



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:20 AM UTC

PDB ID : 8YI1 / pdb_00008yi1
Title : Crystal structure of a BAHD acyltransferase Ep07g04462
Authors : Ren, R.B.; Yu, L.Y.; Pang, B.
Deposited on : 2024-02-28
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

<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

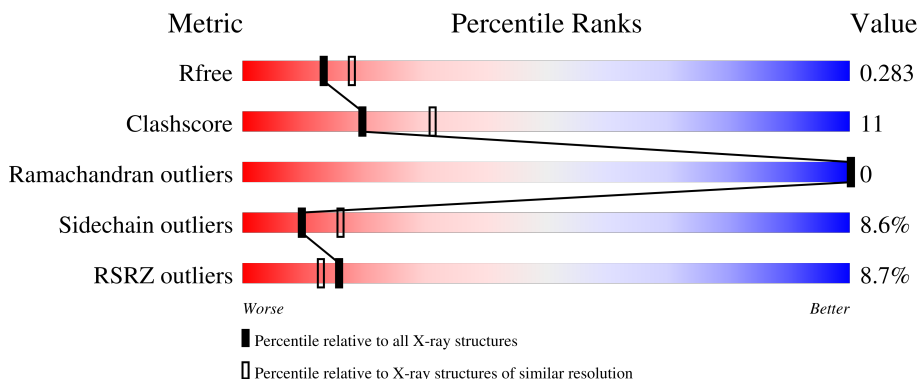
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

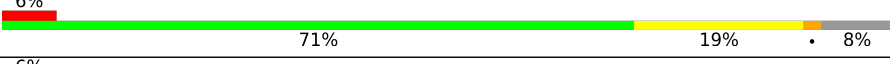
The reported resolution of this entry is 2.40 Å.

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	452	
1	B	452	
1	C	452	
1	D	452	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13199 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.

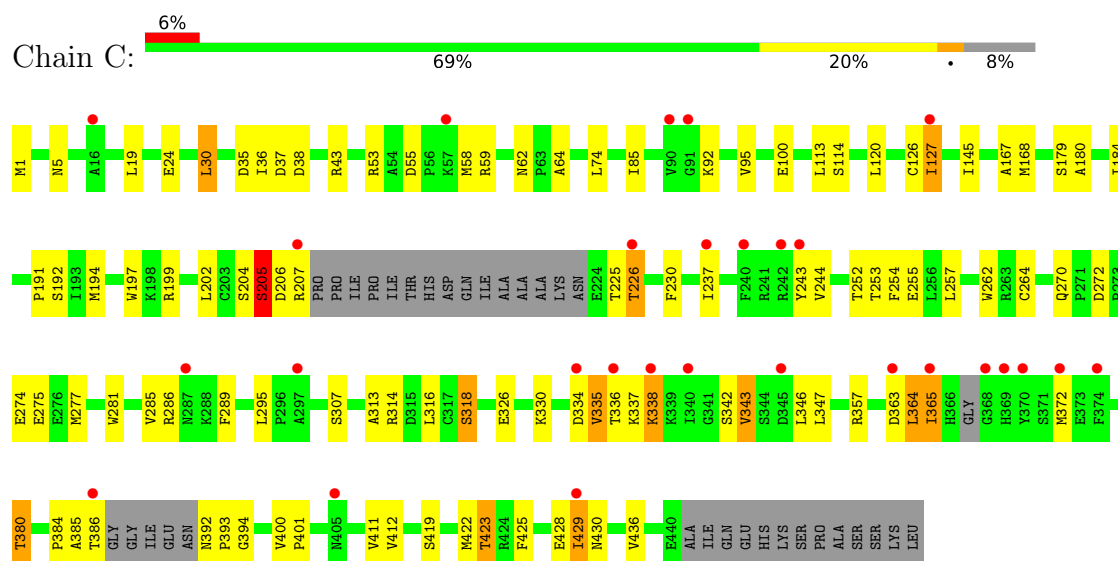
- Molecule 1 is a protein called BAHD acyltransferase Ep07g04462.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3232	2075	542	592	23			
1	B	417	Total	C	N	O	S	0	0	0
			3242	2080	546	593	23			
1	C	418	Total	C	N	O	S	0	0	0
			3237	2076	546	592	23			
1	D	418	Total	C	N	O	S	0	0	0
			3248	2085	547	593	23			

