD11	1.20	1.09
1:A:9:ASN:ND2	1:A:12:CYS:SG	2.25	1.07
1:B:447:PRO:HG2	8:B:656:HOH:O	1.55	1.06
1:B:440:PHE:HE1	8:B:668:HOH:O	1.35	1.05
1:A:64:ILE:HG13	8:A:667:HOH:O	1.55	1.04
1:B:178:ARG:HH21	1:B:182:ASP:HB3	1.23	1.03
1:B:463:VAL:HG23	8:B:650:HOH:O	1.57	1.03
1:B:85:LEU:HA	8:B:833:HOH:O	1.58	1.03
1:A:285:ASN:OD1	1:A:311:HIS:HD2	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:PHE:CE1	1:B:67:PRO:HG2	1.94	1.01
1:B:178:ARG:NH2	1:B:182:ASP:HB3	1.76	1.00
1:B:322:ASP:HA	8:B:631:HOH:O	1.62	1.00
1:A:433:MET:HB2	8:A:895:HOH:O	1.62	1.00
1:A:271:GLN:HG2	1:A:476:ARG:NH2	1.77	0.99
1:B:57:VAL:HG22	8:B:634:HOH:O	1.62	0.99
1:A:382:VAL:HG13	8:A:690:HOH:O	1.63	0.98
1:B:172:ILE:HG13	8:B:643:HOH:O	1.63	0.97
1:B:417:TRP:HD1	8:B:895:HOH:O	1.48	0.97
1:B:46:TRP:HB2	8:B:634:HOH:O	1.66	0.96
1:A:141:PHE:CD1	8:A:642:HOH:O	2.19	0.96
1:A:115:PRO:HD2	8:A:792:HOH:O	1.64	0.96
1:A:309:ILE:HD12	4:A:720:NAG:H81	1.45	0.95
1:B:50:ASP:HB2	8:B:783:HOH:O	1.62	0.95
1:A:388:ILE:CD1	1:A:405:ILE:HD11	1.96	0.95
1:B:19:ILE:HG13	8:B:911:HOH:O	1.65	0.94
1:A:301:SER:HB3	8:A:597:HOH:O	1.66	0.94
1:B:308:ALA:HB2	8:B:923:HOH:O	1.67	0.94
1:B:82:ILE:HG12	1:B:122:GLN:HB2	1.48	0.93
1:B:140:HIS:ND1	8:B:623:HOH:O	1.96	0.92
8:A:696:HOH:O	1:B:191:ALA:HB3	1.69	0.92
1:B:461:PRO:HG3	8:B:652:HOH:O	1.69	0.92
1:A:510:SER:CB	8:A:626:HOH:O	1.96	0.92
1:B:46:TRP:CB	8:B:634:HOH:O	2.18	0.91
1:B:295:GLN:OE1	1:B:452:ALA:HB3	1.68	0.91
1:A:498:ALA:HB2	8:A:818:HOH:O	1.70	0.91
7:B:2001:KIB:H7	8:B:566:HOH:O	1.68	0.91
1:B:107:GLY:HA2	1:B:113:GLU:OE1	1.71	0.90
1:A:388:ILE:HD13	1:A:405:ILE:CD1	2.02	0.90
1:A:358:THR:O	4:A:740:NAG:H82	1.73	0.89
1:A:491:PHE:HB2	8:A:641:HOH:O	1.71	0.89
1:B:460:ASP:HB3	1:B:463:VAL:CG1	2.02	0.89
1:B:261:THR:CG2	8:B:812:HOH:O	1.95	0.87
1:A:438:HIS:NE2	1:A:519:GLU:OE1	2.06	0.87
1:B:428:SER:HB3	1:B:484:GLY:H	1.35	0.87
1:B:540:CYS:HB3	8:B:831:HOH:O	1.74	0.87
1:B:413:GLN:HG2	8:B:909:HOH:O	1.74	0.86
1:A:429:LEU:HD23	8:A:783:HOH:O	1.74	0.86
1:A:43:VAL:HB	1:A:57:VAL:HG23	1.57	0.86
1:B:161:LEU:HG	8:B:820:HOH:O	1.75	0.86
1:B:265:LEU:HB2	8:B:918:HOH:O	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:PHE:HE1	1:B:67:PRO:HG2	1.40	0.86
1:A:314:GLY:HA3	8:A:891:HOH:O	1.76	0.85
1:B:256:PRO:HB3	8:B:584:HOH:O	1.75	0.85
1:B:381:ASN:OD1	1:B:554:LYS:NZ	2.10	0.85
1:A:523:ASP:HA	8:A:902:HOH:O	1.75	0.85
1:A:273:TYR:CZ	8:A:791:HOH:O	2.28	0.84
1:B:267:LEU:HD11	8:B:918:HOH:O	1.77	0.84
1:B:347:PRO:HD3	8:B:897:HOH:O	1.76	0.84
1:B:295:GLN:HG2	8:B:611:HOH:O	1.78	0.84
1:B:228:ARG:HG2	1:B:274:ASP:OD2	1.78	0.84
1:B:455:GLN:HG2	8:B:766:HOH:O	1.77	0.83
1:B:61:ASN:HB3	8:B:884:HOH:O	1.79	0.83
1:B:115:PRO:HA	8:B:747:HOH:O	1.78	0.83
1:A:518:LEU:HG	1:A:521:PRO:HG3	1.58	0.83
1:B:145:TYR:CE2	8:B:599:HOH:O	2.31	0.83
1:A:271:GLN:HG2	1:A:476:ARG:HH21	1.40	0.83
1:B:479:THR:HB	8:B:668:HOH:O	1.79	0.82
1:B:244:ASN:ND2	1:B:281:ARG:HH12	1.78	0.82
1:A:285:ASN:OD1	1:A:311:HIS:CD2	2.31	0.82
1:B:206:ASN:HA	8:B:783:HOH:O	1.78	0.82
1:B:540:CYS:CB	8:B:831:HOH:O	2.28	0.82
1:A:95:HIS:O	1:A:135:SER:HB3	1.80	0.82
1:B:91:SER:HB3	8:B:747:HOH:O	1.79	0.81
7:B:2001:KIB:H7	8:B:819:HOH:O	1.79	0.81
1:B:523:ASP:HA	1:B:526:GLN:HE22	1.43	0.81
1:B:549:THR:HA	8:B:803:HOH:O	1.80	0.81
1:A:201:ASN:ND2	8:A:768:HOH:O	2.13	0.81
1:B:520:ARG:HH21	1:B:523:ASP:CG	1.85	0.80
1:A:306:PRO:CG	8:A:597:HOH:O	2.29	0.80
1:A:302:LEU:HD11	8:B:766:HOH:O	1.81	0.80
1:A:429:LEU:CD2	8:A:783:HOH:O	2.29	0.80
1:B:401:VAL:HG23	1:B:402:SER:H	1.47	0.80
1:A:438:HIS:HA	8:A:621:HOH:O	1.81	0.79
1:B:271:GLN:NE2	1:B:476:ARG:CZ	2.46	0.79
1:A:9:ASN:OD1	1:A:12:CYS:SG	2.41	0.79
1:A:189:ASN:ND2	8:A:632:HOH:O	2.13	0.79
1:B:114:CYS:SG	8:B:831:HOH:O	2.40	0.79
1:B:170:PHE:O	8:B:643:HOH:O	2.01	0.78
1:B:306:PRO:HG3	8:B:591:HOH:O	1.83	0.78
1:A:114:CYS:HB3	8:A:792:HOH:O	1.83	0.78
1:A:484:GLY:HA2	8:A:662:HOH:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TYR:HB2	1:A:79:VAL:HG22	1.65	0.78
1:B:380:ILE:HG13	1:B:402:SER:O	1.83	0.78
1:B:440:PHE:CE1	8:B:668:HOH:O	2.17	0.78
1:A:456:ARG:HD2	8:A:742:HOH:O	1.83	0.78
1:B:95:HIS:CD2	1:B:272:ARG:HH12	2.02	0.77
1:B:267:LEU:CD1	8:B:918:HOH:O	2.32	0.77
1:B:95:HIS:O	1:B:135:SER:HB2	1.84	0.77
1:B:40:LEU:HD22	1:B:60:ILE:HG12	1.66	0.77
1:B:36:TYR:HB2	1:B:79:VAL:HG22	1.65	0.76
1:A:453:SER:HB2	8:A:653:HOH:O	1.84	0.76
1:B:479:THR:HG22	8:B:588:HOH:O	1.83	0.76
1:B:1:GLU:HG3	1:B:2:PRO:HD2	1.68	0.76
1:A:9:ASN:CG	1:A:12:CYS:SG	2.63	0.76
1:B:540:CYS:SG	8:B:831:HOH:O	2.44	0.76
1:B:476:ARG:HG3	8:B:668:HOH:O	1.85	0.75
1:B:290:VAL:HG23	8:B:772:HOH:O	1.87	0.75
1:B:303:ASN:O	8:B:664:HOH:O	2.03	0.75
1:B:393:LEU:HD21	1:B:528:ILE:HD13	1.69	0.75
1:A:249:VAL:HA	1:A:275:VAL:HG12	1.69	0.75
1:A:423:PRO:HA	8:A:662:HOH:O	1.85	0.75
1:B:138:HIS:HE1	8:B:617:HOH:O	1.69	0.74
1:A:65:MET:HB3	1:A:150:VAL:O	1.87	0.74
1:B:200:ILE:HD12	8:B:923:HOH:O	1.87	0.74
1:B:373:TRP:HZ3	8:B:586:HOH:O	1.70	0.74
1:B:393:LEU:HD21	1:B:528:ILE:CD1	2.18	0.73
1:B:4:CYS:HG	1:B:12:CYS:HG	1.31	0.73
1:A:505:ILE:HG23	8:A:665:HOH:O	1.86	0.73
1:A:118:PRO:HG3	1:A:546:TYR:CZ	2.22	0.73
1:B:447:PRO:HD2	8:B:869:HOH:O	1.88	0.73
1:B:138:HIS:CE1	8:B:617:HOH:O	2.42	0.73
1:A:109:ASN:HB2	1:A:115:PRO:HD3	1.71	0.72
1:B:447:PRO:CD	8:B:869:HOH:O	2.35	0.72
1:B:428:SER:CB	1:B:484:GLY:H	2.01	0.72
1:A:95:HIS:CD2	1:A:272:ARG:HH12	2.08	0.72
1:B:439:ASP:HB2	8:B:880:HOH:O	1.89	0.72
1:A:106:ASP:HB3	1:A:112:THR:HG21	1.69	0.72
5:B:710:NAG:H82	8:B:937:HOH:O	1.88	0.71
1:B:113:GLU:OE1	8:B:858:HOH:O	2.06	0.71
1:A:56:LYS:HE3	5:A:710:NAG:O6	1.90	0.71
1:A:479:THR:O	8:A:895:HOH:O	2.09	0.71
