Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 06:20 PM EDT

PDB ID	:	2GRM
Title	:	Crystal structure of PrgX/iCF10 complex
Authors	:	Shi, K.; Kozlowicz, B.K.; Gu, Z.Y.; Ohlendorf, D.H.; Earhart, C.A.; Dunny, G.M.
Deposited on	:	2006-04-24
Resolution	:	3.00 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 ⓘ symbol.

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

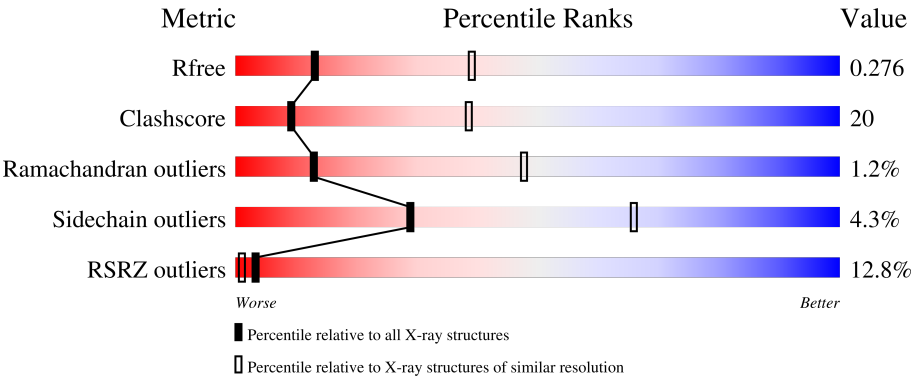
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	A	317	66% 31%
1	B	317	62% 35%
1	C	317	37% 58% 32% 7%
2	D	7	14% 86%
2	E	7	14% 14% 86%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7780 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 PrgX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2599	1685	418	489	7			
1	B	315	Total	C	N	O	S	0	0	0
			2599	1685	418	489	7			
1	C	294	Total	C	N	O	S	0	0	0
			2422	1570	393	453	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	CYS	TYR	engineered mutation	GB 150553
B	231	CYS	TYR	engineered mutation	GB 150553
C	231	CYS	TYR	engineered mutation	GB 150553

- Molecule 2 is a protein called peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	7	Total	C	N	O	0	0	0
			56	40	7	9			
2	E	7	Total	C	N	O	0	0	0
			56	40	7	9			

- Molecule 3 is water.

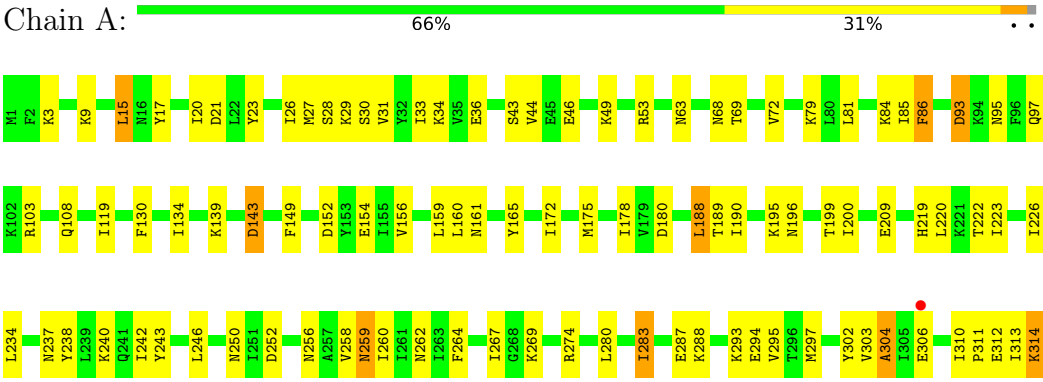
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	19	Total	O	0	0
			19	19		
3	C	7	Total	O	0	0
			7	7		

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.

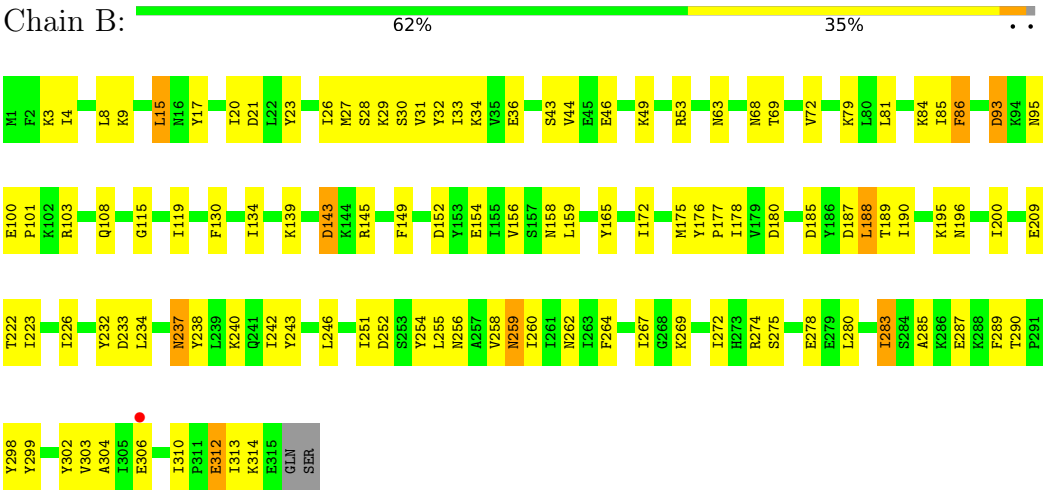
- Molecule 1: PrgX

Chain A:



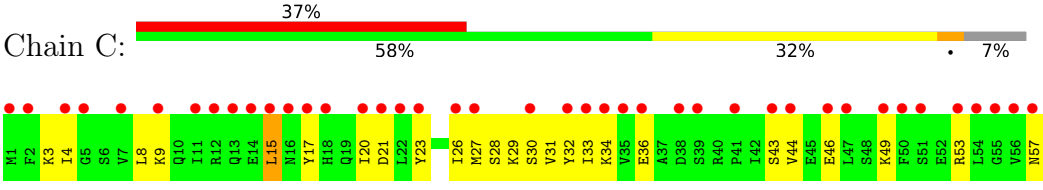
- Molecule 1: PrgX

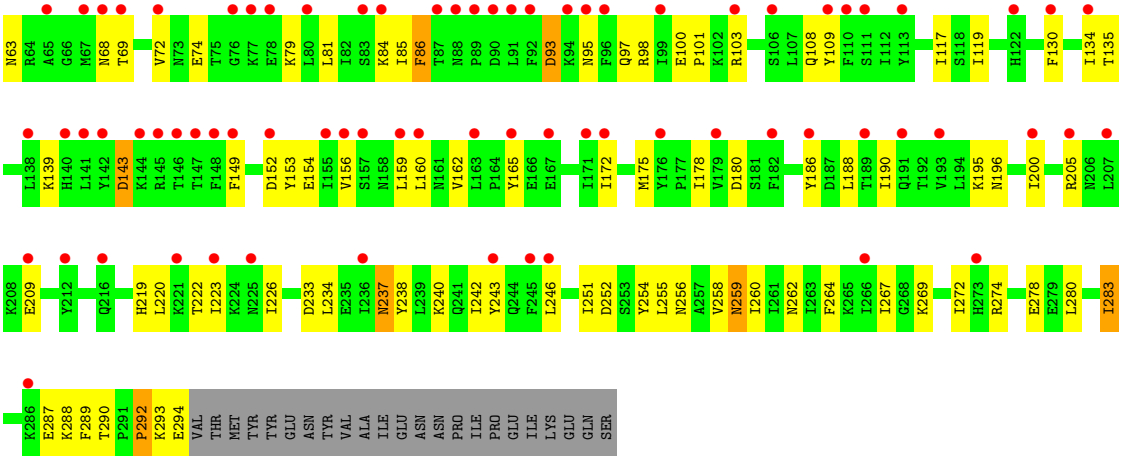
Chain B:



- Molecule 1: PrgX

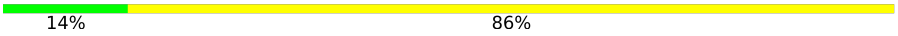
Chain C:





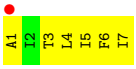
- Molecule 2: peptide

Chain D:



- Molecule 2: peptide

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	93.46Å 134.75Å 192.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.62 – 3.00 49.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.62-3.00) 97.1 (49.24-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.285 0.236 , 0.276	Depositor DCC
R_{free} test set	1184 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 85.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7780	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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

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	0.54	1/2652 (0.0%)	0.60	1/3583 (0.0%)
1	B	0.48	0/2652	0.58	0/3583
1	C	0.34	0/2470	0.51	0/3333
2	D	0.51	0/56	0.57	0/74
2	E	0.53	0/56	0.72	0/74
All	All	0.46	1/7886 (0.0%)	0.57	1/10647 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	CYS	CB-SG	-6.08	1.72	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	231	CYS	CA-CB-SG	-5.08	104.86	114.00

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	2599	0	2639	100	0
1	B	2599	0	2639	110	0
1	C	2422	0	2471	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	56	0	67	12	0
2	E	56	0	67	12	0
3	A	22	0	0	3	0
3	B	19	0	0	1	0
3	C	7	0	0	10	0
All	All	7780	0	7883	311	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 20.

