



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:39 am 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](mailto: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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

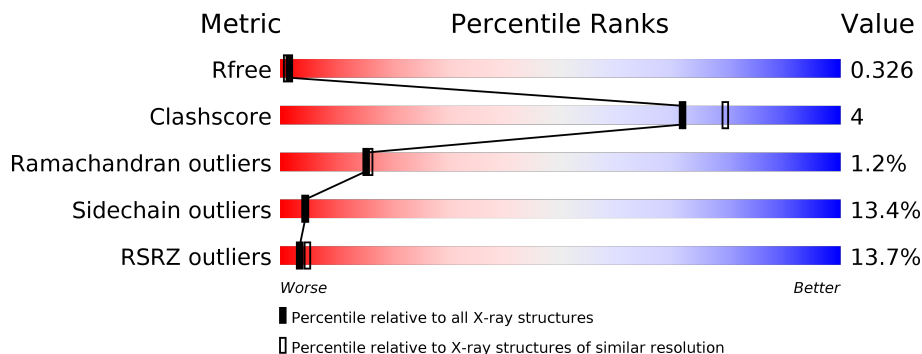
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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  $\geq 3$ , 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>11%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	B	427	<div> <div>15%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
1	C	427	<div> <div>16%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	D	427	<div> <div>12%</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			

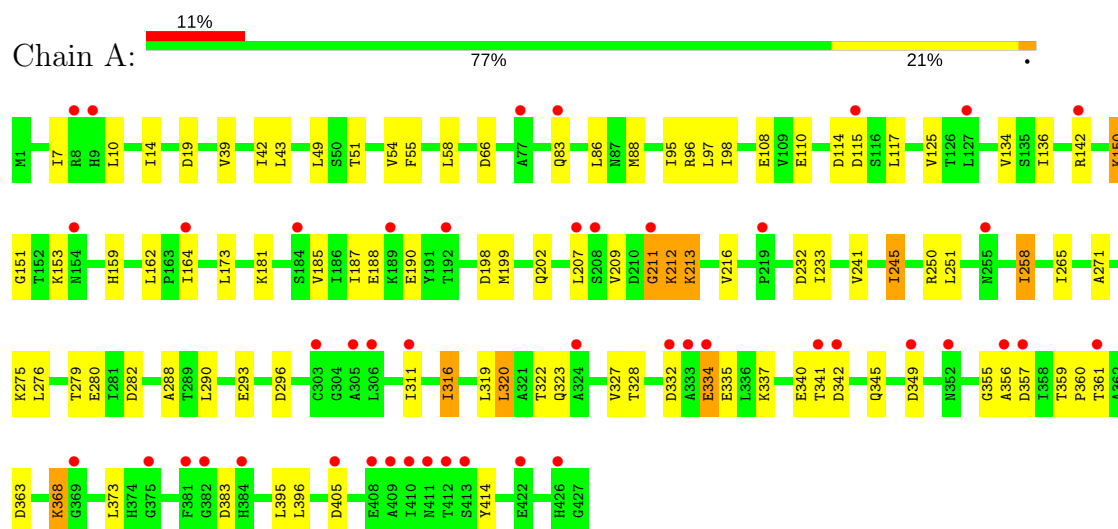
- Molecule 2 is water.

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		

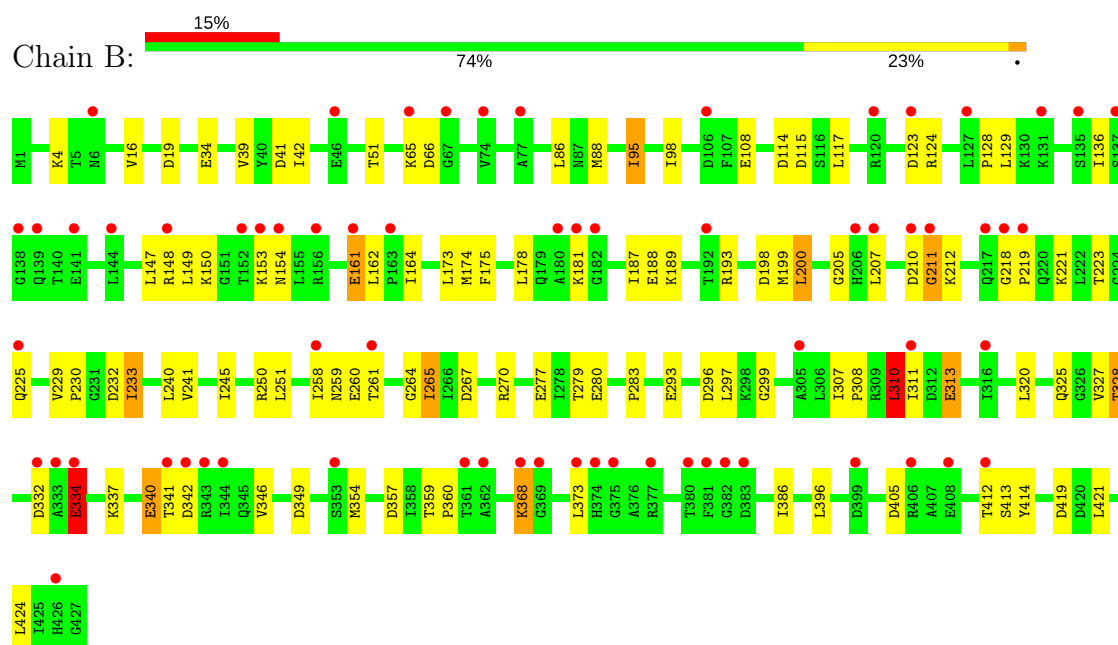
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

