



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2016 – 04:39 AM EST

PDB ID : 4KV8
Title : Crystal structure of HIV RT in complex with BILR0355BS
Authors : Coulombe, R.
Deposited on : 2013-05-22
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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

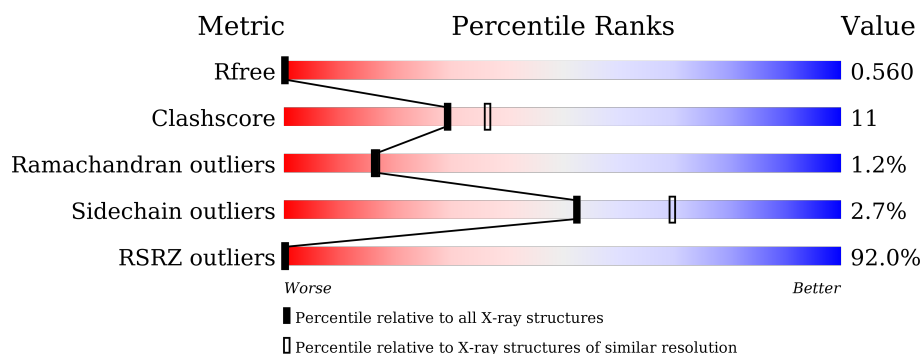
1 Overall quality at a glance ⓘ

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	564	<div> <div>92%</div> <div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
2	B	442	<div> <div>83%</div> <div> <div>68%</div> <div>23%</div> <div>• 8%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	1WT	A	602	-	-	-	X
5	SUC	B	2001	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7964 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 HIV Reverse transcriptase P66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4513	2917	753	835	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P04585
A	561	VAL	-	EXPRESSION TAG	UNP P04585
A	562	PRO	-	EXPRESSION TAG	UNP P04585
A	563	ARG	-	EXPRESSION TAG	UNP P04585

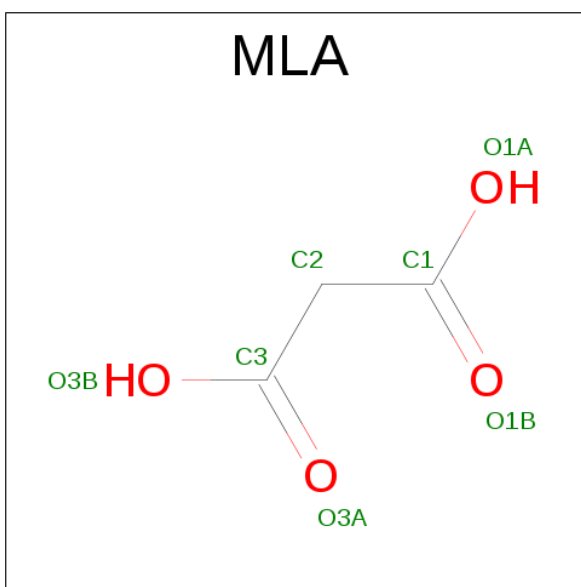
- Molecule 2 is a protein called HIV Reverse transcriptase P51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	407	Total	C	N	O	S	0	0	0
			3370	2197	556	610	7			

There are 2 discrepancies between the modelled and reference sequences:

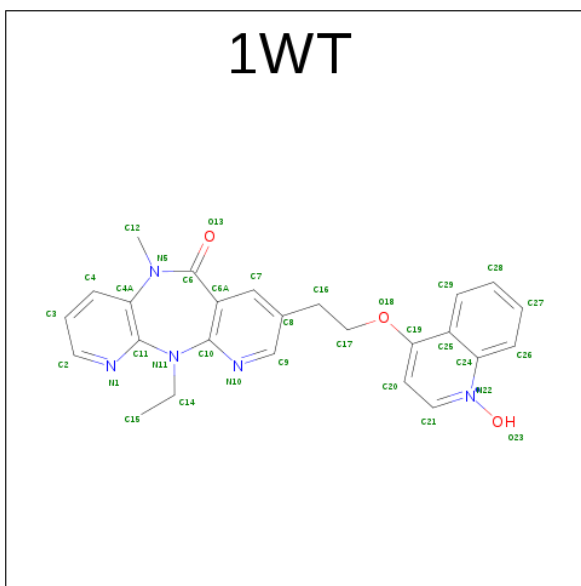
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP P04585
B	0	SER	-	EXPRESSION TAG	UNP P04585

- Molecule 3 is MALONIC ACID (three-letter code: MLA) (formula: C₃H₄O₄).



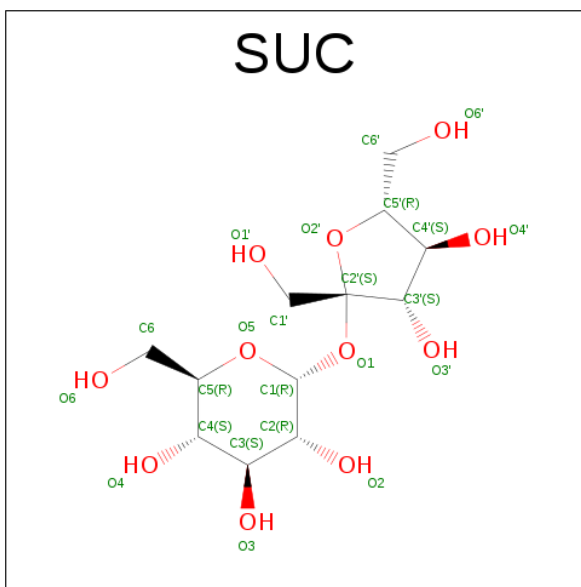
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is 11-ETHYL-5-METHYL-8-[2-(1-OXIDANYLQUINOLIN-4-YL)OXYETHYL]DIPYRIDO[3,2-[1,4]DIAZEPIN-6-ONE (three-letter code: 1WT) (formula: $C_{25}H_{24}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			33	25	5	3		

- Molecule 5 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			23	12	11		

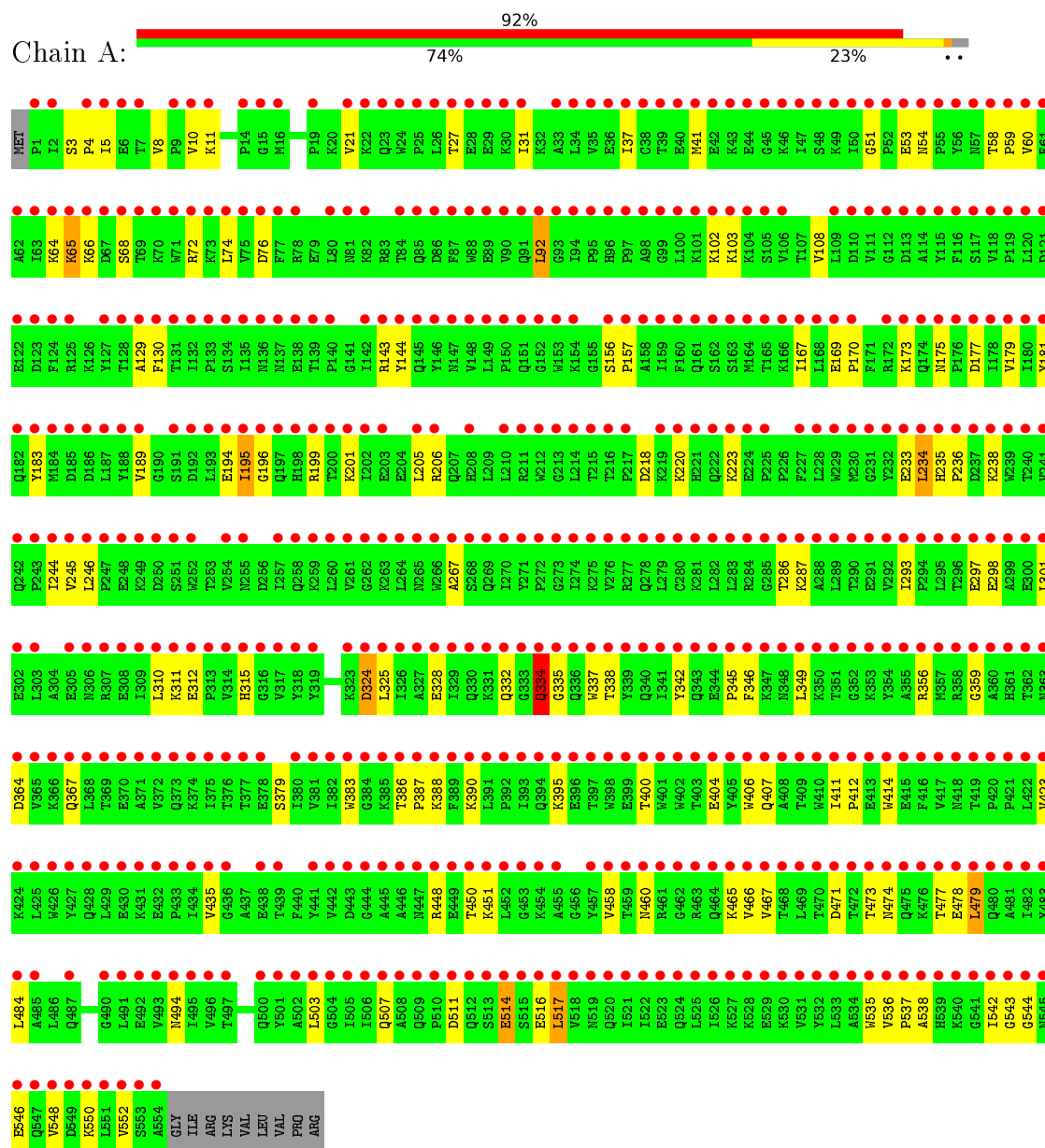
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	9	Total	O	0	0
			9	9		

