



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2017 – 09:11 AM EDT

PDB ID : 5M8Q
Title : Crystal structure of human tyrosinase related protein 1 mutant (T391V-R374S-Y362F) in complex with kojic acid
Authors : Lai, X.; Soler-Lopez, m.; Wichers, h.j.; Dijkstra, b.w.
Deposited on : unknown
Resolution : 2.85 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

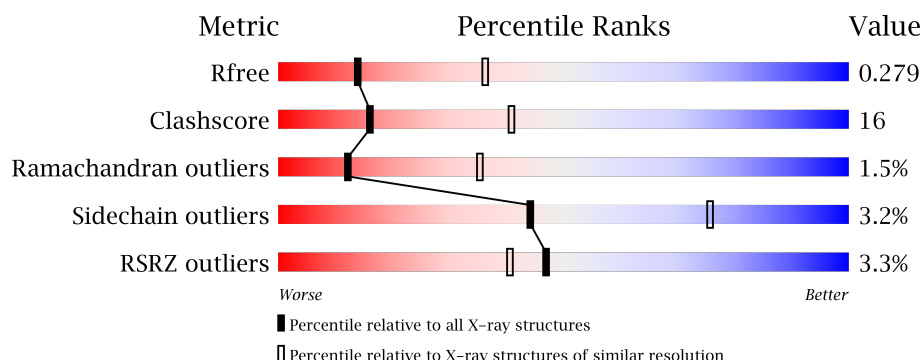
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	100719	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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	446	<div> <div>2%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>
1	B	446	<div> <div>10%</div> <div>54%</div> <div>38%</div> <div>6%</div> <div>.</div> </div>
1	C	446	<div> <div>%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>
1	D	446	<div> <div>74%</div> <div>24%</div> <div>.</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	504	-	-	-	X
6	KOJ	A	516	-	-	-	X
6	KOJ	C	514	-	-	-	X
6	KOJ	D	510	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14735 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 5,6-dihydroxyindole-2-carboxylic acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	B	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	C	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	D	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	PHE	TYR	engineered mutation	UNP P17643
A	374	SER	ARG	engineered mutation	UNP P17643
A	391	VAL	THR	engineered mutation	UNP P17643
B	362	PHE	TYR	engineered mutation	UNP P17643
B	374	SER	ARG	engineered mutation	UNP P17643
B	391	VAL	THR	engineered mutation	UNP P17643
C	362	PHE	TYR	engineered mutation	UNP P17643
C	374	SER	ARG	engineered mutation	UNP P17643
C	391	VAL	THR	engineered mutation	UNP P17643
D	362	PHE	TYR	engineered mutation	UNP P17643
D	374	SER	ARG	engineered mutation	UNP P17643
D	391	VAL	THR	engineered mutation	UNP P17643

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



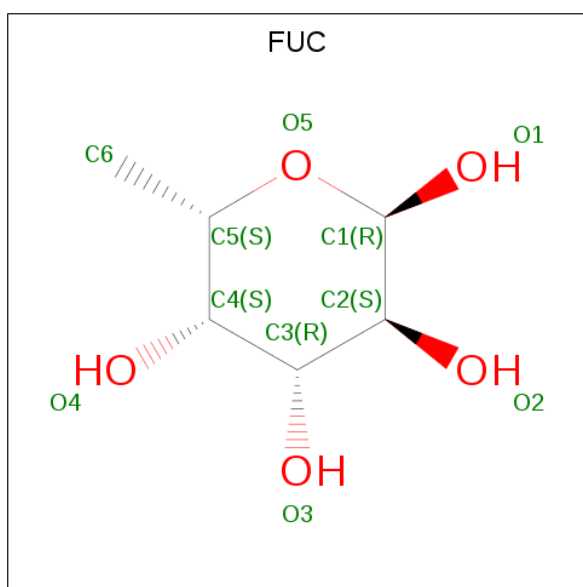
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1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

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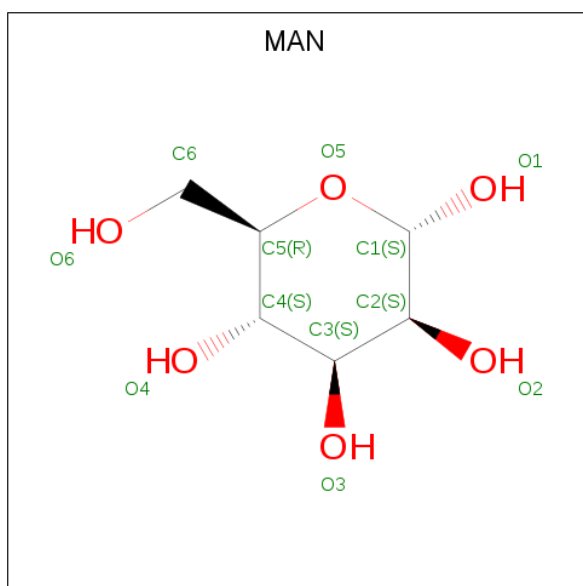
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1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

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).

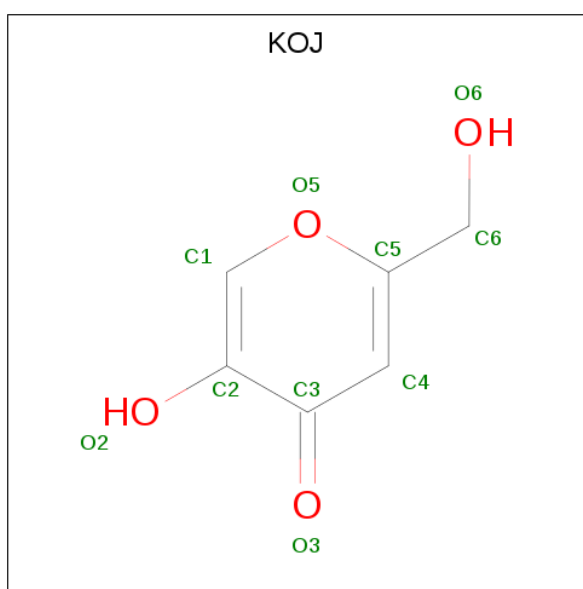


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Zn	0	0
			2	2		
5	A	2	Total	Zn	0	0
			2	2		
5	D	2	Total	Zn	0	0
			2	2		
5	C	3	Total	Zn	0	0
			3	3		

- Molecule 6 is 5-HYDROXY-2-(HYDROXYMETHYL)-4H-PYRAN-4-ONE (three-letter code: KOJ) (formula: C₆H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		

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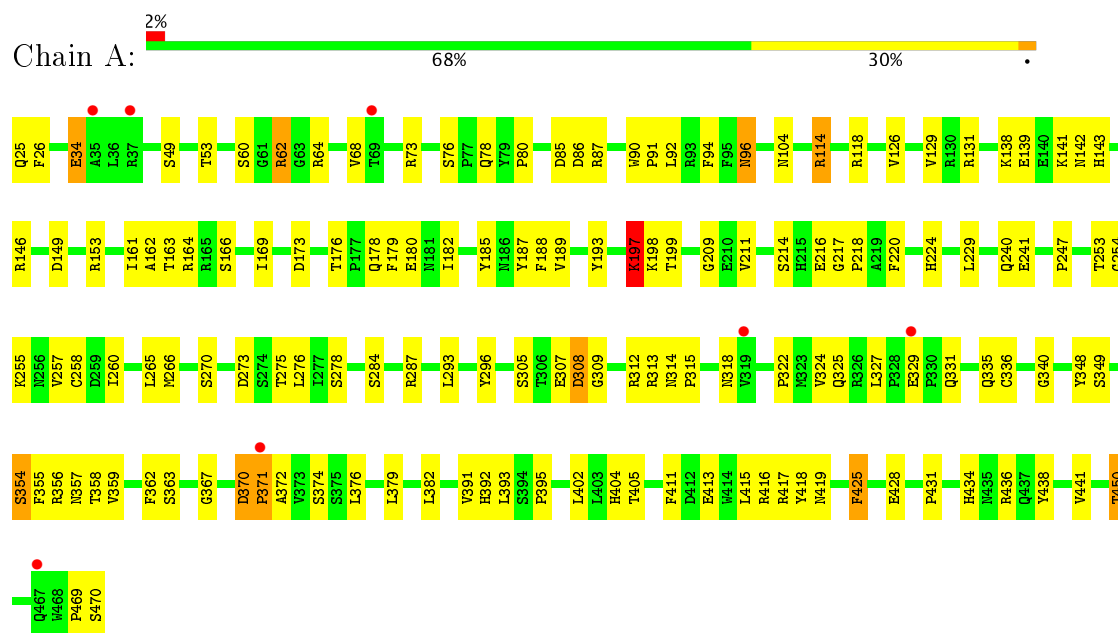
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	O 1	0	0
7	C	1	Total 1	O 1	0	0
7	D	1	Total 1	O 1	0	0

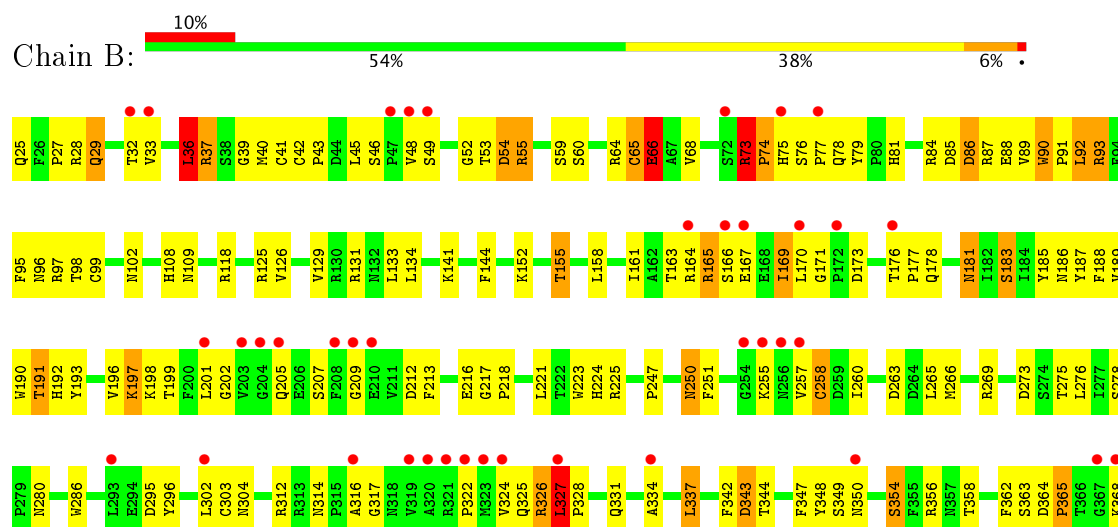
3 Residue-property plots

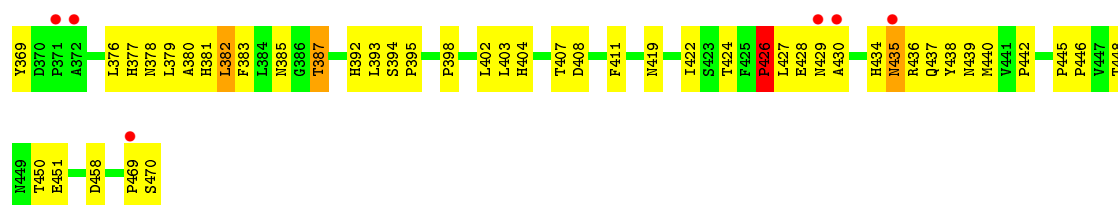
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

