Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2019 – 04:31 PM EDT

PDB ID	:	6DGU
Title	:	PER-2 class A extended-spectrum beta-lactamase crystal structure at 2.69 Angstrom resolution
Authors	:	Power, P.; Ruggiero, M.; Gutkind, G.; Bonomo, R.; Klinke, S.
Deposited on	:	2018-05-18
Resolution	:	2.69 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:

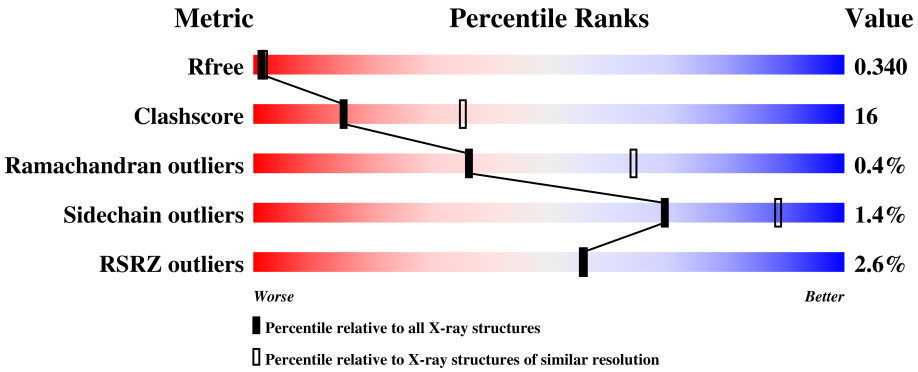
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

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 2.69 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}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)

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 <=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	281	2% 69% 28%
1	B	281	3% 67% 31%
1	C	281	4% 64% 33%
1	D	281	2% 62% 32%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8616 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	277	Total	C	N	O	S	0	0	0
			2126	1350	364	403	9			
1	A	274	Total	C	N	O	S	0	0	0
			2107	1338	361	399	9			
1	C	275	Total	C	N	O	S	0	0	0
			2115	1344	362	400	9			
1	D	272	Total	C	N	O	S	0	0	0
			2094	1330	359	396	9			

- Molecule 2 is water.

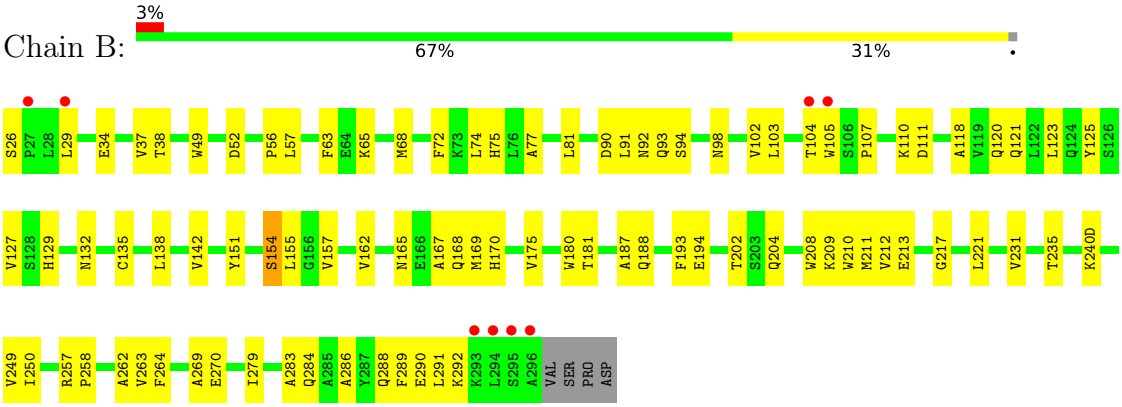
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	56	Total	O	0	0
			56	56		
2	A	45	Total	O	0	0
			45	45		
2	C	48	Total	O	0	0
			48	48		
2	D	25	Total	O	0	0
			25	25		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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.

