



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:05 AM GMT

PDB ID : 2PC4
Title : Crystal structure of fructose-bisphosphate aldolase from Plasmodium falciparum in complex with TRAP-tail determined at 2.4 angstrom resolution
Authors : Bosch, J.; Buscaglia, C.A.; Krumm, B.; Cardozo, T.; Nussenzweig, V.; Hol, W.G.J.; Structural Genomics of Pathogenic Protozoa Consortium (SGPP)
Deposited on : 2007-03-29
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

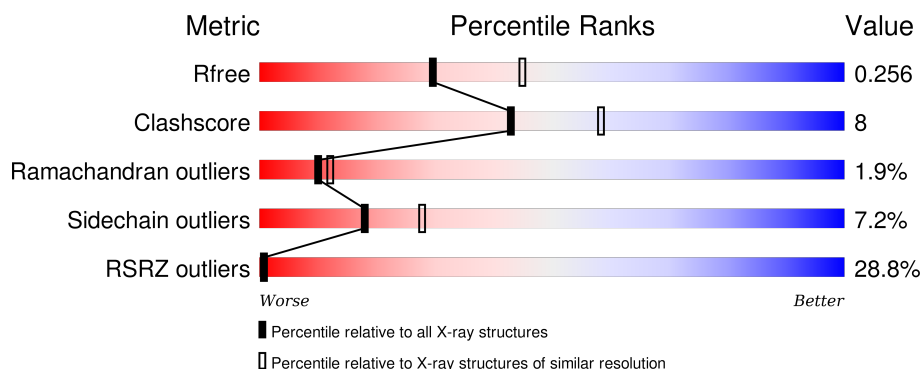
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	369	<div> <div>29%</div> <div>79%</div> <div>16%</div> <div>• •</div> </div>
1	B	369	<div> <div>30%</div> <div>73%</div> <div>18%</div> <div>• 5%</div> </div>
1	C	369	<div> <div>27%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	D	369	<div> <div>25%</div> <div>74%</div> <div>18%</div> <div>• • 5%</div> </div>
2	H	6	<div> <div>17%</div> <div>50%</div> <div>50%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11457 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 Fructose-bisphosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	1	0
			2749	1741	476	522	10			
1	B	351	Total	C	N	O	S	0	2	0
			2688	1702	466	510	10			
1	C	365	Total	C	N	O	S	0	1	0
			2781	1757	484	530	10			
1	D	351	Total	C	N	O	S	0	2	0
			2689	1702	467	510	10			

- Molecule 2 is a protein called PbTRAP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	3	Total	C	N	O	0	0	0
			31	19	5	7			

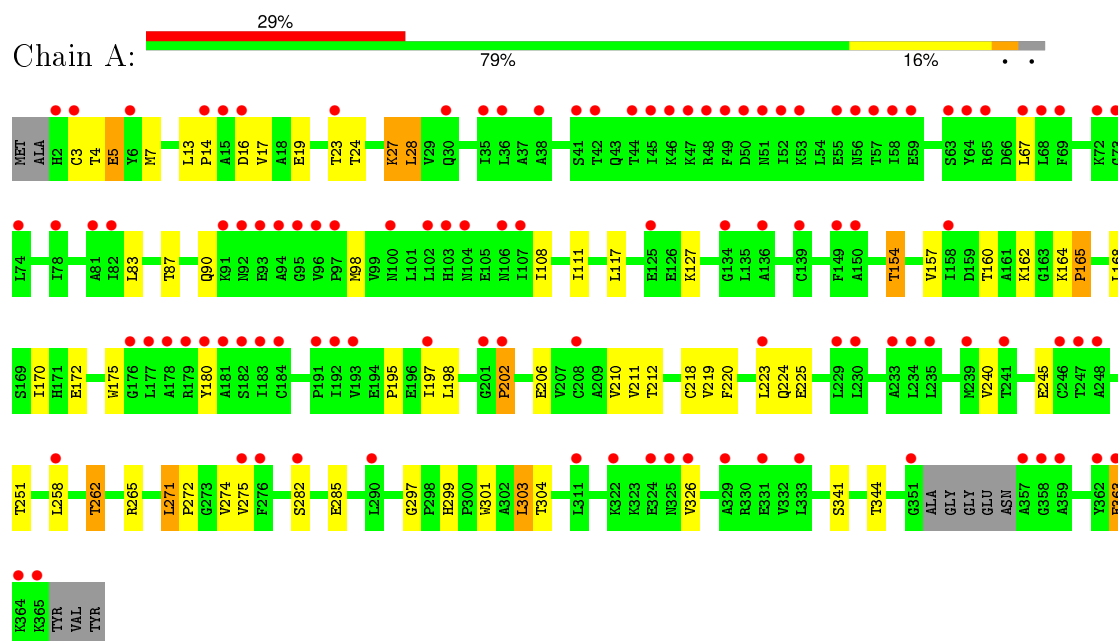
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		
3	B	131	Total	O	0	0
			131	131		
3	C	134	Total	O	0	0
			134	134		
3	D	125	Total	O	0	0
			125	125		
3	H	2	Total	O	0	0
			2	2		

