



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:50 AM UTC

PDB ID : 1NP3 / pdb_00001np3
Title : Crystal structure of class I acetohydroxy acid isomeroreductase from *Pseudomonas aeruginosa*
Authors : Ahn, H.J.; Eom, S.J.; Yoon, H.-J.; Lee, B.I.; Cho, H.; Suh, S.W.
Deposited on : 2003-01-17
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

<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

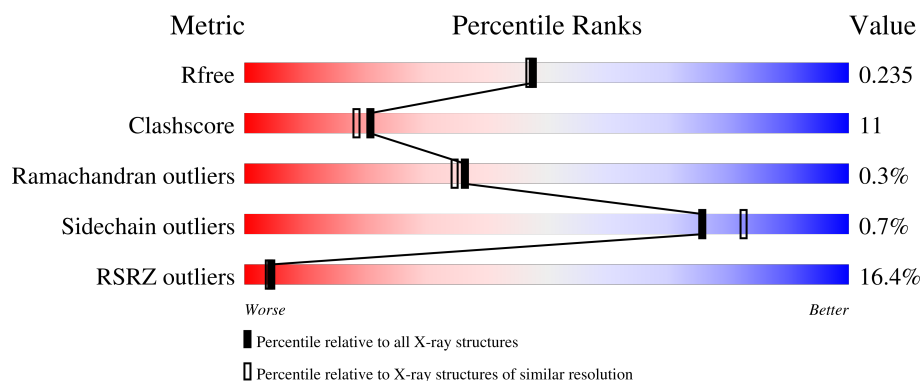
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	338	10% 76% 20% .
1	B	338	37% 70% 26% ..
1	C	338	9% 78% 18% ..
1	D	338	8% 79% 16% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10348 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 Ketol-acid reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2472	1560	421	474	17			
1	B	327	Total	C	N	O	S	0	0	0
			2472	1560	421	474	17			
1	C	327	Total	C	N	O	S	0	0	0
			2472	1560	421	474	17			
1	D	327	Total	C	N	O	S	0	0	0
			2472	1560	421	474	17			

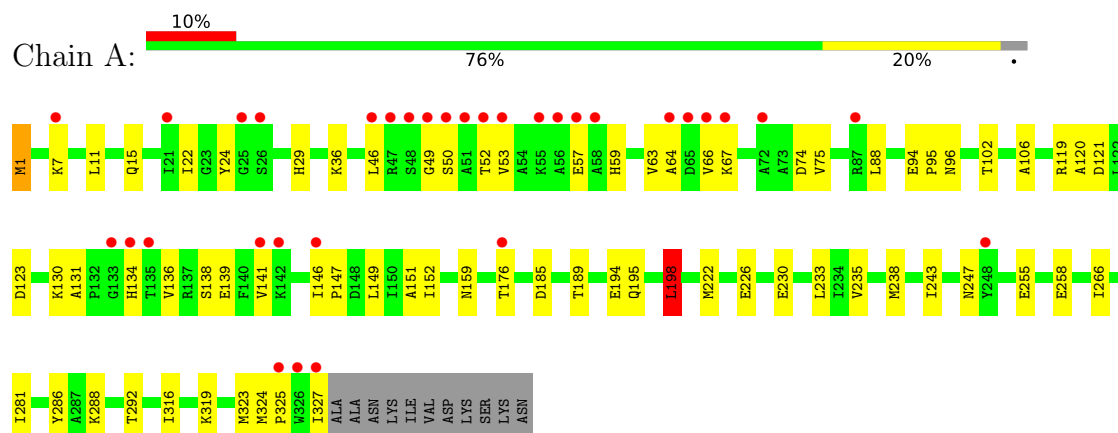
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total	O	0	0
			126	126		
2	B	105	Total	O	0	0
			105	105		
2	C	108	Total	O	0	0
			108	108		
2	D	121	Total	O	0	0
			121	121		