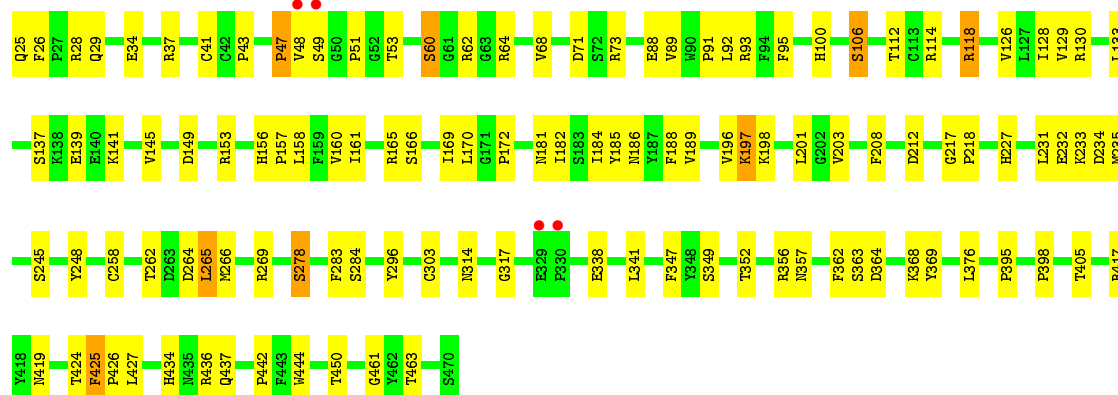
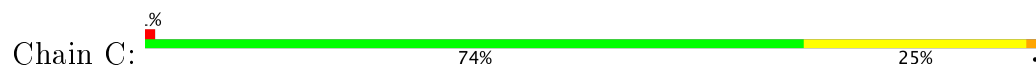


- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

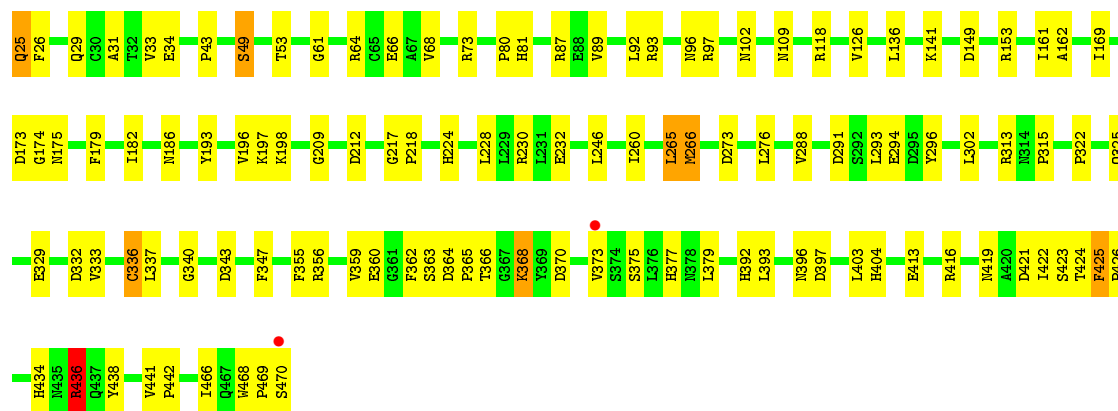




- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.64Å 140.43Å 191.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.88 – 2.85 47.87 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.88-2.85) 92.9 (47.87-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.86Å)	Xtriage
Refinement program	REFMAC, PHENIX	Depositor
R, R_{free}	0.208 , 0.275 0.217 , 0.279	Depositor DCC
R_{free} test set	2855 reflections (5.65%)	DCC
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14735	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, ZN, KOJ, NAG, FUC

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	0.57	5/3661 (0.1%)	0.76	4/4990 (0.1%)
1	B	0.62	5/3661 (0.1%)	0.94	17/4990 (0.3%)
1	C	0.49	0/3661	0.68	2/4990 (0.0%)
1	D	0.49	0/3661	0.65	1/4990 (0.0%)
All	All	0.54	10/14644 (0.1%)	0.76	24/19960 (0.1%)

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	4
1	C	0	1
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	ARG	NE-CZ	-8.60	1.21	1.33
1	B	86	ASP	CB-CG	-7.94	1.35	1.51
1	A	371	PRO	CA-CB	7.03	1.67	1.53
1	B	73	ARG	CZ-NH2	-6.35	1.24	1.33
1	B	66	GLU	CD-OE1	-6.24	1.18	1.25
1	B	73	ARG	CZ-NH1	-5.81	1.25	1.33
1	A	34	GLU	CD-OE2	-5.76	1.19	1.25
1	A	34	GLU	CD-OE1	-5.72	1.19	1.25
1	A	370	ASP	CB-CG	5.08	1.62	1.51
1	A	371	PRO	N-CD	5.02	1.54	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	LEU	CB-CG-CD1	-15.77	84.19	111.00
1	B	327	LEU	CA-CB-CG	15.06	149.94	115.30
1	B	37	ARG	NE-CZ-NH2	14.50	127.55	120.30
1	A	370	ASP	CB-CG-OD1	14.38	131.24	118.30
1	B	73	ARG	NE-CZ-NH2	13.30	126.95	120.30
1	B	92	LEU	CB-CG-CD1	-11.08	92.16	111.00
1	B	169	ILE	CG1-CB-CG2	-10.15	89.06	111.40
1	A	370	ASP	CB-CG-OD2	-8.46	110.69	118.30
1	C	265	LEU	CA-CB-CG	8.44	134.71	115.30
1	B	92	LEU	CB-CG-CD2	7.25	123.32	111.00
1	B	382	LEU	CA-CB-CG	7.05	131.51	115.30
1	A	114	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	B	327	LEU	CB-CG-CD1	6.40	121.88	111.00
1	B	337	LEU	CB-CG-CD2	6.13	121.43	111.00
1	C	64	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	73	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	96	ASN	CB-CA-C	5.68	121.76	110.40
1	B	37	ARG	CG-CD-NE	5.67	123.71	111.80
1	B	90	TRP	C-N-CD	-5.56	108.36	120.60
1	B	36	LEU	CA-CB-CG	5.54	128.03	115.30
1	B	337	LEU	CA-CB-CG	5.28	127.44	115.30
1	D	25	GLN	C-N-CA	-5.18	108.76	121.70
1	B	37	ARG	NH1-CZ-NH2	-5.15	113.73	119.40
1	B	86	ASP	CB-CG-OD1	-5.09	113.72	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	426	PRO	Peptide
1	B	435	ASN	Peptide
1	B	65	CYS	Peptide
1	B	99	CYS	Peptide
1	C	48	VAL	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	3554	0	3319	107	0
1	B	3554	0	3322	198	0
1	C	3554	0	3321	82	0
1	D	3554	0	3320	80	0
2	A	126	0	111	2	0
2	B	56	0	51	3	0
2	C	98	0	87	1	0
2	D	70	0	62	1	0
3	A	10	0	10	1	0
3	B	10	0	10	0	0
3	C	10	0	10	0	0
3	D	20	0	20	0	0
4	A	33	0	28	0	0
4	C	33	0	28	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
6	A	10	0	6	3	0
6	B	10	0	6	3	0
6	C	10	0	6	1	0
6	D	10	0	6	0	0
7	A	1	0	0	2	0
7	B	1	0	0	1	0
7	C	1	0	0	1	0
7	D	1	0	0	0	0
All	All	14735	0	13723	461	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 16.