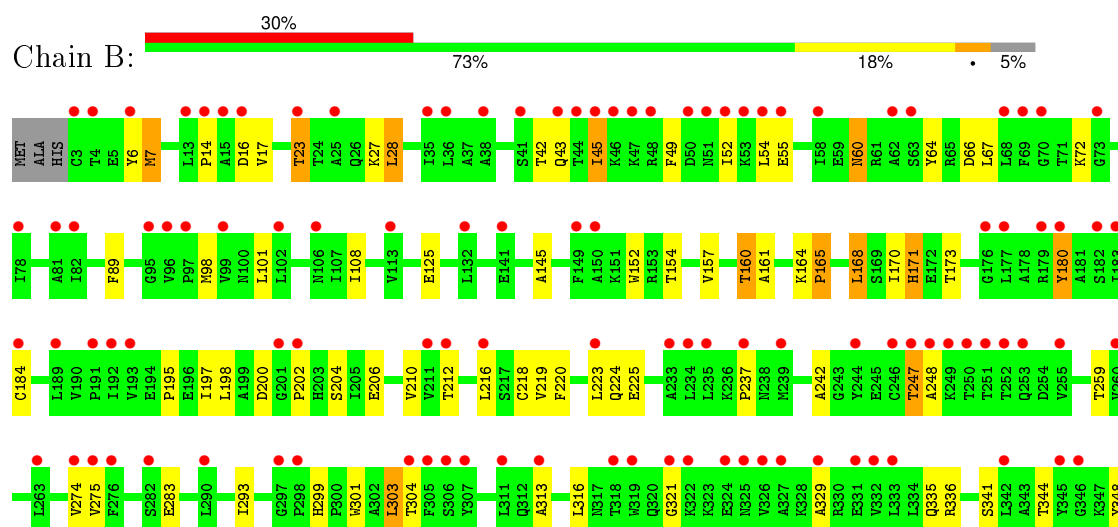
3 Residue-property plots [i](#)

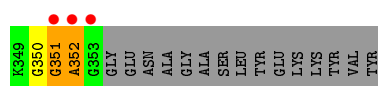
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Fructose-bisphosphate aldolase

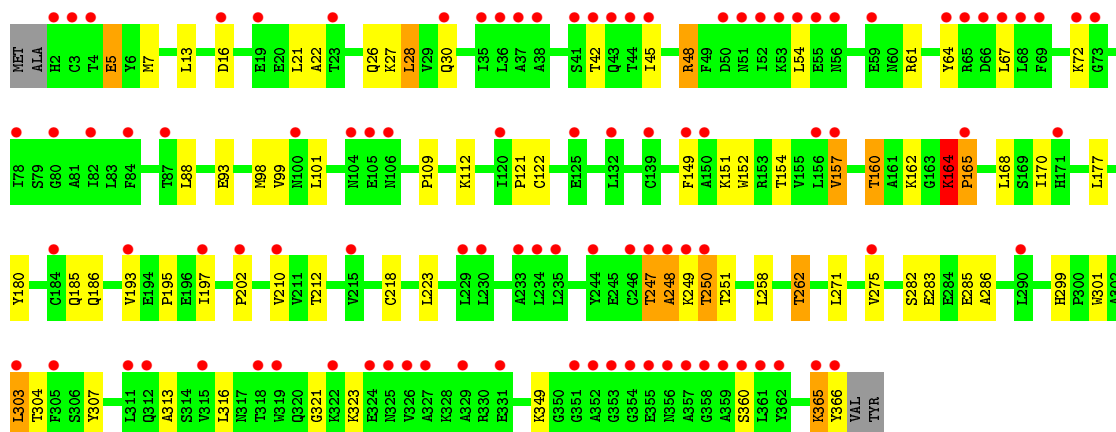
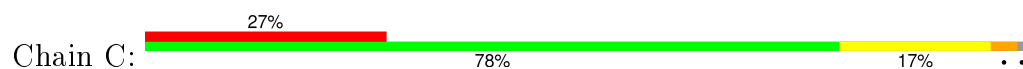


• Molecule 1: Fructose-bisphosphate aldolase

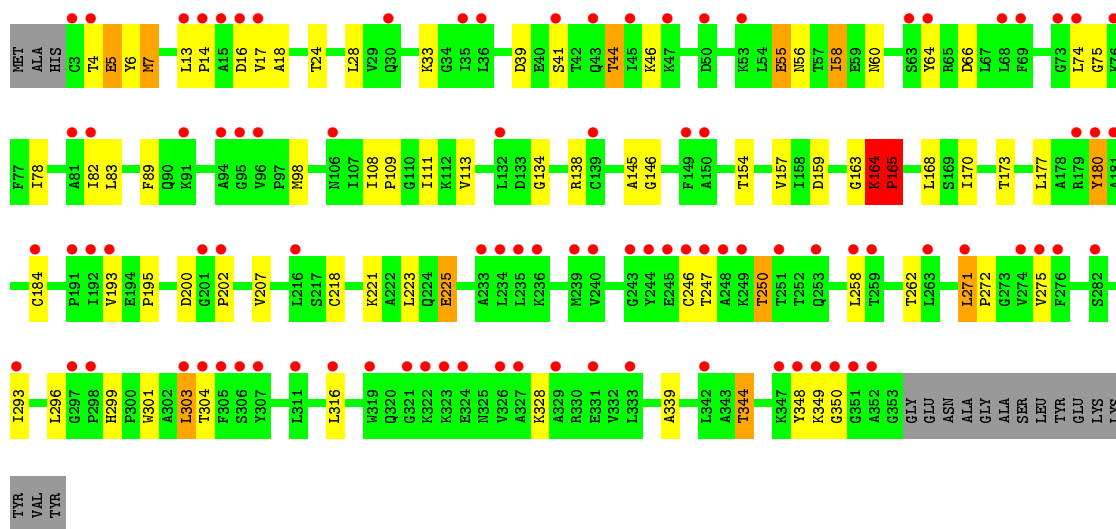




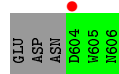
• Molecule 1: Fructose-bisphosphate aldolase



• Molecule 1: Fructose-bisphosphate aldolase



• Molecule 2: PbTRAP



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.39Å 145.52Å 148.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.40 25.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.7 (19.97-2.40) 91.1 (25.61-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.250 0.205 , 0.256	Depositor DCC
R_{free} test set	2910 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.6	EDS
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 62422 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11457	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.43	0/2798	0.55	0/3788
1	B	0.42	0/2740	0.58	0/3713
1	C	0.42	0/2831	0.57	0/3837
1	D	0.42	0/2740	0.56	0/3712
2	H	0.45	0/32	0.45	0/42
All	All	0.42	0/11141	0.56	0/15092

