



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:10 PM UTC

PDB ID : 5JO7 / pdb_00005jo7
Title : Henbane premnaspirodiene synthase (HPS), also known as Henbane vetispiradiene synthase (HVS) from *Hyoscyamus muticus*
Authors : Koo, H.J.; Xu, Y.; Louie, G.V.; Bowman, M.; Noel, J.P.
Deposited on : 2016-05-02
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

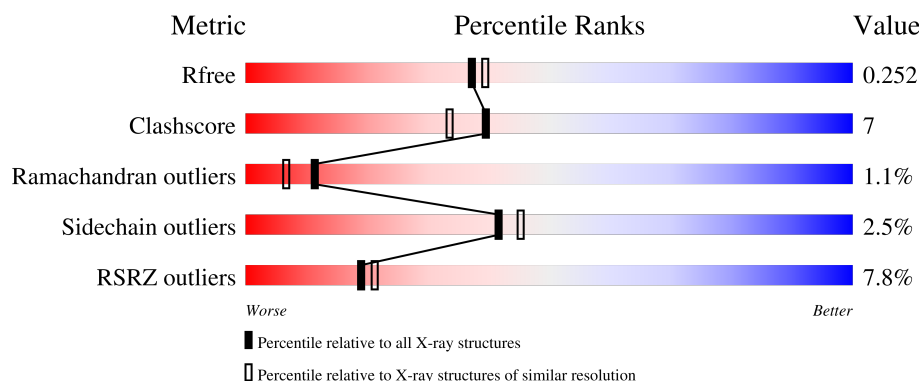
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	538	
1	B	538	
1	C	538	
1	D	538	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17486 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 Vetispiradiene synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	1	0
			4190	2683	690	800	17			
1	B	506	Total	C	N	O	S	0	2	0
			4169	2674	686	792	17			
1	C	503	Total	C	N	O	S	0	2	0
			4141	2658	677	789	17			
1	D	499	Total	C	N	O	S	0	1	0
			4099	2629	672	781	17			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP Q39978
A	19	SER	-	expression tag	UNP Q39978
A	20	HIS	-	expression tag	UNP Q39978
A	21	MET	-	expression tag	UNP Q39978
A	22	ALA	-	expression tag	UNP Q39978
A	30	ARG	HIS	conflict	UNP Q39978
A	381	ARG	GLY	conflict	UNP Q39978
A	387	ALA	GLY	conflict	UNP Q39978
B	18	GLY	-	expression tag	UNP Q39978
B	19	SER	-	expression tag	UNP Q39978
B	20	HIS	-	expression tag	UNP Q39978
B	21	MET	-	expression tag	UNP Q39978
B	22	ALA	-	expression tag	UNP Q39978
B	30	ARG	HIS	conflict	UNP Q39978
B	381	ARG	GLY	conflict	UNP Q39978
B	387	ALA	GLY	conflict	UNP Q39978
C	18	GLY	-	expression tag	UNP Q39978
C	19	SER	-	expression tag	UNP Q39978
C	20	HIS	-	expression tag	UNP Q39978
C	21	MET	-	expression tag	UNP Q39978
C	22	ALA	-	expression tag	UNP Q39978

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Chain	Residue	Modelled	Actual	Comment	Reference
C	30	ARG	HIS	conflict	UNP Q39978
C	381	ARG	GLY	conflict	UNP Q39978
C	387	ALA	GLY	conflict	UNP Q39978
D	18	GLY	-	expression tag	UNP Q39978
D	19	SER	-	expression tag	UNP Q39978
D	20	HIS	-	expression tag	UNP Q39978
D	21	MET	-	expression tag	UNP Q39978
D	22	ALA	-	expression tag	UNP Q39978
D	30	ARG	HIS	conflict	UNP Q39978
D	381	ARG	GLY	conflict	UNP Q39978
D	387	ALA	GLY	conflict	UNP Q39978

