



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:58 PM GMT

PDB ID : 1RF5
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
<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

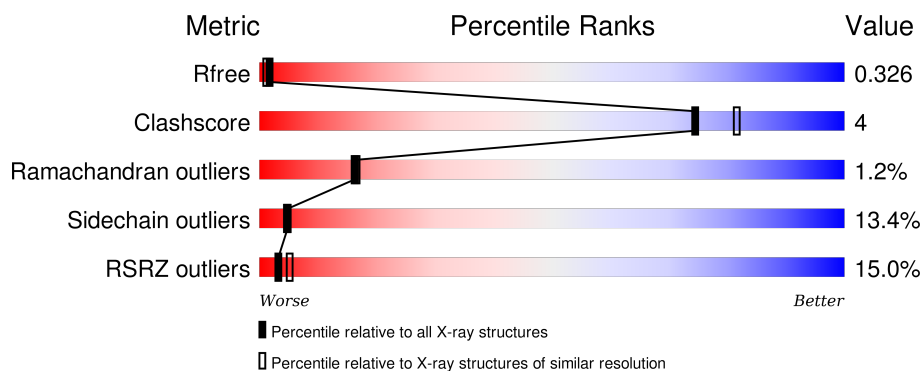
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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	427	<div> <div>12%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	B	427	<div> <div>17%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
1	C	427	<div> <div>17%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	D	427	<div> <div>13%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>

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			

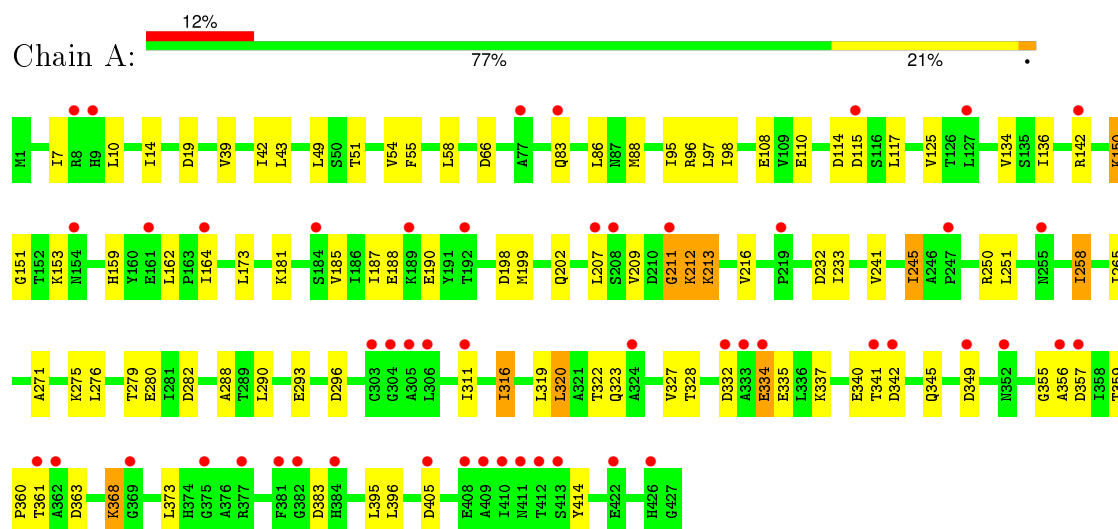
- Molecule 2 is water.