1:B:142:SER:OG	1:B:556:ASP:OD1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HD21	1:A:310:PHE:HD2	1.55	0.71
1:A:95:HIS:CD2	1:A:272:ARG:NH1	2.59	0.71
1:A:31:GLY:CA	8:A:901:HOH:O	2.40	0.70
1:A:115:PRO:CD	8:A:792:HOH:O	2.28	0.70
1:B:200:ILE:CD1	8:B:772:HOH:O	2.40	0.70
1:A:302:LEU:HD21	8:B:766:HOH:O	1.90	0.70
1:B:546:TYR:OH	1:B:550:ASN:ND2	2.25	0.70
1:A:42:GLU:OE1	8:A:615:HOH:O	2.08	0.70
1:B:446:SER:HB2	8:B:869:HOH:O	1.91	0.69
1:B:172:ILE:CG1	8:B:643:HOH:O	2.31	0.69
1:B:50:ASP:CB	8:B:783:HOH:O	2.29	0.69
1:A:43:VAL:HB	1:A:57:VAL:CG2	2.21	0.69
1:A:176:TYR:CE2	1:A:195:SER:HA	2.26	0.69
1:B:306:PRO:CG	8:B:591:HOH:O	2.39	0.69
1:B:285:ASN:OD1	1:B:311:HIS:HD2	1.76	0.68
1:B:520:ARG:NH2	1:B:523:ASP:OD2	2.17	0.68
1:B:244:ASN:O	1:B:281:ARG:NH1	2.24	0.68
1:A:131:GLN:HG2	1:A:254:MET:SD	2.33	0.68
1:A:297:ALA:HB1	8:A:783:HOH:O	1.93	0.68
1:A:445:ARG:HD3	8:A:666:HOH:O	1.93	0.68
1:B:436:HIS:O	8:B:717:HOH:O	2.12	0.68
1:B:554:LYS:NZ	1:B:557:SER:O	2.27	0.68
1:B:254:MET:SD	8:B:917:HOH:O	2.51	0.67
1:B:460:ASP:HB3	1:B:463:VAL:HG12	1.75	0.67
1:B:97:ILE:HA	8:B:917:HOH:O	1.93	0.67
7:B:2001:KIB:O1	7:B:2001:KIB:C7	2.43	0.67
1:B:380:ILE:HD12	8:B:689:HOH:O	1.93	0.67
1:B:515:VAL:C	8:B:689:HOH:O	2.31	0.67
1:A:23:TYR:O	8:A:620:HOH:O	2.11	0.67
1:A:224:ARG:HG3	8:A:588:HOH:O	1.94	0.67
1:B:291:THR:HG21	8:B:762:HOH:O	1.95	0.67
1:A:309:ILE:HD12	4:A:720:NAG:C8	2.22	0.67
1:A:389:ILE:CG2	1:A:389:ILE:O	2.43	0.67
1:A:389:ILE:HG22	1:A:389:ILE:O	1.95	0.67
1:A:306:PRO:HG3	8:A:597:HOH:O	1.89	0.66
1:B:307:ALA:HB2	5:B:730:NAG:H62	1.77	0.66
1:B:196:ASP:OD1	8:B:658:HOH:O	2.13	0.66
1:A:219:LEU:HD21	1:A:310:PHE:CD2	2.30	0.66
1:B:135:SER:N	8:B:636:HOH:O	2.28	0.66
3:A:610:CL:CL	8:A:715:HOH:O	2.51	0.65
1:A:311:HIS:CE1	4:A:720:NAG:O4	2.49	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:CG1	1:A:82:ILE:HD12	2.26	0.65
1:A:301:SER:CB	8:A:597:HOH:O	2.35	0.65
1:B:438:HIS:N	8:B:717:HOH:O	2.18	0.65
1:B:200:ILE:HD11	8:B:772:HOH:O	1.96	0.65
1:B:520:ARG:O	1:B:523:ASP:HB2	1.95	0.65
1:B:117:PRO:HG2	1:B:542:GLU:HB2	1.78	0.65
1:B:107:GLY:CA	1:B:113:GLU:OE1	2.45	0.65
1:A:236:ASN:HB3	1:A:238:PHE:CE1	2.31	0.65
1:B:240:VAL:HG22	8:B:918:HOH:O	1.96	0.64
1:A:543:TRP:CD1	8:A:792:HOH:O	2.49	0.64
1:A:468:LEU:HD13	1:A:488:LEU:CD2	2.27	0.64
1:B:420:GLU:OE2	8:B:633:HOH:O	2.15	0.64
1:B:371:PHE:CG	8:B:819:HOH:O	2.50	0.64
1:A:13:TRP:HB2	1:A:158:PRO:HG3	1.78	0.64
1:A:559:LEU:CD1	8:A:690:HOH:O	2.45	0.64
1:A:31:GLY:HA3	8:A:901:HOH:O	1.97	0.64
1:A:349:ASN:O	1:A:351:PHE:N	2.25	0.64
1:A:222:GLY:N	1:A:279:ALA:O	2.31	0.64
1:A:235:GLU:HB2	8:A:665:HOH:O	1.98	0.64
1:A:289:ASN:HB2	8:A:785:HOH:O	1.97	0.63
1:B:455:GLN:CD	8:B:932:HOH:O	2.35	0.63
1:B:178:ARG:NH2	1:B:182:ASP:CB	2.59	0.63
1:B:303:ASN:HB3	8:B:591:HOH:O	1.97	0.63
1:B:179:ALA:CB	5:B:711:NAG:H81	2.28	0.63
1:B:332:CYS:O	1:B:333:LEU:HD23	1.98	0.63
1:A:68:ASN:OD1	8:A:907:HOH:O	2.15	0.63
1:B:455:GLN:HB2	8:B:932:HOH:O	1.97	0.63
1:B:523:ASP:HA	1:B:526:GLN:NE2	2.12	0.62
1:A:204:ALA:HB1	8:A:625:HOH:O	1.98	0.62
7:B:2001:KIB:O1	7:B:2001:KIB:H7B	1.99	0.62
1:B:347:PRO:HA	8:B:930:HOH:O	1.98	0.62
1:B:500:LEU:HD11	8:B:623:HOH:O	1.99	0.62
1:B:523:ASP:O	1:B:527:ARG:HD2	1.98	0.62
1:A:540:CYS:O	1:A:544:ARG:HG3	1.99	0.62
1:B:382:VAL:HG13	1:B:559:LEU:HD11	1.81	0.62
1:B:179:ALA:HB3	5:B:711:NAG:H81	1.82	0.62
1:B:449:VAL:HG11	8:B:932:HOH:O	1.98	0.61
1:A:484:GLY:C	8:A:662:HOH:O	2.39	0.61
1:B:436:HIS:C	8:B:717:HOH:O	2.37	0.61
1:A:273:TYR:CE1	8:A:791:HOH:O	2.49	0.61
1:B:131:GLN:HE21	1:B:254:MET:HB3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLY:N	8:A:901:HOH:O	2.33	0.61
1:B:286:TYR:HA	8:B:630:HOH:O	1.99	0.61
1:B:455:GLN:CB	8:B:932:HOH:O	2.49	0.60
1:B:209:THR:OG1	1:B:211:GLU:OE2	2.17	0.60
1:B:327:PRO:HA	8:B:685:HOH:O	2.00	0.60
1:B:502:HIS:HB3	1:B:514:SER:OG	2.01	0.60
1:B:95:HIS:CD2	1:B:272:ARG:NH1	2.69	0.60
1:B:382:VAL:CG1	1:B:559:LEU:HD11	2.31	0.60
1:B:371:PHE:HB3	8:B:819:HOH:O	2.01	0.60
1:B:219:LEU:O	1:B:221:PRO:HD3	2.02	0.60
1:B:38:PHE:CE1	1:B:67:PRO:CG	2.80	0.59
1:B:307:ALA:CB	5:B:730:NAG:H62	2.32	0.59
1:B:323:GLU:O	5:B:730:NAG:H83	2.03	0.59
1:B:302:LEU:HD11	8:B:658:HOH:O	2.03	0.59
1:B:196:ASP:O	1:B:197:ASN:HB2	2.03	0.59
1:A:286:TYR:OH	8:A:811:HOH:O	2.16	0.59
5:A:711:NAG:H61	8:A:721:HOH:O	2.02	0.59
1:A:116:ILE:HG22	1:A:117:PRO:O	2.03	0.58
1:B:432:PRO:O	1:B:503:CYS:HA	2.02	0.58
1:B:206:ASN:CA	8:B:783:HOH:O	2.44	0.58
1:A:185:HIS:CD2	8:A:632:HOH:O	2.56	0.58
1:A:546:TYR:OH	1:A:550:ASN:ND2	2.36	0.58
1:B:176:TYR:CE2	1:B:195:SER:HA	2.39	0.58
1:A:231:ASN:HB3	1:A:268:ALA:O	2.03	0.58
1:B:417:TRP:CD1	8:B:895:HOH:O	2.34	0.58
1:B:447:PRO:CG	8:B:656:HOH:O	2.26	0.58
1:A:453:SER:OG	1:A:455:GLN:HG3	2.04	0.57
1:B:353:LYS:HD2	8:B:633:HOH:O	2.03	0.57
1:B:230:LEU:HD21	8:B:636:HOH:O	2.04	0.57
1:B:174:ASP:HB3	1:B:236:ASN:HB2	1.86	0.57
1:B:446:SER:CB	8:B:869:HOH:O	2.48	0.57
1:B:46:TRP:HH2	1:B:64:ILE:HD12	1.70	0.57
1:B:380:ILE:CD1	8:B:689:HOH:O	2.50	0.57
1:A:294:GLY:CA	1:A:331:GLN:HA	2.34	0.57
1:B:46:TRP:HB3	8:B:634:HOH:O	1.98	0.57
1:B:87:THR:HG21	1:B:552:TYR:HE2	1.70	0.57
1:A:436:HIS:HA	3:A:610:CL:CL	2.42	0.57
1:A:174:ASP:HB3	1:A:236:ASN:HB2	1.87	0.57
1:B:174:ASP:HB2	1:B:195:SER:HB3	1.87	0.57
1:B:416:TYR:CD1	1:B:416:TYR:N	2.73	0.57
1:A:141:PHE:HA	8:A:642:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:THR:HG21	1:B:552:TYR:CE2	2.39	0.57
8:A:653:HOH:O	1:B:194:PHE:CD2	2.52	0.56
1:B:95:HIS:C	1:B:95:HIS:CD2	2.79	0.56
1:A:216:ASN:CG	4:A:720:NAG:H82	2.24	0.56
1:A:479:THR:HG22	8:A:895:HOH:O	2.04	0.56
