Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 11:25 PM JST

PDB ID	:	6IEP
Title	:	GAPDH of Streptococcus agalactiae
Authors	:	Ponnuraj, K.; Nagarajan, R.
Deposited on	:	2018-09-15
Resolution	:	2.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

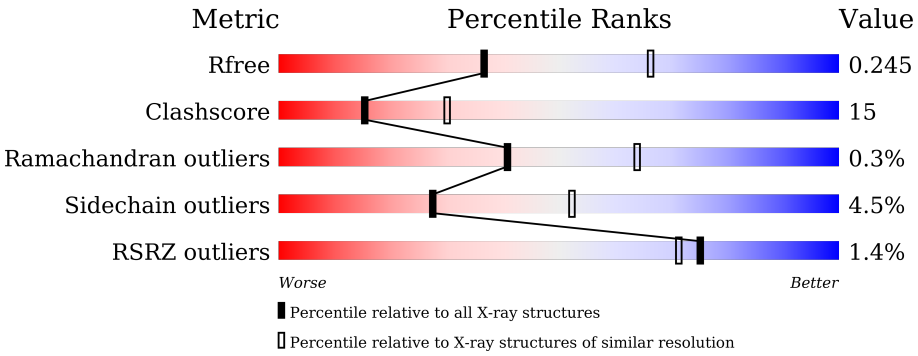
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	344	2% 70% 24%
1	B	344	2% 67% 27%
1	C	344	2% 74% 21%
1	D	344	76% 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10240 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2490	1557	433	492	8			
1	B	332	Total	C	N	O	S	0	0	0
			2477	1549	430	490	8			
1	C	333	Total	C	N	O	S	0	0	0
			2493	1558	434	493	8			
1	D	337	Total	C	N	O	S	0	0	0
			2513	1570	438	497	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	LEU	-	expression tag	UNP Q8E3E8
A	338	GLU	-	expression tag	UNP Q8E3E8
A	339	HIS	-	expression tag	UNP Q8E3E8
A	340	HIS	-	expression tag	UNP Q8E3E8
A	341	HIS	-	expression tag	UNP Q8E3E8
A	342	HIS	-	expression tag	UNP Q8E3E8
A	343	HIS	-	expression tag	UNP Q8E3E8
A	344	HIS	-	expression tag	UNP Q8E3E8
B	337	LEU	-	expression tag	UNP Q8E3E8
B	338	GLU	-	expression tag	UNP Q8E3E8
B	339	HIS	-	expression tag	UNP Q8E3E8
B	340	HIS	-	expression tag	UNP Q8E3E8
B	341	HIS	-	expression tag	UNP Q8E3E8
B	342	HIS	-	expression tag	UNP Q8E3E8
B	343	HIS	-	expression tag	UNP Q8E3E8
B	344	HIS	-	expression tag	UNP Q8E3E8
C	337	LEU	-	expression tag	UNP Q8E3E8
C	338	GLU	-	expression tag	UNP Q8E3E8
C	339	HIS	-	expression tag	UNP Q8E3E8
C	340	HIS	-	expression tag	UNP Q8E3E8
C	341	HIS	-	expression tag	UNP Q8E3E8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	342	HIS	-	expression tag	UNP Q8E3E8
C	343	HIS	-	expression tag	UNP Q8E3E8
C	344	HIS	-	expression tag	UNP Q8E3E8
D	337	LEU	-	expression tag	UNP Q8E3E8
D	338	GLU	-	expression tag	UNP Q8E3E8
D	339	HIS	-	expression tag	UNP Q8E3E8
D	340	HIS	-	expression tag	UNP Q8E3E8
D	341	HIS	-	expression tag	UNP Q8E3E8
D	342	HIS	-	expression tag	UNP Q8E3E8
D	343	HIS	-	expression tag	UNP Q8E3E8
D	344	HIS	-	expression tag	UNP Q8E3E8

- Molecule 2 is water.