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	3
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	LYS	Peptide
1	A	297	GLY	Peptide
1	A	363	GLU	Peptide
1	B	164	LYS	Peptide
1	C	164	LYS	Peptide
1	C	249	LYS	Peptide
1	D	164	LYS	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	2749	0	2805	43	0
1	B	2688	0	2744	56	0
1	C	2781	0	2811	42	0
1	D	2689	0	2750	52	0
2	H	31	0	19	0	0
3	A	127	0	0	3	0
3	B	131	0	0	6	0
3	C	134	0	0	6	0
3	D	125	0	0	3	0
3	H	2	0	0	0	0
All	All	11457	0	11129	180	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 (180) 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:204:SER:HA	1:B:247:THR:HG21	1.26	1.10
1:D:157:VAL:O	1:D:165:PRO:HD3	1.51	1.10
1:C:258:LEU:O	1:C:262:THR:HG23	1.54	1.08
1:A:258:LEU:O	1:A:262:THR:HG23	1.66	0.95
1:B:157:VAL:O	1:B:165:PRO:CD	2.17	0.92
1:B:157:VAL:O	1:B:165:PRO:HD3	1.70	0.91
1:C:250:THR:HG21	3:C:401:HOH:O	1.77	0.84
1:D:262:THR:HG22	3:D:383:HOH:O	1.82	0.79
1:B:6:TYR:HA	1:C:160:THR:HG22	1.70	0.73
1:B:157:VAL:O	1:B:165:PRO:HD2	1.87	0.73
1:B:170:ILE:HG22	1:B:218:CYS:SG	2.32	0.69
1:D:275:VAL:HG12	1:D:304:THR:HG23	1.73	0.69
1:A:258:LEU:O	1:A:262:THR:CG2	2.42	0.68
1:B:219:VAL:O	1:B:223:LEU:HD13	1.95	0.67
1:A:90:GLN:HB3	1:A:98:MET:HE2	1.76	0.67
1:C:262:THR:HG22	3:C:388:HOH:O	1.94	0.67
1:C:157:VAL:O	1:C:164:LYS:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:HIS:CD2	1:D:303:LEU:HD22	2.30	0.66
1:B:242:ALA:HB1	1:B:247:THR:HG22	1.77	0.66
1:D:164:LYS:O	1:D:165:PRO:C	2.34	0.66
1:D:177:LEU:HD22	1:D:193:VAL:HG13	1.78	0.65
1:B:160:THR:HG23	1:C:5:GLU:O	1.97	0.64
1:A:23:THR:HG23	1:A:27:LYS:NZ	2.13	0.64
1:D:250:THR:O	1:D:250:THR:HG23	1.97	0.64
1:D:163:GLY:O	1:D:164:LYS:O	2.15	0.63
1:D:55:GLU:O	1:D:60:ASN:ND2	2.30	0.63
1:A:14:PRO:HB2	1:A:17:VAL:HG12	1.82	0.62
1:A:154:THR:HG22	3:A:370:HOH:O	1.99	0.62
1:A:165:PRO:HD2	1:D:6:TYR:CE1	2.35	0.62
1:B:23:THR:HG21	3:B:375:HOH:O	2.00	0.62
1:A:160:THR:HG21	1:D:4:THR:O	2.00	0.61
1:A:5:GLU:HB2	1:D:207:VAL:HG22	1.82	0.61
1:B:161:ALA:HB2	3:B:452:HOH:O	2.00	0.61
1:B:299:HIS:CD2	1:B:303:LEU:HD22	2.36	0.60
1:A:87:THR:HG23	1:A:98:MET:CE	2.32	0.60
1:A:157:VAL:HG22	1:A:198:LEU:HD12	1.82	0.60
1:B:351:GLY:O	1:B:352:ALA:CB	2.50	0.60
1:D:66:ASP:HA	1:D:98:MET:HE1	1.84	0.60
1:B:54:LEU:HD23	1:B:60:ASN:HD21	1.65	0.59
1:B:6:TYR:CE1	1:C:165:PRO:HD2	2.37	0.59
1:A:271:LEU:HD22	1:A:272:PRO:HD2	1.85	0.59
1:B:242:ALA:HB1	1:B:247:THR:CG2	2.33	0.58
1:B:154:THR:HG21	3:B:369:HOH:O	2.03	0.58
1:C:13:LEU:HD21	3:C:395:HOH:O	2.03	0.58
1:D:299:HIS:CG	1:D:303:LEU:HD22	2.40	0.57
1:A:170:ILE:HG22	1:A:218:CYS:SG	2.44	0.57
1:B:275:VAL:HG12	1:B:304:THR:HG23	1.85	0.57
1:B:28:LEU:HD13	1:B:108:ILE:HD12	1.87	0.57
1:D:154:THR:HG21	3:D:369:HOH:O	2.05	0.56
1:A:23:THR:HG23	1:A:27:LYS:HZ3	1.70	0.56
1:A:299:HIS:CD2	1:A:303:LEU:HD22	2.41	0.56
1:C:64:TYR:CZ	1:C:316:LEU:HD13	2.40	0.56
1:B:54:LEU:HD21	1:B:321:GLY:HA3	1.87	0.55