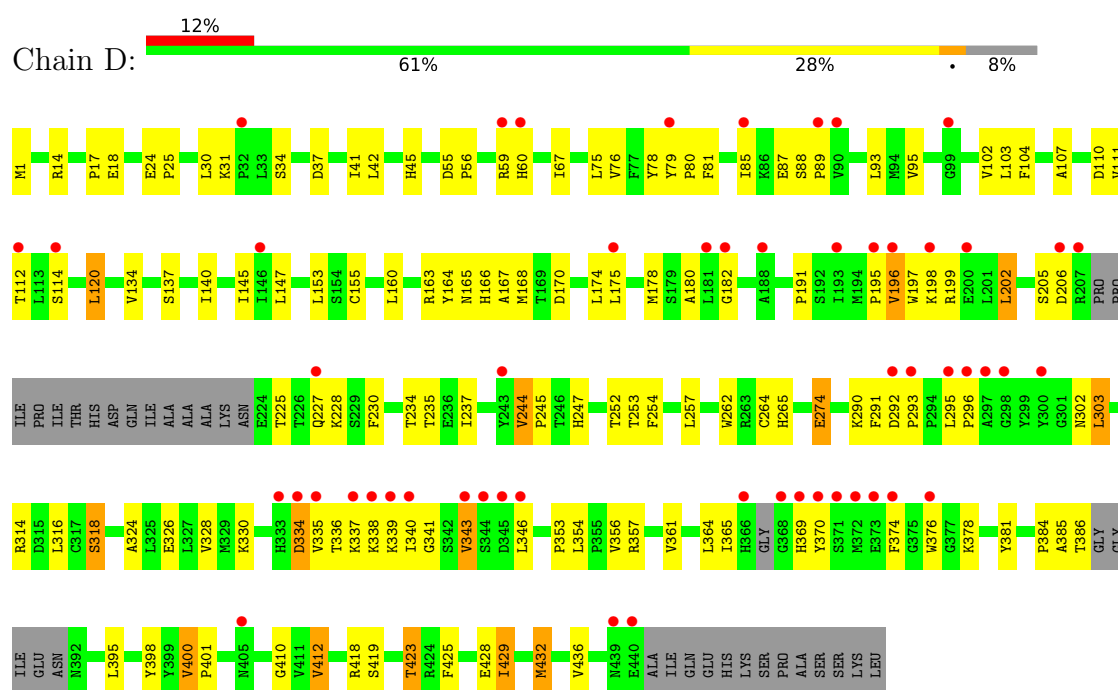
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	66	Total	O	0	0
			66	66		
2	B	62	Total	O	0	0
			62	62		
2	C	64	Total	O	0	0
			64	64		
2	D	48	Total	O	0	0
			48	48		