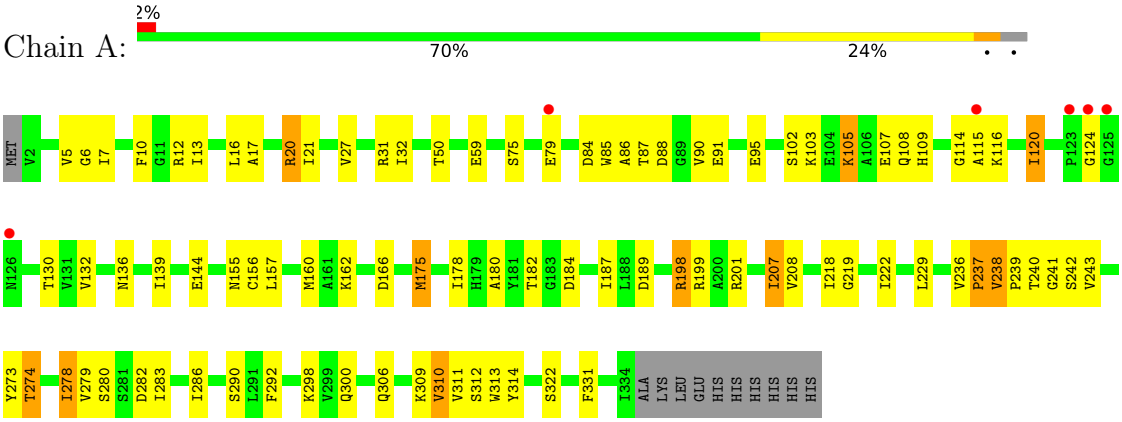
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	73	Total O 73 73	0	0
2	B	53	Total O 53 53	0	0
2	C	60	Total O 60 60	0	0
2	D	81	Total O 81 81	0	0

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.

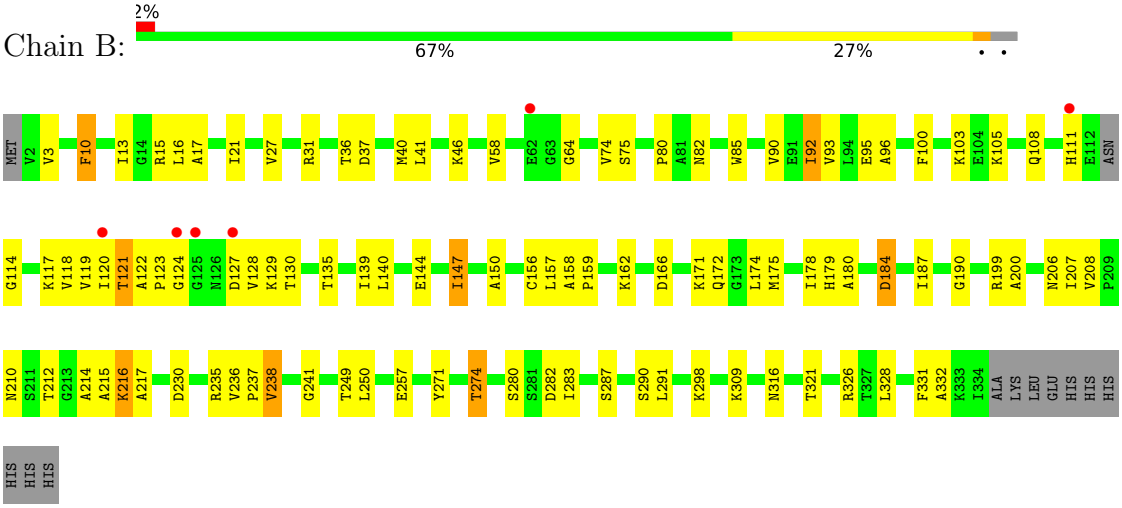
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain A:



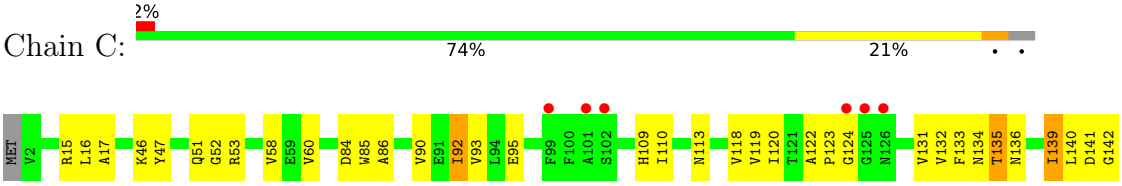
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

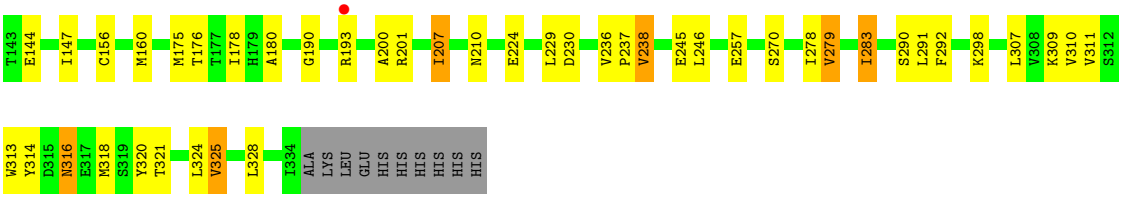
Chain B:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

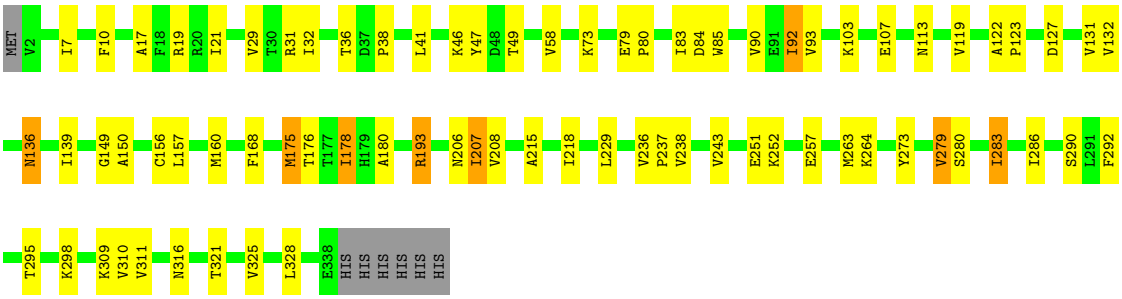
Chain C:





• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

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	88.58Å 124.42Å 125.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 36.17 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.60) 99.9 (36.17-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.94 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.246 0.206 , 0.245	Depositor DCC
R_{free} test set	1306 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10240	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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	0.36	0/2528	0.67	2/3432 (0.1%)
1	B	0.35	0/2514	0.64	1/3413 (0.0%)
1	C	0.35	0/2531	0.64	1/3436 (0.0%)
1	D	0.35	0/2551	0.65	2/3464 (0.1%)
All	All	0.35	0/10124	0.65	6/13745 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	207	ILE	N-CA-C	-6.23	94.18	111.00
1	A	207	ILE	N-CA-C	-6.02	94.74	111.00
1	B	207	ILE	N-CA-C	-5.96	94.89	111.00
1	C	207	ILE	N-CA-C	-5.88	95.11	111.00
1	A	124	GLY	N-CA-C	5.33	126.42	113.10
1	D	178	ILE	N-CA-C	-5.13	97.14	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	2490	0	2457	85	0
1	B	2477	0	2437	87	0
1	C	2493	0	2461	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2513	0	2472	78	0
2	A	73	0	0	5	0
2	B	53	0	0	0	0
2	C	60	0	0	5	0
2	D	81	0	0	2	0
All	All	10240	0	9827	294	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 15.

