Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:06 am BST

PDB ID	:	4ZMU
Title	:	Dcsbis, a diguanylate cyclase from Pseudomonas aeruginosa
Authors	:	Chen, Y.; Liu, C.; Liu, S.; Chi, K.; Gu, L.
Deposited on	:	2015-05-04
Resolution	:	2.50 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:

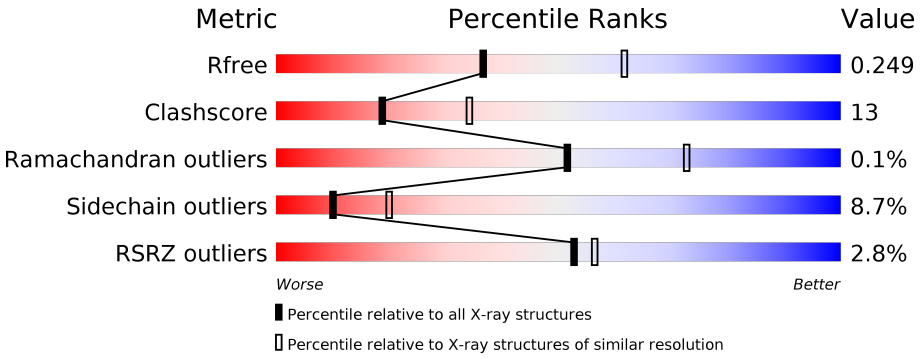
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	345	2% 76% 20%
1	B	345	% 70% 25%
1	C	345	6% 64% 30%
1	D	345	2% 72% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10770 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 diguanylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2674	1665	497	501	11			
1	B	338	Total	C	N	O	S	0	0	0
			2653	1651	494	498	10			
1	C	338	Total	C	N	O	S	0	0	0
			2653	1651	494	498	10			
1	D	338	Total	C	N	O	S	0	0	0
			2653	1651	494	498	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q9I072
A	-2	PRO	-	expression tag	UNP Q9I072
A	-1	GLY	-	expression tag	UNP Q9I072
A	0	SER	-	expression tag	UNP Q9I072
B	-3	GLY	-	expression tag	UNP Q9I072
B	-2	PRO	-	expression tag	UNP Q9I072
B	-1	GLY	-	expression tag	UNP Q9I072
B	0	SER	-	expression tag	UNP Q9I072
C	-3	GLY	-	expression tag	UNP Q9I072
C	-2	PRO	-	expression tag	UNP Q9I072
C	-1	GLY	-	expression tag	UNP Q9I072
C	0	SER	-	expression tag	UNP Q9I072
D	-3	GLY	-	expression tag	UNP Q9I072
D	-2	PRO	-	expression tag	UNP Q9I072
D	-1	GLY	-	expression tag	UNP Q9I072
D	0	SER	-	expression tag	UNP Q9I072

- Molecule 2 is water.

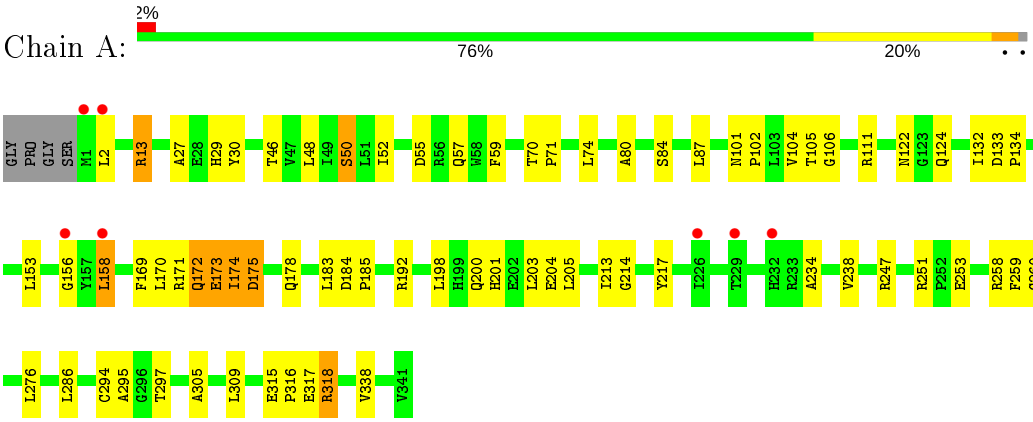
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	66	Total O 66 66	0	0
2	B	39	Total O 39 39	0	0
2	C	13	Total O 13 13	0	0
2	D	19	Total O 19 19	0	0

