



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:24 PM UTC

PDB ID : 5ERY / pdb_00005ery
Title : Crystal Structure of APO MenD from M. tuberculosis - P212121
Authors : Johnston, J.M.; Jirgis, E.N.M.; Bashiri, G.; Bulloch, E.M.M.; Baker, E.N.
Deposited on : 2015-11-16
Resolution : 2.25 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

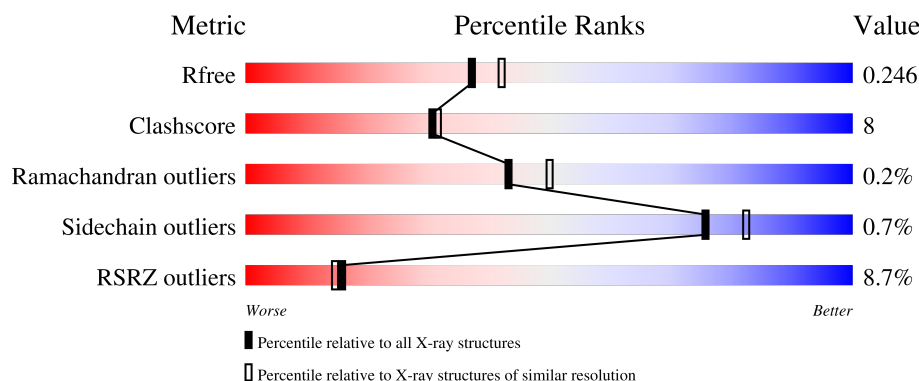
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	574	7% 76% 11% 12%
1	B	574	8% 72% 14% 14%
1	C	574	9% 68% 14% 18%
1	D	574	7% 72% 14% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14779 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	3	0
			3691	2308	684	690	9			
1	D	498	Total	C	N	O	S	0	3	0
			3658	2284	682	683	9			
1	C	473	Total	C	N	O	S	0	3	0
			3478	2179	645	645	9			
1	B	496	Total	C	N	O	S	0	4	0
			3641	2276	676	680	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WK11
A	-18	GLY	-	expression tag	UNP P9WK11
A	-17	SER	-	expression tag	UNP P9WK11
A	-16	SER	-	expression tag	UNP P9WK11
A	-15	HIS	-	expression tag	UNP P9WK11
A	-14	HIS	-	expression tag	UNP P9WK11
A	-13	HIS	-	expression tag	UNP P9WK11
A	-12	HIS	-	expression tag	UNP P9WK11
A	-11	HIS	-	expression tag	UNP P9WK11
A	-10	HIS	-	expression tag	UNP P9WK11
A	-9	SER	-	expression tag	UNP P9WK11
A	-8	SER	-	expression tag	UNP P9WK11
A	-7	GLY	-	expression tag	UNP P9WK11
A	-6	LEU	-	expression tag	UNP P9WK11
A	-5	VAL	-	expression tag	UNP P9WK11
A	-4	PRO	-	expression tag	UNP P9WK11
A	-3	ARG	-	expression tag	UNP P9WK11
A	-2	GLY	-	expression tag	UNP P9WK11
A	-1	SER	-	expression tag	UNP P9WK11
A	0	HIS	-	expression tag	UNP P9WK11

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP P9WK11
D	-18	GLY	-	expression tag	UNP P9WK11
D	-17	SER	-	expression tag	UNP P9WK11
D	-16	SER	-	expression tag	UNP P9WK11
D	-15	HIS	-	expression tag	UNP P9WK11
D	-14	HIS	-	expression tag	UNP P9WK11
D	-13	HIS	-	expression tag	UNP P9WK11
D	-12	HIS	-	expression tag	UNP P9WK11
D	-11	HIS	-	expression tag	UNP P9WK11
D	-10	HIS	-	expression tag	UNP P9WK11
D	-9	SER	-	expression tag	UNP P9WK11
D	-8	SER	-	expression tag	UNP P9WK11
D	-7	GLY	-	expression tag	UNP P9WK11
D	-6	LEU	-	expression tag	UNP P9WK11
D	-5	VAL	-	expression tag	UNP P9WK11
D	-4	PRO	-	expression tag	UNP P9WK11
D	-3	ARG	-	expression tag	UNP P9WK11
D	-2	GLY	-	expression tag	UNP P9WK11
D	-1	SER	-	expression tag	UNP P9WK11
D	0	HIS	-	expression tag	UNP P9WK11
C	-19	MET	-	initiating methionine	UNP P9WK11
C	-18	GLY	-	expression tag	UNP P9WK11
C	-17	SER	-	expression tag	UNP P9WK11