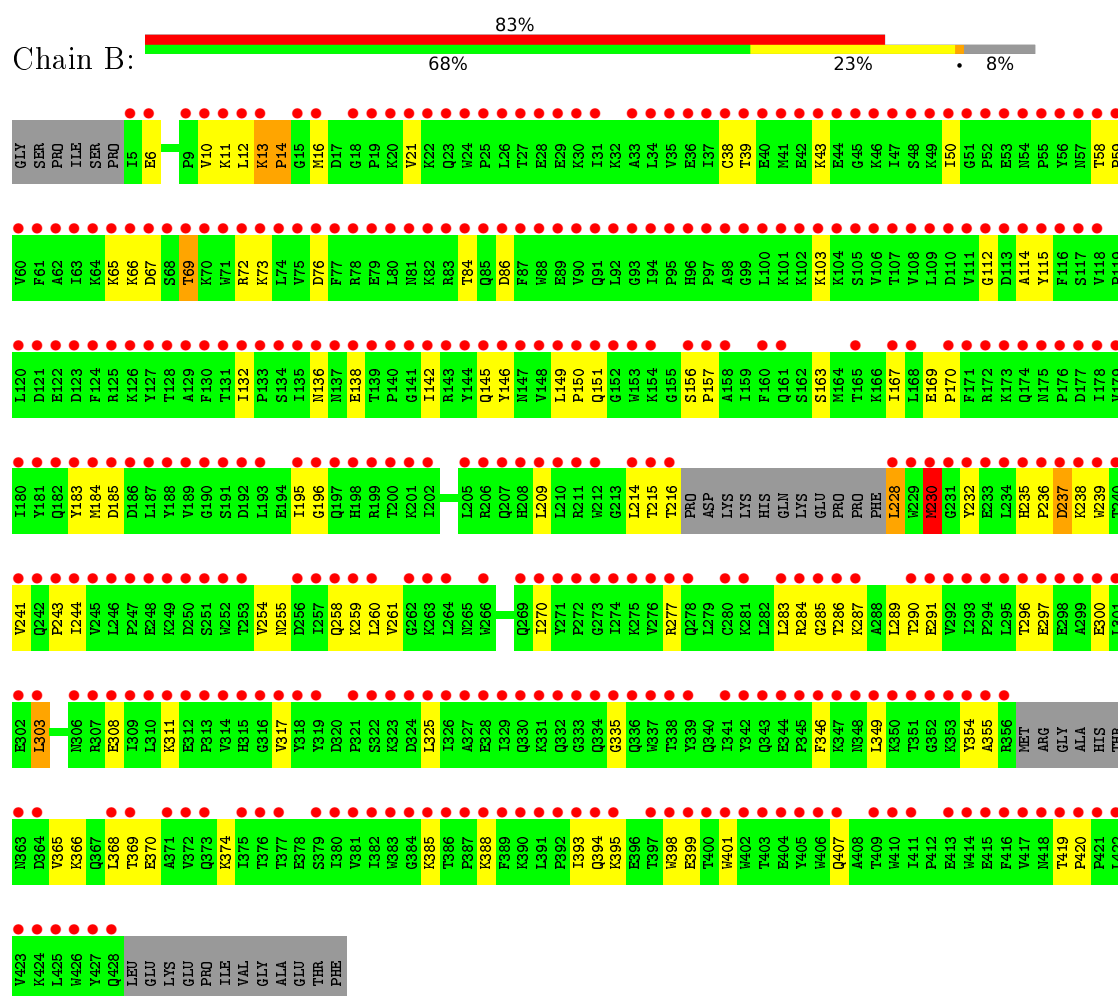
3 Residue-property plots

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 ($RSRZ > 2$). 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: HIV Reverse transcriptase P66



- Molecule 2: HIV Reverse transcriptase P51



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.21Å 154.89Å 154.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 77.14 – 3.08	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.30) 40.3 (77.14-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.07Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.229 , 0.266 0.576 , 0.560	Depositor DCC
R_{free} test set	1087 reflections (10.26%)	DCC
Wilson B-factor (Å ²)	121.0	Xtriage
Anisotropy	1.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 268.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.43	EDS
Total number of atoms	7964	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 1WT, SUC, MLA