1:C:54:LEU:HD22	1:C:321:GLY:HA3	1.89	0.55
1:B:168:LEU:HA	1:B:171[A]:HIS:CE1	2.42	0.55
1:D:33:LYS:HE2	1:D:75:GLY:O	2.07	0.54
1:D:41:SER:OG	1:D:44:THR:HG23	2.08	0.54
1:C:88:LEU:HD12	1:C:99:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:THR:O	1:C:248:ALA:HB2	2.07	0.54
1:A:117:LEU:HD22	1:A:127:LYS:HB3	1.90	0.53
1:B:206:GLU:O	1:B:210:VAL:HG23	2.09	0.53
1:D:271:LEU:HD22	1:D:272:PRO:HD2	1.92	0.52
3:B:373:HOH:O	1:C:210:VAL:HG21	2.10	0.52
1:C:48:ARG:HB3	1:C:316:LEU:HD21	1.91	0.51
1:A:157:VAL:CG2	1:A:198:LEU:HD12	2.39	0.51
1:B:98:MET:CE	1:B:101:LEU:HD12	2.40	0.51
1:A:13:LEU:HD11	3:A:403:HOH:O	2.10	0.51
1:C:28:LEU:HD21	1:C:149:PHE:CD1	2.46	0.51
1:B:66:ASP:HA	1:B:98:MET:HE1	1.93	0.51
1:A:87:THR:HG23	1:A:98:MET:HE1	1.92	0.50
1:C:152:TRP:CD1	1:C:177:LEU:HD23	2.47	0.50
1:B:299:HIS:CG	1:B:303:LEU:HD22	2.46	0.50
1:C:170:ILE:HG22	1:C:218:CYS:SG	2.51	0.50
1:A:282:SER:OG	1:A:285:GLU:HG2	2.11	0.50
1:B:52:ILE:HD12	1:B:54:LEU:HD13	1.93	0.50
1:D:74:LEU:HD11	1:D:78:ILE:HD12	1.94	0.50
1:D:170:ILE:HG22	1:D:218:CYS:SG	2.52	0.50
1:C:42:THR:HG23	1:C:61:ARG:NH1	2.27	0.50
1:C:365:LYS:O	1:C:366:TYR:CB	2.60	0.49
1:C:283:GLU:CD	1:C:313:ALA:HB3	2.32	0.49
1:D:109:PRO:HG2	1:D:146:GLY:O	2.13	0.49
1:C:299:HIS:CD2	1:C:303:LEU:HD22	2.48	0.49
1:A:162:LYS:C	1:B:7:MET:HG2	2.33	0.49
1:D:24:THR:O	1:D:28:LEU:HD13	2.12	0.49
1:D:154:THR:OG1	1:D:173:THR:HG23	2.13	0.49
1:C:64:TYR:CE1	1:C:316:LEU:HD13	2.48	0.49
1:A:219:VAL:O	1:A:223:LEU:HD13	2.14	0.48
1:C:286:ALA:HB1	1:C:307:TYR:CE2	2.47	0.48
1:B:348:TYR:CZ	1:B:350:GLY:HA2	2.48	0.48
1:D:66:ASP:CA	1:D:98:MET:HE1	2.43	0.48
1:D:39:ASP:HB3	1:D:82:ILE:HG22	1.96	0.48
1:D:344:THR:CG2	3:D:370:HOH:O	2.62	0.48
1:B:23:THR:HG22	3:B:424:HOH:O	2.13	0.48
1:D:258:LEU:O	1:D:262:THR:HG23	2.13	0.48
1:B:98:MET:HE1	1:B:101:LEU:HD12	1.96	0.48
1:A:202:PRO:HD2	3:A:456:HOH:O	2.14	0.47
1:D:339:ALA:HB1	1:D:348:TYR:CE1	2.49	0.47
1:C:162:LYS:C	1:D:7:MET:HG2	2.33	0.47
1:B:45:ILE:HD11	1:B:49:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:SER:HA	1:B:247:THR:CG2	2.19	0.47
1:D:293:ILE:HG22	1:D:303:LEU:HD23	1.96	0.47
1:C:275:VAL:HG12	1:C:304:THR:HG23	1.96	0.47
1:C:247:THR:O	1:C:248:ALA:CB	2.62	0.47
1:D:14:PRO:HB2	1:D:17:VAL:HG12	1.96	0.47
1:C:98:MET:HA	1:C:101:LEU:HD12	1.97	0.47
1:B:67:LEU:HD11	1:B:329:ALA:CB	2.45	0.46
1:C:27:LYS:HA	1:C:30:GLN:HG3	1.97	0.46
1:D:89:PHE:CE1	1:D:145:ALA:HB2	2.51	0.46
1:C:22:ALA:O	1:C:26:GLN:HG2	2.16	0.46
1:A:67:LEU:HD12	1:A:326:VAL:HG22	1.98	0.46
1:C:282:SER:OG	1:C:285:GLU:HG2	2.16	0.46
1:C:112:LYS:NZ	3:C:374:HOH:O	2.48	0.46
1:C:177:LEU:HD22	1:C:193:VAL:HG13	1.98	0.46
1:D:164:LYS:HB3	1:D:165:PRO:CD	2.46	0.46
1:B:64:TYR:OH	1:B:316:LEU:HD22	2.16	0.46
1:A:28:LEU:HD13	1:A:108:ILE:HD12	1.99	0.45
1:B:247:THR:O	1:B:247:THR:HG23	2.15	0.45
1:D:64:TYR:CE1	1:D:316:LEU:HD12	2.51	0.45
1:C:67:LEU:HD23	1:C:67:LEU:C	2.37	0.45
1:B:198:LEU:HB3	1:B:200:ASP:OD2	2.16	0.45