All (461) 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:165:ARG:NH2	1:B:167:GLU:OE2	1.62	1.31
1:B:92:LEU:HD11	1:B:96:ASN:HA	1.24	1.20
1:B:327:LEU:HD12	1:B:380:ALA:HA	1.19	1.15
1:B:255:LYS:O	1:B:326:ARG:NH1	1.85	1.09
1:B:350:ASN:HA	1:B:369:TYR:CE2	2.02	0.94
6:A:516:KOJ:O3	7:A:601:HOH:O	1.89	0.91
1:B:439:ASN:HD22	1:B:446:PRO:HB3	1.35	0.90
1:B:165:ARG:NH2	1:B:167:GLU:CD	2.27	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:GLN:HA	1:B:334:ALA:HB3	1.54	0.87
1:B:85:ASP:OD1	1:B:86:ASP:N	2.06	0.87
1:B:337:LEU:HD12	1:B:337:LEU:N	1.90	0.85
1:B:327:LEU:HD13	1:B:383:PHE:HB3	1.58	0.85
1:B:166:SER:HA	1:B:169:ILE:HD13	1.61	0.83
1:B:66:GLU:OE1	1:B:98:THR:N	2.12	0.83
1:C:141:LYS:HD2	1:C:265:LEU:HD11	1.61	0.83
1:B:334:ALA:HA	1:B:337:LEU:HD11	1.62	0.82
1:C:338:GLU:OE1	1:C:417:ARG:NH2	2.12	0.81
1:A:254:GLY:HA3	1:A:329:GLU:OE2	1.81	0.81
1:B:342:PHE:H	1:B:424:THR:HG21	1.43	0.81
1:B:73:ARG:HB3	1:B:74:PRO:HD2	1.63	0.80
1:B:327:LEU:HD12	1:B:380:ALA:CA	2.07	0.80
1:B:337:LEU:HD12	1:B:337:LEU:H	1.42	0.79
1:B:378:ASN:ND2	6:B:508:KOJ:H4	1.96	0.79
1:B:439:ASN:ND2	1:B:446:PRO:HB3	1.97	0.79
1:B:75:HIS:NE2	1:B:79:TYR:HB3	1.97	0.79
1:D:425:PHE:O	1:D:436:ARG:NH1	2.16	0.79
1:B:66:GLU:N	1:B:66:GLU:OE2	2.16	0.79
1:C:89:VAL:HG12	1:C:92:LEU:HB2	1.64	0.78
1:B:218:PRO:HG3	1:B:426:PRO:HG2	1.65	0.78
6:B:508:KOJ:O3	7:B:601:HOH:O	2.00	0.77
1:A:436:ARG:HG2	1:A:450:THR:HG22	1.65	0.77
1:A:49:SER:HB2	1:A:53:THR:HG21	1.66	0.77
1:D:364:ASP:OD1	1:D:368:LYS:HB3	1.84	0.77
1:B:326:ARG:NH2	1:B:327:LEU:HB2	1.99	0.76
1:B:92:LEU:HD11	1:B:96:ASN:CA	2.11	0.76
1:C:73:ARG:HH22	1:D:97:ARG:HH22	1.33	0.75
1:C:28:ARG:NH1	1:C:157:PRO:O	2.20	0.74
1:B:28:ARG:NH2	1:B:181:ASN:OD1	2.20	0.74
1:D:43:PRO:HG2	1:D:109:ASN:HB3	1.68	0.73
1:B:216:GLU:HG2	1:B:362:PHE:HE2	1.52	0.73
1:C:25:GLN:HG2	1:C:161:ILE:HA	1.70	0.73
1:D:425:PHE:HB3	1:D:436:ARG:HH11	1.52	0.73
1:C:363:SER:HB3	1:C:369:TYR:HA	1.71	0.73
1:B:29:GLN:HG3	1:B:43:PRO:HB3	1.72	0.72
1:B:25:GLN:HG2	1:B:161:ILE:HD12	1.72	0.71
1:B:327:LEU:CD1	1:B:380:ALA:HA	2.12	0.71
1:A:293:LEU:HD11	1:A:392:HIS:NE2	2.05	0.71
1:A:118:ARG:HG3	1:A:126:VAL:HG11	1.71	0.71
1:B:378:ASN:HD22	6:B:508:KOJ:H4	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ASP:HB3	1:B:88:GLU:OE2	1.91	0.71
1:D:89:VAL:HG13	1:D:92:LEU:HB2	1.72	0.71
1:B:430:ALA:HB3	1:B:435:ASN:OD1	1.91	0.71
1:B:86:ASP:OD2	1:B:165:ARG:NH1	2.24	0.71
1:D:49:SER:HB2	1:D:53:THR:HG21	1.73	0.70
1:B:66:GLU:OE1	1:B:97:ARG:HA	1.91	0.70
1:B:76:SER:OG	1:B:78:GLN:OE1	2.08	0.70
1:B:76:SER:CB	1:B:78:GLN:OE1	2.40	0.70
1:A:25:GLN:HG2	1:A:161:ILE:HA	1.72	0.70
1:A:413:GLU:OE2	1:A:416:ARG:NH2	2.24	0.70
1:B:96:ASN:HD22	2:B:501:NAG:H83	1.57	0.70
1:B:358:THR:HA	1:B:363:SER:HB2	1.74	0.69
1:C:34:GLU:HG3	1:C:37:ARG:HH21	1.56	0.69
1:A:60:SER:HB2	1:A:62:ARG:HG3	1.75	0.69
1:D:413:GLU:OE2	1:D:416:ARG:NH1	2.26	0.69
1:B:327:LEU:HB3	1:B:328:PRO:HD2	1.75	0.68
1:A:163:THR:HG23	1:A:164:ARG:HG2	1.76	0.68
1:A:73:ARG:NH1	1:A:428:GLU:OE2	2.27	0.68
1:A:138:LYS:H	1:A:138:LYS:HD3	1.58	0.68
1:A:354:SER:O	1:A:358:THR:HG23	1.92	0.68
1:C:106:SER:HB2	1:C:114:ARG:HG2	1.76	0.68
1:B:201:LEU:HD12	1:B:205:GLN:OE1	1.94	0.67
1:B:165:ARG:NH1	1:B:166:SER:OG	2.28	0.67
1:B:250:ASN:O	1:B:250:ASN:ND2	2.29	0.66
1:A:104:ASN:OD1	1:A:114:ARG:NH1	2.24	0.66
1:B:52:GLY:HA2	1:B:55:ARG:NH1	2.11	0.65
1:A:265:LEU:HD12	1:A:265:LEU:O	1.97	0.65
1:A:392:HIS:CD2	1:A:393:LEU:HG	2.31	0.65
1:C:112:THR:OG1	1:C:233:LYS:NZ	2.28	0.65
1:A:218:PRO:HD2	1:A:434:HIS:HB3	1.79	0.65
1:B:152:LYS:HD3	1:B:286:TRP:CD2	2.30	0.65
1:B:349:SER:O	1:B:369:TYR:HE2	1.80	0.64
1:D:25:GLN:HG3	1:D:26:PHE:H	1.62	0.64
1:B:161:ILE:HD11	1:B:190:TRP:CD2	2.31	0.64
1:B:257:VAL:HG12	1:B:258:CYS:H	1.62	0.64
1:B:33:VAL:HG13	1:B:177:PRO:HG3	1.78	0.64
1:D:64:ARG:NH2	1:D:66:GLU:OE2	2.31	0.64
1:C:218:PRO:HD2	1:C:434:HIS:HB3	1.79	0.64
1:C:29:GLN:HG3	1:C:43:PRO:HB3	1.79	0.64
1:D:260:ILE:HD12	1:D:266:MET:HG3	1.80	0.64
1:B:165:ARG:HD2	1:B:166:SER:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:GLY:O	1:D:102:ASN:ND2	2.20	0.64
1:B:170:LEU:HD23	1:B:170:LEU:H	1.63	0.63
1:B:65:CYS:HA	1:B:66:GLU:OE2	1.97	0.63
1:B:328:PRO:CG	1:B:376:LEU:HD23	2.28	0.63
1:B:75:HIS:CE1	1:B:76:SER:O	2.51	0.63
1:A:358:THR:HG22	1:A:363:SER:HB2	1.81	0.63
1:B:87:ARG:HB2	1:B:213:PHE:CZ	2.33	0.63
1:B:32:THR:O	1:B:36:LEU:HD23	1.98	0.63
1:A:85:ASP:HB2	1:A:199:THR:HG23	1.81	0.62
1:C:269:ARG:NH1	1:C:314:ASN:OD1	2.33	0.62
1:A:49:SER:HB3	1:D:93:ARG:HE	1.63	0.62
1:C:436:ARG:HG2	1:C:450:THR:HG23	1.81	0.62
1:B:327:LEU:HA	1:B:379:LEU:HG	1.80	0.62
1:B:108:HIS:HA	1:B:445:PRO:HG3	1.80	0.62
1:C:118:ARG:HD3	1:C:126:VAL:HG11	1.80	0.62
1:B:428:GLU:CD	1:B:435:ASN:HD22	2.03	0.62
1:D:25:GLN:HG2	1:D:161:ILE:HA	1.82	0.61
1:B:324:VAL:HG11	1:B:382:LEU:HB3	1.81	0.61
1:A:49:SER:HB2	1:A:53:THR:CG2	2.30	0.61
1:D:149:ASP:OD1	1:D:153:ARG:NH2	2.34	0.61
1:B:164:ARG:HG3	1:B:178:GLN:HG3	1.83	0.60
1:D:198:LYS:HG2	1:D:209:GLY:HA2	1.82	0.60
1:A:293:LEU:HD11	1:A:392:HIS:CD2	2.35	0.60
1:D:422:ILE:O	1:D:436:ARG:NH1	2.35	0.60
1:D:34:GLU:N	1:D:34:GLU:OE2	2.35	0.60
1:A:273:ASP:HB3	1:A:276:LEU:HD12	1.83	0.60
1:C:25:GLN:HG3	1:C:26:PHE:H	1.67	0.60
1:C:352:THR:HG23	1:C:369:TYR:H	1.65	0.60
1:B:64:ARG:NH2	1:D:366:THR:O	2.32	0.59
1:C:341:LEU:HD22	1:C:424:THR:HG21	1.84	0.59
1:D:118:ARG:HD2	1:D:126:VAL:HG21	1.83	0.59
1:D:96:ASN:HD22	2:D:501:NAG:H83	1.67	0.59
1:A:370:ASP:OD1	1:A:371:PRO:HD2	2.02	0.59
1:B:347:PHE:CG	1:B:426:PRO:HG3	2.37	0.59
1:B:141:LYS:HD3	1:B:265:LEU:HD23	1.84	0.59
1:A:166:SER:HA	1:A:169:ILE:HB	1.85	0.59
1:B:161:ILE:HD11	1:B:190:TRP:CE3	2.38	0.59
1:C:197:LYS:NZ	1:C:198:LYS:O	2.35	0.59
1:B:197:LYS:NZ	1:B:302:LEU:HD13	2.17	0.59
1:B:75:HIS:NE2	1:B:76:SER:O	2.36	0.58
1:B:322:PRO:HA	1:B:325:GLN:NE2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:MET:HA	1:B:97:ARG:HB2	1.84	0.58
1:B:49:SER:HB2	1:B:53:THR:HG21	1.84	0.58
1:B:327:LEU:HD13	1:B:383:PHE:CB	2.31	0.58
1:C:262:THR:HG22	1:C:264:ASP:H	1.66	0.58
1:B:43:PRO:HG2	1:B:109:ASN:HB3	1.86	0.58
1:D:29:GLN:HG3	1:D:43:PRO:HB3	1.85	0.58
1:B:166:SER:HA	1:B:169:ILE:CD1	2.32	0.58
1:B:91:PRO:HG2	1:B:446:PRO:HG3	1.86	0.57
1:C:73:ARG:NH2	1:D:97:ARG:HH22	2.02	0.57
1:B:218:PRO:HG2	1:B:434:HIS:HB3	1.86	0.57
1:A:358:THR:HG21	1:A:367:GLY:HA2	1.87	0.57
1:B:263:ASP:OD2	1:B:280:ASN:HB3	2.05	0.57
1:A:218:PRO:HB2	1:A:425:PHE:CE1	2.39	0.57
1:B:269:ARG:NH1	1:B:314:ASN:OD1	2.37	0.57
1:B:328:PRO:HG3	1:B:376:LEU:HD23	1.87	0.57
1:B:190:TRP:O	1:B:193:TYR:N	2.38	0.57
1:B:326:ARG:HH21	1:B:327:LEU:HB2	1.70	0.57
1:B:304:ASN:HD21	2:B:504:NAG:C1	2.18	0.57
1:B:322:PRO:HA	1:B:325:GLN:CD	2.26	0.56
1:B:276:LEU:HD21	1:B:312:ARG:CZ	2.36	0.56
1:C:425:PHE:O	1:C:436:ARG:NH1	2.39	0.56
1:D:343:ASP:O	1:D:424:THR:HB	2.06	0.56
1:D:392:HIS:CD2	1:D:393:LEU:HG	2.41	0.56