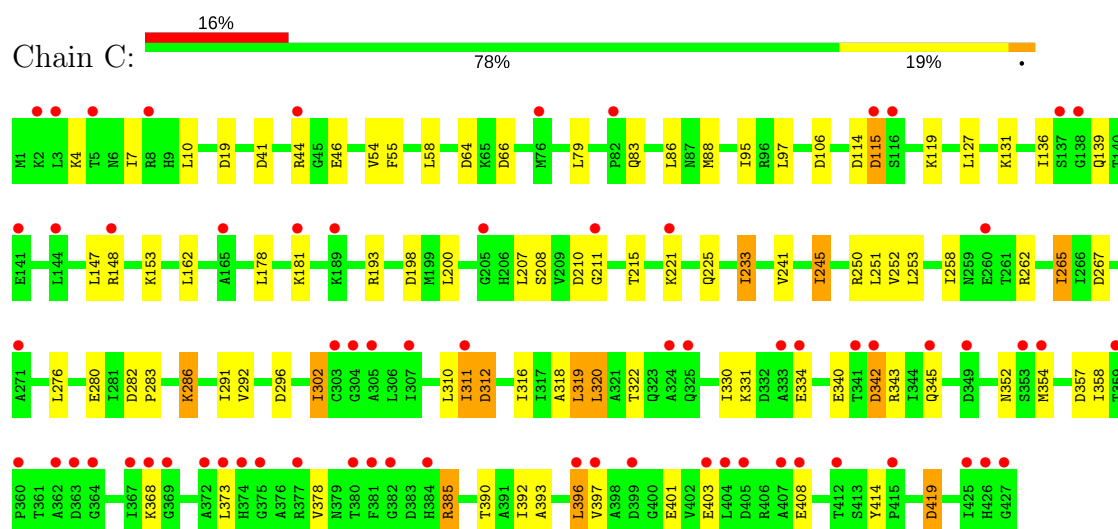
- Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase



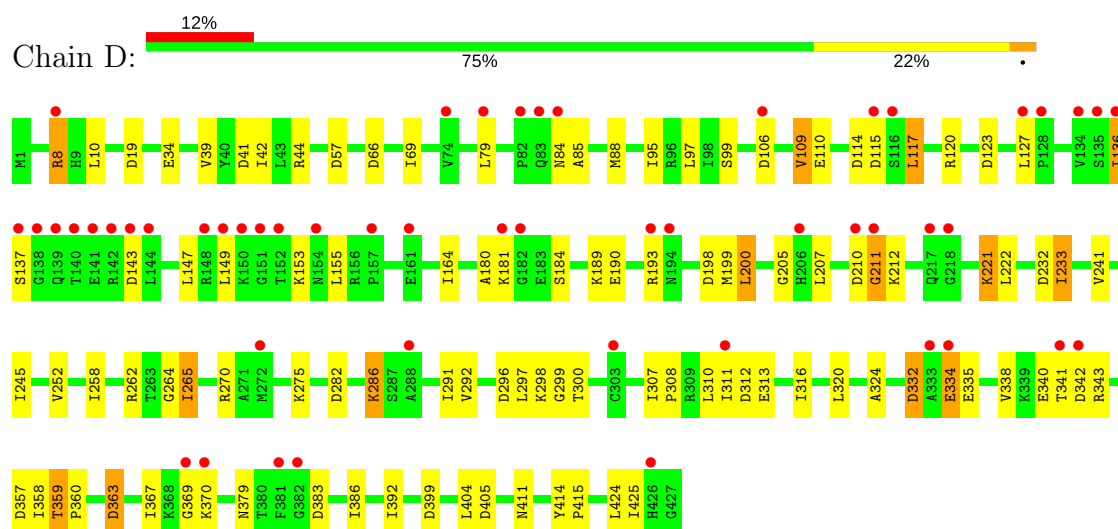
- Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 62.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.53	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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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 [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	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