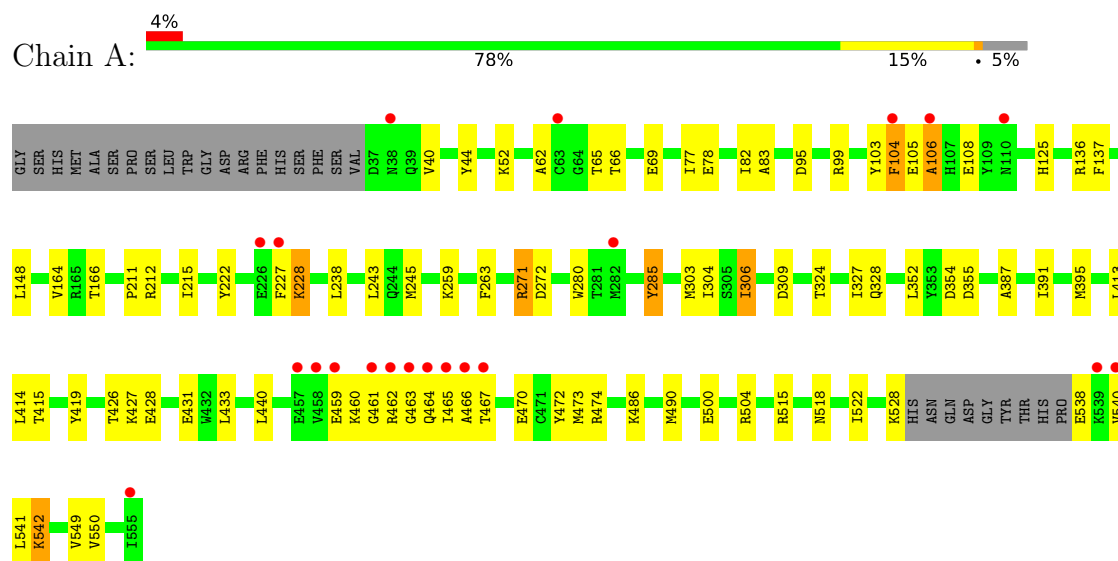
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	306	Total 306	O 306	0	0
2	B	252	Total 252	O 252	0	0
2	C	198	Total 198	O 198	0	0
2	D	131	Total 131	O 131	0	0

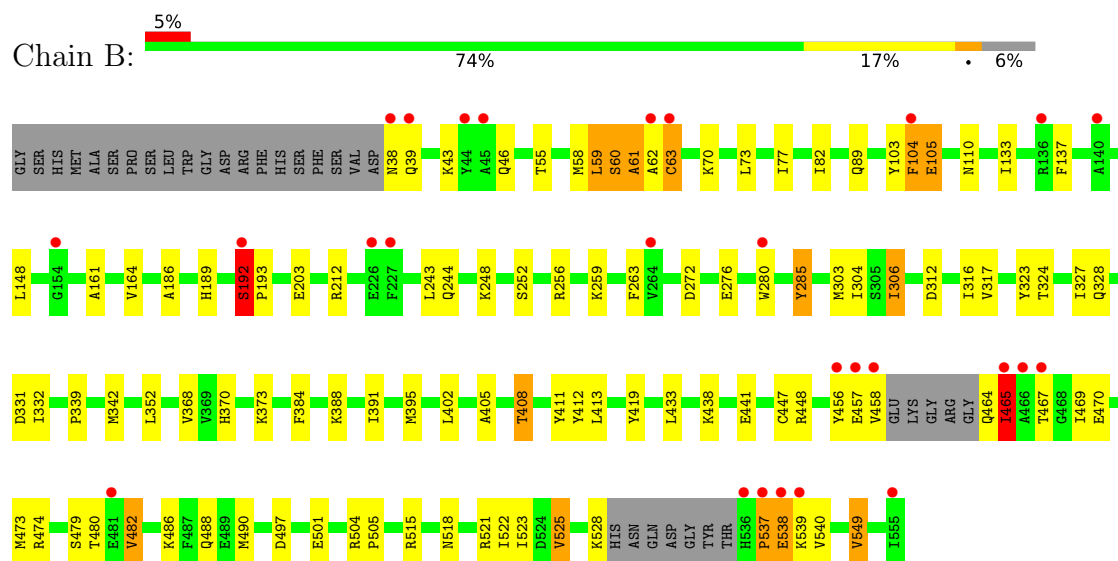
3 Residue-property plots [i](#)