All (311) 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:117:ILE:HG22	3:C:324:HOH:O	1.41	1.20
1:C:162:VAL:HG11	3:C:321:HOH:O	1.45	1.14
1:A:250:ASN:HB3	3:A:336:HOH:O	1.66	0.96
1:C:154:GLU:HG2	3:C:322:HOH:O	1.76	0.85
1:B:31:VAL:HA	1:B:34:LYS:HD2	1.58	0.85
1:C:246:LEU:HD21	1:C:283:ILE:HD11	1.58	0.85
1:A:31:VAL:HA	1:A:34:LYS:HD2	1.57	0.85
1:C:31:VAL:HA	1:C:34:LYS:HD2	1.56	0.84
1:C:172:ILE:HA	1:C:175:MET:HE3	1.59	0.82
1:A:26:ILE:HD12	1:A:49:LYS:HD3	1.62	0.81
1:B:95:ASN:HD22	1:B:98:ARG:HH12	1.29	0.81
1:B:154:GLU:OE2	2:E:7:ILE:HG12	1.80	0.80
1:C:240:LYS:HB3	3:C:320:HOH:O	1.81	0.79
1:B:289:PHE:HZ	1:C:289:PHE:HZ	1.27	0.79
1:A:250:ASN:CB	3:A:336:HOH:O	2.26	0.79
1:A:95:ASN:HD22	1:A:98:ARG:HH12	1.30	0.77
1:B:93:ASP:O	1:B:97:GLN:HG2	1.85	0.77
1:C:26:ILE:HD12	1:C:49:LYS:HD3	1.64	0.77
1:B:246:LEU:HD21	1:B:283:ILE:HD11	1.66	0.77
1:B:172:ILE:HA	1:B:175:MET:HE3	1.65	0.77
1:B:26:ILE:HD12	1:B:49:LYS:HD3	1.67	0.75
1:C:93:ASP:O	1:C:97:GLN:HG2	1.87	0.74
1:C:95:ASN:HD22	1:C:98:ARG:HH12	1.33	0.74
1:A:274:ARG:HD3	1:A:306:GLU:OE2	1.88	0.74
1:A:246:LEU:HD21	1:A:283:ILE:HD11	1.68	0.74
1:A:156:VAL:HG21	1:A:175:MET:CE	2.18	0.73
1:A:93:ASP:O	1:A:97:GLN:HG2	1.88	0.73
1:A:161:ASN:HB2	2:D:2:ILE:HG21	1.68	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PHE:CD1	1:B:119:ILE:HG12	2.24	0.72
1:B:293:LYS:O	1:B:297:MET:HG3	1.90	0.72
1:C:100:GLU:HB3	1:C:101:PRO:HD3	1.72	0.71
1:B:29:LYS:O	1:B:33:ILE:HG13	1.91	0.71
1:A:172:ILE:HA	1:A:175:MET:HE3	1.73	0.70
1:A:100:GLU:HB3	1:A:101:PRO:HD3	1.75	0.69
1:C:29:LYS:O	1:C:33:ILE:HG13	1.93	0.69
1:B:100:GLU:HB3	1:B:101:PRO:HD3	1.75	0.69
1:B:86:PHE:CD2	1:B:310:ILE:HD12	2.28	0.68
1:B:130:PHE:CE1	1:B:134:ILE:HD12	2.29	0.68
1:C:156:VAL:HG21	1:C:175:MET:CE	2.24	0.68
1:B:223:ILE:O	1:B:226:ILE:HG22	1.94	0.67
1:A:189:THR:HG22	2:D:5:ILE:HD13	1.75	0.67
1:C:175:MET:SD	3:C:319:HOH:O	2.53	0.67
1:A:29:LYS:O	1:A:33:ILE:HG13	1.95	0.67
1:A:156:VAL:HG21	1:A:175:MET:HE1	1.75	0.67
1:B:156:VAL:HG21	1:B:175:MET:CE	2.26	0.66
1:A:98:ARG:HB3	1:A:98:ARG:NH1	2.11	0.65
1:A:130:PHE:CE1	1:A:134:ILE:HD12	2.31	0.65
1:A:313:ILE:HG12	2:D:4:LEU:HB2	1.78	0.65
1:A:86:PHE:CD1	1:A:119:ILE:HG12	2.32	0.64
1:C:86:PHE:CD1	1:C:119:ILE:HG12	2.31	0.64
1:C:130:PHE:CE1	1:C:134:ILE:HD12	2.32	0.64
1:C:178:ILE:CD1	1:C:190:ILE:HB	2.27	0.64
1:B:189:THR:HG22	2:E:5:ILE:HD13	1.78	0.63
1:A:293:LYS:O	1:A:297:MET:HB2	1.98	0.63
1:A:130:PHE:CZ	1:A:134:ILE:HD12	2.34	0.62
1:C:134:ILE:HD11	1:C:159:LEU:HD11	1.81	0.62
1:B:130:PHE:CZ	1:B:134:ILE:HD12	2.34	0.62
1:B:178:ILE:CD1	1:B:190:ILE:HB	2.30	0.62
1:B:313:ILE:HG12	2:E:4:LEU:HB2	1.82	0.61
1:C:223:ILE:O	1:C:226:ILE:HG22	2.00	0.61
1:A:178:ILE:CD1	1:A:190:ILE:HB	2.29	0.61
1:A:223:ILE:O	1:A:226:ILE:HG22	2.00	0.61
1:A:250:ASN:CG	3:A:336:HOH:O	2.38	0.61
1:B:289:PHE:HZ	1:C:289:PHE:CZ	2.16	0.60
1:B:98:ARG:NH1	1:B:98:ARG:HB3	2.16	0.60
1:C:242:ILE:HD11	1:C:280:LEU:HD13	1.83	0.60
1:A:134:ILE:HD11	1:A:159:LEU:HD11	1.83	0.60
1:B:72:VAL:HG21	3:B:331:HOH:O	2.00	0.60
1:A:28:SER:O	1:A:31:VAL:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:PHE:CZ	1:C:289:PHE:HZ	2.16	0.60
1:A:220:LEU:O	1:A:226:ILE:HG21	2.02	0.59
1:B:312:GLU:O	1:B:312:GLU:HG3	2.02	0.59
1:C:98:ARG:HB3	1:C:98:ARG:NH1	2.16	0.59
1:B:21:ASP:O	1:B:53:ARG:HD3	2.02	0.59
1:C:283:ILE:HD13	1:C:283:ILE:O	2.03	0.59
1:B:103:ARG:HG2	1:B:103:ARG:HH11	1.65	0.59
1:C:103:ARG:HG2	1:C:103:ARG:HH11	1.67	0.59