1:B:260:ILE:HD12	1:B:266:MET:HG3	1.88	0.56
1:A:25:GLN:N	1:A:187:TYR:HH	2.04	0.55
1:A:25:GLN:OE1	1:A:25:GLN:HA	2.06	0.55
1:B:66:GLU:OE1	1:B:97:ARG:CA	2.54	0.55
1:B:66:GLU:CD	1:B:98:THR:O	2.45	0.55
1:D:291:ASP:HB2	1:D:393:LEU:HD21	1.87	0.55
1:C:182:ILE:HD11	1:C:186:ASN:HB3	1.89	0.55
1:A:161:ILE:HD13	1:A:182:ILE:HD13	1.87	0.55
1:A:241:GLU:HG3	1:C:203:VAL:HG12	1.89	0.55
1:B:328:PRO:HG3	1:B:376:LEU:HA	1.89	0.55
1:D:421:ASP:OD1	1:D:423:SER:OG	2.23	0.55
1:A:78:GLN:O	1:A:80:PRO:HD3	2.07	0.54
1:D:173:ASP:O	1:D:175:ASN:N	2.39	0.54
1:D:218:PRO:HD2	1:D:434:HIS:HB3	1.88	0.54
1:D:232:GLU:HG3	1:D:246:LEU:HG	1.88	0.54
1:B:201:LEU:HB2	1:B:205:GLN:HG2	1.89	0.54
1:B:73:ARG:HB3	1:B:74:PRO:CD	2.37	0.54
1:C:129:VAL:HG22	1:C:463:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLN:O	1:A:335:GLN:HG3	2.07	0.54
1:A:138:LYS:H	1:A:138:LYS:CD	2.21	0.53
1:A:217:GLY:O	1:A:356:ARG:HD3	2.08	0.53
1:B:81:HIS:ND1	1:B:84:ARG:HG3	2.24	0.53
1:D:322:PRO:HA	1:D:325:GLN:HG3	1.90	0.53
1:A:209:GLY:O	1:A:211:VAL:N	2.40	0.53
1:B:266:MET:HE3	1:B:398:PRO:HG2	1.89	0.53
1:B:88:GLU:O	1:B:90:TRP:N	2.41	0.53
1:C:248:TYR:HA	1:C:405:THR:OG1	2.09	0.53
1:D:80:PRO:HG2	1:D:81:HIS:CE1	2.44	0.53
1:A:169:ILE:HD11	1:A:179:PHE:CZ	2.44	0.53
1:D:293:LEU:HD23	1:D:296:TYR:HD2	1.74	0.53
1:A:141:LYS:HD3	1:A:265:LEU:HD23	1.90	0.53
1:B:273:ASP:HB3	1:B:276:LEU:HG	1.91	0.53
1:B:190:TRP:O	1:B:192:HIS:N	2.42	0.52
1:C:34:GLU:OE2	1:C:37:ARG:NE	2.42	0.52
1:B:52:GLY:HA2	1:B:55:ARG:CZ	2.40	0.52
1:B:76:SER:C	1:B:78:GLN:OE1	2.48	0.52
1:A:413:GLU:OE2	1:A:417:ARG:NE	2.42	0.52
1:D:198:LYS:HG2	1:D:209:GLY:CA	2.39	0.52
1:B:327:LEU:HB3	1:B:328:PRO:CD	2.37	0.52
1:B:185:TYR:O	1:B:188:PHE:HB3	2.08	0.52
1:B:216:GLU:HG2	1:B:362:PHE:CE2	2.38	0.52
1:B:29:GLN:CG	1:B:43:PRO:HB3	2.39	0.52
1:C:141:LYS:O	1:C:145:VAL:HG23	2.10	0.52
1:A:275:THR:HG22	1:A:314:ASN:HD22	1.74	0.52
1:D:31:ALA:HB1	1:D:179:PHE:CD2	2.45	0.52
1:B:163:THR:OG1	1:B:178:GLN:HB3	2.10	0.52
1:D:364:ASP:CG	1:D:368:LYS:HB3	2.29	0.52
1:B:73:ARG:HD3	1:B:73:ARG:N	2.24	0.51
1:D:228:LEU:HD11	1:D:404:HIS:HB3	1.91	0.51
1:B:428:GLU:OE1	1:B:429:ASN:N	2.25	0.51
1:A:355:PHE:O	1:A:359:VAL:HG12	2.11	0.51
1:B:39:GLY:O	1:B:96:ASN:N	2.43	0.51
1:A:189:VAL:HG22	1:A:395:PRO:HB2	1.92	0.51
1:C:425:PHE:HB3	1:C:436:ARG:HD3	1.92	0.51
1:C:60:SER:HB2	1:C:62:ARG:HG3	1.91	0.51
1:A:185:TYR:O	1:A:188:PHE:HB3	2.10	0.51
1:B:364:ASP:CG	1:B:368:LYS:HG2	2.31	0.51
1:C:26:PHE:CD1	1:C:95:PHE:HE2	2.28	0.51
1:A:68:VAL:HG12	1:A:96:ASN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:H	1:A:293:LEU:HD12	1.75	0.51
1:B:344:THR:HG23	1:B:354:SER:HB2	1.92	0.51
1:B:155:THR:HA	1:B:183:SER:HA	1.91	0.51
1:B:364:ASP:OD1	1:B:368:LYS:HG2	2.11	0.51
1:B:66:GLU:OE1	1:B:97:ARG:C	2.49	0.51
1:B:328:PRO:CG	1:B:376:LEU:HA	2.41	0.51
1:B:342:PHE:HB3	1:B:424:THR:HG23	1.93	0.50
1:C:118:ARG:HD3	1:C:126:VAL:CG1	2.41	0.50
1:C:436:ARG:HG2	1:C:450:THR:CG2	2.42	0.50
1:B:152:LYS:NZ	1:B:186:ASN:OD1	2.44	0.50
1:A:340:GLY:HA2	1:A:418:TYR:CE2	2.47	0.50
1:A:247:PRO:O	1:A:402:LEU:HD23	2.11	0.50
1:B:41:CYS:HB2	1:B:95:PHE:CD1	2.47	0.50
1:C:196:VAL:HG12	1:C:212:ASP:CG	2.31	0.50
1:D:333:VAL:O	1:D:337:LEU:HD12	2.12	0.50
1:C:185:TYR:O	1:C:188:PHE:HB3	2.12	0.50
1:C:427:LEU:HD11	1:C:436:ARG:NH2	2.26	0.50
1:C:88:GLU:OE1	1:C:93:ARG:NH2	2.45	0.50
1:C:137:SER:O	1:C:141:LYS:HG3	2.12	0.50
1:A:173:ASP:OD2	1:A:176:THR:N	2.44	0.49
1:B:187:TYR:O	1:B:191:THR:HG23	2.11	0.49
1:C:89:VAL:HG12	1:C:89:VAL:O	2.12	0.49
1:A:322:PRO:HA	1:A:325:GLN:HG3	1.94	0.49
1:B:337:LEU:CD1	1:B:337:LEU:H	2.17	0.49
1:D:329:GLU:N	1:D:332:ASP:OD2	2.43	0.49
1:A:293:LEU:HD21	1:A:392:HIS:CG	2.48	0.49
1:B:403:LEU:O	1:B:407:THR:HG23	2.13	0.49
1:B:437:GLN:OE1	1:B:450:THR:HG21	2.12	0.49
1:D:25:GLN:HE21	1:D:162:ALA:H	1.60	0.49
1:C:278:SER:O	1:C:284:SER:HB3	2.13	0.49
1:A:197:LYS:HE2	1:A:198:LYS:O	2.12	0.49
2:A:508:NAG:O7	2:A:508:NAG:O3	2.29	0.49
1:B:347:PHE:CD1	1:B:426:PRO:HG3	2.46	0.49
1:A:293:LEU:HA	1:A:296:TYR:CD2	2.48	0.49
1:D:118:ARG:CD	1:D:126:VAL:HG21	2.42	0.49
1:D:466:ILE:HD13	1:D:468:TRP:CH2	2.47	0.49
1:B:448:THR:OG1	1:B:451:GLU:HG3	2.13	0.49
1:D:336:CYS:SG	1:D:359:VAL:HG22	2.52	0.49
1:B:337:LEU:N	1:B:337:LEU:CD1	2.72	0.48
1:A:370:ASP:C	1:A:372:ALA:H	2.15	0.48
1:B:176:THR:OG1	1:B:178:GLN:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:THR:OG1	1:B:178:GLN:O	2.24	0.48
1:B:217:GLY:O	1:B:356:ARG:HD3	2.13	0.48
1:A:214:SER:O	1:A:220:PHE:HA	2.13	0.48
1:B:224:HIS:CD2	1:B:404:HIS:CE1	3.01	0.48
1:B:73:ARG:O	1:B:74:PRO:O	2.30	0.48
1:C:28:ARG:HH21	1:C:181:ASN:ND2	2.10	0.48
1:C:181:ASN:OD1	2:C:503:NAG:H2	2.13	0.48
1:C:133:LEU:HD21	1:C:265:LEU:HG	1.96	0.48
1:A:275:THR:OG1	1:A:312:ARG:NH1	2.46	0.48
1:A:25:GLN:HG3	1:A:26:PHE:H	1.78	0.48
1:B:350:ASN:HA	1:B:369:TYR:HE2	1.74	0.48
1:B:422:ILE:O	1:B:436:ARG:NH2	2.47	0.48
1:D:260:ILE:O	1:D:266:MET:HB2	2.14	0.48
1:A:260:ILE:HB	1:A:265:LEU:CD1	2.43	0.48
1:C:34:GLU:CG	1:C:37:ARG:HH21	2.25	0.48
1:B:85:ASP:C	1:B:86:ASP:OD1	2.52	0.48
1:D:33:VAL:HG13	1:D:34:GLU:OE2	2.13	0.48
1:A:469:PRO:O	1:A:470:SER:HB2	2.14	0.47
1:B:93:ARG:HE	1:B:93:ARG:HA	1.78	0.47
1:A:216:GLU:HB3	1:A:349:SER:HB3	1.95	0.47
1:C:201:LEU:HD11	1:C:208:PHE:HB2	1.96	0.47
1:B:125:ARG:HD2	1:C:49:SER:HA	1.97	0.47
1:A:182:ILE:HD12	1:A:305:SER:HB3	1.96	0.47
1:D:182:ILE:HD11	1:D:186:ASN:HB3	1.97	0.47
1:D:291:ASP:OD1	1:D:393:LEU:HD11	2.14	0.47
1:A:85:ASP:OD1	1:A:86:ASP:N	2.47	0.47
1:C:71:ASP:HB2	1:C:437:GLN:O	2.15	0.47
1:C:196:VAL:HG12	1:C:212:ASP:OD2	2.15	0.47
1:D:149:ASP:CG	1:D:153:ARG:HH21	2.18	0.47
1:B:134:LEU:HD21	1:B:260:ILE:HG22	1.96	0.47
1:B:76:SER:HB2	1:B:78:GLN:OE1	2.14	0.47
1:D:375:SER:HA	1:D:379:LEU:HB2	1.95	0.47
1:B:42:CYS:O	1:B:55:ARG:HG3	2.16	0.46
1:B:41:CYS:HB2	1:B:95:PHE:CG	2.50	0.46
1:B:255:LYS:N	1:B:326:ARG:NH1	2.64	0.46
1:B:27:PRO:HG3	1:B:158:LEU:HD11	1.97	0.46
1:B:273:ASP:OD1	1:B:275:THR:OG1	2.33	0.46
1:B:133:LEU:HD22	1:B:402:LEU:HD13	1.98	0.46
1:B:430:ALA:H	1:B:435:ASN:HD21	1.63	0.46
1:B:212:ASP:O	1:B:434:HIS:NE2	2.45	0.46
1:D:347:PHE:CG	1:D:426:PRO:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:SER:HA	1:C:169:ILE:HB	1.98	0.46
1:D:313:ARG:HD3	1:D:397:ASP:OD2	2.16	0.46
1:A:416:ARG:NH2	1:A:417:ARG:HE	2.14	0.46
1:C:145:VAL:HG13	1:C:283:PHE:CZ	2.51	0.46
1:C:47:PRO:HB2	1:C:53:THR:OG1	2.15	0.46
1:B:28:ARG:HH22	1:B:181:ASN:CG	2.19	0.45
1:B:45:LEU:HB3	1:B:54:ASP:OD1	2.16	0.45
1:B:314:ASN:ND2	1:B:317:GLY:HA3	2.31	0.45
1:B:66:GLU:OE2	1:B:98:THR:O	2.33	0.45
1:C:156:HIS:CE1	1:C:158:LEU:HB3	2.51	0.45
1:B:49:SER:CB	1:B:53:THR:HG21	2.45	0.45
1:A:138:LYS:HD3	1:A:138:LYS:N	2.28	0.45
1:A:318:ASN:HA	2:A:512:NAG:O6	2.17	0.45
1:B:196:VAL:HG12	1:B:212:ASP:OD1	2.17	0.45
1:B:46:SER:O	1:B:48:VAL:HG23	2.17	0.45
1:B:88:GLU:O	1:B:89:VAL:C	2.54	0.45
1:C:25:GLN:N	1:C:442:PRO:O	2.49	0.45
