Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 01:01 PM EDT

PDB ID	:	2FQZ
Title	:	Metal-depleted Ecl18kI in complex with uncleaved DNA
Authors	:	Bochtler, M.; Szczepanowski, R.H.; Tamulaitis, G.; Grazulis, S.; Czapinska, H.; Manakova, E.; Siksnys, V.
Deposited on	:	2006-01-18
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

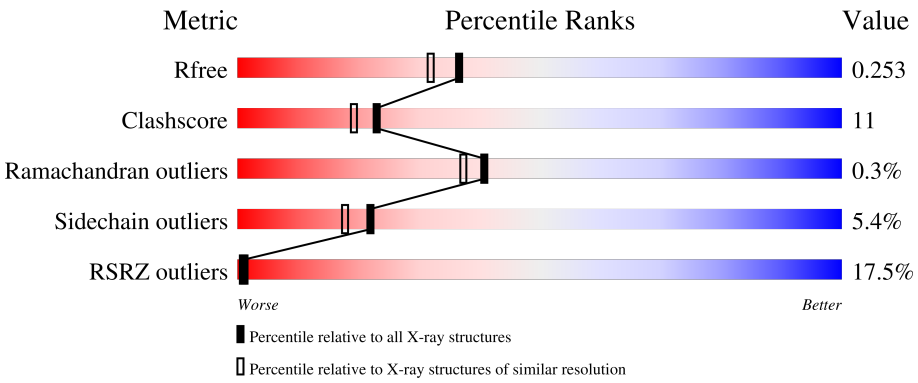
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	E	9	33% 67%
1	G	9	22% 78%
2	F	9	11% 11% 89%
2	H	9	22% 78%
3	A	305	25% 72% 20% • 5%

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Mol	Chain	Length	Quality of chain
3	B	305	15% 71% 23%
3	C	305	16% 73% 20%
3	D	305	12% 73% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11645 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 DNA chain called DNA STRAND 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	9	364	172	74	102	16	0	9	0
1	G	9	364	172	74	102	16	0	9	0

- Molecule 2 is a DNA chain called DNA STRAND 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	9	362	172	68	106	16	0	9	0
2	H	9	362	172	68	106	16	0	9	0

- Molecule 3 is a protein called R.Ecl18kI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	290	2393	1522	396	462	13	21	0	0
3	B	293	2421	1541	399	468	13	15	0	0
3	C	292	2412	1537	398	464	13	19	0	0
3	D	292	2412	1537	398	464	13	11	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	GLN	ARG	engineered mutation	UNP O87963
B	277	GLN	ARG	engineered mutation	UNP O87963
C	277	GLN	ARG	engineered mutation	UNP O87963
D	277	GLN	ARG	engineered mutation	UNP O87963

- Molecule 4 is water.

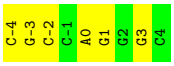
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	16	16	16	0	0
			Total	O		
4	F	15	15	15	0	0
			Total	O		
4	G	24	24	24	0	0
			Total	O		
4	H	20	20	20	0	0
			Total	O		
4	A	83	83	83	0	0
			Total	O		
4	B	133	133	133	0	0
			Total	O		
4	C	135	135	135	0	0
			Total	O		
4	D	129	129	129	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

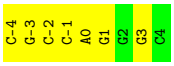
- Molecule 1: DNA STRAND 1

Chain E:



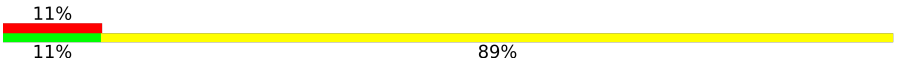
- Molecule 1: DNA STRAND 1

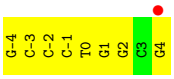
Chain G:



- Molecule 2: DNA STRAND 2

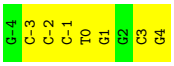
Chain F:





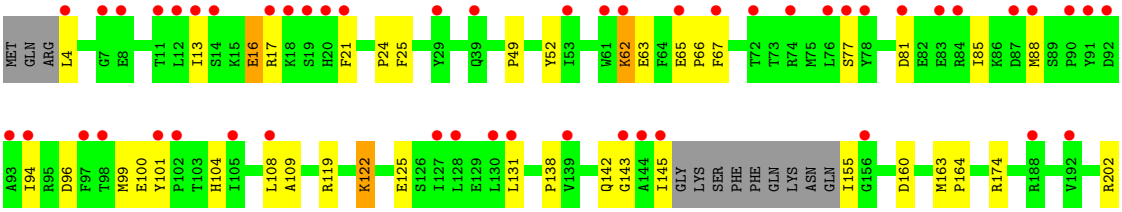
- Molecule 2: DNA STRAND 2

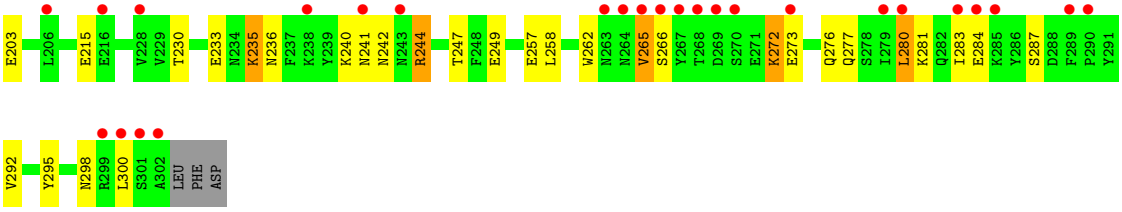
Chain H:



- Molecule 3: R.Ecl18kI

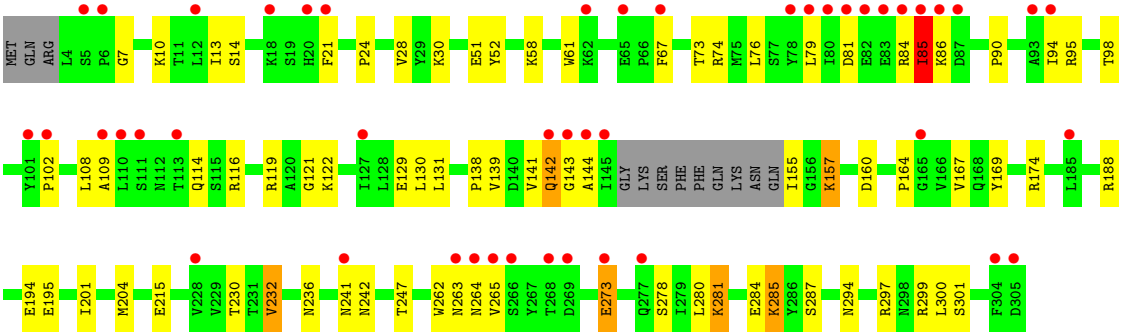
Chain A:





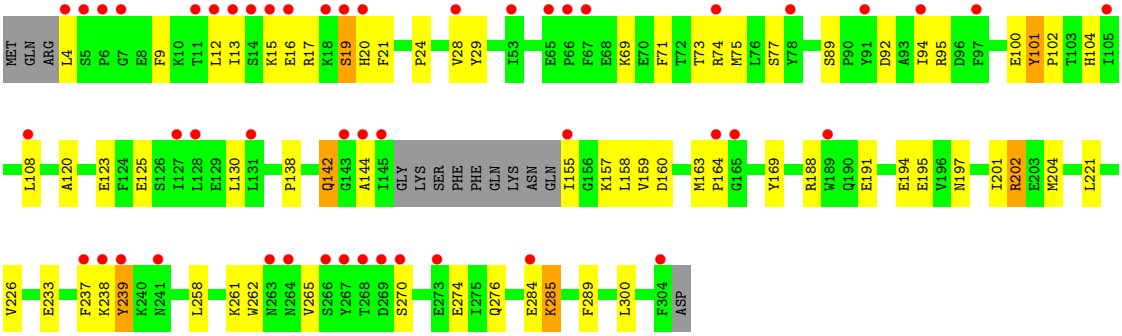
• Molecule 3: R.Ecl18kI

Chain B:



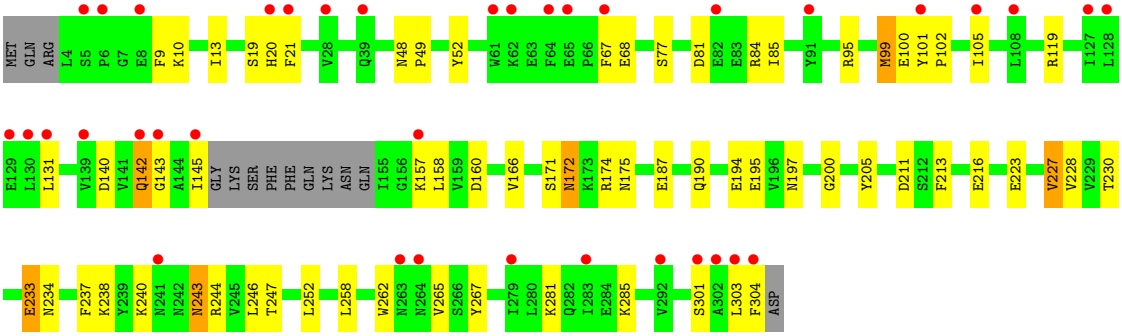
• Molecule 3: R.Ecl18kI

Chain C:



• Molecule 3: R.Ecl18kI

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.37Å 95.52Å 190.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.61 – 1.97	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-2.00) 91.5 (19.61-1.97)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	3.99 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , 0.260 0.210 , 0.253	Depositor DCC
R_{free} test set	4666 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11645	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	E	0.43	0/408	0.69	0/626
1	G	0.59	0/408	0.82	0/626
2	F	0.44	0/404	0.70	0/620
2	H	0.48	0/404	0.76	0/620
3	A	0.52	0/2440	0.65	0/3293
3	B	0.57	0/2469	0.69	1/3331 (0.0%)
3	C	0.59	0/2460	0.70	1/3320 (0.0%)
3	D	0.59	0/2460	0.71	0/3320
All	All	0.56	0/11453	0.70	2/15756 (0.0%)