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		

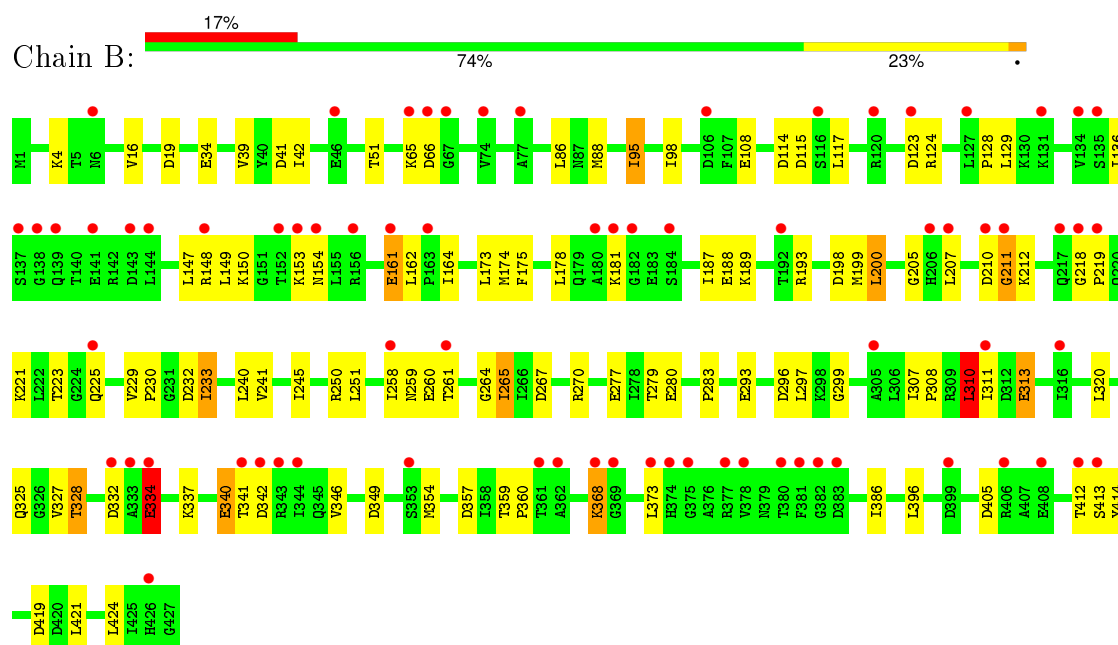
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

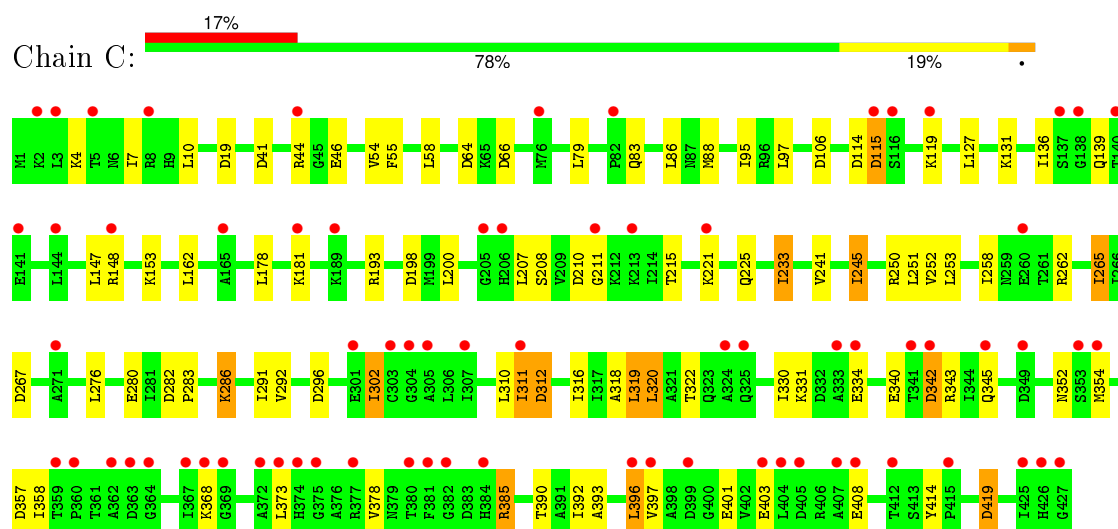
- Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase



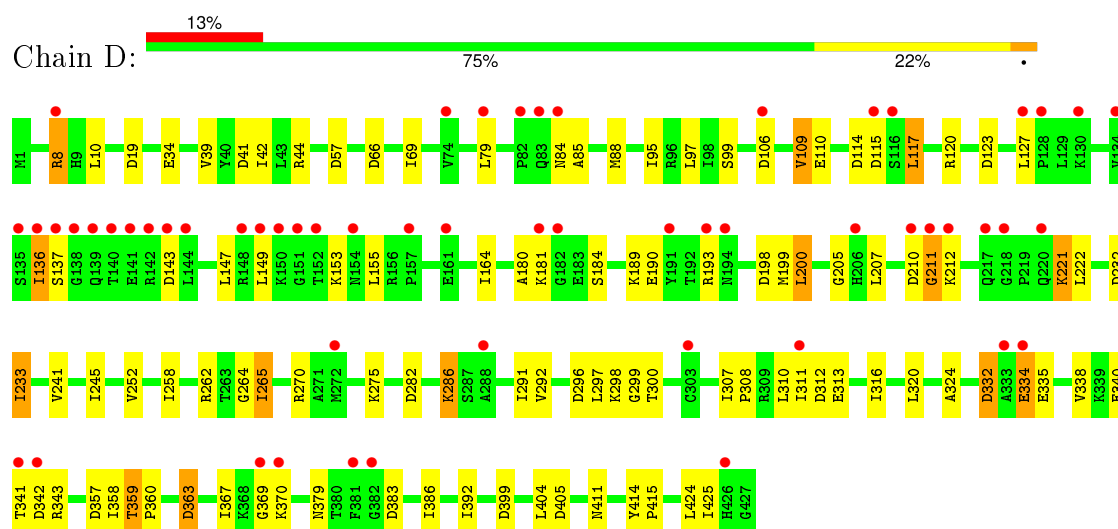
- Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase



- 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 9.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 95.7 (9.99-2.30)	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 0.311 , 0.326	Depositor DCC
R_{free} test set	5013 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 62.2	EDS
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 100263 reflections	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, 0.375 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	0.53	2/3252 (0.1%)	1.02	18/4391 (0.4%)
1	B	0.63	2/3252 (0.1%)	1.25	24/4391 (0.5%)
1	C	0.46	1/3251 (0.0%)	1.15	17/4388 (0.4%)
1	D	0.30	0/3252	1.35	26/4391 (0.6%)
All	All	0.50	5/13007 (0.0%)	1.20	85/17561 (0.5%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	340	GLU	C-N	-29.87	0.65	1.34
1	A	340	GLU	C-N	22.25	1.85	1.34
1	C	334	GLU	C-N	20.19	1.80	1.34
1	A	334	GLU	C-N	-11.84	1.06	1.34
1	B	334	GLU	C-N	-11.61	1.07	1.34

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	334	GLU	O-C-N	-64.31	19.80	122.70
1	C	334	GLU	O-C-N	-59.96	26.76	122.70
1	B	340	GLU	O-C-N	-47.90	46.05	122.70
1	A	334	GLU	O-C-N	-46.96	47.57	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	GLU	O-C-N	-42.94	54.00	122.70
1	D	340	GLU	O-C-N	-32.77	70.27	122.70
1	D	340	GLU	CA-C-N	23.30	168.47	117.20
1	B	334	GLU	CA-C-N	-18.60	76.27	117.20
1	A	340	GLU	C-N-CA	-15.83	82.12	121.70
1	B	340	GLU	CA-C-N	14.68	149.50	117.20
1	C	334	GLU	CA-C-N	-8.64	98.18	117.20
1	B	334	GLU	C-N-CA	-7.53	102.88	121.70
1	B	340	GLU	C-N-CA	-7.26	103.54	121.70
1	D	334	GLU	CA-C-N	-7.00	101.80	117.20
1	C	114	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	114	ASP	CB-CG-OD2	6.47	124.12	118.30
1	C	210	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	114	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	232	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	232	ASP	CB-CG-OD2	6.25	123.92	118.30
1	D	340	GLU	C-N-CA	6.18	137.14	121.70
1	D	106	ASP	CB-CG-OD2	6.15	123.84	118.30
1	D	210	ASP	CB-CG-OD2	6.15	123.83	118.30
1	D	114	ASP	CB-CG-OD2	6.13	123.81	118.30
1	B	198	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	106	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	198	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	357	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	123	ASP	CB-CG-OD2	5.97	123.67	118.30
1	D	399	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	198	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	57	ASP	CB-CG-OD2	5.91	123.62	118.30
1	D	123	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	64	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	282	ASP	CB-CG-OD2	5.89	123.60	118.30
1	D	312	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	349	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	232	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	363	ASP	CB-CG-OD2	5.82	123.53	118.30
1	B	419	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	41	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	342	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	198	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	267	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	357	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	349	ASP	CB-CG-OD2	5.74	123.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	405	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	296	ASP	CB-CG-OD2	5.60	123.34	118.30
1	D	66	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	282	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	115	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	383	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	357	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	383	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	19	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	332	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	405	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	41	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	19	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	310	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	332	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	342	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	210	ASP	CB-CG-OD2	5.20	122.97	118.30
1	A	342	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	19	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	282	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	19	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	267	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	332	ASP	CB-CG-OD2	5.14	122.92	118.30
1	C	115	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	342	ASP	CB-CG-OD2	5.12	122.90	118.30
1	B	296	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	340	GLU	O-C-N	5.08	130.83	122.70
1	B	405	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	296	ASP	CB-CG-OD2	5.06	122.85	118.30
1	D	296	ASP	CB-CG-OD2	5.05	122.85	118.30
1	C	419	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	357	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	66	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	143	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	66	ASP	CB-CG-OD2	5.04	122.83	118.30
1	D	115	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	41	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	66	ASP	CB-CG-OD2	5.00	122.81	118.30