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

• Molecule 1: Vetispiradiene synthase 1



• Molecule 1: Vetispiradiene synthase 1



• Molecule 1: Vetispiradiene synthase 1

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.45Å 100.69Å 222.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.69 – 2.15 74.69 – 2.15	Depositor EDS
% Data completeness (in resolution range)	85.0 (74.69-2.15) 85.1 (74.69-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.191 , 0.250 0.195 , 0.252	Depositor DCC
R_{free} test set	2192 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17486	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.08% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.62	0/4283	0.86	4/5800 (0.1%)
1	B	0.53	0/4267	0.85	9/5781 (0.2%)
1	C	0.52	0/4237	0.90	12/5739 (0.2%)
1	D	0.46	0/4190	0.82	3/5674 (0.1%)
All	All	0.53	0/16977	0.86	28/22994 (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	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	485	GLU	N-CA-C	14.48	127.14	111.36
1	B	60	SER	N-CA-C	9.58	121.72	111.28
1	C	485	GLU	CA-C-N	9.17	138.20	121.70
1	C	485	GLU	C-N-CA	9.17	138.20	121.70
1	B	192	SER	CA-C-N	-7.61	112.00	120.45
1	B	192	SER	C-N-CA	-7.61	112.00	120.45
1	B	105	GLU	N-CA-C	6.80	118.69	111.28
1	A	550	VAL	CB-CA-C	-6.77	105.96	111.71
1	D	192	SER	CA-C-N	-6.55	113.18	120.45
1	D	192	SER	C-N-CA	-6.55	113.18	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	487	PHE	N-CA-C	-6.12	104.69	111.36
1	A	62	ALA	N-CA-C	-5.87	105.70	112.92
1	C	478	VAL	N-CA-C	5.84	117.80	112.43
1	C	457	GLU	CA-C-N	5.78	132.11	121.70
1	C	457	GLU	C-N-CA	5.78	132.11	121.70
1	C	485	GLU	CA-C-O	-5.71	114.37	120.42
1	B	61	ALA	CA-C-N	5.69	131.94	121.70
1	B	61	ALA	C-N-CA	5.69	131.94	121.70
1	C	469	ILE	N-CA-C	-5.63	105.04	110.72
1	C	287	GLU	CA-C-N	5.61	125.27	119.05
1	C	287	GLU	C-N-CA	5.61	125.27	119.05
1	B	549	VAL	CA-C-N	-5.20	117.87	122.97
1	B	549	VAL	C-N-CA	-5.20	117.87	122.97
1	B	540	VAL	N-CA-C	-5.13	104.68	111.09
1	C	480	THR	N-CA-C	5.12	116.94	111.36
1	A	542	LYS	CA-C-N	-5.04	113.85	119.19
1	A	542	LYS	C-N-CA	-5.04	113.85	119.19
1	D	46	GLN	N-CA-C	5.03	117.17	110.53

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ALA	Peptide
1	B	104	PHE	Peptide
1	B	59	LEU	Peptide
1	C	106	ALA	Peptide
1	D	64	GLY	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	4190	0	4135	52	0
1	B	4169	0	4113	73	0
1	C	4141	0	4092	49	0
1	D	4099	0	4050	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	306	0	0	4	0
2	B	252	0	0	7	0
2	C	198	0	0	6	0
2	D	131	0	0	3	0
All	All	17486	0	16390	222	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 7.