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
3	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	188	ARG	NE-CZ-NH1	5.43	123.02	120.30
3	B	188	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	241	ASN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	364	0	193	13	0
1	G	364	0	195	10	0
2	F	362	0	194	15	0
2	H	362	0	196	10	0
3	A	2393	0	2360	57	0
3	B	2421	0	2384	60	0
3	C	2412	0	2380	55	0
3	D	2412	0	2380	57	0
4	A	83	0	0	11	0
4	B	133	0	0	8	0
4	C	135	0	0	8	0
4	D	129	0	0	11	0
4	E	16	0	0	1	0
4	F	15	0	0	1	0
4	G	24	0	0	1	0
4	H	20	0	0	2	0
All	All	11645	0	10282	242	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 (242) 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)
4:H:16:HOH:O	3:D:157:LYS:HG3	1.35	1.26
1:G:-3[A]:DG:H5"	3:C:157:LYS:HB2	1.21	1.20
3:D:160:ASP:HB3	4:D:398:HOH:O	1.52	1.09
2:H:-3[B]:DC:H5"	3:C:157:LYS:HB2	1.41	1.02
3:B:155:ILE:HD11	3:B:169:TYR:CE2	1.97	0.99
3:D:197:ASN:HB3	4:D:379:HOH:O	1.61	0.98
3:B:51:GLU:HB3	4:B:427:HOH:O	1.67	0.95
1:E:-3[B]:DG:H5"	3:B:157:LYS:HB2	1.49	0.95
2:F:-3[A]:DC:H5"	3:B:157:LYS:HB2	1.46	0.94
3:D:262:TRP:O	3:D:265:VAL:HG12	1.66	0.94
3:D:240:LYS:HD3	4:D:407:HOH:O	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:-3[A]:DG:C5'	3:C:157:LYS:HB2	2.02	0.87
3:D:211:ASP:HB2	3:D:234:ASN:OD1	1.75	0.87
3:A:77:SER:HB2	4:A:340:HOH:O	1.75	0.85
3:D:211:ASP:CB	3:D:234:ASN:OD1	2.24	0.85
3:A:272:LYS:O	3:A:276:GLN:HG2	1.78	0.84
4:G:20:HOH:O	2:H:-3[B]:DC:H5	1.59	0.84
3:B:155:ILE:HD11	3:B:169:TYR:CD2	2.12	0.84
3:C:12:LEU:HB2	4:C:426:HOH:O	1.83	0.77
3:A:142:GLN:HG3	3:A:143:GLY:N	2.00	0.76
3:C:155:ILE:HD11	3:C:169:TYR:CE2	2.21	0.76
3:B:284:GLU:HG3	4:B:431:HOH:O	1.83	0.76
3:C:142:GLN:HG2	3:C:159:VAL:O	1.87	0.74
3:C:75:MET:HA	4:C:364:HOH:O	1.87	0.73
3:C:197:ASN:HB3	4:C:379:HOH:O	1.87	0.73
3:A:202:ARG:NH2	4:A:324:HOH:O	2.22	0.73
3:B:144:ALA:HA	3:B:285:LYS:HG2	1.70	0.73
3:C:74:ARG:O	3:C:77:SER:HB2	1.88	0.72
3:C:239:TYR:HD2	4:C:435:HOH:O	1.73	0.72
2:F:-4[B]:DG:H2"	2:F:-3[B]:DC:OP2	1.89	0.71
3:A:202:ARG:HG2	3:C:202:ARG:HG3	1.73	0.70
3:C:94:ILE:HD12	3:D:85:ILE:HD13	1.71	0.70
3:B:102:PRO:HD2	4:B:389:HOH:O	1.92	0.69
3:D:9:PHE:O	3:D:13:ILE:HG12	1.92	0.69
3:D:77:SER:HB2	4:D:359:HOH:O	1.93	0.69
3:D:216:GLU:HG2	4:D:409:HOH:O	1.93	0.69
3:B:74:ARG:HD2	4:B:417:HOH:O	1.93	0.68
3:C:12:LEU:CB	4:C:426:HOH:O	2.40	0.67
3:D:240:LYS:CD	4:D:407:HOH:O	2.34	0.67
3:A:164:PRO:HG3	3:A:262:TRP:CD2	2.31	0.66
3:A:85:ILE:HD13	3:B:94:ILE:HD12	1.77	0.66
3:A:94:ILE:CD1	3:B:85:ILE:HD12	2.26	0.66
3:B:142:GLN:HG3	3:B:143:GLY:N	2.10	0.66
3:D:233:GLU:HB2	4:D:424:HOH:O	1.94	0.65
3:A:142:GLN:HG2	3:A:160:ASP:HA	1.78	0.65
3:B:155:ILE:CD1	3:B:169:TYR:CE2	2.78	0.65
3:C:201:ILE:HD13	3:C:204:MET:HE2	1.78	0.65
3:D:205:TYR:HA	3:D:227:VAL:HG13	1.79	0.64
3:D:140:ASP:OD2	3:D:166:VAL:HG22	1.97	0.64
3:A:203:GLU:OE2	3:C:202:ARG:HD2	1.97	0.63
3:A:63:GLU:CG	3:A:63:GLU:O	2.45	0.63