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	30	0
1	C	3212	0	3323	26	0
1	D	3212	0	3324	26	0
2	A	191	0	0	1	0
2	B	172	0	0	0	0
2	C	203	0	0	1	0
2	D	201	0	0	0	0
All	All	13615	0	13293	102	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 (102) 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:HG2	1:C:286:LYS:O	1.66	0.92
1:D:286:LYS:O	1:D:286:LYS:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:211:GLY:O	1:D:212:LYS:HB2	2.12	0.49
1:D:10:LEU:HG	1:D:424:LEU:HB3	1.95	0.49
1:A:10:LEU:HD23	1:A:251:LEU:HD11	1.93	0.49
1:D:241:VAL:HG22	1:D:320:LEU:HD13	1.95	0.49
1:B:250:ARG:HG3	1:B:293:GLU:HB3	1.93	0.49
1:A:327:VAL:HG22	1:A:368:LYS:HG3	1.95	0.49
1:A:279:THR:HA	1:B:277:GLU:HG2	1.94	0.49
1:C:10:LEU:HB3	1:C:251:LEU:HD21	1.94	0.48
1:B:280:GLU:HG2	1:C:252:VAL:HG11	1.95	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:88:MET:HG3	1:C:95:ILE:HD12	1.99	0.44
1:A:359:THR:HA	1:A:360:PRO:HD3	1.86	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:HG13	1:B:233:ILE:H	1.44	0.43
1:B:128:PRO:HB2	1:B:173:LEU:HD21	2.00	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: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
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:D:252:VAL:HG22	1:D:291:ILE:HG12	2.02	0.42
1:C:233:ILE:H	1:C:233:ILE:HG13	1.43	0.42
1:D:264:GLY:HA3	1:D:310:LEU:HB3	2.01	0.42
1:D:233:ILE:HD13	1:D:262:ARG:HB3	2.01	0.42
1:B:299:GLY:HA2	1:B:328:THR:HG22	2.02	0.42
1:A:316:ILE:HG13	1:A:316:ILE:H	1.43	0.42
1:C:312:ASP:HB3	1:C:385:ARG:HH21	1.85	0.42
1:C:55:PHE:HA	1:C:58:LEU:HD12	2.01	0.42
1:A:233:ILE:HG13	1:A:233:ILE:H	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:D:241:VAL:HG21	1:D:316:ILE:HG22	2.01	0.41
1:C:252:VAL:HG22	1:C:291:ILE:HG12	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LEU:HD23	1:D:120:ARG:HD3	2.03	0.41
1:B:359:THR:HA	1:B:360:PRO:HD3	1.91	0.41
1:D:324:ALA:O	1:D:369:GLY:HA3	2.21	0.41
1:C:245:ILE:HG12	1:C:396:LEU:HD21	2.03	0.40
1:B:307:ILE:HB	1:B:308:PRO:HD3	2.04	0.40
1:B:218:GLY:HA3	1:B:219:PRO:HD2	1.92	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 [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	425/427 (100%)	401 (94%)	19 (4%)	5 (1%)	16	16
1	B	425/427 (100%)	397 (93%)	25 (6%)	3 (1%)	26	31
1	C	423/427 (99%)	395 (93%)	25 (6%)	3 (1%)	26	31
1	D	425/427 (100%)	396 (93%)	20 (5%)	9 (2%)	9	7
All	All	1698/1708 (99%)	1589 (94%)	89 (5%)	20 (1%)	16	16