1:A:163:THR:HG22	1:A:178:GLN:O	2.16	0.45
1:B:161:ILE:HA	1:B:161:ILE:HD12	1.58	0.45
1:A:90:TRP:HA	1:A:91:PRO:HA	1.78	0.45
1:B:37:ARG:HD2	1:B:37:ARG:HA	1.27	0.45
1:D:355:PHE:CE1	1:D:359:VAL:HG21	2.52	0.45
1:D:288:VAL:HA	1:D:396:ASN:OD1	2.15	0.45
1:D:403:LEU:HD23	1:D:403:LEU:O	2.17	0.45
1:B:316:ALA:O	1:B:325:GLN:HB3	2.16	0.45
1:B:91:PRO:CG	1:B:446:PRO:HG3	2.47	0.45
1:C:89:VAL:HG13	1:C:92:LEU:HD12	1.99	0.45
1:B:334:ALA:HB2	1:B:469:PRO:HB2	1.99	0.44
1:B:86:ASP:CG	1:B:165:ARG:NH1	2.70	0.44
1:D:68:VAL:CG2	1:D:92:LEU:HD21	2.47	0.44
1:B:76:SER:O	1:B:78:GLN:N	2.50	0.44
1:B:85:ASP:HB2	1:B:199:THR:HG23	1.98	0.44
1:D:169:ILE:HD11	1:D:179:PHE:CZ	2.53	0.44
1:A:118:ARG:HG3	1:A:126:VAL:CG1	2.42	0.44
1:A:224:HIS:CD2	1:A:404:HIS:CE1	3.05	0.44
1:B:129:VAL:HG12	1:B:131:ARG:HG2	1.99	0.44
1:B:54:ASP:OD2	1:B:59:SER:HB3	2.17	0.44
1:D:92:LEU:HA	1:D:92:LEU:HD23	1.64	0.44
1:C:73:ARG:HH22	1:D:97:ARG:NH2	2.09	0.44
1:D:370:ASP:HB3	1:D:373:VAL:CG2	2.47	0.44
1:A:173:ASP:OD2	1:A:176:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLY:O	1:B:205:GLN:HG3	2.18	0.44
1:C:264:ASP:OD2	1:C:265:LEU:HD13	2.17	0.44
1:B:173:ASP:HB3	1:B:176:THR:HB	1.99	0.44
1:B:221:LEU:HD22	1:B:411:PHE:HB2	1.99	0.44
1:B:324:VAL:HG22	1:B:379:LEU:HD12	2.00	0.44
1:B:144:PHE:HE2	1:B:402:LEU:HD11	1.83	0.44
1:B:265:LEU:HD12	1:B:265:LEU:O	2.17	0.44
1:B:296:TYR:CZ	1:B:303:CYS:HA	2.52	0.44
1:A:260:ILE:HD12	1:A:266:MET:HG3	1.98	0.44
1:C:169:ILE:HG23	1:C:170:LEU:HG	2.00	0.44
1:C:296:TYR:CZ	1:C:303:CYS:HA	2.53	0.44
1:A:391:VAL:HG13	1:A:392:HIS:N	2.32	0.43
1:B:152:LYS:HD3	1:B:286:TRP:CE3	2.53	0.43
1:B:165:ARG:HD2	1:B:166:SER:N	2.30	0.43
1:B:387:THR:O	1:B:394:SER:HA	2.18	0.43
1:B:225:ARG:HB2	1:B:408:ASP:OD1	2.18	0.43
1:B:86:ASP:OD1	1:B:86:ASP:N	2.50	0.43
1:A:357:ASN:OD1	1:A:362:PHE:HB2	2.17	0.43
1:B:86:ASP:CG	1:B:165:ARG:HH11	2.22	0.43
1:C:189:VAL:HG22	1:C:395:PRO:HB2	1.99	0.43
1:D:419:ASN:OD1	1:D:419:ASN:O	2.36	0.43
1:A:253:THR:OG1	1:A:255:LYS:HG3	2.19	0.43
1:A:324:VAL:HA	1:A:379:LEU:CD1	2.48	0.43
1:B:66:GLU:CD	1:B:66:GLU:N	2.71	0.43
1:A:180:GLU:OE1	1:A:305:SER:OG	2.36	0.43
1:B:257:VAL:HG12	1:B:258:CYS:N	2.29	0.43
1:C:357:ASN:OD1	1:C:362:PHE:HB2	2.18	0.43
1:B:189:VAL:HA	1:B:395:PRO:HB2	1.99	0.43
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.73	0.43
1:C:68:VAL:HG11	1:C:91:PRO:HD2	2.01	0.43
1:D:196:VAL:HG12	1:D:212:ASP:OD1	2.19	0.43
1:A:118:ARG:CZ	1:A:126:VAL:HG11	2.49	0.43
1:C:139:GLU:OE1	1:C:139:GLU:N	2.47	0.42
1:B:343:ASP:O	1:B:424:THR:OG1	2.37	0.42
1:B:392:HIS:CD2	1:B:393:LEU:HD22	2.54	0.42
1:C:128:ILE:HG12	1:C:461:GLY:O	2.18	0.42
1:D:332:ASP:OD1	1:D:365:PRO:HG2	2.19	0.42
1:C:129:VAL:HG22	1:C:463:THR:CG2	2.50	0.42
1:D:273:ASP:HB3	1:D:276:LEU:HD12	2.02	0.42
1:A:142:ASN:OD1	1:A:146:ARG:HD2	2.20	0.42
1:A:162:ALA:HB2	1:A:179:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:HG2	1:A:441:VAL:HG11	2.01	0.42
1:C:232:GLU:OE2	1:C:245:SER:HA	2.20	0.42
1:D:87:ARG:NH1	1:D:197:LYS:HG2	2.35	0.42
1:A:104:ASN:CG	1:A:114:ARG:HH11	2.16	0.42
1:A:129:VAL:HG12	1:A:131:ARG:HG2	2.01	0.42
1:A:358:THR:HG22	1:A:363:SER:CB	2.48	0.42
1:B:324:VAL:CG1	1:B:324:VAL:O	2.68	0.42
1:B:85:ASP:C	1:B:88:GLU:OE1	2.58	0.42
1:D:265:LEU:O	1:D:265:LEU:HD12	2.19	0.42
1:A:308:ASP:HB3	1:A:309:GLY:H	1.76	0.42
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.80	0.42
1:C:266:MET:CE	1:C:398:PRO:HB2	2.49	0.42
1:B:65:CYS:CA	1:B:66:GLU:OE2	2.67	0.42
1:C:149:ASP:CG	1:C:153:ARG:HH12	2.23	0.42
6:C:514:KOJ:O2	7:C:601:HOH:O	2.21	0.42
1:A:149:ASP:O	1:A:153:ARG:HG3	2.19	0.42
1:C:347:PHE:CG	1:C:426:PRO:HG3	2.55	0.42
6:A:516:KOJ:O2	7:A:601:HOH:O	2.21	0.42
1:A:76:SER:OG	1:A:431:PRO:HA	2.20	0.42
1:C:130:ARG:HH21	1:C:232:GLU:CD	2.17	0.42
1:A:143:HIS:CE1	1:A:241:GLU:OE2	2.73	0.42
1:A:229:LEU:HA	1:A:229:LEU:HD12	1.87	0.42
1:A:348:TYR:CG	1:A:349:SER:N	2.88	0.42
1:A:392:HIS:NE2	1:A:393:LEU:HG	2.34	0.42
1:B:102:ASN:OD1	1:D:340:GLY:HA3	2.20	0.42
1:C:41:CYS:HB3	1:C:444:TRP:CZ2	2.55	0.42
1:D:224:HIS:CD2	1:D:404:HIS:CE1	3.08	0.42
1:A:278:SER:O	1:A:284:SER:HB3	2.20	0.41
1:B:436:ARG:HG2	1:B:450:THR:CG2	2.50	0.41
1:A:257:VAL:HG22	1:A:258:CYS:N	2.35	0.41
1:A:34:GLU:H	1:A:34:GLU:HG3	1.71	0.41
1:B:458:ASP:OD2	1:C:51:PRO:HG2	2.20	0.41
1:A:25:GLN:HG3	1:A:26:PHE:N	2.34	0.41
1:D:136:LEU:O	1:D:141:LYS:HE3	2.20	0.41
1:D:313:ARG:HG2	1:D:315:PRO:HD3	2.02	0.41
1:A:313:ARG:HG2	1:A:315:PRO:HD3	2.03	0.41
1:B:247:PRO:O	1:B:402:LEU:HD23	2.20	0.41
1:C:100:HIS:ND1	1:D:64:ARG:NH2	2.69	0.41
1:C:217:GLY:O	1:C:356:ARG:HD3	2.20	0.41
1:B:348:TYR:CG	1:B:349:SER:N	2.89	0.41
1:A:68:VAL:HG13	1:A:92:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:VAL:HG12	1:C:181:ASN:HD22	1.86	0.41
1:C:188:PHE:CE1	1:C:227:HIS:CE1	3.08	0.41
1:A:143:HIS:HE1	1:A:241:GLU:OE2	2.04	0.41
1:A:260:ILE:O	1:A:266:MET:HB2	2.21	0.41
1:D:359:VAL:O	1:D:377:HIS:HB3	2.20	0.41
1:D:441:VAL:HA	1:D:442:PRO:HA	1.90	0.41
1:A:391:VAL:CG1	1:A:392:HIS:N	2.84	0.41
1:A:382:LEU:CD2	6:A:516:KOJ:H6C2	2.51	0.41
1:B:37:ARG:C	1:B:39:GLY:H	2.24	0.41
1:B:304:ASN:HD21	2:B:504:NAG:C2	2.33	0.41
1:C:231:LEU:O	1:C:235:MET:HG3	2.21	0.41
1:D:80:PRO:HG2	1:D:81:HIS:ND1	2.36	0.41
1:A:138:LYS:HE2	1:A:139:GLU:OE2	2.21	0.41
1:B:198:LYS:HD2	1:B:209:GLY:HA3	2.03	0.41
1:B:364:ASP:HB2	1:B:365:PRO:HD2	2.02	0.41
1:B:223:TRP:CD1	1:B:440:MET:HB3	2.56	0.41
1:C:368:LYS:HE2	1:C:368:LYS:HB3	1.94	0.41
1:D:197:LYS:HE3	1:D:302:LEU:HD23	2.02	0.41
1:A:287:ARG:HB2	1:A:307:GLU:OE1	2.21	0.41
1:A:418:TYR:N	1:A:418:TYR:CD1	2.89	0.41
1:B:170:LEU:HA	1:B:176:THR:O	2.21	0.41
1:B:440:MET:H	1:B:440:MET:HG3	1.69	0.41
1:B:68:VAL:HG23	1:B:96:ASN:C	2.40	0.41
1:C:314:ASN:ND2	1:C:317:GLY:HA3	2.36	0.41
1:C:89:VAL:CG1	1:C:89:VAL:O	2.69	0.41
1:B:118:ARG:HG3	1:B:126:VAL:CG1	2.51	0.40
1:D:73:ARG:HG2	1:D:73:ARG:H	1.64	0.40
1:B:251:PHE:HB2	1:B:327:LEU:HG	2.03	0.40
1:D:469:PRO:O	1:D:470:SER:HB2	2.21	0.40
1:B:328:PRO:HG3	1:B:376:LEU:H	1.86	0.40
1:A:240:GLN:OE1	1:C:165:ARG:NH2	2.53	0.40
1:D:217:GLY:O	1:D:356:ARG:HD3	2.22	0.40
1:D:25:GLN:HG3	1:D:26:PHE:N	2.31	0.40
1:A:411:PHE:CZ	1:A:415:LEU:HD11	2.56	0.40
1:A:94:PHE:O	3:A:503:FUC:H61	2.21	0.40
1:B:192:HIS:O	1:B:196:VAL:HG22	2.21	0.40
1:B:197:LYS:HZ3	1:B:302:LEU:HD13	1.83	0.40
1:C:184:ILE:CG2	1:C:234:ASP:HB3	2.51	0.40
1:C:92:LEU:HA	1:C:92:LEU:HD23	1.69	0.40
1:D:360:GLU:OE2	1:D:362:PHE:HE2	2.05	0.40
1:D:370:ASP:HB3	1:D:373:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLY:HA2	1:A:327:LEU:O	2.21	0.40
1:B:377:HIS:O	1:B:381:HIS:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	402 (90%)	40 (9%)	2 (0%)	32	64
1	B	444/446 (100%)	377 (85%)	51 (12%)	16 (4%)	4	14
1	C	444/446 (100%)	409 (92%)	31 (7%)	4 (1%)	20	49
1	D	444/446 (100%)	403 (91%)	37 (8%)	4 (1%)	20	49
All	All	1776/1784 (100%)	1591 (90%)	159 (9%)	26 (2%)	12	35