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	0.35	0/4630	0.58	0/6291
2	B	0.36	0/3465	0.61	1/4708 (0.0%)
All	All	0.36	0/8095	0.59	1/10999 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	244	ILE	N-CA-C	-5.86	95.17	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4513	0	4563	107	0
2	B	3370	0	3398	83	0
3	A	7	0	2	2	0
4	A	33	0	24	0	0
5	B	23	0	22	0	0
6	A	9	0	0	0	0
6	B	9	0	0	0	0
All	All	7964	0	8009	180	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.59	0.99
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.00	0.94
1:A:195:ILE:HD11	1:A:199:ARG:HE	1.37	0.86
1:A:92:LEU:HD12	1:A:92:LEU:H	1.40	0.85
1:A:342:TYR:HA	1:A:349:LEU:HD23	1.61	0.82
1:A:514:GLU:H	1:A:514:GLU:CD	1.83	0.80
2:B:209:LEU:HD22	2:B:214:LEU:HD12	1.66	0.78
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.68	0.75
2:B:241:VAL:O	2:B:243:PRO:HD3	1.86	0.75
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.68	0.74
2:B:260:LEU:HD21	2:B:303:LEU:HD21	1.72	0.71
2:B:395:LYS:O	2:B:399:GLU:HG3	1.91	0.70
1:A:536:VAL:HG13	1:A:542:ILE:HD12	1.73	0.70
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.06	0.70
2:B:114:ALA:HB2	2:B:214:LEU:HD21	1.76	0.67
2:B:12:LEU:HD23	2:B:84:THR:HG22	1.76	0.67
1:A:287:LYS:HD3	1:A:293:ILE:HD11	1.76	0.66
2:B:228:LEU:N	2:B:228:LEU:HD12	2.10	0.66
1:A:195:ILE:HD11	1:A:199:ARG:NE	2.10	0.66
2:B:112:GLY:HA3	2:B:151:GLN:HE21	1.62	0.65
2:B:354:TYR:HD2	2:B:374:LYS:HD3	1.63	0.64
1:A:400:THR:O	1:A:404:GLU:HG2	1.98	0.63
1:A:514:GLU:N	1:A:514:GLU:CD	2.52	0.63
1:A:66:LYS:HE3	1:A:68:SER:HB3	1.81	0.62
2:B:236:PRO:C	2:B:238:LYS:H	2.03	0.62
1:A:108:VAL:HG11	1:A:223:LYS:HE3	1.80	0.61
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.83	0.60
1:A:450:THR:O	1:A:451:LYS:HB2	2.02	0.60
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.37	0.60
2:B:58:THR:HG23	2:B:76:ASP:O	2.02	0.59
1:A:332:GLN:NE2	1:A:338:THR:HB	2.17	0.59
1:A:324:ASP:OD2	1:A:388:LYS:HD3	2.03	0.59
1:A:66:LYS:C	1:A:68:SER:H	2.05	0.59
2:B:354:TYR:CD2	2:B:374:LYS:HD3	2.38	0.59
1:A:332:GLN:HE21	1:A:338:THR:HB	1.68	0.59
1:A:474:ASN:O	1:A:478:GLU:HG2	2.03	0.59
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.36	0.56
1:A:548:VAL:O	1:A:552:VAL:HG23	2.05	0.56
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.87	0.56
2:B:10:VAL:C	2:B:11:LYS:HD3	2.26	0.55
1:A:298:GLU:CD	1:A:298:GLU:H	2.10	0.55
2:B:39:THR:HG22	2:B:43:LYS:HE3	1.87	0.55
2:B:209:LEU:HB3	2:B:214:LEU:HB2	1.89	0.55
1:A:218:ASP:OD1	1:A:220:LYS:HB2	2.07	0.54
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.89	0.54
2:B:103:LYS:O	2:B:236:PRO:HG2	2.07	0.54
2:B:308:GLU:HA	2:B:311:LYS:HE2	1.88	0.54
2:B:230:MET:HE1	2:B:232:TYR:HB3	1.89	0.54
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.91	0.53
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.89	0.53
1:A:65:LYS:O	1:A:65:LYS:HD3	2.09	0.53
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.43	0.53
2:B:11:LYS:HD3	2:B:11:LYS:N	2.24	0.53
2:B:112:GLY:HA3	2:B:151:GLN:NE2	2.24	0.53
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.91	0.52
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.91	0.52
2:B:366:LYS:O	2:B:370:GLU:HG3	2.10	0.52
1:A:129:ALA:HA	1:A:144:TYR:O	2.10	0.51
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.39	0.51
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.91	0.51
1:A:173:LYS:NZ	1:A:173:LYS:HB3	2.24	0.51
1:A:234:LEU:N	1:A:234:LEU:HD23	2.26	0.51
1:A:37:ILE:HG22	1:A:41:MET:CE	2.39	0.51
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.46	0.51
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.46	0.51
1:A:460:ASN:HD21	3:A:601:MLA:HC22	1.75	0.51
1:A:175:ASN:OD1	1:A:201:LYS:HE3	2.11	0.51
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.93	0.50
1:A:51:GLY:HA3	1:A:53:GLU:OE2	2.11	0.50
2:B:346:PHE:N	2:B:346:PHE:CD2	2.77	0.50
1:A:335:GLY:HA3	1:A:356:ARG:HD3	1.94	0.49
1:A:411:ILE:HG22	1:A:412:PRO:O	2.12	0.49
1:A:54:ASN:O	1:A:143:ARG:NH2	2.45	0.49
1:A:233:GLU:C	1:A:234:LEU:HD23	2.32	0.49
1:A:542:ILE:HD11	2:B:261:VAL:HG11	1.94	0.49
2:B:157:PRO:HG2	2:B:184:MET:HA	1.94	0.49
1:A:473:THR:O	1:A:477:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ALA:CB	2:B:214:LEU:HD21	2.43	0.49
1:A:325:LEU:HD21	1:A:383:TRP:CD2	2.48	0.48
1:A:334:GLN:H	1:A:334:GLN:CD	2.17	0.48
1:A:287:LYS:HD3	1:A:293:ILE:CD1	2.44	0.48
2:B:114:ALA:HB2	2:B:214:LEU:CD2	2.42	0.48
2:B:136:ASN:HB3	2:B:138:GLU:HG3	1.96	0.48
2:B:335:GLY:O	2:B:355:ALA:HA	2.12	0.48
1:A:169:GLU:CB	1:A:170:PRO:HD3	2.43	0.48
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.47	0.48
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.44	0.48
1:A:334:GLN:NE2	1:A:334:GLN:H	2.12	0.47
1:A:3:SER:HA	1:A:4:PRO:HD3	1.68	0.47
1:A:544:GLY:N	2:B:285:GLY:O	2.47	0.47
1:A:467:VAL:CG2	1:A:484:LEU:HD11	2.44	0.47
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.94	0.47
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.54	0.47
2:B:325:LEU:HD12	2:B:385:LYS:HG3	1.97	0.47
2:B:254:VAL:O	2:B:258:GLN:HG3	2.15	0.47
2:B:13:LYS:HE3	2:B:86:ASP:OD1	2.16	0.46
1:A:66:LYS:HE3	1:A:66:LYS:HB2	1.67	0.46
2:B:388:LYS:HE3	2:B:388:LYS:HB2	1.69	0.46
1:A:5:ILE:HD12	1:A:167:ILE:HG13	1.96	0.46
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.42	0.46
2:B:236:PRO:O	2:B:238:LYS:N	2.49	0.46
1:A:503:LEU:O	1:A:507:GLN:HG3	2.15	0.46
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.50	0.46
1:A:8:VAL:O	1:A:10:VAL:HG23	2.16	0.46
1:A:37:ILE:HG22	1:A:41:MET:HE2	1.98	0.46
1:A:66:LYS:CE	1:A:68:SER:HB3	2.43	0.46
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.98	0.45
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.99	0.45
1:A:406:TRP:CZ3	1:A:407:GLN:NE2	2.83	0.45
2:B:215:THR:O	2:B:216:THR:C	2.54	0.45
2:B:65:LYS:CG	2:B:66:LYS:H	2.30	0.45
1:A:379:SER:CB	1:A:387:PRO:HD3	2.47	0.45
2:B:65:LYS:HG2	2:B:66:LYS:N	2.32	0.45
1:A:74:LEU:C	1:A:74:LEU:HD23	2.37	0.45
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.52	0.45
1:A:53:GLU:H	1:A:53:GLU:CD	2.20	0.44
2:B:277:ARG:HG2	2:B:277:ARG:HH11	1.83	0.44
2:B:228:LEU:C	2:B:230:MET:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG12	1:A:11:LYS:N	2.32	0.44
2:B:65:LYS:HG2	2:B:66:LYS:H	1.82	0.44
1:A:311:LYS:HG3	1:A:312:GLU:HG2	2.00	0.44
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.48	0.44
2:B:297:GLU:HA	2:B:300:GLU:HG3	1.99	0.44
1:A:194:GLU:OE1	1:A:194:GLU:N	2.36	0.43
2:B:365:VAL:O	2:B:369:THR:HG23	2.17	0.43
1:A:66:LYS:C	1:A:68:SER:N	2.72	0.43
1:A:479:LEU:HA	1:A:479:LEU:HD12	1.86	0.43
2:B:236:PRO:C	2:B:238:LYS:N	2.69	0.43
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.00	0.43
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.54	0.43
2:B:296:THR:O	2:B:300:GLU:HG3	2.18	0.43
1:A:173:LYS:NZ	1:A:173:LYS:CB	2.81	0.43
1:A:359:GLY:HA2	1:A:514:GLU:HG3	2.00	0.42
1:A:465:LYS:HG2	1:A:466:VAL:N	2.33	0.42
2:B:11:LYS:HE2	2:B:13:LYS:NZ	2.34	0.42
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.52	0.42
2:B:12:LEU:HD23	2:B:84:THR:CG2	2.47	0.42
1:A:467:VAL:HG22	1:A:484:LEU:HD11	2.02	0.42
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.49	0.42
2:B:195:ILE:HG23	2:B:196:GLY:N	2.34	0.42
2:B:235:HIS:HB3	2:B:238:LYS:HD3	2.00	0.42
2:B:317:VAL:HG12	2:B:349:LEU:HD23	2.00	0.42
2:B:72:ARG:HG2	2:B:73:LYS:N	2.33	0.42
1:A:64:LYS:HE2	1:A:68:SER:O	2.20	0.42
2:B:270:ILE:HG12	2:B:346:PHE:O	2.20	0.42
2:B:69:THR:HG23	2:B:69:THR:O	2.19	0.42
2:B:65:LYS:CG	2:B:66:LYS:N	2.83	0.42
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.02	0.42
1:A:346:PHE:N	1:A:346:PHE:CD2	2.85	0.42
2:B:277:ARG:HG2	2:B:277:ARG:NH1	2.34	0.42
2:B:230:MET:CE	2:B:232:TYR:HB3	2.50	0.42
1:A:58:THR:HG23	1:A:76:ASP:O	2.20	0.41
1:A:286:THR:C	1:A:287:LYS:HG3	2.40	0.41
1:A:297:GLU:O	1:A:301:LEU:HG	2.21	0.41
1:A:543:GLY:HA3	2:B:283:LEU:O	2.21	0.41
2:B:255:ASN:HD21	2:B:259:LYS:NZ	2.18	0.41
1:A:64:LYS:O	1:A:66:LYS:N	2.53	0.41
1:A:102:LYS:C	1:A:103:LYS:HD2	2.41	0.41
1:A:179:VAL:O	1:A:189:VAL:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASN:ND2	3:A:601:MLA:HC22	2.35	0.41
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.21	0.41
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.51	0.41
2:B:419:THR:HA	2:B:420:PRO:HD3	1.90	0.41
2:B:195:ILE:HD12	2:B:195:ILE:HA	1.89	0.41
1:A:386:THR:HG21	2:B:401:TRP:CH2	2.56	0.41
1:A:194:GLU:O	1:A:196:GLY:N	2.54	0.40
2:B:228:LEU:HD11	2:B:407:GLN:HE22	1.85	0.40
1:A:286:THR:O	1:A:286:THR:HG23	2.21	0.40
1:A:537:PRO:HD2	1:A:542:ILE:CD1	2.52	0.40
2:B:393:ILE:HG12	2:B:394:GLN:N	2.36	0.40
1:A:460:ASN:HA	2:B:286:THR:O	2.22	0.40
1:A:546:GLU:O	1:A:550:LYS:HG3	2.21	0.40
1:A:27:THR:O	1:A:31:ILE:HG13	2.21	0.40
1:A:328:GLU:OE1	1:A:342:TYR:OH	2.28	0.40
2:B:142:ILE:HG13	2:B:142:ILE:H	1.69	0.40
2:B:163:SER:O	2:B:167:ILE:HG13	2.22	0.40
2:B:287:LYS:HD3	2:B:291:GLU:OE2	2.21	0.40
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.56	0.40
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.02	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	552/564 (98%)	524 (95%)	23 (4%)	5 (1%)	21	24
2	B	401/442 (91%)	375 (94%)	20 (5%)	6 (2%)	13	12
All	All	953/1006 (95%)	899 (94%)	43 (4%)	11 (1%)	16	16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	A	538	ALA
2	B	67	ASP
1	A	65	LYS
2	B	6	GLU
2	B	14	PRO
2	B	230	MET
2	B	237	ASP
1	A	345	PRO
1	A	195	ILE
2	B	13	LYS