All (294) 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:120:ILE:HD11	1:C:124:GLY:HA2	1.34	1.06
1:B:171:LYS:HB2	1:B:249:THR:HG23	1.47	0.95
1:C:120:ILE:HD11	1:C:124:GLY:CA	1.99	0.91
1:B:85:TRP:HB3	1:B:90:VAL:HB	1.54	0.90
1:C:92:ILE:HD13	1:C:93:VAL:N	1.88	0.88
1:C:136:ASN:O	1:C:139:ILE:HD12	1.73	0.87
1:C:283:ILE:HD11	1:C:291:LEU:HD23	1.56	0.87
1:A:279:VAL:HG21	1:D:208:VAL:HG22	1.60	0.84
1:B:119:VAL:HG22	1:B:147:ILE:HD11	1.58	0.84
1:C:120:ILE:CD1	1:C:124:GLY:HA2	2.08	0.83
1:D:193:ARG:HH11	1:D:193:ARG:HA	1.44	0.82
1:D:132:VAL:H	1:D:136:ASN:HD21	1.27	0.82
1:A:187:ILE:HD13	1:B:187:ILE:HA	1.63	0.81
1:C:86:ALA:HB3	1:C:113:ASN:HA	1.62	0.80
1:B:100:PHE:HD1	1:B:105:LYS:HB3	1.48	0.79
1:A:208:VAL:HG22	1:D:279:VAL:HG21	1.66	0.77
1:C:92:ILE:HD13	1:C:93:VAL:H	1.46	0.77
1:C:84:ASP:HA	1:C:113:ASN:O	1.86	0.76
1:C:85:TRP:HB3	1:C:90:VAL:HB	1.67	0.76
1:A:207:ILE:HD12	1:A:236:VAL:HG12	1.67	0.75
1:D:132:VAL:H	1:D:136:ASN:ND2	1.86	0.74
1:D:92:ILE:HD13	1:D:93:VAL:N	2.02	0.74
1:C:224:GLU:CD	1:C:224:GLU:H	1.92	0.73
1:C:16:LEU:HD21	1:C:51:GLN:HG3	1.69	0.72
1:A:13:ILE:HD12	1:A:13:ILE:H	1.53	0.72
1:B:280:SER:HB3	1:C:207:ILE:H	1.55	0.71
1:B:147:ILE:HD13	1:B:147:ILE:H	1.56	0.71
1:C:119:VAL:HG22	1:C:147:ILE:HD11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HD22	1:A:175:MET:CE	2.20	0.71
1:D:122:ALA:HB1	1:D:123:PRO:HD2	1.72	0.71
1:A:160:MET:HE1	1:A:311:VAL:N	2.05	0.70
1:A:237:PRO:HB2	1:D:237:PRO:HB2	1.72	0.70
1:B:129:LYS:HD3	1:B:139:ILE:HD13	1.74	0.70
1:A:279:VAL:CG2	1:D:208:VAL:HG22	2.22	0.70
1:A:157:LEU:HD22	1:A:175:MET:HE3	1.74	0.69
1:C:156:CYS:HA	1:C:290:SER:HB2	1.75	0.69
1:A:85:TRP:HB3	1:A:90:VAL:HB	1.76	0.68
1:D:92:ILE:HD12	1:D:328:LEU:HD22	1.75	0.68
1:C:160:MET:HE1	1:C:311:VAL:C	2.15	0.66
1:C:193:ARG:HG2	2:C:428:HOH:O	1.94	0.66
1:C:85:TRP:HE1	1:C:109:HIS:HD2	1.43	0.66
1:B:236:VAL:HG11	1:C:236:VAL:HG11	1.78	0.65
1:B:117:LYS:HB3	1:B:331:PHE:CE2	2.31	0.65