1:C:154:THR:HG21	3:C:371:HOH:O	2.16	0.45
1:B:220:PHE:O	1:B:224:GLN:HG2	2.17	0.45
1:D:74:LEU:CD1	1:D:78:ILE:HD12	2.46	0.44
1:B:67:LEU:HD11	1:B:329:ALA:HB3	1.99	0.44
1:B:64:TYR:OH	1:B:316:LEU:CD2	2.65	0.44
1:B:283:GLU:OE2	1:B:313:ALA:HB3	2.18	0.44
1:B:180:TYR:CE1	1:B:184:CYS:SG	3.10	0.44
1:D:28:LEU:HD12	1:D:108:ILE:HD12	1.99	0.44
1:A:83:LEU:O	1:A:111:ILE:HD12	2.18	0.44
1:C:197:ILE:CD1	1:C:212:THR:HA	2.48	0.44
1:A:275:VAL:HG12	1:A:304:THR:HG23	1.99	0.44
1:C:275:VAL:O	1:C:275:VAL:HG23	2.18	0.44
1:B:275:VAL:O	1:B:275:VAL:HG23	2.17	0.44
1:D:113:VAL:O	1:D:138[B]:ARG:NH2	2.51	0.44
1:A:240:VAL:HG21	1:A:262:THR:HG21	2.00	0.44
1:A:206:GLU:O	1:A:210:VAL:HG23	2.18	0.43
1:C:21:LEU:HD13	1:C:185:GLN:HG2	1.99	0.43
1:A:175:TRP:HH2	1:B:171[A]:HIS:CE1	2.36	0.43
1:A:197:ILE:CD1	1:A:212:THR:HA	2.49	0.43
1:B:237:PRO:HD3	1:B:274:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:HG21	1:D:4:THR:HG23	2.01	0.43
1:A:220:PHE:O	1:A:224:GLN:HG2	2.19	0.43
1:B:54:LEU:CD2	1:B:321:GLY:HA3	2.49	0.43
1:A:341:SER:O	1:A:344:THR:HB	2.18	0.43
1:D:159:ASP:HB3	1:D:164:LYS:HB2	2.01	0.43
1:A:165:PRO:HG2	1:A:211:VAL:HG13	2.01	0.43
1:B:154:THR:OG1	1:B:173:THR:HG23	2.18	0.43
1:C:299:HIS:CG	1:C:303:LEU:HD22	2.53	0.43
1:C:121:PRO:O	1:C:122:CYS:HB2	2.19	0.43
1:A:274:VAL:HB	1:A:303:LEU:HD12	2.01	0.42
3:B:437:HOH:O	1:C:210:VAL:HG22	2.19	0.42
1:B:14:PRO:HG2	1:B:17:VAL:HG22	2.00	0.42
1:A:275:VAL:O	1:A:275:VAL:HG23	2.19	0.42
1:C:45:ILE:HG21	1:C:61:ARG:HD3	2.01	0.42
1:B:216:LEU:HA	1:B:216:LEU:HD23	1.91	0.42
1:B:64:TYR:CE1	1:B:316:LEU:HD13	2.55	0.42
1:B:259:THR:HB	1:B:293:ILE:CD1	2.50	0.42
1:A:160:THR:CG2	1:D:5:GLU:O	2.68	0.42
1:B:42:THR:HA	1:B:45:ILE:HG22	2.02	0.42
1:B:341:SER:O	1:B:344:THR:HB	2.20	0.42
1:D:46:LYS:HD2	1:D:56:ASN:HD22	1.85	0.41
1:A:165:PRO:CD	1:D:6:TYR:CE1	3.03	0.41
1:A:24:THR:HG22	1:A:28:LEU:HD22	2.01	0.41
1:D:163:GLY:C	1:D:164:LYS:O	2.57	0.41
1:D:159:ASP:H	1:D:164:LYS:HB2	1.84	0.41
1:C:164:LYS:NZ	3:C:446:HOH:O	2.50	0.41
1:A:299:HIS:CG	1:A:303:LEU:HD22	2.56	0.41
1:D:180:TYR:CE1	1:D:184:CYS:SG	3.14	0.41
1:B:89:PHE:CE1	1:B:145:ALA:HB2	2.56	0.41
1:A:160:THR:HG23	1:D:5:GLU:O	2.21	0.41
1:D:58:ILE:O	1:D:58:ILE:HD13	2.21	0.41
1:D:28:LEU:CD1	1:D:108:ILE:HD12	2.51	0.40
1:B:152:TRP:HB3	1:B:180:TYR:CE2	2.56	0.40
1:D:134:GLY:O	1:D:138[A]:ARG:HG3	2.21	0.40
1:A:23:THR:HG23	1:A:27:LYS:HZ2	1.84	0.40
1:D:13:LEU:HB2	1:D:18:ALA:HB2	2.03	0.40
1:B:351:GLY:O	1:B:352:ALA:HB3	2.22	0.40
1:B:197:ILE:CD1	1:B:212:THR:HA	2.51	0.40
1:D:83:LEU:O	1:D:111:ILE:HD12	2.21	0.40
1:D:221:LYS:NZ	1:D:225:GLU:OE1	2.49	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	356/369 (96%)	334 (94%)	18 (5%)	4 (1%)	17	25
1	B	351/369 (95%)	326 (93%)	17 (5%)	8 (2%)	8	8
1	C	364/369 (99%)	336 (92%)	22 (6%)	6 (2%)	12	16
1	D	351/369 (95%)	326 (93%)	16 (5%)	9 (3%)	7	6
2	H	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1423/1482 (96%)	1323 (93%)	73 (5%)	27 (2%)	10	12

