



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:13 PM UTC

PDB ID : 1RF5 / pdb_00001rf5
Title : Structural Studies of Streptococcus pneumoniae EPSP Synthase in Unliganded State
Authors : Park, H.; Hilsenbeck, J.L.; Kim, H.J.; Shuttleworth, W.A.; Park, Y.H.; Evans, J.N.; Kang, C.
Deposited on : 2003-11-07
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

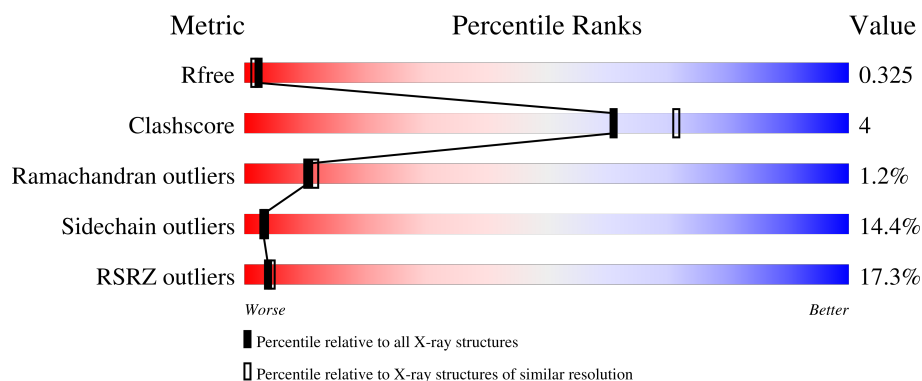
1 Overall quality at a glance

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	427	17% 79% 18% .
1	B	427	18% 77% 20% .
1	C	427	18% 80% 18% .
1	D	427	15% 78% 19% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13615 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 5-enolpyruvylshikimate-3-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	51	0	0
			3212	2019	559	619	15			
1	B	427	Total	C	N	O	S	51	0	0
			3212	2019	559	619	15			
1	C	427	Total	C	N	O	S	51	0	0
			3212	2019	559	619	15			
1	D	427	Total	C	N	O	S	51	0	0
			3212	2019	559	619	15			

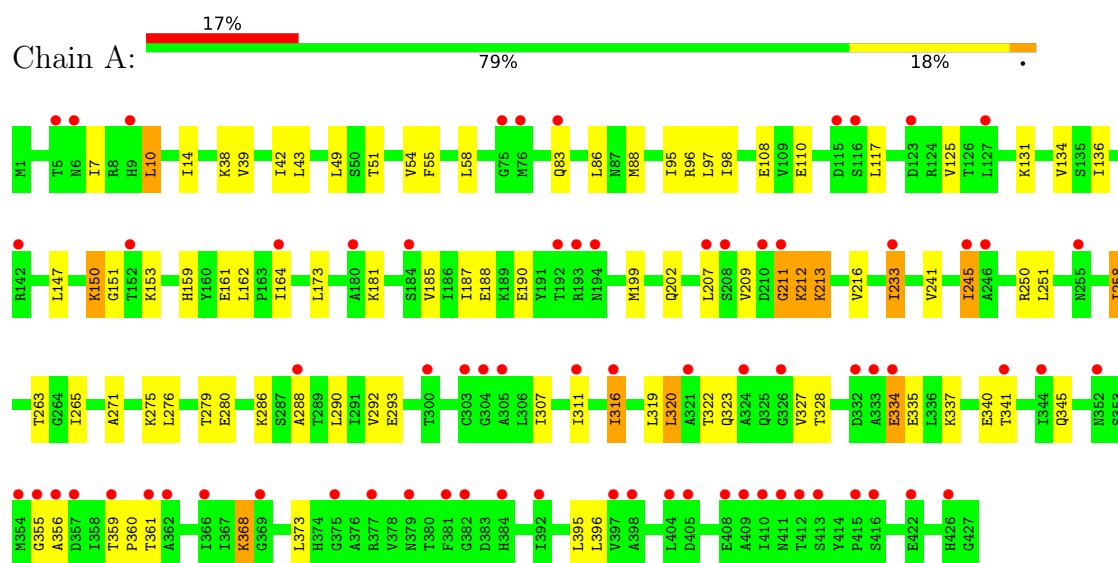
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	191	Total	O	0	0
			191	191		
2	B	172	Total	O	0	0
			172	172		
2	C	203	Total	O	0	0
			203	203		
2	D	201	Total	O	0	0
			201	201		