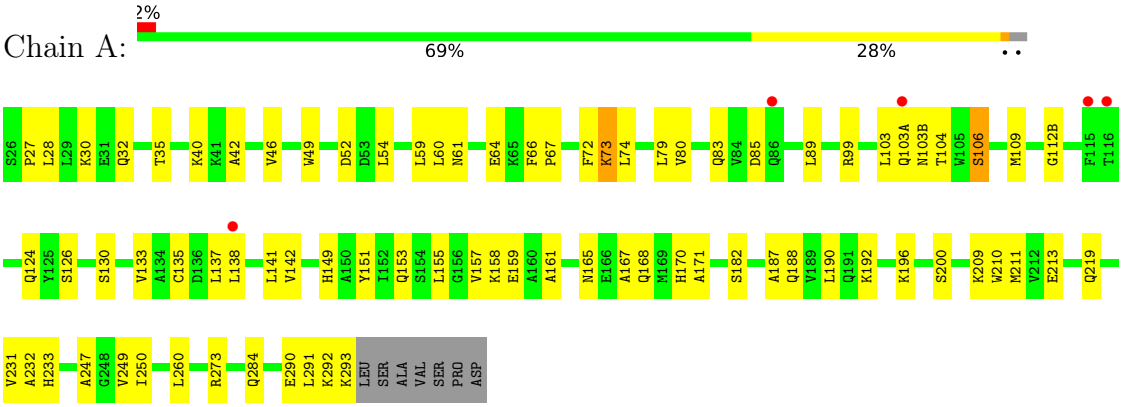
• Molecule 1: Beta-lactamase

Chain B:



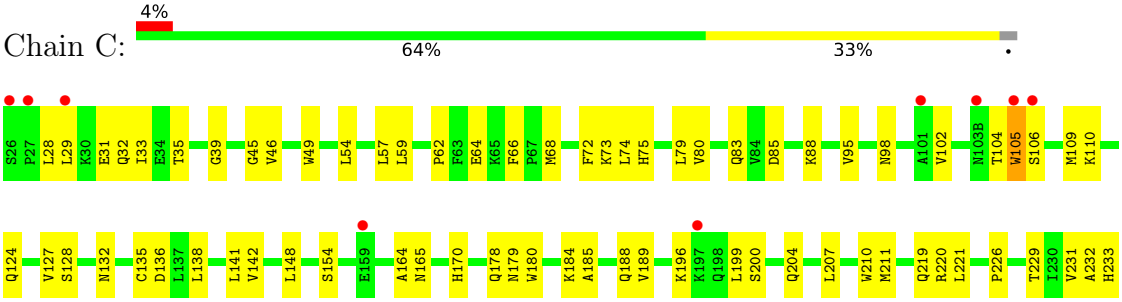
• Molecule 1: Beta-lactamase

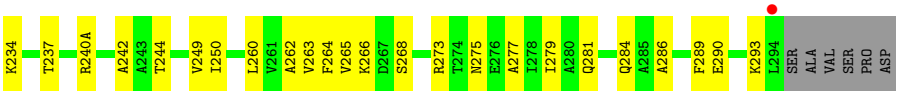
Chain A:



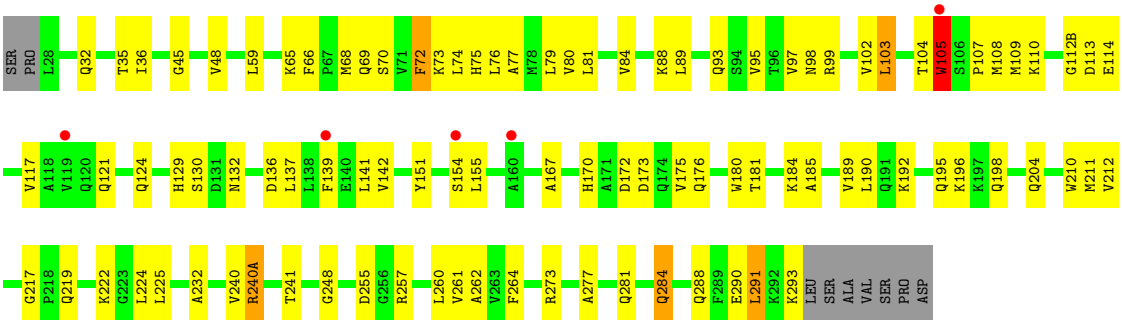
• Molecule 1: Beta-lactamase

Chain C:





• Molecule 1: Beta-lactamase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.37Å 82.58Å 174.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.29 – 2.69 41.29 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.3 (41.29-2.69) 96.9 (41.29-2.69)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.267 , 0.340 0.267 , 0.340	Depositor DCC
R_{free} test set	1980 reflections (6.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 3.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	0.160 for k,h,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	8616	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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	0.47	0/2146	0.75	1/2915 (0.0%)
1	B	0.49	0/2165	0.73	0/2941
1	C	0.50	0/2154	0.76	2/2926 (0.1%)
1	D	0.50	1/2132 (0.0%)	0.76	5/2895 (0.2%)
All	All	0.49	1/8597 (0.0%)	0.75	8/11677 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	105	TRP	CB-CG	-6.17	1.39	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	105	TRP	CB-CG-CD2	-8.61	115.41	126.60
1	A	28	LEU	CB-CG-CD2	8.25	125.02	111.00
1	D	105	TRP	N-CA-CB	-6.74	98.48	110.60
1	C	124	GLN	CA-CB-CG	6.20	127.04	113.40
1	D	105	TRP	CB-CA-C	6.14	122.67	110.40
1	C	57	LEU	CA-CB-CG	6.02	129.15	115.30
1	D	105	TRP	CA-CB-CG	5.67	124.47	113.70
1	D	291	LEU	CA-CB-CG	-5.04	103.72	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103(A)	GLN	Peptide
1	D	105	TRP	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	A	2107	0	2130	63	0
1	B	2126	0	2151	63	0
1	C	2115	0	2141	77	0
1	D	2094	0	2118	75	0
2	A	45	0	0	9	0
2	B	56	0	0	10	0
2	C	48	0	0	17	0
2	D	25	0	0	4	0
All	All	8616	0	8540	272	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 16.