All (222) 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:464:GLN:NE2	1:B:465:ILE:O	2.09	0.85
1:A:271:ARG:NH1	1:A:309:ASP:OD1	2.11	0.84
1:D:203:GLU:O	1:D:528:LYS:NZ	2.16	0.79
1:A:395:MET:HE3	1:A:474:ARG:HD3	1.67	0.77
1:D:340:GLU:OE1	2:D:601:HOH:O	2.03	0.77
1:C:395:MET:HG2	1:C:474:ARG:HD3	1.68	0.76
1:B:61:ALA:HB1	1:B:63:CYS:H	1.51	0.75
1:C:225:GLU:O	1:C:228:LYS:NZ	2.19	0.74
1:D:63:CYS:SG	1:D:70:LYS:NZ	2.59	0.74
1:B:61:ALA:HA	1:B:62:ALA:HB3	1.72	0.70
1:A:465:ILE:O	1:A:467:THR:N	2.22	0.69
1:D:395:MET:HG2	1:D:474:ARG:HD3	1.74	0.68
1:A:104:PHE:H	1:A:104:PHE:HD1	1.42	0.67
1:A:271:ARG:HG3	1:A:271:ARG:HH11	1.59	0.67
1:B:486:LYS:NZ	2:B:601:HOH:O	2.19	0.67
1:A:104:PHE:O	1:A:136:ARG:NH2	2.24	0.66
1:B:339:PRO:HD2	1:B:342:MET:HE2	1.78	0.66
1:B:408:THR:HG21	2:B:628:HOH:O	1.96	0.65
1:D:64:GLY:H	1:D:65:THR:HA	1.61	0.65
1:B:537:PRO:O	1:B:539:LYS:N	2.30	0.64
1:B:456:TYR:C	1:B:458:VAL:H	2.06	0.64
1:A:103:TYR:O	1:A:105:GLU:N	2.31	0.63
1:A:472:TYR:CZ	1:A:486:LYS:HG2	2.32	0.63
1:C:153:ARG:NH2	2:C:606:HOH:O	2.30	0.62
1:C:358:LYS:NZ	2:C:608:HOH:O	2.32	0.61
1:D:192:SER:OG	1:D:193:PRO:HD2	2.01	0.61
1:B:192:SER:OG	1:B:193:PRO:HD2	2.00	0.60
1:B:285:TYR:CD2	1:B:515:ARG:HD2	2.36	0.60
1:B:61:ALA:HB1	1:B:63:CYS:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:LEU:HD21	1:D:288:PRO:HG3	1.82	0.59
1:B:60:SER:N	1:B:61:ALA:HB2	2.17	0.58
1:C:188:PRO:O	2:C:601:HOH:O	2.17	0.58
1:C:66:THR:HG23	1:C:68:THR:H	1.68	0.58
1:B:408:THR:HG22	1:B:448:ARG:NH2	2.18	0.58
1:D:74:ILE:HD12	1:D:90:ILE:HG23	1.86	0.58
1:D:456:TYR:HD1	1:D:467:THR:HG21	1.68	0.57
1:A:303:MET:HG3	1:A:352:LEU:HD22	1.87	0.57
1:D:109:TYR:O	1:D:115:SER:OG	2.20	0.57
1:D:334:GLN:OE1	1:D:337:ARG:NH1	2.34	0.56
1:B:43:LYS:NZ	2:B:609:HOH:O	2.37	0.56
1:B:304:ILE:HD11	1:B:413:LEU:HD23	1.88	0.56
1:A:538:GLU:HB2	1:A:540:VAL:HG23	1.88	0.56
1:B:55:THR:HA	1:B:58:MET:HE3	1.88	0.56
1:D:98:TYR:CE1	1:D:129:VAL:HG12	2.41	0.56
1:A:463:GLY:HA3	1:A:464:GLN:C	2.29	0.56
1:B:408:THR:HG22	1:B:448:ARG:HH21	1.70	0.56
1:B:323:TYR:CD1	1:B:342:MET:HE3	2.41	0.55
1:B:303:MET:HG3	1:B:352:LEU:HD22	1.87	0.55
1:D:64:GLY:N	1:D:65:THR:HA	2.21	0.55
1:A:137:PHE:HB3	1:A:148:LEU:HD11	1.88	0.55
1:A:285:TYR:CD2	1:A:515:ARG:HD2	2.41	0.55
1:C:61:ALA:C	1:C:63:CYS:H	2.15	0.54
1:C:52:LYS:NZ	2:C:614:HOH:O	2.40	0.54
1:B:203:GLU:O	1:B:528:LYS:NZ	2.40	0.54
1:C:106:ALA:CB	1:C:107:HIS:HA	2.37	0.54
1:C:518:ASN:O	1:C:522[B]:ILE:HG13	2.07	0.54
1:A:125:HIS:O	1:A:504:ARG:NH1	2.37	0.54
1:A:78:GLU:HA	1:A:83:ALA:HB2	1.89	0.54
1:A:515:ARG:NH2	2:A:619:HOH:O	2.40	0.54
1:C:104:PHE:CG	1:C:133:ILE:HG13	2.43	0.54
1:B:467:THR:HG23	1:B:470:GLU:H	1.73	0.53
1:A:66:THR:N	1:A:69:GLU:OE2	2.41	0.53
1:B:419:TYR:CE2	1:B:433:LEU:HD11	2.44	0.53
1:D:258:TRP:NE1	1:D:272:ASP:OD1	2.40	0.53
1:B:518:ASN:O	1:B:522:ILE:HG13	2.09	0.53
1:A:263:PHE:CE2	1:A:306:ILE:HG13	2.45	0.52
1:B:395:MET:HE3	1:B:474:ARG:HD3	1.90	0.52
1:D:419:TYR:CE2	1:D:433:LEU:HD11	2.44	0.52
1:D:472:TYR:CZ	1:D:486:LYS:HG2	2.45	0.52
1:B:373:LYS:NZ	2:B:612:HOH:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASP:O	1:A:99:ARG:HG2	2.11	0.51
1:B:469:ILE:O	1:B:473:MET:HG3	2.11	0.51
1:C:77:ILE:HG23	1:C:82:ILE:HG13	1.91	0.51
1:C:426:THR:OG1	1:C:428:GLU:HG2	2.11	0.51
1:B:456:TYR:O	1:B:458:VAL:N	2.43	0.51