● Molecule 1: BAHD acyltransferase Ep07g04462



● Molecule 1: BAHD acyltransferase Ep07g04462



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.27Å 89.64Å 99.06Å 70.87° 89.61° 89.69°	Depositor
Resolution (Å)	32.99 – 2.40 32.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.3 (32.99-2.40) 97.3 (32.99-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.232 , 0.284 0.233 , 0.283	Depositor DCC
R_{free} test set	1969 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13199	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5160e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.42	0/3310	0.64	1/4503 (0.0%)
1	B	0.44	1/3320 (0.0%)	0.77	5/4516 (0.1%)
1	C	0.44	0/3314	0.69	3/4508 (0.1%)
1	D	0.42	0/3326	0.67	2/4523 (0.0%)
All	All	0.43	1/13270 (0.0%)	0.70	11/18050 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	24	GLU	C-O	-5.22	1.18	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	TYR	N-CA-C	20.37	132.87	111.07
1	B	371	SER	N-CA-C	14.31	126.88	111.28
1	C	206	ASP	N-CA-C	8.45	120.26	111.14
1	D	205	SER	N-CA-C	7.04	122.12	112.90
1	B	369	HIS	CA-C-N	6.61	129.03	120.44
1	B	369	HIS	C-N-CA	6.61	129.03	120.44
1	A	369	HIS	N-CA-C	-6.44	102.58	111.28
1	C	243	TYR	CA-CB-CG	5.38	123.58	113.90
1	B	370	TYR	N-CA-CB	-5.29	102.35	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	SER	N-CA-C	-5.26	105.44	111.07
1	D	369	HIS	N-CA-C	-5.10	101.34	108.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	ASP	Peptide
1	D	17	PRO	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	3232	0	3238	80	0
1	B	3242	0	3249	55	0
1	C	3237	0	3240	70	0
1	D	3248	0	3258	95	0
2	A	66	0	0	0	0
2	B	62	0	0	1	0
2	C	64	0	0	5	0
2	D	48	0	0	4	0
All	All	13199	0	12985	298	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 (298) 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:364:LEU:HD23	1:C:384:PRO:CG	1.94	0.98
1:C:364:LEU:HD23	1:C:384:PRO:HG2	1.49	0.93
1:A:277:MET:HE3	1:A:313:ALA:HB2	1.53	0.91
1:A:38:ASP:O	1:A:43:ARG:NH1	2.05	0.89
1:D:112:THR:HG22	1:D:114:SER:H	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ASP:O	1:B:43:ARG:NH1	2.10	0.85
1:B:37:ASP:HB3	1:B:302:ASN:HD22	1.43	0.83
1:C:53:ARG:NH2	2:C:501:HOH:O	2.11	0.83
1:A:1:MET:HB2	1:A:429:ILE:HD11	1.60	0.82
1:A:363:ASP:OD1	1:A:365:ILE:HG13	1.80	0.82
1:C:1:MET:HB2	1:C:429:ILE:HD11	1.67	0.76
1:C:364:LEU:HD23	1:C:384:PRO:HG3	1.66	0.76
1:B:295:LEU:HD12	1:B:296:PRO:HD2	1.67	0.75
1:A:244:VAL:HG21	1:A:325:LEU:HD23	1.66	0.75
1:D:1:MET:HB2	1:D:429:ILE:HD11	1.68	0.74
1:C:38:ASP:C	1:C:43:ARG:HH12	1.96	0.73
1:D:295:LEU:HD22	1:D:303:LEU:HD11	1.71	0.72
1:B:239:ALA:HB1	1:B:436:VAL:HG11	1.70	0.72
1:D:59:ARG:HD2	1:D:60:HIS:H	1.55	0.72
1:A:13:ARG:NH1	1:A:108:GLU:OE1	2.21	0.72
1:D:191:PRO:O	2:D:501:HOH:O	2.08	0.71
1:B:35:ASP:OD1	1:B:92:LYS:NZ	2.23	0.71
1:C:365:ILE:HA	1:C:401:PRO:HD3	1.72	0.71
1:A:148:TYR:HE2	1:A:178:MET:HE1	1.57	0.68
1:D:170:ASP:HB3	1:D:302:ASN:ND2	2.07	0.68
1:D:365:ILE:HA	1:D:401:PRO:HD3	1.74	0.68
1:D:134:VAL:O	1:D:137:SER:OG	2.10	0.68
1:A:38:ASP:OD2	1:A:92:LYS:NZ	2.28	0.67
1:A:314:ARG:O	1:A:318:SER:HB2	1.94	0.67
1:B:14:ARG:NH2	2:B:501:HOH:O	2.25	0.67
1:C:365:ILE:HD13	1:C:401:PRO:HD3	1.76	0.67
1:D:140:ILE:HG23	1:D:165:ASN:HD21	1.59	0.67
1:D:14:ARG:HB3	1:D:107:ALA:HB2	1.78	0.66
1:B:207:ARG:HH11	1:B:207:ARG:CG	2.08	0.65
1:A:237:ILE:HG21	1:A:253:THR:HG23	1.79	0.65
1:A:62:ASN:ND2	1:A:152:ARG:HD2	2.11	0.65
1:A:364:LEU:HG	1:A:384:PRO:HG3	1.78	0.65
1:C:314:ARG:O	1:C:318:SER:OG	2.15	0.65
1:B:419:SER:O	1:B:423:THR:HG22	1.98	0.64
1:C:252:THR:HG22	1:C:254:PHE:H	1.63	0.64
1:C:226:THR:HG22	1:C:422:MET:HE3	1.78	0.64
1:D:145:ILE:HD13	1:D:168:MET:HE3	1.78	0.64
1:B:207:ARG:HH11	1:B:207:ARG:HG3	1.63	0.63