1:B:385:GLY:O	1:B:544:ARG:NH1	2.31	0.56
1:A:60:ILE:HD11	1:A:149:VAL:HG13	1.88	0.56
1:A:100:LYS:HG3	8:A:680:HOH:O	2.05	0.56
1:A:103:ASN:HB2	8:A:635:HOH:O	2.05	0.56
1:A:117:PRO:HG3	1:A:543:TRP:HA	1.88	0.56
1:A:42:GLU:OE2	1:A:56:LYS:NZ	2.33	0.55
1:B:184:VAL:O	1:B:188:GLN:HG3	2.05	0.55
1:B:220:THR:HB	1:B:223:LYS:HG3	1.88	0.55
1:B:249:VAL:HG21	1:B:265:LEU:HD21	1.88	0.55
1:B:360:PRO:HG2	1:B:376:ASN:HA	1.88	0.55
1:B:237:HIS:HE1	1:B:505:ILE:HD11	1.71	0.55
5:B:711:NAG:H61	8:B:734:HOH:O	2.06	0.55
1:B:464:ASP:OD1	1:B:467:ARG:HD3	2.06	0.55
1:B:145:TYR:CD2	8:B:599:HOH:O	2.57	0.55
1:A:555:ILE:HD11	8:A:571:HOH:O	2.06	0.55
1:A:90:THR:O	1:A:91:SER:HB3	2.07	0.55
1:B:302:LEU:CD1	8:B:658:HOH:O	2.55	0.55
1:B:373:TRP:CZ3	8:B:586:HOH:O	2.53	0.55
1:B:162:PRO:HG2	8:B:820:HOH:O	2.07	0.55
1:A:388:ILE:HD12	1:A:516:ASP:OD2	2.08	0.54
1:B:35:SER:HB3	8:B:764:HOH:O	2.07	0.54
1:B:315:ALA:HB1	1:B:316:PRO:HD2	1.90	0.54
1:A:34:GLN:HA	8:A:593:HOH:O	2.06	0.54
1:B:427:PHE:HA	1:B:456:ARG:HH22	1.73	0.54
1:B:100:LYS:HE3	8:B:576:HOH:O	2.07	0.54
1:A:27:THR:OG1	1:A:130:ARG:NH1	2.40	0.54
1:A:290:VAL:HB	1:A:306:PRO:HB2	1.89	0.54
1:A:306:PRO:HG2	8:A:597:HOH:O	2.00	0.54
1:A:223:LYS:O	1:A:225:HIS:CE1	2.60	0.54
1:B:348:VAL:HG21	1:B:470:GLY:H	1.72	0.54
1:A:422:ASP:N	1:A:423:PRO:CD	2.69	0.54
1:B:36:TYR:O	1:B:79:VAL:HA	2.08	0.54
5:B:710:NAG:H62	8:B:560:HOH:O	2.07	0.54
1:B:559:LEU:HD22	8:B:623:HOH:O	2.08	0.54
1:A:559:LEU:HD11	8:A:690:HOH:O	2.04	0.54
1:A:292:PHE:CE1	1:A:300:GLY:HA2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:2001:KIB:C7	8:B:819:HOH:O	2.45	0.54
1:B:104:LEU:HD22	1:B:532:ASP:HB3	1.89	0.53
1:B:117:PRO:O	1:B:121:GLY:HA3	2.08	0.53
1:B:371:PHE:CB	8:B:819:HOH:O	2.55	0.53
1:B:64:ILE:HG13	1:B:64:ILE:O	2.08	0.53
1:A:384:TRP:NE1	8:A:642:HOH:O	2.39	0.53
1:A:311:HIS:NE2	1:A:316:PRO:O	2.40	0.53
1:B:354:ARG:CB	1:B:356:ASP:OD1	2.57	0.53
1:A:413:GLN:NE2	8:A:806:HOH:O	2.39	0.53
1:A:419:ILE:N	1:A:419:ILE:HD12	2.23	0.53
1:A:424:GLU:HB3	8:A:904:HOH:O	2.08	0.53
1:B:163:TYR:HA	1:B:224:ARG:HB2	1.91	0.53
1:A:302:LEU:CD1	8:B:766:HOH:O	2.47	0.53
1:B:217:VAL:HG13	8:B:744:HOH:O	2.09	0.53
1:B:104:LEU:CD2	1:B:528:ILE:HG23	2.39	0.52
1:B:82:ILE:CD1	1:B:122:GLN:NE2	2.72	0.52
1:B:263:ASP:HB2	8:B:805:HOH:O	2.09	0.52
1:B:520:ARG:NH2	1:B:523:ASP:CG	2.59	0.52
1:B:438:HIS:NE2	1:B:519:GLU:OE1	2.34	0.52
1:B:308:ALA:CA	8:B:923:HOH:O	2.58	0.52
1:B:87:THR:HG23	8:B:560:HOH:O	2.09	0.52
1:A:19:ILE:HG13	1:A:341:VAL:HG11	1.92	0.52
1:B:384:TRP:HH2	8:B:937:HOH:O	1.93	0.52
1:B:355:PRO:HB3	8:B:622:HOH:O	2.09	0.52
1:A:406:VAL:HB	8:A:888:HOH:O	2.10	0.52
1:B:39:ASN:OD1	1:B:84:ASN:ND2	2.39	0.52
1:A:344:ARG:NH2	8:A:605:HOH:O	2.42	0.51
1:B:450:PRO:HB2	1:B:453:SER:HB3	1.91	0.51
1:A:384:TRP:CZ2	8:A:642:HOH:O	2.62	0.51
1:B:487:LEU:HD21	8:B:588:HOH:O	2.09	0.51
1:B:249:VAL:CG2	1:B:265:LEU:HD21	2.41	0.51
1:B:200:ILE:HD13	8:B:772:HOH:O	2.04	0.51
1:A:423:PRO:CA	8:A:662:HOH:O	2.49	0.51
5:A:711:NAG:C6	8:A:721:HOH:O	2.58	0.51
1:B:321:THR:HG21	8:B:933:HOH:O	2.11	0.51
1:B:174:ASP:CG	1:B:233:SER:HB3	2.30	0.51
1:B:493:THR:O	1:B:520:ARG:HD2	2.11	0.51
1:B:104:LEU:HD22	1:B:528:ILE:HG23	1.93	0.51
1:A:58:MET:HG2	1:A:85:LEU:HD22	1.92	0.51
1:A:302:LEU:CD2	8:B:766:HOH:O	2.56	0.50
1:A:371:PHE:CD1	7:A:1001:KIB:C8	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:HD11	1:B:122:GLN:NE2	2.26	0.50
1:A:46:TRP:CE3	1:A:57:VAL:HG11	2.46	0.50
1:B:267:LEU:N	1:B:267:LEU:HD12	2.26	0.50
1:A:416:TYR:HD1	8:A:787:HOH:O	1.94	0.50
1:B:393:LEU:HD21	1:B:528:ILE:HD12	1.93	0.50
1:B:346:VAL:O	8:B:698:HOH:O	2.19	0.50
1:A:440:PHE:O	1:A:475:ARG:HA	2.12	0.50
1:B:23:TYR:N	1:B:23:TYR:CD2	2.78	0.50
1:B:552:TYR:OH	8:B:692:HOH:O	2.15	0.50
1:B:559:LEU:O	8:B:921:HOH:O	2.19	0.50
1:B:271:GLN:HE21	1:B:476:ARG:NE	2.09	0.50
5:A:710:NAG:H61	8:A:786:HOH:O	2.11	0.50
1:A:490:ALA:CB	8:A:852:HOH:O	2.60	0.50
1:B:99:GLN:HB3	1:B:102:THR:O	2.12	0.50
1:A:250:ILE:O	1:A:251:ALA:HB2	2.12	0.50
1:B:295:GLN:CD	8:B:769:HOH:O	2.49	0.50
1:B:245:HIS:CE1	1:B:281:ARG:HG3	2.47	0.50
1:A:239:GLN:HG2	1:A:330:HIS:CD2	2.47	0.50
1:B:98:HIS:NE2	1:B:131:GLN:OE1	2.45	0.50
1:B:46:TRP:CE3	1:B:57:VAL:HG11	2.47	0.50
1:B:234:THR:O	1:B:505:ILE:HA	2.12	0.49
1:A:141:PHE:CG	8:A:642:HOH:O	2.58	0.49
1:A:428:SER:CB	1:A:484:GLY:H	2.24	0.49
1:A:131:GLN:HB2	8:A:561:HOH:O	2.11	0.49
1:B:473:PRO:O	1:B:474:PRO:C	2.47	0.49
1:A:543:TRP:CG	8:A:792:HOH:O	2.65	0.49
1:B:95:HIS:O	1:B:135:SER:CB	2.58	0.49
1:B:331:GLN:O	1:B:332:CYS:HB2	2.11	0.49
1:A:546:TYR:O	1:A:549:THR:OG1	2.26	0.49
1:A:169:VAL:HA	1:A:228:ARG:HB2	1.94	0.49
1:B:122:GLN:CG	8:B:832:HOH:O	2.61	0.49
1:B:285:ASN:OD1	1:B:311:HIS:CD2	2.62	0.49
1:B:355:PRO:CB	8:B:622:HOH:O	2.60	0.49
1:A:134:THR:HG21	1:A:228:ARG:HB3	1.94	0.49
1:A:552:TYR:CD1	5:A:711:NAG:H62	2.48	0.49
1:A:287:TRP:CE2	1:A:320:PRO:HB2	2.48	0.49
1:B:209:THR:CB	1:B:211:GLU:OE2	2.61	0.49
1:A:64:ILE:CG2	8:A:821:HOH:O	2.61	0.49
1:B:435:LEU:HG	8:B:717:HOH:O	2.13	0.49
1:A:454:GLN:HG2	8:B:660:HOH:O	2.13	0.49
1:B:237:HIS:NE2	1:B:432:PRO:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:GLN:N	1:B:531:GLU:OE1	2.46	0.48
1:A:427:PHE:HA	1:A:456:ARG:HH12	1.78	0.48
1:A:523:ASP:O	1:A:527:ARG:HG3	2.13	0.48
1:A:393:LEU:CD2	8:A:890:HOH:O	2.62	0.48
1:B:200:ILE:CD1	8:B:923:HOH:O	2.54	0.48
1:B:428:SER:HB3	1:B:484:GLY:N	2.16	0.48
1:B:544:ARG:NH1	8:B:831:HOH:O	2.46	0.48
1:B:467:ARG:NH2	8:B:900:HOH:O	2.34	0.48
1:B:103:ASN:HB2	8:B:748:HOH:O	2.12	0.48
1:B:447:PRO:CB	8:B:656:HOH:O	2.57	0.48
1:A:103:ASN:N	8:A:635:HOH:O	2.46	0.48
1:B:76:THR:CG2	1:B:126:ARG:HG3	2.43	0.48