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	74	PRO
1	B	191	THR
1	B	197	LYS
1	B	327	LEU
1	B	427	LEU
1	D	174	GLY
1	A	197	LYS
1	B	171	GLY
1	B	385	ASN
1	B	419	ASN
1	A	419	ASN
1	B	54	ASP
1	B	181	ASN

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Mol	Chain	Res	Type
1	B	326	ARG
1	B	387	THR
1	C	47	PRO
1	C	172	PRO
1	D	368	LYS
1	D	436	ARG
1	C	376	LEU
1	B	426	PRO
1	D	266	MET
1	B	77	PRO
1	C	364	ASP
1	B	365	PRO
1	B	442	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	395/395 (100%)	382 (97%)	13 (3%)	43	74
1	B	395/395 (100%)	376 (95%)	19 (5%)	30	61
1	C	395/395 (100%)	386 (98%)	9 (2%)	56	83
1	D	395/395 (100%)	385 (98%)	10 (2%)	53	81
All	All	1580/1580 (100%)	1529 (97%)	51 (3%)	44	76

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	A	64	ARG
1	A	193	TYR
1	A	197	LYS
1	A	270	SER
1	A	308	ASP
1	A	336	CYS
1	A	354	SER

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Mol	Chain	Res	Type
1	A	374	SER
1	A	405	THR
1	A	425	PHE
1	A	438	TYR
1	A	450	THR
1	B	29	GLN
1	B	36	LEU
1	B	55	ARG
1	B	60	SER
1	B	66	GLU
1	B	73	ARG
1	B	93	ARG
1	B	155	THR
1	B	165	ARG
1	B	183	SER
1	B	207	SER
1	B	250	ASN
1	B	258	CYS
1	B	278	SER
1	B	295	ASP
1	B	343	ASP
1	B	354	SER
1	B	438	TYR
1	B	470	SER
1	C	60	SER
1	C	106	SER
1	C	118	ARG
1	C	197	LYS
1	C	258	CYS
1	C	278	SER
1	C	349	SER
1	C	419	ASN
1	C	425	PHE
1	D	49	SER
1	D	193	TYR
1	D	230	ARG
1	D	265	LEU
1	D	294	GLU
1	D	336	CYS
1	D	363	SER
1	D	425	PHE
1	D	436	ARG