2:F:4[A]:DG:H5"	3:A:119:ARG:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:200:GLY:HA2	4:D:363:HOH:O	1.99	0.63
3:D:211:ASP:HB3	3:D:234:ASN:OD1	1.98	0.63
4:E:574:HOH:O	2:F:-3[B]:DC:H5	1.80	0.62
3:D:20:HIS:O	3:D:67:PHE:HE2	1.82	0.62
3:D:240:LYS:CE	4:D:407:HOH:O	2.49	0.61
3:A:21:PHE:CE1	3:A:67:PHE:HD2	2.19	0.61
3:C:258:LEU:HG	4:C:433:HOH:O	2.02	0.60
3:A:138:PRO:O	3:A:163:MET:HG2	2.02	0.59
3:A:96:ASP:O	3:A:100:GLU:HB2	2.02	0.59
3:D:101:TYR:N	3:D:102:PRO:HD2	2.18	0.59
2:F:-3[B]:DC:N4	4:F:222:HOH:O	2.36	0.58
3:A:174:ARG:NH1	4:A:376:HOH:O	2.36	0.58
1:E:0[A]:DA:N3	1:E:0[A]:DA:H2'	2.18	0.58
3:A:62:LYS:O	3:A:66:PRO:HD2	2.04	0.58
3:A:292:VAL:O	3:A:295:TYR:HB3	2.04	0.57
3:B:74:ARG:HB2	3:B:74:ARG:CZ	2.34	0.57
1:G:-3[A]:DG:H5"	3:C:157:LYS:CB	2.15	0.57
3:A:142:GLN:HG3	3:A:143:GLY:H	1.68	0.56
3:D:171:SER:O	3:D:172:ASN:HB2	2.05	0.56
3:A:94:ILE:HD11	3:B:85:ILE:HD12	1.86	0.56
3:A:298:ASN:HB2	4:A:346:HOH:O	2.05	0.56
3:D:68:GLU:HG3	4:D:317:HOH:O	2.06	0.55
3:A:230:THR:O	3:A:247:THR:HA	2.06	0.55
3:D:101:TYR:N	3:D:102:PRO:CD	2.69	0.55
3:B:139:VAL:O	3:B:299:ARG:NH1	2.33	0.55
3:C:9:PHE:HA	4:C:426:HOH:O	2.05	0.55
3:C:13:ILE:HD12	3:C:108:LEU:HD13	1.89	0.55
3:A:99:MET:HG3	3:B:73:THR:HG21	1.89	0.55
3:C:89:SER:HB3	3:C:92:ASP:H	1.72	0.55
3:B:24:PRO:HG3	3:B:119:ARG:HG2	1.89	0.54
1:E:-4[B]:DC:N4	2:F:4[B]:DG:H1	2.06	0.54
3:B:144:ALA:CA	3:B:285:LYS:HG2	2.38	0.54
3:C:276:GLN:HG3	3:C:300:LEU:HD11	1.89	0.54
3:C:4:LEU:O	3:C:104:HIS:NE2	2.32	0.54
1:E:-3[B]:DG:C5'	3:B:157:LYS:HB2	2.24	0.54
3:C:15:LYS:HB3	3:C:16:GLU:OE1	2.08	0.54
3:C:262:TRP:O	3:C:265:VAL:HB	2.09	0.53
3:A:280:LEU:HD13	3:A:284:GLU:OE2	2.08	0.53
3:C:201:ILE:HD13	3:C:204:MET:CE	2.38	0.53
3:A:13:ILE:HD12	3:A:108:LEU:HD13	1.90	0.53
3:B:142:GLN:HG3	3:B:143:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:237:PHE:CD2	3:C:238:LYS:HE3	2.43	0.53
2:F:4[A]:DG:H5"	3:A:119:ARG:CG	2.39	0.53
2:H:-2[A]:DC:H2'	2:H:-1[A]:DC:C6	2.44	0.53
3:B:144:ALA:O	3:B:285:LYS:HE2	2.09	0.52
3:D:142:GLN:HG3	3:D:143:GLY:N	2.24	0.52
1:G:-2[A]:DC:H2'	1:G:-1[A]:DC:C6	2.44	0.52
3:D:10:LYS:HA	3:D:13:ILE:HG13	1.91	0.52
3:D:21:PHE:CE1	3:D:67:PHE:HD2	2.28	0.52
3:A:242:ASN:OD1	3:A:244:ARG:HG3	2.10	0.52
3:C:144:ALA:HA	3:C:285:LYS:HE2	1.92	0.52
1:E:-4[B]:DC:H2"	1:E:-3[B]:DG:OP2	2.11	0.51
3:B:81:ASP:HB3	3:B:84:ARG:HB2	1.92	0.51
3:D:52:TYR:CE2	3:D:131:LEU:HB2	2.45	0.51
3:D:227:VAL:HG21	3:D:246:LEU:HD12	1.92	0.51
1:E:-4[A]:DC:H2"	1:E:-3[A]:DG:OP2	2.10	0.51
3:D:84:ARG:NH2	3:D:100:GLU:HG3	2.26	0.51
3:D:243:ASN:C	3:D:243:ASN:HD22	2.14	0.51
3:A:63:GLU:O	3:A:63:GLU:HG2	2.10	0.50
3:B:164:PRO:HG3	3:B:262:TRP:CD2	2.46	0.50
3:B:142:GLN:NE2	3:B:157:LYS:O	2.45	0.50
1:G:-2[B]:DC:H2'	1:G:-1[B]:DC:C6	2.46	0.50
3:D:84:ARG:NH2	3:D:100:GLU:CG	2.75	0.50
3:A:276:GLN:O	3:A:280:LEU:HB2	2.11	0.50
3:C:100:GLU:OE1	3:C:100:GLU:HA	2.12	0.50
3:C:16:GLU:HA	3:C:19:SER:OG	2.11	0.50
3:B:144:ALA:O	3:B:285:LYS:HG2	2.11	0.49
3:D:142:GLN:HG2	3:D:160:ASP:HA	1.95	0.49
2:H:3[B]:DC:H5	4:H:19:HOH:O	1.94	0.49