1:C:286:ARG:NH2	2:C:505:HOH:O	2.31	0.63
1:D:264:CYS:SG	1:D:428:GLU:HG3	2.38	0.63
1:C:127:ILE:HD13	1:C:386:THR:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:ASN:HB2	1:C:393:PRO:HD3	1.81	0.63
1:D:400:VAL:HG12	1:D:401:PRO:HD2	1.81	0.62
1:A:133:ASP:HA	1:A:163:ARG:NH2	2.14	0.62
1:B:386:THR:O	1:B:398:TYR:OH	2.07	0.61
1:C:38:ASP:O	1:C:43:ARG:NH1	2.32	0.61
1:C:197:TRP:CE2	1:C:199:ARG:HG3	2.34	0.61
1:B:240:PHE:HD1	1:B:436:VAL:HG21	1.65	0.61
1:C:85:ILE:HG13	1:C:145:ILE:HD11	1.82	0.61
1:D:166:HIS:CE1	1:D:302:ASN:HD21	2.18	0.61
1:A:6:THR:HG23	1:A:6:THR:O	2.00	0.61
1:A:275:GLU:HB2	1:A:277:MET:CE	2.31	0.61
1:D:170:ASP:HB3	1:D:302:ASN:HD22	1.64	0.60
1:D:262:TRP:CE2	1:D:316:LEU:HD11	2.37	0.60
1:D:34:SER:OG	1:D:37:ASP:OD1	2.12	0.60
1:D:112:THR:HG22	1:D:114:SER:N	2.16	0.59
1:D:314:ARG:O	1:D:318:SER:OG	2.18	0.59
1:C:394:GLY:O	2:C:502:HOH:O	2.16	0.59
1:B:148:TYR:HH	1:B:177:PHE:HE2	1.50	0.59
1:D:244:VAL:HG22	1:D:245:PRO:HD2	1.84	0.59
1:A:277:MET:SD	1:A:357:ARG:HG2	2.43	0.58
1:C:113:LEU:HD21	1:C:380:THR:HG21	1.85	0.58
1:A:71:LEU:HD21	1:A:148:TYR:CZ	2.38	0.58
1:A:56:PRO:HB3	1:D:247:HIS:HB2	1.84	0.58
1:B:336:THR:O	1:B:339:LYS:NZ	2.32	0.58
1:D:18:GLU:HB3	1:D:104:PHE:O	2.03	0.58
1:A:37:ASP:HB3	1:A:167:ALA:O	2.04	0.58
1:C:272:ASP:HB2	1:C:275:GLU:HG3	1.84	0.58
1:D:252:THR:HG22	1:D:254:PHE:H	1.69	0.58
1:D:370:TYR:O	1:D:378:LYS:HG2	2.03	0.57
1:A:148:TYR:CE2	1:A:178:MET:HE1	2.40	0.57
1:A:364:LEU:C	1:A:366:HIS:H	2.13	0.57
1:C:285:VAL:HG11	1:C:347:LEU:HD21	1.87	0.57
1:B:244:VAL:HG23	1:B:245:PRO:HD2	1.86	0.56
1:A:62:ASN:HD22	1:A:152:ARG:HD2	1.69	0.56
1:B:290:LYS:O	1:B:340:ILE:HD12	2.05	0.56
1:C:37:ASP:HB3	1:C:167:ALA:O	2.05	0.56
1:D:78:TYR:CE1	1:D:195:PRO:HG3	2.41	0.56
1:D:370:TYR:CD2	1:D:378:LYS:HE3	2.40	0.56
1:B:264:CYS:SG	1:B:428:GLU:HG3	2.45	0.56
1:A:365:ILE:HA	1:A:401:PRO:HD3	1.87	0.56
1:B:365:ILE:HA	1:B:401:PRO:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:O	1:A:137:SER:OG	2.20	0.56
1:A:145:ILE:HD13	1:A:168:MET:HE2	1.88	0.56
1:B:200:GLU:CD	1:B:200:GLU:H	2.13	0.56
1:B:227:GLN:O	1:B:228:LYS:HG3	2.05	0.56
1:B:37:ASP:HB2	1:B:167:ALA:O	2.06	0.56
1:D:326:GLU:OE2	1:D:330:LYS:NZ	2.36	0.56
1:D:237:ILE:HG21	1:D:253:THR:HG23	1.87	0.56
1:C:204:SER:HB2	1:C:207:ARG:HD2	1.87	0.55
1:B:404:ASN:ND2	1:B:408:GLU:OE1	2.39	0.55
1:C:364:LEU:CD2	1:C:384:PRO:HG3	2.33	0.55
1:A:272:ASP:HB2	1:A:275:GLU:HG3	1.89	0.55
1:B:112:THR:HG22	1:B:154:SER:HB2	1.89	0.55
1:A:62:ASN:HD22	1:A:152:ARG:NH1	2.05	0.54
1:B:127:ILE:HG21	1:B:386:THR:HG22	1.89	0.54
1:B:262:TRP:CE2	1:B:316:LEU:HD11	2.42	0.54
1:B:170:ASP:HB3	1:B:302:ASN:OD1	2.06	0.54
1:C:338:LYS:HB3	1:C:346:LEU:HD22	1.90	0.54
1:D:425:PHE:O	1:D:429:ILE:HG23	2.08	0.54
1:A:86:LYS:NZ	1:A:96:ASP:OD2	2.41	0.54
1:C:274:GLU:CD	1:C:274:GLU:H	2.17	0.53
1:D:384:PRO:O	2:D:502:HOH:O	2.19	0.53
1:A:244:VAL:HG21	1:A:325:LEU:CD2	2.36	0.53
1:B:364:LEU:HG	1:B:384:PRO:HG3	1.91	0.53
1:C:204:SER:OG	1:C:207:ARG:NE	2.41	0.52
1:D:227:GLN:C	1:D:228:LYS:HG2	2.35	0.52
1:A:361:VAL:HG11	1:A:399:TYR:CZ	2.44	0.52
1:D:197:TRP:CE2	1:D:199:ARG:HG3	2.43	0.52
1:C:365:ILE:HD11	1:C:411:VAL:HG22	1.91	0.52
1:B:239:ALA:HB1	1:B:436:VAL:CG1	2.39	0.52
1:D:302:ASN:O	1:D:303:LEU:HD23	2.09	0.52
1:A:267:ILE:O	1:A:270:GLN:NE2	2.31	0.52
1:A:370:TYR:HD1	1:A:370:TYR:H	1.58	0.52
1:B:247:HIS:HB2	1:D:56:PRO:HB3	1.92	0.52
1:C:1:MET:HE3	1:C:230:PHE:CD2	2.44	0.51
1:D:166:HIS:HE1	1:D:302:ASN:HD21	1.57	0.51
1:A:133:ASP:HA	1:A:163:ARG:HH22	1.75	0.51
1:D:339:LYS:HG3	1:D:340:ILE:HG22	1.92	0.51
1:A:262:TRP:CE2	1:A:316:LEU:HD11	2.45	0.51
1:B:439:ASN:N	1:B:439:ASN:OD1	2.42	0.51
1:C:385:ALA:O	1:C:386:THR:OG1	2.27	0.51
1:B:37:ASP:CB	1:B:302:ASN:HD22	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ILE:HD13	1:C:401:PRO:CD	2.41	0.51