*Continued on next page...*

*Continued from previous page...*

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: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
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: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

*Continued on next page...*

*Continued from previous page...*

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: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:HG13	1:B:233:ILE:H	1.44	0.43
1:A:108:GLU:HG3	1:A:150:LYS:HG3	2.00	0.43
1:A:55:PHE:HA	1:A:58:LEU:HD12	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
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:D:252:VAL:HG22	1:D:291:ILE:HG12	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: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: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

*Continued on next page...*

*Continued from previous page...*

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: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: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%)	15	16
1	B	425/427 (100%)	397 (93%)	25 (6%)	3 (1%)	25	30
1	C	423/427 (99%)	395 (93%)	25 (6%)	3 (1%)	25	30
1	D	425/427 (100%)	396 (93%)	20 (5%)	9 (2%)	8	6
All	All	1698/1708 (99%)	1589 (94%)	89 (5%)	20 (1%)	15	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

*Continued on next page...*

*Continued from previous page...*

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%)	4	4

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	421/427 (98%)	0.83	46 (10%) 6 9	19, 32, 59, 80	0
1	B	421/427 (98%)	1.03	66 (15%) 2 3	19, 39, 60, 87	0
1	C	421/427 (98%)	0.93	67 (15%) 2 3	19, 36, 61, 90	0
1	D	421/427 (98%)	0.76	52 (12%) 4 7	17, 33, 57, 72	0
All	All	1684/1708 (98%)	0.89	231 (13%) 3 5	17, 35, 60, 90	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	THR	14.9
1	B	382	GLY	10.5
1	A	356	ALA	9.6
1	B	341	THR	8.9
1	B	342	ASP	7.7
1	C	342	ASP	6.5
1	C	381	PHE	6.0
1	A	341	THR	6.0
1	C	405	ASP	5.8
1	B	381	PHE	5.7
1	D	154	ASN	5.6
1	D	341	THR	5.6
1	A	369	GLY	5.4
1	D	142	ARG	5.1
1	D	369	GLY	4.9
1	C	382	GLY	4.8
1	A	334	GLU	4.8
1	A	412	THR	4.7
1	D	342	ASP	4.7
1	C	311	ILE	4.6
1	C	362	ALA	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	362	ALA	4.6
1	B	383	ASP	4.5
1	D	144	LEU	4.4
1	B	217	GLN	4.3
1	B	139	GLN	4.3
1	B	344	ILE	4.2
1	A	83	GLN	4.2
1	B	334	GLU	4.2
1	D	148	ARG	4.2
1	C	211	GLY	4.2
1	C	399	ASP	4.1
1	C	305	ALA	4.0
1	C	115	ASP	4.0
1	B	152	THR	3.9
1	A	357	ASP	3.9
1	C	408	GLU	3.8
1	C	377	ARG	3.8
1	A	382	GLY	3.8
1	D	127	LEU	3.8
1	A	381	PHE	3.7
1	B	218	GLY	3.7
1	D	218	GLY	3.7
1	A	192	THR	3.7
1	D	152	THR	3.7
1	A	208	SER	3.7
1	D	194	ASN	3.6
1	B	138	GLY	3.5
1	D	311	ILE	3.5
1	B	374	HIS	3.5
1	B	144	LEU	3.5
1	C	303	CYS	3.5
1	B	380	THR	3.5
1	D	84	ASN	3.5
1	C	397	VAL	3.5
1	D	150	LYS	3.5
1	A	303	CYS	3.4
1	A	411	ASN	3.4
1	A	408	GLU	3.4
1	A	255	ASN	3.4
1	C	369	GLY	3.4
1	A	410	ILE	3.4