2:H:3[B]:DC:H2"	2:H:4[B]:DG:C8	2.47	0.49
3:B:142:GLN:HG2	3:B:160:ASP:HA	1.94	0.49
3:B:232:VAL:HG23	3:B:236:ASN:ND2	2.27	0.49
3:A:49:PRO:HD2	3:A:249:GLU:HG3	1.93	0.49
3:C:20:HIS:HB2	4:C:384:HOH:O	2.13	0.49
3:D:142:GLN:HG3	3:D:143:GLY:H	1.78	0.49
3:B:273:GLU:HG2	4:B:413:HOH:O	2.11	0.48
3:B:24:PRO:HB2	3:B:122:LYS:HG3	1.95	0.48
3:C:29:TYR:CE1	3:C:289:PHE:HB3	2.48	0.48
3:C:17:ARG:HG3	3:C:21:PHE:CD2	2.48	0.48
3:C:155:ILE:HD11	3:C:169:TYR:CD2	2.48	0.48
3:A:215:GLU:OE1	3:A:242:ASN:ND2	2.47	0.48
3:A:257:GLU:OE1	3:C:261:LYS:NZ	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:285:LYS:N	3:B:285:LYS:HD3	2.29	0.48
3:A:235:LYS:NZ	4:A:321:HOH:O	2.47	0.48
3:D:243:ASN:HD22	3:D:244:ARG:N	2.12	0.48
3:A:265:VAL:HG22	4:A:384:HOH:O	2.13	0.47
3:C:71:PHE:O	3:C:75:MET:HG2	2.14	0.47
3:C:73:THR:HG21	3:D:99:MET:HG3	1.95	0.47
1:G:-4[A]:DC:H1'	1:G:-3[A]:DG:C8	2.50	0.47
3:D:175:ASN:HA	3:D:258:LEU:HD22	1.96	0.47
1:G:0[B]:DA:H2'	1:G:0[B]:DA:N3	2.30	0.47
3:B:167:VAL:HG23	4:B:350:HOH:O	2.14	0.47
3:A:24:PRO:HB2	3:A:122:LYS:HG3	1.97	0.47
2:H:0[A]:DT:OP2	2:H:1[A]:DG:H2'	2.15	0.47
3:A:277:GLN:HA	3:A:277:GLN:OE1	2.14	0.46
3:B:280:LEU:CD2	3:B:300:LEU:HD21	2.46	0.46
3:B:280:LEU:HD23	3:B:300:LEU:HD21	1.98	0.46
3:C:69:LYS:HE3	3:D:102:PRO:HG2	1.98	0.46
1:E:-4[B]:DC:N3	2:F:4[B]:DG:N2	2.57	0.46
3:B:94:ILE:O	3:B:98:THR:HG23	2.15	0.46
1:G:0[B]:DA:OP2	1:G:1[B]:DG:H2'	2.15	0.46
3:A:81:ASP:O	3:A:85:ILE:HG12	2.15	0.46
3:B:30:LYS:HE3	4:B:421:HOH:O	2.15	0.46
3:A:164:PRO:HG3	3:A:262:TRP:CE2	2.50	0.46
3:B:52:TYR:CE2	3:B:131:LEU:HB2	2.51	0.46
3:B:230:THR:O	3:B:247:THR:HA	2.16	0.46
3:D:237:PHE:CE2	3:D:238:LYS:HE3	2.51	0.46
3:A:101:TYR:HB3	3:A:104:HIS:HB2	1.97	0.45
3:C:221:LEU:HD22	3:C:226:VAL:HG11	1.98	0.45
2:H:4[B]:DG:H5"	3:D:119:ARG:HG3	1.98	0.45
3:A:174:ARG:CZ	4:A:376:HOH:O	2.64	0.45
3:B:294:ASN:ND2	4:B:411:HOH:O	2.50	0.45
3:D:223:GLU:HB2	4:D:432:HOH:O	2.15	0.45
3:A:109:ALA:HB3	3:B:109:ALA:CB	2.47	0.45
2:H:0[B]:DT:H72	3:C:120:ALA:HA	1.99	0.45
2:H:4[B]:DG:H5"	3:D:119:ARG:CG	2.47	0.45
3:C:194:GLU:OE1	3:C:195:GLU:OE2	2.35	0.45
3:D:303:LEU:HD23	3:D:304:PHE:CE1	2.52	0.45
3:C:191:GLU:HG2	3:D:190:GLN:HB2	1.99	0.44
3:A:283:ILE:HD11	3:A:300:LEU:HD22	1.99	0.44
3:C:74:ARG:O	3:C:77:SER:CB	2.63	0.44
2:F:-2[A]:DC:H2'	2:F:-1[A]:DC:C6	2.53	0.44
3:B:13:ILE:HD13	3:B:108:LEU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:PRO:HB3	3:C:123:GLU:HG3	1.99	0.44
3:C:28:VAL:HG12	3:C:130:LEU:HD12	1.99	0.44
3:D:100:GLU:C	3:D:102:PRO:HD2	2.39	0.44
1:E:0[A]:DA:OP2	1:E:1[A]:DG:H2'	2.18	0.43
3:B:90:PRO:O	3:B:94:ILE:HG13	2.18	0.43
3:A:25:PHE:HZ	3:A:292:VAL:HG21	1.82	0.43
3:B:28:VAL:HG12	3:B:130:LEU:HD12	1.99	0.43
3:D:101:TYR:O	3:D:105:ILE:HG13	2.17	0.43
3:D:265:VAL:HG11	3:D:267:TYR:CZ	2.53	0.43
1:E:0[B]:DA:N6	3:B:61:TRP:HB2	2.33	0.43
3:D:48:ASN:N	3:D:49:PRO:CD	2.82	0.43
3:C:163:MET:HE1	3:C:258:LEU:HB3	1.99	0.43
3:B:7:GLY:HA2	3:B:10:LYS:HE2	2.00	0.43