1:C:303:MET:HG3	1:C:352:LEU:HD22	1.92	0.51
1:A:486:LYS:O	1:A:490:MET:HG3	2.11	0.51
1:C:106:ALA:HB1	1:C:107:HIS:HA	1.92	0.51
1:A:472:TYR:CE2	1:A:486:LYS:HG2	2.46	0.50
1:C:485:GLU:N	1:C:486:LYS:HB3	2.26	0.50
1:A:65:THR:HB	1:A:69:GLU:HG3	1.94	0.50
1:B:137:PHE:HB3	1:B:148:LEU:HD11	1.94	0.50
1:C:110:ASN:OD1	1:C:136:ARG:HD3	2.12	0.50
1:C:104:PHE:HZ	1:C:129:VAL:HG23	1.77	0.50
1:C:113:ASN:OD1	1:C:157:ASN:ND2	2.38	0.49
1:A:212:ARG:HD2	2:A:744:HOH:O	2.12	0.49
1:D:123:ARG:HG2	1:D:129:VAL:HG22	1.93	0.49
1:A:166:THR:OG1	1:A:500:GLU:HB2	2.13	0.49
1:C:427:LYS:O	1:C:431:GLU:HG2	2.12	0.49
1:A:280[B]:TRP:HZ3	1:A:541:LEU:HD11	1.78	0.49
1:B:497:ASP:O	1:B:501:GLU:HG2	2.13	0.49
1:C:280[B]:TRP:HZ3	1:C:541:LEU:HD11	1.78	0.49
1:D:107:HIS:HA	1:D:108:GLU:C	2.37	0.49
1:D:469:ILE:O	1:D:473:MET:HG3	2.12	0.49
1:B:285:TYR:CE2	1:B:515:ARG:HD2	2.48	0.49
1:C:469:ILE:O	1:C:473:MET:HG3	2.13	0.49
1:D:48:ILE:HG23	1:D:235:PHE:CE1	2.48	0.48
1:B:60:SER:OG	1:B:61:ALA:HA	2.14	0.48
1:D:107:HIS:HA	1:D:109:TYR:N	2.28	0.48
1:B:212:ARG:HD2	2:B:770:HOH:O	2.14	0.48
1:A:463:GLY:HA3	1:A:464:GLN:O	2.14	0.48
1:C:485:GLU:O	1:C:488:GLN:HB2	2.14	0.48
1:D:304:ILE:HD11	1:D:413:LEU:HD23	1.95	0.48
1:A:272:ASP:HB3	1:B:272:ASP:HB3	1.96	0.48
1:C:489:GLU:O	1:C:493:ILE:HG12	2.14	0.47
1:C:233:LEU:HG	1:C:237:LYS:HE2	1.96	0.47
1:D:329:ARG:NE	2:D:604:HOH:O	2.29	0.47
1:B:323:TYR:HB2	1:B:342:MET:CE	2.45	0.47
1:B:323:TYR:HD1	1:B:342:MET:HE3	1.79	0.47
1:C:138:GLN:NE2	1:C:142:GLY:O	2.48	0.47
1:C:272:ASP:HB3	1:D:272:ASP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:GLU:OE2	2:C:602:HOH:O	2.20	0.47
1:B:263:PHE:CE2	1:B:306:ILE:HG13	2.49	0.47
1:A:66:THR:O	1:A:69:GLU:HG2	2.15	0.47
1:B:479:SER:OG	1:B:482:VAL:HG12	2.15	0.47
1:A:324:THR:O	1:A:328:GLN:HG2	2.15	0.47
1:B:252:SER:OG	1:B:256:ARG:NH1	2.48	0.47
1:D:211:PRO:O	1:D:215:ILE:HG12	2.15	0.47
1:A:355:ASP:OD1	2:A:601:HOH:O	2.20	0.46
1:B:259:LYS:HA	1:B:259:LYS:HD3	1.69	0.46
1:D:70:LYS:HA	1:D:70:LYS:HD3	1.58	0.46
1:D:107:HIS:HB2	1:D:110:ASN:OD1	2.15	0.46
1:B:60:SER:HA	1:B:89:GLN:HE21	1.81	0.46
1:C:467:THR:OG1	1:C:468:GLY:HA3	2.15	0.46
1:D:389:TRP:CZ3	1:D:396:PRO:HG3	2.51	0.46
1:B:384:PHE:CZ	1:B:388:LYS:HD2	2.51	0.46
1:D:427:LYS:O	1:D:431:GLU:HG2	2.16	0.46
1:A:542:LYS:NZ	1:B:312:ASP:OD2	2.48	0.45
1:B:61:ALA:HB3	1:B:70:LYS:NZ	2.31	0.45
1:D:108:GLU:H	1:D:108:GLU:CD	2.25	0.45
1:B:317:VAL:CG2	1:B:391:ILE:HG13	2.47	0.45
1:B:521:ARG:O	1:B:525:VAL:HG13	2.16	0.45
1:C:252:SER:O	1:C:256:ARG:HG3	2.16	0.45
1:A:304:ILE:HD11	1:A:413:LEU:HD23	1.98	0.45
1:C:486:LYS:N	1:C:489:GLU:H	2.15	0.45
1:B:324:THR:O	1:B:328:GLN:HG2	2.16	0.45
1:B:488:GLN:NE2	2:B:624:HOH:O	2.49	0.45
1:D:331:ASP:OD1	1:D:332:ILE:N	2.50	0.45
1:C:61:ALA:C	1:C:63:CYS:N	2.75	0.44
1:B:104:PHE:HD2	1:B:133:ILE:O	2.00	0.44
1:B:70:LYS:HA	1:B:70:LYS:HD3	1.74	0.44
1:C:95:ASP:O	1:C:99:ARG:HG2	2.17	0.44
1:C:104:PHE:O	1:C:136:ARG:NH2	2.47	0.44
1:C:149:ARG:HA	1:C:155:LEU:HD11	1.99	0.44
1:A:427:LYS:O	1:A:431:GLU:HG2	2.17	0.44
1:B:161:ALA:O	1:B:164:VAL:HG22	2.18	0.44
1:C:445:THR:O	1:C:449:VAL:HB	2.17	0.44
1:D:106:ALA:O	1:D:107:HIS:C	2.60	0.44
1:C:395:MET:HG2	1:C:474:ARG:CD	2.44	0.44
1:A:459:GLU:O	1:A:461:GLY:N	2.51	0.44
1:B:59:LEU:C	1:B:61:ALA:HB2	2.43	0.44
1:B:38:ASN:HA	1:B:39:GLN:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ASN:O	1:A:522:ILE:HG13	2.18	0.43