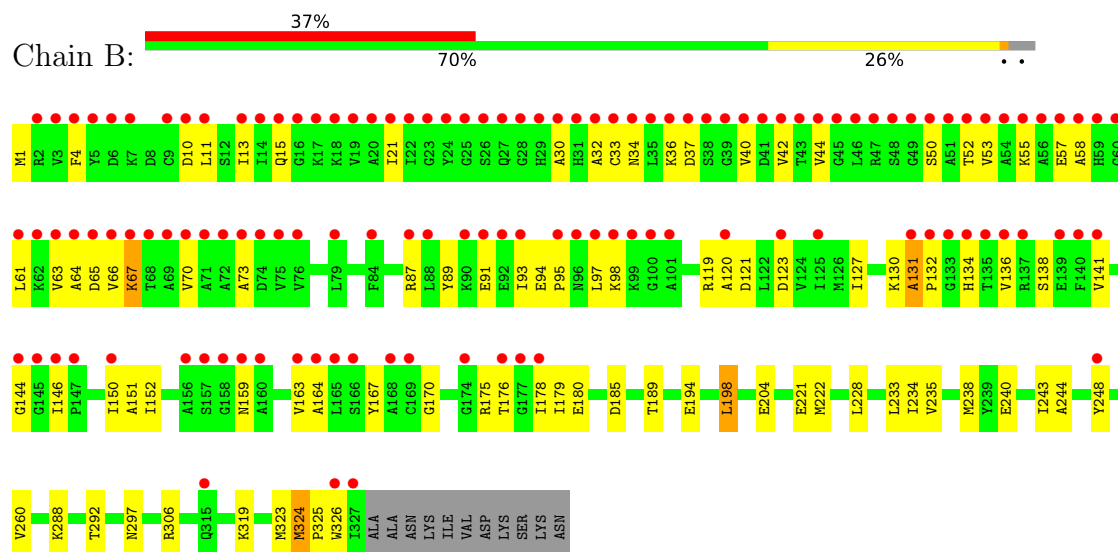
3 Residue-property plots

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.

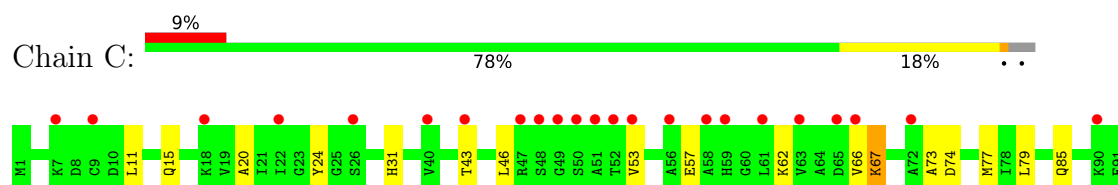
• Molecule 1: Ketol-acid reductoisomerase

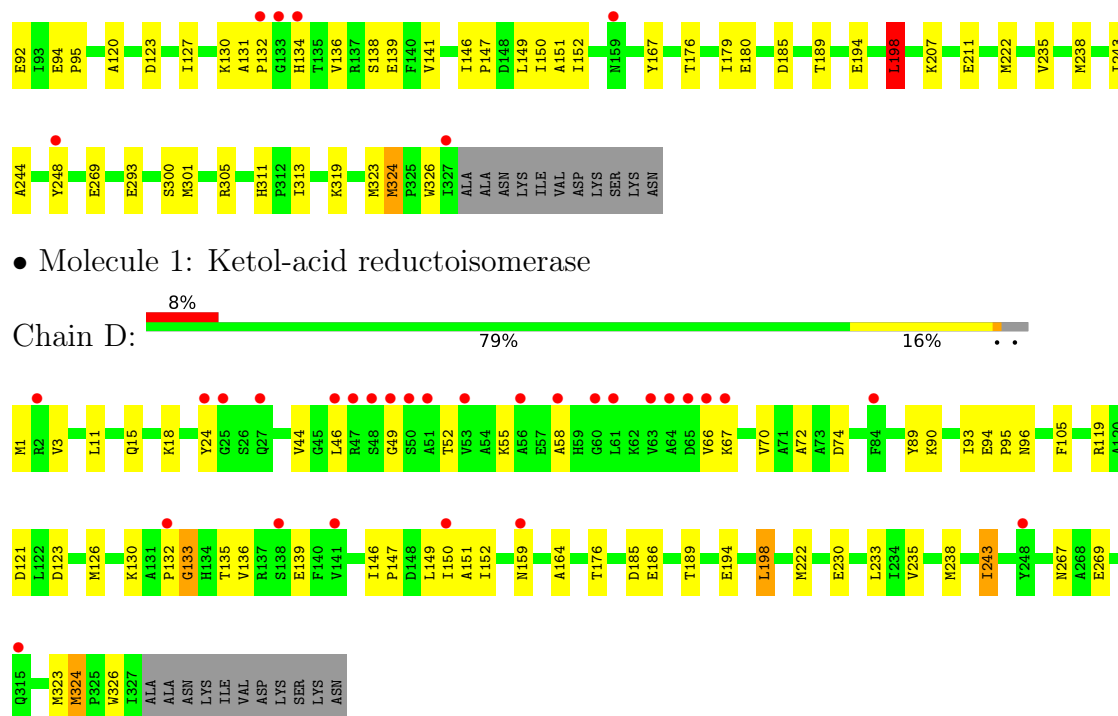


• Molecule 1: Ketol-acid reductoisomerase



• Molecule 1: Ketol-acid reductoisomerase





● Molecule 1: Ketol-acid reductoisomerase

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	184.38Å 184.38Å 184.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.00) 97.0 (20.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.64 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.235 0.212 , 0.235	Depositor DCC
R_{free} test set	13545 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10348	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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