1:D:103:LYS:HD2	1:D:127:ASP:O	1.97	0.65
1:C:201:ARG:HH21	1:D:47:TYR:HB3	1.62	0.65
2:A:450:HOH:O	1:C:53:ARG:HD2	1.96	0.64
1:A:207:ILE:H	1:D:280:SER:CB	2.10	0.64
1:C:283:ILE:HG12	1:C:313:TRP:HB3	1.80	0.64
1:D:21:ILE:HD13	1:D:325:VAL:HG13	1.79	0.64
1:A:274:THR:HG21	2:C:425:HOH:O	1.98	0.63
1:B:171:LYS:HB2	1:B:249:THR:CG2	2.25	0.63
1:D:46:LYS:HG2	1:D:58:VAL:HB	1.78	0.63
1:B:282:ASP:OD1	1:C:201:ARG:NH2	2.32	0.63
1:B:206:ASN:HB3	1:C:279:VAL:HG13	1.81	0.62
1:A:298:LYS:HB2	1:A:309:LYS:HB3	1.81	0.62
1:B:280:SER:O	1:B:283:ILE:HG13	1.99	0.62
1:B:274:THR:OG1	1:B:291:LEU:HD11	2.00	0.62
1:B:215:ALA:HB1	1:B:230:ASP:HA	1.80	0.61
1:A:208:VAL:HG22	1:D:279:VAL:CG2	2.29	0.61
1:B:298:LYS:HB2	1:B:309:LYS:HB3	1.82	0.61
1:C:160:MET:HE3	1:C:292:PHE:HD1	1.65	0.61
1:B:129:LYS:HD3	1:B:139:ILE:CD1	2.30	0.61
1:A:156:CYS:HA	1:A:290:SER:HB2	1.83	0.60
1:B:139:ILE:HD12	1:B:139:ILE:C	2.21	0.60
1:A:160:MET:CE	1:A:310:VAL:HB	2.32	0.60
1:C:160:MET:HE2	1:C:310:VAL:HB	1.82	0.60
1:B:180:ALA:HB1	1:B:238:VAL:O	2.02	0.60
1:D:193:ARG:HA	1:D:193:ARG:NH1	2.15	0.59
1:A:273:TYR:HB2	2:A:440:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ALA:CB	1:C:113:ASN:HA	2.30	0.59
1:C:92:ILE:HD12	1:C:328:LEU:HD22	1.84	0.59
1:C:132:VAL:O	1:C:135:THR:HG23	2.02	0.59
1:B:147:ILE:HD13	1:B:147:ILE:N	2.18	0.59
1:D:157:LEU:CD2	1:D:218:ILE:HD12	2.33	0.59
1:B:178:ILE:N	1:B:178:ILE:HD12	2.18	0.58
1:A:207:ILE:HD11	1:D:236:VAL:HG21	1.85	0.58
1:A:17:ALA:O	1:A:21:ILE:HG12	2.04	0.58
1:B:3:VAL:CG1	1:B:92:ILE:HD11	2.33	0.58
1:A:13:ILE:HD12	1:A:13:ILE:N	2.18	0.58
1:A:189:ASP:OD2	1:A:201:ARG:NH1	2.37	0.58
1:B:13:ILE:HD12	1:B:13:ILE:N	2.19	0.57
1:D:180:ALA:HB1	1:D:238:VAL:O	2.03	0.57
1:D:17:ALA:O	1:D:21:ILE:HG12	2.05	0.57
1:C:278:ILE:HD12	1:C:283:ILE:HD13	1.85	0.57
1:A:280:SER:HB3	1:D:207:ILE:HB	1.87	0.56
1:C:135:THR:HG22	2:C:419:HOH:O	2.04	0.56
1:C:178:ILE:HD12	1:C:178:ILE:N	2.19	0.56
