



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 10:28 AM JST

PDB ID : 7Y3Z / pdb_00007y3z
Title : Structure of a novel carboxylesterase FEH from Rhodococcus sp. T1
Authors : Huang, Y.; Liu, W.D.; Zhang, Y.J.; Duan, Y.J.; Lu, M.L.
Deposited on : 2022-06-13
Resolution : 2.30 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

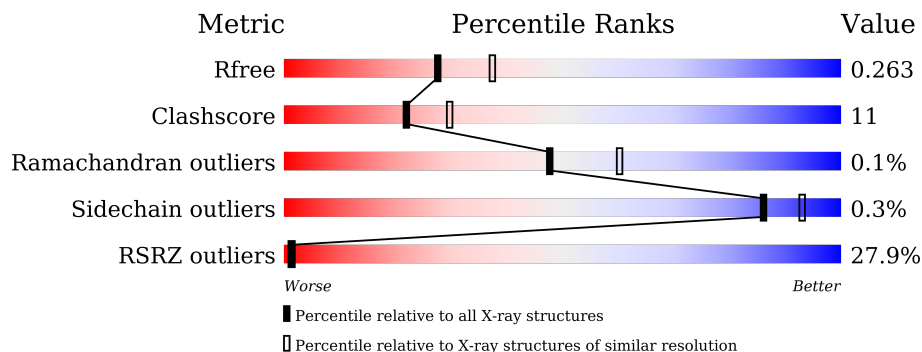
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	387	13% 83% 14% ..
1	B	387	38% 73% 24% ..
1	C	387	44% 68% 29% ..
1	D	387	14% 83% 14% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11467 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 Fenoxaprop-p-ethyl hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	377	Total	C	N	O	S	0	0	0
			2865	1813	493	547	12			
1	A	377	Total	C	N	O	S	0	0	0
			2865	1813	493	547	12			
1	B	377	Total	C	N	O	S	0	0	0
			2865	1813	493	547	12			
1	C	377	Total	C	N	O	S	0	0	0
			2865	1813	493	547	12			

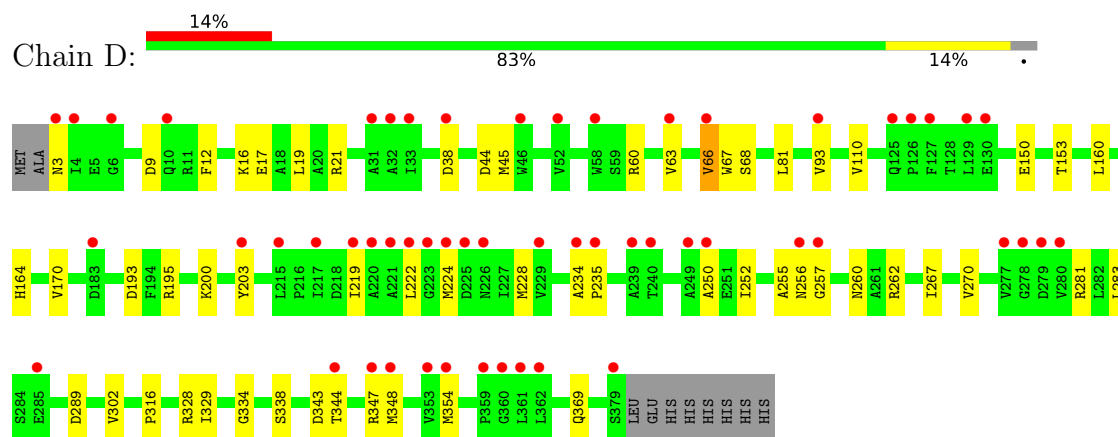
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	3	Total	O	0	0
			3	3		
2	A	4	Total	O	0	0
			4	4		

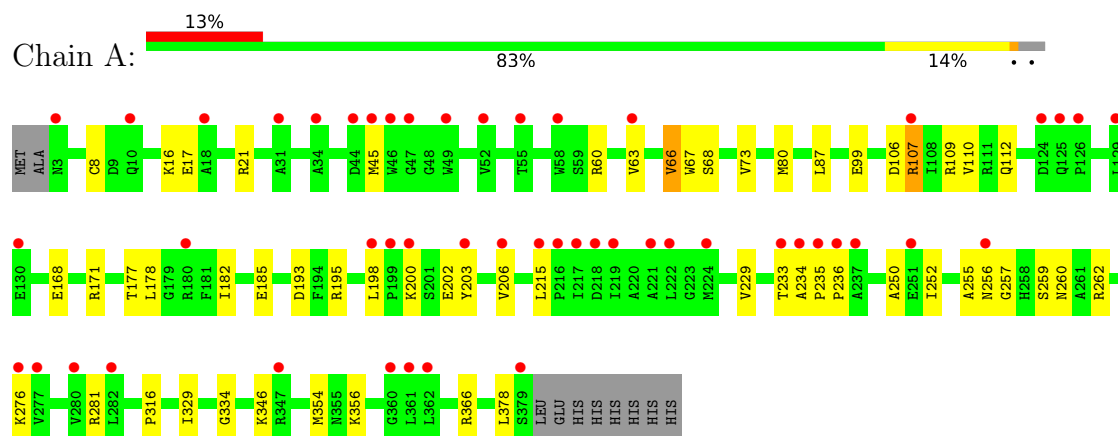
3 Residue-property plots [i](#)

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.