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	0.37	0/2517	0.90	9/3403 (0.3%)
1	B	0.36	0/2517	0.87	7/3403 (0.2%)
1	C	0.36	0/2517	0.88	11/3403 (0.3%)
1	D	0.38	0/2517	0.88	7/3403 (0.2%)
All	All	0.37	0/10068	0.88	34/13612 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	ASP	N-CA-C	-7.00	98.29	109.76
1	A	123	ASP	N-CA-C	-6.73	98.72	109.76
1	B	198	LEU	N-CA-C	6.67	119.16	111.02
1	D	74	ASP	N-CA-C	-6.54	105.84	113.88
1	D	149	LEU	N-CA-C	-6.43	99.82	110.17
1	B	131	ALA	CA-C-N	6.22	126.41	119.32
1	B	131	ALA	C-N-CA	6.22	126.41	119.32
1	C	123	ASP	N-CA-C	-6.08	99.79	109.76
1	A	120	ALA	N-CA-C	6.02	119.45	111.75
1	B	324	MET	CA-C-N	6.01	126.44	119.47
1	B	324	MET	C-N-CA	6.01	126.44	119.47
1	A	149	LEU	N-CA-C	-5.92	100.02	109.96
1	D	198	LEU	N-CA-C	5.90	118.19	111.11
1	C	198	LEU	N-CA-C	5.86	118.17	111.02
1	C	74	ASP	N-CA-C	-5.82	106.34	113.50
1	C	131	ALA	CA-C-N	5.79	127.08	119.84
1	C	131	ALA	C-N-CA	5.79	127.08	119.84
1	A	198	LEU	N-CA-C	5.67	117.92	111.11
1	C	120	ALA	N-CA-C	5.59	118.14	111.71
1	D	324	MET	CA-C-N	5.44	125.26	119.28
1	D	324	MET	C-N-CA	5.44	125.26	119.28
1	A	131	ALA	CA-C-N	5.43	126.62	119.84
1	A	131	ALA	C-N-CA	5.43	126.62	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ASP	N-CA-C	-5.42	106.79	113.41
1	B	260	VAL	N-CA-C	5.40	115.61	110.53
1	D	243	ILE	N-CA-C	5.36	115.57	110.53
1	A	134	HIS	N-CA-C	-5.35	105.85	112.38
1	A	106	ALA	N-CA-C	-5.29	106.84	113.72
1	C	85	GLN	N-CA-C	5.26	117.69	111.33
1	C	134	HIS	N-CA-C	-5.24	105.74	111.82
1	C	324	MET	CA-C-N	5.21	125.01	119.28
1	C	324	MET	C-N-CA	5.21	125.01	119.28
1	B	120	ALA	N-CA-C	5.15	116.90	111.28
1	C	149	LEU	N-CA-C	-5.00	101.55	109.76

There are no chirality outliers.

There are no planarity outliers.

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	2472	0	2447	54	0
1	B	2472	0	2447	82	0
1	C	2472	0	2447	56	0
1	D	2472	0	2447	54	0
2	A	126	0	0	1	0
2	B	105	0	0	6	0
2	C	108	0	0	1	0
2	D	121	0	0	5	0
All	All	10348	0	9788	219	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 11.