1:C:365:ARG:HD3	2:C:702:HOH:O	2.17	0.43
1:C:523:ILE:HD11	1:C:527:TYR:HE2	1.83	0.43
1:A:40:VAL:HG12	1:A:245:MET:HE1	2.00	0.43
1:A:77:ILE:HG23	1:A:82:ILE:HG13	2.01	0.43
1:C:470:GLU:HA	1:C:473:MET:HE3	2.01	0.43
1:A:105:GLU:O	1:A:106:ALA:HB3	2.18	0.43
1:B:331:ASP:OD1	1:B:332:ILE:N	2.52	0.43
1:B:339:PRO:HD2	1:B:342:MET:CE	2.48	0.43
1:D:245:MET:HE2	1:D:245:MET:HB3	1.81	0.43
1:C:228:LYS:HD3	1:C:233:LEU:HD22	2.00	0.43
1:A:65:THR:HB	1:A:69:GLU:CG	2.49	0.43
1:C:486:LYS:H	1:C:489:GLU:CB	2.31	0.43
1:B:186:ALA:HA	1:B:189[A]:HIS:NE2	2.34	0.43
1:C:263:PHE:CE2	1:C:306:ILE:HG13	2.53	0.43
1:D:105:GLU:HA	1:D:106:ALA:HA	1.90	0.43
1:D:329:ARG:HD3	2:D:608:HOH:O	2.18	0.43
1:A:222:TYR:CZ	1:A:228:LYS:HB2	2.54	0.43
1:A:415:THR:HG21	1:A:440:LEU:HD13	2.01	0.42
1:B:316:ILE:N	2:B:621:HOH:O	2.48	0.42
1:B:280[A]:TRP:HZ3	1:B:411:TYR:OH	2.03	0.42
1:D:104:PHE:N	1:D:104:PHE:CD2	2.87	0.42
1:A:528:LYS:HD2	1:A:528:LYS:HA	1.83	0.42
1:B:412:TYR:OH	1:B:441:GLU:OE1	2.23	0.42
1:D:293:ALA:HA	1:D:421:GLY:HA3	2.01	0.42
1:D:390:PHE:CD1	1:D:465:ILE:HG23	2.54	0.42
1:D:259:LYS:HA	1:D:259:LYS:HD3	1.82	0.42
1:A:263:PHE:CD2	1:A:306:ILE:HG13	2.53	0.42
1:D:415:THR:HG21	1:D:440:LEU:HD13	2.00	0.42
1:A:419:TYR:CE2	1:A:433:LEU:HD11	2.54	0.42
1:B:469:ILE:HG22	1:B:473:MET:HE3	2.01	0.42
1:D:104:PHE:N	1:D:104:PHE:HD2	2.18	0.42
1:D:243:LEU:HD23	1:D:243:LEU:HA	1.65	0.42
1:B:456:TYR:C	1:B:458:VAL:N	2.73	0.42
1:C:409:SER:O	1:C:410:THR:OG1	2.35	0.42
1:D:486:LYS:O	1:D:490:MET:HG3	2.20	0.42
1:B:447:CYS:HA	1:B:523:ILE:HG12	2.02	0.41
1:D:216:ARG:HD3	1:D:240:TYR:CZ	2.55	0.41
1:D:261:LEU:HD23	1:D:261:LEU:HA	1.89	0.41
1:D:72:ASN:O	1:D:76:ILE:HG12	2.19	0.41
1:D:544:HIS:O	1:D:548:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:SER:HA	1:B:89:GLN:NE2	2.35	0.41
1:B:248:LYS:HE2	1:B:549:VAL:O	2.21	0.41
1:C:66:THR:O	1:C:69:GLU:HG2	2.20	0.41
1:D:412:TYR:OH	1:D:441:GLU:OE1	2.33	0.41
1:B:103:TYR:HB3	1:B:105:GLU:HG3	2.02	0.41
1:B:73:LEU:O	1:B:77:ILE:HG12	2.19	0.41
1:B:276:GLU:OE2	1:B:538:GLU:HG3	2.21	0.41
1:A:44:TYR:CD1	1:A:238:LEU:HD22	2.56	0.41
1:A:306:ILE:HD13	1:A:306:ILE:HA	1.93	0.41
1:B:43:LYS:O	1:B:46:GLN:HB2	2.21	0.41
1:B:405:ALA:HA	1:B:408:THR:HB	2.02	0.41
1:D:280[B]:TRP:HZ3	1:D:541:LEU:HD11	1.85	0.41
1:D:385:ILE:HA	1:D:385:ILE:HD13	1.85	0.41
1:B:77:ILE:HG23	1:B:82:ILE:HG13	2.03	0.41
1:B:104:PHE:HZ	1:B:110:ASN:HA	1.85	0.41
1:B:486:LYS:O	1:B:490:MET:HG3	2.21	0.41
1:A:426:THR:OG1	1:A:428:GLU:HG2	2.21	0.40
1:A:470:GLU:HA	1:A:473:MET:CE	2.52	0.40
1:B:244:GLN:HG2	1:B:248:LYS:HE3	2.03	0.40
1:D:52:LYS:HG2	1:D:235:PHE:CZ	2.56	0.40
1:A:211:PRO:O	1:A:215:ILE:HG12	2.21	0.40
1:A:259:LYS:NZ	1:A:272:ASP:OD2	2.55	0.40
1:C:459:GLU:OE2	1:C:459:GLU:N	2.44	0.40
1:C:312:ASP:OD2	1:D:542:LYS:NZ	2.54	0.40
1:A:387:ALA:O	1:A:391:ILE:HG12	2.22	0.40
1:B:504:ARG:HA	1:B:505:PRO:C	2.46	0.40
1:C:261:LEU:HD23	1:C:261:LEU:HA	1.93	0.40
1:C:304:ILE:HD12	1:C:304:ILE:HG23	1.88	0.40
1:A:52:LYS:NZ	2:A:640:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/538 (94%)	489 (96%)	14 (3%)	4 (1%)	16	10
1	B	502/538 (93%)	485 (97%)	12 (2%)	5 (1%)	12	8
1	C	499/538 (93%)	479 (96%)	15 (3%)	5 (1%)	12	8
1	D	494/538 (92%)	471 (95%)	15 (3%)	8 (2%)	7	3
All	All	2002/2152 (93%)	1924 (96%)	56 (3%)	22 (1%)	11	7