1:C:233:ASP:O	1:C:237:ASN:HB2	2.03	0.59
1:A:154:GLU:OE2	2:D:7:ILE:HG13	2.03	0.59
1:B:3:LYS:HD3	1:B:3:LYS:N	2.17	0.59
1:B:242:ILE:HD11	1:B:280:LEU:HD13	1.84	0.59
1:B:28:SER:O	1:B:31:VAL:HG12	2.03	0.58
1:C:21:ASP:O	1:C:53:ARG:HD3	2.03	0.58
1:A:209:GLU:HA	1:A:209:GLU:OE2	2.04	0.58
1:C:30:SER:O	1:C:34:LYS:HG3	2.04	0.58
1:C:28:SER:O	1:C:31:VAL:HG12	2.03	0.58
1:C:220:LEU:O	1:C:226:ILE:HG21	2.03	0.58
1:A:30:SER:O	1:A:34:LYS:HG3	2.04	0.58
1:A:233:ASP:O	1:A:237:ASN:HB2	2.04	0.58
1:A:69:THR:O	1:A:72:VAL:HG13	2.04	0.58
1:A:242:ILE:HD11	1:A:280:LEU:HD13	1.85	0.58
1:B:209:GLU:OE2	1:B:209:GLU:HA	2.03	0.57
1:C:242:ILE:CG1	3:C:323:HOH:O	2.53	0.56
1:A:21:ASP:O	1:A:53:ARG:HD3	2.06	0.56
1:B:30:SER:O	1:B:34:LYS:HG3	2.05	0.56
1:C:172:ILE:HA	1:C:175:MET:CE	2.34	0.56
1:B:69:THR:O	1:B:72:VAL:HG13	2.05	0.56
1:C:130:PHE:CZ	1:C:134:ILE:HD12	2.40	0.56
1:A:3:LYS:HD3	1:A:3:LYS:N	2.20	0.56
1:C:156:VAL:HG21	1:C:175:MET:HE2	1.87	0.56
1:A:189:THR:HG22	2:D:5:ILE:CD1	2.35	0.56
1:B:3:LYS:HD3	1:B:3:LYS:H	1.69	0.56
1:A:283:ILE:HD13	1:A:283:ILE:O	2.05	0.56
1:B:134:ILE:HD11	1:B:159:LEU:HD11	1.87	0.56
1:B:185:ASP:HB3	2:E:7:ILE:HD12	1.88	0.56
1:C:3:LYS:HD3	1:C:3:LYS:N	2.20	0.56
1:B:234:LEU:HD23	1:B:264:PHE:CZ	2.41	0.56
1:C:15:LEU:HB3	1:C:17:TYR:CD1	2.41	0.55
1:B:251:ILE:HG22	1:C:290:THR:O	2.06	0.55
1:C:69:THR:O	1:C:72:VAL:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ILE:HG13	1:B:269:LYS:HG2	1.87	0.55
1:C:178:ILE:HD11	1:C:190:ILE:HB	1.87	0.55
1:A:310:ILE:N	1:A:310:ILE:HD12	2.20	0.55
1:B:233:ASP:O	1:B:237:ASN:HB2	2.05	0.55
1:A:178:ILE:HD11	1:A:190:ILE:HB	1.88	0.55
1:C:267:ILE:HG13	1:C:269:LYS:HG2	1.88	0.55
1:C:43:SER:OG	1:C:46:GLU:HG3	2.07	0.55
1:C:242:ILE:HG13	3:C:323:HOH:O	2.07	0.55
1:B:43:SER:OG	1:B:46:GLU:HG3	2.06	0.54
1:B:256:ASN:O	1:B:260:ILE:HG12	2.08	0.54
1:A:95:ASN:HA	1:A:98:ARG:HH12	1.72	0.54
1:B:158:ASN:HD21	2:E:5:ILE:H	1.54	0.54
1:A:219:HIS:O	1:A:222:THR:HB	2.08	0.54
1:C:209:GLU:OE2	1:C:209:GLU:HA	2.07	0.54
1:C:165:TYR:HB2	1:C:200:ILE:HG21	1.90	0.53
1:C:95:ASN:HA	1:C:98:ARG:HH12	1.73	0.53
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.72	0.53
1:B:283:ILE:HD13	1:B:283:ILE:O	2.08	0.53
1:B:15:LEU:HB3	1:B:17:TYR:CD1	2.43	0.53
1:C:196:ASN:O	1:C:200:ILE:HG12	2.09	0.53
1:B:178:ILE:HD11	1:B:190:ILE:HB	1.90	0.52
1:C:219:HIS:O	1:C:222:THR:HB	2.09	0.52
1:C:9:LYS:HB2	1:C:36:GLU:CG	2.39	0.52
1:B:3:LYS:H	1:B:3:LYS:CD	2.23	0.52
1:C:15:LEU:HB3	1:C:17:TYR:HD1	1.75	0.52
1:A:15:LEU:HB3	1:A:17:TYR:CD1	2.44	0.52
1:A:79:LYS:NZ	1:A:108:GLN:HE22	2.08	0.52
1:B:172:ILE:HA	1:B:175:MET:CE	2.36	0.52
1:B:86:PHE:CE2	1:B:310:ILE:HD12	2.45	0.52
1:C:280:LEU:HA	1:C:283:ILE:HG22	1.92	0.52
1:A:149:PHE:O	1:A:152:ASP:HB2	2.10	0.52
1:C:3:LYS:HD3	1:C:3:LYS:H	1.74	0.52
1:A:3:LYS:HD3	1:A:3:LYS:H	1.75	0.51
1:A:172:ILE:HA	1:A:175:MET:CE	2.40	0.51
1:B:20:ILE:HA	1:B:23:TYR:CE1	2.44	0.51
1:A:267:ILE:HG13	1:A:269:LYS:HG2	1.91	0.51
1:B:9:LYS:HB2	1:B:36:GLU:CG	2.41	0.51
1:B:226:ILE:O	1:B:226:ILE:HG23	2.09	0.51
1:A:43:SER:OG	1:A:46:GLU:HG3	2.10	0.51
1:A:313:ILE:HA	2:D:4:LEU:O	2.11	0.51
1:B:219:HIS:O	1:B:222:THR:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LYS:HB2	1:C:36:GLU:HG2	1.93	0.51
1:C:79:LYS:NZ	1:C:108:GLN:HE22	2.07	0.51
1:C:149:PHE:O	1:C:152:ASP:HB2	2.11	0.51
1:C:20:ILE:HA	1:C:23:TYR:CE1	2.46	0.51
1:A:20:ILE:HA	1:A:23:TYR:CE1	2.46	0.51
1:A:98:ARG:CB	1:A:98:ARG:HH11	2.24	0.51
1:B:95:ASN:HA	1:B:98:ARG:HH12	1.76	0.51