3:B:79:LEU:HD12	3:B:79:LEU:C	2.39	0.43
3:B:201:ILE:HD13	3:B:204:MET:CE	2.48	0.43
3:C:101:TYR:N	3:C:102:PRO:CD	2.82	0.43
3:D:230:THR:O	3:D:247:THR:HA	2.18	0.43
2:F:-4[B]:DG:C2'	2:F:-3[B]:DC:OP2	2.64	0.43
3:C:164:PRO:HG3	3:C:262:TRP:CD2	2.54	0.43
1:E:0[B]:DA:H4'	1:E:0[B]:DA:OP2	2.19	0.42
3:D:265:VAL:HG11	3:D:267:TYR:OH	2.19	0.42
1:G:3[B]:DG:O6	2:H:-3[B]:DC:N4	2.51	0.42
3:B:21:PHE:CE1	3:B:67:PHE:HD2	2.37	0.42
3:D:84:ARG:CZ	3:D:100:GLU:HG3	2.49	0.42
1:G:-3[A]:DG:C5'	3:C:157:LYS:CB	2.87	0.42
3:A:52:TYR:CE2	3:A:131:LEU:HB2	2.54	0.42
3:A:236:ASN:HB3	3:A:240:LYS:HE2	2.01	0.42
3:B:215:GLU:OE1	3:B:242:ASN:ND2	2.52	0.42
3:A:163:MET:HE1	3:A:258:LEU:HB3	2.02	0.42
3:B:281:LYS:O	3:B:284:GLU:HB3	2.20	0.42
3:C:238:LYS:HB2	3:C:239:TYR:CE1	2.54	0.42
3:D:281:LYS:HE2	3:D:281:LYS:HB2	1.64	0.42
2:F:-4[A]:DG:H2"	2:F:-3[A]:DC:OP2	2.18	0.42
3:A:287:SER:HB3	4:A:343:HOH:O	2.19	0.42
3:B:300:LEU:HD12	3:B:300:LEU:HA	1.91	0.42
3:C:125:GLU:HG2	3:C:160:ASP:OD2	2.20	0.42
3:B:129:GLU:OE2	3:B:141:VAL:HG21	2.20	0.42
3:B:138:PRO:O	3:B:164:PRO:HA	2.20	0.42
3:C:300:LEU:HD12	3:C:300:LEU:HA	1.91	0.42
3:C:138:PRO:O	3:C:163:MET:HG2	2.20	0.41
1:E:-2[B]:DC:O3'	3:B:121:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:LEU:O	3:C:262:TRP:HD1	2.03	0.41
3:A:258:LEU:O	3:A:262:TRP:HD1	2.03	0.41
3:A:85:ILE:O	3:A:88:MET:HB2	2.21	0.41
3:B:194:GLU:OE1	3:B:195:GLU:OE2	2.38	0.41
1:E:3[B]:DG:O6	2:F:-3[B]:DC:N4	2.54	0.41
3:D:194:GLU:OE1	3:D:195:GLU:OE2	2.39	0.41
3:D:237:PHE:CZ	3:D:238:LYS:HE3	2.55	0.41
1:E:0[A]:DA:H2	4:A:329:HOH:O	2.03	0.41
2:F:0[B]:DT:OP2	2:F:1[B]:DG:H2'	2.20	0.41
3:A:63:GLU:O	3:A:63:GLU:HG3	2.20	0.41
3:A:13:ILE:CD1	3:A:108:LEU:HD13	2.50	0.41
3:A:16:GLU:HG3	4:A:375:HOH:O	2.20	0.41
3:A:125:GLU:HG2	3:A:160:ASP:OD2	2.21	0.41
3:B:76:LEU:O	3:B:79:LEU:CD1	2.69	0.41
3:C:270:SER:O	3:C:274:GLU:HG3	2.20	0.41
3:D:81:ASP:HB3	3:D:84:ARG:HB3	2.03	0.41
3:A:17:ARG:NH1	4:A:331:HOH:O	2.27	0.41
3:B:144:ALA:HA	3:B:285:LYS:CG	2.44	0.41
2:F:0[A]:DT:H2"	3:B:116:ARG:HD3	2.03	0.40
3:A:99:MET:CG	3:B:73:THR:HG21	2.51	0.40
3:D:157:LYS:HA	3:D:157:LYS:HD3	1.92	0.40
3:A:202:ARG:HG2	3:C:202:ARG:CG	2.48	0.40
3:D:20:HIS:O	3:D:67:PHE:CE2	2.68	0.40
3:D:213:PHE:CZ	3:D:228:VAL:HG11	2.56	0.40
3:A:24:PRO:HG3	3:A:119:ARG:HG2	2.04	0.40
2:F:2[B]:DG:O4'	3:B:114:GLN:HG3	2.21	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	
3	A	286/305 (94%)	275 (96%)	11 (4%)	0	100	100
3	B	289/305 (95%)	278 (96%)	10 (4%)	1 (0%)	41	37
3	C	288/305 (94%)	274 (95%)	13 (4%)	1 (0%)	41	37
3	D	288/305 (94%)	283 (98%)	4 (1%)	1 (0%)	41	37
All	All	1151/1220 (94%)	1110 (96%)	38 (3%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	172	ASN
3	B	85	ILE
3	C	101	TYR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	269/283 (95%)	252 (94%)	17 (6%)	18	13
3	B	272/283 (96%)	253 (93%)	19 (7%)	15	10
3	C	271/283 (96%)	262 (97%)	9 (3%)	38	37
3	D	271/283 (96%)	257 (95%)	14 (5%)	23	19
All	All	1083/1132 (96%)	1024 (95%)	59 (5%)	22	18