1:A:86:ALA:H	1:A:114:GLY:HA2	1.70	0.56
1:B:237:PRO:HB2	1:C:237:PRO:HB2	1.87	0.56
1:D:178:ILE:HB	1:D:243:VAL:HG12	1.88	0.56
1:B:13:ILE:HD12	1:B:13:ILE:H	1.69	0.56
1:C:201:ARG:NH2	1:D:47:TYR:HB3	2.21	0.56
1:A:207:ILE:CD1	1:D:236:VAL:HG21	2.35	0.56
1:D:92:ILE:HD11	1:D:119:VAL:HG23	1.88	0.55
1:B:93:VAL:HB	1:B:118:VAL:HG22	1.87	0.55
1:C:119:VAL:HG21	1:C:328:LEU:HD23	1.88	0.55
1:D:160:MET:HE1	1:D:311:VAL:N	2.21	0.55
1:A:180:ALA:HB1	1:A:238:VAL:O	2.07	0.55
1:B:100:PHE:CD1	1:B:105:LYS:HB3	2.37	0.55
1:D:17:ALA:HA	1:D:321:THR:HG23	1.89	0.55
1:B:298:LYS:HE3	1:C:230:ASP:OD2	2.07	0.55
1:A:198:ARG:NH2	1:D:295:THR:OG1	2.40	0.54
1:C:313:TRP:O	1:C:314:TYR:HB3	2.07	0.54
1:D:298:LYS:HB2	1:D:309:LYS:HB3	1.89	0.54
1:A:207:ILE:H	1:D:280:SER:HB3	1.73	0.54
1:D:218:ILE:HD13	1:D:229:LEU:HD12	1.87	0.54
1:A:236:VAL:HG11	1:D:236:VAL:HG11	1.90	0.54
1:B:128:VAL:CG1	1:B:147:ILE:HA	2.38	0.54
1:B:3:VAL:HG12	1:B:92:ILE:HD11	1.89	0.54
1:B:21:ILE:HG23	1:B:27:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LYS:HB2	1:C:309:LYS:HB3	1.90	0.54
1:B:103:LYS:HB2	1:B:127:ASP:CB	2.38	0.53
1:D:168:PHE:O	1:D:251:GLU:HB2	2.09	0.53
1:B:124:GLY:CA	1:B:128:VAL:HB	2.38	0.53
1:A:95:GLU:HB3	1:A:120:ILE:HA	1.89	0.53
1:A:278:ILE:HD13	1:A:278:ILE:H	1.71	0.53
1:B:280:SER:HB2	1:C:207:ILE:HB	1.90	0.53
1:A:207:ILE:HD11	1:D:236:VAL:CG2	2.38	0.53
1:A:136:ASN:O	1:A:139:ILE:HG12	2.09	0.52
1:B:147:ILE:HD12	1:B:331:PHE:CE2	2.44	0.52
1:A:162:LYS:HE2	1:A:166:ASP:OD1	2.09	0.52
1:B:156:CYS:HA	1:B:290:SER:HB2	1.90	0.52
1:D:132:VAL:N	1:D:136:ASN:HD21	2.04	0.52
1:D:178:ILE:N	1:D:178:ILE:HD12	2.24	0.52
1:A:280:SER:O	1:A:283:ILE:HG13	2.10	0.52
1:D:160:MET:HE1	1:D:310:VAL:HB	1.92	0.52
1:A:31:ARG:HD2	1:A:88:ASP:OD2	2.10	0.52
1:A:207:ILE:H	1:D:280:SER:HB2	1.74	0.52
1:B:174:LEU:HA	1:B:230:ASP:O	2.10	0.52
1:D:157:LEU:HD21	1:D:218:ILE:HD12	1.92	0.51
1:A:207:ILE:HB	1:D:280:SER:HB2	1.91	0.51
1:D:7:ILE:HD12	1:D:7:ILE:N	2.25	0.51