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Mol	Chain	Res	Type
1	D	438	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	B	178	GLN
1	B	304	ASN
1	B	378	ASN
1	D	419	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 9 are monoatomic - leaving 40 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	501	1,3,2	14,14,15	1.14	2 (14%)	15,19,21	1.26	1 (6%)
2	NAG	A	502	2	14,14,15	0.98	1 (7%)	15,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUC	A	503	2	9,10,11	1.43	0	13,14,16	1.44	2 (15%)
2	NAG	A	504	1	14,14,15	1.66	2 (14%)	15,19,21	1.03	2 (13%)
2	NAG	A	505	1,2	14,14,15	0.96	1 (7%)	15,19,21	0.93	1 (6%)
2	NAG	A	506	2	14,14,15	0.44	0	15,19,21	0.72	0
2	NAG	A	507	1,2	14,14,15	0.84	1 (7%)	15,19,21	1.00	1 (6%)
2	NAG	A	508	2,4	14,14,15	0.68	1 (7%)	15,19,21	1.35	2 (13%)
4	MAN	A	509	2,4	11,11,12	1.19	1 (9%)	13,15,17	1.95	3 (23%)
4	MAN	A	510	4	11,11,12	1.59	3 (27%)	13,15,17	1.84	3 (23%)
4	MAN	A	511	4	11,11,12	1.06	1 (9%)	13,15,17	2.03	4 (30%)
2	NAG	A	512	1,2	14,14,15	0.55	0	15,19,21	0.61	0
2	NAG	A	513	2	14,14,15	0.80	1 (7%)	15,19,21	0.51	0
6	KOJ	A	516	-	7,10,10	4.45	5 (71%)	5,13,13	1.39	1 (20%)
2	NAG	B	501	1	14,14,15	1.83	1 (7%)	15,19,21	1.32	3 (20%)
2	NAG	B	502	1,3	14,14,15	1.22	3 (21%)	15,19,21	1.20	1 (6%)
3	FUC	B	503	2	9,10,11	1.70	3 (33%)	13,14,16	1.66	3 (23%)
2	NAG	B	504	-	14,14,15	1.17	1 (7%)	15,19,21	0.62	0
2	NAG	B	505	1	14,14,15	0.81	1 (7%)	15,19,21	0.59	0
6	KOJ	B	508	-	7,10,10	4.26	4 (57%)	5,13,13	0.76	0
2	NAG	C	501	1,3	14,14,15	0.67	0	15,19,21	0.64	0
3	FUC	C	502	2	9,10,11	1.22	2 (22%)	13,14,16	2.13	2 (15%)
2	NAG	C	503	-	14,14,15	1.05	1 (7%)	15,19,21	1.70	3 (20%)
2	NAG	C	504	1,2	14,14,15	0.81	1 (7%)	15,19,21	0.77	0
2	NAG	C	505	2	14,14,15	0.52	0	15,19,21	0.47	0
2	NAG	C	506	1,2	14,14,15	1.82	2 (14%)	15,19,21	2.51	4 (26%)
2	NAG	C	507	2,4	14,14,15	0.99	1 (7%)	15,19,21	1.29	2 (13%)
4	MAN	C	508	2,4	11,11,12	1.25	1 (9%)	13,15,17	1.78	2 (15%)
4	MAN	C	509	4	11,11,12	1.22	1 (9%)	13,15,17	1.73	1 (7%)
4	MAN	C	510	4	11,11,12	0.72	0	13,15,17	1.78	3 (23%)
2	NAG	C	511	1	14,14,15	0.66	1 (7%)	15,19,21	0.75	1 (6%)
6	KOJ	C	514	-	7,10,10	4.13	4 (57%)	5,13,13	1.43	1 (20%)
2	NAG	D	501	1,3	14,14,15	0.55	0	15,19,21	0.80	0
3	FUC	D	502	2	9,10,11	2.58	5 (55%)	13,14,16	2.31	5 (38%)
2	NAG	D	503	1,3	14,14,15	1.95	3 (21%)	15,19,21	1.08	1 (6%)
3	FUC	D	504	2	9,10,11	2.17	3 (33%)	13,14,16	1.74	3 (23%)
2	NAG	D	505	1,2	14,14,15	0.33	0	15,19,21	0.71	0
2	NAG	D	506	2	14,14,15	0.54	0	15,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	507	1	14,14,15	1.03	1 (7%)	15,19,21	0.95	1 (6%)
6	KOJ	D	510	-	7,10,10	4.47	5 (71%)	5,13,13	1.51	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	501	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
3	FUC	A	503	2	-	0/0/17/20	0/1/1/1
2	NAG	A	504	1	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	506	2	-	0/6/23/26	0/1/1/1
2	NAG	A	507	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	508	2,4	-	0/6/23/26	0/1/1/1
4	MAN	A	509	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	510	4	-	0/2/19/22	0/1/1/1
4	MAN	A	511	4	-	0/2/19/22	0/1/1/1
2	NAG	A	512	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	513	2	-	0/6/23/26	0/1/1/1
6	KOJ	A	516	-	-	0/1/2/2	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1,3	-	0/6/23/26	0/1/1/1
3	FUC	B	503	2	-	0/0/17/20	0/1/1/1
2	NAG	B	504	-	-	0/6/23/26	0/1/1/1
2	NAG	B	505	1	-	0/6/23/26	0/1/1/1
6	KOJ	B	508	-	-	0/1/2/2	0/1/1/1
2	NAG	C	501	1,3	-	0/6/23/26	0/1/1/1
3	FUC	C	502	2	-	0/0/17/20	0/1/1/1
2	NAG	C	503	-	-	0/6/23/26	0/1/1/1
2	NAG	C	504	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	505	2	-	0/6/23/26	0/1/1/1
2	NAG	C	506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	507	2,4	-	0/6/23/26	0/1/1/1
4	MAN	C	508	2,4	-	0/2/19/22	1/1/1/1
4	MAN	C	509	4	-	0/2/19/22	0/1/1/1
4	MAN	C	510	4	-	0/2/19/22	0/1/1/1
2	NAG	C	511	1	-	0/6/23/26	0/1/1/1
6	KOJ	C	514	-	-	0/1/2/2	0/1/1/1
2	NAG	D	501	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	D	502	2	-	0/0/17/20	0/1/1/1
2	NAG	D	503	1,3	-	0/6/23/26	0/1/1/1
3	FUC	D	504	2	-	0/0/17/20	0/1/1/1
2	NAG	D	505	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	506	2	-	0/6/23/26	0/1/1/1
2	NAG	D	507	1	-	0/6/23/26	0/1/1/1
6	KOJ	D	510	-	-	0/1/2/2	0/1/1/1

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAG	O5-C1	-6.37	1.33	1.43
2	D	503	NAG	O5-C1	-4.44	1.36	1.43
2	B	504	NAG	O5-C1	-4.21	1.36	1.43
2	C	507	NAG	O5-C1	-3.62	1.37	1.43
2	A	505	NAG	O5-C1	-3.48	1.38	1.43
2	C	503	NAG	O5-C1	-3.43	1.38	1.43
2	B	502	NAG	O5-C1	-3.01	1.38	1.43
2	C	504	NAG	O5-C1	-2.86	1.39	1.43
6	D	510	KOJ	C4-C5	-2.77	1.31	1.35
2	A	508	NAG	C1-C2	-2.38	1.49	1.52
6	A	516	KOJ	C4-C5	-2.28	1.32	1.35
6	B	508	KOJ	O3-C3	-2.20	1.19	1.23
6	D	510	KOJ	O3-C3	-2.19	1.19	1.23
6	A	516	KOJ	O3-C3	-2.09	1.19	1.23
4	A	509	MAN	O3-C3	-2.02	1.38	1.43
6	B	508	KOJ	O2-C2	2.01	1.41	1.35
3	D	502	FUC	O3-C3	2.01	1.47	1.43
2	A	504	NAG	C3-C2	2.01	1.56	1.52
2	C	511	NAG	O5-C1	2.05	1.47	1.43
2	B	502	NAG	C3-C2	2.06	1.57	1.52
3	B	503	FUC	O5-C1	2.09	1.47	1.43
6	C	514	KOJ	C3-C2	2.10	1.48	1.41
2	A	501	NAG	C8-C7	2.13	1.55	1.50
6	D	510	KOJ	O2-C2	2.16	1.41	1.35
2	D	503	NAG	C3-C2	2.20	1.57	1.52
3	B	503	FUC	C4-C5	2.25	1.57	1.53
3	D	502	FUC	C4-C3	2.26	1.58	1.52
4	A	510	MAN	C1-C2	2.30	1.57	1.52
3	C	502	FUC	C2-C3	2.32	1.55	1.52
6	A	516	KOJ	O2-C2	2.37	1.42	1.35
3	C	502	FUC	C4-C5	2.39	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	505	NAG	O5-C1	2.48	1.47	1.43
3	D	504	FUC	C2-C3	2.61	1.56	1.52
2	B	502	NAG	C1-C2	2.61	1.56	1.52
4	C	509	MAN	O5-C5	2.62	1.49	1.43
4	A	510	MAN	C4-C3	2.62	1.59	1.52
6	C	514	KOJ	O2-C2	2.65	1.42	1.35
4	A	511	MAN	C2-C3	2.68	1.56	1.52
2	A	513	NAG	C1-C2	2.75	1.56	1.52
2	A	501	NAG	O5-C1	2.93	1.48	1.43
4	A	510	MAN	C2-C3	2.94	1.56	1.52
3	D	502	FUC	O4-C4	3.00	1.49	1.43
2	A	507	NAG	O5-C1	3.06	1.48	1.43
4	C	508	MAN	O5-C5	3.17	1.50	1.43
3	D	502	FUC	C1-C2	3.26	1.59	1.52
2	D	507	NAG	O5-C1	3.35	1.49	1.43
3	B	503	FUC	C1-C2	3.45	1.60	1.52
2	A	502	NAG	C1-C2	3.50	1.57	1.52
2	C	506	NAG	C1-C2	3.56	1.57	1.52
3	D	504	FUC	C1-C2	3.80	1.61	1.52
3	D	504	FUC	C4-C5	3.91	1.60	1.53
6	A	516	KOJ	C4-C3	4.89	1.47	1.37
6	B	508	KOJ	C4-C3	5.06	1.47	1.37
3	D	502	FUC	C2-C3	5.08	1.59	1.52
6	D	510	KOJ	C4-C3	5.17	1.48	1.37
2	D	503	NAG	C1-C2	5.18	1.59	1.52
2	C	506	NAG	O5-C1	5.59	1.52	1.43
6	C	514	KOJ	C4-C3	5.64	1.49	1.37
2	A	504	NAG	C1-C2	5.72	1.60	1.52
6	C	514	KOJ	O5-C5	8.44	1.46	1.35
6	B	508	KOJ	O5-C5	9.27	1.47	1.35
6	D	510	KOJ	O5-C5	9.67	1.47	1.35
6	A	516	KOJ	O5-C5	9.84	1.48	1.35