C	-16	SER	-	expression tag	UNP P9WK11
C	-15	HIS	-	expression tag	UNP P9WK11
C	-14	HIS	-	expression tag	UNP P9WK11
C	-13	HIS	-	expression tag	UNP P9WK11
C	-12	HIS	-	expression tag	UNP P9WK11
C	-11	HIS	-	expression tag	UNP P9WK11
C	-10	HIS	-	expression tag	UNP P9WK11
C	-9	SER	-	expression tag	UNP P9WK11
C	-8	SER	-	expression tag	UNP P9WK11
C	-7	GLY	-	expression tag	UNP P9WK11
C	-6	LEU	-	expression tag	UNP P9WK11
C	-5	VAL	-	expression tag	UNP P9WK11
C	-4	PRO	-	expression tag	UNP P9WK11
C	-3	ARG	-	expression tag	UNP P9WK11
C	-2	GLY	-	expression tag	UNP P9WK11
C	-1	SER	-	expression tag	UNP P9WK11
C	0	HIS	-	expression tag	UNP P9WK11
B	-19	MET	-	initiating methionine	UNP P9WK11
B	-18	GLY	-	expression tag	UNP P9WK11

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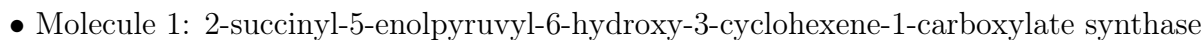
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP P9WK11
B	-16	SER	-	expression tag	UNP P9WK11
B	-15	HIS	-	expression tag	UNP P9WK11
B	-14	HIS	-	expression tag	UNP P9WK11
B	-13	HIS	-	expression tag	UNP P9WK11
B	-12	HIS	-	expression tag	UNP P9WK11
B	-11	HIS	-	expression tag	UNP P9WK11
B	-10	HIS	-	expression tag	UNP P9WK11
B	-9	SER	-	expression tag	UNP P9WK11
B	-8	SER	-	expression tag	UNP P9WK11
B	-7	GLY	-	expression tag	UNP P9WK11
B	-6	LEU	-	expression tag	UNP P9WK11
B	-5	VAL	-	expression tag	UNP P9WK11
B	-4	PRO	-	expression tag	UNP P9WK11
B	-3	ARG	-	expression tag	UNP P9WK11
B	-2	GLY	-	expression tag	UNP P9WK11
B	-1	SER	-	expression tag	UNP P9WK11
B	0	HIS	-	expression tag	UNP P9WK11

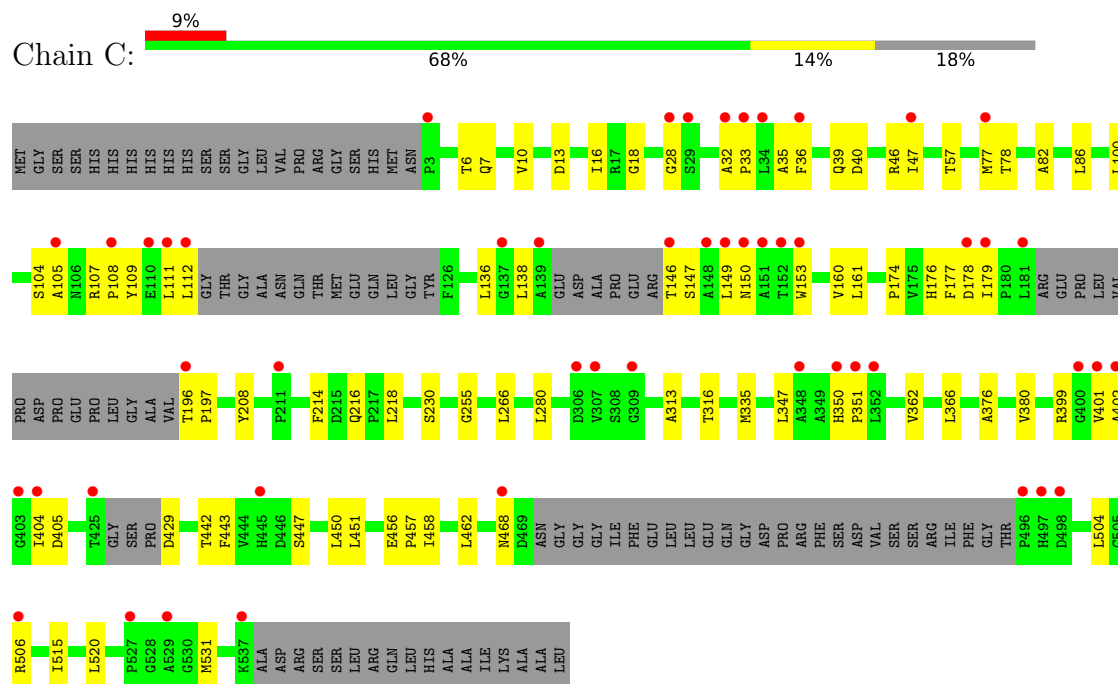
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	85	Total O 85 85	0	0
2	D	86	Total O 86 86	0	0
2	C	58	Total O 58 58	0	0
2	B	82	Total O 82 82	0	0

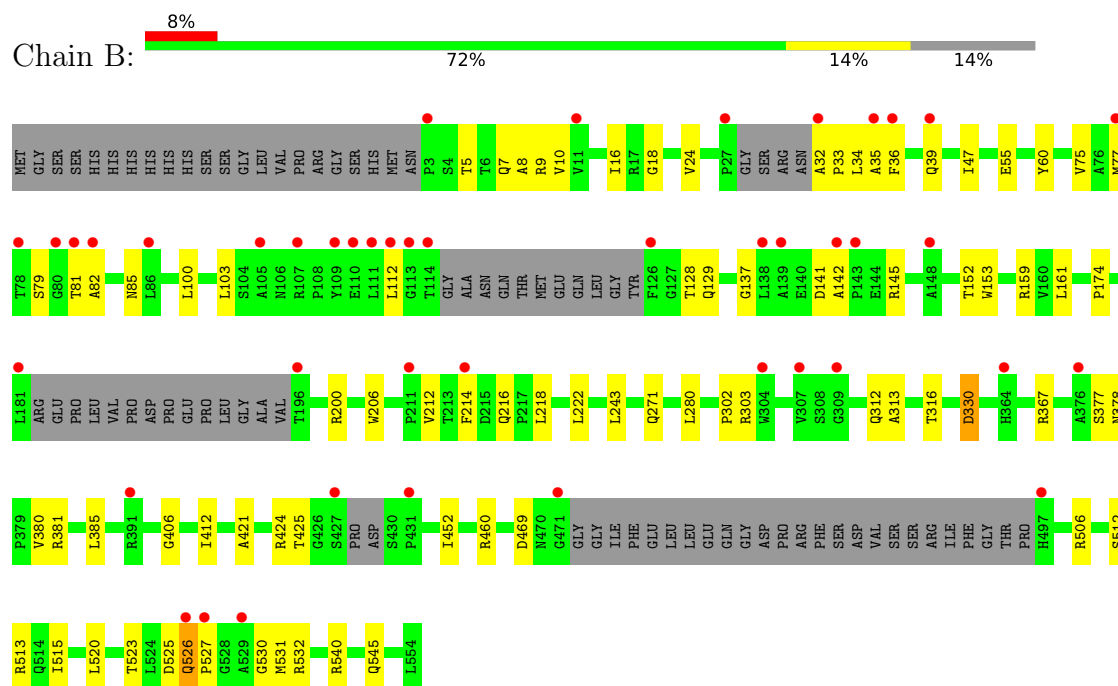
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.41Å 137.28Å 164.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.25 49.70 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.70-2.25) 99.9 (49.70-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.25Å)	Xtriage
Refinement program	PHENIX, REFMAC	Depositor
R, R_{free}	0.212 , 0.246 0.214 , 0.246	Depositor DCC
R_{free} test set	5380 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14779	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	0.30	0/3771	0.55	0/5161
1	B	0.31	0/3722	0.55	0/5096
1	C	0.31	0/3556	0.61	0/4873
1	D	0.29	0/3743	0.58	2/5126 (0.0%)
All	All	0.30	0/14792	0.57	2/20256 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	145	ARG	CA-C-N	5.34	130.92	120.99