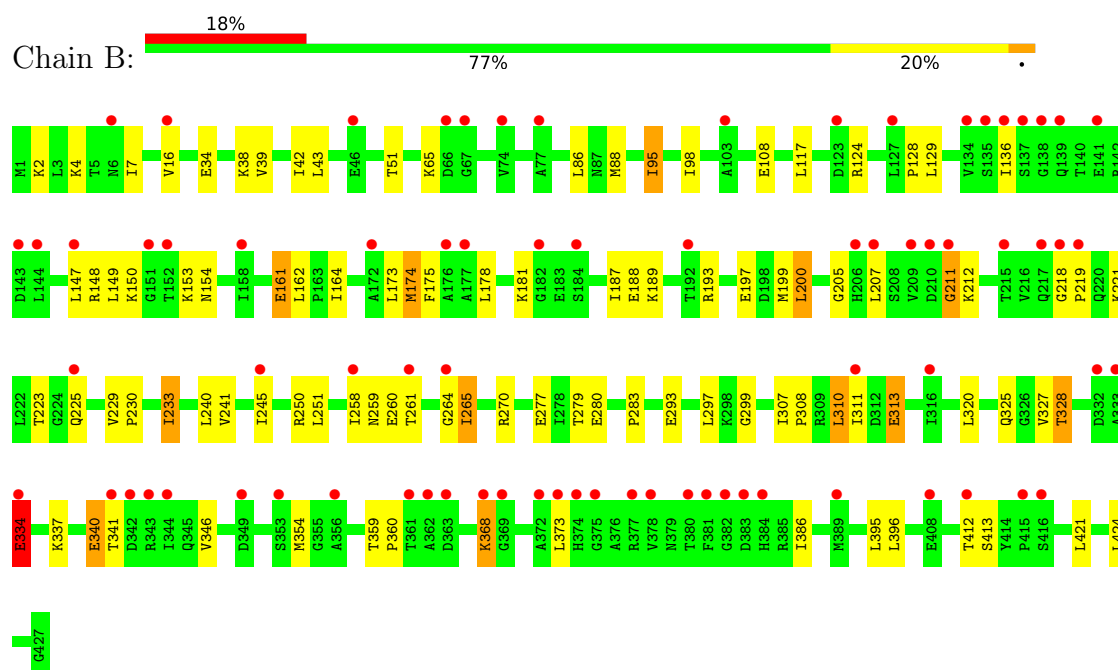
3 Residue-property plots [i](#)

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.

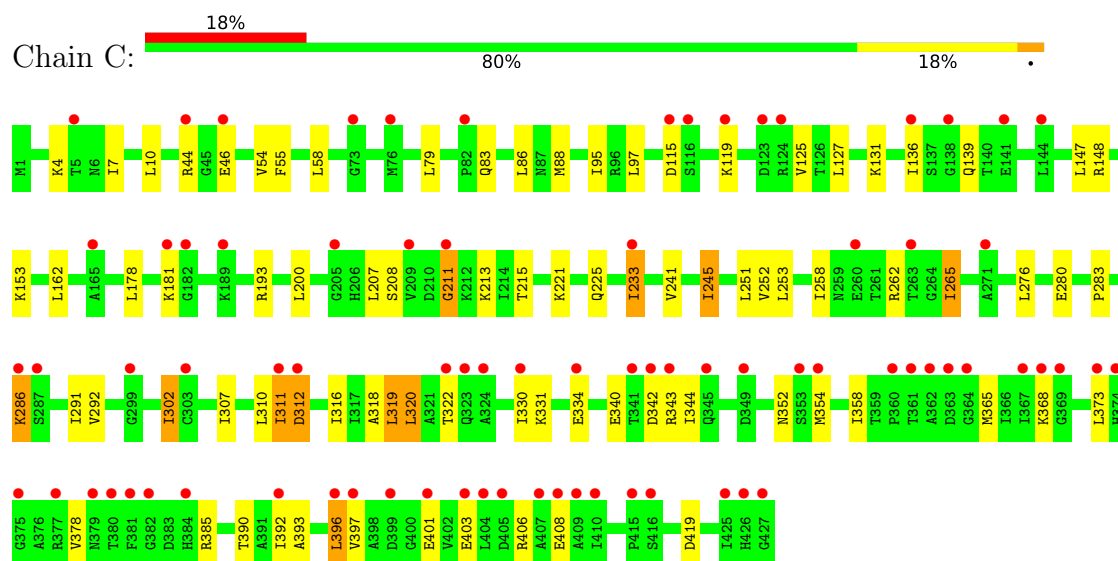
- Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase



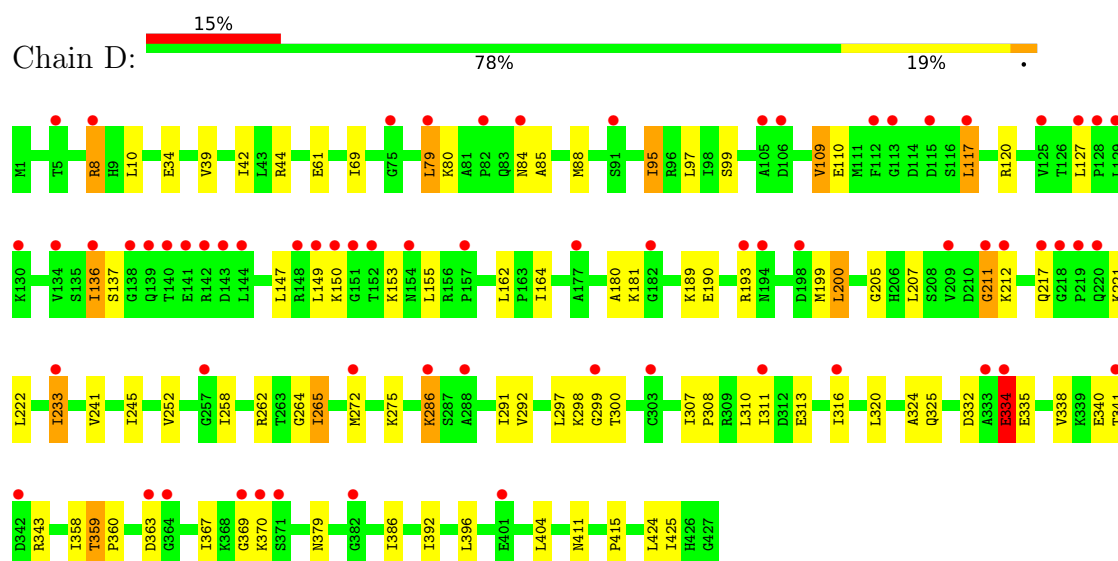
- Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase



• Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase



• Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.59Å 116.48Å 176.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 94.4 (10.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	19.68 (at 2.31Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.277 0.312 , 0.325	Depositor DCC
R_{free} test set	5011 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13615	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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	0.92	3/3252 (0.1%)	1.27	4/4391 (0.1%)
1	B	1.01	2/3252 (0.1%)	1.33	6/4391 (0.1%)
1	C	0.73	2/3251 (0.1%)	1.36	1/4388 (0.0%)
1	D	0.43	1/3252 (0.0%)	1.59	6/4391 (0.1%)
All	All	0.80	8/13007 (0.1%)	1.39	17/17561 (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	B	0	3
1	D	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	340	GLU	C-N	-48.81	0.65	1.33
1	A	340	GLU	C-N	41.32	1.85	1.33
1	C	334	GLU	C-N	33.43	1.80	1.33
1	A	334	GLU	C-N	-20.82	1.06	1.33
1	B	334	GLU	C-N	-19.47	1.07	1.33
1	D	340	GLU	C-N	5.37	1.40	1.33
1	A	307	ILE	CA-CB	5.22	1.57	1.54
1	C	307	ILE	CA-CB	5.18	1.57	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	334	GLU	O-C-N	-76.35	19.80	122.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	GLU	O-C-N	-72.05	26.76	122.59
1	B	340	GLU	O-C-N	-58.28	46.05	122.40
1	A	334	GLU	O-C-N	-55.01	47.57	121.83
1	D	340	GLU	O-C-N	-46.63	70.27	122.96
1	B	334	GLU	O-C-N	-31.33	54.00	121.35
1	A	340	GLU	CA-C-N	-22.45	82.12	121.85
1	A	340	GLU	C-N-CA	-22.45	82.12	121.85
1	B	334	GLU	CA-C-N	-10.24	102.88	122.53
1	B	334	GLU	C-N-CA	-10.24	102.88	122.53
1	B	340	GLU	CA-C-N	-9.42	103.54	121.54
1	B	340	GLU	C-N-CA	-9.42	103.54	121.54
1	D	340	GLU	CA-C-N	8.58	137.14	121.70
1	D	340	GLU	C-N-CA	8.58	137.14	121.70
1	A	340	GLU	O-C-N	6.52	130.83	123.27
1	D	334	GLU	CA-C-N	-5.34	111.35	121.54
1	D	334	GLU	C-N-CA	-5.34	111.35	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	GLU	Mainchain
1	B	334	GLU	Mainchain
1	B	340	GLU	Mainchain,Peptide
1	D	334	GLU	Mainchain

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	3212	0	3323	26	0
1	B	3212	0	3323	32	0
1	C	3212	0	3323	28	0
1	D	3212	0	3324	27	0
2	A	191	0	0	1	0
2	B	172	0	0	0	0
2	C	203	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	201	0	0	0	0
All	All	13615	0	13293	107	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 4.