1:B:479:THR:CG2	8:B:588:HOH:O	2.54	0.48
1:A:484:GLY:CA	8:A:662:HOH:O	2.46	0.48
1:B:543:TRP:CZ2	1:B:547:TRP:CE3	3.02	0.48
1:A:449:VAL:HB	1:A:455:GLN:NE2	2.29	0.48
1:A:331:GLN:OE1	1:A:450:PRO:HA	2.13	0.48
1:A:266:PHE:CE1	1:A:332:CYS:HA	2.49	0.48
1:B:174:ASP:OD1	1:B:233:SER:HB3	2.14	0.47
1:B:97:ILE:CD1	8:B:917:HOH:O	2.23	0.47
1:B:308:ALA:CB	8:B:923:HOH:O	2.40	0.47
1:A:434:HIS:CD2	1:A:504:HIS:HD2	2.32	0.47
1:A:529:SER:OG	1:A:531:GLU:HG2	2.14	0.47
1:B:184:VAL:HG12	1:B:185:HIS:N	2.29	0.47
1:A:530:GLN:OE1	1:A:530:GLN:HA	2.14	0.47
1:B:304:PRO:O	8:B:914:HOH:O	2.20	0.47
1:B:268:ALA:O	1:B:269:VAL:C	2.50	0.47
1:A:384:TRP:CZ3	1:A:554:LYS:HD2	2.49	0.47
1:A:267:LEU:HG	1:A:273:TYR:HD2	1.79	0.47
1:B:445:ARG:HD3	8:B:582:HOH:O	2.13	0.47
1:B:476:ARG:CG	8:B:668:HOH:O	2.55	0.47
1:B:336:LEU:HD22	1:B:474:PRO:HG2	1.96	0.47
1:B:7:PRO:HB3	1:B:164:ASP:HA	1.95	0.47
1:A:95:HIS:O	1:A:135:SER:CB	2.56	0.47
5:B:711:NAG:C6	8:B:734:HOH:O	2.63	0.47
1:A:1:GLU:HG3	8:A:777:HOH:O	2.13	0.47
1:B:381:ASN:O	1:B:402:SER:HB3	2.14	0.47
1:A:245:HIS:CE1	1:A:281:ARG:HG3	2.49	0.47
1:A:336:LEU:HD21	1:A:442:VAL:HG11	1.96	0.47
1:B:449:VAL:CG2	8:B:932:HOH:O	2.28	0.47
1:A:305:HIS:O	1:A:306:PRO:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:VAL:CG2	8:B:756:HOH:O	2.63	0.47
1:A:449:VAL:HG21	8:A:796:HOH:O	2.14	0.47
1:A:100:LYS:HE3	1:A:100:LYS:HB2	1.82	0.47
1:B:354:ARG:HB3	1:B:356:ASP:OD1	2.14	0.47
1:B:248:THR:CG2	1:B:259:ALA:HB1	2.44	0.47
1:B:228:ARG:O	1:B:230:LEU:HD12	2.14	0.47
1:A:4:CYS:SG	8:A:628:HOH:O	2.11	0.47
1:A:115:PRO:HG2	8:A:792:HOH:O	2.14	0.47
1:A:434:HIS:HD2	1:A:504:HIS:HD2	1.63	0.47
1:B:111:VAL:HG21	1:B:500:LEU:HD21	1.97	0.47
1:A:251:ALA:HA	1:A:257:VAL:HG22	1.95	0.47
1:B:22:ASP:HB3	1:B:25:VAL:HG22	1.96	0.47
1:B:500:LEU:CD1	8:B:623:HOH:O	2.60	0.46
1:A:64:ILE:HA	8:A:667:HOH:O	2.15	0.46
1:B:306:PRO:O	8:B:624:HOH:O	2.20	0.46
1:A:434:HIS:HE1	3:A:610:CL:CL	2.35	0.46
1:B:93:HIS:HA	1:B:106:ASP:O	2.15	0.46
1:A:359:LEU:HD22	1:A:515:VAL:HG11	1.97	0.46
1:B:104:LEU:CD2	1:B:532:ASP:HB3	2.45	0.46
1:B:100:LYS:HD3	1:B:100:LYS:HA	1.52	0.46
1:B:58:MET:HG3	1:B:147:ASN:HB3	1.97	0.46
1:B:142:SER:HG	1:B:556:ASP:CG	2.14	0.46
1:A:434:HIS:HA	1:A:477:ASP:O	2.15	0.46
1:A:533:GLU:O	1:A:536:PHE:HB3	2.16	0.46
1:B:131:GLN:O	1:B:254:MET:CE	2.64	0.46
1:B:122:GLN:HG2	8:B:832:HOH:O	2.15	0.46
1:B:91:SER:O	1:B:91:SER:OG	2.33	0.46
1:A:354:ARG:NH1	1:A:356:ASP:OD1	2.49	0.46
1:B:386:LYS:HE3	1:B:390:ASP:OD2	2.15	0.46
1:B:332:CYS:C	1:B:333:LEU:HD23	2.35	0.46
1:A:253:ASP:OD2	1:A:476:ARG:HB2	2.15	0.46
1:B:19:ILE:CG1	8:B:911:HOH:O	2.44	0.46
1:B:349:ASN:HB3	8:B:661:HOH:O	2.16	0.46
1:B:91:SER:CB	8:B:747:HOH:O	2.52	0.46
1:B:315:ALA:HB1	1:B:316:PRO:CD	2.46	0.46
1:A:138:HIS:HB2	1:A:145:TYR:CB	2.46	0.46
1:B:131:GLN:HB3	8:B:629:HOH:O	2.16	0.45
1:B:215:ALA:HB3	1:B:308:ALA:HB2	1.97	0.45
1:A:335:THR:CG2	8:A:791:HOH:O	2.65	0.45
1:B:348:VAL:HG21	1:B:470:GLY:N	2.31	0.45
1:A:344:ARG:CZ	8:A:605:HOH:O	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLN:HB3	8:A:645:HOH:O	2.16	0.45
1:A:145:TYR:OH	1:A:234:THR:HA	2.15	0.45
1:B:1:GLU:HG3	1:B:2:PRO:CD	2.42	0.45
1:A:138:HIS:HE1	8:A:568:HOH:O	1.99	0.45
1:B:23:TYR:CB	8:B:627:HOH:O	2.32	0.45
1:A:468:LEU:CD1	1:A:488:LEU:CD2	2.94	0.45
1:A:111:VAL:HG13	1:A:516:ASP:OD2	2.17	0.45
1:A:13:TRP:CE3	1:A:157:GLY:HA2	2.52	0.45
1:B:223:LYS:O	1:B:225:HIS:CE1	2.70	0.45
1:A:248:THR:HA	1:A:261:THR:HA	1.98	0.45
1:B:244:ASN:HA	1:B:244:ASN:HD22	1.59	0.45
1:A:271:GLN:CG	1:A:476:ARG:NH2	2.66	0.45
1:A:384:TRP:CE2	8:A:642:HOH:O	2.55	0.45
1:B:76:THR:HG21	1:B:126:ARG:HG3	1.98	0.45
1:A:118:PRO:CG	1:A:546:TYR:CE1	2.99	0.45
1:B:432:PRO:O	1:B:504:HIS:N	2.45	0.45
1:A:384:TRP:CE3	1:A:554:LYS:HD2	2.52	0.45
1:A:64:ILE:HG21	8:A:821:HOH:O	2.16	0.44
1:B:215:ALA:HB3	1:B:308:ALA:CB	2.47	0.44
1:B:122:GLN:NE2	8:B:832:HOH:O	2.50	0.44
1:A:118:PRO:HG3	1:A:546:TYR:CE1	2.52	0.44
1:A:391:TYR:OH	1:A:400:PRO:HD3	2.17	0.44
1:B:132:TYR:CD1	1:B:132:TYR:N	2.85	0.44
1:B:192:PRO:HD3	7:B:2001:KIB:C1	2.47	0.44
1:A:468:LEU:HD13	1:A:488:LEU:HD23	1.99	0.44
1:A:386:LYS:N	1:A:387:PRO:HD3	2.32	0.44
1:A:206:ASN:C	1:A:208:ASN:H	2.20	0.44
1:B:86:VAL:O	1:B:119:LYS:HE2	2.18	0.44
1:B:19:ILE:CD1	8:B:911:HOH:O	2.64	0.44
1:B:325:THR:HG23	8:B:859:HOH:O	2.17	0.44
1:A:94:TRP:O	8:A:782:HOH:O	2.21	0.44
1:B:136:TRP:CZ3	1:B:138:HIS:CD2	3.05	0.44
1:B:111:VAL:HG21	1:B:500:LEU:CD2	2.48	0.44
1:B:440:PHE:O	1:B:475:ARG:HA	2.18	0.44
1:A:427:PHE:HB3	8:A:696:HOH:O	2.17	0.44
1:A:287:TRP:CH2	5:A:730:NAG:H62	2.52	0.44
1:B:209:THR:HG21	1:B:211:GLU:OE2	2.18	0.44
1:B:136:TRP:CH2	1:B:138:HIS:CD2	3.06	0.44
1:A:518:LEU:CG	1:A:521:PRO:HG3	2.41	0.44
1:B:182:ASP:OD1	8:B:841:HOH:O	2.21	0.44
1:B:177:TYR:CE2	1:B:196:ASP:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LEU:CD2	8:B:835:HOH:O	2.66	0.43
1:B:482:PRO:HA	8:B:835:HOH:O	2.16	0.43
1:B:552:TYR:CD1	5:B:711:NAG:H62	2.52	0.43
1:B:443:LEU:HD11	1:B:490:ALA:HB2	1.99	0.43
1:B:230:LEU:HG	1:B:272:ARG:HG2	2.00	0.43
1:B:449:VAL:HB	1:B:455:GLN:NE2	2.33	0.43
1:A:287:TRP:CZ2	5:A:730:NAG:H62	2.53	0.43
1:A:490:ALA:HB1	8:A:852:HOH:O	2.18	0.43
1:A:427:PHE:CA	1:A:456:ARG:HH12	2.31	0.43
1:A:453:SER:CB	8:A:653:HOH:O	2.55	0.43
1:A:292:PHE:CD1	1:A:300:GLY:HA2	2.53	0.43
1:A:58:MET:HG2	1:A:85:LEU:CD2	2.47	0.43
1:B:15:ASP:HA	8:B:929:HOH:O	2.19	0.43
1:A:393:LEU:HD23	8:A:890:HOH:O	2.19	0.43
1:B:253:ASP:OD2	1:B:476:ARG:HB2	2.19	0.43
1:B:389:ILE:O	1:B:393:LEU:HG	2.18	0.43
1:A:37:VAL:CG1	1:A:82:ILE:CD1	2.95	0.43
1:B:218:THR:CG2	1:B:313:ALA:HB2	2.48	0.43