1	D	145	ARG	C-N-CA	5.34	130.92	120.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	255	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3691	0	3722	57	0
1	B	3641	0	3682	71	0
1	C	3478	0	3514	68	0
1	D	3658	0	3698	71	0
2	A	85	0	0	4	0
2	B	82	0	0	5	0
2	C	58	0	0	1	0
2	D	86	0	0	1	0
All	All	14779	0	14616	240	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 8.

All (240) 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:367:ARG:NH1	1:B:525:ASP:OD1	1.90	1.05
1:A:39[B]:GLN:OE1	1:A:43:ARG:NH2	2.05	0.89
1:C:36:PHE:O	1:C:39:GLN:HG2	1.74	0.87
1:B:280:LEU:O	1:B:381:ARG:NH2	2.10	0.85
1:B:142:ALA:HB1	1:B:145:ARG:HB2	1.62	0.81
1:C:108:PRO:HG2	1:C:138:LEU:HD22	1.63	0.81
1:C:32:ALA:HB3	1:C:35:ALA:HB2	1.65	0.78
1:A:7:GLN:NE2	1:A:137:GLY:O	2.17	0.77
1:A:40:ASP:OD1	1:A:43:ARG:NH1	2.18	0.77
1:D:9:ARG:NH2	1:D:40:ASP:OD2	2.13	0.77
1:A:488:VAL:HG21	1:D:39:GLN:HB2	1.67	0.76
1:C:13:ASP:OD1	1:C:46:ARG:NH2	2.16	0.76
1:C:456:GLU:O	1:C:458:ILE:CD1	2.37	0.73
1:A:498:ASP:OD1	1:D:509:HIS:HD2	1.71	0.72
1:B:330:ASP:OD1	2:B:601:HOH:O	2.08	0.72
1:C:77:MET:HE2	1:C:104:SER:HB3	1.72	0.71
1:C:33:PRO:HB3	1:C:105:ALA:HB2	1.73	0.70
1:A:498:ASP:OD1	1:D:509:HIS:CD2	2.45	0.69
1:A:218:LEU:HD22	1:A:313:ALA:HB1	1.75	0.69
1:C:405:ASP:OD1	1:B:85:ASN:ND2	2.26	0.69
1:C:149:LEU:HD21	1:C:153:TRP:CZ2	2.28	0.69
1:B:39:GLN:OE1	1:B:39:GLN:N	2.26	0.67
1:D:214[B]:PHE:HE1	1:B:212:VAL:HG21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:SER:HB3	1:C:112:LEU:HB2	1.77	0.66
1:D:178:ASP:O	1:D:179:ILE:HD13	1.96	0.66
1:A:274:MET:HE3	1:A:305:PRO:HG2	1.77	0.66
1:D:469:ASP:HB2	1:D:540:ARG:HG2	1.77	0.66
1:D:32:ALA:H	1:D:33:PRO:HD2	1.60	0.66
1:C:32:ALA:HA	1:C:78:THR:HG22	1.76	0.66
1:C:515:ILE:HD11	1:C:520:LEU:HD12	1.77	0.65
1:B:424:ARG:NH1	2:B:603:HOH:O	2.29	0.65
1:D:149:LEU:HD21	1:D:153:TRP:CZ2	2.32	0.65
1:B:35:ALA:O	1:B:39:GLN:NE2	2.29	0.65
1:D:468:ASN:HB3	1:D:537:LYS:HD3	1.79	0.65
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.79	0.64
1:D:212:VAL:HG21	1:B:214[A]:PHE:CE1	2.33	0.64
1:B:367:ARG:HH12	1:B:525:ASP:CG	2.06	0.63
1:C:146:THR:O	1:C:150:ASN:N	2.31	0.63
1:C:456:GLU:O	1:C:458:ILE:HD12	1.98	0.63
1:A:488:VAL:CG2	1:D:39:GLN:HB2	2.29	0.63
1:A:363:SER:HA	1:A:366:LEU:HD12	1.82	0.62
1:A:109:TYR:CE1	1:B:152:THR:HG21	2.35	0.62
1:A:109:TYR:OH	1:B:137:GLY:HA3	2.00	0.62
1:C:376:ALA:O	1:C:399:ARG:NH1	2.33	0.62
1:C:7:GLN:HB3	1:C:153:TRP:CH2	2.35	0.61
1:D:214[B]:PHE:CE1	1:B:212:VAL:HG21	2.36	0.61
1:C:266:LEU:HB3	1:C:335:MET:HE3	1.82	0.61
1:B:10:VAL:HG11	1:B:153:TRP:HE3	1.65	0.61