1:B:36:THR:HB	1:B:41:LEU:HD21	1.93	0.51
1:A:91:GLU:O	1:A:116:LYS:HB3	2.11	0.51
1:B:31:ARG:HH21	1:B:75:SER:CB	2.24	0.51
1:D:7:ILE:HD13	1:D:29:VAL:CG1	2.41	0.50
1:B:241:GLY:HA2	1:B:283:ILE:HD11	1.94	0.50
1:C:119:VAL:HG13	1:C:147:ILE:CD1	2.42	0.50
1:B:280:SER:CB	1:C:207:ILE:H	2.23	0.49
1:C:46:LYS:CG	1:C:58:VAL:HB	2.43	0.49
1:D:160:MET:HE1	1:D:310:VAL:C	2.32	0.49
1:A:120:ILE:HG12	1:A:120:ILE:O	2.12	0.49
1:B:140:LEU:HA	1:B:144:GLU:OE2	2.12	0.49
1:C:131:VAL:HG22	1:C:139:ILE:HD11	1.95	0.49
1:B:36:THR:HG22	1:B:37:ASP:N	2.27	0.49
1:B:119:VAL:HG21	1:B:328:LEU:HD23	1.94	0.49
1:B:216:LYS:HG3	1:B:217:ALA:H	1.78	0.48
1:C:257:GLU:CD	1:C:257:GLU:H	2.16	0.48
1:D:21:ILE:CD1	1:D:325:VAL:HG13	2.42	0.48
1:A:109:HIS:O	1:A:115:ALA:HB3	2.13	0.48
1:B:212:THR:HG22	1:B:214:ALA:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:ASP:HA	1:D:113:ASN:O	2.14	0.48
1:D:119:VAL:HG21	1:D:328:LEU:HD23	1.96	0.48
1:B:122:ALA:HB1	1:B:123:PRO:HD2	1.94	0.48
1:A:31:ARG:HH21	1:A:75:SER:CB	2.27	0.48
1:A:103:LYS:O	1:A:107:GLU:HG3	2.14	0.48
1:A:184:ASP:OD2	1:A:199:ARG:HD3	2.13	0.48
1:D:283:ILE:O	1:D:286:ILE:HG12	2.13	0.48
1:C:134:ASN:HD22	1:C:270:SER:CB	2.27	0.48
1:A:13:ILE:H	1:A:13:ILE:CD1	2.24	0.47
1:A:84:ASP:HB2	1:A:87:THR:HG23	1.95	0.47
1:A:282:ASP:OD1	1:C:47:TYR:HB3	2.14	0.47
1:B:179:HIS:HB3	1:B:235:ARG:HD3	1.96	0.47
1:D:257:GLU:CD	1:D:257:GLU:H	2.17	0.47
1:B:119:VAL:CG2	1:B:147:ILE:HD11	2.37	0.47
1:B:135:THR:HG21	1:B:158:ALA:HB1	1.96	0.47
1:C:92:ILE:HD11	1:C:119:VAL:HG23	1.95	0.47
1:A:178:ILE:N	1:A:178:ILE:HD12	2.29	0.47
1:B:96:ALA:HA	1:B:121:THR:OG1	2.14	0.47
1:A:278:ILE:HD13	1:A:278:ILE:N	2.29	0.47
1:A:160:MET:HE3	1:A:292:PHE:HD1	1.80	0.47
1:D:29:VAL:HG11	1:D:32:ILE:HD11	1.96	0.47
1:D:85:TRP:HB3	1:D:90:VAL:HB	1.97	0.47
1:D:103:LYS:O	1:D:107:GLU:HG3	2.14	0.47
1:C:122:ALA:O	1:C:123:PRO:C	2.53	0.47
1:C:190:GLY:O	1:C:200:ALA:HB1	2.14	0.47
1:A:218:ILE:HG21	1:A:229:LEU:HD12	1.96	0.46