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

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Mol	Chain	Res	Type
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%)	308 (88%)	42 (12%)	6	6
1	B	350/350 (100%)	301 (86%)	49 (14%)	4	4
1	C	350/350 (100%)	297 (85%)	53 (15%)	3	3
1	D	350/350 (100%)	306 (87%)	44 (13%)	5	5
All	All	1400/1400 (100%)	1212 (87%)	188 (13%)	5	5

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	14	ILE
1	A	43	LEU
1	A	49	LEU
1	A	83	GLN
1	A	88	MET
1	A	95	ILE
1	A	97	LEU

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Mol	Chain	Res	Type
1	A	110	GLU
1	A	117	LEU
1	A	136	ILE
1	A	142	ARG
1	A	150	LYS
1	A	153	LYS
1	A	162	LEU
1	A	164	ILE
1	A	173	LEU
1	A	181	LYS
1	A	190	GLU
1	A	199	MET
1	A	207	LEU
1	A	213	LYS
1	A	216	VAL
1	A	245	ILE
1	A	258	ILE
1	A	265	ILE
1	A	276	LEU
1	A	290	LEU
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	A	414	TYR
1	B	4	LYS
1	B	16	VAL
1	B	34	GLU
1	B	65	LYS
1	B	86	LEU
1	B	95	ILE
1	B	117	LEU
1	B	124	ARG

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Mol	Chain	Res	Type
1	B	129	LEU
1	B	136	ILE
1	B	147	LEU
1	B	148	ARG
1	B	149	LEU
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	412	THR
1	B	413	SER
1	B	414	TYR
1	B	421	LEU
1	C	4	LYS

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Mol	Chain	Res	Type
1	C	7	ILE
1	C	44	ARG
1	C	46	GLU
1	C	79	LEU
1	C	83	GLN
1	C	97	LEU
1	C	115	ASP
1	C	119	LYS
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	250	ARG
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	345	GLN

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Mol	Chain	Res	Type
1	C	354	MET
1	C	368	LYS
1	C	385	ARG
1	C	392	ILE
1	C	396	LEU
1	C	401	GLU
1	C	403	GLU
1	C	408	GLU
1	C	414	TYR
1	C	419	ASP
1	D	8	ARG
1	D	34	GLU
1	D	44	ARG
1	D	84	ASN
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	153	LYS
1	D	164	ILE
1	D	181	LYS
1	D	184	SER
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	221	LYS
1	D	222	LEU
1	D	233	ILE
1	D	245	ILE
1	D	258	ILE
1	D	265	ILE
1	D	270	ARG
1	D	286	LYS
1	D	292	VAL
1	D	297	LEU