1:C:39:GLN:HG3	1:C:40:ASP:N	2.14	0.61
1:B:77:MET:HE2	1:B:82:ALA:HB1	1.82	0.61
1:B:7:GLN:NE2	1:B:137:GLY:O	2.34	0.61
1:C:457:PRO:C	1:C:458:ILE:HD12	2.26	0.60
1:A:138:LEU:HD13	1:A:180:PRO:HB2	1.83	0.60
1:D:14:GLU:HB3	1:D:157:THR:HG21	1.84	0.59
1:C:77:MET:HE2	1:C:104:SER:CB	2.32	0.59
1:B:24:VAL:HB	1:B:75:VAL:HG22	1.85	0.59
1:C:462:LEU:HD23	1:C:531:MET:HE3	1.84	0.59
1:D:77:MET:SD	1:D:86:LEU:HD12	2.43	0.58
1:A:212:VAL:HG21	1:C:214[A]:PHE:CE1	2.39	0.58
1:C:429:ASP:OD1	1:C:429:ASP:N	2.37	0.58
1:A:212:VAL:HG21	1:C:214[A]:PHE:HE1	1.69	0.57
1:C:104:SER:HG	1:C:178:ASP:CG	2.12	0.57
1:A:40:ASP:O	1:A:44:SER:OG	2.21	0.57
1:A:544:ARG:NH2	1:A:547:HIS:HB2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:MET:HB3	1:A:82:ALA:HB1	1.86	0.57
1:C:7:GLN:HB3	1:C:153:TRP:CZ2	2.40	0.57
1:C:196:THR:HB	1:C:197:PRO:HD3	1.86	0.57
1:C:376:ALA:HB1	1:C:402:ALA:HA	1.87	0.57
1:B:34:LEU:HD21	1:B:103:LEU:HD13	1.86	0.57
1:B:421:ALA:O	1:B:425:THR:HG23	2.05	0.57
1:D:136:LEU:HD23	1:D:179:ILE:HD12	1.86	0.56
1:A:303:ARG:NH1	2:A:605:HOH:O	2.37	0.56
1:B:55:GLU:HG2	1:B:77:MET:CE	2.34	0.56
1:B:377:SER:OG	1:B:378:ASN:N	2.36	0.56
1:D:33:PRO:HA	1:D:36:PHE:CD2	2.41	0.56
1:B:302:PRO:HG2	2:B:641:HOH:O	2.05	0.56
1:B:39:GLN:H	1:B:39:GLN:CD	2.13	0.55
1:D:200:ARG:HH12	1:B:312:GLN:HA	1.70	0.55
1:A:216:GLN:HB3	1:A:316:THR:HG23	1.87	0.55
1:D:18:GLY:HA3	1:D:161:LEU:HD13	1.88	0.55
1:B:303:ARG:NH2	2:B:602:HOH:O	2.20	0.54
1:C:36:PHE:O	1:C:39:GLN:CG	2.53	0.54
1:B:128:THR:HG23	1:B:129:GLN:HE21	1.73	0.54
1:C:6:THR:O	1:C:10:VAL:HG23	2.08	0.54
1:D:494:GLY:O	1:D:495:THR:OG1	2.24	0.54
1:C:401:VAL:HG11	1:B:81:THR:HG23	1.90	0.54
1:B:10:VAL:HG11	1:B:153:TRP:CE3	2.44	0.53
1:A:441:LEU:HD12	1:A:497[B]:HIS:CE1	2.44	0.53
1:C:107:ARG:HD3	1:C:107:ARG:N	2.24	0.53
1:A:265:PRO:HG3	1:A:283:PRO:HB3	1.91	0.53
1:B:460:ARG:O	1:B:530:GLY:HA2	2.09	0.52
1:A:55:GLU:HG2	1:A:77:MET:HE1	1.90	0.52
1:A:40:ASP:HA	1:A:43:ARG:NH1	2.25	0.52
1:D:32:ALA:H	1:D:33:PRO:CD	2.23	0.52
1:B:222:LEU:HD22	1:B:243:LEU:HD11	1.92	0.52
1:D:200:ARG:NH2	1:D:206:TRP:CE2	2.78	0.51
1:C:136:LEU:HD22	1:C:153:TRP:HD1	1.74	0.51
1:D:27:PRO:HD2	1:D:52:ARG:O	2.10	0.51
1:D:30:ARG:O	1:D:31:ASN:HB3	2.10	0.51
1:B:525:ASP:O	1:B:527:PRO:HD3	2.09	0.51
1:C:401:VAL:CG1	1:B:81:THR:HG23	2.40	0.51
1:C:447:SER:HB3	1:C:504:LEU:HD21	1.91	0.51
1:B:526:GLN:O	1:B:532:ARG:NH1	2.44	0.51
1:A:441:LEU:HD12	1:A:497[B]:HIS:NE2	2.26	0.51
1:B:218:LEU:HD11	1:B:313:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLU:HG2	1:B:77:MET:HE3	1.93	0.51
1:D:196:THR:N	1:D:197:PRO:HD3	2.26	0.51