All (219) 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:C:238:MET:HE3	1:C:243:ILE:HG12	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:VAL:HA	1:D:146:ILE:HD13	1.49	0.92
1:B:238:MET:HE3	1:B:243:ILE:HG12	1.60	0.83
1:D:238:MET:HE3	1:D:243:ILE:HG12	1.59	0.82
1:A:119:ARG:HD2	1:A:121:ASP:OD1	1.79	0.81
1:B:324:MET:HE2	1:B:326:TRP:HZ2	1.48	0.78
1:C:66:VAL:HG13	1:C:67:LYS:HD3	1.66	0.77
1:B:130:LYS:HE2	1:B:130:LYS:HA	1.65	0.77
1:B:136:VAL:HA	1:B:146:ILE:HD13	1.66	0.76
1:A:176:THR:HG23	1:B:323:MET:O	1.86	0.76
1:A:147:PRO:HD3	1:A:176:THR:HG21	1.68	0.75
1:A:185:ASP:O	1:A:189:THR:HG22	1.87	0.74
1:D:119:ARG:NH1	1:D:121:ASP:OD1	2.22	0.73
1:D:324:MET:HE2	1:D:326:TRP:CZ2	2.23	0.73
1:C:136:VAL:HA	1:C:146:ILE:HD13	1.69	0.73
1:B:66:VAL:HG13	1:B:67:LYS:HD3	1.71	0.72
1:B:185:ASP:O	1:B:189:THR:HG22	1.92	0.70
1:D:238:MET:CE	1:D:243:ILE:HG12	2.22	0.70
1:C:324:MET:HE2	1:C:326:TRP:CZ2	2.27	0.69
1:D:324:MET:HE2	1:D:326:TRP:HZ2	1.56	0.68
1:B:11:LEU:O	1:B:15:GLN:HG3	1.94	0.68
1:A:11:LEU:O	1:A:15:GLN:HG3	1.95	0.66
1:B:194:GLU:HA	1:B:198:LEU:HB2	1.77	0.66
1:A:222:MET:HE3	1:B:189:THR:HG21	1.77	0.65
1:C:319:LYS:HB3	1:C:319:LYS:NZ	2.11	0.65
1:D:194:GLU:HA	1:D:198:LEU:HB2	1.78	0.65
1:A:238:MET:HE3	1:A:243:ILE:HG12	1.79	0.65
1:A:130:LYS:HA	1:A:130:LYS:HE2	1.78	0.65
1:B:10:ASP:OD2	1:B:13:ILE:HG13	1.97	0.65
1:B:167:TYR:HA	2:B:384:HOH:O	1.96	0.65
1:C:189:THR:HG21	1:D:222:MET:HE3	1.77	0.65
1:C:244:ALA:O	1:C:248:TYR:HD1	1.80	0.64
1:A:194:GLU:HA	1:A:198:LEU:HB2	1.79	0.64
1:C:185:ASP:O	1:C:189:THR:HG22	1.97	0.64
1:B:65:ASP:HB3	1:B:67:LYS:NZ	2.13	0.64
1:A:235:VAL:HG21	1:B:235:VAL:HG21	1.80	0.64
1:C:132:PRO:HG3	1:D:233:LEU:HD22	1.80	0.63
1:B:159:ASN:O	1:B:163:VAL:HG23	1.99	0.63
1:C:130:LYS:HA	1:C:130:LYS:HE2	1.80	0.63
1:C:324:MET:HE2	1:C:326:TRP:HZ2	1.63	0.63
1:D:126:MET:HE1	1:D:186:GLU:HG3	1.80	0.63
1:C:147:PRO:HG3	1:D:324:MET:HE3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HB2	1:B:221:GLU:OE1	1.99	0.62
1:B:66:VAL:HG12	1:B:67:LYS:NZ	2.14	0.62
1:D:133:GLY:N	2:D:343:HOH:O	2.32	0.62
1:A:195:GLN:HE22	1:A:281:ILE:HD11	1.65	0.61
1:A:151:ALA:C	1:A:152:ILE:HD12	2.24	0.61
1:A:323:MET:O	1:B:176:THR:HG23	2.01	0.61
1:C:235:VAL:HG21	1:D:235:VAL:HG21	1.82	0.60
1:D:185:ASP:O	1:D:189:THR:HG22	2.01	0.60
1:C:139:GLU:HB2	1:C:146:ILE:CD1	2.31	0.60
1:D:130:LYS:HE2	1:D:130:LYS:HA	1.84	0.60
1:A:327:ILE:HG23	1:B:240:GLU:HA	1.83	0.59
1:B:306:ARG:HD2	2:B:366:HOH:O	2.02	0.59