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Mol	Chain	Res	Type
1	D	298	LYS
1	D	300	THR
1	D	311	ILE
1	D	343	ARG
1	D	359	THR
1	D	363	ASP
1	D	370	LYS
1	D	379	ASN
1	D	386	ILE
1	D	392	ILE
1	D	404	LEU
1	D	414	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	159	HIS
1	A	255	ASN
1	A	259	ASN
1	A	325	GLN
1	B	6	ASN
1	B	325	GLN
1	C	83	GLN
1	C	90	ASN
1	C	220	GLN
1	C	259	ASN
1	C	352	ASN
1	C	411	ASN
1	D	254	GLN
1	D	259	ASN
1	D	379	ASN
1	D	411	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	421/427 (98%)	0.91	51 (12%) 6 9	19, 32, 59, 80	0
1	B	421/427 (98%)	1.11	73 (17%) 2 3	19, 39, 60, 87	0
1	C	421/427 (98%)	1.00	72 (17%) 2 3	19, 36, 61, 90	0
1	D	421/427 (98%)	0.84	56 (13%) 4 7	17, 33, 57, 72	0
All	All	1684/1708 (98%)	0.96	252 (14%) 3 5	17, 35, 60, 90	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	THR	15.4
1	B	382	GLY	10.8
1	A	356	ALA	9.9
1	B	341	THR	9.2
1	B	342	ASP	8.0
1	C	342	ASP	6.7
1	C	381	PHE	6.2
1	A	341	THR	6.2
1	C	405	ASP	6.0
1	B	381	PHE	5.9
1	D	341	THR	5.8
1	D	154	ASN	5.8
1	A	369	GLY	5.6
1	D	142	ARG	5.2
1	D	369	GLY	5.1
1	C	382	GLY	5.0
1	A	334	GLU	4.9
1	A	412	THR	4.9
1	D	342	ASP	4.8
1	C	311	ILE	4.8
1	C	362	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	362	ALA	4.7
1	B	383	ASP	4.7
1	D	144	LEU	4.6
1	B	217	GLN	4.4
1	B	139	GLN	4.4
1	B	344	ILE	4.4
1	A	83	GLN	4.4
1	C	211	GLY	4.3
1	B	334	GLU	4.3
1	C	399	ASP	4.3
1	D	148	ARG	4.3
1	C	305	ALA	4.2
1	C	115	ASP	4.2
1	B	152	THR	4.1
1	A	357	ASP	4.0
1	C	408	GLU	4.0
1	A	382	GLY	4.0
1	D	127	LEU	4.0
1	C	377	ARG	3.9
1	A	381	PHE	3.9
1	B	218	GLY	3.9
1	A	192	THR	3.9
1	D	218	GLY	3.9
1	D	152	THR	3.8
1	A	208	SER	3.8
1	D	194	ASN	3.7
1	D	311	ILE	3.7
1	C	303	CYS	3.7
1	B	138	GLY	3.7
1	B	374	HIS	3.7
1	B	380	THR	3.7
1	B	144	LEU	3.6
1	C	397	VAL	3.6
1	A	303	CYS	3.6
1	D	84	ASN	3.6
1	A	411	ASN	3.6
1	A	410	ILE	3.5
1	D	150	LYS	3.5
1	C	369	GLY	3.5
1	A	255	ASN	3.5
1	A	408	GLU	3.5
1	B	182	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	333	ALA	3.5
1	D	115	ASP	3.5
1	A	426	HIS	3.5
1	A	333	ALA	3.5
1	B	211	GLY	3.4
1	B	210	ASP	3.4
1	A	352	ASN	3.4
1	B	206	HIS	3.3
1	B	219	PRO	3.3
1	D	139	GLN	3.3
1	D	382	GLY	3.3
1	B	412	THR	3.2
1	C	380	THR	3.2
1	C	425	ILE	3.2
1	D	211	GLY	3.2
1	B	399	ASP	3.2
1	B	156	ARG	3.2
1	D	141	GLU	3.2
1	C	5	THR	3.2
1	B	361	THR	3.2
1	C	141	GLU	3.2
1	C	427	GLY	3.1
1	C	353	SER	3.1
1	C	426	HIS	3.1
1	D	106	ASP	3.1
1	B	137	SER	3.1
1	C	407	ALA	3.0
1	C	144	LEU	3.0
1	B	181	LYS	3.0
1	C	368	LYS	3.0
1	D	138	GLY	3.0
1	C	334	GLU	3.0
1	B	127	LEU	3.0
1	C	404	LEU	3.0
1	A	405	ASP	3.0
1	B	375	GLY	3.0
1	A	211	GLY	3.0
1	B	141	GLU	2.9
1	C	333	ALA	2.9
1	C	44	ARG	2.9
1	C	325	GLN	2.9