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	PHE
1	A	460	LYS
1	A	462	ARG
1	A	466	ALA
1	B	192	SER
1	B	465	ILE
1	C	62	ALA
1	C	104	PHE
1	C	457	GLU
1	C	458	VAL
1	C	486	LYS
1	D	47	GLU
1	D	60	SER
1	D	467	THR
1	B	457	GLU
1	B	537	PRO
1	B	538	GLU
1	D	110	ASN
1	D	192	SER
1	D	457	GLU
1	D	459	GLU
1	D	107	HIS

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	458/481 (95%)	446 (97%)	12 (3%)	40	43
1	B	457/481 (95%)	443 (97%)	14 (3%)	35	37
1	C	454/481 (94%)	445 (98%)	9 (2%)	48	54
1	D	449/481 (93%)	438 (98%)	11 (2%)	43	47
All	All	1818/1924 (94%)	1772 (98%)	46 (2%)	42	45

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLU
1	A	164	VAL
1	A	227	PHE
1	A	228	LYS
1	A	243	LEU
1	A	271	ARG
1	A	285	TYR
1	A	306	ILE
1	A	327	ILE
1	A	354	ASP
1	A	414	LEU
1	A	549	VAL
1	B	63	CYS
1	B	243	LEU
1	B	285	TYR
1	B	306	ILE
1	B	327	ILE
1	B	368	VAL
1	B	370	HIS
1	B	402	LEU
1	B	408	THR
1	B	438	LYS
1	B	465	ILE
1	B	480	THR
1	B	482	VAL
1	B	525	VAL
1	C	66	THR
1	C	129	VAL
1	C	285	TYR
1	C	306	ILE
1	C	327	ILE
1	C	433	LEU
1	C	449	VAL