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	4	LEU
3	A	16	GLU
3	A	62	LYS
3	A	65	GLU
3	A	122	LYS
3	A	145	ILE
3	A	155	ILE
3	A	233	GLU

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Mol	Chain	Res	Type
3	A	235	LYS
3	A	241	ASN
3	A	244	ARG
3	A	265	VAL
3	A	266	SER
3	A	272	LYS
3	A	273	GLU
3	A	280	LEU
3	A	281	LYS
3	B	14	SER
3	B	58	LYS
3	B	85	ILE
3	B	86	LYS
3	B	95	ARG
3	B	142	GLN
3	B	157	LYS
3	B	174	ARG
3	B	232	VAL
3	B	263	ASN
3	B	264	ASN
3	B	265	VAL
3	B	273	GLU
3	B	278	SER
3	B	281	LYS
3	B	285	LYS
3	B	287	SER
3	B	297	ARG
3	B	301	SER
3	C	19	SER
3	C	95	ARG
3	C	142	GLN
3	C	158	LEU
3	C	202	ARG
3	C	233	GLU
3	C	239	TYR
3	C	284	GLU
3	C	285	LYS
3	D	19	SER
3	D	95	ARG
3	D	99	MET
3	D	142	GLN
3	D	145	ILE

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Mol	Chain	Res	Type
3	D	158	LEU
3	D	174	ARG
3	D	187	GLU
3	D	227	VAL
3	D	233	GLU
3	D	243	ASN
3	D	252	LEU
3	D	285	LYS
3	D	301	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	190	GLN
3	A	219	ASN
3	B	175	ASN
3	B	197	ASN
3	B	277	GLN
3	B	294	ASN
3	C	142	GLN
3	D	47	ASN
3	D	225	ASN
3	D	243	ASN
3	D	277	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	E	9/9 (100%)	0.54	0	100	100	33, 36, 42, 50	0
1	G	9/9 (100%)	0.36	0	100	100	26, 27, 36, 42	0
2	F	9/9 (100%)	0.59	1 (11%)	5	4	29, 32, 46, 47	0
2	H	9/9 (100%)	0.32	0	100	100	27, 29, 37, 39	0
3	A	290/305 (95%)	1.44	77 (26%)	0	0	25, 44, 65, 69	5 (1%)
3	B	293/305 (96%)	1.10	46 (15%)	2	1	21, 34, 53, 65	3 (1%)
3	C	292/305 (95%)	1.04	49 (16%)	1	1	22, 33, 53, 66	5 (1%)
3	D	292/305 (95%)	0.85	37 (12%)	3	3	21, 35, 51, 58	3 (1%)
All	All	1203/1256 (95%)	1.09	210 (17%)	1	1	21, 36, 57, 69	16 (1%)