1:A:369:HIS:O	1:A:372:MET:HE1	2.10	0.51
1:D:24:GLU:HG2	1:D:25:PRO:HD2	1.93	0.51
1:B:80:PRO:HB2	1:B:168:MET:HE1	1.92	0.51
1:C:62:ASN:HD21	1:C:64:ALA:HB3	1.76	0.51
1:C:35:ASP:OD2	1:C:204:SER:N	2.44	0.50
1:D:88:SER:OG	1:D:89:PRO:HD2	2.12	0.50
1:A:183:GLU:OE2	1:A:192:SER:OG	2.24	0.50
1:C:289:PHE:HB3	1:C:346:LEU:HD13	1.93	0.50
1:D:364:LEU:HG	1:D:384:PRO:HG3	1.94	0.50
1:B:148:TYR:OH	1:B:177:PHE:HE2	1.94	0.49
1:C:425:PHE:O	1:C:429:ILE:HG23	2.12	0.49
1:D:41:ILE:HG13	1:D:354:LEU:HD21	1.94	0.49
1:D:291:PHE:HA	1:D:341:GLY:O	2.13	0.49
1:A:62:ASN:HD22	1:A:152:ARG:HH11	1.58	0.49
1:C:36:ILE:HG13	1:C:202:LEU:HD13	1.93	0.49
1:D:164:TYR:CE1	1:D:174:LEU:HD22	2.48	0.49
1:B:243:TYR:HB2	1:B:436:VAL:HG22	1.95	0.49
1:C:43:ARG:NH2	2:C:507:HOH:O	2.36	0.49
1:A:364:LEU:C	1:A:366:HIS:N	2.69	0.49
1:D:292:ASP:HB3	1:D:293:PRO:HD2	1.95	0.49
1:B:197:TRP:CE2	1:B:199:ARG:HG3	2.48	0.48
1:C:180:ALA:O	1:C:184:ILE:HG12	2.13	0.48
1:A:127:ILE:HD11	1:A:385:ALA:HB1	1.95	0.48
1:B:281:TRP:CE2	1:B:307:SER:OG	2.67	0.48
1:C:419:SER:O	1:C:423:THR:HG23	2.14	0.48
1:D:103:LEU:HB3	1:D:147:LEU:HD13	1.96	0.48
1:D:182:GLY:HA2	1:D:374:PHE:CD1	2.49	0.48
1:A:244:VAL:HG22	1:A:245:PRO:HD2	1.95	0.48
1:B:103:LEU:HB3	1:B:147:LEU:HD23	1.96	0.48
1:A:197:TRP:CE2	1:A:199:ARG:HG3	2.49	0.48
1:A:264:CYS:SG	1:A:428:GLU:HG3	2.54	0.48
1:B:337:LYS:O	1:B:338:LYS:HD2	2.12	0.48
1:D:419:SER:O	1:D:423:THR:HG23	2.13	0.48
1:A:292:ASP:HB3	1:A:293:PRO:HD3	1.94	0.48
1:D:111:VAL:HG13	1:D:153:LEU:HD22	1.95	0.48
1:D:79:TYR:CG	1:D:80:PRO:HD3	2.48	0.47
1:A:231:PHE:CE2	1:A:233:THR:HG22	2.50	0.47
1:C:281:TRP:CE2	1:C:307:SER:OG	2.68	0.47
1:A:433:LEU:O	1:A:436:VAL:HG12	2.14	0.47
1:A:34:SER:HB2	1:A:202:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:GLU:HB3	1:D:93:LEU:HD23	1.97	0.47
1:D:160:LEU:HD21	1:D:178:MET:HE1	1.95	0.47
1:A:58:MET:HE3	1:A:375:GLY:O	2.15	0.47
1:A:275:GLU:HB2	1:A:277:MET:HE2	1.96	0.47
1:C:237:ILE:HG21	1:C:253:THR:HG23	1.95	0.47
1:C:277:MET:HE3	1:C:313:ALA:HB2	1.97	0.47
1:D:81:PHE:HE1	1:D:168:MET:HG2	1.79	0.47
1:A:65:SER:O	1:A:69:GLU:HG2	2.16	0.46
1:B:37:ASP:HA	1:B:42:LEU:HD12	1.96	0.46
1:D:198:LYS:HA	1:D:198:LYS:HD3	1.68	0.46
1:C:197:TRP:NE1	1:C:199:ARG:HG3	2.30	0.46
1:C:277:MET:HE1	1:C:357:ARG:HG3	1.96	0.46
1:A:166:HIS:ND1	1:A:166:HIS:O	2.47	0.46
1:D:324:ALA:O	1:D:328:VAL:HG23	2.16	0.46
1:B:28:ARG:HD2	1:B:97:CYS:O	2.14	0.46
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.77	0.46
1:A:198:LYS:HA	1:A:198:LYS:HD3	1.68	0.46
1:C:95:VAL:HG21	1:C:168:MET:HE1	1.98	0.46
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.74	0.45
1:C:295:LEU:HD21	1:C:343:VAL:HG11	1.99	0.45
1:D:34:SER:HB2	1:D:202:LEU:HB2	1.99	0.45
1:B:244:VAL:CG2	1:B:248:LEU:HB2	2.46	0.45
1:C:30:LEU:HD23	1:C:30:LEU:HA	1.76	0.45
1:C:252:THR:HB	1:C:255:GLU:H	1.81	0.45
1:D:95:VAL:HG21	1:D:168:MET:HE1	1.97	0.45
1:A:432:MET:HE2	1:A:432:MET:HB3	1.73	0.45
1:B:231:PHE:CE2	1:B:233:THR:HG22	2.52	0.45
1:C:43:ARG:NE	2:C:507:HOH:O	2.41	0.45
1:A:79:TYR:CG	1:A:80:PRO:HD3	2.52	0.45
1:A:339:LYS:HE2	1:A:339:LYS:HB3	1.79	0.45
1:D:81:PHE:CE1	1:D:168:MET:HG2	2.52	0.45
1:D:292:ASP:HB3	1:D:293:PRO:CD	2.46	0.45
1:B:71:LEU:HD21	1:B:148:TYR:CD2	2.52	0.45
1:D:42:LEU:HD22	1:D:166:HIS:CE1	2.52	0.45
1:D:385:ALA:O	1:D:386:THR:OG1	2.30	0.45
1:D:330:LYS:O	1:D:334:ASP:OD1	2.34	0.44
1:D:353:PRO:O	2:D:504:HOH:O	2.21	0.44
1:C:180:ALA:HB1	1:C:191:PRO:HB3	1.99	0.44
1:A:122:PRO:HG2	1:A:400:VAL:HG21	1.99	0.44
1:B:240:PHE:O	1:B:244:VAL:HG12	2.16	0.44
1:D:180:ALA:HB1	1:D:191:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:THR:HG23	2:D:505:HOH:O	2.18	0.44
1:D:202:LEU:HD11	1:D:343:VAL:HG12	1.99	0.44