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Mol	Chain	Res	Type
1	C	486	LYS
1	C	549	VAL
1	D	65	THR
1	D	67	LEU
1	D	88	LYS
1	D	228	LYS
1	D	266	THR
1	D	285	TYR
1	D	306	ILE
1	D	327	ILE
1	D	399	SER
1	D	411	TYR
1	D	522	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	124	GLN
1	A	404	ASN
1	B	89	GLN
1	B	124	GLN
1	B	138	GLN
1	D	124	GLN
1	D	182	HIS
1	D	404	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	510/538 (94%)	-0.12	21 (4%)	41	46	12, 26, 58, 133	1 (0%)
1	B	506/538 (94%)	0.16	27 (5%)	32	36	17, 33, 65, 116	2 (0%)
1	C	503/538 (93%)	0.29	34 (6%)	23	26	15, 38, 76, 106	2 (0%)
1	D	499/538 (92%)	0.92	75 (15%)	5	6	21, 52, 95, 126	1 (0%)
All	All	2018/2152 (93%)	0.31	157 (7%)	19	21	12, 37, 81, 133	6 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	ILE	6.6
1	C	227	PHE	6.3
1	A	466	ALA	6.3
1	D	45	ALA	6.1
1	D	65	THR	6.0
1	A	104	PHE	5.9
1	D	465	ILE	5.7
1	D	458	VAL	5.5
1	B	227	PHE	5.4
1	D	555	ILE	5.3
1	A	227	PHE	5.2
1	D	466	ALA	5.1
1	D	62	ALA	5.0
1	A	465	ILE	4.9
1	D	64	GLY	4.7
1	D	227	PHE	4.7
1	C	467	THR	4.7
1	C	537	PRO	4.7
1	C	106	ALA	4.6
1	D	61	ALA	4.5
1	C	63	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	468	GLY	4.4
1	D	461	GLY	4.2
1	B	44	TYR	4.1
1	D	540	VAL	4.0
1	D	107	HIS	3.9
1	D	55	THR	3.8
1	D	460	LYS	3.8
1	D	264	VAL	3.8
1	C	64	GLY	3.7
1	B	466	ALA	3.7
1	D	231	LEU	3.7
1	C	528	LYS	3.7
1	B	537	PRO	3.6
1	A	63	CYS	3.5
1	A	462	ARG	3.5
1	C	458	VAL	3.5
1	A	282	MET	3.5
1	B	539	LYS	3.4
1	D	189	HIS	3.3
1	D	63	CYS	3.3
1	B	555	ILE	3.3
1	D	68	THR	3.3
1	C	555	ILE	3.3
1	D	106	ALA	3.3
1	D	538	GLU	3.3
1	C	104	PHE	3.3
1	C	478	VAL	3.2
1	D	190	LEU	3.2
1	A	106	ALA	3.1
1	D	140	ALA	3.1
1	B	136	ARG	3.1
1	D	67	LEU	3.1
1	C	264	VAL	3.0
1	D	198	VAL	3.0
1	C	477	GLY	3.0
1	A	464	GLN	3.0
1	B	264	VAL	3.0
1	D	147	SER	3.0
1	D	192	SER	3.0
1	D	459	GLU	3.0
1	D	51	LEU	2.9
1	D	50	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	104	PHE	2.9
1	A	461	GLY	2.9
1	A	458	VAL	2.9
1	D	456	TYR	2.9
1	D	188	PRO	2.9
1	B	226	GLU	2.9
1	B	457	GLU	2.9
1	D	158	LEU	2.8
1	C	105	GLU	2.8
1	C	367	ASP	2.8
1	D	235	PHE	2.8
1	D	467	THR	2.8
1	D	187	ALA	2.8
1	C	66	THR	2.8
1	D	46	GLN	2.7
1	C	459	GLU	2.7
1	D	76	ILE	2.7
1	D	145	LYS	2.7
1	D	71	LEU	2.6
1	B	458	VAL	2.6
1	D	539	LYS	2.6
1	C	65	THR	2.6
1	D	59	LEU	2.6
1	D	528	LYS	2.6
1	B	536	HIS	2.6
1	C	390	PHE	2.6
1	C	107	HIS	2.6
1	B	38	ASN	2.6
1	A	539	LYS	2.6
1	C	483	ALA	2.6
1	D	541	LEU	2.6
1	C	69	GLU	2.5
1	D	86	PHE	2.5
1	B	192	SER	2.5
1	D	193	PRO	2.5
1	D	112	LEU	2.5
1	A	467	THR	2.4
1	B	456	TYR	2.4
1	C	456	TYR	2.4
1	D	150	SER	2.4
1	B	45	ALA	2.4
1	D	186	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	457	GLU	2.4
1	A	459	GLU	2.4
1	D	115	SER	2.4
1	D	100	ALA	2.4
1	A	226	GLU	2.4
1	C	39	GLN	2.4
1	D	119	PHE	2.4
1	D	137	PHE	2.4
1	C	482	VAL	2.4
1	D	66	THR	2.4
1	C	387	ALA	2.3
1	B	154	GLY	2.3
1	D	181	GLY	2.3
1	D	171	ILE	2.3
1	D	549	VAL	2.3
1	B	538	GLU	2.3
1	B	140	ALA	2.3
1	C	466	ALA	2.3
1	A	555	ILE	2.3
1	B	481	GLU	2.3
1	D	110	ASN	2.3
1	D	58	MET	2.3
1	C	472	TYR	2.3
1	B	39	GLN	2.2
1	D	56	SER	2.2
1	D	141	ASN	2.2
1	C	540	VAL	2.2
1	D	96	HIS	2.2
1	D	238	LEU	2.2
1	D	109	TYR	2.2
1	B	280[A]	TRP	2.2
1	D	111	ASP	2.2
1	D	178	PHE	2.1
1	A	540	VAL	2.1
1	B	62	ALA	2.1
1	D	99	ARG	2.1
1	C	476	TYR	2.1
1	D	260	ASP	2.1
1	D	48	ILE	2.1
1	C	454	ALA	2.1
1	A	110	ASN	2.1
1	A	38	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	57	THR	2.1
1	D	142	GLY	2.1
1	D	183	LEU	2.0
1	C	103	TYR	2.0
1	C	539	LYS	2.0
1	D	97	ILE	2.0
1	D	280[A]	TRP	2.0
1	B	63	CYS	2.0
1	B	467	THR	2.0
1	A	463	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.