1:A:213:GLN:NE2	8:A:708:HOH:O	2.35	0.43
1:A:37:VAL:HG13	1:A:82:ILE:HD12	1.97	0.43
1:B:354:ARG:HB2	1:B:356:ASP:OD1	2.18	0.43
1:B:446:SER:OG	1:B:482:PRO:HG2	2.18	0.43
1:A:479:THR:HG23	1:A:487:LEU:HD21	2.00	0.43
1:A:103:ASN:ND2	1:A:499:TRP:CZ3	2.82	0.43
1:B:440:PHE:CD1	1:B:489:LEU:HD22	2.53	0.43
1:A:10:ARG:O	1:A:158:PRO:HA	2.19	0.43
1:B:531:GLU:N	1:B:531:GLU:OE1	2.48	0.42
1:B:339:ARG:HG3	8:B:706:HOH:O	2.17	0.42
1:B:446:SER:CA	8:B:869:HOH:O	2.67	0.42
1:B:271:GLN:NE2	1:B:476:ARG:NE	2.65	0.42
1:A:105:HIS:ND1	1:A:125:TYR:HA	2.34	0.42
1:B:131:GLN:O	1:B:254:MET:HE2	2.18	0.42
1:B:244:ASN:ND2	1:B:281:ARG:NH1	2.58	0.42
1:A:36:TYR:O	1:A:79:VAL:HA	2.19	0.42
1:A:11:ALA:O	1:A:158:PRO:HB3	2.20	0.42
1:B:38:PHE:HE1	1:B:67:PRO:CG	2.21	0.42
1:B:200:ILE:O	1:B:215:ALA:HB2	2.18	0.42
1:A:206:ASN:OD1	1:A:208:ASN:HB2	2.19	0.42
1:A:334:ASP:N	1:A:334:ASP:OD1	2.51	0.42
1:A:93:HIS:O	1:A:137:TYR:HA	2.20	0.42
1:B:526:GLN:HE21	1:B:526:GLN:HB2	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:HIS:HA	1:B:477:ASP:O	2.20	0.42
1:A:385:GLY:N	8:A:853:HOH:O	2.52	0.42
1:B:48:GLY:HA3	8:B:567:HOH:O	2.19	0.42
1:B:197:ASN:ND2	8:B:783:HOH:O	2.48	0.42
1:B:244:ASN:OD1	8:B:826:HOH:O	2.22	0.42
1:B:185:HIS:CD2	1:B:185:HIS:C	2.93	0.42
1:B:295:GLN:CG	8:B:611:HOH:O	2.48	0.42
1:B:311:HIS:NE2	1:B:316:PRO:O	2.53	0.42
1:B:353:LYS:CD	8:B:633:HOH:O	2.65	0.42
1:B:283:PRO:HA	1:B:312:TYR:CD2	2.54	0.42
1:A:95:HIS:HD2	1:A:272:ARG:HH12	1.61	0.42
8:A:653:HOH:O	1:B:194:PHE:HD2	1.95	0.42
1:A:100:LYS:CG	8:A:680:HOH:O	2.68	0.42
1:B:456:ARG:CG	8:B:881:HOH:O	2.67	0.42
1:B:11:ALA:HB2	8:B:777:HOH:O	2.20	0.42
1:A:380:ILE:HG23	1:A:557:SER:HB2	2.01	0.42
1:B:461:PRO:HG2	8:B:824:HOH:O	2.20	0.41
1:B:233:SER:O	1:B:269:VAL:HG13	2.20	0.41
1:B:508:HIS:NE2	7:B:2001:KIB:H7B	2.36	0.41
1:A:46:TRP:CG	1:A:57:VAL:HG21	2.55	0.41
1:A:360:PRO:HG2	1:A:376:ASN:HA	2.02	0.41
1:B:135:SER:HB2	1:B:136:TRP:H	1.68	0.41
1:B:104:LEU:HD21	1:B:528:ILE:CG2	2.50	0.41
1:B:56:LYS:HE3	5:B:710:NAG:O6	2.20	0.41
1:A:346:VAL:HG21	8:A:852:HOH:O	2.21	0.41
1:A:340:PRO:HG2	8:A:631:HOH:O	2.19	0.41
1:A:423:PRO:HG3	8:A:765:HOH:O	2.20	0.41
1:A:36:TYR:CB	1:A:79:VAL:HG22	2.43	0.41
1:B:471:ASP:OD2	8:B:872:HOH:O	2.20	0.41
1:B:289:ASN:OD1	5:B:730:NAG:H82	2.20	0.41
1:A:12:CYS:CB	8:A:628:HOH:O	1.97	0.41
1:B:81:VAL:HG21	1:B:125:TYR:HE1	1.85	0.41
1:B:305:HIS:O	1:B:306:PRO:C	2.59	0.41
1:A:87:THR:O	1:A:550:ASN:ND2	2.53	0.41
1:B:197:ASN:ND2	1:B:205:VAL:O	2.51	0.41
1:A:428:SER:OG	1:A:484:GLY:N	2.44	0.41
1:B:237:HIS:CD2	1:B:268:ALA:CB	3.03	0.41
1:B:505:ILE:CD1	8:B:684:HOH:O	2.22	0.41
1:B:97:ILE:CA	8:B:917:HOH:O	2.60	0.41
1:A:481:LEU:HA	1:A:487:LEU:HD22	2.02	0.41
1:B:401:VAL:HG23	1:B:402:SER:N	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TYR:CE1	1:A:69:ILE:HG23	2.56	0.41
1:B:99:GLN:OE1	1:B:127:TRP:HB3	2.21	0.41
1:A:454:GLN:NE2	8:A:884:HOH:O	2.53	0.41
1:B:282:ALA:HA	1:B:283:PRO:HD3	1.77	0.41
1:B:555:ILE:HD13	8:B:608:HOH:O	2.20	0.41
1:B:94:TRP:CD1	1:B:94:TRP:N	2.86	0.41
1:B:460:ASP:HA	1:B:461:PRO:HD2	1.88	0.41
1:B:401:VAL:CG2	1:B:402:SER:H	2.22	0.41
1:A:521:PRO:HA	1:A:524:LEU:HD23	2.03	0.41
1:A:291:THR:HG23	8:A:596:HOH:O	2.21	0.41
1:A:14:SER:OG	1:A:17:PHE:HB2	2.21	0.41
1:B:94:TRP:O	1:B:97:ILE:HB	2.21	0.40
1:B:78:GLU:HA	1:B:125:TYR:O	2.21	0.40
1:B:159:ALA:HB1	1:B:250:ILE:HD12	2.03	0.40
1:A:28:PRO:HD3	1:A:73:TRP:CE2	2.56	0.40
1:B:397:THR:OG1	1:B:397:THR:O	2.34	0.40
1:B:207:PRO:HG3	1:B:303:ASN:HA	2.04	0.40
1:A:176:TYR:CB	1:A:183:LEU:HD11	2.52	0.40
1:B:131:GLN:NE2	1:B:254:MET:HB3	2.35	0.40
1:A:521:PRO:O	1:A:524:LEU:HB3	2.21	0.40
1:B:479:THR:HG21	1:B:489:LEU:HD21	2.03	0.40
1:A:265:LEU:CD2	8:A:791:HOH:O	2.70	0.40
1:A:206:ASN:HB3	1:A:209:THR:OG1	2.21	0.40
1:B:236:ASN:HB3	1:B:238:PHE:CE1	2.55	0.40
1:A:399:TYR:CZ	1:A:518:LEU:CD2	3.04	0.40
1:A:555:ILE:HG12	8:A:867:HOH:O	2.21	0.40
1:A:18:ASP:HB2	1:A:19:ILE:H	1.67	0.40
1:A:287:TRP:CE2	5:A:730:NAG:H5	2.57	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)
1:B:78:GLU:OE2	4:A:700:NAG:O7[3_545]	2.04	0.16

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	557/559 (100%)	504 (90%)	47 (8%)	6 (1%)	17	9
1	B	557/559 (100%)	502 (90%)	50 (9%)	5 (1%)	21	13
All	All	1114/1118 (100%)	1006 (90%)	97 (9%)	11 (1%)	19	11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	SER
1	B	402	SER
1	A	91	SER
1	A	493	THR
1	B	15	ASP
1	B	100	LYS
1	B	484	GLY
1	A	268	ALA
1	B	401	VAL
1	A	100	LYS
1	A	149	VAL

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	478/478 (100%)	444 (93%)	34 (7%)	18	12
1	B	478/478 (100%)	447 (94%)	31 (6%)	21	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	956/956 (100%)	891 (93%)	65 (7%)	20	13

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	40	LEU
1	A	59	LEU
1	A	65	MET
1	A	80	THR
1	A	88	ASN
1	A	91	SER
1	A	100	LYS
1	A	109	ASN
1	A	123	ARG
1	A	140	HIS
1	A	144	GLN
1	A	150	VAL
1	A	189	ASN
1	A	211	GLU
1	A	224	ARG
1	A	230	LEU
1	A	254	MET
1	A	272	ARG
1	A	277	ILE
1	A	295	GLN
1	A	349	ASN
1	A	355	PRO
1	A	422	ASP
1	A	424	GLU
1	A	434	HIS
1	A	454	GLN
1	A	456	ARG
1	A	465	LEU
1	A	477	ASP
1	A	487	LEU
1	A	503	CYS
1	A	507	TRP
1	A	513	LEU
1	B	1	GLU
1	B	9	ASN
1	B	12	CYS

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Mol	Chain	Res	Type
1	B	40	LEU
1	B	64	ILE
1	B	95	HIS
1	B	100	LYS
1	B	109	ASN
1	B	122	GLN
1	B	123	ARG
1	B	135	SER
1	B	140	HIS
1	B	223	LYS
1	B	244	ASN
1	B	254	MET
1	B	272	ARG
1	B	281	ARG
1	B	338	VAL
1	B	340	PRO
1	B	355	PRO
1	B	397	THR
1	B	440	PHE
1	B	450	PRO
1	B	487	LEU
1	B	493	THR
1	B	507	TRP
1	B	510	SER
1	B	513	LEU
1	B	520	ARG
1	B	526	GLN