1:D:274:GLU:H	1:D:274:GLU:HG2	1.54	0.44
1:A:324:ALA:O	1:A:328:VAL:HG23	2.18	0.44
1:D:112:THR:HG23	1:D:155:CYS:HB3	1.99	0.44
1:D:196:VAL:HG21	1:D:296:PRO:HB2	2.00	0.44
1:B:237:ILE:HG21	1:B:253:THR:HG23	2.00	0.44
1:A:373:GLU:HG2	1:A:377:GLY:C	2.42	0.43
1:B:342:SER:HB2	1:B:345:ASP:HB2	2.00	0.43
1:A:146:ILE:HG13	1:A:147:LEU:N	2.33	0.43
1:A:415:LEU:HA	1:A:415:LEU:HD23	1.71	0.43
1:A:18:GLU:HG3	1:A:104:PHE:HB3	2.01	0.43
1:B:35:ASP:OD2	1:B:204:SER:N	2.52	0.43
1:B:207:ARG:CG	1:B:207:ARG:NH1	2.72	0.43
1:A:281:TRP:CE2	1:A:307:SER:OG	2.71	0.43
1:B:240:PHE:CD1	1:B:436:VAL:HG21	2.50	0.43
1:D:79:TYR:CD2	1:D:80:PRO:HD3	2.54	0.43
1:D:432:MET:O	1:D:436:VAL:HG23	2.19	0.43
1:A:58:MET:O	1:A:61:LYS:HB2	2.19	0.43
1:A:398:TYR:O	1:A:414:PRO:HD2	2.18	0.43
1:D:111:VAL:O	1:D:153:LEU:HB3	2.19	0.43
1:A:295:LEU:HD13	1:A:295:LEU:HA	1.87	0.43
1:D:31:LYS:HE3	1:D:197:TRP:CG	2.53	0.43
1:A:50:GLN:HA	1:A:381:TYR:O	2.19	0.42
1:C:191:PRO:HD2	1:C:194:MET:SD	2.59	0.42
1:C:204:SER:CB	1:C:207:ARG:CD	2.97	0.42
1:C:338:LYS:HB3	1:C:346:LEU:CD2	2.50	0.42
1:C:347:LEU:HD23	1:C:347:LEU:HA	1.85	0.42
1:B:148:TYR:OH	1:B:177:PHE:CE2	2.72	0.42
1:D:166:HIS:HE1	1:D:302:ASN:ND2	2.18	0.42
1:D:364:LEU:HD23	1:D:398:TYR:HB2	2.01	0.42
1:A:6:THR:O	1:A:6:THR:CG2	2.65	0.42
1:A:347:LEU:HD23	1:A:347:LEU:HA	1.87	0.42
1:D:418:ARG:HG3	1:D:418:ARG:HH11	1.84	0.42
1:C:19:LEU:HD13	1:C:100:GLU:O	2.20	0.42
1:D:37:ASP:HB3	1:D:167:ALA:O	2.19	0.42
1:D:168:MET:HE2	1:D:168:MET:HB2	1.90	0.42
1:B:47:LYS:HE3	1:B:131:LEU:HD23	2.02	0.42
1:B:337:LYS:C	1:B:338:LYS:HD2	2.44	0.42
1:C:38:ASP:CA	1:C:43:ARG:HH12	2.33	0.42
1:C:204:SER:O	1:C:205:SER:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:HIS:CE1	1:D:395:LEU:HB2	2.55	0.42
1:D:291:PHE:CE1	1:D:343:VAL:HA	2.55	0.42
1:A:269:LEU:HA	1:A:269:LEU:HD23	1.65	0.42
1:A:413:VAL:HG23	1:A:413:VAL:O	2.20	0.42
1:C:204:SER:CB	1:C:207:ARG:HD2	2.50	0.42
1:C:429:ILE:HG13	1:C:430:ASN:N	2.35	0.42
1:A:137:SER:C	1:A:139:ALA:H	2.28	0.41
1:C:62:ASN:ND2	1:C:64:ALA:HB3	2.34	0.41
1:D:234:THR:HG23	1:D:410:GLY:HA2	2.01	0.41
1:D:356:VAL:HG13	1:D:357:ARG:N	2.35	0.41
1:C:55:ASP:OD2	1:C:58:MET:HG2	2.20	0.41
1:C:254:PHE:CD1	1:C:254:PHE:C	2.98	0.41
1:D:55:ASP:H	1:D:376:TRP:CD1	2.38	0.41
1:C:264:CYS:SG	1:C:428:GLU:HG3	2.61	0.41
1:A:237:ILE:O	1:A:240:PHE:HB2	2.21	0.41
1:A:292:ASP:O	1:A:294:PRO:HD3	2.21	0.41
1:C:262:TRP:CE2	1:C:316:LEU:HD11	2.55	0.41
1:D:103:LEU:HD23	1:D:103:LEU:HA	1.73	0.41
1:D:290:LYS:O	1:D:340:ILE:HG13	2.21	0.41
1:A:339:LYS:HG2	1:A:340:ILE:N	2.36	0.41
1:A:372:MET:HB2	1:A:372:MET:HE3	1.62	0.41
1:B:58:MET:HE3	1:B:58:MET:HB3	1.91	0.41
1:C:254:PHE:CE2	1:C:363:ASP:HB2	2.56	0.41
1:C:307:SER:HB3	1:C:335:VAL:CG2	2.50	0.41
1:C:330:LYS:O	1:C:334:ASP:OD1	2.39	0.41
1:A:252:THR:HG22	1:A:254:PHE:H	1.86	0.41
1:A:1:MET:CE	1:A:429:ILE:HG12	2.51	0.41
1:A:228:LYS:HD2	1:A:422:MET:HE3	2.03	0.41
1:C:326:GLU:OE2	1:C:330:LYS:NZ	2.40	0.41
1:C:372:MET:HE2	1:C:372:MET:HB2	1.68	0.41
1:D:120:LEU:HD21	1:D:381:TYR:HB2	2.03	0.41
1:D:264:CYS:SG	1:D:429:ILE:HG22	2.61	0.41
1:D:291:PHE:CE1	1:D:343:VAL:HG13	2.56	0.41
1:A:337:LYS:HB2	1:A:337:LYS:HE2	1.89	0.41
1:B:94:MET:HE3	1:B:94:MET:HB3	1.88	0.41
1:D:230:PHE:O	1:D:412:VAL:HA	2.21	0.41
1:D:87:GLU:CB	1:D:93:LEU:HD23	2.50	0.40
1:D:257:LEU:HD23	1:D:257:LEU:HA	1.81	0.40
1:D:338:LYS:HB3	1:D:346:LEU:HD21	2.03	0.40
1:A:1:MET:SD	1:A:232:LEU:HD21	2.61	0.40
1:B:37:ASP:HB3	1:B:302:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:HIS:HB3	1:D:163:ARG:HD3	2.02	0.40
1:D:75:LEU:HD21	1:D:102:VAL:HG13	2.03	0.40
1:D:197:TRP:NE1	1:D:199:ARG:HG3	2.35	0.40
1:D:334:ASP:OD1	1:D:334:ASP:N	2.53	0.40
1:D:34:SER:HB2	1:D:202:LEU:CB	2.51	0.40
1:C:365:ILE:O	1:C:365:ILE:CG2	2.70	0.40