1:B:31:VAL:O	1:B:34:LYS:HB2	2.11	0.51
1:B:63:ASN:HD22	1:B:68:ASN:HB2	1.76	0.51
1:B:156:VAL:HG21	1:B:175:MET:HE2	1.91	0.51
1:B:290:THR:O	1:C:251:ILE:HG22	2.10	0.50
1:A:31:VAL:O	1:A:34:LYS:HB2	2.11	0.50
1:A:9:LYS:HB2	1:A:36:GLU:CG	2.42	0.50
1:A:31:VAL:HA	1:A:34:LYS:CD	2.38	0.50
1:A:256:ASN:O	1:A:260:ILE:HG12	2.12	0.50
1:B:15:LEU:HB3	1:B:17:TYR:HD1	1.77	0.50
1:C:256:ASN:O	1:C:260:ILE:HG12	2.11	0.50
1:B:259:ASN:O	1:B:262:ASN:HB3	2.12	0.50
1:A:86:PHE:CE2	1:A:310:ILE:HG23	2.46	0.49
1:A:283:ILE:HD13	1:A:283:ILE:C	2.33	0.49
1:B:220:LEU:O	1:B:226:ILE:HG21	2.13	0.49
1:B:27:MET:SD	1:B:31:VAL:HG13	2.53	0.49
1:C:283:ILE:HD13	1:C:283:ILE:C	2.32	0.49
1:A:165:TYR:HB2	1:A:200:ILE:HG21	1.95	0.49
1:B:79:LYS:NZ	1:B:108:GLN:HE22	2.11	0.49
1:B:280:LEU:HA	1:B:283:ILE:HG22	1.94	0.49
1:B:188:LEU:HD13	2:E:5:ILE:HD12	1.95	0.49
1:B:23:TYR:CZ	1:B:29:LYS:HB2	2.47	0.48
1:B:98:ARG:CB	1:B:98:ARG:HH11	2.26	0.48
1:C:81:LEU:HD12	1:C:84:LYS:HB3	1.95	0.48
1:C:153:TYR:HA	3:C:319:HOH:O	2.13	0.48
1:C:259:ASN:O	1:C:262:ASN:HB3	2.14	0.48
1:A:9:LYS:HB2	1:A:36:GLU:HG2	1.95	0.48
1:C:240:LYS:O	1:C:243:TYR:HB3	2.13	0.48
1:B:86:PHE:CE2	1:B:310:ILE:HG23	2.49	0.48
1:A:3:LYS:H	1:A:3:LYS:CD	2.26	0.48
1:B:165:TYR:HB2	1:B:200:ILE:HG21	1.95	0.48
1:C:3:LYS:H	1:C:3:LYS:CD	2.27	0.48
1:B:275:SER:OG	2:E:1:ALA:HB2	2.13	0.48
1:C:23:TYR:CZ	1:C:29:LYS:HB2	2.49	0.48
1:A:139:LYS:O	1:A:143:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ASN:HB3	1:B:68:ASN:HB3	1.96	0.47
1:B:283:ILE:HD13	1:B:283:ILE:C	2.34	0.47
1:B:196:ASN:O	1:B:200:ILE:HG12	2.13	0.47
1:B:9:LYS:HB2	1:B:36:GLU:HG2	1.95	0.47
1:A:196:ASN:HB3	2:D:2:ILE:HD12	1.96	0.47
1:B:23:TYR:CE2	1:B:29:LYS:HB2	2.49	0.47
1:B:156:VAL:HG11	1:B:172:ILE:HG12	1.96	0.47
1:B:240:LYS:O	1:B:243:TYR:HB3	2.15	0.47
1:B:298:TYR:HB3	1:B:302:TYR:CE2	2.49	0.47
1:A:199:THR:HG21	2:D:1:ALA:HA	1.95	0.47
1:A:234:LEU:HD23	1:A:264:PHE:CZ	2.49	0.47
1:B:28:SER:OG	1:B:31:VAL:HG12	2.14	0.47
1:C:156:VAL:HG21	1:C:175:MET:HE1	1.95	0.47
1:A:15:LEU:HB3	1:A:17:TYR:HD1	1.78	0.47
1:C:27:MET:SD	1:C:31:VAL:HG13	2.55	0.47
1:A:156:VAL:HG21	1:A:175:MET:HE2	1.97	0.47
1:C:31:VAL:O	1:C:34:LYS:HB2	2.14	0.47
1:A:23:TYR:CZ	1:A:29:LYS:HB2	2.50	0.46
1:C:23:TYR:CE2	1:C:29:LYS:HB2	2.50	0.46
1:A:311:PRO:HB2	2:D:4:LEU:HD23	1.97	0.46
1:B:85:ILE:HD11	1:B:95:ASN:OD1	2.15	0.46
1:C:160:LEU:HD21	1:C:172:ILE:HD11	1.96	0.46
1:A:280:LEU:HA	1:A:283:ILE:HG22	1.97	0.46
1:C:98:ARG:CB	1:C:98:ARG:HH11	2.29	0.46
1:A:26:ILE:CD1	1:A:49:LYS:HD3	2.40	0.46
1:B:115:GLY:HA2	2:E:6:PHE:HZ	1.80	0.46
1:A:98:ARG:NH1	1:A:98:ARG:CB	2.77	0.46
1:A:196:ASN:O	1:A:200:ILE:HG12	2.16	0.46
1:B:274:ARG:HD3	1:B:306:GLU:OE2	2.16	0.46
1:B:156:VAL:HG21	1:B:175:MET:HE1	1.96	0.46
1:C:139:LYS:O	1:C:143:ASP:HB2	2.16	0.46
1:C:292:PRO:O	1:C:294:GLU:N	2.49	0.46
1:A:81:LEU:HD12	1:A:84:LYS:HB3	1.97	0.45
1:C:186:TYR:O	1:C:190:ILE:HG23	2.16	0.45
1:A:63:ASN:HD22	1:A:68:ASN:HB2	1.81	0.45
1:C:280:LEU:HA	1:C:283:ILE:CG2	2.46	0.45
1:A:23:TYR:CE2	1:A:29:LYS:HB2	2.51	0.45
1:B:3:LYS:N	1:B:3:LYS:CD	2.79	0.45
1:B:145:ARG:NH2	1:B:152:ASP:OD1	2.47	0.45
1:C:26:ILE:CD1	1:C:49:LYS:HD3	2.40	0.45
1:A:294:GLU:HG2	1:A:295:VAL:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LEU:HD12	1:B:84:LYS:HB3	1.97	0.45
1:C:234:LEU:HD23	1:C:264:PHE:CZ	2.51	0.45
1:B:264:PHE:CE1	1:B:272:ILE:HG21	2.52	0.45
1:B:274:ARG:O	1:B:278:GLU:HG3	2.17	0.45
1:C:63:ASN:HD22	1:C:68:ASN:HB2	1.82	0.45