1:C:146:THR:OG1	1:C:147:SER:N	2.43	0.50
1:A:470:ASN:O	1:A:497[A]:HIS:HD2	1.94	0.50
1:D:54:ASP:HB3	1:D:57:THR:HB	1.94	0.50
1:D:7:GLN:HA	1:D:153:TRP:CZ3	2.47	0.50
1:A:404:ILE:HG12	2:A:628:HOH:O	2.11	0.49
1:B:18:GLY:HA3	1:B:161:LEU:HD13	1.94	0.49
1:D:212:VAL:HG21	1:B:214[A]:PHE:CD1	2.46	0.49
1:D:32:ALA:HB1	1:D:36:PHE:CZ	2.48	0.49
1:B:5:THR:HG22	1:B:9:ARG:NH1	2.28	0.49
1:D:142:ALA:HB1	1:D:144:GLU:HG2	1.95	0.49
1:C:506:ARG:HH22	1:B:506:ARG:HH11	1.59	0.49
1:B:513:ARG:NH1	1:B:523:THR:HG23	2.28	0.49
1:B:39:GLN:N	1:B:39:GLN:CD	2.70	0.49
1:A:544:ARG:O	1:A:544:ARG:NH1	2.46	0.48
1:C:77:MET:HB3	1:C:82:ALA:HB1	1.94	0.48
1:D:140:GLU:HB2	1:C:109:TYR:CD2	2.48	0.48
1:C:16:ILE:HG12	1:C:47:ILE:HG13	1.96	0.48
1:D:526:GLN:HB3	1:D:527:PRO:HD2	1.94	0.48
1:A:77:MET:SD	1:A:86:LEU:HD11	2.54	0.48
1:A:256:ASP:OD2	1:A:391:ARG:CZ	2.62	0.48
1:B:141:ASP:N	1:B:141:ASP:OD1	2.44	0.48
1:D:25:LEU:HD23	1:D:26:CYS:N	2.29	0.48
1:B:79:SER:OG	1:B:82:ALA:HB2	2.13	0.48
1:A:497[A]:HIS:CE1	1:A:499:VAL:H	2.31	0.47
1:A:288:LEU:HD13	1:A:307:VAL:HG21	1.97	0.47
1:D:290:ASP:O	1:D:310:ASN:ND2	2.47	0.47
1:B:280:LEU:HD11	1:B:380:VAL:HG22	1.97	0.47
1:A:313:ALA:HA	1:C:208:TYR:O	2.15	0.47
1:D:60:TYR:CG	1:D:406:GLY:HA3	2.50	0.47
1:D:513:ARG:HG3	1:D:515:ILE:HG23	1.95	0.47
1:D:281:HIS:HB3	1:D:283:PRO:HD2	1.96	0.47
1:C:451:LEU:HD23	2:C:605:HOH:O	2.15	0.47
1:C:176:HIS:NE2	1:C:178:ASP:OD2	2.49	0.46
1:B:142:ALA:HB1	1:B:145:ARG:CB	2.40	0.46
1:A:470:ASN:O	1:A:497[A]:HIS:CD2	2.69	0.46
1:C:401:VAL:HG12	1:C:401:VAL:O	2.15	0.46
1:B:36:PHE:HA	1:B:39:GLN:OE1	2.15	0.46
1:D:10:VAL:HG11	1:D:150:ASN:OD1	2.15	0.46
1:B:412:ILE:HD13	1:B:452:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:HD3	1:B:112:LEU:HD11	1.97	0.46
1:D:100:LEU:O	1:D:174:PRO:HA	2.15	0.46
1:D:280:LEU:HD23	1:D:280:LEU:HA	1.71	0.46
1:D:212:VAL:HG21	1:B:214[A]:PHE:HE1	1.79	0.46
1:A:60:TYR:CG	1:A:406:GLY:HA3	2.51	0.45
1:A:460:ARG:O	1:A:530:GLY:HA2	2.16	0.45
1:D:492:ILE:HD11	1:D:493:PHE:CD2	2.51	0.45
1:B:100:LEU:O	1:B:174:PRO:HA	2.15	0.45
1:B:216:GLN:HB3	1:B:316:THR:HG23	1.98	0.45
1:B:77:MET:HE2	1:B:77:MET:HB3	1.66	0.45
1:C:32:ALA:CA	1:C:78:THR:HG22	2.46	0.45
1:D:212:VAL:HG22	1:D:213:THR:N	2.31	0.45
1:B:55:GLU:HB2	1:B:85:ASN:HB3	1.98	0.45
1:A:325:ARG:HE	1:A:325:ARG:HB2	1.59	0.44
1:A:74:CYS:HB3	1:A:103:LEU:HD12	1.99	0.44
1:A:497[A]:HIS:O	1:A:498:ASP:CG	2.60	0.44
1:A:109:TYR:CD1	1:B:152:THR:HG21	2.53	0.44
1:D:373:VAL:O	1:D:436:ALA:HA	2.17	0.44
1:A:270:GLN:HG3	2:A:669:HOH:O	2.16	0.44
1:D:7:GLN:HE21	1:D:153:TRP:NE1	2.16	0.44
1:D:302:PRO:HG3	2:D:623:HOH:O	2.17	0.44