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	495/504 (98%)	481 (97%)	14 (3%)	51	68
2	B	370/401 (92%)	361 (98%)	9 (2%)	57	74
All	All	865/905 (96%)	842 (97%)	23 (3%)	52	70

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	92	LEU
1	A	177	ASP
1	A	205	LEU
1	A	234	LEU
1	A	245	VAL
1	A	324	ASP
1	A	334	GLN
1	A	448	ARG
1	A	479	LEU
1	A	511	ASP
1	A	514	GLU
1	A	516	GLU

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Mol	Chain	Res	Type
1	A	517	LEU
2	B	14	PRO
2	B	16	MET
2	B	69	THR
2	B	228	LEU
2	B	230	MET
2	B	237	ASP
2	B	284	ARG
2	B	303	LEU
2	B	368	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	258	GLN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN
1	A	348	ASN
1	A	367	GLN
1	A	407	GLN
1	A	475	GLN
1	A	480	GLN
1	A	500	GLN
1	A	524	GLN
2	B	151	GLN
2	B	161	GLN
2	B	208	HIS
2	B	242	GLN
2	B	255	ASN
2	B	269	GLN
2	B	348	ASN
2	B	394	GLN
2	B	407	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	MLA	A	601	-	0,6,6	0.00	-	0,7,7	0.00	-
4	1WT	A	602	-	28,37,37	3.00	17 (60%)	28,53,53	4.51	18 (64%)
5	SUC	B	2001	-	24,24,24	0.66	1 (4%)	36,36,36	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLA	A	601	-	-	0/0/4/4	0/0/0/0
4	1WT	A	602	-	-	0/6/32/32	0/4/5/5
5	SUC	B	2001	-	-	0/12/51/51	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	1WT	C25-C19	-5.42	1.42	1.52
4	A	602	1WT	C29-C25	-5.18	1.43	1.53
4	A	602	1WT	O23-N22	-5.08	1.31	1.45
4	A	602	1WT	C20-C21	-4.97	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	1WT	C28-C29	-4.33	1.41	1.53
4	A	602	1WT	C27-C26	-4.16	1.42	1.53
4	A	602	1WT	C25-C24	-4.13	1.46	1.54
4	A	602	1WT	C26-C24	-3.67	1.43	1.52
4	A	602	1WT	C20-C19	-3.51	1.44	1.52
4	A	602	1WT	C27-C28	-2.23	1.42	1.51
4	A	602	1WT	O18-C19	-2.16	1.39	1.43
4	A	602	1WT	C3-C4	2.07	1.41	1.36
5	B	2001	SUC	O5-C1	2.22	1.47	1.41
4	A	602	1WT	C9-N10	2.67	1.36	1.31
4	A	602	1WT	C7-C8	2.68	1.43	1.37
4	A	602	1WT	C11-N1	2.81	1.39	1.35
4	A	602	1WT	C2-N1	2.86	1.38	1.32
4	A	602	1WT	C10-N10	3.56	1.40	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	1WT	C6A-C10-N10	-2.43	120.58	123.55
4	A	602	1WT	C17-O18-C19	2.14	118.73	113.86
4	A	602	1WT	C9-N10-C10	2.28	119.89	116.89
4	A	602	1WT	C2-N1-C11	2.31	119.80	116.96
4	A	602	1WT	C26-C24-C25	3.44	117.76	111.09
4	A	602	1WT	C27-C28-C29	3.68	119.06	111.44
4	A	602	1WT	C19-C25-C24	3.81	118.61	109.63
4	A	602	1WT	C29-C25-C24	3.82	119.26	110.85
4	A	602	1WT	O18-C19-C25	4.00	116.07	107.91
4	A	602	1WT	C27-C26-C24	4.39	121.58	110.32
4	A	602	1WT	C28-C27-C26	4.47	120.68	111.44
4	A	602	1WT	C21-N22-C24	4.58	119.12	111.72
4	A	602	1WT	O18-C19-C20	5.15	124.25	110.08
4	A	602	1WT	C28-C29-C25	5.41	121.66	111.75
4	A	602	1WT	C20-C19-C25	5.45	119.68	112.65
4	A	602	1WT	C29-C25-C19	6.31	122.14	112.25
4	A	602	1WT	C21-C20-C19	8.99	120.89	111.83
4	A	602	1WT	O23-N22-C24	14.13	123.13	105.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	MLA	2	0