1:C:156:VAL:CG2	3:C:319:HOH:O	2.65	0.45
1:A:3:LYS:N	1:A:3:LYS:CD	2.80	0.45
1:B:4:ILE:HG22	1:B:8:LEU:CD2	2.47	0.45
1:B:98:ARG:NH1	1:B:98:ARG:CB	2.79	0.45
1:B:31:VAL:HA	1:B:34:LYS:CD	2.39	0.44
1:C:226:ILE:O	1:C:226:ILE:HG23	2.16	0.44
1:B:26:ILE:CD1	1:B:49:LYS:HD3	2.42	0.44
1:C:205:ARG:HG2	1:C:205:ARG:HH11	1.82	0.44
1:A:160:LEU:HD21	1:A:172:ILE:HD11	2.00	0.44
1:C:292:PRO:C	1:C:294:GLU:H	2.21	0.44
1:A:79:LYS:HZ2	1:A:108:GLN:HE22	1.66	0.44
1:A:312:GLU:OE2	1:A:314:LYS:HE2	2.18	0.44
1:C:31:VAL:HA	1:C:34:LYS:CD	2.37	0.44
1:C:156:VAL:HG11	1:C:172:ILE:HG12	1.98	0.44
1:A:259:ASN:O	1:A:262:ASN:HB3	2.18	0.44
1:C:98:ARG:NH1	1:C:98:ARG:CB	2.81	0.44
2:E:5:ILE:HD11	2:E:7:ILE:HG23	2.00	0.44
1:C:4:ILE:HG22	1:C:8:LEU:CD2	2.48	0.43
1:A:280:LEU:HA	1:A:283:ILE:CG2	2.48	0.43
1:B:108:GLN:HA	1:B:108:GLN:NE2	2.32	0.43
1:B:176:TYR:HB3	1:B:177:PRO:HA	2.00	0.43
1:A:302:TYR:O	1:A:304:ALA:N	2.52	0.43
1:C:3:LYS:N	1:C:3:LYS:CD	2.82	0.43
1:A:258:VAL:HG22	1:A:280:LEU:HD21	2.00	0.43
1:B:103:ARG:HG2	1:B:103:ARG:NH1	2.33	0.43
1:C:85:ILE:HD11	1:C:95:ASN:OD1	2.19	0.43
1:B:255:LEU:HD21	1:C:255:LEU:HD21	2.01	0.43
1:C:139:LYS:HE2	1:C:139:LYS:HB2	1.88	0.43
1:A:226:ILE:O	1:A:226:ILE:HG23	2.19	0.43
1:B:149:PHE:O	1:B:152:ASP:HB2	2.19	0.43
2:D:7:ILE:HD12	2:D:7:ILE:C	2.39	0.43
1:B:187:ASP:O	1:B:190:ILE:HG12	2.19	0.43
1:A:302:TYR:O	1:A:306:GLU:HB3	2.18	0.42
1:C:264:PHE:CE1	1:C:272:ILE:HG21	2.54	0.42
1:C:237:ASN:O	1:C:240:LYS:HB2	2.19	0.42
1:C:242:ILE:HD12	3:C:323:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ARG:O	1:C:278:GLU:HG3	2.19	0.42
1:B:189:THR:CG2	2:E:7:ILE:HD13	2.49	0.42
1:A:95:ASN:HD22	1:A:95:ASN:HA	1.62	0.42
1:B:254:TYR:O	1:B:258:VAL:HG23	2.20	0.42
1:C:23:TYR:HB3	1:C:32:TYR:CD2	2.55	0.42
1:A:85:ILE:HD11	1:A:95:ASN:OD1	2.19	0.42
1:B:23:TYR:HB3	1:B:32:TYR:CD2	2.55	0.42
1:B:188:LEU:HD13	2:E:5:ILE:CD1	2.49	0.42
1:C:254:TYR:O	1:C:258:VAL:HG23	2.19	0.42
1:C:287:GLU:O	1:C:288:LYS:HB2	2.20	0.42
1:B:86:PHE:HD2	1:B:310:ILE:HD12	1.78	0.42
1:B:285:ALA:C	1:B:287:GLU:H	2.23	0.42
1:C:134:ILE:HG23	1:C:135:THR:N	2.35	0.42
1:A:26:ILE:HD12	1:A:49:LYS:CD	2.41	0.42
1:A:63:ASN:HB3	1:A:68:ASN:HB3	2.02	0.42
1:B:95:ASN:HD22	1:B:95:ASN:HA	1.64	0.42
1:B:232:TYR:OH	2:E:3:THR:HG21	2.20	0.42
1:A:28:SER:OG	1:A:31:VAL:HG12	2.20	0.41
1:C:63:ASN:HB3	1:C:68:ASN:HB3	2.02	0.41
1:A:188:LEU:HD13	2:D:5:ILE:CD1	2.50	0.41
1:B:139:LYS:O	1:B:143:ASP:HB2	2.20	0.41
1:C:28:SER:OG	1:C:31:VAL:HG12	2.19	0.41
1:C:57:ASN:O	1:C:61:ILE:HG13	2.21	0.41
1:C:74:GLU:HG2	1:C:109:TYR:OH	2.21	0.41
1:B:63:ASN:CB	1:B:68:ASN:HB3	2.50	0.41
1:A:274:ARG:HA	1:A:302:TYR:CE2	2.55	0.41
1:C:27:MET:HB2	1:C:31:VAL:CG1	2.51	0.41
1:B:285:ALA:C	1:B:287:GLU:N	2.73	0.41
1:C:26:ILE:HD12	1:C:49:LYS:CD	2.43	0.41
1:A:287:GLU:O	1:A:288:LYS:HB2	2.21	0.40
1:A:240:LYS:O	1:A:243:TYR:HB3	2.21	0.40
1:B:86:PHE:CE1	1:B:119:ILE:HG12	2.56	0.40
1:A:27:MET:SD	1:A:31:VAL:HG13	2.61	0.40
1:A:108:GLN:HA	1:A:108:GLN:NE2	2.35	0.40
1:A:156:VAL:HG11	1:A:172:ILE:HG12	2.03	0.40
1:A:232:TYR:OH	2:D:3:THR:HG21	2.22	0.40
1:C:108:GLN:NE2	1:C:108:GLN:HA	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	313/317 (99%)	285 (91%)	25 (8%)	3 (1%)	15 53
1	B	313/317 (99%)	280 (90%)	28 (9%)	5 (2%)	9 40
1	C	292/317 (92%)	265 (91%)	24 (8%)	3 (1%)	15 53
2	D	5/7 (71%)	4 (80%)	1 (20%)	0	100 100
2	E	5/7 (71%)	3 (60%)	2 (40%)	0	100 100
All	All	928/965 (96%)	837 (90%)	80 (9%)	11 (1%)	13 48