3 Residue-property plots (i)

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

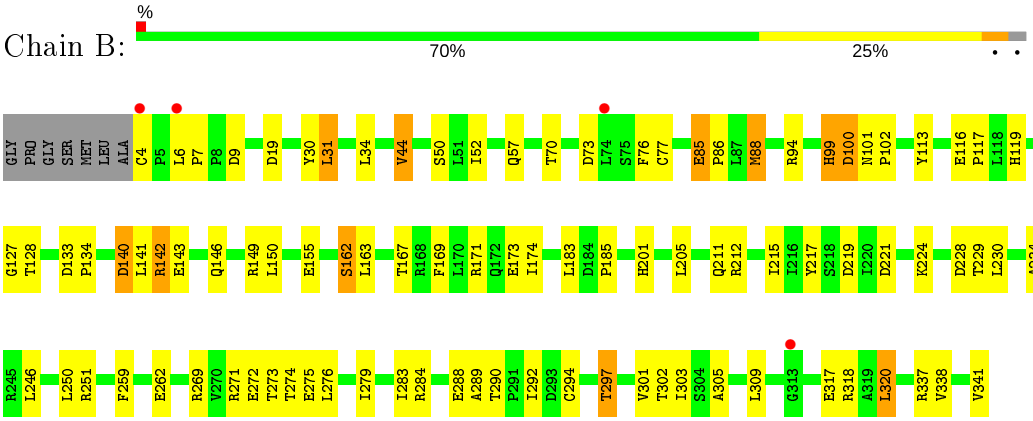
- Molecule 1: diguanylate cyclase

Chain A:



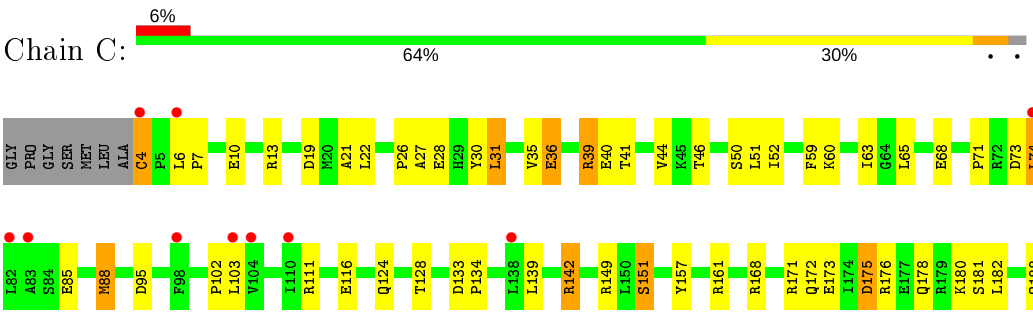
- Molecule 1: diguanylate cyclase

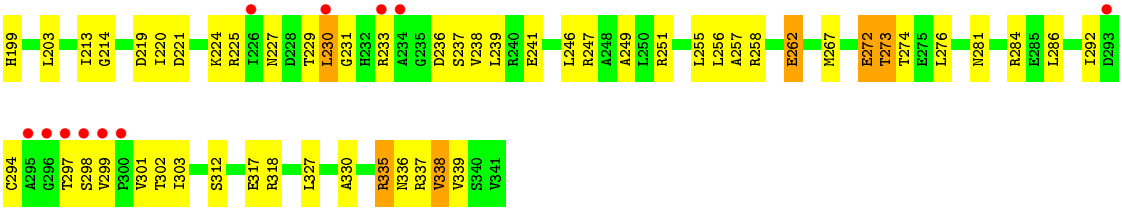
Chain B:



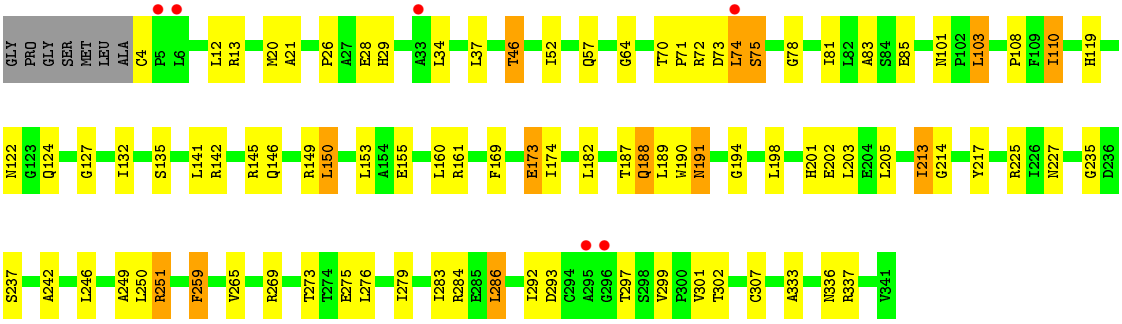
- Molecule 1: diguanylate cyclase

Chain C:





- Molecule 1: diguanylate cyclase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.61Å 109.08Å 111.85Å 90.00° 95.88° 90.00°	Depositor
Resolution (Å)	42.26 – 2.50 49.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.26-2.50) 90.9 (49.56-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.188 , 0.246 0.194 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (3.41%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10770	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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	0.50	0/2722	0.69	3/3688 (0.1%)
1	B	0.46	0/2701	0.64	0/3660
1	C	0.40	0/2701	0.58	0/3660
1	D	0.40	0/2701	0.59	0/3660
All	All	0.44	0/10825	0.63	3/14668 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	PHE	CB-CA-C	-6.55	97.30	110.40
1	A	260	GLY	N-CA-C	-5.99	98.14	113.10
1	A	259	PHE	N-CA-C	5.89	126.91	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	2674	0	2674	53	0
1	B	2653	0	2646	75	0
1	C	2653	0	2646	89	0
1	D	2653	0	2646	72	0
2	A	66	0	0	3	0
2	B	39	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	13	0	0	0	0
2	D	19	0	0	2	0
All	All	10770	0	10612	279	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 13.