All (272) 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:B:135:CYS:SG	2:B:453:HOH:O	2.17	1.02
1:B:165:ASN:OD1	1:B:168:GLN:NE2	2.07	0.87
1:B:52:ASP:OD2	2:B:401:HOH:O	1.99	0.79
1:D:217:GLY:O	2:D:401:HOH:O	2.03	0.76
1:C:207:LEU:O	2:C:401:HOH:O	2.02	0.76
1:C:95:VAL:HG21	1:C:141:LEU:HD11	1.66	0.75
1:A:67:PRO:O	2:A:401:HOH:O	2.04	0.75
1:C:29:LEU:HD23	1:C:33:ILE:HG13	1.67	0.74
1:D:262:ALA:HB1	1:D:264:PHE:HE1	1.52	0.74
1:A:219:GLN:NE2	2:A:404:HOH:O	2.21	0.74
1:D:80:VAL:HG22	1:D:142:VAL:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:HD13	1:B:211:MET:SD	2.28	0.73
1:D:173:ASP:HB3	1:D:240(A):ARG:HH21	1.55	0.72
1:D:112(B):GLY:O	1:D:114:GLU:N	2.22	0.72
1:D:288:GLN:NE2	2:D:402:HOH:O	2.22	0.72
1:C:39:GLY:O	2:C:402:HOH:O	2.08	0.71
1:D:79:LEU:HD12	1:D:151:TYR:HB2	1.73	0.71
1:C:83:GLN:N	2:C:408:HOH:O	2.24	0.70
1:C:105:TRP:O	2:C:403:HOH:O	2.10	0.70
1:D:81:LEU:HA	1:D:84:VAL:HB	1.72	0.70
1:B:231:VAL:HG22	1:B:250:ILE:HG12	1.72	0.70
1:B:94:SER:O	2:B:402:HOH:O	2.10	0.70
1:A:80:VAL:HG21	1:A:138:LEU:HD22	1.74	0.70
1:A:126:SER:O	2:A:402:HOH:O	2.08	0.69
1:C:249:VAL:HG22	1:C:260:LEU:HD12	1.74	0.69
1:C:28:LEU:O	1:C:28:LEU:HD22	1.92	0.69
1:C:64:GLU:O	2:C:404:HOH:O	2.11	0.69
1:B:92:ASN:HA	1:B:118:ALA:HB1	1.74	0.68
1:B:91:LEU:O	1:B:120:GLN:N	2.25	0.67
1:C:240(A):ARG:HH22	1:C:242:ALA:HB2	1.59	0.67
1:B:240(D):LYS:HE3	1:B:269:ALA:HB2	1.78	0.66
1:C:32:GLN:HA	1:C:35:THR:HG22	1.76	0.66
1:A:249:VAL:HG12	1:A:260:LEU:HD22	1.77	0.66
1:B:111:ASP:O	2:B:404:HOH:O	2.13	0.66
1:A:130:SER:HA	2:A:402:HOH:O	1.97	0.65
1:D:196:LYS:HG2	1:D:204:GLN:CD	2.16	0.64
1:C:29:LEU:HD11	1:C:286:ALA:HA	1.79	0.64
1:C:104:THR:HG21	1:C:132:ASN:HB2	1.78	0.64
1:C:59:LEU:O	2:C:407:HOH:O	2.14	0.64
1:C:106:SER:HB3	1:C:109:MET:HG2	1.79	0.64
1:D:79:LEU:HD22	1:D:142:VAL:CG1	2.28	0.64
1:D:103:LEU:HD13	1:D:167:ALA:HA	1.78	0.64
1:D:73:LYS:NZ	1:D:132:ASN:OD1	2.31	0.64
1:A:290:GLU:OE1	1:A:293:LYS:HD2	1.98	0.63
1:B:104:THR:HG21	1:B:132:ASN:HB2	1.79	0.63
1:D:192:LYS:HD3	1:D:198:GLN:NE2	2.15	0.62
1:B:104:THR:HB	1:B:170:HIS:HE1	1.65	0.61
1:A:284:GLN:NE2	1:D:35:THR:O	2.34	0.61
1:B:34:GLU:HA	1:B:37:VAL:HG22	1.83	0.60
1:B:72:PHE:HA	1:B:75:HIS:ND1	2.16	0.60
1:D:79:LEU:CD2	1:D:142:VAL:HG13	2.31	0.60
1:D:88:LYS:O	1:D:89:LEU:HD23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LEU:HA	1:C:31:GLU:HG3	1.83	0.60
1:C:85:ASP:OD2	1:C:200:SER:N	2.33	0.60
1:D:80:VAL:O	1:D:84:VAL:N	2.35	0.59
1:D:48:VAL:HG12	1:D:261:VAL:HG13	1.84	0.59
1:C:184:LYS:HE2	1:C:188:GLN:NE2	2.17	0.59
1:C:220:ARG:HH22	1:C:237:THR:CG2	2.16	0.59
1:D:99:ARG:NH2	1:D:109:MET:O	2.36	0.59
1:A:64:GLU:HB3	1:A:66:PHE:CE2	2.38	0.58
1:B:65:LYS:NZ	2:B:409:HOH:O	2.36	0.58
1:C:231:VAL:HG22	1:C:250:ILE:HG12	1.84	0.58
1:D:277:ALA:O	1:D:281:GLN:HG3	2.03	0.58
1:B:127:VAL:CG1	1:B:211:MET:HG3	2.34	0.58
1:C:221:LEU:HB2	2:C:412:HOH:O	2.02	0.58
1:C:184:LYS:HE2	1:C:188:GLN:HE22	1.69	0.57
1:C:45:GLY:HA3	1:C:66:PHE:CE2	2.39	0.57
1:C:79:LEU:O	2:C:408:HOH:O	2.17	0.57
1:C:74:LEU:HD13	1:C:211:MET:SD	2.45	0.57
1:B:286:ALA:O	1:B:290:GLU:HG2	2.04	0.57