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	554/564 (98%)	8.67	517 (93%)  	45, 67, 101, 115	0
2	B	407/442 (92%)	7.79	367 (90%)  	45, 66, 104, 116	0
All	All	961/1006 (95%)	8.30	884 (91%)  	45, 66, 102, 116	0

All (884) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	326	ILE	53.2
1	A	427	TYR	44.6
1	A	348	ASN	44.6
2	B	141	GLY	43.8
1	A	39	THR	42.3
1	A	268	SER	42.0
1	A	548	VAL	37.1
1	A	100	LEU	35.9
1	A	433	PRO	35.6
1	A	496	VAL	35.4
1	A	446	ALA	34.4
1	A	469	LEU	34.4
1	A	338	THR	34.1
2	B	135	ILE	33.2
1	A	58	THR	32.1
2	B	387	PRO	31.1
2	B	185	ASP	30.9
2	B	144	TYR	29.4
1	A	273	GLY	29.4
1	A	532	TYR	28.8
1	A	468	THR	28.4
1	A	544	GLY	28.3
1	A	533	LEU	26.8
1	A	128	THR	26.3

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Mol	Chain	Res	Type	RSRZ
2	B	323	LYS	25.7
1	A	6	GLU	25.1
1	A	390	LYS	24.8
1	A	448	ARG	24.0
1	A	342	TYR	23.7
2	B	299	ALA	23.7
1	A	458	VAL	23.6
2	B	252	TRP	23.4
2	B	186	ASP	23.0
2	B	134	SER	23.0
1	A	495	ILE	22.9
2	B	35	VAL	22.7
2	B	98	ALA	22.7
1	A	148	VAL	22.6
2	B	41	MET	22.5
1	A	349	LEU	22.4
1	A	329	ILE	22.0
1	A	462	GLY	21.8
2	B	108	VAL	21.8
1	A	477	THR	21.8
1	A	339	TYR	21.2
2	B	380	ILE	21.0
1	A	95	PRO	20.8
1	A	233	GLU	20.7
1	A	267	ALA	20.2
2	B	34	LEU	19.8
2	B	393	ILE	19.7
2	B	325	LEU	19.7
1	A	63	ILE	19.4
1	A	550	LYS	19.4
2	B	87	PHE	19.4
1	A	132	ILE	19.4
1	A	316	GLY	19.3
2	B	99	GLY	19.3
1	A	317	VAL	19.3
2	B	142	ILE	19.1
1	A	318	TYR	19.0
1	A	24	TRP	19.0
1	A	352	GLY	19.0
1	A	522	ILE	18.7
2	B	19	PRO	18.6
2	B	330	GLN	18.6

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Mol	Chain	Res	Type	RSRZ
1	A	493	VAL	18.5
2	B	84	THR	18.4
2	B	353	LYS	18.3
1	A	357	MET	18.2
1	A	272	PRO	18.2
1	A	7	THR	18.1
1	A	314	VAL	18.1
2	B	101	LYS	18.1
2	B	183	TYR	17.9
1	A	99	GLY	17.7
1	A	481	ALA	17.5
2	B	338	THR	17.5
2	B	100	LEU	17.4
1	A	40	GLU	17.3
1	A	1	PRO	17.2
2	B	390	LYS	17.2
1	A	57	ASN	17.2
2	B	152	GLY	17.1
1	A	475	GLN	17.1
1	A	114	ALA	17.1
1	A	22	LYS	17.0
2	B	92	LEU	16.8
1	A	118	VAL	16.7
1	A	502	ALA	16.6
1	A	525	LEU	16.6
1	A	59	PRO	16.5
1	A	119	PRO	16.5
1	A	549	ASP	16.5
2	B	296	THR	16.3
1	A	315	HIS	16.3
2	B	215	THR	16.1
2	B	109	LEU	16.1
2	B	71	TRP	16.1
1	A	160	PHE	16.0
1	A	193	LEU	15.9
1	A	467	VAL	15.8
1	A	117	SER	15.8
1	A	251	SER	15.8
1	A	64	LYS	15.7
1	A	455	ALA	15.6
1	A	543	GLY	15.6
1	A	234	LEU	15.6

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Mol	Chain	Res	Type	RSRZ
1	A	459	THR	15.5
1	A	439	THR	15.5
2	B	69	THR	15.4
1	A	552	VAL	15.3
1	A	454	LYS	15.2
1	A	271	TYR	15.1
1	A	169	GLU	15.1
2	B	405	TYR	15.0
2	B	329	ILE	14.9
2	B	350	LYS	14.9
1	A	471	ASP	14.9
1	A	331	LYS	14.9
1	A	474	ASN	14.8
2	B	93	GLY	14.8
1	A	43	LYS	14.8
2	B	116	PHE	14.7
1	A	144	TYR	14.7
2	B	244	ILE	14.7
2	B	28	GLU	14.7
2	B	53	GLU	14.6
1	A	137	ASN	14.5
1	A	98	ALA	14.5
1	A	175	ASN	14.4
1	A	182	GLN	14.3
1	A	362	THR	14.3
1	A	231	GLY	14.3
2	B	326	ILE	14.3
1	A	297	GLU	14.2
2	B	105	SER	14.2
1	A	229	TRP	14.1
2	B	184	MET	14.1
2	B	145	GLN	14.1
1	A	228	LEU	14.0
1	A	150	PRO	14.0
1	A	545	ASN	13.9
1	A	23	GLN	13.8
1	A	105	SER	13.8
1	A	452	LEU	13.7
1	A	48	SER	13.7
2	B	310	LEU	13.7
2	B	120	LEU	13.7
1	A	384	GLY	13.7

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Mol	Chain	Res	Type	RSRZ
2	B	112	GLY	13.7
2	B	423	VAL	13.7
1	A	380	ILE	13.6
1	A	147	ASN	13.6
2	B	386	THR	13.6
1	A	101	LYS	13.5
1	A	37	ILE	13.5
2	B	416	PHE	13.4
1	A	239	TRP	13.3
1	A	453	GLY	13.3
2	B	137	ASN	13.3
2	B	309	ILE	13.3
2	B	47	ILE	13.2
2	B	81	ASN	13.0
2	B	48	SER	13.0
2	B	372	VAL	13.0
2	B	308	GLU	13.0
2	B	399	GLU	12.9
2	B	42	GLU	12.8
2	B	324	ASP	12.8
1	A	142	ILE	12.8
2	B	238	LYS	12.7
1	A	407	GLN	12.7
1	A	398	TRP	12.7
2	B	210	LEU	12.6
2	B	67	ASP	12.5
1	A	424	LYS	12.4
2	B	91	GLN	12.4
2	B	187	LEU	12.4
1	A	133	PRO	12.4
1	A	510	PRO	12.4
2	B	211	ARG	12.4
2	B	342	TYR	12.3
1	A	149	LEU	12.3
1	A	161	GLN	12.3
1	A	44	GLU	12.2
2	B	24	TRP	12.2
2	B	95	PRO	12.1
1	A	521	ILE	12.0
2	B	56	TYR	12.0
2	B	190	GLY	12.0
2	B	59	PRO	12.0