All (279) 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:230:LEU:HD12	1:C:230:LEU:O	1.38	1.24
1:C:225:ARG:O	1:C:229:THR:HG22	1.44	1.18
1:C:39:ARG:HH11	1:C:39:ARG:HG2	1.02	1.13
1:C:142:ARG:HH11	1:C:142:ARG:HG2	1.07	1.11
1:B:4:CYS:HB2	1:B:73:ASP:HA	1.40	1.04
1:B:77:CYS:SG	1:B:128:THR:HG21	2.05	0.96
1:B:229:THR:HB	1:B:230:LEU:HD12	1.48	0.92
1:C:39:ARG:NH1	1:C:39:ARG:HG2	1.83	0.91
1:B:50:SER:HB3	1:B:128:THR:HG22	1.55	0.88
1:C:142:ARG:NH1	1:C:142:ARG:HG2	1.88	0.86
1:C:142:ARG:CG	1:C:142:ARG:HH11	1.88	0.86
1:D:203:LEU:HD12	1:D:213:ILE:HD13	1.56	0.84
1:D:13:ARG:HA	1:D:124:GLN:HG3	1.58	0.84
1:D:4:CYS:HB2	1:D:73:ASP:HA	1.61	0.83
1:C:88:MET:HE1	1:C:139:LEU:H	1.42	0.82
1:C:13:ARG:HA	1:C:124:GLN:CG	2.12	0.79
1:D:284:ARG:HD2	1:D:336:ASN:O	1.83	0.79
1:C:203:LEU:HD23	1:C:213:ILE:HG13	1.65	0.78
1:C:39:ARG:CG	1:C:39:ARG:HH11	1.92	0.78
1:C:13:ARG:HA	1:C:124:GLN:HG2	1.65	0.78
1:A:13:ARG:HA	1:A:124:GLN:CG	2.13	0.78
1:D:13:ARG:HA	1:D:124:GLN:CG	2.14	0.76
1:B:221:ASP:HB2	1:B:302:THR:HG23	1.65	0.76
1:B:85:GLU:HG3	1:B:86:PRO:HD2	1.68	0.76
1:A:203:LEU:HD23	1:A:213:ILE:HG13	1.67	0.76
1:C:330:ALA:HB2	1:C:339:VAL:HG23	1.70	0.74
1:C:230:LEU:CD1	1:C:230:LEU:O	2.30	0.71
1:D:57:GLN:HE21	1:D:70:THR:HB	1.54	0.71
1:D:227:ASN:HD21	1:D:235:GLY:HA3	1.55	0.70
1:A:57:GLN:HE21	1:A:70:THR:HB	1.56	0.70
1:A:175:ASP:OD1	1:A:178:GLN:CB	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ILE:HD13	1:D:81:ILE:HD13	1.73	0.70
1:D:214:GLY:HA3	1:D:276:LEU:HD13	1.73	0.70
1:A:141:LEU:HD23	1:A:141:LEU:H	1.58	0.69
1:C:230:LEU:HD12	1:C:230:LEU:C	2.10	0.69
1:D:52:ILE:HD12	1:D:127:GLY:HA2	1.74	0.69
1:A:13:ARG:NH2	1:A:52:ILE:O	2.26	0.69
1:D:75:SER:HB3	1:D:78:GLY:H	1.57	0.69
1:A:175:ASP:OD1	1:A:178:GLN:HB3	1.93	0.68
1:B:122:ASN:ND2	1:B:124:GLN:H	1.92	0.68
1:D:250:LEU:HD21	1:D:283:ILE:HD11	1.73	0.68
1:C:39:ARG:HD3	1:C:63:ILE:HD13	1.75	0.68
1:D:74:LEU:HD21	1:D:103:LEU:HD13	1.76	0.67
1:C:44:VAL:HG23	1:C:46:THR:H	1.60	0.67
1:A:156:GLY:HA2	1:B:30:TYR:CE2	2.29	0.67
1:C:40:GLU:HG2	1:D:149:ARG:HH12	1.57	0.67
1:A:30:TYR:OH	2:A:401:HOH:O	2.11	0.67
1:B:52:ILE:HD12	1:B:127:GLY:HA2	1.75	0.66
1:C:30:TYR:HD2	1:C:31:LEU:HD13	1.59	0.66
1:C:4:CYS:HB2	1:C:73:ASP:HA	1.78	0.65
1:A:156:GLY:HA2	1:B:30:TYR:CZ	2.32	0.65
1:C:302:THR:OG1	1:C:336:ASN:OD1	2.15	0.65
1:D:141:LEU:HG	1:D:142:ARG:N	2.12	0.65
1:A:133:ASP:CG	1:A:134:PRO:HD2	2.17	0.65
1:B:341:VAL:OXT	2:B:401:HOH:O	2.14	0.65
1:A:13:ARG:HA	1:A:124:GLN:HG3	1.79	0.64
1:C:281:ASN:OD1	1:C:338:VAL:HG11	1.98	0.64
1:B:294:CYS:O	1:B:297:THR:HG23	1.98	0.64
1:C:157:TYR:CE1	1:D:160:LEU:HD22	2.33	0.64
1:B:119:HIS:HD2	1:B:155:GLU:OE1	1.80	0.63
1:D:187:THR:O	1:D:188:GLN:HB2	1.97	0.63
1:C:88:MET:HE1	1:C:139:LEU:N	2.10	0.63
1:C:297:THR:HG22	1:C:298:SER:H	1.64	0.62
1:A:175:ASP:N	1:A:175:ASP:OD1	2.30	0.62
1:B:99:HIS:HD2	1:B:100:ASP:N	1.98	0.62
1:B:140:ASP:HB3	1:B:143:GLU:H	1.65	0.61
1:B:250:LEU:HD21	1:B:283:ILE:HD11	1.82	0.61
1:C:221:ASP:HB2	1:C:302:THR:HG23	1.82	0.61
1:D:191:ASN:ND2	1:D:194:GLY:H	1.99	0.61
1:B:86:PRO:HB2	1:B:88:MET:CE	2.31	0.60
1:C:297:THR:HG22	1:C:298:SER:N	2.17	0.60