1:B:49:TRP:CE2	1:B:56:PRO:HD3	2.40	0.57
1:B:107:PRO:HG2	1:B:129:HIS:HB3	1.85	0.57
1:B:138:LEU:O	1:B:142:VAL:HG22	2.04	0.57
1:A:32:GLN:O	1:A:35:THR:HG22	2.05	0.57
1:D:185:ALA:O	1:D:189:VAL:HG23	2.04	0.57
1:B:221:LEU:HD23	1:B:283:ALA:HB2	1.87	0.56
1:B:193:PHE:O	1:B:204:GLN:NE2	2.31	0.56
1:A:284:GLN:HE22	1:D:36:ILE:HA	1.69	0.56
1:D:79:LEU:HD22	1:D:142:VAL:HG11	1.87	0.56
1:B:284:GLN:O	1:B:288:GLN:HG2	2.06	0.56
1:A:159:GLU:OE2	2:A:403:HOH:O	2.18	0.56
1:B:105:TRP:HD1	1:B:107:PRO:HD3	1.71	0.56
1:C:128:SER:OG	1:C:210:TRP:O	2.23	0.55
1:C:185:ALA:O	1:C:189:VAL:HG23	2.05	0.55
1:C:284:GLN:NE2	2:C:406:HOH:O	2.12	0.55
1:D:74:LEU:HD13	1:D:211:MET:SD	2.47	0.55
1:A:52:ASP:HB2	1:A:293:LYS:HE2	1.88	0.55
1:C:79:LEU:HD12	2:C:408:HOH:O	2.07	0.54
1:D:172:ASP:O	1:D:175:VAL:HG23	2.07	0.54
1:B:29:LEU:HD12	1:B:289:PHE:CD2	2.43	0.54
1:C:220:ARG:HH12	1:C:237:THR:HG23	1.72	0.54
1:D:290:GLU:HA	1:D:293:LYS:HB2	1.88	0.54
1:C:138:LEU:O	1:C:142:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD13	1:A:211:MET:SD	2.47	0.54
1:C:226:PRO:O	1:C:229:THR:OG1	2.20	0.54
1:A:46:VAL:HB	1:A:60:LEU:HB3	1.90	0.53
1:D:59:LEU:HD11	1:D:184:LYS:HG3	1.89	0.53
1:C:59:LEU:HD13	1:C:62:PRO:HB3	1.90	0.53
1:D:75:HIS:HE2	1:D:189:VAL:HG21	1.74	0.53
1:D:79:LEU:HD12	1:D:151:TYR:CB	2.38	0.53
1:A:153:GLN:NE2	1:A:157:VAL:O	2.42	0.52
1:C:290:GLU:CD	1:C:293:LYS:HE3	2.29	0.52
1:B:49:TRP:CZ2	1:B:56:PRO:HD3	2.44	0.52
1:C:234:LYS:HA	2:C:410:HOH:O	2.10	0.52
1:D:76:LEU:HD22	1:D:139:PHE:CE1	2.44	0.52
1:A:85:ASP:OD2	1:A:200:SER:N	2.37	0.52
1:A:103:LEU:HD13	1:A:167:ALA:HA	1.92	0.52
1:C:199:LEU:O	2:C:409:HOH:O	2.19	0.52
1:C:240(A):ARG:NH2	1:C:242:ALA:HB2	2.22	0.52
1:A:190:LEU:HD11	1:A:247:ALA:HB1	1.92	0.52
1:D:76:LEU:HD13	1:D:139:PHE:HE1	1.75	0.52
1:C:73:LYS:HE2	1:C:135:CYS:CB	2.40	0.52
1:D:89:LEU:HD11	1:D:141:LEU:HB3	1.91	0.51
1:D:151:TYR:CE1	1:D:155:LEU:HD21	2.45	0.51
1:D:79:LEU:HD22	1:D:142:VAL:HG13	1.92	0.51
1:C:277:ALA:O	1:C:281:GLN:HG3	2.10	0.51
1:B:121:GLN:O	1:B:125:TYR:HD2	1.94	0.51
1:B:72:PHE:HZ	1:B:169:MET:HE1	1.76	0.51
1:C:273:ARG:O	1:C:277:ALA:N	2.43	0.51
1:D:80:VAL:HG22	1:D:142:VAL:CG2	2.39	0.51
1:D:211:MET:O	1:D:232:ALA:HA	2.10	0.51
1:B:52:ASP:CG	1:B:257:ARG:HH12	2.14	0.51
1:B:68:MET:HG2	1:B:181:THR:HG22	1.93	0.51
1:D:72:PHE:HA	1:D:75:HIS:ND1	2.26	0.51
1:B:169:MET:HA	1:B:175:VAL:CG2	2.41	0.51
1:C:265:VAL:HG12	1:C:268:SER:HB2	1.93	0.50
1:D:240:VAL:HG12	1:D:241:THR:OG1	2.12	0.50
1:C:164:ALA:HB3	1:C:179:ASN:HD21	1.76	0.50
1:C:263:VAL:HB	1:C:279:ILE:HG23	1.94	0.50
1:D:195:GLN:HB2	2:D:412:HOH:O	2.10	0.50
1:B:270:GLU:OE2	2:B:406:HOH:O	2.20	0.50
1:D:107:PRO:HG2	1:D:129:HIS:HB3	1.94	0.50
1:A:188:GLN:O	1:A:192:LYS:HG2	2.12	0.49
1:D:192:LYS:HA	2:D:412:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:ASP:OD2	1:D:257:ARG:NE	2.44	0.49
1:A:153:GLN:HE22	1:A:158:LYS:HA	1.77	0.49
1:A:292:LYS:HG2	1:A:292:LYS:O	2.11	0.49
1:D:69:GLN:NE2	1:D:176:GLN:OE1	2.39	0.49
1:B:217:GLY:HA3	1:B:235:THR:HG21	1.94	0.49
1:B:249:VAL:O	2:B:405:HOH:O	2.19	0.49