1	B	556	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	95	HIS
1	A	122	GLN
1	A	154	GLN
1	A	156	ASN
1	A	185	HIS
1	A	236	ASN
1	A	295	GLN
1	A	311	HIS
1	A	349	ASN

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Mol	Chain	Res	Type
1	B	63	ASN
1	B	122	GLN
1	B	131	GLN
1	B	185	HIS
1	B	244	ASN
1	B	271	GLN
1	B	311	HIS
1	B	455	GLN
1	B	526	GLN
1	B	550	ASN

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 ⓘ

8 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$
5	NAG	A	710	1,5	14,14,15	1.16	1 (7%)	15,19,21	3.22	5 (33%)
5	NAG	A	711	5	14,14,15	0.98	1 (7%)	15,19,21	1.97	4 (26%)
5	NAG	A	730	1,5	14,14,15	1.34	2 (14%)	15,19,21	3.49	8 (53%)
5	NAG	A	731	5	14,14,15	1.61	4 (28%)	15,19,21	2.37	5 (33%)
5	NAG	B	710	1,5	14,14,15	1.10	1 (7%)	15,19,21	2.16	4 (26%)
5	NAG	B	711	5	14,14,15	0.88	0	15,19,21	1.05	0
5	NAG	B	730	1,5	14,14,15	1.58	3 (21%)	15,19,21	5.08	11 (73%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	731	5	14,14,15	1.45	2 (14%)	15,19,21	3.73	8 (53%)

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
5	NAG	A	710	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	711	5	-	0/6/23/26	0/1/1/1
5	NAG	A	730	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	731	5	-	0/6/23/26	0/1/1/1
5	NAG	B	710	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	711	5	-	0/6/23/26	0/1/1/1
5	NAG	B	730	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	731	5	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	730	NAG	O5-C5	-3.58	1.35	1.43
5	A	731	NAG	C1-C2	-3.39	1.47	1.52
5	B	731	NAG	O5-C5	-3.13	1.36	1.43
5	B	731	NAG	O5-C1	-3.09	1.38	1.43
5	A	730	NAG	O5-C1	-2.86	1.38	1.43
5	B	730	NAG	O5-C1	-2.79	1.39	1.43
5	B	730	NAG	C3-C2	-2.75	1.46	1.52
5	A	731	NAG	O5-C1	-2.46	1.39	1.43
5	A	731	NAG	C2-N2	-2.46	1.42	1.46
5	A	711	NAG	O3-C3	-2.09	1.38	1.43
5	A	731	NAG	O7-C7	2.17	1.28	1.23
5	A	710	NAG	C1-C2	2.32	1.55	1.52
5	B	710	NAG	C1-C2	2.43	1.55	1.52
5	A	730	NAG	C2-N2	3.63	1.52	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	731	NAG	C1-O5-C5	-10.00	99.56	112.25
5	B	730	NAG	O4-C4-C3	-8.01	92.31	110.34
5	A	731	NAG	C2-N2-C7	-7.35	113.59	123.04
5	A	730	NAG	C3-C2-N2	-7.25	93.20	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	730	NAG	C2-N2-C7	-5.43	116.07	123.04
5	B	731	NAG	O6-C6-C5	-5.17	94.24	111.33
5	B	730	NAG	O7-C7-C8	-4.91	113.05	122.06
5	A	710	NAG	C2-N2-C7	-4.81	116.86	123.04
5	B	730	NAG	C3-C2-N2	-4.42	99.98	110.56
5	A	711	NAG	C3-C4-C5	-4.05	103.14	110.20
5	B	730	NAG	O5-C5-C6	-3.97	98.75	107.35
5	B	710	NAG	O5-C5-C6	-3.96	98.77	107.35
5	A	730	NAG	O7-C7-C8	-3.73	115.21	122.06
5	B	731	NAG	O4-C4-C3	-3.72	101.95	110.34
5	B	710	NAG	C4-C3-C2	-3.51	105.77	111.23
5	A	730	NAG	C1-O5-C5	-3.51	107.80	112.25
5	A	710	NAG	O7-C7-C8	-3.35	115.91	122.06
5	A	711	NAG	O3-C3-C2	-3.23	102.72	109.11
5	A	731	NAG	C3-C4-C5	-2.81	105.29	110.20
5	B	710	NAG	C8-C7-N2	-2.46	111.40	116.11
5	A	711	NAG	C3-C2-N2	-2.22	105.25	110.56
5	B	730	NAG	O3-C3-C2	-2.15	104.86	109.11
5	A	710	NAG	O3-C3-C4	-2.07	105.67	110.34
5	A	731	NAG	C8-C7-N2	-2.00	112.27	116.11
5	A	731	NAG	C3-C2-N2	2.07	115.53	110.56
5	A	730	NAG	C4-C3-C2	2.39	114.94	111.23
5	B	731	NAG	C8-C7-N2	2.62	121.12	116.11
5	A	731	NAG	C6-C5-C4	2.70	119.68	113.02
5	B	731	NAG	O3-C3-C2	2.91	114.88	109.11
5	B	730	NAG	O3-C3-C4	3.07	117.25	110.34
5	B	731	NAG	C2-N2-C7	3.09	127.00	123.04
5	B	730	NAG	C4-C3-C2	3.10	116.05	111.23
5	A	730	NAG	O5-C5-C6	3.23	114.35	107.35
5	B	731	NAG	C4-C3-C2	3.29	116.34	111.23
5	A	710	NAG	C3-C4-C5	3.44	116.19	110.20
5	B	730	NAG	O7-C7-N2	3.56	129.12	121.86
5	A	711	NAG	O4-C4-C5	3.57	118.71	109.24
5	B	730	NAG	C6-C5-C4	3.92	122.69	113.02
5	B	710	NAG	C1-O5-C5	3.99	117.31	112.25
5	A	730	NAG	O3-C3-C2	4.08	117.19	109.11
5	B	731	NAG	C6-C5-C4	4.47	124.05	113.02
5	A	730	NAG	C8-C7-N2	5.59	126.81	116.11
5	B	730	NAG	C2-N2-C7	8.10	133.44	123.04
5	A	710	NAG	C1-O5-C5	9.76	124.64	112.25
5	B	730	NAG	C1-O5-C5	11.78	127.20	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	710	NAG	2	0
5	A	711	NAG	3	0
5	A	730	NAG	3	0
5	B	710	NAG	3	0
5	B	711	NAG	5	0
5	B	730	NAG	4	0

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 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
7	KIB	A	1001	-	12,12,12	3.13	4 (33%)	16,16,16	2.07	7 (43%)
4	NAG	A	700	1	14,14,15	1.06	1 (7%)	15,19,21	1.12	2 (13%)
4	NAG	A	720	1	14,14,15	1.05	0	15,19,21	2.47	7 (46%)
4	NAG	A	740	1	14,14,15	0.75	0	15,19,21	2.40	5 (33%)
6	SO4	A	8002	-	4,4,4	0.29	0	6,6,6	0.96	1 (16%)
7	KIB	B	2001	-	12,12,12	3.68	6 (50%)	16,16,16	1.99	5 (31%)
4	NAG	B	700	1	14,14,15	1.00	1 (7%)	15,19,21	2.72	8 (53%)
4	NAG	B	720	1	14,14,15	0.72	0	15,19,21	1.09	1 (6%)
4	NAG	B	740	1	14,14,15	0.82	1 (7%)	15,19,21	2.34	5 (33%)
4	NAG	B	760	1	14,14,15	0.90	1 (7%)	15,19,21	1.72	4 (26%)
6	SO4	B	8001	-	4,4,4	0.21	0	6,6,6	0.84	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
7	KIB	A	1001	-	-	0/4/4/4	0/1/1/1
4	NAG	A	700	1	-	0/6/23/26	0/1/1/1
4	NAG	A	720	1	-	0/6/23/26	0/1/1/1
4	NAG	A	740	1	-	0/6/23/26	0/1/1/1
6	SO4	A	8002	-	-	0/0/0/0	0/0/0/0
7	KIB	B	2001	-	-	0/4/4/4	0/1/1/1
4	NAG	B	700	1	-	0/6/23/26	0/1/1/1
4	NAG	B	720	1	-	0/6/23/26	0/1/1/1
4	NAG	B	740	1	-	0/6/23/26	0/1/1/1
4	NAG	B	760	1	-	0/6/23/26	0/1/1/1
6	SO4	B	8001	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1001	KIB	O1-C1	-4.36	1.26	1.37
7	A	1001	KIB	O2-C4	-3.73	1.28	1.37
4	A	700	NAG	O5-C1	-3.03	1.38	1.43
7	B	2001	KIB	O2-C4	-2.93	1.30	1.37
4	B	700	NAG	C4-C3	-2.15	1.46	1.52
4	B	740	NAG	C1-C2	2.00	1.55	1.52
4	B	760	NAG	C1-C2	2.32	1.55	1.52