1:C:239:LEU:HD21	1:C:258:ARG:NH2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:LEU:O	1:D:250:LEU:HG	2.03	0.59
1:D:13:ARG:HG3	1:D:124:GLN:HE21	1.67	0.59
1:D:275:GLU:O	1:D:279:ILE:HG13	2.01	0.59
1:B:173:GLU:HB2	1:B:174:ILE:HD12	1.85	0.59
1:C:30:TYR:CE2	1:C:157:TYR:HB2	2.38	0.59
1:D:203:LEU:HD12	1:D:213:ILE:CD1	2.28	0.59
1:B:201:HIS:CE1	1:B:205:LEU:HD11	2.38	0.59
1:C:178:GLN:O	1:C:181:SER:HB3	2.03	0.59
1:D:119:HIS:CD2	1:D:155:GLU:OE2	2.56	0.58
1:A:175:ASP:OD1	1:A:178:GLN:HB2	2.02	0.58
1:A:200:GLN:O	1:A:204:GLU:HG3	2.03	0.58
1:D:191:ASN:C	1:D:191:ASN:HD22	2.07	0.58
1:A:317:GLU:HB2	2:A:413:HOH:O	2.04	0.58
1:A:318:ARG:HB2	1:A:318:ARG:CZ	2.33	0.58
1:B:140:ASP:HB2	1:B:143:GLU:OE2	2.03	0.58
1:D:276:LEU:HD21	1:D:307:CYS:HB2	1.86	0.58
1:B:224:LYS:HE3	1:B:228:ASP:OD1	2.04	0.57
1:B:211:GLN:HE22	1:B:269:ARG:HE	1.51	0.57
1:B:275:GLU:O	1:B:279:ILE:HG13	2.03	0.57
1:B:85:GLU:CG	1:B:86:PRO:HD2	2.35	0.57
1:A:253:GLU:HB3	1:B:163:LEU:HD11	1.86	0.57
1:C:149:ARG:HB2	1:D:37:LEU:HD23	1.87	0.56
1:C:40:GLU:HG2	1:D:149:ARG:NH1	2.21	0.56
1:D:46:THR:OG1	1:D:132:ILE:HB	2.06	0.56
1:C:21:ALA:O	1:C:161:ARG:NH2	2.39	0.56
1:B:146:GLN:OE1	1:B:149:ARG:NH1	2.38	0.56
1:B:44:VAL:HG22	1:B:133:ASP:HB2	1.88	0.55
1:A:27:ALA:HB3	1:A:247:ARG:CZ	2.36	0.55
1:C:284:ARG:HD3	1:C:337:ARG:HA	1.89	0.55
1:A:46:THR:HB	1:A:132:ILE:HB	1.88	0.55
1:D:249:ALA:HB2	1:D:286:LEU:HD12	1.89	0.55
1:C:76:PHE:HD1	1:C:76:PHE:H	1.55	0.54
1:B:122:ASN:HD21	1:B:124:GLN:HB2	1.71	0.54
1:B:7:PRO:HB2	1:B:9:ASP:OD2	2.08	0.54
1:C:52:ILE:HD11	1:C:77:CYS:HB3	1.88	0.54
1:B:57:GLN:NE2	1:B:70:THR:OG1	2.40	0.54
1:A:13:ARG:HA	1:A:124:GLN:HG2	1.89	0.54
1:B:251:ARG:HH12	1:B:279:ILE:CD1	2.21	0.54
1:D:71:PRO:HG2	1:D:74:LEU:HB2	1.89	0.54
1:D:292:ILE:HD12	1:D:301:VAL:HG21	1.89	0.53
1:C:13:ARG:HA	1:C:124:GLN:HG3	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ARG:O	1:D:75:SER:HB2	2.08	0.53
1:A:201:HIS:CE1	1:A:205:LEU:HD11	2.44	0.53
1:A:203:LEU:HD11	1:A:316:PRO:HG3	1.91	0.53
1:B:119:HIS:CD2	1:B:155:GLU:OE1	2.60	0.53
1:A:169:PHE:CE1	1:A:198:LEU:HD23	2.44	0.53
1:A:294:CYS:HB2	1:A:297:THR:HG23	1.90	0.53
1:D:203:LEU:HA	1:D:213:ILE:CD1	2.38	0.53
1:A:178:GLN:NE2	2:A:406:HOH:O	2.42	0.53
1:A:70:THR:HG22	1:A:71:PRO:O	2.09	0.52
1:D:85:GLU:O	2:D:401:HOH:O	2.19	0.52
1:B:86:PRO:HB2	1:B:88:MET:HE3	1.90	0.52
1:D:203:LEU:HA	1:D:213:ILE:HD11	1.90	0.52
1:C:41:THR:HA	1:D:146:GLN:HE22	1.75	0.52
1:C:272:GLU:HG2	1:C:273:THR:N	2.24	0.52
1:D:182:LEU:HB3	1:D:194:GLY:HA2	1.90	0.51
1:D:242:ALA:O	1:D:246:LEU:HD23	2.10	0.51
1:B:292:ILE:HD12	1:B:301:VAL:HG21	1.91	0.51
1:C:272:GLU:HG2	1:C:273:THR:H	1.75	0.51
1:D:70:THR:HG23	1:D:71:PRO:HD2	1.92	0.51
1:D:108:PRO:HG2	1:D:110:ILE:HG22	1.93	0.51
1:D:70:THR:HG22	1:D:71:PRO:O	2.11	0.51
1:D:191:ASN:HD22	1:D:194:GLY:H	1.58	0.51
1:B:99:HIS:CD2	1:B:100:ASP:N	2.78	0.51
1:C:219:ASP:HB2	1:C:327:LEU:HD21	1.93	0.51
1:D:333:ALA:HB3	1:D:337:ARG:HD2	1.93	0.51
1:A:104:VAL:HG13	1:A:111:ARG:NH1	2.26	0.50
1:C:214:GLY:HA3	1:C:276:LEU:HD13	1.92	0.50
1:C:19:ASP:O	1:C:171:ARG:HD3	2.11	0.50
1:C:249:ALA:HB2	1:C:286:LEU:HD12	1.93	0.50
1:C:36:GLU:HG3	1:C:36:GLU:O	2.08	0.50
1:B:183:LEU:O	1:B:185:PRO:HD3	2.11	0.50