All (107) 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:286:LYS:O	1:C:286:LYS:HG2	1.66	0.92
1:D:286:LYS:HG2	1:D:286:LYS:O	1.82	0.78
1:C:311:ILE:O	1:C:312:ASP:HB2	1.92	0.70
1:B:88:MET:HG3	1:B:95:ILE:HG23	1.74	0.68
1:B:193:ARG:HA	1:B:261:THR:HG21	1.76	0.68
1:C:241:VAL:HG22	1:C:320:LEU:HG	1.74	0.67
1:C:378:VAL:HG11	1:C:390:THR:HG21	1.79	0.63
1:A:211:GLY:O	1:A:212:LYS:HB2	1.99	0.61
1:C:193:ARG:HH21	1:C:262:ARG:HH11	1.50	0.59
1:C:397:VAL:HG11	2:C:598:HOH:O	2.03	0.58
1:D:109:VAL:HG12	1:D:149:LEU:HB3	1.84	0.58
1:A:245:ILE:HG12	1:A:323:GLN:HG3	1.85	0.58
1:C:352:ASN:HD21	1:C:358:ILE:H	1.52	0.57
1:D:79:LEU:H	1:D:79:LEU:HD23	1.69	0.57
1:B:245:ILE:HG22	1:B:396:LEU:HD21	1.88	0.55
1:D:272:MET:HE1	1:D:320:LEU:HG	1.87	0.55
1:C:302:ILE:O	1:C:302:ILE:HG13	2.05	0.55
1:A:51:THR:HG23	1:A:98:ILE:HD11	1.90	0.53
1:B:264:GLY:HA3	1:B:310:LEU:HB3	1.91	0.53
1:C:319:LEU:HD11	1:C:393:ALA:HB2	1.91	0.52
1:D:358:ILE:HG12	1:D:367:ILE:HG12	1.92	0.52
1:D:411:ASN:HD22	1:D:415:PRO:HA	1.76	0.51
1:B:108:GLU:HG3	1:B:150:LYS:HB2	1.92	0.51
1:D:332:ASP:H	1:D:363:ASP:HB2	1.75	0.51
1:B:211:GLY:O	1:B:212:LYS:HB2	2.11	0.51
1:A:188:GLU:HB2	1:A:212:LYS:HG2	1.93	0.51
1:A:96:ARG:HG2	1:A:125:VAL:HG21	1.92	0.50
1:D:39:VAL:HB	1:D:69:ILE:HB	1.94	0.50
1:A:54:VAL:HG13	1:A:86:LEU:HD22	1.93	0.50
1:D:8:ARG:HH22	1:D:425:ILE:HG23	1.77	0.49
1:D:10:LEU:HG	1:D:424:LEU:HB3	1.95	0.49
1:D:211:GLY:O	1:D:212:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HD23	1:A:251:LEU:HD11	1.93	0.49
1:B:250:ARG:HG3	1:B:293:GLU:HB3	1.93	0.49
1:D:241:VAL:HG22	1:D:320:LEU:HD13	1.95	0.49
1:A:279:THR:HA	1:B:277:GLU:HG2	1.94	0.49
1:A:327:VAL:HG22	1:A:368:LYS:HG3	1.95	0.49
1:B:280:GLU:HG2	1:C:252:VAL:HG11	1.95	0.48
1:C:10:LEU:HB3	1:C:251:LEU:HD21	1.94	0.48
1:C:283:PRO:HG3	1:D:275:LYS:HE2	1.94	0.48
1:B:241:VAL:HG22	1:B:320:LEU:HD13	1.95	0.48
1:B:51:THR:HG23	1:B:98:ILE:HD11	1.95	0.48
1:B:174:MET:HE2	1:B:200:LEU:HD12	1.96	0.48
1:C:311:ILE:O	1:C:312:ASP:CB	2.61	0.48
1:C:302:ILE:HG12	1:C:330:ILE:HG12	1.95	0.48
1:B:327:VAL:HG22	1:B:368:LYS:HG3	1.95	0.48
1:C:245:ILE:HD12	1:C:320:LEU:HD23	1.96	0.47
1:D:88:MET:HG3	1:D:95:ILE:HD12	1.97	0.47
1:B:251:LEU:HD22	1:B:424:LEU:HD22	1.96	0.47
1:D:265:ILE:HG12	1:D:313:GLU:HG2	1.96	0.47
1:C:241:VAL:HG21	1:C:316:ILE:HG13	1.97	0.47
1:A:39:VAL:HG11	1:A:42:ILE:HD12	1.98	0.46
1:A:134:VAL:HG13	1:A:151:GLY:HA2	1.97	0.46
1:D:307:ILE:HB	1:D:308:PRO:HD3	1.96	0.46
1:B:265:ILE:H	1:B:265:ILE:HG13	1.35	0.46
1:B:161:GLU:HG2	1:B:187:ILE:HB	1.97	0.46
1:D:200:LEU:HD22	1:D:205:GLY:HA3	1.98	0.45
1:C:54:VAL:HG13	1:C:86:LEU:HD22	1.99	0.45
1:A:202:GLN:HA	2:A:550:HOH:O	2.16	0.45
1:B:95:ILE:H	1:B:95:ILE:HG13	1.34	0.45
1:A:359:THR:HA	1:A:360:PRO:HD3	1.86	0.44
1:C:88:MET:HG3	1:C:95:ILE:HD12	1.99	0.44
1:A:271:ALA:HA	1:B:260:GLU:HG3	1.98	0.44
1:C:208:SER:HB3	1:C:215:THR:HB	2.00	0.44
1:D:155:LEU:HD23	1:D:180:ALA:HB2	1.99	0.44
1:B:39:VAL:HG11	1:B:42:ILE:HD12	1.99	0.44
1:A:258:ILE:HD13	1:A:288:ALA:HB3	1.99	0.43
1:B:233:ILE:H	1:B:233:ILE:HG13	1.44	0.43
1:A:55:PHE:HA	1:A:58:LEU:HD12	2.00	0.43
1:A:108:GLU:HG3	1:A:150:LYS:HG3	2.00	0.43
1:B:128:PRO:HB2	1:B:173:LEU:HD21	2.00	0.43
1:A:280:GLU:HG2	1:D:252:VAL:HG11	2.01	0.43
1:C:318:ALA:O	1:C:322:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LEU:HD22	1:B:205:GLY:HA3	2.01	0.43
1:A:159:HIS:CD2	1:A:185:VAL:HG22	2.53	0.43
1:D:39:VAL:HG11	1:D:42:ILE:HD12	2.01	0.42
1:C:233:ILE:H	1:C:233:ILE:HG13	1.43	0.42
1:C:344:ILE:HG23	1:C:365:MET:HE2	2.00	0.42
1:D:252:VAL:HG22	1:D:291:ILE:HG12	2.02	0.42
1:B:174:MET:HE1	1:B:197:GLU:HG3	2.02	0.42
1:D:264:GLY:HA3	1:D:310:LEU:HB3	2.01	0.42
1:B:299:GLY:HA2	1:B:328:THR:HG22	2.02	0.42
1:D:233:ILE:HD13	1:D:262:ARG:HB3	2.01	0.42
1:A:316:ILE:H	1:A:316:ILE:HG13	1.43	0.42
1:C:55:PHE:HA	1:C:58:LEU:HD12	2.01	0.42
1:C:312:ASP:HB3	1:C:385:ARG:HH21	1.85	0.42
1:A:233:ILE:H	1:A:233:ILE:HG13	1.70	0.42
1:A:355:GLY:HA3	1:A:373:LEU:HD23	2.01	0.41
1:B:175:PHE:HA	1:B:178:LEU:HD12	2.03	0.41
1:B:229:VAL:HA	1:B:230:PRO:HD3	1.89	0.41
1:B:354:MET:HB3	1:B:373:LEU:HD22	2.02	0.41
1:A:241:VAL:HG22	1:A:320:LEU:HG	2.03	0.41
1:A:187:ILE:HG12	1:A:213:LYS:HG3	2.03	0.41
1:C:265:ILE:H	1:C:265:ILE:HG13	1.57	0.41
1:A:250:ARG:HG3	1:A:293:GLU:HB3	2.02	0.41
1:A:275:LYS:HE2	1:B:283:PRO:HG3	2.03	0.41
1:B:359:THR:HA	1:B:360:PRO:HD3	1.91	0.41
1:C:252:VAL:HG22	1:C:291:ILE:HG12	2.03	0.41
1:D:117:LEU:HD23	1:D:120:ARG:HD3	2.03	0.41
1:D:241:VAL:HG21	1:D:316:ILE:HG22	2.01	0.41
1:D:324:ALA:O	1:D:369:GLY:HA3	2.21	0.41
1:C:211:GLY:C	1:C:213:LYS:H	2.28	0.40
1:B:218:GLY:HA3	1:B:219:PRO:HD2	1.92	0.40
1:B:307:ILE:HB	1:B:308:PRO:HD3	2.04	0.40
1:C:245:ILE:HG12	1:C:396:LEU:HD21	2.03	0.40
1:B:265:ILE:HG12	1:B:313:GLU:HG2	2.02	0.40
1:D:359:THR:HA	1:D:360:PRO:HD3	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	425/427 (100%)	401 (94%)	19 (4%)	5 (1%)	10	12
1	B	425/427 (100%)	397 (93%)	25 (6%)	3 (1%)	18	23
1	C	423/427 (99%)	395 (93%)	25 (6%)	3 (1%)	18	23
1	D	425/427 (100%)	396 (93%)	20 (5%)	9 (2%)	5	4
All	All	1698/1708 (99%)	1589 (94%)	89 (5%)	20 (1%)	10	12