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	B	165	PRO
1	B	247	THR
1	B	352	ALA
1	C	247	THR
1	C	248	ALA
1	C	365	LYS
1	D	164	LYS
1	D	349	LYS
1	A	165	PRO
1	C	165	PRO
1	D	165	PRO
1	B	351	GLY
1	D	246	CYS
1	B	248	ALA
1	D	250	THR
1	D	350	GLY
1	B	160	THR
1	C	202	PRO
1	D	296	LEU
1	B	195	PRO

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Mol	Chain	Res	Type
1	D	195	PRO
1	A	195	PRO
1	B	202	PRO
1	C	195	PRO
1	A	202	PRO
1	D	202	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	293/298 (98%)	273 (93%)	20 (7%)	20	31
1	B	287/298 (96%)	267 (93%)	20 (7%)	19	29
1	C	293/298 (98%)	268 (92%)	25 (8%)	13	20
1	D	287/298 (96%)	268 (93%)	19 (7%)	21	32
2	H	3/6 (50%)	3 (100%)	0	100	100
All	All	1163/1198 (97%)	1079 (93%)	84 (7%)	18	28

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	CYS
1	A	5	GLU
1	A	7	MET
1	A	16	ASP
1	A	19	GLU
1	A	27	LYS
1	A	28	LEU
1	A	154	THR
1	A	168	LEU
1	A	172	GLU
1	A	180	TYR
1	A	225	GLU
1	A	245	GLU

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Mol	Chain	Res	Type
1	A	251	THR
1	A	262	THR
1	A	265	ARG
1	A	271	LEU
1	A	301	TRP
1	A	303	LEU
1	A	363	GLU
1	B	7	MET
1	B	16	ASP
1	B	23	THR
1	B	27	LYS
1	B	28	LEU
1	B	43	GLN
1	B	45	ILE
1	B	55	GLU
1	B	60	ASN
1	B	72	LYS
1	B	125	GLU
1	B	168	LEU
1	B	171[A]	HIS
1	B	171[B]	HIS
1	B	180	TYR
1	B	225	GLU
1	B	301	TRP
1	B	303	LEU
1	B	335	GLN
1	B	336	ARG
1	C	5	GLU
1	C	7	MET
1	C	16	ASP
1	C	28	LEU
1	C	48	ARG
1	C	72	LYS
1	C	93	GLU
1	C	109	PRO
1	C	151	LYS
1	C	157	VAL
1	C	160	THR
1	C	164	LYS
1	C	168	LEU
1	C	180	TYR
1	C	186	GLN

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Mol	Chain	Res	Type
1	C	223	LEU
1	C	250	THR
1	C	251	THR
1	C	262	THR
1	C	271	LEU
1	C	301	TRP
1	C	303	LEU
1	C	323	LYS
1	C	349	LYS
1	C	360	SER
1	D	5	GLU
1	D	7	MET
1	D	16	ASP
1	D	44	THR
1	D	55	GLU
1	D	58	ILE
1	D	164	LYS
1	D	165	PRO
1	D	168	LEU
1	D	180	TYR
1	D	200	ASP
1	D	223	LEU
1	D	225	GLU
1	D	247	THR
1	D	271	LEU
1	D	301	TRP
1	D	303	LEU
1	D	328	LYS
1	D	344	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	312	GLN
1	D	56	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	359/369 (97%)	1.41	108 (30%)  	59, 66, 83, 111	0
1	B	351/369 (95%)	1.68	111 (31%)  	58, 66, 88, 97	0
1	C	365/369 (98%)	1.46	98 (26%)  	50, 66, 89, 105	0
1	D	351/369 (95%)	1.42	94 (26%)  	55, 65, 81, 95	0
2	H	3/6 (50%)	2.03	1 (33%)  	73, 73, 76, 77	3 (100%)
All	All	1429/1482 (96%)	1.50	412 (28%)  	50, 66, 86, 111	3 (0%)

All (412) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	351	GLY	14.3
1	B	3	CYS	12.6
1	D	3	CYS	12.3
1	C	3	CYS	11.8
1	D	350	GLY	11.0
1	A	365	LYS	10.4
1	B	63	SER	10.2
1	A	2	HIS	9.7
1	B	352	ALA	9.6
1	C	354	GLY	8.9
1	B	351	GLY	8.7
1	C	362	TYR	8.2
1	C	248	ALA	8.2
1	C	353	GLY	8.1
1	C	2	HIS	7.9
1	B	326	VAL	7.5
1	C	358	GLY	7.4
1	D	95	GLY	7.3
1	B	321	GLY	7.2
1	B	47	LYS	7.2