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	510	MAN	O2-C2-C3	-3.69	102.92	110.17
4	A	509	MAN	O2-C2-C3	-3.69	102.93	110.17
2	C	503	NAG	C1-O5-C5	-3.32	107.58	112.17
4	C	508	MAN	O2-C2-C3	-3.23	103.83	110.17
2	C	506	NAG	C4-C3-C2	-3.20	106.32	111.02
2	B	501	NAG	O6-C6-C5	-2.77	102.03	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	508	NAG	O4-C4-C5	-2.60	102.72	109.28
2	A	507	NAG	O4-C4-C3	-2.58	104.75	110.36
2	C	507	NAG	C3-C4-C5	-2.45	105.89	110.22
6	C	514	KOJ	O5-C5-C4	-2.39	117.45	119.85
4	A	511	MAN	C3-C4-C5	-2.31	106.16	110.22
6	A	516	KOJ	O2-C2-C3	-2.15	115.30	119.52
2	C	507	NAG	C4-C3-C2	-2.08	107.98	111.02
6	D	510	KOJ	O6-C6-C5	-2.04	107.58	112.18
2	B	501	NAG	C1-O5-C5	-2.01	109.40	112.17
2	C	511	NAG	C1-O5-C5	2.10	115.06	112.17
6	D	510	KOJ	C4-C3-C2	2.17	121.34	118.21
4	A	509	MAN	O5-C1-C2	2.19	114.22	110.79
2	A	505	NAG	C1-O5-C5	2.27	115.29	112.17
2	A	504	NAG	C2-N2-C7	2.27	126.26	122.94
3	B	503	FUC	O2-C2-C1	2.40	114.07	109.18
2	A	501	NAG	O4-C4-C5	2.42	115.37	109.28
3	D	504	FUC	O5-C5-C4	2.47	113.69	109.62
3	D	502	FUC	C2-C3-C4	2.54	115.30	110.88
2	D	507	NAG	C1-O5-C5	2.71	115.90	112.17
2	B	501	NAG	O4-C4-C5	2.74	116.20	109.28
3	D	502	FUC	C1-O5-C5	2.76	118.50	112.39
2	A	504	NAG	C4-C3-C2	2.81	115.14	111.02
3	D	502	FUC	O5-C1-C2	2.83	115.22	110.79
3	A	503	FUC	C1-O5-C5	2.84	118.67	112.39
3	D	504	FUC	C1-O5-C5	2.91	118.82	112.39
4	A	510	MAN	C3-C4-C5	2.92	115.36	110.22
3	D	502	FUC	O5-C5-C4	2.96	114.50	109.62
2	A	508	NAG	C2-N2-C7	2.99	127.30	122.94
4	C	510	MAN	C1-O5-C5	3.02	116.32	112.17
3	B	503	FUC	O5-C5-C4	3.06	114.67	109.62
2	C	506	NAG	C1-C2-N2	3.12	115.81	110.49
2	C	503	NAG	C4-C3-C2	3.20	115.70	111.02
3	B	503	FUC	C1-O5-C5	3.22	119.51	112.39
3	A	503	FUC	O5-C5-C4	3.22	114.93	109.62
4	C	510	MAN	C1-C2-C3	3.26	113.78	109.65
4	A	510	MAN	C1-C2-C3	3.44	114.02	109.65
4	A	511	MAN	O5-C1-C2	3.50	116.27	110.79
4	A	510	MAN	C2-C3-C4	3.51	117.00	110.88
4	A	511	MAN	C1-C2-C3	3.61	114.23	109.65
2	C	503	NAG	C3-C4-C5	3.69	116.73	110.22
3	D	504	FUC	O2-C2-C1	3.70	116.69	109.18
2	D	503	NAG	C4-C3-C2	3.80	116.58	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	NAG	C4-C3-C2	3.87	116.68	111.02
3	C	502	FUC	C1-O5-C5	4.12	121.50	112.39
4	A	509	MAN	C1-O5-C5	4.19	117.95	112.17
4	A	511	MAN	C1-O5-C5	4.20	117.95	112.17
4	C	508	MAN	C1-O5-C5	4.72	118.67	112.17
3	D	502	FUC	C1-C2-C3	5.34	116.42	109.65
4	C	509	MAN	C1-O5-C5	5.35	119.54	112.17
2	C	506	NAG	O4-C4-C5	5.58	123.33	109.28
3	C	502	FUC	O5-C5-C4	5.61	118.86	109.62
2	C	506	NAG	C1-O5-C5	5.68	120.00	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	508	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	FUC	1	0
2	A	508	NAG	1	0
2	A	512	NAG	1	0
6	A	516	KOJ	3	0
2	B	501	NAG	1	0
2	B	504	NAG	2	0
6	B	508	KOJ	3	0
2	C	503	NAG	1	0
6	C	514	KOJ	1	0
2	D	501	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	446/446 (100%)	0.10	7 (1%) 72 70	33, 51, 66, 79	0
1	B	446/446 (100%)	0.60	45 (10%) 8 5	42, 71, 95, 108	0
1	C	446/446 (100%)	0.00	4 (0%) 84 83	38, 54, 69, 90	0
1	D	446/446 (100%)	-0.05	2 (0%) 92 92	34, 49, 66, 81	0
All	All	1784/1784 (100%)	0.16	58 (3%) 47 40	33, 54, 87, 108	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	320	ALA	5.4
1	B	164	ARG	5.2
1	B	48	VAL	4.9
1	B	256	ASN	4.8
1	B	327	LEU	4.6
1	B	49	SER	4.4
1	B	203	VAL	4.1
1	B	47	PRO	4.1
1	B	72	SER	4.1
1	B	430	ALA	4.1
1	B	204	GLY	3.8
1	B	208	PHE	3.4
1	B	302	LEU	3.4
1	B	429	ASN	3.3
1	B	170	LEU	3.2
1	B	166	SER	3.2
1	B	33	VAL	3.1
1	B	32	THR	3.1
1	B	316	ALA	3.1
1	B	172	PRO	3.1
1	B	334	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	367	GLY	2.9
1	A	371	PRO	2.9
1	C	330	PRO	2.8
1	A	69	THR	2.8
1	B	324	VAL	2.7
1	B	201	LEU	2.7
1	B	293	LEU	2.6
1	B	323	MET	2.6
1	A	319	VAL	2.6
1	B	209	GLY	2.6
1	D	373	VAL	2.5
1	B	350	ASN	2.5
1	B	469	PRO	2.5
1	B	254	GLY	2.5
1	B	321	ARG	2.4
1	C	48	VAL	2.4
1	B	372	ALA	2.4
1	B	371	PRO	2.4
1	B	435	ASN	2.4
1	B	368	LYS	2.4
1	D	470	SER	2.3
1	B	176	THR	2.3
1	B	75	HIS	2.3
1	C	49	SER	2.2
1	B	255	LYS	2.2
1	B	319	VAL	2.2
1	B	257	VAL	2.2
1	C	329	GLU	2.2
1	B	210	GLU	2.2
1	B	77	PRO	2.1
1	A	467	GLN	2.1
1	A	37	ARG	2.0
1	A	329	GLU	2.0
1	B	167	GLU	2.0
1	B	205	GLN	2.0
1	B	322	PRO	2.0
1	A	35	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
6	KOJ	D	510	10/10	0.85	0.29	5.62	45,50,56,56	0
2	NAG	A	504	14/15	0.74	0.34	5.28	41,67,75,76	0
6	KOJ	C	514	10/10	0.89	0.22	2.71	50,54,57,59	0
6	KOJ	A	516	10/10	0.90	0.24	2.29	50,54,56,62	0
6	KOJ	B	508	10/10	0.90	0.28	1.60	74,75,82,83	0
2	NAG	C	506	14/15	0.88	0.26	0.83	43,49,57,58	0
2	NAG	C	511	14/15	0.92	0.21	0.30	50,57,67,68	0
2	NAG	B	501	14/15	0.67	0.34	0.24	68,87,95,95	0
2	NAG	C	507	14/15	0.93	0.21	0.24	33,53,62,68	0
3	FUC	D	502	10/11	0.85	0.21	0.15	57,63,67,67	0
2	NAG	B	505	14/15	0.72	0.31	0.02	76,87,93,94	0
2	NAG	C	504	14/15	0.93	0.18	-0.02	53,58,65,66	0
3	FUC	C	502	10/11	0.91	0.21	-0.03	65,68,72,84	0
2	NAG	D	501	14/15	0.89	0.19	-0.06	44,60,69,71	0
2	NAG	D	507	14/15	0.91	0.21	-0.10	43,59,64,64	0
5	ZN	A	515	1/1	0.98	0.15	-0.15	51,51,51,51	0
2	NAG	A	512	14/15	0.90	0.17	-0.28	55,61,71,75	0
2	NAG	A	508	14/15	0.95	0.17	-0.34	45,50,58,70	0
2	NAG	A	505	14/15	0.92	0.17	-0.40	56,61,64,65	0
3	FUC	A	503	10/11	0.89	0.24	-0.53	59,61,67,72	0
5	ZN	D	508	1/1	0.99	0.18	-0.59	39,39,39,39	0
2	NAG	B	504	14/15	0.88	0.21	-0.59	59,70,81,82	0
5	ZN	C	513	1/1	0.99	0.14	-0.67	60,60,60,60	0
2	NAG	C	501	14/15	0.92	0.17	-0.82	54,64,71,72	0
2	NAG	D	505	14/15	0.93	0.15	-0.95	49,56,62,62	0
5	ZN	C	512	1/1	1.00	0.14	-1.09	42,42,42,42	0
4	MAN	C	508	11/12	0.93	0.16	-1.40	45,52,58,60	0
5	ZN	B	506	1/1	0.97	0.14	-1.43	78,78,78,78	0
4	MAN	A	509	11/12	0.96	0.16	-1.50	53,58,67,68	0
5	ZN	A	514	1/1	0.97	0.12	-1.87	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ZN	D	509	1/1	0.99	0.14	-2.03	53,53,53,53	0
5	ZN	B	507	1/1	0.97	0.13	-2.34	68,68,68,68	0
2	NAG	A	507	14/15	0.92	0.14	-2.34	44,49,52,52	0
5	ZN	C	515	1/1	0.99	0.08	-3.26	58,58,58,58	0
2	NAG	C	505	14/15	0.82	0.26	-	56,63,68,69	0
2	NAG	D	503	14/15	0.84	0.24	-	53,68,79,79	0
3	FUC	B	503	10/11	0.78	0.31	-	69,83,89,90	0
2	NAG	D	506	14/15	0.89	0.24	-	64,72,75,76	0
3	FUC	D	504	10/11	0.85	0.36	-	58,76,83,87	0
2	NAG	A	513	14/15	0.82	0.38	-	77,84,93,93	0
4	MAN	A	511	11/12	0.86	0.26	-	65,71,85,88	0
4	MAN	C	509	11/12	0.91	0.21	-	50,58,65,67	0
2	NAG	B	502	14/15	0.88	0.20	-	71,78,86,88	0
4	MAN	C	510	11/12	0.92	0.20	-	52,59,63,67	0
2	NAG	A	506	14/15	0.86	0.26	-	57,66,73,78	0
2	NAG	A	501	14/15	0.93	0.17	-	60,70,72,73	0
4	MAN	A	510	11/12	0.86	0.24	-	63,67,75,75	0
2	NAG	A	502	14/15	0.90	0.34	-	66,78,87,88	0
2	NAG	C	503	14/15	0.64	0.29	-	54,71,85,87	0

6.5 Other polymers

There are no such residues in this entry.