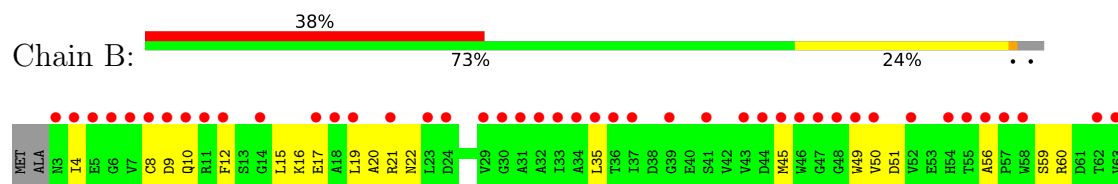
• Molecule 1: Fenoxaprop-p-ethyl hydrolase

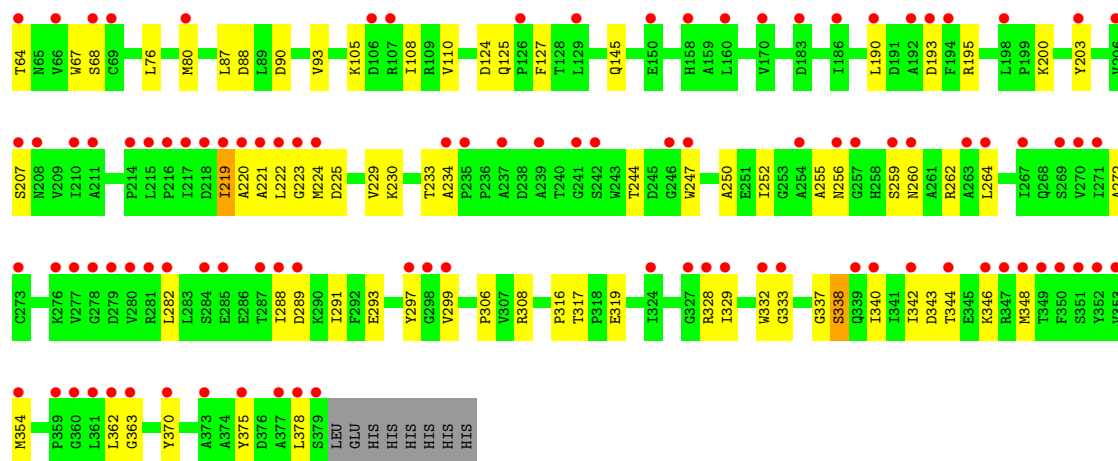


• Molecule 1: Fenoxaprop-p-ethyl hydrolase

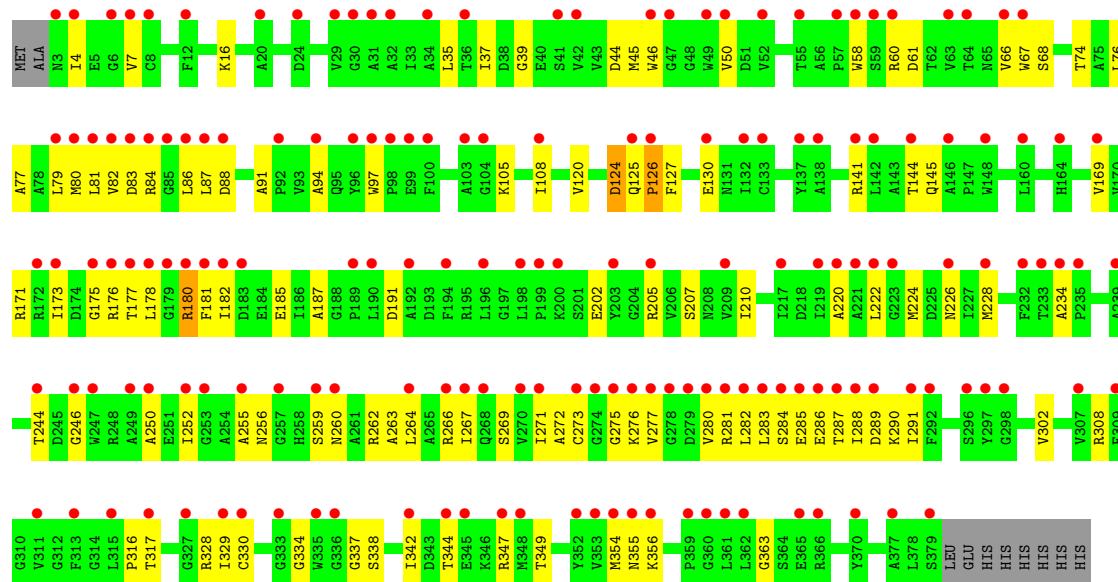
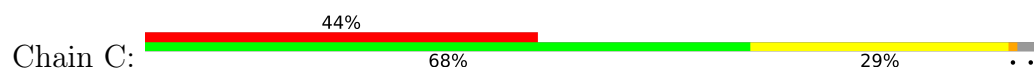