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	ALA
1	B	341	THR
1	D	335	GLU
1	A	337	LYS
1	B	337	LYS
1	A	212	LYS
1	C	312	ASP
1	D	85	ALA
1	D	338	VAL
1	D	341	THR
1	A	209	VAL
1	C	373	LEU
1	D	137	SER
1	D	221	LYS
1	D	299	GLY
1	C	211	GLY
1	D	211	GLY
1	D	136	ILE
1	A	211	GLY
1	B	211	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	350/350 (100%)	301 (86%)	49 (14%)	3	3
1	B	350/350 (100%)	297 (85%)	53 (15%)	3	3
1	C	350/350 (100%)	299 (85%)	51 (15%)	3	3
1	D	350/350 (100%)	301 (86%)	49 (14%)	3	3
All	All	1400/1400 (100%)	1198 (86%)	202 (14%)	3	3

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	10	LEU
1	A	14	ILE
1	A	38	LYS
1	A	43	LEU
1	A	49	LEU
1	A	83	GLN
1	A	88	MET
1	A	95	ILE
1	A	97	LEU
1	A	110	GLU
1	A	117	LEU
1	A	131	LYS
1	A	136	ILE
1	A	147	LEU
1	A	150	LYS
1	A	153	LYS
1	A	161	GLU
1	A	162	LEU
1	A	164	ILE
1	A	173	LEU
1	A	181	LYS
1	A	190	GLU
1	A	199	MET

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Mol	Chain	Res	Type
1	A	207	LEU
1	A	213	LYS
1	A	216	VAL
1	A	233	ILE
1	A	245	ILE
1	A	258	ILE
1	A	263	THR
1	A	265	ILE
1	A	276	LEU
1	A	286	LYS
1	A	290	LEU
1	A	292	VAL
1	A	311	ILE
1	A	316	ILE
1	A	319	LEU
1	A	320	LEU
1	A	322	THR
1	A	328	THR
1	A	335	GLU
1	A	341	THR
1	A	345	GLN
1	A	361	THR
1	A	368	LYS
1	A	395	LEU
1	A	396	LEU
1	B	2	LYS
1	B	4	LYS
1	B	7	ILE
1	B	16	VAL
1	B	34	GLU
1	B	38	LYS
1	B	43	LEU
1	B	65	LYS
1	B	86	LEU
1	B	95	ILE
1	B	117	LEU
1	B	124	ARG
1	B	129	LEU
1	B	136	ILE
1	B	147	LEU
1	B	148	ARG
1	B	149	LEU