1:C:116:GLU:HB2	1:C:151:SER:HB2	1.93	0.50
1:B:251:ARG:NH1	1:B:279:ILE:HD13	2.26	0.50
1:D:297:THR:O	1:D:299:VAL:HG23	2.12	0.50
1:B:174:ILE:HD12	1:B:174:ILE:N	2.27	0.49
1:B:85:GLU:O	2:B:402:HOH:O	2.20	0.49
1:C:168:ARG:HE	1:C:172:GLN:NE2	2.11	0.49
1:A:234:ALA:O	1:A:238:VAL:HG23	2.13	0.49
1:C:195:PHE:O	1:C:199:HIS:HB3	2.12	0.48
1:C:27:ALA:HB3	1:C:247:ARG:CZ	2.42	0.48
1:B:251:ARG:NH1	1:B:279:ILE:CD1	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ASP:O	1:B:171:ARG:NH1	2.37	0.48
1:C:276:LEU:HG	1:C:276:LEU:O	2.11	0.48
1:D:251:ARG:NH1	1:D:279:ILE:HD11	2.27	0.48
1:C:297:THR:CG2	1:C:298:SER:H	2.23	0.48
1:D:119:HIS:HD2	1:D:155:GLU:OE2	1.96	0.48
1:A:74:LEU:HD22	1:A:102:PRO:HD2	1.96	0.47
1:C:6:LEU:HD23	1:C:6:LEU:N	2.30	0.47
1:B:34:LEU:C	1:B:34:LEU:HD23	2.34	0.47
1:C:111:ARG:HG2	1:C:134:PRO:O	2.14	0.47
1:C:224:LYS:HB3	1:C:224:LYS:NZ	2.30	0.47
1:C:225:ARG:O	1:C:229:THR:CG2	2.37	0.47
1:D:122:ASN:OD1	1:D:124:GLN:HB2	2.14	0.47
1:D:214:GLY:HA3	1:D:276:LEU:CD1	2.41	0.47
1:C:238:VAL:HA	1:C:292:ILE:HG21	1.97	0.47
1:B:86:PRO:HB2	1:B:88:MET:HE1	1.95	0.47
1:C:76:PHE:CD1	1:C:76:PHE:N	2.83	0.47
1:D:83:ALA:HB1	1:D:85:GLU:OE1	2.15	0.47
1:C:175:ASP:OD2	1:C:175:ASP:N	2.48	0.46
1:D:37:LEU:HD12	1:D:150:LEU:HD11	1.97	0.46
1:A:105:THR:HG22	1:A:106:GLY:N	2.30	0.46
1:B:169:PHE:CE2	1:B:173:GLU:HG3	2.51	0.46
1:C:294:CYS:SG	1:C:299:VAL:HG21	2.55	0.46
1:A:172:GLN:HE21	1:A:172:GLN:HB3	1.61	0.46
1:D:74:LEU:CD2	1:D:103:LEU:HD22	2.45	0.46
1:B:140:ASP:OD2	1:B:142:ARG:HB2	2.15	0.46
1:D:74:LEU:CD2	1:D:103:LEU:HD13	2.44	0.46
1:B:234:ALA:O	1:B:238:VAL:HG23	2.16	0.46
1:C:221:ASP:CG	1:C:335:ARG:HB3	2.37	0.46
1:D:26:PRO:HG2	1:D:190:TRP:NE1	2.31	0.46
1:B:122:ASN:ND2	1:B:122:ASN:C	2.69	0.46
1:C:41:THR:HA	1:D:146:GLN:NE2	2.31	0.46
1:C:142:ARG:NH1	1:C:142:ARG:CG	2.57	0.45
1:C:301:VAL:HG12	1:C:302:THR:N	2.32	0.45
1:C:220:ILE:HA	1:C:303:ILE:HG13	1.98	0.45
1:A:122:ASN:OD1	1:A:124:GLN:HB2	2.16	0.45
1:B:162:SER:HA	1:B:167:THR:HG21	1.98	0.45
1:C:272:GLU:OE2	1:C:274:THR:OG1	2.33	0.45
1:D:141:LEU:HG	1:D:142:ARG:H	1.81	0.45
1:A:80:ALA:HB2	1:A:87:LEU:HD23	1.97	0.45
1:B:284:ARG:HD3	1:B:337:ARG:HA	1.98	0.45
1:B:76:PHE:H	1:B:76:PHE:HD2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:GLU:HG2	1:C:262:GLU:O	2.15	0.45
1:C:299:VAL:O	1:C:301:VAL:HG23	2.16	0.45
1:A:101:ASN:HA	1:A:102:PRO:HD3	1.85	0.45
1:B:229:THR:CB	1:B:230:LEU:HD12	2.34	0.44
1:B:99:HIS:CD2	1:B:99:HIS:C	2.91	0.44
1:C:281:ASN:OD1	1:C:338:VAL:CG1	2.65	0.44
1:C:7:PRO:HD2	1:C:10:GLU:HB2	1.99	0.44
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.82	0.44
1:D:259:PHE:CG	1:D:265:VAL:HG13	2.51	0.44
1:B:31:LEU:HD12	1:B:31:LEU:HA	1.80	0.44
1:A:214:GLY:HA3	1:A:276:LEU:HD13	2.00	0.44
1:A:294:CYS:O	1:A:297:THR:HG22	2.17	0.44
1:B:85:GLU:OE2	1:B:85:GLU:HA	2.17	0.44
1:D:202:GLU:O	1:D:269:ARG:HD3	2.17	0.44
1:B:101:ASN:HA	1:B:102:PRO:HD2	1.65	0.44
1:B:215:ILE:HG21	1:B:320:LEU:HD13	2.00	0.44
1:B:4:CYS:CB	1:B:73:ASP:HA	2.28	0.44
1:A:172:GLN:O	1:A:172:GLN:HG2	2.17	0.43
1:A:318:ARG:NE	1:A:318:ARG:HA	2.33	0.43
1:C:168:ARG:HE	1:C:172:GLN:HE22	1.66	0.43
1:D:20:MET:O	1:D:21:ALA:C	2.57	0.43