1:A:79:LEU:HD21	1:A:142:VAL:HB	1.95	0.49
1:A:27:PRO:HA	1:A:30:LYS:HB3	1.93	0.49
1:D:121:GLN:HA	1:D:124:GLN:HG2	1.95	0.49
1:B:288:GLN:O	1:B:291:LEU:HB2	2.12	0.49
1:D:68:MET:HG2	1:D:181:THR:HG22	1.95	0.48
1:A:232:ALA:HB3	1:A:249:VAL:HG22	1.94	0.48
1:A:35:THR:HG21	1:D:32:GLN:OE1	2.13	0.48
1:C:98:ASN:O	1:C:102:VAL:HG23	2.14	0.48
1:C:233:HIS:O	2:C:410:HOH:O	2.20	0.48
1:D:98:ASN:O	1:D:102:VAL:HG22	2.13	0.48
1:D:77:ALA:O	1:D:81:LEU:HD12	2.14	0.48
1:B:105:TRP:CD1	1:B:107:PRO:HD3	2.49	0.48
1:C:33:ILE:HD13	1:C:46:VAL:HG11	1.95	0.48
1:D:89:LEU:HD22	1:D:93:GLN:HE22	1.78	0.48
1:A:99:ARG:NH1	1:A:112(B):GLY:O	2.47	0.47
1:A:149:HIS:CE1	1:A:161:ALA:HA	2.49	0.47
1:B:202:THR:HG22	2:B:416:HOH:O	2.15	0.47
1:B:263:VAL:HB	1:B:279:ILE:HG12	1.96	0.47
1:B:26:SER:N	2:B:412:HOH:O	2.46	0.47
1:A:273:ARG:HD3	1:D:219:GLN:OE1	2.14	0.47
1:D:190:LEU:CB	1:D:260:LEU:HD23	2.44	0.47
1:C:136:ASP:OD1	1:C:165:ASN:HB2	2.15	0.47
1:A:103(B):ASN:OD1	1:A:103(B):ASN:N	2.48	0.47
1:A:231:VAL:HG22	1:A:250:ILE:HG12	1.96	0.47
1:C:132:ASN:ND2	1:C:170:HIS:CE1	2.83	0.47
1:C:66:PHE:HD1	1:C:266:LYS:HB2	1.80	0.47
1:D:79:LEU:HD21	1:D:142:VAL:HG13	1.96	0.47
1:B:157:VAL:HG22	1:B:188:GLN:HB2	1.98	0.46
1:D:124:GLN:HB3	1:D:210:TRP:NE1	2.30	0.46
1:C:79:LEU:HD22	1:C:148:LEU:HA	1.98	0.46
1:D:97:VAL:HG13	1:D:137:LEU:HD11	1.97	0.46
1:A:151:TYR:CZ	1:A:155:LEU:HD11	2.50	0.46
1:A:54:LEU:HA	1:A:54:LEU:HD23	1.77	0.46
1:B:49:TRP:CE3	1:B:187:ALA:HB1	2.50	0.46
1:A:83:GLN:HE21	1:A:89:LEU:CD1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:LEU:HD13	1:D:139:PHE:CE1	2.50	0.46
1:C:132:ASN:HD22	1:C:170:HIS:CE1	2.34	0.46
1:D:104:THR:HB	1:D:170:HIS:NE2	2.31	0.46
1:B:63:PHE:CG	1:A:59:LEU:HD12	2.51	0.46
1:A:209:LYS:HE2	1:A:213:GLU:OE2	2.15	0.46
1:A:182:SER:HB2	2:A:407:HOH:O	2.16	0.45
1:B:292:LYS:O	1:B:292:LYS:HG2	2.16	0.45
1:C:211:MET:HG2	1:C:233:HIS:O	2.16	0.45
1:A:170:HIS:HB3	2:A:418:HOH:O	2.16	0.45
1:D:45:GLY:HA3	1:D:66:PHE:CZ	2.52	0.45
1:A:249:VAL:HG12	1:A:260:LEU:CD2	2.46	0.45
1:B:165:ASN:H	1:B:168:GLN:NE2	2.15	0.45
1:B:29:LEU:HD22	1:B:57:LEU:CD2	2.47	0.45
1:B:68:MET:SD	1:B:72:PHE:HB3	2.56	0.45
1:C:127:VAL:HG11	2:C:401:HOH:O	2.16	0.45
1:C:262:ALA:HB1	1:C:264:PHE:HE1	1.80	0.45
1:D:73:LYS:HE3	1:D:130:SER:HA	1.98	0.45
1:A:211:MET:HG2	1:A:233:HIS:O	2.17	0.45
1:A:79:LEU:HB2	1:A:151:TYR:CD2	2.51	0.44
1:B:165:ASN:ND2	2:B:413:HOH:O	2.48	0.44
1:B:90:ASP:O	1:B:93:GLN:HB3	2.18	0.44
1:D:136:ASP:OD2	1:D:167:ALA:N	2.48	0.44
1:A:124:GLN:HG3	1:A:210:TRP:CD1	2.53	0.44
1:A:73:LYS:HE2	1:A:135:CYS:SG	2.57	0.44
1:C:289:PHE:CD2	1:C:293:LYS:HE2	2.52	0.44
1:C:29:LEU:CD2	1:C:33:ILE:HG13	2.42	0.44
1:A:79:LEU:HD23	1:A:80:VAL:N	2.32	0.44
1:A:60:LEU:O	1:A:61:ASN:HB2	2.17	0.44
1:D:212:VAL:HG22	1:D:232:ALA:HB2	2.00	0.44
1:C:106:SER:CB	1:C:109:MET:HG2	2.46	0.44
1:C:219:GLN:OE1	1:C:273:ARG:NH2	2.51	0.44
1:C:249:VAL:HG13	1:C:260:LEU:HD13	2.00	0.43
1:D:75:HIS:NE2	1:D:189:VAL:HG21	2.33	0.43
1:B:208:TRP:O	1:B:212:VAL:N	2.47	0.43
1:C:80:VAL:HG21	1:C:138:LEU:HD13	1.99	0.43
1:C:72:PHE:HA	1:C:75:HIS:ND1	2.33	0.43