There are no symmetry-related clashes.

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	408/452 (90%)	391 (96%)	17 (4%)	0	100	100
1	B	409/452 (90%)	400 (98%)	9 (2%)	0	100	100
1	C	410/452 (91%)	400 (98%)	10 (2%)	0	100	100
1	D	410/452 (91%)	393 (96%)	17 (4%)	0	100	100
All	All	1637/1808 (90%)	1584 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	356/388 (92%)	321 (90%)	35 (10%)	7	12
1	B	357/388 (92%)	328 (92%)	29 (8%)	11	18
1	C	355/388 (92%)	322 (91%)	33 (9%)	8	14
1	D	357/388 (92%)	331 (93%)	26 (7%)	13	22
All	All	1425/1552 (92%)	1302 (91%)	123 (9%)	10	16

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	28	ARG
1	A	37	ASP
1	A	50	GLN
1	A	58	MET
1	A	62	ASN
1	A	67	ILE
1	A	74	LEU
1	A	90	VAL
1	A	121	GLN
1	A	127	ILE
1	A	138	SER
1	A	146	ILE
1	A	189	THR
1	A	192	SER
1	A	196	VAL
1	A	202	LEU
1	A	235	THR
1	A	244	VAL
1	A	295	LEU
1	A	318	SER
1	A	337	LYS
1	A	339	LYS
1	A	340	ILE
1	A	342	SER
1	A	343	VAL
1	A	344	SER
1	A	347	LEU
1	A	364	LEU
1	A	365	ILE
1	A	372	MET
1	A	386	THR
1	A	423	THR

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Mol	Chain	Res	Type
1	A	429	ILE
1	A	436	VAL
1	B	6	THR
1	B	24	GLU
1	B	37	ASP
1	B	67	ILE
1	B	74	LEU
1	B	90	VAL
1	B	94	MET
1	B	114	SER
1	B	121	GLN
1	B	147	LEU
1	B	175	LEU
1	B	202	LEU
1	B	207	ARG
1	B	225	THR
1	B	238	SER
1	B	244	VAL
1	B	250	SER
1	B	290	LYS
1	B	335	VAL
1	B	338	LYS
1	B	343	VAL
1	B	356	VAL
1	B	361	VAL
1	B	372	MET
1	B	386	THR
1	B	403	THR
1	B	423	THR
1	B	433	LEU
1	B	439	ASN
1	C	5	ASN
1	C	24	GLU
1	C	30	LEU
1	C	59	ARG
1	C	74	LEU
1	C	92	LYS
1	C	114	SER
1	C	120	LEU
1	C	126	CYS
1	C	127	ILE
1	C	179	SER

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Mol	Chain	Res	Type
1	C	192	SER
1	C	205	SER
1	C	225	THR
1	C	226	THR
1	C	244	VAL
1	C	257	LEU
1	C	270	GLN
1	C	318	SER
1	C	335	VAL
1	C	336	THR
1	C	337	LYS
1	C	338	LYS
1	C	342	SER
1	C	343	VAL
1	C	364	LEU
1	C	365	ILE
1	C	380	THR
1	C	400	VAL
1	C	412	VAL
1	C	423	THR
1	C	429	ILE
1	C	436	VAL
1	D	30	LEU
1	D	67	ILE
1	D	76	VAL
1	D	85	ILE
1	D	110	ASP
1	D	120	LEU
1	D	175	LEU
1	D	196	VAL
1	D	202	LEU
1	D	206	ASP
1	D	225	THR
1	D	244	VAL
1	D	274	GLU
1	D	303	LEU
1	D	318	SER
1	D	334	ASP
1	D	335	VAL
1	D	336	THR
1	D	337	LYS
1	D	343	VAL

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Mol	Chain	Res	Type
1	D	361	VAL
1	D	400	VAL
1	D	412	VAL
1	D	423	THR
1	D	429	ILE
1	D	432	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	278	ASN
1	C	5	ASN
1	C	45	HIS
1	C	176	GLN
1	C	437	GLN
1	D	45	HIS
1	D	50	GLN
1	D	176	GLN
1	D	247	HIS
1	D	302	ASN