1:D:28:GLU:OE1	1:D:161:ARG:HD2	2.18	0.43
1:D:302:THR:HA	2:D:408:HOH:O	2.17	0.43
1:B:212:ARG:HA	1:B:212:ARG:HD2	1.79	0.43
1:B:288:GLU:HG2	1:B:288:GLU:O	2.19	0.43
1:C:51:LEU:N	1:C:51:LEU:HD22	2.34	0.43
1:A:272:GLU:HG2	1:A:273:THR:N	2.34	0.43
1:B:122:ASN:HD22	1:B:122:ASN:C	2.22	0.43
1:D:141:LEU:HD12	1:D:145:ARG:NH1	2.34	0.43
1:B:320:LEU:HD13	1:B:320:LEU:HA	1.73	0.43
1:B:276:LEU:HD22	1:B:309:LEU:HD23	2.00	0.43
1:C:7:PRO:HG2	1:C:10:GLU:HB2	2.01	0.43
1:B:289:ALA:O	1:B:290:THR:CG2	2.67	0.42
1:C:227:ASN:O	1:C:231:GLY:N	2.51	0.42
1:B:289:ALA:O	1:B:290:THR:HG23	2.19	0.42
1:B:50:SER:HB3	1:B:128:THR:CG2	2.39	0.42
1:D:201:HIS:O	1:D:205:LEU:HG	2.19	0.42
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.72	0.42
1:C:262:GLU:CG	1:C:262:GLU:O	2.68	0.42
1:B:229:THR:HB	1:B:230:LEU:CD1	2.35	0.42
1:C:241:GLU:O	1:C:241:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLU:OE2	1:D:145:ARG:NH2	2.53	0.42
1:A:183:LEU:O	1:A:185:PRO:HD3	2.19	0.42
1:A:111:ARG:HD3	1:A:111:ARG:HA	1.89	0.42
1:B:141:LEU:HD12	1:B:141:LEU:HA	1.85	0.42
1:D:227:ASN:HD21	1:D:235:GLY:CA	2.25	0.42
1:A:294:CYS:O	1:A:295:ALA:HB3	2.19	0.42
1:A:29:HIS:HB2	1:A:247:ARG:O	2.19	0.42
1:B:113:TYR:CD2	1:B:113:TYR:C	2.93	0.42
1:B:116:GLU:HA	1:B:117:PRO:HD3	1.92	0.42
1:A:48:LEU:HD13	1:A:59:PHE:CE1	2.55	0.42
1:C:59:PHE:CD2	1:C:68:GLU:O	2.72	0.42
1:D:169:PHE:HE2	1:D:198:LEU:HD23	1.85	0.42
1:C:26:PRO:HA	1:C:188:GLN:O	2.20	0.42
1:C:102:PRO:HB2	1:C:103:LEU:HD12	2.01	0.41
1:C:133:ASP:HA	1:C:134:PRO:HD2	1.95	0.41
1:C:28:GLU:HG3	1:C:60:LYS:HE3	2.02	0.41
1:D:29:HIS:O	1:D:29:HIS:CD2	2.73	0.41
1:C:22:LEU:HA	1:C:161:ARG:NH2	2.34	0.41
1:C:255:LEU:HB3	1:C:267:MET:HB3	2.02	0.41
1:B:305:ALA:HB3	1:B:338:VAL:HG22	2.01	0.41
1:C:111:ARG:CG	1:C:134:PRO:O	2.69	0.41
1:D:173:GLU:O	1:D:174:ILE:HD13	2.20	0.41
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.93	0.41
1:A:305:ALA:O	1:A:338:VAL:HA	2.19	0.41
1:C:256:LEU:HD12	1:C:257:ALA:H	1.85	0.41
1:C:71:PRO:HD2	1:C:74:LEU:HD12	2.02	0.41
1:B:211:GLN:NE2	1:B:269:ARG:HE	2.17	0.41
1:A:50:SER:OG	1:A:57:GLN:HG3	2.21	0.41
1:B:6:LEU:HB2	1:B:7:PRO:HD2	2.02	0.41
1:C:180:LYS:HB2	1:C:180:LYS:HE2	1.74	0.41
1:D:12:LEU:HD23	1:D:12:LEU:HA	1.71	0.41
1:D:292:ILE:HD12	1:D:301:VAL:CG2	2.50	0.41
1:D:74:LEU:HD22	1:D:103:LEU:HD22	2.03	0.41
1:A:272:GLU:HG2	1:A:273:THR:H	1.86	0.40
1:D:74:LEU:HD23	1:D:101:ASN:OD1	2.21	0.40
1:A:173:GLU:C	1:A:174:ILE:HG12	2.42	0.40
1:B:133:ASP:HA	1:B:134:PRO:HD3	1.88	0.40
1:C:39:ARG:CG	1:C:39:ARG:NH1	2.61	0.40
1:A:184:ASP:OD2	1:A:258:ARG:HD2	2.21	0.40
1:B:219:ASP:OD1	1:B:262:GLU:HG3	2.22	0.40
1:B:94:ARG:HB3	1:B:94:ARG:HE	1.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:LEU:HB3	1:C:194:GLY:CA	2.51	0.40
1:D:46:THR:CG2	1:D:64:GLY:O	2.69	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	339/345 (98%)	322 (95%)	17 (5%)	0	100 100
1	B	336/345 (97%)	320 (95%)	16 (5%)	0	100 100
1	C	336/345 (97%)	310 (92%)	24 (7%)	2 (1%)	25 43
1	D	336/345 (97%)	318 (95%)	18 (5%)	0	100 100
All	All	1347/1380 (98%)	1270 (94%)	75 (6%)	2 (0%)	51 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	335	ARG
1	C	233	ARG