1	B	182	GLY	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	333	ALA	3.4
1	D	115	ASP	3.3
1	A	426	HIS	3.3
1	A	333	ALA	3.3
1	B	210	ASP	3.3
1	B	211	GLY	3.3
1	A	352	ASN	3.3
1	B	206	HIS	3.2
1	B	219	PRO	3.2
1	D	139	GLN	3.2
1	B	156	ARG	3.1
1	D	382	GLY	3.1
1	D	141	GLU	3.1
1	D	211	GLY	3.1
1	B	399	ASP	3.1
1	B	412	THR	3.1
1	C	380	THR	3.1
1	C	425	ILE	3.1
1	C	141	GLU	3.1
1	C	5	THR	3.1
1	B	361	THR	3.0
1	C	427	GLY	3.0
1	B	181	LYS	3.0
1	C	353	SER	3.0
1	D	106	ASP	3.0
1	C	368	LYS	3.0
1	C	426	HIS	3.0
1	B	137	SER	2.9
1	C	334	GLU	2.9
1	C	144	LEU	2.9
1	C	407	ALA	2.9
1	D	138	GLY	2.9
1	A	405	ASP	2.9
1	B	127	LEU	2.9
1	C	404	LEU	2.9
1	B	375	GLY	2.9
1	C	44	ARG	2.9
1	B	141	GLU	2.8
1	A	211	GLY	2.8
1	C	325	GLN	2.8
1	C	333	ALA	2.8
1	D	161	GLU	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	415	PRO	2.8
1	B	353	SER	2.8
1	A	77	ALA	2.7
1	A	384	HIS	2.7
1	D	206	HIS	2.7
1	A	311	ILE	2.7
1	A	184	SER	2.7
1	D	79	LEU	2.7
1	B	343	ARG	2.7
1	B	106	ASP	2.7
1	D	140	THR	2.7
1	B	408	GLU	2.7
1	B	311	ILE	2.7
1	A	142	ARG	2.7
1	B	377	ARG	2.7
1	D	426	HIS	2.7
1	B	406	ARG	2.6
1	C	148	ARG	2.6
1	D	151	GLY	2.6
1	D	210	ASP	2.6
1	C	304	GLY	2.6
1	A	413	SER	2.6
1	B	225	GLN	2.6
1	B	261	THR	2.6
1	D	157	PRO	2.6
1	A	9	HIS	2.6
1	C	354	MET	2.6
1	C	374	HIS	2.6
1	C	364	GLY	2.6
1	B	46	GLU	2.6
1	A	207	LEU	2.5
1	C	375	GLY	2.5
1	B	135	SER	2.5
1	C	359	THR	2.5
1	A	332	ASP	2.5
1	C	138	GLY	2.5
1	C	384	HIS	2.5
1	B	161	GLU	2.5
1	D	137	SER	2.5
1	D	136	ILE	2.5
1	B	67	GLY	2.5
1	C	363	ASP	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	137	SER	2.4
1	A	305	ALA	2.4
1	A	409	ALA	2.4
1	B	74	VAL	2.4
1	D	8	ARG	2.4
1	B	6	ASN	2.4
1	C	165	ALA	2.4
1	B	65	LYS	2.4
1	B	131	LYS	2.4
1	D	181	LYS	2.4
1	C	349	ASP	2.4
1	D	193	ARG	2.4
1	B	154	ASN	2.4
1	D	334	GLU	2.4
1	B	332	ASP	2.4
1	C	2	LYS	2.4
1	C	360	PRO	2.4
1	A	361	THR	2.4
1	D	135	SER	2.4
1	C	205	GLY	2.3
1	B	120	ARG	2.3
1	A	375	GLY	2.3
1	B	77	ALA	2.3
1	C	8	ARG	2.3
1	D	143	ASP	2.3
1	A	154	ASN	2.3
1	C	221	LYS	2.3
1	D	182	GLY	2.3
1	C	82	PRO	2.3
1	D	128	PRO	2.3
1	D	303	CYS	2.3
1	D	333	ALA	2.3
1	C	116	SER	2.3
1	D	82	PRO	2.3
1	A	8	ARG	2.3
1	C	372	ALA	2.3
1	B	305	ALA	2.2
1	A	127	LEU	2.2
1	B	207	LEU	2.2
1	B	369	GLY	2.2
1	B	368	LYS	2.2
1	B	123	ASP	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	258	ILE	2.2
1	B	316	ILE	2.2
1	C	324	ALA	2.2
1	C	403	GLU	2.2
1	A	342	ASP	2.2
1	C	345	GLN	2.2
1	C	412	THR	2.2
1	C	307	ILE	2.2
1	D	272	MET	2.2
1	A	349	ASP	2.2
1	D	288	ALA	2.2
1	B	148	ARG	2.2
1	C	3	LEU	2.2
1	C	260	GLU	2.2
1	C	189	LYS	2.1
1	D	370	LYS	2.1
1	D	74	VAL	2.1
1	D	134	VAL	2.1
1	B	163	PRO	2.1
1	C	76	MET	2.1
1	D	381	PHE	2.1
1	A	164	ILE	2.1
1	A	115	ASP	2.1
1	B	192	THR	2.1
1	C	367	ILE	2.1
1	B	153	LYS	2.1
1	C	181	LYS	2.1
1	D	217	GLN	2.1
1	A	422	GLU	2.1
1	B	373	LEU	2.1
1	C	396	LEU	2.1
1	A	219	PRO	2.1
1	C	373	LEU	2.0
1	A	324	ALA	2.0
1	B	180	ALA	2.0
1	C	271	ALA	2.0
1	B	426	HIS	2.0
1	A	306	LEU	2.0
1	A	189	LYS	2.0
1	D	149	LEU	2.0
1	D	83	GLN	2.0
1	D	116	SER	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.