1:D:537:LYS:HD3	1:D:537:LYS:HA	1.80	0.44
1:C:28:GLY:HA3	1:C:78:THR:HB	1.99	0.44
1:C:404:ILE:O	1:C:442:THR:HG23	2.17	0.44
1:B:35:ALA:O	1:B:39:GLN:OE1	2.36	0.44
1:C:149:LEU:HD21	1:C:153:TRP:CH2	2.53	0.44
1:A:404:ILE:HG13	1:A:405:ASP:N	2.32	0.43
1:B:60:TYR:CG	1:B:406:GLY:HA3	2.53	0.43
1:B:512:SER:C	1:B:513:ARG:HG2	2.43	0.43
1:A:222:LEU:HD22	1:A:243:LEU:HD11	2.00	0.43
1:C:136:LEU:HD12	1:C:179:ILE:HD12	2.00	0.43
1:D:10:VAL:HG13	1:D:154:ARG:NH2	2.33	0.43
1:D:440:ASP:OD2	1:D:497:HIS:NE2	2.43	0.43
1:A:441:LEU:HD11	1:D:53:ILE:HD13	2.00	0.43
1:D:6:THR:O	1:D:10:VAL:HG23	2.18	0.43
1:C:100:LEU:O	1:C:174:PRO:HA	2.17	0.43
1:B:7:GLN:HG3	1:B:153:TRP:CE2	2.54	0.43
1:C:362:VAL:O	1:C:366:LEU:HG	2.18	0.43
1:D:354:THR:HB	1:D:543:LEU:HD13	2.01	0.43
1:D:471:GLY:C	1:D:540:ARG:NH1	2.77	0.43
1:D:513:ARG:HG3	1:D:515:ILE:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:LEU:HD23	1:C:347:LEU:HA	1.88	0.43
1:D:418:TYR:CE2	1:D:432:PRO:HG2	2.53	0.42
1:C:280:LEU:HD11	1:C:380:VAL:HG22	2.01	0.42
1:A:404:ILE:HG23	2:A:628:HOH:O	2.19	0.42
1:B:8:ALA:HB1	1:B:34:LEU:HA	2.01	0.42
1:A:421:ALA:O	1:A:425:THR:HG23	2.19	0.42
1:B:531:MET:HE2	1:B:531:MET:HB3	1.81	0.42
1:D:3:PRO:HG2	1:D:4:SER:H	1.85	0.42
1:B:271:GLN:NE2	2:B:604:HOH:O	2.32	0.42
1:A:8:ALA:HB1	1:A:34:LEU:HA	2.02	0.42
1:D:200:ARG:NH1	1:D:206:TRP:O	2.53	0.42
1:C:7:GLN:HE21	1:C:153:TRP:NE1	2.16	0.42
1:A:544:ARG:NH2	1:A:547:HIS:CB	2.83	0.42
1:D:3:PRO:CG	1:D:4:SER:H	2.33	0.41
1:D:5:THR:O	1:D:9:ARG:HG3	2.20	0.41
1:B:515:ILE:HD11	1:B:520:LEU:HD13	2.01	0.41
1:A:106:ASN:O	1:A:180:PRO:HA	2.19	0.41
1:A:373:VAL:O	1:A:436:ALA:HA	2.20	0.41
1:A:218:LEU:HD11	1:A:314:THR:C	2.46	0.41
1:A:497[B]:HIS:O	1:A:498:ASP:CG	2.63	0.41
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.86	0.41
1:C:33:PRO:HG3	1:C:104:SER:HA	2.02	0.41
1:C:218:LEU:HD11	1:C:313:ALA:HB1	2.02	0.41
1:D:136:LEU:CD2	1:D:179:ILE:HD12	2.49	0.41
1:D:156:ALA:HB2	1:C:111:LEU:HD11	2.02	0.41
1:D:350:HIS:CE1	1:D:546:LEU:HB2	2.56	0.41
1:B:280:LEU:HD23	1:B:280:LEU:HA	1.78	0.41
1:D:3:PRO:HD2	1:D:5:THR:HG23	2.03	0.41
1:D:178:ASP:C	1:D:179:ILE:HD13	2.46	0.41
1:C:160:VAL:HG21	1:C:177:PHE:CG	2.54	0.41
1:A:59:GLY:O	1:A:63:ILE:HG12	2.20	0.41
1:A:77:MET:HE3	1:A:82:ALA:HB1	2.03	0.41
1:D:136:LEU:HD12	1:D:136:LEU:HA	1.90	0.41
1:C:149:LEU:HD21	1:C:153:TRP:CE2	2.55	0.41
1:C:149:LEU:HD23	1:C:149:LEU:C	2.46	0.41
1:B:381:ARG:O	1:B:385:LEU:HG	2.20	0.41
1:D:140:GLU:HA	1:C:109:TYR:HE2	1.86	0.41
1:C:350:HIS:HA	1:C:351:PRO:HD3	1.98	0.41
1:B:200:ARG:HE	1:B:206:TRP:HA	1.85	0.41