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	416/452 (92%)	0.71	37 (8%)	15 12	24, 49, 84, 111	0
1	B	417/452 (92%)	0.66	27 (6%)	25 21	26, 47, 78, 100	0
1	C	418/452 (92%)	0.62	28 (6%)	24 20	27, 47, 76, 98	0
1	D	418/452 (92%)	1.01	54 (12%)	7 5	26, 55, 98, 121	0
All	All	1669/1808 (92%)	0.75	146 (8%)	16 13	24, 49, 87, 121	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	372	MET	5.5
1	D	340	ILE	4.9
1	B	225	THR	4.6
1	B	372	MET	4.3
1	B	244	VAL	4.1
1	D	334	ASP	3.8
1	D	295	LEU	3.8
1	A	372	MET	3.8
1	D	374	PHE	3.7
1	A	369	HIS	3.7
1	C	369	HIS	3.7
1	D	293	PRO	3.6
1	A	295	LEU	3.6
1	D	333	HIS	3.5
1	C	243	TYR	3.5
1	B	369	HIS	3.5
1	C	207	ARG	3.5
1	C	372	MET	3.5
1	C	237	ILE	3.5
1	D	297	ALA	3.4
1	D	207	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	386	THR	3.4
1	C	340	ILE	3.4
1	D	369	HIS	3.3
1	C	370	TYR	3.3
1	D	373	GLU	3.1
1	A	370	TYR	3.1
1	A	375	GLY	3.1
1	B	386	THR	3.1
1	A	374	PHE	3.1
1	D	300	TYR	3.0
1	A	334	ASP	3.0
1	B	365	ILE	3.0
1	A	293	PRO	3.0
1	A	337	LYS	3.0
1	A	225	THR	3.0
1	D	440	GLU	3.0
1	B	243	TYR	3.0
1	B	405	ASN	3.0
1	D	298	GLY	3.0
1	C	336	THR	2.9
1	A	243	TYR	2.9
1	C	240	PHE	2.9
1	B	438	ASN	2.9
1	D	368	GLY	2.9
1	B	90	VAL	2.9
1	D	296	PRO	2.9
1	D	243	TYR	2.9
1	A	438	ASN	2.9
1	A	429	ILE	2.9
1	D	60	HIS	2.9
1	D	335	VAL	2.9
1	C	334	ASP	2.9
1	C	386	THR	2.8
1	D	405	ASN	2.8
1	C	363	ASP	2.8
1	B	368	GLY	2.8
1	A	244	VAL	2.8
1	A	368	GLY	2.7
1	D	89	PRO	2.7
1	C	338	LYS	2.7
1	D	99	GLY	2.7
1	A	439	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	287	ASN	2.7
1	C	405	ASN	2.7
1	A	90	VAL	2.7
1	B	57	LYS	2.7
1	B	370	TYR	2.7
1	B	437	GLN	2.7
1	A	345	ASP	2.7
1	C	345	ASP	2.7
1	A	340	ILE	2.7
1	C	91	GLY	2.6
1	D	370	TYR	2.6
1	D	292	ASP	2.6
1	D	345	ASP	2.6
1	B	237	ILE	2.6
1	C	127	ILE	2.6
1	B	385	ALA	2.6
1	C	16	ALA	2.6
1	D	200	GLU	2.6
1	D	371	SER	2.6
1	B	394	GLY	2.6
1	A	270	GLN	2.6
1	B	11	THR	2.6
1	A	292	ASP	2.5
1	D	343	VAL	2.5
1	C	374	PHE	2.5
1	D	181	LEU	2.5
1	D	196	VAL	2.5
1	D	439	ASN	2.5
1	D	188	ALA	2.5
1	A	60	HIS	2.4
1	A	343	VAL	2.4
1	C	368	GLY	2.4
1	A	371	SER	2.4
1	D	366	HIS	2.4
1	C	297	ALA	2.4
1	D	339	LYS	2.4
1	D	114	SER	2.3
1	A	339	LYS	2.3
1	C	90	VAL	2.3
1	B	297	ALA	2.3
1	A	376	TRP	2.3
1	D	206	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	338	LYS	2.3
1	B	439	ASN	2.3
1	D	195	PRO	2.3
1	A	237	ILE	2.3
1	D	346	LEU	2.3
1	D	198	LYS	2.3
1	D	337	LYS	2.3
1	B	380	THR	2.2
1	B	69	GLU	2.2
1	B	373	GLU	2.2
1	A	405	ASN	2.2
1	B	366	HIS	2.2
1	C	226	THR	2.2
1	D	182	GLY	2.2
1	D	90	VAL	2.2
1	A	287	ASN	2.2
1	B	435	GLN	2.2
1	D	112	THR	2.2
1	A	365	ILE	2.2
1	D	32	PRO	2.2
1	C	57	LYS	2.2
1	A	366	HIS	2.1
1	B	371	SER	2.1
1	C	242	ARG	2.1
1	D	227	GLN	2.1
1	A	336	THR	2.1
1	D	85	ILE	2.1
1	D	79	TYR	2.1
1	D	376	TRP	2.1
1	C	429	ILE	2.1
1	D	344	SER	2.1
1	A	226	THR	2.1
1	A	146	ILE	2.1
1	C	365	ILE	2.1
1	D	193	ILE	2.1
1	A	57	LYS	2.1
1	B	416	LEU	2.0
1	D	146	ILE	2.0
1	D	59	ARG	2.0
1	A	172	ALA	2.0
1	D	175	LEU	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.