1:D:70:SER:CB	1:D:73:LYS:HZ3	2.31	0.43
1:A:106:SER:OG	1:A:109:MET:HG2	2.19	0.43
1:B:98:ASN:O	1:B:102:VAL:HG13	2.19	0.43
1:B:104:THR:HB	1:B:170:HIS:CE1	2.50	0.43
1:C:83:GLN:HA	1:C:88:LYS:HZ2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD22	1:B:167:ALA:HA	2.00	0.43
1:C:68:MET:CE	1:C:72:PHE:HB3	2.49	0.43
1:B:77:ALA:O	1:B:81:LEU:HD12	2.18	0.43
1:C:54:LEU:N	2:C:416:HOH:O	2.41	0.43
1:A:209:LYS:HG2	1:A:213:GLU:CD	2.39	0.43
1:A:79:LEU:HD12	1:A:151:TYR:CB	2.48	0.43
1:A:165:ASN:OD1	1:A:168:GLN:NE2	2.32	0.42
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.83	0.42
1:B:65:LYS:HD3	1:B:180:TRP:CE2	2.54	0.42
1:D:84:VAL:HA	1:D:89:LEU:O	2.18	0.42
1:C:211:MET:O	1:C:232:ALA:HA	2.20	0.42
1:D:103:LEU:HD22	1:D:167:ALA:HB2	2.01	0.42
1:D:291:LEU:HD23	1:D:291:LEU:HA	1.62	0.42
1:C:66:PHE:CD1	1:C:266:LYS:HB2	2.54	0.42
1:B:123:LEU:HB3	1:B:210:TRP:CZ3	2.55	0.42
1:B:194:GLU:CD	1:B:258:PRO:HB3	2.39	0.42
1:C:29:LEU:CD2	1:C:33:ILE:HD11	2.49	0.42
1:A:106:SER:HB2	1:A:133:VAL:HG23	2.01	0.42
1:A:137:LEU:O	1:A:141:LEU:HD23	2.20	0.42
1:B:68:MET:HE1	1:B:162:VAL:HG22	2.01	0.42
1:B:90:ASP:HB3	1:B:93:GLN:HB2	2.02	0.42
1:D:65:LYS:HD3	1:D:180:TRP:CE2	2.54	0.42
1:D:198:GLN:OE1	1:D:198:GLN:N	2.53	0.42
1:D:190:LEU:HD13	1:D:248:GLY:O	2.19	0.42
1:C:178:GLN:HA	1:C:180:TRP:HD1	1.85	0.42
1:C:196:LYS:HG2	1:C:204:GLN:NE2	2.35	0.42
1:D:224:LEU:HB3	1:D:284:GLN:OE1	2.20	0.42
1:D:69:GLN:O	1:D:72:PHE:CD2	2.73	0.42
1:A:83:GLN:NE2	1:A:89:LEU:HD11	2.36	0.41
1:D:108:MET:SD	1:D:117:VAL:HG21	2.60	0.41
1:A:106:SER:O	1:A:106:SER:OG	2.33	0.41
1:C:68:MET:N	2:C:418:HOH:O	2.50	0.41
1:A:49:TRP:CE3	1:A:187:ALA:HB1	2.55	0.41
1:C:49:TRP:HB3	1:C:260:LEU:HD23	2.03	0.41
1:A:83:GLN:HE21	1:A:89:LEU:HD11	1.85	0.41
1:D:255:ASP:OD1	1:D:257:ARG:HB2	2.21	0.41
1:D:95:VAL:HG22	1:D:141:LEU:HD11	2.02	0.41
1:D:222:LYS:HA	1:D:225:LEU:HG	2.02	0.41
1:A:40:LYS:O	1:A:42:ALA:N	2.53	0.41
1:C:104:THR:HG21	1:C:132:ASN:CB	2.47	0.41
1:A:153:GLN:NE2	1:A:158:LYS:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LYS:O	1:B:213:GLU:HG3	2.22	0.40
1:B:262:ALA:HB1	1:B:264:PHE:HE1	1.86	0.40
1:C:234:LYS:HD2	2:C:410:HOH:O	2.21	0.40
1:B:151:TYR:O	1:B:154:SER:HB3	2.21	0.40
1:B:34:GLU:O	1:B:38:THR:OG1	2.23	0.40
1:C:244:THR:HG21	1:C:275:ASN:HB3	2.03	0.40
1:C:29:LEU:HD23	1:C:29:LEU:O	2.22	0.40
1:A:211:MET:O	1:A:232:ALA:HA	2.20	0.40
1:A:209:LYS:O	1:A:213:GLU:HG3	2.21	0.40
1:A:219:GLN:HE22	1:D:273:ARG:HG2	1.87	0.40
1:A:171:ALA:HB2	2:A:405:HOH:O	2.22	0.40
1:A:196:LYS:NZ	2:A:413:HOH:O	2.55	0.40
1:B:151:TYR:CZ	1:B:155:LEU:HD21	2.57	0.40
1:C:29:LEU:CD2	1:C:33:ILE:CD1	3.00	0.40
1:C:73:LYS:HE2	1:C:135:CYS:HB2	2.03	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	272/281 (97%)	263 (97%)	7 (3%)	2 (1%)	24	50
1	B	275/281 (98%)	266 (97%)	9 (3%)	0	100	100
1	C	273/281 (97%)	266 (97%)	6 (2%)	1 (0%)	36	64
1	D	270/281 (96%)	262 (97%)	7 (3%)	1 (0%)	36	64
All	All	1090/1124 (97%)	1057 (97%)	29 (3%)	4 (0%)	36	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	105	TRP
1	D	113	ASP
1	A	104	THR
1	A	106	SER