1:D:10:VAL:HG13	1:D:154:ARG:CZ	2.51	0.40
1:D:304:TRP:O	1:B:159:ARG:NH1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:MET:HG2	1:C:86:LEU:CD1	2.51	0.40
1:C:216:GLN:HB3	1:C:316:THR:HG23	2.03	0.40
1:C:515:ILE:HD11	1:C:520:LEU:CD1	2.47	0.40
1:C:108:PRO:CG	1:C:138:LEU:HD22	2.41	0.40
1:D:492:ILE:HD11	1:D:493:PHE:CE2	2.56	0.40
1:C:443:PHE:CZ	1:C:450:LEU:HD11	2.56	0.40
1:B:16:ILE:HG12	1:B:47:ILE:HG23	2.03	0.40
1:A:100:LEU:O	1:A:174:PRO:HA	2.21	0.40
1:B:35:ALA:O	1:B:39:GLN:CD	2.64	0.40
1:B:469:ASP:HB2	1:B:540:ARG:HB2	2.03	0.40
1:D:419:GLU:HG2	1:D:431:PRO:HB2	2.04	0.40
1:C:18:GLY:HA3	1:C:161:LEU:HD13	2.03	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	493/574 (86%)	477 (97%)	16 (3%)	0	100	100
1	B	488/574 (85%)	473 (97%)	14 (3%)	1 (0%)	43	50
1	C	464/574 (81%)	455 (98%)	9 (2%)	0	100	100
1	D	493/574 (86%)	482 (98%)	9 (2%)	2 (0%)	30	31
All	All	1938/2296 (84%)	1887 (97%)	48 (2%)	3 (0%)	43	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	31	ASN
1	D	32	ALA
1	B	526	GLN

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	386/445 (87%)	383 (99%)	3 (1%)	73	80
1	B	381/445 (86%)	378 (99%)	3 (1%)	73	80
1	C	365/445 (82%)	362 (99%)	3 (1%)	73	80
1	D	384/445 (86%)	382 (100%)	2 (0%)	81	87
All	All	1516/1780 (85%)	1505 (99%)	11 (1%)	76	82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	48	ARG
1	A	57	THR
1	D	57	THR
1	D	230	SER
1	C	57	THR
1	C	230	SER
1	C	468	ASN
1	B	330	ASP
1	B	545[A]	GLN
1	B	545[B]	GLN

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	445	HIS
1	A	547	HIS
1	D	7	GLN
1	D	470	ASN
1	D	547	HIS
1	C	7	GLN
1	C	271	GLN
1	C	445	HIS

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Mol	Chain	Res	Type
1	B	547	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	504/574 (87%)	0.42	38 (7%)	20	18	28, 50, 93, 119	3 (0%)
1	B	496/574 (86%)	0.53	44 (8%)	15	14	25, 52, 100, 138	4 (0%)
1	C	473/574 (82%)	0.56	50 (10%)	11	11	28, 51, 100, 126	3 (0%)
1	D	498/574 (86%)	0.51	40 (8%)	18	16	29, 50, 97, 137	3 (0%)
All	All	1971/2296 (85%)	0.51	172 (8%)	16	15	25, 51, 98, 138	13 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	ALA	6.5
1	B	111	LEU	5.9
1	B	32	ALA	5.9
1	D	3	PRO	5.8
1	B	81	THR	5.7
1	A	111	LEU	5.7
1	B	82	ALA	5.3
1	A	496	PRO	4.7
1	B	36	PHE	4.6
1	B	109	TYR	4.5
1	B	527	PRO	4.4
1	B	80	GLY	4.4
1	B	3	PRO	4.4
1	A	125	TYR	4.3
1	A	112	LEU	4.3
1	C	111	LEU	4.3
1	C	139	ALA	4.1
1	B	113	GLY	4.0
1	D	77	MET	3.9
1	C	112	LEU	3.9
1	C	404	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	139	ALA	3.9
1	A	78	THR	3.9
1	A	81	THR	3.8
1	D	493	PHE	3.8
1	D	528	GLY	3.8