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Mol	Chain	Res	Type	RSRZ
1	A	429	LEU	12.0
1	A	383	TRP	12.0
1	A	447	ASN	12.0
2	B	154	LYS	11.9
2	B	337	TRP	11.9
1	A	363	ASN	11.9
1	A	15	GLY	11.8
1	A	116	PHE	11.8
2	B	426	TRP	11.8
2	B	30	LYS	11.8
1	A	551	LEU	11.8
2	B	351	THR	11.7
1	A	167	ILE	11.7
1	A	466	VAL	11.6
2	B	94	ILE	11.6
2	B	253	THR	11.6
2	B	300	GLU	11.6
2	B	29	GLU	11.5
1	A	90	VAL	11.5
2	B	82	LYS	11.5
2	B	197	GLN	11.4
1	A	188	TYR	11.4
1	A	343	GLN	11.4
1	A	47	ILE	11.4
1	A	330	GLN	11.3
1	A	337	TRP	11.3
2	B	176	PRO	11.3
1	A	537	PRO	11.2
2	B	345	PRO	11.2
1	A	113	ASP	11.2
2	B	86	ASP	11.2
1	A	103	LYS	11.2
2	B	72	ARG	11.2
1	A	354	TYR	11.1
1	A	178	ILE	11.1
1	A	319	TYR	11.1
1	A	269	GLN	11.0
1	A	185	ASP	11.0
1	A	327	ALA	11.0
1	A	547	GLN	11.0
1	A	56	TYR	10.9
1	A	311	LYS	10.9

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Mol	Chain	Res	Type	RSRZ
2	B	235	HIS	10.9
2	B	121	ASP	10.9
2	B	233	GLU	10.9
1	A	381	VAL	10.8
2	B	125	ARG	10.8
2	B	10	VAL	10.8
2	B	401	TRP	10.8
2	B	167	ILE	10.8
2	B	158	ALA	10.8
1	A	389	PHE	10.7
1	A	423	VAL	10.7
2	B	110	ASP	10.7
2	B	150	PRO	10.7
2	B	411	ILE	10.7
1	A	328	GLU	10.7
1	A	180	ILE	10.7
2	B	298	GLU	10.6
2	B	70	LYS	10.6
1	A	503	LEU	10.6
1	A	33	ALA	10.6
1	A	168	LEU	10.5
1	A	434	ILE	10.5
1	A	286	THR	10.5
1	A	341	ILE	10.5
2	B	336	GLN	10.5
2	B	382	ILE	10.5
2	B	157	PRO	10.4
2	B	202	ILE	10.4
2	B	78	ARG	10.4
1	A	87	PHE	10.4
2	B	236	PRO	10.4
1	A	21	VAL	10.4
1	A	417	VAL	10.3
1	A	131	THR	10.3
1	A	426	TRP	10.3
1	A	154	LYS	10.2
1	A	230	MET	10.2
1	A	290	THR	10.2
1	A	263	LYS	10.2
2	B	146	TYR	10.1
1	A	358	ARG	10.1
1	A	399	GLU	10.1

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Mol	Chain	Res	Type	RSRZ
2	B	314	VAL	10.0
1	A	96	HIS	10.0
1	A	71	TRP	10.0
2	B	143	ARG	10.0
2	B	133	PRO	10.0
1	A	91	GLN	9.9
1	A	153	TRP	9.9
1	A	443	ASP	9.9
2	B	170	PRO	9.9
1	A	345	PRO	9.9
2	B	240	THR	9.9
2	B	239	TRP	9.8
2	B	136	ASN	9.7
1	A	238	LYS	9.7
1	A	410	TRP	9.6
2	B	250	ASP	9.5
1	A	81	ASN	9.4
1	A	325	LEU	9.4
1	A	500	GLN	9.4
2	B	126	LYS	9.4
1	A	227	PHE	9.4
2	B	241	VAL	9.3
2	B	80	LEU	9.3
2	B	66	LYS	9.3
1	A	270	ILE	9.3
1	A	346	PHE	9.3
2	B	114	ALA	9.3
1	A	292	VAL	9.3
1	A	215	THR	9.3
1	A	196	GLY	9.2
1	A	194	GLU	9.2
1	A	336	GLN	9.2
1	A	274	ILE	9.2
2	B	148	VAL	9.1
1	A	445	ALA	9.1
2	B	417	VAL	9.1
2	B	349	LEU	9.1
2	B	402	TRP	9.1
2	B	102	LYS	9.1
2	B	317	VAL	9.1
1	A	406	TRP	9.1
1	A	146	TYR	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	183	TYR	9.0
2	B	400	THR	9.0
1	A	391	LEU	9.0
2	B	25	PRO	9.0
2	B	276	VAL	9.0
1	A	92	LEU	8.9
1	A	212	TRP	8.9
1	A	435	VAL	8.9
1	A	282	LEU	8.9
1	A	422	LEU	8.8
1	A	296	THR	8.8
1	A	181	TYR	8.8
2	B	373	GLN	8.8
1	A	134	SER	8.8
1	A	106	VAL	8.7
1	A	397	THR	8.7
1	A	538	ALA	8.7
2	B	88	TRP	8.7
1	A	431	LYS	8.7
1	A	232	TYR	8.7
1	A	385	LYS	8.7
1	A	472	THR	8.6
1	A	484	LEU	8.6
2	B	151	GLN	8.6
2	B	398	TRP	8.6
2	B	228	LEU	8.5
1	A	519	ASN	8.5
1	A	373	GLN	8.5
1	A	524	GLN	8.5
1	A	38	CYS	8.5
1	A	34	LEU	8.5
2	B	140	PRO	8.5
1	A	360	ALA	8.5
1	A	416	PHE	8.4
2	B	243	PRO	8.4
2	B	115	TYR	8.4
2	B	147	ASN	8.4
2	B	209	LEU	8.4
1	A	222	GLN	8.3
1	A	470	THR	8.3
2	B	307	ARG	8.3
2	B	343	GLN	8.3

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Mol	Chain	Res	Type	RSRZ
2	B	131	THR	8.3
2	B	182	GLN	8.3
1	A	542	ILE	8.3
1	A	310	LEU	8.3
2	B	297	GLU	8.3
1	A	449	GLU	8.2
2	B	214	LEU	8.2
1	A	164	MET	8.2
2	B	26	LEU	8.2
2	B	208	HIS	8.2
2	B	68	SER	8.2
1	A	483	TYR	8.1
2	B	107	THR	8.1
1	A	377	THR	8.1
2	B	237	ASP	8.1
2	B	54	ASN	8.1
1	A	246	LEU	8.1
1	A	70	LYS	8.1
1	A	244	ILE	8.1
1	A	505	ILE	8.1
2	B	375	ILE	8.1
2	B	344	GLU	8.0
1	A	480	GLN	8.0
1	A	102	LYS	8.0
1	A	240	THR	8.0
1	A	436	GLY	7.9
1	A	347	LYS	7.9
1	A	285	GLY	7.9
2	B	352	GLY	7.9
2	B	177	ASP	7.8
2	B	49	LYS	7.8
1	A	110	ASP	7.8
1	A	491	LEU	7.7
1	A	432	GLU	7.7
1	A	165	THR	7.7
1	A	535	TRP	7.7
2	B	39	THR	7.7
1	A	124	PHE	7.7
1	A	487	GLN	7.7
1	A	152	GLY	7.6
2	B	195	ILE	7.6
2	B	113	ASP	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	355	ALA	7.6
1	A	418	ASN	7.6
1	A	61	PHE	7.5
1	A	139	THR	7.5
2	B	55	PRO	7.5
2	B	123	ASP	7.5
1	A	136	ASN	7.5
2	B	229	TRP	7.5
2	B	394	GLN	7.4
2	B	270	ILE	7.4
1	A	80	LEU	7.4
2	B	97	PRO	7.4
1	A	457	TYR	7.4
2	B	174	GLN	7.3
1	A	97	PRO	7.3
1	A	376	THR	7.3
1	A	200	THR	7.3
1	A	359	GLY	7.3
1	A	187	LEU	7.2
2	B	23	GLN	7.2
1	A	36	GLU	7.2
1	A	490	GLY	7.2
2	B	428	GLN	7.2
1	A	284	ARG	7.2
1	A	291	GLU	7.2
1	A	554	ALA	7.2
1	A	287	LYS	7.2
1	A	517	LEU	7.1
1	A	504	GLY	7.1
1	A	476	LYS	7.1
1	A	210	LEU	7.0
2	B	422	LEU	7.0
1	A	216	THR	7.0
2	B	354	TYR	7.0
1	A	451	LYS	7.0
2	B	388	LYS	7.0
1	A	77	PHE	7.0
1	A	283	LEU	7.0
1	A	501	TYR	7.0
2	B	272	PRO	6.9
1	A	45	GLY	6.9
2	B	356	ARG	6.9