7	B	2001	KIB	C3-C4	3.00	1.43	1.39
7	B	2001	KIB	O4-C2	3.61	1.42	1.37
7	B	2001	KIB	C5-C4	3.96	1.45	1.39
7	A	1001	KIB	C6-C1	4.01	1.45	1.40
7	B	2001	KIB	C2-C1	6.03	1.48	1.40
7	A	1001	KIB	C2-C1	7.74	1.50	1.40
7	B	2001	KIB	C6-C1	8.46	1.51	1.40

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	700	NAG	O4-C4-C3	-6.96	94.67	110.34
4	A	740	NAG	C3-C4-C5	-5.92	99.88	110.20
4	B	740	NAG	C2-N2-C7	-5.75	115.65	123.04
7	B	2001	KIB	C3-C2-C1	-4.40	116.13	120.56
4	A	720	NAG	O7-C7-C8	-4.21	114.34	122.06
4	A	740	NAG	C1-O5-C5	-3.85	107.36	112.25
7	A	1001	KIB	C5-C6-C1	-3.53	117.01	120.56
4	B	700	NAG	O3-C3-C4	-3.36	102.78	110.34
4	B	760	NAG	C2-N2-C7	-3.12	119.03	123.04
4	B	700	NAG	C3-C2-N2	-3.07	103.21	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	760	NAG	C1-O5-C5	-2.91	108.55	112.25
4	B	700	NAG	O6-C6-C5	-2.75	102.23	111.33
4	A	720	NAG	O3-C3-C2	-2.66	103.84	109.11
4	B	700	NAG	C3-C4-C5	-2.42	105.97	110.20
4	B	720	NAG	O7-C7-C8	-2.22	117.98	122.06
4	B	740	NAG	O7-C7-N2	-2.17	117.43	121.86
4	B	700	NAG	C2-N2-C7	-2.11	120.33	123.04
4	B	700	NAG	C1-O5-C5	-2.10	109.59	112.25
4	B	740	NAG	O6-C6-C5	-2.03	104.64	111.33
4	A	700	NAG	C8-C7-N2	2.01	119.95	116.11
4	A	740	NAG	O7-C7-N2	2.01	125.97	121.86
6	A	8002	SO4	O2-S-O1	2.04	115.95	109.50
7	A	1001	KIB	C6-C5-C4	2.11	122.73	119.12
7	B	2001	KIB	C5-C6-C1	2.11	122.69	120.56
4	A	700	NAG	O3-C3-C2	2.20	113.47	109.11
7	A	1001	KIB	O3-C6-C1	2.32	116.81	114.47
7	B	2001	KIB	C7-O3-C6	2.33	121.07	117.54
7	A	1001	KIB	O1-C1-C2	2.35	124.47	119.33
4	A	740	NAG	C6-C5-C4	2.36	118.83	113.02
4	B	760	NAG	O5-C5-C6	2.60	112.99	107.35
4	A	720	NAG	C2-N2-C7	2.77	126.59	123.04
7	B	2001	KIB	C2-C3-C4	2.92	124.13	119.12
4	A	720	NAG	C3-C4-C5	3.03	115.48	110.20
4	A	720	NAG	O5-C5-C6	3.11	114.08	107.35
7	A	1001	KIB	C8-O4-C2	3.13	122.29	117.54
4	A	720	NAG	O7-C7-N2	3.21	128.41	121.86
4	B	760	NAG	O3-C3-C2	3.28	115.61	109.11
4	B	700	NAG	O3-C3-C2	3.34	115.73	109.11
7	A	1001	KIB	C7-O3-C6	3.37	122.65	117.54
4	A	740	NAG	C2-N2-C7	3.45	127.47	123.04
7	B	2001	KIB	O4-C2-C1	3.56	118.06	114.47
4	B	740	NAG	C3-C4-C5	3.57	116.43	110.20
7	A	1001	KIB	O4-C2-C1	3.67	118.16	114.47
4	B	740	NAG	C8-C7-N2	3.68	123.15	116.11
4	A	720	NAG	C4-C3-C2	4.16	117.70	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1001	KIB	1	0
4	A	700	NAG	0	1
4	A	720	NAG	4	0
4	A	740	NAG	1	0
7	B	2001	KIB	7	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	559/559 (100%)	1.82	211 (37%)  	2, 12, 24, 31	0
1	B	559/559 (100%)	1.76	181 (32%)  	3, 13, 23, 32	0
All	All	1118/1118 (100%)	1.79	392 (35%)  	2, 13, 24, 32	0

All (392) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	ILE	5.1
1	A	191	ALA	5.0
1	B	547	TRP	5.0
1	B	12	CYS	4.9
1	B	391	TYR	4.9
1	A	555	ILE	4.8
1	A	552	TYR	4.8
1	A	338	VAL	4.7
1	A	111	VAL	4.7
1	A	396	ASN	4.6
1	A	547	TRP	4.5
1	A	12	CYS	4.5
1	A	394	THR	4.4
1	B	352	VAL	4.3
1	B	210	GLY	4.2
1	A	372	VAL	4.2
1	B	543	TRP	4.2
1	A	414	TRP	4.1
1	B	408	VAL	4.1
1	B	136	TRP	4.1
1	A	528	ILE	4.0
1	A	373	TRP	3.9
1	A	255	VAL	3.9
1	A	114	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	526	GLN	3.9
1	A	368	THR	3.9
1	B	87	THR	3.9
1	A	546	TYR	3.8
1	A	499	TRP	3.8
1	B	393	LEU	3.8
1	A	543	TRP	3.8
1	B	410	ALA	3.8
1	B	423	PRO	3.8
1	A	367	GLY	3.8
1	A	143	ALA	3.8
1	B	316	PRO	3.7
1	B	120	GLY	3.7
1	B	369	PRO	3.7
1	A	82	ILE	3.7
1	A	363	LEU	3.7
1	A	401	VAL	3.7
1	B	389	ILE	3.7
1	B	536	PHE	3.6
1	A	133	GLY	3.6
1	A	524	LEU	3.6
1	B	524	LEU	3.6
1	A	2	PRO	3.6
1	A	406	VAL	3.5
1	A	293	GLY	3.5
1	B	91	SER	3.5
1	A	39	ASN	3.5
1	A	551	PRO	3.4
1	B	399	TYR	3.4
1	A	136	TRP	3.4
1	B	401	VAL	3.4
1	A	553	PRO	3.4
1	A	328	VAL	3.4
1	B	238	PHE	3.3
1	B	280	SER	3.3
1	B	489	LEU	3.3
1	B	505	ILE	3.3
1	A	399	TYR	3.3
1	A	348	VAL	3.3
1	A	351	PHE	3.3
1	B	73	TRP	3.3
1	B	509	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	116	ILE	3.3
1	B	59	LEU	3.3
1	A	354	ARG	3.3
1	B	348	VAL	3.2
1	A	282	ALA	3.2
1	A	321	THR	3.2
1	A	447	PRO	3.2
1	B	551	PRO	3.2
1	A	131	GLN	3.2
1	B	396	ASN	3.2
1	A	486	TRP	3.2
1	B	378	SER	3.2
1	B	207	PRO	3.2
1	A	203	THR	3.2
1	A	443	LEU	3.2
1	B	486	TRP	3.1
1	A	298	CYS	3.1
1	A	121	GLY	3.1
1	B	28	PRO	3.1
1	B	4	CYS	3.1
1	A	366	THR	3.1
1	A	283	PRO	3.1
1	A	59	LEU	3.1
1	A	336	LEU	3.1
1	A	491	PHE	3.1
1	A	378	SER	3.1
1	A	309	ILE	3.1
1	B	309	ILE	3.1
1	A	62	GLY	3.0
1	B	425	GLY	3.0
1	A	159	ALA	3.0
1	A	548	PRO	3.0
1	B	457	PHE	3.0
1	B	397	THR	3.0
1	A	463	VAL	3.0
1	B	143	ALA	3.0
1	A	51	GLY	2.9
1	B	456	ARG	2.9
1	A	204	ALA	2.9
1	A	192	PRO	2.9
1	B	217	VAL	2.9
1	B	23	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	380	ILE	2.9
1	B	60	ILE	2.9
1	A	184	VAL	2.9
1	A	141	PHE	2.9
1	B	349	ASN	2.9
1	A	26	SER	2.9
1	A	534	ASP	2.9
1	A	539	VAL	2.9
1	B	94	TRP	2.9
1	A	545	ALA	2.9
1	A	369	PRO	2.9
1	A	536	PHE	2.9
1	B	394	THR	2.9
1	B	539	VAL	2.9
1	A	115	PRO	2.9
1	A	179	ALA	2.9
1	B	384	TRP	2.9
1	A	347	PRO	2.8
1	B	490	ALA	2.8
1	B	26	SER	2.8
1	B	175	TYR	2.8
1	B	214	TYR	2.8
1	A	417	TRP	2.8
1	B	95	HIS	2.8
1	A	87	THR	2.8
1	A	395	GLY	2.8
1	B	83	ASN	2.8
1	B	380	ILE	2.8
1	A	124	THR	2.8
1	B	205	VAL	2.8
1	B	367	GLY	2.8
1	B	292	PHE	2.8
1	A	259	ALA	2.8
1	A	104	LEU	2.8
1	A	117	PRO	2.8
1	B	283	PRO	2.8
1	A	127	TRP	2.8
1	A	540	CYS	2.8
1	B	74	GLY	2.8
1	A	391	TYR	2.7
1	B	379	ASP	2.7
1	B	46	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	290	VAL	2.7
1	A	316	PRO	2.7
1	A	411	VAL	2.7
1	B	338	VAL	2.7
1	B	372	VAL	2.7
1	A	137	TYR	2.7
1	A	397	THR	2.7
1	B	108	ALA	2.7
1	B	522	ALA	2.7
1	A	95	HIS	2.7
1	A	287	TRP	2.7
1	B	513	LEU	2.7
1	B	14	SER	2.7
1	A	150	VAL	2.7
1	B	503	CYS	2.7
1	A	134	THR	2.7
1	A	325	THR	2.7