1:B:66:VAL:HG12	1:B:67:LYS:HZ1	1.67	0.59
1:B:73:ALA:O	1:B:98:LYS:HD3	2.02	0.59
1:D:90:LYS:HG3	2:D:423:HOH:O	2.03	0.59
1:B:53:VAL:HG22	1:B:63:VAL:HG11	1.84	0.59
1:A:22:ILE:HG21	1:A:88:LEU:HD21	1.83	0.59
1:C:324:MET:HE3	1:D:147:PRO:HG3	1.85	0.58
1:B:33:CYS:HA	1:B:36:LYS:HE2	1.85	0.57
1:C:301:MET:O	1:C:305:ARG:HG3	2.04	0.57
1:A:7:LYS:HG3	2:A:448:HOH:O	2.05	0.56
1:D:151:ALA:C	1:D:152:ILE:HD12	2.30	0.56
1:B:65:ASP:HB3	1:B:67:LYS:HZ2	1.71	0.56
1:B:179:ILE:HD12	1:B:179:ILE:N	2.21	0.56
1:A:53:VAL:O	1:A:57:GLU:HG2	2.06	0.56
1:C:53:VAL:O	1:C:57:GLU:HG3	2.06	0.56
1:D:139:GLU:HB2	1:D:146:ILE:CD1	2.36	0.56
1:D:139:GLU:HB2	1:D:146:ILE:HD12	1.89	0.55
1:C:138:SER:O	1:C:141:VAL:HG22	2.07	0.55
1:C:222:MET:HE3	1:D:189:THR:HG21	1.88	0.55
1:B:324:MET:HE2	1:B:326:TRP:CZ2	2.36	0.55
1:C:238:MET:HE3	1:C:243:ILE:CG1	2.28	0.55
1:C:11:LEU:O	1:C:15:GLN:HG3	2.06	0.54
1:C:194:GLU:HA	1:C:198:LEU:HB2	1.88	0.54
1:B:94:GLU:N	1:B:95:PRO:HD2	2.22	0.54
1:D:267:ASN:OD1	1:D:269:GLU:HB2	2.08	0.54
1:D:126:MET:HE1	1:D:186:GLU:CG	2.37	0.54
1:A:24:TYR:HB3	1:A:52:THR:HG21	1.89	0.54
1:D:126:MET:CE	1:D:186:GLU:HG3	2.38	0.54
1:B:66:VAL:O	1:B:70:VAL:HG23	2.07	0.53
1:C:147:PRO:CG	1:D:324:MET:HE3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:LEU:O	1:D:15:GLN:HG3	2.08	0.53
1:C:152:ILE:HD12	1:C:152:ILE:N	2.23	0.53
1:D:24:TYR:HB2	1:D:46:LEU:HD21	1.91	0.53
1:B:89:TYR:HA	1:B:93:ILE:HB	1.91	0.53
1:D:152:ILE:HD12	1:D:152:ILE:N	2.24	0.52
1:B:4:PHE:HB2	1:B:178:ILE:HB	1.91	0.52
1:B:233:LEU:HD23	2:B:412:HOH:O	2.09	0.52
1:D:24:TYR:HB3	1:D:52:THR:HG21	1.89	0.52
1:B:146:ILE:N	1:B:146:ILE:HD12	2.25	0.52
1:B:70:VAL:HG12	1:B:97:LEU:HA	1.91	0.52
1:B:36:LYS:HE3	1:B:37:ASP:OD2	2.10	0.52
1:C:198:LEU:HD21	1:D:230:GLU:HB2	1.92	0.52
1:B:152:ILE:N	1:B:152:ILE:HD12	2.25	0.52
1:C:24:TYR:HB2	1:C:46:LEU:HD21	1.91	0.51
1:A:152:ILE:HD12	1:A:152:ILE:N	2.26	0.51
1:A:189:THR:HG21	1:B:222:MET:HE3	1.93	0.51
1:A:67:LYS:HG2	1:A:96:ASN:HD21	1.76	0.51
1:A:138:SER:O	1:A:141:VAL:HG22	2.11	0.50
1:B:119:ARG:NH1	1:B:121:ASP:OD2	2.45	0.50
1:B:234:ILE:N	1:B:234:ILE:HD12	2.25	0.50
1:D:18:LYS:HD3	1:D:72:ALA:O	2.11	0.50
1:B:93:ILE:O	1:B:97:LEU:HB2	2.12	0.50
1:A:136:VAL:HA	1:A:146:ILE:HD13	1.94	0.50
1:C:244:ALA:O	1:C:248:TYR:CD1	2.63	0.50
1:C:293:GLU:OE1	1:C:300:SER:HB3	2.11	0.49
1:C:150:ILE:HG22	1:C:179:ILE:O	2.13	0.49
1:A:195:GLN:NE2	1:A:281:ILE:HD11	2.27	0.49
1:A:67:LYS:HG2	1:A:96:ASN:ND2	2.28	0.49
1:B:50:SER:C	1:B:52:THR:H	2.21	0.49