• Molecule 1: Fenoxaprop-p-ethyl hydrolase





• Molecule 1: Fenoxaprop-p-ethyl hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	129.96Å 148.96Å 156.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.48 – 2.30 74.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (74.48-2.30) 86.9 (74.48-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.33 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.238 , 0.257 0.244 , 0.263	Depositor DCC
R_{free} test set	2006 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11467	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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	0.13	0/2934	0.33	0/3999
1	B	0.18	0/2934	0.39	1/3999 (0.0%)
1	C	0.27	1/2934 (0.0%)	0.50	0/3999
1	D	0.16	0/2934	0.36	0/3999
All	All	0.19	1/11736 (0.0%)	0.40	1/15996 (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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	ARG	CG-CD	-5.37	1.36	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	ILE	CB-CG1-CD1	-5.05	103.20	113.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	ALA	Peptide
1	A	66	VAL	Peptide
1	B	124	ASP	Peptide
1	B	234	ALA	Peptide
1	C	124	ASP	Peptide
1	C	66	VAL	Peptide
1	D	234	ALA	Peptide
1	D	66	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	2865	0	2784	36	0
1	B	2865	0	2784	65	1
1	C	2865	0	2784	109	0
1	D	2865	0	2784	38	0
2	A	4	0	0	0	0
2	D	3	0	0	1	0
All	All	11467	0	11136	241	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (241) 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:16:LYS:HG3	1:B:45:MET:HE1	1.42	0.99
1:B:8:CYS:SG	1:B:16:LYS:NZ	2.36	0.98
1:C:126:PRO:O	1:C:141:ARG:NH2	1.95	0.98
1:B:362:LEU:HD13	1:B:363:GLY:H	1.28	0.98
1:B:219:ILE:O	1:B:222:LEU:N	2.00	0.93
1:C:80:MET:HG2	1:C:282:LEU:HG	1.55	0.88
1:B:378:LEU:HD23	1:B:378:LEU:O	1.75	0.86
1:C:79:LEU:HB3	1:C:287:THR:HG21	1.58	0.85
1:C:77:ALA:HA	1:C:80:MET:SD	2.18	0.82
1:A:276:LYS:HB2	1:A:281:ARG:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD11	1:A:202:GLU:HB2	1.61	0.80
1:C:130:GLU:OE1	1:C:130:GLU:N	2.16	0.76
1:D:289:ASP:OD1	1:D:328:ARG:NH2	2.18	0.73
1:D:219:ILE:HD11	1:C:222:LEU:HD11	1.70	0.73
1:B:8:CYS:SG	1:B:9:ASP:N	2.62	0.72
1:C:202:GLU:HG2	1:C:205:ARG:HE	1.55	0.71
1:C:61:ASP:O	1:C:205:ARG:NH1	2.23	0.71
1:C:125:GLN:HE22	1:C:234:ALA:HA	1.57	0.70
1:C:286:GLU:OE2	1:C:287:THR:N	2.25	0.69
1:B:362:LEU:CD1	1:B:363:GLY:H	2.04	0.69
1:C:210:ILE:HB	1:C:356:LYS:HA	1.73	0.68
1:C:275:GLY:HA2	1:C:283:LEU:HD12	1.75	0.67
1:C:125:GLN:O	1:C:127:PHE:N	2.28	0.67
1:C:171:ARG:HA	1:C:176:ARG:O	1.94	0.67
1:A:356:LYS:O	1:A:366:ARG:NH2	2.25	0.66
1:C:269:SER:HA	1:C:272:ALA:HB3	1.78	0.65
1:C:182:ILE:O	1:C:187:ALA:N	2.24	0.65
1:D:193:ASP:OD1	1:D:195:ARG:NH2	2.29	0.64
1:A:109:ARG:H	1:A:112:GLN:NE2	1.96	0.64
1:B:67:TRP:O	1:B:255:ALA:HA	1.97	0.64
1:A:252:ILE:HB	1:A:256:ASN:HB2	1.78	0.64
1:D:3:ASN:N	2:D:401:HOH:O	2.31	0.64
1:C:44:ASP:OD1	1:C:262:ARG:NE	2.29	0.64
1:A:16:LYS:HB2	1:A:45:MET:HE1	1.78	0.64
1:C:125:GLN:HE21	1:C:125:GLN:HA	1.64	0.63
1:B:60:ARG:O	1:B:262:ARG:NH2	2.27	0.63
1:C:86:LEU:N	1:C:86:LEU:HD22	2.14	0.63
1:A:109:ARG:H	1:A:112:GLN:HE21	1.45	0.62
1:C:176:ARG:HB3	1:C:180:ARG:HG2	1.81	0.62
1:B:87:LEU:HD11	1:B:110:VAL:HG11	1.82	0.62
1:A:68:SER:HB2	1:A:334:GLY:HA2	1.83	0.60
1:C:61:ASP:HB3	1:C:205:ARG:NH1	2.17	0.60
1:B:289:ASP:OD1	1:B:328:ARG:NH2	2.34	0.60
1:C:46:TRP:HB2	1:C:58:TRP:CD1	2.36	0.60
1:A:200:LYS:HA	1:A:203:TYR:CD2	2.36	0.60
1:B:12:PHE:HB3	1:B:15:LEU:HD12	1.84	0.60
1:C:285:GLU:OE2	1:C:289:ASP:N	2.35	0.60
1:D:228:MET:HG3	1:D:302:VAL:O	2.02	0.59
1:B:219:ILE:HD12	1:B:219:ILE:H	1.66	0.59
1:C:271:ILE:HD11	1:C:342:ILE:HG21	1.84	0.59
1:A:178:LEU:O	1:A:182:ILE:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:GLY:HA2	1:B:363:GLY:HA2	1.84	0.58
1:B:16:LYS:O	1:B:20:ALA:N	2.27	0.58
1:C:79:LEU:HD13	1:C:291:ILE:HD11	1.86	0.58
1:C:287:THR:O	1:C:290:LYS:N	2.36	0.58
1:B:252:ILE:HB	1:B:256:ASN:HB2	1.85	0.57