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Mol	Chain	Res	Type	RSRZ
1	C	352	ALA	7.1
1	C	366	TYR	7.1
1	A	357	ALA	7.0
1	C	355	GLU	7.0
1	D	352	ALA	6.5
1	B	318	THR	6.4
1	C	359	ALA	6.4
1	B	106	ASN	6.4
1	B	55	GLU	6.3
1	B	46	LYS	6.2
1	C	247	THR	6.1
1	C	68	LEU	6.1
1	D	36	LEU	6.1
1	C	351	GLY	6.1
1	D	248	ALA	6.1
1	D	106	ASN	6.1
1	A	68	LEU	6.0
1	B	247	THR	5.9
1	B	36	LEU	5.9
1	A	202	PRO	5.9
1	B	246	CYS	5.8
1	D	276	PHE	5.7
1	A	358	GLY	5.6
1	A	351	GLY	5.6
1	B	35	ILE	5.5
1	A	248	ALA	5.5
1	C	329	ALA	5.3
1	A	359	ALA	5.3
1	D	275	VAL	5.3
1	C	356	ASN	5.3
1	D	247	THR	5.3
1	C	104	ASN	5.2
1	B	331	GLU	5.1
1	B	96	VAL	5.1
1	A	331	GLU	5.0
1	C	64	TYR	5.0
1	D	35	ILE	5.0
1	B	313	ALA	5.0
1	A	104	ASN	5.0
1	A	41	SER	5.0
1	A	106	ASN	5.0
1	A	64	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	50	ASP	4.8
1	D	201	GLY	4.7
1	A	65	ARG	4.7
1	A	96	VAL	4.7
1	A	42	THR	4.7
1	B	248	ALA	4.7
1	C	357	ALA	4.6
1	D	14	PRO	4.6
1	B	346	GLY	4.6
1	C	246	CYS	4.5
1	C	324	GLU	4.5
1	B	58	ILE	4.5
1	B	251	THR	4.5
1	B	325	ASN	4.4
1	D	4	THR	4.4
1	B	276	PHE	4.4
1	C	106	ASN	4.4
1	D	68	LEU	4.4
1	B	192	ILE	4.4
1	B	102	LEU	4.3
1	B	311	LEU	4.3
1	D	82	ILE	4.3
1	C	69	PHE	4.3
1	C	35	ILE	4.2
1	A	50	ASP	4.2
1	C	365	LYS	4.2
1	B	275	VAL	4.2
1	A	46	LYS	4.2
1	A	3	CYS	4.2
1	C	54	LEU	4.2
1	C	59	GLU	4.1
1	B	41	SER	4.1
1	D	263	LEU	4.1
1	D	253	GLN	4.1
1	B	234	LEU	4.1
1	B	99	VAL	4.0
1	C	331	GLU	4.0
1	C	30	GLN	4.0
1	C	36	LEU	4.0
1	D	239	MET	4.0
1	B	333	LEU	4.0
1	D	349	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	4	THR	3.9
1	D	342	LEU	3.9
1	D	306	SER	3.9
1	D	96	VAL	3.9
1	A	35	ILE	3.9
1	A	47	LYS	3.8
1	C	360	SER	3.8
1	D	303	LEU	3.8
1	B	305	PHE	3.8
1	A	201	GLY	3.8
1	D	321	GLY	3.8
1	B	249	LYS	3.8
1	A	58	ILE	3.8
1	C	327	ALA	3.8
1	A	333	LEU	3.8
1	B	327	ALA	3.7
1	D	324	GLU	3.7
1	D	192	ILE	3.7
1	D	53	LYS	3.7
1	D	64	TYR	3.7
1	C	23	THR	3.7
1	D	307	TYR	3.7
1	B	324	GLU	3.7
1	C	67	LEU	3.7
1	D	179	ARG	3.7
1	D	81	ALA	3.7
1	D	234	LEU	3.7
1	B	183	ILE	3.6
1	B	307	TYR	3.6
1	B	263	LEU	3.6
1	C	361	LEU	3.6
1	B	353	GLY	3.6
1	C	82	ILE	3.6
1	A	59	GLU	3.6
1	D	235	LEU	3.6
1	D	15	ALA	3.6
1	A	325	ASN	3.6
1	B	322	LYS	3.5
1	C	16	ASP	3.5
1	D	193	VAL	3.5
1	B	202	PRO	3.5
1	B	297	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	235	LEU	3.5
1	B	180	TYR	3.5
1	B	51	ASN	3.5
1	B	201	GLY	3.5
1	D	30	GLN	3.5
1	C	65	ARG	3.4
1	A	36	LEU	3.4
1	A	95	GLY	3.4
1	B	54	LEU	3.4
1	A	363	GLU	3.4
1	B	179	ARG	3.4
1	B	290	LEU	3.4
1	C	171[A]	HIS	3.4
1	A	44	THR	3.4
1	C	233	ALA	3.4
1	B	329	ALA	3.4
1	D	191	PRO	3.4
1	B	82	ILE	3.4
1	C	249	LYS	3.4
1	A	192	ILE	3.4
1	A	239	MET	3.3
1	D	45	ILE	3.3
1	A	51	ASN	3.3
1	D	322	LYS	3.3
1	B	298	PRO	3.3
2	H	604	ASP	3.3
1	A	176	GLY	3.3
1	D	297	GLY	3.3
1	C	53	LYS	3.3
1	D	274	VAL	3.3
1	B	250	THR	3.3
1	C	42	THR	3.3
1	D	282	SER	3.3
1	B	48	ARG	3.3
1	B	95	GLY	3.3
1	A	183	ILE	3.2
1	A	234	LEU	3.2
1	C	43	GLN	3.2
1	A	73	GLY	3.2
1	C	290	LEU	3.2
1	A	197	ILE	3.2
1	D	202	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	315	VAL	3.2
1	D	47	LYS	3.2
1	A	69	PHE	3.2
1	C	41	SER	3.2
1	B	23	THR	3.2
1	D	94	ALA	3.2
1	B	132	LEU	3.2
1	D	43	GLN	3.2
1	C	45	ILE	3.2
1	B	44	THR	3.2
1	C	325	ASN	3.2
1	C	38	ALA	3.2
1	D	331	GLU	3.1
1	B	282	SER	3.1
1	B	45	ILE	3.1
1	D	305	PHE	3.1
1	B	237	PRO	3.1
1	C	73	GLY	3.1
1	B	306	SER	3.1
1	C	234	LEU	3.0
1	B	141	GLU	3.0
1	B	38	ALA	3.0
1	A	364	LYS	3.0
1	C	326	VAL	3.0
1	D	347	LYS	3.0
1	B	319	TRP	3.0
1	A	74	LEU	3.0
1	D	150	ALA	3.0
1	A	177	LEU	3.0
1	B	233	ALA	3.0
1	C	52	ILE	3.0