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Mol	Chain	Res	Type
1	B	153	LYS
1	B	154	ASN
1	B	161	GLU
1	B	162	LEU
1	B	164	ILE
1	B	174	MET
1	B	181	LYS
1	B	188	GLU
1	B	189	LYS
1	B	199	MET
1	B	200	LEU
1	B	207	LEU
1	B	221	LYS
1	B	223	THR
1	B	225	GLN
1	B	233	ILE
1	B	240	LEU
1	B	258	ILE
1	B	259	ASN
1	B	265	ILE
1	B	270	ARG
1	B	279	THR
1	B	297	LEU
1	B	310	LEU
1	B	311	ILE
1	B	313	GLU
1	B	325	GLN
1	B	328	THR
1	B	334	GLU
1	B	346	VAL
1	B	368	LYS
1	B	386	ILE
1	B	395	LEU
1	B	412	THR
1	B	413	SER
1	B	421	LEU
1	C	4	LYS
1	C	7	ILE
1	C	44	ARG
1	C	46	GLU
1	C	79	LEU
1	C	83	GLN

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Mol	Chain	Res	Type
1	C	97	LEU
1	C	115	ASP
1	C	119	LYS
1	C	125	VAL
1	C	127	LEU
1	C	131	LYS
1	C	136	ILE
1	C	139	GLN
1	C	147	LEU
1	C	148	ARG
1	C	153	LYS
1	C	162	LEU
1	C	178	LEU
1	C	181	LYS
1	C	200	LEU
1	C	207	LEU
1	C	221	LYS
1	C	225	GLN
1	C	233	ILE
1	C	245	ILE
1	C	253	LEU
1	C	258	ILE
1	C	265	ILE
1	C	276	LEU
1	C	280	GLU
1	C	286	LYS
1	C	292	VAL
1	C	302	ILE
1	C	310	LEU
1	C	311	ILE
1	C	319	LEU
1	C	320	LEU
1	C	331	LYS
1	C	340	GLU
1	C	342	ASP
1	C	343	ARG
1	C	354	MET
1	C	368	LYS
1	C	392	ILE
1	C	396	LEU
1	C	401	GLU
1	C	403	GLU

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Mol	Chain	Res	Type
1	C	406	ARG
1	C	408	GLU
1	C	419	ASP
1	D	8	ARG
1	D	34	GLU
1	D	44	ARG
1	D	61	GLU
1	D	79	LEU
1	D	80	LYS
1	D	84	ASN
1	D	95	ILE
1	D	97	LEU
1	D	99	SER
1	D	109	VAL
1	D	110	GLU
1	D	117	LEU
1	D	127	LEU
1	D	136	ILE
1	D	147	LEU
1	D	150	LYS
1	D	153	LYS
1	D	162	LEU
1	D	164	ILE
1	D	181	LYS
1	D	189	LYS
1	D	190	GLU
1	D	193	ARG
1	D	199	MET
1	D	200	LEU
1	D	207	LEU
1	D	217	GLN
1	D	222	LEU
1	D	233	ILE
1	D	245	ILE
1	D	258	ILE
1	D	265	ILE
1	D	286	LYS
1	D	292	VAL
1	D	297	LEU
1	D	298	LYS
1	D	300	THR
1	D	311	ILE

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Mol	Chain	Res	Type
1	D	325	GLN
1	D	334	GLU
1	D	343	ARG
1	D	359	THR
1	D	370	LYS
1	D	379	ASN
1	D	386	ILE
1	D	392	ILE
1	D	396	LEU
1	D	404	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	11	HIS
1	A	53	GLN
1	A	83	GLN
1	A	139	GLN
1	A	159	HIS
1	A	179	GLN
1	A	201	GLN
1	A	217	GLN
1	A	255	ASN
1	A	259	ASN
1	A	325	GLN
1	B	6	ASN
1	B	154	ASN
1	B	168	GLN
1	B	179	GLN
1	B	259	ASN
1	B	325	GLN
1	B	426	HIS
1	C	83	GLN
1	C	90	ASN
1	C	139	GLN
1	C	201	GLN
1	C	220	GLN
1	C	323	GLN
1	C	352	ASN
1	C	411	ASN
1	D	6	ASN

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Mol	Chain	Res	Type
1	D	159	HIS
1	D	201	GLN
1	D	206	HIS
1	D	254	GLN
1	D	259	ASN
1	D	325	GLN
1	D	379	ASN
1	D	411	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	A	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	340:GLU	C	341:THR	N	2.02
1	A	340:GLU	C	341:THR	N	1.85
1	C	334:GLU	C	335:GLU	N	1.80
1	B	334:GLU	C	335:GLU	N	1.07
1	A	334:GLU	C	335:GLU	N	1.06
1	B	340:GLU	C	341:THR	N	0.65