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	227/233 (97%)	225 (99%)	2 (1%)	81 93
1	B	229/233 (98%)	227 (99%)	2 (1%)	81 93
1	C	228/233 (98%)	226 (99%)	2 (1%)	81 93
1	D	225/233 (97%)	218 (97%)	7 (3%)	43 73
All	All	909/932 (98%)	896 (99%)	13 (1%)	69 89

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	110	LYS
1	B	154	SER
1	A	72	PHE
1	A	73	LYS
1	C	110	LYS
1	C	154	SER
1	D	72	PHE
1	D	103	LEU
1	D	105	TRP
1	D	110	LYS
1	D	154	SER
1	D	240(A)	ARG
1	D	284	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	92	ASN
1	B	120	GLN
1	A	83	GLN
1	A	153	GLN
1	C	86	GLN
1	C	188	GLN
1	D	168	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

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	274/281 (97%)	0.05	5 (1%) 68 69	18, 21, 27, 29	0
1	B	277/281 (98%)	0.06	8 (2%) 51 51	18, 20, 25, 27	0
1	C	275/281 (97%)	0.15	10 (3%) 42 42	21, 24, 28, 30	0
1	D	272/281 (96%)	0.29	5 (1%) 68 69	22, 29, 36, 39	0
All	All	1098/1124 (97%)	0.14	28 (2%) 56 56	18, 23, 31, 39	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	27	PRO	5.1
1	B	29	LEU	4.8
1	D	119	VAL	4.2
1	C	105	TRP	4.1
1	D	105	TRP	4.0
1	B	104	THR	3.9
1	D	160	ALA	3.4
1	B	294	LEU	3.4
1	C	159	GLU	3.4
1	D	154	SER	3.4
1	C	103(B)	ASN	3.3
1	B	27	PRO	3.3
1	B	296	ALA	3.2
1	C	294	LEU	3.0
1	A	86	GLN	2.8
1	A	115	PHE	2.8
1	C	26	SER	2.7
1	C	29	LEU	2.5
1	B	295	SER	2.5
1	B	293	LYS	2.5
1	C	101	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	116	THR	2.4
1	B	105	TRP	2.4
1	A	138	LEU	2.3
1	C	106	SER	2.3
1	C	197	LYS	2.3
1	D	139	PHE	2.2
1	A	103(A)	GLN	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.