1	D	161	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	415	PRO	2.9
1	A	77	ALA	2.9
1	B	353	SER	2.9
1	A	311	ILE	2.9
1	A	384	HIS	2.8
1	D	206	HIS	2.8
1	D	79	LEU	2.8
1	A	184	SER	2.8
1	D	140	THR	2.8
1	B	311	ILE	2.8
1	B	106	ASP	2.8
1	D	426	HIS	2.8
1	B	408	GLU	2.8
1	B	343	ARG	2.8
1	A	142	ARG	2.8
1	B	377	ARG	2.8
1	D	151	GLY	2.7
1	D	210	ASP	2.7
1	C	304	GLY	2.7
1	A	413	SER	2.7
1	B	261	THR	2.7
1	D	157	PRO	2.7
1	B	406	ARG	2.7
1	C	148	ARG	2.7
1	A	9	HIS	2.7
1	C	374	HIS	2.7
1	C	364	GLY	2.7
1	B	225	GLN	2.7
1	A	207	LEU	2.7
1	C	354	MET	2.7
1	C	375	GLY	2.7
1	B	46	GLU	2.6
1	C	359	THR	2.6
1	B	135	SER	2.6
1	C	138	GLY	2.6
1	A	332	ASP	2.6
1	C	384	HIS	2.6
1	D	136	ILE	2.6
1	D	137	SER	2.6
1	B	74	VAL	2.6
1	B	67	GLY	2.6
1	B	161	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	305	ALA	2.6
1	A	409	ALA	2.6
1	C	137	SER	2.6
1	C	363	ASP	2.6
1	C	165	ALA	2.6
1	B	6	ASN	2.6
1	D	8	ARG	2.5
1	C	349	ASP	2.5
1	B	154	ASN	2.5
1	B	65	LYS	2.5
1	B	131	LYS	2.5
1	B	332	ASP	2.5
1	A	361	THR	2.5
1	C	360	PRO	2.5
1	D	181	LYS	2.5
1	D	193	ARG	2.5
1	D	334	GLU	2.5
1	C	205	GLY	2.5
1	D	135	SER	2.5
1	C	2	LYS	2.4
1	A	375	GLY	2.4
1	B	77	ALA	2.4
1	D	303	CYS	2.4
1	D	143	ASP	2.4
1	D	182	GLY	2.4
1	A	154	ASN	2.4
1	B	120	ARG	2.4
1	D	333	ALA	2.4
1	C	82	PRO	2.4
1	D	128	PRO	2.4
1	C	8	ARG	2.4
1	C	116	SER	2.4
1	D	82	PRO	2.4
1	C	372	ALA	2.4
1	C	221	LYS	2.4
1	B	305	ALA	2.4
1	A	127	LEU	2.3
1	B	207	LEU	2.3
1	B	369	GLY	2.3
1	B	258	ILE	2.3
1	B	316	ILE	2.3
1	A	8	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	123	ASP	2.3
1	C	324	ALA	2.3
1	C	307	ILE	2.3
1	C	412	THR	2.3
1	B	368	LYS	2.3
1	A	342	ASP	2.3
1	D	288	ALA	2.3
1	C	403	GLU	2.3
1	A	349	ASP	2.3
1	C	3	LEU	2.3
1	D	272	MET	2.3
1	C	345	GLN	2.3
1	D	74	VAL	2.3
1	D	134	VAL	2.3
1	C	260	GLU	2.2
1	B	148	ARG	2.2
1	B	163	PRO	2.2
1	A	164	ILE	2.2
1	D	381	PHE	2.2
1	C	189	LYS	2.2
1	D	370	LYS	2.2
1	C	76	MET	2.2
1	B	192	THR	2.2
1	C	367	ILE	2.2
1	A	115	ASP	2.2
1	B	373	LEU	2.2
1	C	396	LEU	2.2
1	A	219	PRO	2.2
1	D	217	GLN	2.2
1	A	422	GLU	2.2
1	C	373	LEU	2.2
1	A	324	ALA	2.2
1	B	180	ALA	2.2
1	C	271	ALA	2.2
1	B	153	LYS	2.1
1	C	181	LYS	2.1
1	A	306	LEU	2.1
1	B	426	HIS	2.1
1	D	149	LEU	2.1
1	B	134	VAL	2.1
1	B	378	VAL	2.1
1	D	116	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	304	GLY	2.1
1	D	83	GLN	2.1
1	A	189	LYS	2.1
1	C	301	GLU	2.1
1	B	66	ASP	2.1
1	B	116	SER	2.1
1	A	161	GLU	2.1
1	D	191	TYR	2.1
1	D	220	GLN	2.1
1	C	119	LYS	2.1
1	D	212	LYS	2.1
1	D	130	LYS	2.0
1	A	247	PRO	2.0
1	B	184	SER	2.0
1	C	213	LYS	2.0
1	A	362	ALA	2.0
1	C	206	HIS	2.0
1	A	377	ARG	2.0
1	B	143	ASP	2.0
1	C	140	THR	2.0
1	B	413	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.