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	421/427 (98%)	1.19	72 (17%) 4 5	19, 32, 59, 80	0
1	B	421/427 (98%)	1.31	76 (18%) 3 4	19, 39, 60, 87	0
1	C	421/427 (98%)	1.21	78 (18%) 3 4	19, 36, 61, 90	0
1	D	421/427 (98%)	1.09	66 (15%) 5 6	17, 33, 57, 72	0
All	All	1684/1708 (98%)	1.20	292 (17%) 4 4	17, 35, 60, 90	0

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	THR	8.4
1	D	369	GLY	7.8
1	C	211	GLY	7.7
1	A	369	GLY	7.7
1	A	356	ALA	7.5
1	B	382	GLY	7.4
1	B	218	GLY	6.1
1	C	369	GLY	6.1
1	D	194	ASN	5.8
1	C	311	ILE	5.8
1	A	255	ASN	5.7
1	B	211	GLY	5.7
1	A	341	THR	5.6
1	D	211	GLY	5.3
1	C	405	ASP	5.2
1	B	341	THR	4.9
1	C	115	ASP	4.9
1	B	342	ASP	4.6
1	C	342	ASP	4.6
1	D	151	GLY	4.6
1	B	383	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	412	THR	4.6
1	C	397	VAL	4.6
1	A	333	ALA	4.5
1	B	138	GLY	4.4
1	A	83	GLN	4.4
1	C	5	THR	4.4
1	C	381	PHE	4.4
1	A	355	GLY	4.4
1	A	192	THR	4.3
1	A	211	GLY	4.3
1	B	369	GLY	4.3
1	A	352	ASN	4.3
1	A	303	CYS	4.2
1	D	341	THR	4.2
1	A	410	ILE	4.1
1	A	411	ASN	4.1
1	B	380	THR	4.0
1	B	381	PHE	4.0
1	C	399	ASP	3.9
1	C	375	GLY	3.8
1	D	127	LEU	3.8
1	B	152	THR	3.7
1	C	364	GLY	3.7
1	D	152	THR	3.7
1	B	258	ILE	3.7
1	D	134	VAL	3.7
1	D	142	ARG	3.7
1	A	208	SER	3.7
1	D	144	LEU	3.6
1	C	324	ALA	3.6
1	C	362	ALA	3.6
1	B	139	GLN	3.6
1	D	311	ILE	3.5
1	B	217	GLN	3.5
1	C	425	ILE	3.5
1	C	407	ALA	3.5
1	A	304	GLY	3.5
1	B	67	GLY	3.5
1	D	218	GLY	3.5
1	B	344	ILE	3.5
1	A	382	GLY	3.4
1	A	408	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	75	GLY	3.4
1	C	144	LEU	3.3
1	C	373	LEU	3.3
1	D	193	ARG	3.3
1	B	368	LYS	3.3
1	C	354	MET	3.3
1	B	334	GLU	3.3
1	B	408	GLU	3.3
1	B	210	ASP	3.3
1	B	333	ALA	3.3
1	C	299	GLY	3.3
1	C	408	GLU	3.3
1	D	150	LYS	3.3
1	A	413	SER	3.3
1	D	299	GLY	3.2
1	A	357	ASP	3.2
1	B	144	LEU	3.2
1	B	316	ILE	3.2
1	A	375	GLY	3.2
1	D	154	ASN	3.2
1	D	342	ASP	3.1
1	B	46	GLU	3.1
1	D	382	GLY	3.1
1	B	378	VAL	3.1
1	D	84	ASN	3.0
1	D	138	GLY	3.0
1	D	303	CYS	3.0
1	B	361	THR	3.0
1	B	135	SER	3.0
1	B	143	ASP	3.0
1	C	138	GLY	3.0
1	A	415	PRO	3.0
1	A	184	SER	3.0
1	C	427	GLY	3.0
1	B	362	ALA	2.9
1	D	333	ALA	2.9
1	B	374	HIS	2.9
1	C	303	CYS	2.9
1	D	370	LYS	2.9
1	B	245	ILE	2.9
1	D	82	PRO	2.9
1	D	79	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	66	ASP	2.9
1	C	401	GLU	2.9
1	B	137	SER	2.9
1	B	375	GLY	2.9
1	C	382	GLY	2.9
1	A	384	HIS	2.9
1	A	409	ALA	2.9
1	C	260	GLU	2.9
1	A	416	SER	2.8
1	D	139	GLN	2.8
1	B	176	ALA	2.8
1	A	392	ILE	2.8
1	C	44	ARG	2.8
1	B	103	ALA	2.8
1	A	300	THR	2.8
1	C	377	ARG	2.8
1	B	225	GLN	2.8
1	D	157	PRO	2.8
1	A	324	ALA	2.8
1	C	380	THR	2.8
1	D	5	THR	2.8
1	D	149	LEU	2.8
1	A	381	PHE	2.8
1	B	332	ASP	2.7
1	A	9	HIS	2.7
1	A	115	ASP	2.7
1	A	361	THR	2.7
1	C	392	ILE	2.7
1	D	233	ILE	2.7
1	B	184	SER	2.7
1	C	181	LYS	2.7
1	D	288	ALA	2.7