1:D:38:ASP:HB3	1:D:347:ARG:HH21	1.69	0.57
1:A:60:ARG:O	1:A:262:ARG:NH2	2.37	0.57
1:C:354:MET:HG2	1:C:355:ASN:O	2.04	0.57
1:D:60:ARG:O	1:D:262:ARG:NH2	2.37	0.57
1:A:215:LEU:HD12	1:A:215:LEU:H	1.69	0.57
1:B:10:GLN:N	1:B:10:GLN:OE1	2.38	0.56
1:C:276:LYS:HD3	1:C:281:ARG:HB2	1.87	0.56
1:A:200:LYS:HA	1:A:203:TYR:CE2	2.41	0.55
1:A:250:ALA:O	1:A:256:ASN:ND2	2.38	0.55
1:A:8:CYS:HB2	1:A:45:MET:HE3	1.88	0.55
1:B:378:LEU:O	1:B:378:LEU:CD2	2.52	0.55
1:C:283:LEU:HD22	1:C:287:THR:OG1	2.05	0.55
1:C:176:ARG:CB	1:C:180:ARG:HG2	2.36	0.54
1:C:286:GLU:OE2	1:C:287:THR:HG23	2.07	0.54
1:D:222:LEU:HD21	1:C:228:MET:SD	2.47	0.54
1:C:330:CYS:O	1:C:342:ILE:HG13	2.07	0.54
1:C:276:LYS:HG2	1:C:281:ARG:HH21	1.73	0.54
1:A:73:VAL:HG12	1:A:182:ILE:HD13	1.90	0.54
1:B:250:ALA:O	1:B:256:ASN:ND2	2.41	0.54
1:A:99:GLU:OE1	1:A:99:GLU:N	2.28	0.53
1:C:67:TRP:CD1	1:C:67:TRP:H	2.25	0.53
1:C:277:VAL:H	1:C:280:VAL:CG2	2.21	0.53
1:D:16:LYS:HA	1:D:45:MET:HE1	1.89	0.53
1:B:362:LEU:HD13	1:B:363:GLY:N	2.11	0.53
1:B:35:LEU:HD21	1:B:348:MET:HG2	1.91	0.53
1:D:160:LEU:HD13	1:D:235:PRO:HG2	1.90	0.53
1:D:250:ALA:O	1:D:256:ASN:ND2	2.42	0.52
1:B:219:ILE:C	1:B:222:LEU:H	2.08	0.52
1:C:288:ILE:HG22	1:C:328:ARG:HH22	1.74	0.52
1:D:219:ILE:HD12	1:D:222:LEU:HB2	1.92	0.52
1:D:67:TRP:H	1:D:67:TRP:CD1	2.26	0.52
1:C:68:SER:HB2	1:C:334:GLY:HA2	1.92	0.52
1:D:67:TRP:O	1:D:255:ALA:HA	2.10	0.52
1:C:81:LEU:HD21	1:C:181:PHE:CZ	2.44	0.52
1:B:343:ASP:OD2	1:B:375:TYR:OH	2.25	0.52
1:C:228:MET:HG3	1:C:302:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LEU:HD13	1:B:45:MET:HE2	1.91	0.51
1:B:200:LYS:HA	1:B:203:TYR:CD1	2.46	0.51
1:C:250:ALA:O	1:C:256:ASN:ND2	2.44	0.51
1:C:169:VAL:O	1:C:173:ILE:HG13	2.10	0.51
1:B:190:LEU:HD11	1:B:282:LEU:HD11	1.93	0.51
1:A:354:MET:HG3	1:A:366:ARG:HH21	1.74	0.51
1:C:269:SER:O	1:C:273:CYS:N	2.41	0.51
1:D:338:SER:CA	1:D:354:MET:HE1	2.41	0.50
1:C:284:SER:OG	1:C:285:GLU:N	2.44	0.50
1:B:17:GLU:O	1:B:21:ARG:HG2	2.12	0.50
1:D:222:LEU:HA	1:C:226:ASN:ND2	2.26	0.50
1:D:9:ASP:HB3	1:D:12:PHE:HD2	1.76	0.50
1:B:272:ALA:HB2	1:B:342:ILE:HG23	1.93	0.50
1:D:219:ILE:CD1	1:C:222:LEU:HD11	2.37	0.50
1:B:308:ARG:H	1:B:317:THR:HG21	1.76	0.50
1:C:171:ARG:O	1:C:175:GLY:N	2.38	0.49
1:C:252:ILE:HB	1:C:256:ASN:HB2	1.94	0.49
1:C:316:PRO:HD3	1:C:329:ILE:O	2.11	0.49
1:C:259:SER:OG	1:C:260:ASN:N	2.45	0.49
1:A:193:ASP:OD1	1:A:195:ARG:NH2	2.43	0.49
1:C:176:ARG:HB3	1:C:180:ARG:CG	2.41	0.49
1:B:22:ASN:ND2	1:B:370:TYR:OH	2.44	0.49
1:C:286:GLU:OE2	1:C:286:GLU:C	2.56	0.49
1:C:182:ILE:HD12	1:C:182:ILE:H	1.76	0.49
1:A:63:VAL:O	1:A:206:VAL:HA	2.12	0.49
1:B:219:ILE:O	1:B:221:ALA:N	2.46	0.49
1:C:191:ASP:O	1:C:266:ARG:NH2	2.46	0.48
1:B:219:ILE:HG23	1:B:223:GLY:O	2.13	0.48
1:C:342:ILE:HG22	1:C:349:THR:HG22	1.95	0.48
1:C:125:GLN:HA	1:C:125:GLN:NE2	2.27	0.48
1:B:88:ASP:OD1	1:B:90:ASP:N	2.44	0.48
1:C:344:THR:HG22	1:C:347:ARG:HH21	1.79	0.48
1:D:316:PRO:HD3	1:D:329:ILE:O	2.14	0.48
1:C:84:ARG:HB2	1:C:86:LEU:CD2	2.43	0.48
1:A:67:TRP:O	1:A:255:ALA:HA	2.13	0.47
1:C:80:MET:HE3	1:C:282:LEU:HD11	1.95	0.47
1:C:284:SER:C	1:C:286:GLU:N	2.73	0.47
1:B:4:ILE:HG21	1:B:45:MET:HE3	1.95	0.47
1:C:35:LEU:HD21	1:C:37:ILE:HG13	1.96	0.47
1:C:80:MET:HE2	1:C:181:PHE:HE2	1.80	0.47
1:C:124:ASP:N	1:C:145:GLN:OE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:THR:HA	1:C:347:ARG:HE	1.78	0.47
1:B:346:LYS:HD3	1:B:378:LEU:HD13	1.96	0.47
1:A:67:TRP:H	1:A:67:TRP:CD1	2.31	0.46
1:C:277:VAL:H	1:C:280:VAL:HG22	1.79	0.46
1:B:316:PRO:HD3	1:B:329:ILE:O	2.15	0.46
1:C:74:THR:HG23	1:C:178:LEU:HD21	1.97	0.46
1:B:60:ARG:HG2	1:B:262:ARG:NH2	2.30	0.46
1:C:276:LYS:CD	1:C:281:ARG:HB2	2.46	0.46
1:D:63:VAL:HG12	1:D:260:ASN:ND2	2.29	0.46
1:B:50:VAL:HG22	1:B:56:ALA:O	2.15	0.46
1:C:39:GLY:HA3	1:C:277:VAL:HG21	1.97	0.46
1:D:200:LYS:HA	1:D:203:TYR:CD1	2.50	0.46
1:A:259:SER:OG	1:A:260:ASN:N	2.49	0.46
1:B:64:THR:OG1	1:B:207:SER:O	2.27	0.46
1:B:299:VAL:HA	1:B:306:PRO:HA	1.98	0.46
1:B:328:ARG:HH11	1:B:344:THR:HG21	1.80	0.46
1:A:17:GLU:O	1:A:21:ARG:HG3	2.16	0.46