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	282/284 (99%)	259 (92%)	23 (8%)	11 22
1	B	280/284 (99%)	256 (91%)	24 (9%)	10 20
1	C	280/284 (99%)	251 (90%)	29 (10%)	7 13
1	D	280/284 (99%)	258 (92%)	22 (8%)	12 24
All	All	1122/1136 (99%)	1024 (91%)	98 (9%)	10 20

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	13	ARG
1	A	50	SER
1	A	55	ASP
1	A	84	SER
1	A	141	LEU
1	A	149	ARG
1	A	150	LEU
1	A	153	LEU
1	A	158	LEU
1	A	171	ARG
1	A	172	GLN
1	A	173	GLU
1	A	174	ILE
1	A	175	ASP
1	A	192	ARG
1	A	217	TYR
1	A	251	ARG
1	A	271	ARG
1	A	272	GLU
1	A	309	LEU
1	A	315	GLU
1	A	318	ARG
1	B	31	LEU
1	B	44	VAL
1	B	85	GLU
1	B	88	MET
1	B	99	HIS
1	B	100	ASP
1	B	122	ASN
1	B	140	ASP
1	B	142	ARG
1	B	150	LEU

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Mol	Chain	Res	Type
1	B	162	SER
1	B	217	TYR
1	B	244	SER
1	B	246	LEU
1	B	259	PHE
1	B	271	ARG
1	B	272	GLU
1	B	273	THR
1	B	274	THR
1	B	297	THR
1	B	303	ILE
1	B	317	GLU
1	B	318	ARG
1	B	320	LEU
1	C	4	CYS
1	C	31	LEU
1	C	35	VAL
1	C	36	GLU
1	C	39	ARG
1	C	50	SER
1	C	65	LEU
1	C	74	LEU
1	C	85	GLU
1	C	88	MET
1	C	95	ASP
1	C	128	THR
1	C	142	ARG
1	C	151	SER
1	C	173	GLU
1	C	175	ASP
1	C	176	ARG
1	C	230	LEU
1	C	236	ASP
1	C	237	SER
1	C	246	LEU
1	C	251	ARG
1	C	262	GLU
1	C	272	GLU
1	C	273	THR
1	C	312	SER
1	C	317	GLU
1	C	318	ARG