1	C	374	HIS	2.7
1	B	209	VAL	2.7
1	D	209	VAL	2.7
1	C	379	ASN	2.7
1	D	91	SER	2.7
1	D	401	GLU	2.7
1	D	106	ASP	2.7
1	C	46	GLU	2.7
1	C	119	LYS	2.6
1	C	334	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	403	GLU	2.6
1	C	345	GLN	2.6
1	A	246	ALA	2.6
1	B	356	ALA	2.6
1	D	143	ASP	2.6
1	D	128	PRO	2.6
1	C	189	LYS	2.6
1	A	152	THR	2.6
1	D	257	GLY	2.6
1	A	207	LEU	2.5
1	C	363	ASP	2.5
1	D	125	VAL	2.5
1	A	233	ILE	2.5
1	B	343	ARG	2.5
1	A	332	ASP	2.5
1	B	136	ILE	2.5
1	D	105	ALA	2.5
1	D	286	LYS	2.5
1	B	219	PRO	2.5
1	B	264	GLY	2.5
1	D	140	THR	2.5
1	A	334	GLU	2.5
1	A	311	ILE	2.5
1	C	271	ALA	2.5
1	A	75	GLY	2.5
1	D	182	GLY	2.5
1	A	344	ILE	2.4
1	B	147	LEU	2.4
1	C	396	LEU	2.4
1	D	115	ASP	2.4
1	D	363	ASP	2.4
1	C	205	GLY	2.4
1	A	359	THR	2.4
1	B	192	THR	2.4
1	C	233	ILE	2.4
1	A	76	MET	2.4
1	B	363	ASP	2.4
1	B	151	GLY	2.4
1	C	353	SER	2.4
1	A	366	ILE	2.4
1	C	330	ILE	2.4
1	C	368	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	141	GLU	2.4
1	D	334	GLU	2.4
1	D	177	ALA	2.4
1	B	416	SER	2.4
1	B	16	VAL	2.4
1	C	136	ILE	2.4
1	A	127	LEU	2.4
1	B	127	LEU	2.4
1	C	404	LEU	2.4
1	D	141	GLU	2.4
1	A	398	ALA	2.3
1	D	272	MET	2.3
1	A	404	LEU	2.3
1	B	373	LEU	2.3
1	A	405	ASP	2.3
1	B	134	VAL	2.3
1	B	384	HIS	2.3
1	B	207	LEU	2.3
1	C	349	ASP	2.3
1	A	326	GLY	2.3
1	D	113	GLY	2.3
1	D	364	GLY	2.3
1	A	362	ALA	2.3
1	B	177	ALA	2.3
1	C	76	MET	2.3
1	B	353	SER	2.3
1	C	116	SER	2.3
1	A	426	HIS	2.3
1	C	426	HIS	2.3
1	B	141	GLU	2.3
1	D	220	GLN	2.3
1	D	136	ILE	2.3
1	C	415	PRO	2.3
1	A	116	SER	2.3
1	C	416	SER	2.3
1	D	371	SER	2.3
1	A	6	ASN	2.2
1	B	123	ASP	2.2
1	D	198	ASP	2.2
1	C	124	ARG	2.2
1	C	343	ARG	2.2
1	A	422	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	311	ILE	2.2
1	B	6	ASN	2.2
1	A	142	ARG	2.2
1	C	360	PRO	2.2
1	B	206	HIS	2.2
1	D	217	GLN	2.2
1	A	316	ILE	2.2
1	C	209	VAL	2.2
1	D	112	PHE	2.2
1	A	123	ASP	2.2
1	A	379	ASN	2.2
1	B	349	ASP	2.2
1	D	148	ARG	2.2
1	C	286	LYS	2.2
1	D	130	LYS	2.2
1	B	412	THR	2.2
1	C	322	THR	2.2
1	A	377	ARG	2.2
1	B	377	ARG	2.2
1	C	323	GLN	2.2
1	A	180	ALA	2.2
1	A	164	ILE	2.1
1	D	212	LYS	2.1
1	C	182	GLY	2.1
1	A	193	ARG	2.1
1	B	415	PRO	2.1
1	C	82	PRO	2.1
1	D	219	PRO	2.1
1	B	182	GLY	2.1
1	A	5	THR	2.1
1	A	305	ALA	2.1
1	B	77	ALA	2.1
1	B	172	ALA	2.1
1	C	409	ALA	2.1
1	C	410	ILE	2.1
1	D	316	ILE	2.1
1	C	73	GLY	2.1
1	A	288	ALA	2.1
1	B	372	ALA	2.1
1	C	165	ALA	2.1
1	A	354	MET	2.1
1	B	389	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	123	ASP	2.1
1	C	384	HIS	2.1
1	D	129	LEU	2.1
1	A	210	ASP	2.1
1	B	215	THR	2.0
1	B	261	THR	2.0
1	C	263	THR	2.0
1	C	312	ASP	2.0
1	A	245	ILE	2.0
1	B	158	ILE	2.0
1	A	397	VAL	2.0
1	B	74	VAL	2.0
1	C	287	SER	2.0
1	C	361	THR	2.0
1	A	321	ALA	2.0
1	A	194	ASN	2.0
1	D	117	LEU	2.0
1	C	367	ILE	2.0
1	D	8	ARG	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.