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Mol	Chain	Res	Type	RSRZ
2	B	168	LEU	6.9
1	A	353	LYS	6.9
1	A	156	SER	6.8
2	B	201	LYS	6.8
2	B	383	TRP	6.8
2	B	335	GLY	6.8
1	A	506	ILE	6.8
1	A	289	LEU	6.7
2	B	230	MET	6.7
1	A	35	VAL	6.7
2	B	281	LYS	6.7
1	A	441	TYR	6.7
2	B	331	LYS	6.7
1	A	162	SER	6.7
2	B	414	TRP	6.7
1	A	94	ILE	6.7
2	B	57	ASN	6.7
2	B	64	LYS	6.7
2	B	205	LEU	6.7
1	A	179	VAL	6.7
1	A	130	PHE	6.7
2	B	216	THR	6.7
1	A	125	ARG	6.6
1	A	151	GLN	6.6
1	A	266	TRP	6.6
2	B	419	THR	6.6
1	A	425	LEU	6.6
2	B	40	GLU	6.6
1	A	386	THR	6.5
1	A	367	GLN	6.5
1	A	309	ILE	6.5
1	A	553	SER	6.5
1	A	143	ARG	6.5
1	A	258	GLN	6.5
1	A	88	TRP	6.5
2	B	5	ILE	6.4
1	A	405	TYR	6.4
1	A	46	LYS	6.4
2	B	45	GLY	6.4
2	B	83	ARG	6.4
1	A	250	ASP	6.4
2	B	198	HIS	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	293	ILE	6.4
2	B	391	LEU	6.4
2	B	106	VAL	6.4
1	A	243	PRO	6.3
1	A	74	LEU	6.3
1	A	115	TYR	6.3
2	B	318	TYR	6.3
1	A	67	ASP	6.3
2	B	421	PRO	6.3
2	B	251	SER	6.2
2	B	200	THR	6.2
2	B	389	PHE	6.2
2	B	295	LEU	6.2
1	A	242	GLN	6.2
1	A	411	ILE	6.2
1	A	302	GLU	6.2
1	A	276	VAL	6.2
2	B	377	THR	6.2
1	A	312	GLU	6.1
1	A	2	ILE	6.1
1	A	370	GLU	6.1
2	B	127	TYR	6.1
2	B	363	ASN	6.1
2	B	291	GLU	6.1
1	A	369	THR	6.1
2	B	175	ASN	6.1
2	B	418	ASN	6.1
1	A	129	ALA	6.1
1	A	402	TRP	6.1
2	B	245	VAL	6.1
1	A	225	PRO	6.1
1	A	307	ARG	6.0
1	A	534	ALA	6.0
1	A	294	PRO	6.0
2	B	74	LEU	6.0
2	B	132	ILE	6.0
1	A	536	VAL	6.0
2	B	111	VAL	6.0
1	A	30	LYS	6.0
1	A	245	VAL	6.0
2	B	232	TYR	6.0
1	A	5	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	478	GLU	6.0
2	B	138	GLU	5.9
2	B	156	SER	5.9
2	B	339	TYR	5.9
1	A	374	LYS	5.9
1	A	408	ALA	5.9
1	A	368	LEU	5.9
1	A	382	ILE	5.9
1	A	145	GLN	5.9
1	A	444	GLY	5.9
1	A	492	GLU	5.9
2	B	89	GLU	5.9
2	B	368	LEU	5.9
2	B	63	ILE	5.9
2	B	44	GLU	5.8
2	B	427	TYR	5.8
2	B	420	PRO	5.8
1	A	430	GLU	5.8
1	A	264	LEU	5.8
2	B	257	ILE	5.8
2	B	180	ILE	5.8
2	B	269	GLN	5.8
1	A	75	VAL	5.8
1	A	140	PRO	5.8
1	A	442	VAL	5.8
1	A	356	ARG	5.7
2	B	355	ALA	5.7
2	B	341	ILE	5.7
1	A	409	THR	5.7
2	B	346	PHE	5.7
1	A	299	ALA	5.6
1	A	159	ILE	5.6
1	A	198	HIS	5.6
1	A	516	GLU	5.6
2	B	312	GLU	5.6
1	A	350	LYS	5.6
1	A	298	GLU	5.6
2	B	424	LYS	5.6
2	B	294	PRO	5.5
1	A	170	PRO	5.5
2	B	316	GLY	5.5
1	A	277	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	410	TRP	5.5
1	A	223	LYS	5.5
2	B	36	GLU	5.5
1	A	419	THR	5.5
1	A	206	ARG	5.5
1	A	334	GLN	5.5
1	A	280	CYS	5.4
2	B	38	CYS	5.4
1	A	112	GLY	5.4
1	A	69	THR	5.4
1	A	520	GLN	5.4
1	A	401	TRP	5.4
2	B	124	PHE	5.4
2	B	311	LYS	5.4
2	B	264	LEU	5.4
1	A	82	LYS	5.3
1	A	25	PRO	5.3
2	B	406	TRP	5.3
1	A	205	LEU	5.3
1	A	281	LYS	5.3
1	A	465	LYS	5.3
2	B	11	LYS	5.3
1	A	109	LEU	5.3
1	A	375	ILE	5.3
2	B	290	THR	5.3
2	B	392	PRO	5.3
2	B	181	TYR	5.2
2	B	79	GLU	5.2
1	A	262	GLY	5.2
1	A	361	HIS	5.2
1	A	512	GLN	5.2
2	B	283	LEU	5.2
2	B	397	THR	5.2
1	A	219	LYS	5.2
2	B	149	LEU	5.2
2	B	193	LEU	5.2
2	B	13	LYS	5.2
2	B	321	PRO	5.2
1	A	527	LYS	5.1
2	B	271	TYR	5.1
2	B	274	ILE	5.1
1	A	404	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	392	PRO	5.1
2	B	20	LYS	5.1
2	B	128	THR	5.1
2	B	50	ILE	5.1
1	A	332	GLN	5.1
2	B	334	GLN	5.1
2	B	306	ASN	5.1
1	A	403	THR	5.0
1	A	184	MET	5.0
1	A	86	ASP	5.0
2	B	369	THR	5.0
2	B	403	THR	5.0
2	B	104	LYS	5.0
2	B	60	VAL	4.9
1	A	473	THR	4.9
1	A	41	MET	4.9
2	B	258	GLN	4.9
1	A	255	ASN	4.9
1	A	265	ASN	4.9
2	B	96	HIS	4.9
1	A	65	LYS	4.9
2	B	192	ASP	4.9
1	A	93	GLY	4.9
1	A	157	PRO	4.9
2	B	413	GLU	4.8
1	A	278	GLN	4.8
1	A	104	LYS	4.8
1	A	16	MET	4.7
1	A	72	ARG	4.7
1	A	217	PRO	4.7
1	A	461	ARG	4.7
2	B	301	LEU	4.7
1	A	340	GLN	4.7
1	A	463	ARG	4.7
1	A	68	SER	4.6
2	B	315	HIS	4.6
2	B	247	PRO	4.6
2	B	385	LYS	4.6
2	B	58	THR	4.6
1	A	201	LYS	4.6
1	A	89	GLU	4.6
1	A	333	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	497	THR	4.5
2	B	260	LEU	4.5
1	A	395	LYS	4.5
1	A	211	ARG	4.5
2	B	262	GLY	4.5
2	B	51	GLY	4.5
2	B	285	GLY	4.5
2	B	234	LEU	4.5
2	B	292	VAL	4.5
2	B	153	TRP	4.4
1	A	541	GLY	4.4
1	A	191	SER	4.4
1	A	11	LYS	4.4
1	A	275	LYS	4.4
1	A	237	ASP	4.4
1	A	428	GLN	4.4