1:C:67:TRP:O	1:C:255:ALA:HA	2.15	0.46
1:C:141:ARG:HG3	1:C:144:THR:HG21	1.97	0.46
1:C:285:GLU:OE2	1:C:288:ILE:HB	2.16	0.46
1:D:19:LEU:HD23	1:D:45:MET:HE2	1.98	0.46
1:B:76:LEU:O	1:B:80:MET:HG3	2.17	0.45
1:A:316:PRO:HD3	1:A:329:ILE:O	2.17	0.45
1:B:229:VAL:O	1:B:233:THR:HG23	2.16	0.45
1:C:264:LEU:HA	1:C:267:ILE:HG22	1.98	0.45
1:A:80:MET:HE1	1:A:185:GLU:HB3	1.98	0.45
1:D:21:ARG:NH2	1:D:369:GLN:OE1	2.49	0.45
1:D:164:HIS:NE2	1:D:252:ILE:HG23	2.31	0.45
1:C:35:LEU:CD2	1:C:37:ILE:HG13	2.47	0.45
1:D:150:GLU:O	1:D:153:THR:HB	2.17	0.45
1:D:338:SER:N	1:D:354:MET:HE1	2.32	0.45
1:C:88:ASP:HB3	1:C:91:ALA:HB2	1.98	0.45
1:C:60:ARG:HG3	1:C:262:ARG:NH2	2.32	0.45
1:D:68:SER:HB2	1:D:334:GLY:HA2	1.99	0.45
1:B:317:THR:O	1:B:317:THR:OG1	2.32	0.45
1:D:222:LEU:O	1:C:222:LEU:HD21	2.17	0.45
1:C:120:VAL:O	1:C:120:VAL:HG23	2.17	0.44
1:A:168:GLU:OE1	1:A:171:ARG:NH1	2.50	0.44
1:B:93:VAL:HG12	1:B:108:ILE:O	2.18	0.44
1:B:297:TYR:OH	1:B:319:GLU:OE2	2.28	0.44
1:B:288:ILE:HG23	1:B:291:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PRO:HA	1:A:236:PRO:HD3	1.87	0.44
1:A:346:LYS:HE2	1:A:378:LEU:HB3	2.00	0.44
1:B:225:ASP:HA	1:B:230:LYS:HD2	2.00	0.44
1:B:49:TRP:HB3	1:B:51:ASP:H	1.83	0.43
1:C:94:ALA:HA	1:C:97:TRP:O	2.18	0.43
1:C:342:ILE:CD1	1:C:344:THR:HG23	2.48	0.43
1:C:284:SER:C	1:C:286:GLU:H	2.25	0.43
1:A:87:LEU:HD11	1:A:110:VAL:HG11	2.00	0.43
1:C:338:SER:N	1:C:354:MET:HE1	2.33	0.43
1:B:259:SER:OG	1:B:260:ASN:N	2.51	0.43
1:C:105:LYS:HB3	1:C:108:ILE:HD12	2.00	0.43
1:C:210:ILE:HD12	1:C:356:LYS:HB2	2.01	0.43
1:C:344:THR:HA	1:C:347:ARG:NE	2.34	0.43
1:D:224:MET:SD	1:D:224:MET:N	2.91	0.43
1:C:329:ILE:HG23	1:C:342:ILE:O	2.18	0.43
1:B:244:THR:HG23	1:B:247:TRP:H	1.83	0.43
1:B:289:ASP:O	1:B:293:GLU:HG3	2.18	0.43
1:D:81:LEU:HD11	1:D:170:VAL:HG13	2.00	0.43
1:B:219:ILE:O	1:B:220:ALA:C	2.60	0.43
1:C:16:LYS:HA	1:C:45:MET:HE1	2.01	0.43
1:C:226:ASN:OD1	1:C:228:MET:N	2.41	0.43
1:C:276:LYS:HD3	1:C:281:ARG:HE	1.84	0.43
1:C:337:GLY:HA2	1:C:363:GLY:HA2	2.01	0.43
1:B:68:SER:HB2	1:B:333:GLY:O	2.19	0.42
1:C:308:ARG:H	1:C:317:THR:HG21	1.84	0.42
1:C:127:PHE:HD1	1:C:141:ARG:NH2	2.17	0.42
1:B:21:ARG:HG2	1:B:21:ARG:H	1.71	0.42
1:D:281:ARG:NH1	1:D:283:LEU:O	2.52	0.42
1:C:272:ALA:O	1:C:347:ARG:NE	2.53	0.42
1:D:328:ARG:HD3	1:D:344:THR:HG21	2.00	0.42
1:A:106:ASP:OD2	1:C:125:GLN:HG2	2.19	0.42
1:A:171:ARG:HG3	1:A:177:THR:HA	2.02	0.42
1:C:7:VAL:CG1	1:C:44:ASP:HB3	2.49	0.42
1:C:202:GLU:HG2	1:C:205:ARG:NE	2.29	0.42
1:D:93:VAL:HG12	1:D:110:VAL:HA	2.01	0.42
1:B:332:TRP:CE3	1:B:332:TRP:HA	2.54	0.42
1:B:338:SER:HA	1:B:354:MET:HE1	2.01	0.42
1:C:76:LEU:O	1:C:80:MET:HG3	2.20	0.42
1:C:176:ARG:NH2	1:C:185:GLU:OE1	2.47	0.42
1:C:220:ALA:C	1:C:222:LEU:H	2.27	0.42
1:A:107:ARG:HD3	1:C:224:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:THR:HG22	1:C:246:GLY:N	2.35	0.42
1:D:267:ILE:O	1:D:270:VAL:HG22	2.19	0.41
1:B:264:LEU:HB3	1:B:340:ILE:HD13	2.00	0.41
1:C:4:ILE:HG12	1:C:45:MET:HE2	2.02	0.41
1:C:83:ASP:OD1	1:C:283:LEU:HA	2.20	0.41
1:D:338:SER:HA	1:D:354:MET:HE1	2.01	0.41
1:B:45:MET:H	1:B:45:MET:HG2	1.59	0.41
1:C:84:ARG:HB2	1:C:86:LEU:HD21	2.01	0.41
1:D:343:ASP:HB3	1:D:348:MET:HG3	2.02	0.41
1:C:263:ALA:O	1:C:267:ILE:HG22	2.20	0.41
1:B:125:GLN:O	1:B:127:PHE:N	2.54	0.41
1:C:82:VAL:HG12	1:C:87:LEU:O	2.20	0.41
1:A:229:VAL:O	1:A:233:THR:HB	2.20	0.41
1:B:219:ILE:C	1:B:221:ALA:N	2.76	0.41
1:C:50:VAL:HG13	1:C:207:SER:HA	2.03	0.41
1:D:44:ASP:OD2	1:D:262:ARG:HD3	2.20	0.41
1:D:66:VAL:HG22	1:D:257:GLY:O	2.20	0.41
1:A:63:VAL:HG13	1:A:259:SER:N	2.36	0.41
1:B:105:LYS:NZ	1:B:145:GLN:O	2.44	0.41
1:C:334:GLY:N	1:C:338:SER:O	2.54	0.41
1:B:59:SER:OG	1:B:60:ARG:N	2.54	0.40
1:B:193:ASP:OD1	1:B:195:ARG:NH2	2.47	0.40
1:C:277:VAL:N	1:C:280:VAL:HG22	2.37	0.40
1:A:66:VAL:HG22	1:A:257:GLY:O	2.21	0.40
1:C:342:ILE:HD13	1:C:344:THR:HG23	2.04	0.40
1:B:354:MET:HE3	1:B:354:MET:HB3	1.76	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:MET:SD	1:B:224:MET:CE[2_556]	1.79	0.41