1:B:67:LYS:CD	1:B:67:LYS:H	2.26	0.49
1:C:31:HIS:HD2	1:C:167:TYR:OH	1.96	0.49
1:B:44:VAL:O	1:B:63:VAL:HA	2.12	0.49
1:B:150:ILE:HD11	1:B:164:ALA:HB3	1.94	0.48
1:B:234:ILE:HD12	1:B:234:ILE:H	1.78	0.48
1:C:43:THR:HG22	1:C:62:LYS:HE2	1.95	0.48
1:A:22:ILE:HD12	1:A:22:ILE:N	2.27	0.48
1:C:269:GLU:HG2	1:D:269:GLU:HG2	1.95	0.48
1:B:297:ASN:HB2	2:B:410:HOH:O	2.13	0.48
1:A:94:GLU:N	1:A:95:PRO:HD2	2.29	0.48
1:D:55:LYS:O	1:D:58:ALA:HB3	2.13	0.48
1:B:66:VAL:CG1	1:B:67:LYS:HD3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LYS:O	1:C:211:GLU:HG3	2.14	0.47
1:D:94:GLU:N	1:D:95:PRO:HD2	2.28	0.47
1:B:67:LYS:HD3	1:B:67:LYS:H	1.79	0.47
1:C:20:ALA:HB2	1:C:73:ALA:HB2	1.96	0.47
1:B:144:GLY:O	1:B:175:ARG:HD2	2.15	0.47
1:C:305:ARG:CZ	2:C:391:HOH:O	2.63	0.47
1:D:119:ARG:HH12	1:D:121:ASP:CG	2.21	0.47
1:A:281:ILE:HD13	1:A:286:TYR:HB3	1.96	0.47
1:B:288:LYS:O	1:B:292:THR:HG23	2.14	0.47
1:C:150:ILE:HG23	1:C:180:GLU:HA	1.96	0.47
1:D:135:THR:HB	2:D:343:HOH:O	2.15	0.47
1:D:150:ILE:HD11	1:D:164:ALA:HB3	1.96	0.47
1:A:238:MET:HE3	1:A:243:ILE:CG1	2.45	0.46
1:B:40:VAL:O	1:B:42:VAL:HG23	2.15	0.46
1:A:36:LYS:NZ	1:A:59:HIS:O	2.48	0.46
1:A:255:GLU:O	1:A:258:GLU:HB3	2.16	0.46
1:A:66:VAL:HG13	1:A:67:LYS:N	2.31	0.46
1:A:1:MET:HB2	1:B:221:GLU:CD	2.41	0.46
1:A:288:LYS:O	1:A:292:THR:HG23	2.16	0.46
1:B:244:ALA:O	1:B:248:TYR:HD1	1.99	0.46
1:B:150:ILE:HG23	1:B:180:GLU:HA	1.98	0.46
1:B:138:SER:O	1:B:141:VAL:HG22	2.15	0.46
1:B:63:VAL:HG12	1:B:64:ALA:N	2.31	0.45
1:A:319:LYS:HE2	1:B:1:MET:HE3	1.99	0.45
1:D:1:MET:HG3	1:D:3:VAL:HG23	1.98	0.45
1:C:176:THR:HG23	1:D:323:MET:O	2.15	0.45
1:A:24:TYR:HB2	1:A:46:LEU:HD21	1.98	0.45
1:A:94:GLU:C	1:A:94:GLU:CD	2.85	0.45
1:B:131:ALA:CB	1:B:146:ILE:HG12	2.47	0.45
1:D:67:LYS:HG2	1:D:96:ASN:ND2	2.31	0.45
1:B:55:LYS:O	1:B:58:ALA:HB3	2.18	0.44
1:B:132:PRO:HB2	1:B:134:HIS:CE1	2.53	0.44
1:C:324:MET:HE3	1:D:147:PRO:CG	2.47	0.44
1:A:22:ILE:N	1:A:22:ILE:CD1	2.80	0.44
1:D:24:TYR:HB3	1:D:52:THR:CG2	2.48	0.44
1:C:139:GLU:HB2	1:C:146:ILE:HD12	1.98	0.44
1:D:159:ASN:HB3	2:D:359:HOH:O	2.18	0.44
1:C:319:LYS:NZ	1:C:319:LYS:CB	2.79	0.44
1:D:126:MET:HE1	1:D:186:GLU:CB	2.48	0.44
1:D:119:ARG:HH11	1:D:119:ARG:CB	2.31	0.43
1:B:15:GLN:HA	1:B:40:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ILE:HD12	1:C:146:ILE:N	2.33	0.43
1:A:233:LEU:HD22	1:B:132:PRO:HG3	1.99	0.43
1:D:146:ILE:HD12	1:D:146:ILE:N	2.33	0.43
1:D:66:VAL:O	1:D:70:VAL:HG23	2.18	0.43
1:B:30:ALA:O	1:B:34:ASN:HB2	2.18	0.43