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	ALA
1	B	304	ALA
1	A	93	ASP
1	C	93	ASP
1	C	293	LYS
1	A	303	VAL
1	B	93	ASP
1	B	299	TYR
1	C	292	PRO
1	B	292	PRO
1	B	303	VAL

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
1	A	297/299 (99%)	285 (96%)	12 (4%)	31 68
1	B	297/299 (99%)	283 (95%)	14 (5%)	26 63
1	C	277/299 (93%)	265 (96%)	12 (4%)	29 66
2	D	6/6 (100%)	6 (100%)	0	100 100
2	E	6/6 (100%)	6 (100%)	0	100 100
All	All	883/909 (97%)	845 (96%)	38 (4%)	29 66

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	44	VAL
1	A	86	PHE
1	A	143	ASP
1	A	180	ASP
1	A	188	LEU
1	A	195	LYS
1	A	238	TYR
1	A	252	ASP
1	A	259	ASN
1	A	283	ILE
1	A	314	LYS
1	B	15	LEU
1	B	44	VAL
1	B	86	PHE
1	B	143	ASP
1	B	180	ASP
1	B	188	LEU
1	B	195	LYS
1	B	237	ASN
1	B	238	TYR
1	B	252	ASP
1	B	259	ASN
1	B	283	ILE
1	B	312	GLU
1	B	314	LYS
1	C	15	LEU
1	C	44	VAL
1	C	86	PHE
1	C	143	ASP
1	C	180	ASP