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	375/387 (97%)	360 (96%)	15 (4%)	0	100	100
1	B	375/387 (97%)	355 (95%)	20 (5%)	0	100	100
1	C	375/387 (97%)	350 (93%)	23 (6%)	2 (0%)	24	31
1	D	375/387 (97%)	359 (96%)	16 (4%)	0	100	100
All	All	1500/1548 (97%)	1424 (95%)	74 (5%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	177	THR
1	C	126	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	296/305 (97%)	295 (100%)	1 (0%)	86	93
1	B	296/305 (97%)	295 (100%)	1 (0%)	86	93
1	C	296/305 (97%)	296 (100%)	0	100	100
1	D	296/305 (97%)	295 (100%)	1 (0%)	86	93
All	All	1184/1220 (97%)	1181 (100%)	3 (0%)	86	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	17	GLU
1	A	107	ARG
1	B	338	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	95	GLN
1	D	125	GLN
1	D	258	HIS
1	A	54	HIS
1	A	112	GLN
1	A	256	ASN
1	A	258	HIS
1	B	22	ASN
1	B	95	GLN
1	C	54	HIS
1	C	125	GLN
1	C	339	GLN

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	377/387 (97%)	1.11	50 (13%) 7 8	54, 73, 95, 110	0
1	B	377/387 (97%)	1.83	146 (38%) 1 0	63, 92, 124, 145	0
1	C	377/387 (97%)	2.12	170 (45%) 0 0	69, 105, 131, 149	0
1	D	377/387 (97%)	1.08	55 (14%) 6 6	52, 73, 95, 141	0
All	All	1508/1548 (97%)	1.54	421 (27%) 1 1	52, 84, 123, 149	0