1	B	537	ASN	2.7
1	B	487	LEU	2.7
1	A	77	VAL	2.7
1	A	456	ARG	2.7
1	B	356	ASP	2.7
1	A	376	ASN	2.7
1	A	158	PRO	2.7
1	B	350	SER	2.7
1	A	527	ARG	2.6
1	B	499	TRP	2.6
1	A	462	ALA	2.6
1	B	102	THR	2.6
1	B	321	THR	2.6
1	B	325	THR	2.6
1	A	207	PRO	2.6
1	B	158	PRO	2.6
1	A	1	GLU	2.6
1	A	518	LEU	2.6
1	B	97	ILE	2.6
1	B	555	ILE	2.6
1	B	43	VAL	2.6
1	B	213	GLN	2.6
1	A	333	LEU	2.6
1	A	500	LEU	2.6
1	B	518	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	549	THR	2.6
1	A	388	ILE	2.6
1	B	525	ARG	2.6
1	A	507	TRP	2.6
1	A	307	ALA	2.6
1	B	32	VAL	2.6
1	B	110	GLY	2.5
1	B	414	TRP	2.5
1	B	342	VAL	2.5
1	B	382	VAL	2.5
1	B	27	THR	2.5
1	B	179	ALA	2.5
1	A	199	LEU	2.5
1	B	85	LEU	2.5
1	B	465	LEU	2.5
1	B	540	CYS	2.5
1	A	221	PRO	2.5
1	A	497	GLY	2.5
1	B	155	ILE	2.5
1	A	355	PRO	2.5
1	B	90	THR	2.5
1	B	137	TYR	2.5
1	A	427	PHE	2.5
1	B	552	TYR	2.5
1	B	400	PRO	2.5
1	A	153	ILE	2.5
1	B	64	ILE	2.5
1	A	232	THR	2.5
1	B	13	TRP	2.5
1	B	25	VAL	2.4
1	A	35	SER	2.4
1	A	230	LEU	2.4
1	B	351	PHE	2.4
1	B	365	LEU	2.4
1	B	3	THR	2.4
1	B	111	VAL	2.4
1	B	403	ASP	2.4
1	A	522	ALA	2.4
1	A	384	TRP	2.4
1	A	167	LEU	2.4
1	A	465	LEU	2.4
1	B	40	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	535	ASP	2.4
1	A	424	GLU	2.4
1	B	507	TRP	2.4
1	A	299	GLY	2.4
1	A	11	ALA	2.4
1	A	320	PRO	2.4
1	B	208	ASN	2.4
1	A	218	THR	2.4
1	A	377	GLY	2.4
1	A	481	LEU	2.4
1	B	416	TYR	2.4
1	B	346	VAL	2.3
1	A	116	ILE	2.3
1	A	25	VAL	2.3
1	B	37	VAL	2.3
1	A	505	ILE	2.3
1	B	82	ILE	2.3
1	A	185	HIS	2.3
1	B	488	LEU	2.3
1	B	114	CYS	2.3
1	B	287	TRP	2.3
1	B	184	VAL	2.3
1	A	277	ILE	2.3
1	B	18	ASP	2.3
1	B	29	ASP	2.3
1	B	549	THR	2.3
1	B	162	PRO	2.3
1	A	85	LEU	2.3
1	A	175	TYR	2.3
1	A	29	ASP	2.3
1	A	352	VAL	2.3
1	A	65	MET	2.3
1	A	155	ILE	2.3
1	B	480	MET	2.3
1	B	548	PRO	2.3
1	A	180	ALA	2.3
1	A	265	LEU	2.3
1	B	204	ALA	2.3
1	B	429	LEU	2.3
1	B	66	GLY	2.3
1	A	458	VAL	2.3
1	A	387	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	313	ALA	2.3
1	A	91	SER	2.2
1	A	202	GLY	2.2
1	A	266	PHE	2.2
1	A	310	PHE	2.2
1	B	427	PHE	2.2
1	A	28	PRO	2.2
1	A	400	PRO	2.2
1	B	298	CYS	2.2
1	B	544	ARG	2.2
1	A	15	ASP	2.2
1	A	92	ILE	2.2
1	B	550	ASN	2.2
1	B	317	GLY	2.2
1	B	510	SER	2.2
1	B	267	LEU	2.2
1	A	132	TYR	2.2
1	A	254	MET	2.2
1	A	198	VAL	2.2
1	A	269	VAL	2.2
1	B	269	VAL	2.2
1	B	93	HIS	2.2
1	B	405	ILE	2.2
1	A	473	PRO	2.2
1	A	177	TYR	2.2
1	A	57	VAL	2.2
1	A	509	VAL	2.2
1	A	558	GLY	2.2
1	A	60	ILE	2.2
1	B	528	ILE	2.2
1	A	503	CYS	2.2
1	A	73	TRP	2.2
1	A	370	LEU	2.2
1	B	118	PRO	2.2
1	A	214	TYR	2.2
1	B	141	PHE	2.2
1	B	138	HIS	2.2
1	B	176	TYR	2.2
1	B	436	HIS	2.2
1	A	146	GLY	2.2
1	B	466	ALA	2.2
1	A	326	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	387	PRO	2.2
1	B	521	PRO	2.2
1	A	267	LEU	2.2
1	B	127	TRP	2.2
1	B	373	TRP	2.2
1	A	107	GLY	2.2
1	A	437	GLY	2.2
1	A	466	ALA	2.2
1	B	231	ASN	2.2
1	A	151	GLY	2.1
1	A	403	ASP	2.1
1	B	243	VAL	2.1
1	A	489	LEU	2.1
1	A	94	TRP	2.1
1	A	454	GLN	2.1
1	A	457	PHE	2.1
1	A	125	TYR	2.1
1	A	176	TYR	2.1
1	A	315	ALA	2.1
1	B	1	GLU	2.1
1	B	132	TYR	2.1
1	B	451	ALA	2.1
1	A	432	PRO	2.1
1	A	389	ILE	2.1
1	A	76	THR	2.1
1	A	358	THR	2.1
1	A	418	LEU	2.1
1	B	161	LEU	2.1
1	B	211	GLU	2.1
1	A	182	ASP	2.1
1	B	461	PRO	2.1
1	A	286	TYR	2.1
1	B	140	HIS	2.1
1	B	434	HIS	2.1
1	A	444	GLY	2.1
1	A	405	ILE	2.1
1	A	419	ILE	2.1
1	B	218	THR	2.1
1	A	441	LEU	2.1
1	A	468	LEU	2.1
1	B	7	PRO	2.1
1	A	186	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	190	ASN	2.1
1	B	10	ARG	2.1
1	A	342	VAL	2.1
1	A	515	VAL	2.1
1	B	368	THR	2.1
1	A	434	HIS	2.1
1	B	504	HIS	2.1
1	A	108	ALA	2.1
1	A	215	ALA	2.1
1	A	308	ALA	2.1
1	A	410	ALA	2.1
1	A	425	GLY	2.1
1	A	511	GLY	2.1
1	B	300	GLY	2.1
1	A	170	PHE	2.1
1	B	491	PHE	2.1
1	B	192	PRO	2.0
1	B	159	ALA	2.0
1	A	460	ASP	2.0
1	B	278	ASP	2.0
1	A	459	PHE	2.0
1	A	86	VAL	2.0
1	B	546	TYR	2.0
1	B	133	GLY	2.0
1	B	153	ILE	2.0
1	B	200	ILE	2.0
1	A	291	THR	2.0
1	A	305	HIS	2.0
1	A	32	VAL	2.0
1	B	77	VAL	2.0
1	B	31	GLY	2.0
1	B	229	ILE	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](#)

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
5	NAG	A	731	14/15	0.74	0.28	3.43	16,22,28,28	0
5	NAG	B	730	14/15	0.84	0.24	1.51	5,12,23,23	0
5	NAG	A	730	14/15	0.71	0.26	1.40	10,13,19,20	0
5	NAG	A	710	14/15	0.80	0.20	-0.72	8,16,18,18	0
5	NAG	B	710	14/15	0.81	0.20	-0.99	8,15,16,17	0
5	NAG	B	711	14/15	0.78	0.21	-1.64	9,14,18,22	0
5	NAG	A	711	14/15	0.82	0.17	-1.70	9,15,19,19	0
5	NAG	B	731	14/15	0.69	0.23	-	7,18,24,25	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	CL	A	610	1/1	0.68	0.33	4.25	41,41,41,41	0
4	NAG	A	700	14/15	0.53	0.29	0.93	26,29,32,34	0
4	NAG	B	740	14/15	0.74	0.24	0.85	17,20,25,26	0
4	NAG	B	760	14/15	0.72	0.21	0.55	8,15,27,28	0
4	NAG	A	740	14/15	0.66	0.26	0.50	8,23,27,28	0
7	KIB	A	1001	12/12	0.70	0.26	0.44	7,17,20,23	0
4	NAG	A	720	14/15	0.77	0.21	0.07	16,22,33,33	0
4	NAG	B	700	14/15	0.76	0.21	-0.10	9,17,19,24	0
7	KIB	B	2001	12/12	0.86	0.21	-0.25	2,7,15,16	0
4	NAG	B	720	14/15	0.79	0.18	-0.99	13,19,24,24	0
3	CL	B	610	1/1	0.97	0.09	-4.97	26,26,26,26	0
2	CU	B	601	1/1	0.99	0.07	-5.37	12,12,12,12	0
2	CU	A	604	1/1	0.99	0.04	-5.84	14,14,14,14	0
2	CU	B	602	1/1	0.95	0.06	-6.89	18,18,18,18	0
2	CU	A	602	1/1	0.87	0.08	-6.96	22,22,22,22	0
2	CU	A	603	1/1	0.96	0.06	-7.00	11,11,11,11	0
2	CU	A	601	1/1	0.93	0.08	-7.62	15,15,15,15	0
2	CU	B	604	1/1	0.96	0.06	-8.02	15,15,15,15	0
2	CU	B	603	1/1	0.99	0.04	-12.03	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	SO4	A	8002	5/5	0.90	0.15	-	22,23,26,29	0
6	SO4	B	8001	5/5	0.77	0.24	-	17,25,25,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.