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Mol	Chain	Res	Type
1	C	188	LEU
1	C	195	LYS
1	C	237	ASN
1	C	238	TYR
1	C	252	ASP
1	C	259	ASN
1	C	283	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	63	ASN
1	A	95	ASN
1	A	108	GLN
1	A	124	ASN
1	A	158	ASN
1	A	204	ASN
1	A	215	ASN
1	A	256	ASN
1	A	259	ASN
1	B	63	ASN
1	B	95	ASN
1	B	108	GLN
1	B	124	ASN
1	B	158	ASN
1	B	161	ASN
1	B	204	ASN
1	B	215	ASN
1	B	256	ASN
1	B	259	ASN
1	C	63	ASN
1	C	95	ASN
1	C	108	GLN
1	C	124	ASN
1	C	204	ASN
1	C	215	ASN
1	C	256	ASN
1	C	259	ASN
1	C	273	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	315/317 (99%)	-0.37	1 (0%) 94 84	28, 55, 119, 195	0
1	B	315/317 (99%)	-0.27	1 (0%) 94 84	30, 62, 126, 195	0
1	C	294/317 (92%)	1.91	117 (39%) 0 0	77, 179, 202, 202	0
2	D	7/7 (100%)	0.03	0 100 100	65, 80, 96, 113	0
2	E	7/7 (100%)	0.35	1 (14%) 2 1	60, 80, 126, 145	0
All	All	938/965 (97%)	0.39	120 (12%) 3 1	28, 78, 201, 202	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	56	VAL	12.4
1	C	44	VAL	11.3
1	C	142	TYR	10.2
1	C	89	PRO	8.9
1	C	55	GLY	7.1
1	C	106	SER	7.0
1	C	92	PHE	6.8
1	C	17	TYR	6.6
1	C	182	PHE	6.6
1	C	2	PHE	6.5
1	C	80	LEU	6.4
1	C	140	HIS	6.3
1	C	109	TYR	6.3
1	C	146	THR	6.2
1	C	38	ASP	6.0
1	C	51	SER	5.9
1	C	65	ALA	5.8
1	C	149	PHE	5.6
1	C	36	GLU	5.5
1	C	144	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	160	LEU	5.4
1	C	130	PHE	5.3
1	C	111	SER	5.2
1	C	69	THR	5.1
1	C	7	VAL	5.0
1	C	35	VAL	5.0
1	C	141	LEU	5.0
1	C	72	VAL	4.9
1	C	87	THR	4.9
1	C	30	SER	4.9
1	C	58	PHE	4.8
1	C	22	LEU	4.8
1	C	50	PHE	4.8
1	C	90	ASP	4.8
1	C	39	SER	4.8
1	C	152	ASP	4.5
1	C	20	ILE	4.4
1	C	207	LEU	4.4
1	C	23	TYR	4.4
1	C	95	ASN	4.3
1	C	88	ASN	4.3
1	C	193	VAL	4.2
1	C	76	GLY	4.1
1	C	68	ASN	4.1
1	C	167	GLU	4.1
1	C	138	LEU	4.1
1	C	46	GLU	4.1
1	C	94	LYS	4.1
1	C	147	THR	4.0
1	C	165	TYR	3.9
1	C	34	LYS	3.8
1	C	171	ILE	3.8
1	C	21	ASP	3.7
1	C	32	TYR	3.7
1	C	148	PHE	3.7
1	C	163	LEU	3.6
1	C	33	ILE	3.6
1	C	91	LEU	3.6
1	C	103	ARG	3.5
1	C	5	GLY	3.5
1	C	286	LYS	3.4
1	C	99	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	200	ILE	3.4
1	C	27	MET	3.4
1	C	53	ARG	3.3
1	C	78	GLU	3.3
1	C	26	ILE	3.2
1	C	189	THR	3.2
1	C	145	ARG	3.2
1	C	134	ILE	3.2
1	A	306	GLU	3.2
1	C	41	PRO	3.2
1	C	4	ILE	3.2
1	C	122	HIS	3.2
1	C	159	LEU	3.0
1	C	9	LYS	2.9
1	C	110	PHE	2.9
1	C	266	ILE	2.9
1	C	186	TYR	2.9
1	C	96	PHE	2.9
1	C	172	ILE	2.7
1	C	83	SER	2.7
1	C	155	ILE	2.7
1	C	191	GLN	2.7
1	C	209	GLU	2.7
1	C	77	LYS	2.7
1	C	246	LEU	2.7
1	C	245	PHE	2.7
1	C	14	GLU	2.7
1	C	113	TYR	2.7
1	C	47	LEU	2.6
1	C	49	LYS	2.6
1	C	16	ASN	2.6
1	C	221	LYS	2.6
1	C	157	SER	2.6
1	C	179	VAL	2.5
1	B	306	GLU	2.5
1	C	216	GLN	2.5
1	C	205	ARG	2.5
1	C	11	ILE	2.4
1	C	61	ILE	2.4
1	C	15	LEU	2.4
1	C	223	ILE	2.4
1	C	12	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	67	MET	2.3
1	C	273	HIS	2.3
1	C	1	MET	2.3
1	C	212	TYR	2.3
1	C	57	ASN	2.2
1	C	18	HIS	2.2
1	C	84	LYS	2.2
1	C	156	VAL	2.1
1	C	225	ASN	2.1
1	C	54	LEU	2.1
1	C	176	TYR	2.1
1	C	13	GLN	2.1
1	C	43	SER	2.1
1	C	243	TYR	2.0
1	C	236	ILE	2.0
2	E	1	ALA	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.