All (421) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	222	LEU	8.8
1	D	220	ALA	8.6
1	C	222	LEU	8.2
1	B	362	LEU	7.4
1	C	280	VAL	7.0
1	A	234	ALA	6.8
1	D	221	ALA	6.7
1	D	224	MET	6.6
1	D	234	ALA	6.5
1	C	282	LEU	6.1
1	C	234	ALA	5.9
1	B	49	TRP	5.7
1	C	31	ALA	5.4
1	B	220	ALA	5.4
1	C	287	THR	5.3
1	A	280	VAL	5.2
1	C	277	VAL	5.2
1	B	8	CYS	5.1
1	C	221	ALA	5.0
1	B	234	ALA	4.9
1	C	247	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	126	PRO	4.8
1	D	249	ALA	4.8
1	B	219	ILE	4.8
1	B	344	THR	4.8
1	A	125	GLN	4.8
1	B	221	ALA	4.8
1	D	219	ILE	4.7
1	B	379	SER	4.7
1	D	223	GLY	4.6
1	B	7	VAL	4.6
1	C	177	THR	4.6
1	C	275	GLY	4.6
1	C	47	GLY	4.5
1	B	34	ALA	4.5
1	A	216	PRO	4.5
1	B	378	LEU	4.5
1	B	210	ILE	4.4
1	B	216	PRO	4.4
1	B	5	GLU	4.4
1	C	356	LYS	4.4
1	B	222	LEU	4.4
1	C	342	ILE	4.3
1	C	80	MET	4.3
1	C	181	PHE	4.3
1	A	224	MET	4.3
1	C	273	CYS	4.3
1	B	47	GLY	4.2
1	A	217	ILE	4.2
1	C	81	LEU	4.2
1	C	283	LEU	4.2
1	C	347	ARG	4.2
1	B	50	VAL	4.2
1	B	56	ALA	4.2
1	B	126	PRO	4.2
1	B	4	ILE	4.2
1	A	44	ASP	4.2
1	C	288	ILE	4.1
1	A	126	PRO	4.1
1	C	98	PRO	4.1
1	B	66	VAL	4.1
1	C	199	PRO	4.1
1	C	96	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	125	GLN	4.1
1	B	23	LEU	4.0
1	C	298	GLY	4.0
1	C	189	PRO	4.0
1	B	237	ALA	4.0
1	C	264	LEU	4.0
1	C	285	GLU	4.0
1	B	52	VAL	3.9
1	C	87	LEU	3.9
1	B	278	GLY	3.9
1	C	223	GLY	3.9
1	B	208	ASN	3.9
1	C	284	SER	3.9
1	B	18	ALA	3.9
1	B	235	PRO	3.9
1	C	360	GLY	3.9
1	A	233	THR	3.9
1	C	7	VAL	3.8
1	D	362	LEU	3.8
1	A	215	LEU	3.8
1	A	235	PRO	3.8
1	C	292	PHE	3.8
1	C	278	GLY	3.8
1	B	48	GLY	3.7
1	A	379	SER	3.7
1	C	274	GLY	3.7
1	B	31	ALA	3.7
1	D	126	PRO	3.7
1	C	276	LYS	3.7
1	B	3	ASN	3.6
1	A	31	ALA	3.6
1	C	125	GLN	3.6
1	B	55	THR	3.6
1	B	106	ASP	3.6
1	C	103	ALA	3.6
1	B	353	VAL	3.5
1	A	221	ALA	3.5
1	B	298	GLY	3.5
1	C	6	GLY	3.5
1	C	266	ARG	3.5
1	C	4	ILE	3.5
1	A	219	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	315	LEU	3.5
1	C	50	VAL	3.4
1	C	60	ARG	3.4
1	B	224	MET	3.4
1	C	377	ALA	3.4
1	B	39	GLY	3.4
1	B	46	TRP	3.4
1	B	186	ILE	3.4
1	C	279	ASP	3.4
1	B	57	PRO	3.4
1	C	354	MET	3.4
1	D	360	GLY	3.4
1	A	129	LEU	3.4
1	C	79	LEU	3.4
1	D	58	TRP	3.4
1	B	361	LEU	3.3
1	C	271	ILE	3.3
1	C	67	TRP	3.3
1	D	379	SER	3.3
1	B	339	GLN	3.3
1	B	327	GLY	3.3
1	C	46	TRP	3.3
1	C	41	SER	3.3
1	C	66	VAL	3.3
1	C	311	VAL	3.3
1	C	183	ASP	3.3
1	C	182	ILE	3.3
1	B	287	THR	3.3
1	B	241	GLY	3.3
1	D	215	LEU	3.2
1	C	291	ILE	3.2
1	D	46	TRP	3.2
1	C	34	ALA	3.2
1	D	250	ALA	3.2
1	B	223	GLY	3.2
1	D	285	GLU	3.2
1	C	219	ILE	3.2
1	C	55	THR	3.2
1	B	360	GLY	3.2
1	C	64	THR	3.2
1	C	281	ARG	3.1
1	B	269	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	285	GLU	3.1
1	B	211	ALA	3.1
1	B	217	ILE	3.1
1	D	344	THR	3.1
1	C	355	ASN	3.1
1	C	63	VAL	3.1
1	B	328	ARG	3.1
1	B	352	TYR	3.1
1	C	200	LYS	3.1
1	C	309	PHE	3.1
1	C	352	TYR	3.0
1	C	379	SER	3.0
1	B	32	ALA	3.0
1	A	58	TRP	3.0
1	C	259	SER	3.0
1	C	84	ARG	3.0
1	A	199	PRO	3.0
1	B	354	MET	3.0
1	B	277	VAL	3.0
1	B	299	VAL	3.0
1	D	256	ASN	3.0
1	C	97	TRP	3.0
1	C	235	PRO	3.0
1	C	345	GLU	3.0
1	B	10	GLN	3.0
1	B	284	SER	3.0
1	C	257	GLY	3.0
1	A	222	LEU	2.9
1	A	362	LEU	2.9
1	D	63	VAL	2.9
1	B	218	ASP	2.9
1	B	58	TRP	2.9
1	C	94	ALA	2.9
1	A	52	VAL	2.9
1	C	82	VAL	2.9
1	B	33	ILE	2.9
1	D	38	ASP	2.9
1	C	359	PRO	2.9
1	C	12	PHE	2.9
1	B	340	ILE	2.9
1	A	361	LEU	2.9
1	B	12	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	280	VAL	2.9
1	C	297	TYR	2.8
1	C	142	LEU	2.8
1	A	63	VAL	2.8
1	B	29	VAL	2.8
1	D	4	ILE	2.8
1	C	88	ASP	2.8
1	B	107	ARG	2.8
1	B	207	SER	2.8
1	B	359	PRO	2.8
1	C	196	LEU	2.8
1	C	270	VAL	2.8
1	B	346	LYS	2.8
1	B	64	THR	2.8
1	B	273	CYS	2.8
1	A	203	TYR	2.8
1	C	178	LEU	2.8
1	A	47	GLY	2.7
1	C	99	GLU	2.7
1	A	237	ALA	2.7
1	B	279	ASP	2.7
1	C	3	ASN	2.7