1:B:57:GLU:HG3	1:B:63:VAL:CG2	2.47	0.43
1:C:94:GLU:N	1:C:95:PRO:HD2	2.33	0.43
1:A:238:MET:HE2	1:B:228:LEU:CD1	2.48	0.43
1:B:94:GLU:C	1:B:94:GLU:CD	2.86	0.43
1:B:119:ARG:HH11	1:B:121:ASP:CG	2.26	0.43
1:C:319:LYS:HB3	1:C:319:LYS:HZ2	1.82	0.43
1:D:89:TYR:HA	1:D:93:ILE:HB	2.01	0.43
1:B:36:LYS:HD3	1:B:61:LEU:CD2	2.49	0.43
1:B:170:GLY:HA3	2:B:384:HOH:O	2.19	0.43
1:A:63:VAL:HG12	1:A:64:ALA:N	2.34	0.43
1:B:136:VAL:HA	1:B:146:ILE:CD1	2.43	0.43
1:C:67:LYS:HE3	1:C:92:GLU:OE2	2.19	0.43
1:B:87:ARG:HG2	1:B:91:GLU:OE1	2.19	0.42
1:A:29:HIS:HE1	1:A:59:HIS:CD2	2.36	0.42
1:A:266:ILE:HB	1:B:204:GLU:CG	2.49	0.42
1:A:316:ILE:HD11	1:B:1:MET:HE2	2.00	0.42
1:C:67:LYS:HD3	1:C:67:LYS:N	2.34	0.42
1:D:66:VAL:HG13	1:D:67:LYS:N	2.35	0.42
1:A:230:GLU:HB2	1:B:198:LEU:HD21	2.00	0.42
1:C:66:VAL:HG12	1:C:67:LYS:NZ	2.34	0.42
1:C:323:MET:O	1:D:176:THR:HG23	2.18	0.42
1:C:150:ILE:CG2	1:C:180:GLU:HA	2.50	0.42
1:C:151:ALA:C	1:C:152:ILE:HD12	2.45	0.42
1:A:139:GLU:HB2	1:A:146:ILE:CD1	2.49	0.42
1:C:77:MET:HG3	1:C:79:LEU:HG	2.02	0.42
1:A:50:SER:H	1:A:53:VAL:HG23	1.85	0.42
1:B:324:MET:HA	1:B:325:PRO:HD2	1.84	0.41
1:D:44:VAL:HG12	1:D:46:LEU:HG	2.02	0.41
1:C:269:GLU:H	1:C:269:GLU:CD	2.27	0.41
1:D:119:ARG:NH1	1:D:121:ASP:CG	2.78	0.41
1:A:119:ARG:CD	1:A:121:ASP:OD1	2.61	0.41
1:B:67:LYS:HD3	1:B:67:LYS:N	2.35	0.41
1:A:247:ASN:OD1	1:A:258:GLU:OE1	2.38	0.41
1:B:151:ALA:C	1:B:152:ILE:HD12	2.46	0.41
1:C:319:LYS:HB3	1:C:319:LYS:HZ3	1.81	0.41
1:D:136:VAL:HG23	2:D:343:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLU:HG3	1:B:189:THR:HG23	2.03	0.41
1:B:319:LYS:NZ	2:B:395:HOH:O	2.53	0.41
1:C:311:HIS:ND1	1:C:313:ILE:HG22	2.36	0.41
1:A:75:VAL:HG22	1:A:102:THR:HB	2.02	0.41
1:B:127:ILE:HD12	1:B:127:ILE:N	2.35	0.41
1:A:46:LEU:HD12	1:A:53:VAL:HA	2.03	0.41
1:B:21:ILE:HD12	1:B:32:ALA:HA	2.02	0.40
1:B:119:ARG:HD2	1:B:121:ASP:OD1	2.21	0.40
1:A:324:MET:HA	1:A:325:PRO:HD2	1.91	0.40
1:D:105:PHE:O	1:D:126:MET:HG3	2.22	0.40
1:C:127:ILE:HD12	1:C:127:ILE:N	2.36	0.40
1:C:293:GLU:CD	1:C:300:SER:HB3	2.47	0.40
1:C:67:LYS:HD3	1:C:67:LYS:H	1.87	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	325/338 (96%)	311 (96%)	13 (4%)	1 (0%)	36	35
1	B	325/338 (96%)	308 (95%)	17 (5%)	0	100	100
1	C	325/338 (96%)	312 (96%)	13 (4%)	0	100	100
1	D	325/338 (96%)	307 (94%)	15 (5%)	3 (1%)	14	9
All	All	1300/1352 (96%)	1238 (95%)	58 (4%)	4 (0%)	36	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	132	PRO
1	A	49	GLY