1	C	19	GLU	2.9
1	C	51	ASN	2.9
1	B	193	VAL	2.9
1	D	271	LEU	2.9
1	A	63	SER	2.9
1	D	251	THR	2.9
1	B	78	ILE	2.9
1	B	332	VAL	2.9
1	C	275	VAL	2.9
1	B	149	PHE	2.9
1	A	247	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	233	ALA	2.9
1	B	81	ALA	2.9
1	D	16	ASP	2.9
1	B	69	PHE	2.9
1	D	304	THR	2.9
1	A	362	TYR	2.9
1	A	322	LYS	2.9
1	B	211	VAL	2.8
1	D	258	LEU	2.8
1	A	57	THR	2.8
1	A	184	CYS	2.8
1	D	329	ALA	2.8
1	A	52	ILE	2.8
1	D	333	LEU	2.8
1	C	84	PHE	2.8
1	B	342	LEU	2.8
1	A	94	ALA	2.8
1	D	41	SER	2.8
1	C	132	LEU	2.8
1	D	74	LEU	2.8
1	A	81	ALA	2.8
1	B	62	ALA	2.8
1	C	165	PRO	2.8
1	D	50	ASP	2.8
1	C	184	CYS	2.8
1	B	212	THR	2.8
1	A	329	ALA	2.7
1	D	139	CYS	2.7
1	A	82	ILE	2.7
1	D	319	TRP	2.7
1	A	229	LEU	2.7
1	C	193	VAL	2.7
1	B	184	CYS	2.7
1	C	322	LYS	2.7
1	C	197	ILE	2.7
1	D	293	ILE	2.7
1	C	235	LEU	2.7
1	C	150	ALA	2.7
1	C	50	ASP	2.7
1	D	76	LYS	2.7
1	C	318	THR	2.7
1	B	25	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	156	LEU	2.7
1	A	178	ALA	2.6
1	A	139	CYS	2.6
1	D	246	CYS	2.6
1	A	230	LEU	2.6
1	B	52	ILE	2.6
1	A	276	PHE	2.6
1	A	324	GLU	2.6
1	C	44	THR	2.6
1	A	136	ALA	2.6
1	B	244	TYR	2.6
1	A	102	LEU	2.6
1	B	304	THR	2.6
1	B	6	TYR	2.6
1	D	326	VAL	2.6
1	B	191	PRO	2.6
1	C	312	GLN	2.6
1	B	182	SER	2.5
1	D	243	GLY	2.5
1	B	68	LEU	2.5
1	C	230	LEU	2.5
1	B	253	GLN	2.5
1	B	176	GLY	2.5
1	D	17	VAL	2.5
1	A	92	ASN	2.5
1	C	305	PHE	2.5
1	D	149	PHE	2.5
1	C	311	LEU	2.5
1	A	53	LYS	2.5
1	A	14	PRO	2.5
1	A	6	TYR	2.5
1	D	245	GLU	2.5
1	A	91	LYS	2.5
1	A	223	LEU	2.5
1	C	4	THR	2.5
1	D	348	TYR	2.5
1	D	298	PRO	2.4
1	A	67	LEU	2.4
1	A	149	PHE	2.4
1	A	93	GLU	2.4
1	A	326	VAL	2.4
1	B	274	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	210	VAL	2.4
1	B	73	GLY	2.4
1	B	216	LEU	2.4
1	C	87	THR	2.4
1	A	78	ILE	2.4
1	B	53	LYS	2.4
1	D	181	ALA	2.4
1	B	255	VAL	2.4
1	A	179	ARG	2.4
1	A	241	THR	2.4
1	B	239	MET	2.4
1	D	184	CYS	2.4
1	B	97	PRO	2.4
1	A	193	VAL	2.4
1	B	113	VAL	2.4
1	C	72	LYS	2.4
1	B	189	LEU	2.4
1	A	150	ALA	2.4
1	A	181	ALA	2.4
1	C	120	ILE	2.3
1	D	91	LYS	2.3
1	C	78	ILE	2.3
1	A	97	PRO	2.3
1	C	55	GLU	2.3
1	B	13	LEU	2.3
1	A	56	ASN	2.3
1	A	134	GLY	2.3
1	B	16	ASP	2.3
1	A	180	TYR	2.3
1	B	345	TYR	2.3
1	D	180	TYR	2.3
1	C	250	THR	2.3
1	A	38	ALA	2.3
1	B	150	ALA	2.3
1	C	37	ALA	2.3
1	C	125	GLU	2.3
1	A	23	THR	2.3
1	C	215	VAL	2.3
1	C	319	TRP	2.3
1	D	233	ALA	2.3
1	D	316	LEU	2.3
1	C	157	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	244	TYR	2.2
1	C	202	PRO	2.2
1	A	15	ALA	2.2
1	D	259	THR	2.2
1	D	240	VAL	2.2
1	A	49	PHE	2.2
1	A	72	LYS	2.2
1	D	236	LYS	2.2
1	D	323	LYS	2.2
1	A	208	CYS	2.2
1	A	275	VAL	2.2
1	A	16	ASP	2.2
1	C	80	GLY	2.2
1	A	290	LEU	2.2
1	D	132	LEU	2.2
1	A	107	ILE	2.2
1	A	48	ARG	2.2
1	B	177	LEU	2.2
1	A	311	LEU	2.1
1	C	303	LEU	2.1
1	C	100	ASN	2.1
1	B	15	ALA	2.1
1	B	223	LEU	2.1
1	D	13	LEU	2.1
1	A	103	HIS	2.1
1	B	260	VAL	2.1
1	A	100	ASN	2.1
1	A	235	LEU	2.1
1	C	229	LEU	2.1
1	C	139	CYS	2.1
1	A	191	PRO	2.1
1	D	73	GLY	2.1
1	A	45	ILE	2.1
1	B	14	PRO	2.1
1	D	69	PHE	2.1
1	A	125	GLU	2.1
1	A	282	SER	2.1
1	D	249	LYS	2.1
1	D	327	ALA	2.1
1	B	43	GLN	2.1
1	C	56	ASN	2.1
1	A	158	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	258	LEU	2.1
1	A	30	GLN	2.0
1	A	55	GLU	2.0
1	A	246	CYS	2.0
1	D	311	LEU	2.0
1	B	252	THR	2.0
1	B	70	GLY	2.0
1	D	244	TYR	2.0
1	C	105	GLU	2.0
1	C	66	ASP	2.0
1	A	182	SER	2.0
1	D	63	SER	2.0
1	D	216	LEU	2.0
1	C	149	PHE	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 carbohydrates 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.