1	C	36	THR	2.7
1	C	179	GLY	2.7
1	B	242	SER	2.7
1	C	100	PHE	2.7
1	C	313	PHE	2.7
1	C	24	ASP	2.7
1	B	363	GLY	2.7
1	C	217	ILE	2.7
1	C	327	GLY	2.7
1	B	35	LEU	2.7
1	C	86	LEU	2.7
1	C	190	LEU	2.7
1	D	31	ALA	2.7
1	B	158	HIS	2.7
1	C	138	ALA	2.7
1	D	226	ASN	2.7
1	A	256	ASN	2.7
1	B	24	ASP	2.7
1	C	205	ARG	2.7
1	A	282	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	10	GLN	2.6
1	B	370	TYR	2.6
1	A	251	GLU	2.6
1	D	93	VAL	2.6
1	B	256	ASN	2.6
1	B	260	ASN	2.6
1	C	173	ILE	2.6
1	C	296	SER	2.6
1	A	49	TRP	2.6
1	C	32	ALA	2.6
1	C	146	ALA	2.6
1	B	375	TYR	2.6
1	B	30	GLY	2.6
1	C	85	GLY	2.6
1	D	130	GLU	2.6
1	C	176	ARG	2.6
1	B	44	ASP	2.6
1	B	214	PRO	2.6
1	B	342	ILE	2.6
1	B	215	LEU	2.6
1	C	83	ASP	2.6
1	C	30	GLY	2.6
1	D	277	VAL	2.6
1	C	52	VAL	2.6
1	C	329	ILE	2.6
1	B	264	LEU	2.5
1	C	172	ARG	2.5
1	A	34	ALA	2.5
1	C	8	CYS	2.5
1	C	20	ALA	2.5
1	C	133	CYS	2.5
1	B	247	TRP	2.5
1	B	350	PHE	2.5
1	C	144	THR	2.5
1	D	66	VAL	2.5
1	B	351	SER	2.5
1	C	29	VAL	2.5
1	C	267	ILE	2.5
1	B	129	LEU	2.5
1	B	192	ALA	2.5
1	C	260	ASN	2.5
1	C	289	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	278	GLY	2.5
1	B	14	GLY	2.5
1	C	58	TRP	2.5
1	B	206	VAL	2.5
1	C	209	VAL	2.5
1	C	180	ARG	2.5
1	C	226	ASN	2.5
1	B	62	THR	2.5
1	B	41	SER	2.5
1	A	107	ARG	2.5
1	B	63	VAL	2.5
1	B	288	ILE	2.5
1	A	3	ASN	2.5
1	B	289	ASP	2.5
1	B	239	ALA	2.5
1	C	255	ALA	2.5
1	D	257	GLY	2.5
1	B	43	VAL	2.4
1	B	333	GLY	2.4
1	C	141	ARG	2.4
1	C	246	GLY	2.4
1	C	244	THR	2.4
1	B	267	ILE	2.4
1	C	42	VAL	2.4
1	C	232	PHE	2.4
1	C	348	MET	2.4
1	A	198	LEU	2.4
1	B	19	LEU	2.4
1	C	203	TYR	2.4
1	C	220	ALA	2.4
1	C	49	TRP	2.4
1	B	203	TYR	2.4
1	A	130	GLU	2.4
1	C	57	PRO	2.4
1	A	360	GLY	2.4
1	C	192	ALA	2.4
1	C	333	GLY	2.4
1	B	349	THR	2.4
1	B	348	MET	2.4
1	C	361	LEU	2.4
1	A	218	ASP	2.3
1	C	370	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	276	LYS	2.3
1	D	348	MET	2.3
1	C	194	PHE	2.3
1	C	362	LEU	2.3
1	B	297	TYR	2.3
1	D	217	ILE	2.3
1	C	268	GLN	2.3
1	D	129	LEU	2.3
1	D	361	LEU	2.3
1	D	3	ASN	2.3
1	D	279	ASP	2.3
1	C	92	PRO	2.3
1	B	332	TRP	2.3
1	B	377	ALA	2.3
1	B	281	ARG	2.3
1	C	252	ILE	2.3
1	B	280	VAL	2.3
1	A	200	LYS	2.3
1	C	160	LEU	2.3
1	C	198	LEU	2.3
1	B	193	ASP	2.3
1	C	336	GLY	2.3
1	A	46	TRP	2.3
1	A	180	ARG	2.3
1	B	11	ARG	2.3
1	B	263	ALA	2.3
1	C	335	TRP	2.3
1	B	36	THR	2.3
1	B	329	ILE	2.3
1	D	127	PHE	2.2
1	B	194	PHE	2.2
1	D	359	PRO	2.2
1	D	6	GLY	2.2
1	B	80	MET	2.2
1	B	347	ARG	2.2
1	A	55	THR	2.2
1	B	271	ILE	2.2
1	A	277	VAL	2.2
1	B	170	VAL	2.2
1	D	347	ARG	2.2
1	B	259	SER	2.2
1	B	190	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	169	VAL	2.2
1	C	307	VAL	2.2
1	C	253	GLY	2.2
1	C	330	CYS	2.2
1	B	17	GLU	2.2
1	D	240	THR	2.2
1	B	373	ALA	2.2
1	D	183	ASP	2.2
1	B	246	GLY	2.2
1	B	257	GLY	2.2
1	C	104	GLY	2.2
1	C	175	GLY	2.2
1	C	233	THR	2.2
1	C	250	ALA	2.2
1	D	203	TYR	2.1
1	C	148	TRP	2.1
1	D	52	VAL	2.1
1	D	229	VAL	2.1
1	B	54	HIS	2.1
1	B	68	SER	2.1
1	B	254	ALA	2.1
1	C	59	SER	2.1
1	C	344	THR	2.1
1	B	324	ILE	2.1
1	C	108	ILE	2.1
1	D	225	ASP	2.1
1	A	124	ASP	2.1
1	B	270	VAL	2.1
1	C	164	HIS	2.1
1	B	6	GLY	2.1
1	C	317	THR	2.1
1	D	32	ALA	2.1
1	B	160	LEU	2.1
1	B	282	LEU	2.1
1	C	130	GLU	2.1
1	C	132	ILE	2.1
1	D	353	VAL	2.1
1	A	236	PRO	2.1
1	A	347	ARG	2.1
1	B	69	CYS	2.1
1	C	239	ALA	2.1
1	D	354	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	45	MET	2.1
1	B	45	MET	2.1
1	C	286	GLU	2.1
1	B	37	ILE	2.1
1	C	353	VAL	2.1
1	B	21	ARG	2.1
1	A	276	LYS	2.0
1	D	239	ALA	2.0
1	A	18	ALA	2.0
1	C	228	MET	2.0
1	C	249	ALA	2.0
1	C	365	GLU	2.0
1	A	10	GLN	2.0
1	B	9	ASP	2.0
1	B	183	ASP	2.0
1	B	198	LEU	2.0
1	D	33	ILE	2.0
1	D	235	PRO	2.0
1	C	137	TYR	2.0
1	A	206	VAL	2.0
1	C	366	ARG	2.0
1	B	150	GLU	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.