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	145	ILE	12.2
3	C	78	TYR	7.8
3	B	144	ALA	7.1
3	A	264	ASN	7.0
3	C	4	LEU	6.8
3	B	83	GLU	6.2
3	A	267	TYR	6.1
3	B	264	ASN	5.7
3	C	16	GLU	5.7
3	B	265	VAL	5.5
3	B	18	LYS	5.4
3	B	6	PRO	5.3
3	C	264	ASN	5.3
3	B	305	ASP	5.3
3	A	144	ALA	5.2
3	A	67	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
3	B	143	GLY	5.1
3	C	145	ILE	5.0
3	A	143	GLY	5.0
3	A	265	VAL	5.0
3	A	94	ILE	4.9
3	A	7	GLY	4.8
3	B	101	TYR	4.7
3	B	268	THR	4.7
3	C	268	THR	4.6
3	B	5	SER	4.6
3	A	8	GLU	4.6
3	C	6	PRO	4.5
3	B	85	ILE	4.5
3	B	94	ILE	4.5
3	C	66	PRO	4.4
3	A	93	ALA	4.4
3	A	19	SER	4.3
3	A	18	LYS	4.2
3	B	241	ASN	4.2
3	C	238	LYS	4.2
3	A	14	SER	4.1
3	A	280	LEU	4.1
3	C	5	SER	4.0
3	C	14	SER	4.0
3	C	67	PHE	4.0
3	B	87	ASP	3.9
3	B	79	LEU	3.9
3	A	97	PHE	3.9
3	A	279	ILE	3.9
3	A	266	SER	3.8
3	B	81	ASP	3.8
3	B	266	SER	3.8
3	A	11	THR	3.8
3	D	127	ILE	3.8
3	D	157	LYS	3.7
3	A	87	ASP	3.7
3	D	20	HIS	3.7
3	D	304	PHE	3.7
3	B	93	ALA	3.7
3	A	61	TRP	3.7
3	A	302	ALA	3.7
3	A	65	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
3	B	62	LYS	3.6
3	A	130	LEU	3.6
3	B	86	LYS	3.6
3	D	6	PRO	3.6
3	A	83	GLU	3.6
3	B	263	ASN	3.6
3	D	65	GLU	3.6
3	A	301	SER	3.6
3	D	283	ILE	3.5
3	D	108	LEU	3.5
3	C	269	ASP	3.5
3	C	239	TYR	3.5
3	C	144	ALA	3.5
3	A	90	PRO	3.4
3	A	300	LEU	3.4
3	D	142	GLN	3.4
3	C	266	SER	3.3
3	C	18	LYS	3.3
3	C	273	GLU	3.3
3	A	263	ASN	3.3
3	C	13	ILE	3.3
3	A	78	TYR	3.2
3	C	263	ASN	3.2
3	C	7	GLY	3.2
3	C	20	HIS	3.2
3	A	131	LEU	3.2
3	C	270	SER	3.2
3	D	130	LEU	3.2
3	A	20	HIS	3.2
3	A	4	LEU	3.2
3	B	20	HIS	3.2
3	A	269	ASP	3.1
3	A	270	SER	3.1
3	D	264	ASN	3.1
3	C	267	TYR	3.1
3	A	12	LEU	3.1
3	B	277	GLN	3.1
3	A	76	LEU	3.1
3	A	39	GLN	3.0
3	C	237	PHE	3.0
3	D	131	LEU	3.0
3	D	5	SER	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	67	PHE	3.0
3	C	15	LYS	3.0
3	D	143	GLY	2.9
3	A	101	TYR	2.9
3	B	82	GLU	2.9
3	D	292	VAL	2.9
3	D	128	LEU	2.9
3	A	139	VAL	2.8
3	D	301	SER	2.8
3	A	105	ILE	2.8
3	A	21	PHE	2.8
3	A	268	THR	2.8
3	A	92	ASP	2.8
3	B	304	PHE	2.8
3	C	74	ARG	2.8
3	A	88	MET	2.8
3	D	61	TRP	2.7
3	D	241	ASN	2.7
3	D	91	TYR	2.7
3	A	273	GLU	2.7
3	B	228	VAL	2.7
3	A	108	LEU	2.7
3	B	110	LEU	2.7
3	B	102	PRO	2.7
3	B	78	TYR	2.6
3	A	53	ILE	2.6
3	B	165	GLY	2.6
3	C	131	LEU	2.6
3	A	84	ARG	2.6
3	C	143	GLY	2.6
3	C	94	ILE	2.6
3	A	62	LYS	2.6
3	A	91	TYR	2.6
3	A	206	LEU	2.6
3	D	139	VAL	2.5
3	C	11	THR	2.5
3	A	127	ILE	2.5
3	C	241	ASN	2.5
3	A	102	PRO	2.5
3	C	155	ILE	2.5
3	C	12	LEU	2.5
3	A	77	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	127	ILE	2.5
3	A	74	ARG	2.5
3	A	283	ILE	2.5
3	A	285	LYS	2.4
3	B	80	ILE	2.4
3	A	241	ASN	2.4
3	B	269	ASP	2.4
3	D	145	ILE	2.4
3	D	303	LEU	2.4
3	A	290	PRO	2.4
3	C	65	GLU	2.3
3	A	13	ILE	2.3
3	B	185	LEU	2.3
3	B	67	PHE	2.3
3	D	101	TYR	2.3
3	C	128	LEU	2.3
3	C	19	SER	2.3
3	D	279	ILE	2.3
3	A	29	TYR	2.3
3	B	109	ALA	2.3
3	C	284	GLU	2.3
3	A	192	VAL	2.3
3	B	65	GLU	2.3
3	D	21	PHE	2.2
3	B	84	ARG	2.2
3	B	142	GLN	2.2
3	A	81	ASP	2.2
3	A	98	THR	2.2
3	C	97	PHE	2.2
3	D	82	GLU	2.2
3	A	188	ARG	2.2
3	A	238	LYS	2.2
3	C	105	ILE	2.2
3	C	108	LEU	2.2
3	B	111	SER	2.2
3	C	164	PRO	2.2
3	D	62	LYS	2.2
3	C	28	VAL	2.2
3	A	72	THR	2.2
3	D	302	ALA	2.2
3	C	189	TRP	2.1
3	B	113	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	12	LEU	2.1
3	C	165	GLY	2.1
3	D	8	GLU	2.1
3	D	129	GLU	2.1
3	A	289	PHE	2.1
3	C	304	PHE	2.1
3	A	145	ILE	2.1
3	D	105	ILE	2.1
3	A	216	GLU	2.1
3	C	53	ILE	2.1
3	D	263	ASN	2.1
3	A	299	ARG	2.1
3	B	21	PHE	2.1
3	A	17	ARG	2.0
3	A	243	ASN	2.0
3	B	127	ILE	2.0
3	D	39	GLN	2.0
3	D	28	VAL	2.0
3	B	273	GLU	2.0
2	F	4[A]	DG	2.0
3	A	228	VAL	2.0
3	A	284	GLU	2.0
3	D	64	PHE	2.0
3	C	91	TYR	2.0
3	A	128	LEU	2.0
3	A	156	GLY	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 monosaccharides 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.