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Mol	Chain	Res	Type
1	C	338	VAL
1	D	34	LEU
1	D	46	THR
1	D	74	LEU
1	D	75	SER
1	D	103	LEU
1	D	110	ILE
1	D	135	SER
1	D	150	LEU
1	D	153	LEU
1	D	173	GLU
1	D	188	GLN
1	D	189	LEU
1	D	191	ASN
1	D	213	ILE
1	D	217	TYR
1	D	225	ARG
1	D	237	SER
1	D	251	ARG
1	D	259	PHE
1	D	273	THR
1	D	286	LEU
1	D	293	ASP

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	57	GLN
1	A	172	GLN
1	A	201	HIS
1	A	211	GLN
1	B	57	GLN
1	B	99	HIS
1	B	119	HIS
1	B	122	ASN
1	B	172	GLN
1	B	178	GLN
1	B	201	HIS
1	B	211	GLN
1	C	29	HIS
1	C	119	HIS
1	C	172	GLN

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Mol	Chain	Res	Type
1	D	57	GLN
1	D	119	HIS
1	D	124	GLN
1	D	146	GLN
1	D	191	ASN
1	D	227	ASN

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	341/345 (98%)	-0.08	7 (2%) 63 66	29, 42, 69, 80	0
1	B	338/345 (97%)	-0.11	4 (1%) 79 80	29, 48, 76, 89	0
1	C	338/345 (97%)	0.31	21 (6%) 20 21	41, 64, 92, 111	0
1	D	338/345 (97%)	0.15	6 (1%) 68 71	39, 58, 81, 91	0
All	All	1355/1380 (98%)	0.07	38 (2%) 53 56	29, 53, 83, 111	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	LEU	5.9
1	A	2	LEU	5.3
1	C	4	CYS	5.2
1	C	297	THR	4.8
1	C	234	ALA	4.4
1	D	6	LEU	3.8
1	D	74	LEU	3.8
1	C	233	ARG	3.6
1	A	1	MET	3.2
1	C	299	VAL	3.0
1	C	6	LEU	3.0
1	C	83	ALA	2.9
1	C	226	ILE	2.8
1	C	300	PRO	2.8
1	B	74	LEU	2.8
1	C	296	GLY	2.7
1	A	229	THR	2.7
1	C	298	SER	2.7
1	B	4	CYS	2.6
1	A	226	ILE	2.5
1	B	313	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	293	ASP	2.5
1	C	138	LEU	2.4
1	D	296	GLY	2.4
1	D	5	PRO	2.3
1	C	110	ILE	2.3
1	C	295	ALA	2.3
1	C	230	LEU	2.3
1	B	6	LEU	2.2
1	A	232	HIS	2.2
1	A	156	GLY	2.1
1	D	33	ALA	2.1
1	C	98	PHE	2.1
1	A	158	LEU	2.1
1	C	82	LEU	2.1
1	C	104	VAL	2.1
1	C	103	LEU	2.1
1	D	295	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.