1	B	181	LEU	3.8
1	A	3	PRO	3.7
1	C	148	ALA	3.7
1	A	80	GLY	3.7
1	B	307	VAL	3.6
1	A	498	ASP	3.6
1	C	402	ALA	3.6
1	D	5	THR	3.5
1	C	77	MET	3.5
1	B	304	TRP	3.5
1	C	497	HIS	3.4
1	C	153	TRP	3.4
1	C	181	LEU	3.4
1	C	307	VAL	3.4
1	B	214[A]	PHE	3.3
1	A	488	VAL	3.3
1	A	489	SER	3.3
1	C	146	THR	3.3
1	D	149	LEU	3.2
1	D	211	PRO	3.2
1	D	307	VAL	3.2
1	C	529	ALA	3.2
1	C	445	HIS	3.2
1	C	3	PRO	3.2
1	B	39	GLN	3.2
1	B	110	GLU	3.1
1	D	34	LEU	3.1
1	D	146	THR	3.1
1	A	182	ARG	3.0
1	A	402	ALA	3.0
1	B	112	LEU	3.0
1	C	29	SER	3.0
1	C	178	ASP	3.0
1	D	529	ALA	3.0
1	B	114	THR	3.0
1	B	376	ALA	2.9
1	C	350	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	47	ILE	2.9
1	A	109	TYR	2.9
1	B	86	LEU	2.9
1	A	146	THR	2.9
1	A	307	VAL	2.9
1	A	404	ILE	2.9
1	D	33	PRO	2.9
1	D	492	ILE	2.9
1	B	126	PHE	2.8
1	C	496	PRO	2.8
1	B	526	GLN	2.8
1	D	29	SER	2.8
1	C	28	GLY	2.7
1	A	291	ALA	2.7
1	C	196	THR	2.7
1	D	180	PRO	2.7
1	D	138	LEU	2.7
1	D	32	ALA	2.7
1	B	138	LEU	2.7
1	D	126	PHE	2.7
1	A	29	SER	2.7
1	C	33	PRO	2.7
1	B	139	ALA	2.6
1	C	537	LYS	2.6
1	C	34	LEU	2.6
1	B	148	ALA	2.6
1	C	468	ASN	2.6
1	B	78	THR	2.6
1	C	352	LEU	2.6
1	B	35	ALA	2.6
1	A	115	GLY	2.6
1	D	145	ARG	2.6
1	C	306	ASP	2.6
1	B	427	SER	2.6
1	D	80	GLY	2.5
1	C	36	PHE	2.5
1	C	32	ALA	2.5
1	B	105	ALA	2.5
1	D	496	PRO	2.5
1	B	211	PRO	2.5
1	C	211	PRO	2.5
1	B	471	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	107	ARG	2.5
1	D	280	LEU	2.5
1	C	400	GLY	2.5
1	A	490	SER	2.4
1	D	36	PHE	2.4
1	C	137	GLY	2.4
1	A	105	ALA	2.4
1	A	137	GLY	2.4
1	B	143	PRO	2.3
1	A	28	GLY	2.3
1	A	113	GLY	2.3
1	A	309	GLY	2.3
1	D	142	ALA	2.3
1	C	348	ALA	2.3
1	D	196	THR	2.3
1	C	179	ILE	2.3
1	D	498	ASP	2.3
1	D	495	THR	2.3
1	D	541	SER	2.3
1	D	527	PRO	2.3
1	C	527	PRO	2.3
1	B	431	PRO	2.3
1	B	309	GLY	2.3
1	D	148	ALA	2.3
1	C	105	ALA	2.3
1	D	515	ILE	2.3
1	A	138	LEU	2.2
1	C	401	VAL	2.3
1	C	498	ASP	2.2
1	C	506	ARG	2.2
1	B	391	ARG	2.2
1	B	529	ALA	2.2
1	B	196	THR	2.2
1	B	364[A]	HIS	2.2
1	D	104	SER	2.2
1	A	310	ASN	2.2
1	D	470	ASN	2.2
1	A	181	LEU	2.2
1	A	126	PHE	2.2
1	C	108	PRO	2.2
1	B	142	ALA	2.2
1	C	403	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	4	SER	2.1
1	D	81	THR	2.1
1	C	110	GLU	2.1
1	B	27	PRO	2.1
1	A	114	THR	2.1
1	A	497[A]	HIS	2.1
1	D	428	PRO	2.1
1	C	152	THR	2.1
1	C	425	THR	2.1
1	B	497	HIS	2.1
1	C	351	PRO	2.1
1	A	530	GLY	2.1
1	A	303	ARG	2.1
1	D	490	SER	2.0
1	C	151	ALA	2.0
1	B	77	MET	2.0
1	D	210	PRO	2.0
1	A	491	ARG	2.0
1	B	11	VAL	2.0
1	D	203	GLY	2.0
1	C	309	GLY	2.0
1	A	308	SER	2.0
1	C	149	LEU	2.0
1	C	150	ASN	2.0
1	A	107	ARG	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.