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Mol	Chain	Res	Type
1	D	49	GLY
1	D	133	GLY

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	253/262 (97%)	250 (99%)	3 (1%)	63	70
1	B	253/262 (97%)	251 (99%)	2 (1%)	73	80
1	C	253/262 (97%)	251 (99%)	2 (1%)	73	80
1	D	253/262 (97%)	253 (100%)	0	100	100
All	All	1012/1048 (97%)	1005 (99%)	7 (1%)	76	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	159	ASN
1	A	198	LEU
1	B	67	LYS
1	B	123	ASP
1	C	67	LYS
1	C	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	159	ASN
1	A	162	ASN
1	A	247	ASN
1	A	252	ASN
1	B	31	HIS
1	B	247	ASN

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Mol	Chain	Res	Type
1	B	282	GLN
1	B	315	GLN
1	C	31	HIS
1	C	247	ASN
1	D	96	ASN
1	D	315	GLN

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	327/338 (96%)	0.23	33 (10%)	12 11	11, 24, 52, 90	0
1	B	327/338 (96%)	1.32	125 (38%)	1 1	12, 35, 79, 102	0
1	C	327/338 (96%)	0.26	29 (8%)	15 14	12, 27, 50, 86	0
1	D	327/338 (96%)	0.12	28 (8%)	16 15	12, 24, 54, 88	0
All	All	1308/1352 (96%)	0.48	215 (16%)	4 4	11, 25, 65, 102	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	TYR	7.5
1	B	64	ALA	6.9
1	B	51	ALA	6.7
1	B	53	VAL	6.7
1	B	40	VAL	6.6
1	B	56	ALA	6.5
1	B	24	TYR	6.4
1	A	248	TYR	6.1
1	B	66	VAL	5.9
1	D	51	ALA	5.9
1	B	54	ALA	5.6
1	A	51	ALA	5.4
1	B	27	GLN	5.3
1	B	61	LEU	5.3
1	B	70	VAL	5.2
1	B	159	ASN	5.2
1	B	72	ALA	5.2
1	D	248	TYR	5.2
1	B	58	ALA	5.1
1	B	71	ALA	5.1
1	B	140	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	48	SER	5.0
1	B	39	GLY	4.9
1	A	48	SER	4.9
1	B	141	VAL	4.9
1	B	44	VAL	4.8
1	B	4	PHE	4.8
1	B	84	PHE	4.8
1	B	23	GLY	4.8
1	C	51	ALA	4.8
1	B	248	TYR	4.8
1	A	65	ASP	4.7
1	B	73	ALA	4.7
1	B	9	CYS	4.7
1	B	55	LYS	4.7
1	B	150	ILE	4.6
1	B	169	CYS	4.6
1	B	47	ARG	4.6
1	B	75	VAL	4.5
1	B	63	VAL	4.4
1	B	38	SER	4.4
1	B	59	HIS	4.3
1	A	50	SER	4.3
1	B	5	TYR	4.3
1	B	15	GLN	4.3
1	B	41	ASP	4.2
1	B	19	VAL	4.2
1	D	47	ARG	4.2
1	B	90	LYS	4.2
1	B	30	ALA	4.1
1	B	26	SER	4.1
1	B	65	ASP	4.1
1	B	7	LYS	4.0
1	D	53	VAL	4.0
1	B	43	THR	4.0
1	B	50	SER	4.0
1	A	47	ARG	4.0
1	A	7	LYS	4.0
1	A	49	GLY	4.0
1	B	46	LEU	4.0
1	C	48	SER	4.0
1	B	35	LEU	4.0
1	B	96	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	11	LEU	3.9
1	B	22	ILE	3.9
1	D	65	ASP	3.9
1	B	160	ALA	3.9
1	A	327	ILE	3.9
1	C	7	LYS	3.9
1	D	66	VAL	3.8
1	B	3	VAL	3.8
1	B	32	ALA	3.7
1	B	29	HIS	3.7
1	D	67	LYS	3.7
1	B	20	ALA	3.6
1	B	42	VAL	3.6
1	B	100	GLY	3.6
1	B	21	ILE	3.5
1	B	34	ASN	3.5
1	B	133	GLY	3.5
1	B	98	LYS	3.5
1	B	18	LYS	3.5
1	C	61	LEU	3.5
1	B	132	PRO	3.4
1	C	132	PRO	3.4
1	B	101	ALA	3.4
1	B	157	SER	3.4
1	B	136	VAL	3.4
1	B	62	LYS	3.4
1	B	36	LYS	3.3
1	B	67	LYS	3.3
1	B	134	HIS	3.3
1	B	52	THR	3.3
1	A	133	GLY	3.3
1	B	49	GLY	3.3
1	D	50	SER	3.3
1	B	28	GLY	3.3
1	C	52	THR	3.2
1	D	48	SER	3.2
1	B	163	VAL	3.2
1	B	93	ILE	3.2
1	A	52	THR	3.2
1	B	57	GLU	3.2
1	B	69	ALA	3.2
1	B	13	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	33	CYS	3.2
1	B	165	LEU	3.2
1	C	50	SER	3.2
1	B	25	GLY	3.2
1	C	43	THR	3.2
1	B	60	GLY	3.1
1	C	58	ALA	3.1
1	D	132	PRO	3.1
1	A	72	ALA	3.1
1	C	53	VAL	3.1
1	B	2	ARG	3.0
1	B	76	VAL	3.0
1	B	92	GLU	3.0
1	A	134	HIS	3.0
1	B	31	HIS	3.0
1	B	45	GLY	3.0
1	B	135	THR	3.0
1	C	65	ASP	3.0
1	D	63	VAL	3.0
1	B	14	ILE	3.0
1	A	326	TRP	3.0
1	C	47	ARG	2.9
1	B	174	GLY	2.9
1	B	68	THR	2.9
1	D	2	ARG	2.9
1	D	24	TYR	2.9
1	B	156	ALA	2.9
1	B	97	LEU	2.9
1	C	159	ASN	2.9
1	D	84	PHE	2.8
1	B	74	ASP	2.8
1	A	141	VAL	2.8
1	C	49	GLY	2.8
1	D	64	ALA	2.8
1	D	141	VAL	2.8
1	D	315	GLN	2.8
1	D	150	ILE	2.7
1	A	67	LYS	2.7
1	B	164	ALA	2.7
1	B	327	ILE	2.7
1	C	66	VAL	2.7
1	B	87	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	6	ASP	2.6
1	B	37	ASP	2.6
1	C	18	LYS	2.6
1	B	146	ILE	2.6
1	B	158	GLY	2.6
1	A	176	THR	2.6
1	A	142	LYS	2.6
1	A	66	VAL	2.6
1	C	40	VAL	2.5
1	B	16	GLY	2.5
1	D	49	GLY	2.5
1	B	144	GLY	2.5
1	A	325	PRO	2.5
1	A	57	GLU	2.5
1	B	139	GLU	2.5
1	A	56	ALA	2.5
1	B	17	LYS	2.5
1	B	145	GLY	2.5
1	B	123	ASP	2.4
1	D	27	GLN	2.4
1	D	138	SER	2.4
1	A	58	ALA	2.4
1	C	56	ALA	2.4
1	C	22	ILE	2.4
1	B	326	TRP	2.4
1	B	147	PRO	2.4
1	C	63	VAL	2.4
1	A	55	LYS	2.4
1	B	166	SER	2.4
1	C	90	LYS	2.4
1	B	176	THR	2.4
1	D	58	ALA	2.3
1	D	46	LEU	2.3
1	D	159	ASN	2.3
1	B	137	ARG	2.3
1	C	26	SER	2.3
1	B	120	ALA	2.3
1	B	168	ALA	2.3
1	A	25	GLY	2.3
1	A	46	LEU	2.3
1	B	177	GLY	2.3
1	B	91	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	10	ASP	2.3
1	D	61	LEU	2.3
1	B	178	ILE	2.2
1	C	327	ILE	2.2
1	A	53	VAL	2.2
1	B	95	PRO	2.2
1	B	131	ALA	2.2
1	B	99	LYS	2.2
1	D	25	GLY	2.2
1	B	315	GLN	2.2
1	A	26	SER	2.2
1	A	146	ILE	2.2
1	C	133	GLY	2.2
1	D	56	ALA	2.2
1	C	9	CYS	2.1
1	A	87	ARG	2.1
1	A	135	THR	2.1
1	C	72	ALA	2.1
1	C	59	HIS	2.1
1	A	64	ALA	2.1
1	B	79	LEU	2.0
1	A	21	ILE	2.0
1	B	125	ILE	2.0
1	B	88	LEU	2.0
1	C	134	HIS	2.0
1	D	60	GLY	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.