2	B	43	LYS	4.4
1	A	60	VAL	4.4
1	A	378	GLU	4.4
1	A	526	ILE	4.3
2	B	371	ALA	4.3
1	A	241	VAL	4.3
1	A	197	GLN	4.3
1	A	73	LYS	4.3
2	B	249	LYS	4.3
1	A	135	ILE	4.3
1	A	186	ASP	4.3
1	A	394	GLN	4.3
2	B	161	GLN	4.3
1	A	303	LEU	4.3
1	A	173	LYS	4.3
1	A	10	VAL	4.3
1	A	189	VAL	4.3
2	B	381	VAL	4.3
1	A	371	ALA	4.2
1	A	260	LEU	4.2
2	B	313	PRO	4.2
1	A	460	ASN	4.2
1	A	252	TRP	4.2
1	A	288	ALA	4.2
2	B	207	GLN	4.2
2	B	280	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	172	ARG	4.2
1	A	123	ASP	4.2
2	B	27	THR	4.1
1	A	479	LEU	4.1
2	B	319	TYR	4.1
2	B	404	GLU	4.1
1	A	76	ASP	4.1
2	B	160	PHE	4.1
1	A	138	GLU	4.1
1	A	539	HIS	4.1
1	A	52	PRO	4.1
1	A	421	PRO	4.0
1	A	485	ALA	4.0
2	B	90	VAL	4.0
1	A	344	GLU	4.0
2	B	171	PHE	4.0
2	B	347	LYS	4.0
1	A	279	LEU	3.9
2	B	206	ARG	3.9
1	A	531	VAL	3.9
2	B	103	LYS	3.9
2	B	379	SER	3.9
1	A	400	THR	3.9
2	B	61	PHE	3.9
1	A	508	ALA	3.9
1	A	192	ASP	3.9
2	B	73	LYS	3.9
1	A	14	PRO	3.8
2	B	21	VAL	3.8
2	B	425	LEU	3.8
1	A	351	THR	3.8
2	B	196	GLY	3.8
1	A	324	ASP	3.8
2	B	117	SER	3.8
2	B	266	TRP	3.8
1	A	507	GLN	3.8
2	B	275	LYS	3.8
1	A	166	LYS	3.8
1	A	26	LEU	3.8
1	A	176	PRO	3.8
2	B	199	ARG	3.8
2	B	130	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	121	ASP	3.8
2	B	259	LYS	3.8
1	A	450	THR	3.7
1	A	414	TRP	3.7
2	B	409	THR	3.7
2	B	327	ALA	3.7
1	A	235	HIS	3.7
1	A	438	GLU	3.7
1	A	120	LEU	3.7
1	A	387	PRO	3.6
2	B	52	PRO	3.6
1	A	482	ILE	3.6
2	B	77	PHE	3.6
2	B	322	SER	3.5
2	B	348	ASN	3.5
2	B	172	ARG	3.5
2	B	287	LYS	3.5
1	A	528	LYS	3.4
2	B	212	TRP	3.4
1	A	540	LYS	3.4
1	A	163	SER	3.4
2	B	179	VAL	3.4
2	B	188	TYR	3.4
1	A	66	LYS	3.4
1	A	111	VAL	3.3
1	A	415	GLU	3.3
1	A	50	ILE	3.3
1	A	301	LEU	3.3
1	A	313	PRO	3.3
1	A	420	PRO	3.3
1	A	396	GLU	3.3
2	B	384	GLY	3.3
1	A	515	SER	3.3
1	A	28	GLU	3.3
1	A	42	GLU	3.3
1	A	464	GLN	3.2
2	B	278	GLN	3.2
1	A	158	ALA	3.2
1	A	177	ASP	3.2
1	A	335	GLY	3.2
1	A	412	PRO	3.2
1	A	523	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	246	LEU	3.2
2	B	333	GLY	3.2
2	B	395	LYS	3.2
2	B	12	LEU	3.1
1	A	366	LYS	3.1
2	B	277	ARG	3.1
2	B	22	LYS	3.1
1	A	249	LYS	3.1
2	B	303	LEU	3.0
1	A	254	VAL	3.0
2	B	415	GLU	3.0
1	A	530	LYS	3.0
2	B	178	ILE	3.0
1	A	248	GLU	3.0
1	A	393	ILE	3.0
2	B	33	ALA	3.0
2	B	189	VAL	3.0
1	A	364	ASP	3.0
1	A	62	ALA	3.0
2	B	85	GLN	3.0
1	A	518	VAL	2.9
1	A	127	TYR	2.9
1	A	174	GLN	2.9
2	B	173	LYS	2.9
2	B	139	THR	2.9
2	B	191	SER	2.9
2	B	31	ILE	2.8
1	A	224	GLU	2.8
1	A	308	GLU	2.8
1	A	295	LEU	2.8
2	B	302	GLU	2.8
1	A	214	LEU	2.8
1	A	208	HIS	2.8
1	A	213	GLY	2.8
2	B	46	LYS	2.7
1	A	203	GLU	2.7
1	A	365	VAL	2.7
2	B	293	ILE	2.7
1	A	54	ASN	2.7
2	B	129	ALA	2.7
1	A	413	GLU	2.7
2	B	263	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	273	GLY	2.7
1	A	511	ASP	2.6
1	A	513	SER	2.6
1	A	9	PRO	2.6
1	A	85	GLN	2.6
1	A	509	GLN	2.6
1	A	494	ASN	2.6
2	B	75	VAL	2.6
1	A	300	GLU	2.5
1	A	221	HIS	2.5
1	A	514	GLU	2.5
2	B	328	GLU	2.5
2	B	332	GLN	2.5
2	B	231	GLY	2.4
1	A	51	GLY	2.4
1	A	31	ILE	2.4
1	A	305	GLU	2.4
1	A	55	PRO	2.4
2	B	9	PRO	2.4
2	B	15	GLY	2.4
1	A	257	ILE	2.4
1	A	388	LYS	2.4
1	A	53	GLU	2.4
2	B	284	ARG	2.3
1	A	236	PRO	2.3
2	B	242	GLN	2.3
1	A	247	PRO	2.3
1	A	372	VAL	2.3
1	A	306	ASN	2.3
1	A	259	LYS	2.3
2	B	37	ILE	2.3
2	B	65	LYS	2.3
2	B	122	GLU	2.2
2	B	364	ASP	2.2
1	A	122	GLU	2.2
2	B	118	VAL	2.2
1	A	261	VAL	2.2
2	B	18	GLY	2.2
1	A	84	THR	2.2
2	B	16	MET	2.2
1	A	546	GLU	2.2
2	B	248	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	202	ILE	2.2
2	B	6	GLU	2.2
1	A	220	LYS	2.1
1	A	195	ILE	2.1
2	B	62	ALA	2.1
2	B	165	THR	2.1
1	A	49	LYS	2.1
2	B	76	ASP	2.1
2	B	407	GLN	2.1
2	B	286	THR	2.1
2	B	376	THR	2.1
2	B	256	ASP	2.1
1	A	78	ARG	2.1
1	A	27	THR	2.1
1	A	4	PRO	2.1
1	A	529	GLU	2.1
1	A	323	LYS	2.1
1	A	199	ARG	2.0
1	A	29	GLU	2.0
1	A	19	PRO	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SUC	B	2001	23/23	0.52	0.68	0.20	64,70,75,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	1WT	A	602	33/33	0.34	0.72	-0.11	50,55,71,79	0
3	MLA	A	601	7/7	0.47	0.38	-0.47	94,96,99,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.