1:A:219:GLY:HA2	1:A:222:ILE:O	2.15	0.46
1:B:80:PRO:HB2	1:B:108:GLN:CB	2.45	0.46
1:A:102:SER:OG	1:A:105:LYS:HB2	2.15	0.46
1:A:105:LYS:O	1:A:108:GLN:HG3	2.15	0.46
1:B:119:VAL:CG2	1:B:328:LEU:HD23	2.46	0.46
1:C:135:THR:HB	2:C:457:HOH:O	2.14	0.46
1:C:175:MET:HG2	1:C:176:THR:N	2.30	0.46
1:C:201:ARG:NH1	1:D:49:THR:OG1	2.48	0.46
1:B:159:PRO:HB2	1:B:271:TYR:CG	2.51	0.46
1:A:278:ILE:H	1:A:278:ILE:CD1	2.28	0.46
1:A:84:ASP:OD2	1:A:87:THR:HG21	2.15	0.46
1:B:216:LYS:HG3	1:B:217:ALA:N	2.31	0.46
1:A:79:GLU:HB3	2:A:410:HOH:O	2.16	0.46
1:A:300:GLN:O	1:A:306:GLN:HA	2.15	0.46
1:D:263:MET:HG3	1:D:292:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLY:HA2	1:B:128:VAL:HB	1.96	0.46
1:B:147:ILE:N	1:B:147:ILE:CD1	2.78	0.46
1:C:92:ILE:HD12	1:C:328:LEU:CD2	2.45	0.46
1:C:133:PHE:O	1:C:134:ASN:HB2	2.15	0.46
1:A:157:LEU:HD22	1:A:175:MET:HE1	1.97	0.46
1:C:160:MET:HE3	1:C:292:PHE:CD1	2.50	0.46
1:B:92:ILE:HD13	1:B:332:ALA:HB2	1.97	0.45
1:C:15:ARG:HG3	1:C:15:ARG:HH11	1.81	0.45
1:B:190:GLY:O	1:B:200:ALA:HB1	2.17	0.45
1:D:131:VAL:HA	1:D:136:ASN:HD21	1.81	0.45
1:A:105:LYS:NZ	2:A:403:HOH:O	2.46	0.45
1:A:160:MET:HE1	1:A:310:VAL:HB	1.97	0.45
1:A:144:GLU:HG2	1:A:331:PHE:HE1	1.82	0.45
1:B:172:GLN:HG3	1:C:307:LEU:HD22	1.98	0.45
1:A:7:ILE:HB	1:A:32:ILE:HD13	1.99	0.45
1:D:273:TYR:HB2	2:D:466:HOH:O	2.16	0.45
1:A:160:MET:HE1	1:A:310:VAL:C	2.37	0.45
1:A:241:GLY:HA2	1:A:283:ILE:HD11	1.99	0.45
1:B:287:SER:O	1:B:326:ARG:NH2	2.40	0.45
1:A:160:MET:HE2	1:A:310:VAL:HB	1.98	0.44
1:A:189:ASP:CG	1:A:201:ARG:NH1	2.70	0.44
1:D:36:THR:HB	1:D:41:LEU:HD21	1.99	0.44
1:A:7:ILE:HB	1:A:32:ILE:CD1	2.47	0.44
1:C:141:ASP:OD1	1:C:142:GLY:N	2.50	0.44
1:D:92:ILE:HD12	1:D:328:LEU:CD2	2.45	0.44
1:C:110:ILE:HD11	1:C:118:VAL:HG23	2.00	0.44
1:C:160:MET:HE2	1:C:311:VAL:N	2.33	0.44
1:A:283:ILE:C	1:A:283:ILE:HD12	2.38	0.44
1:B:157:LEU:HD22	1:B:175:MET:SD	2.57	0.44
1:B:162:LYS:HE2	1:B:166:ASP:OD2	2.18	0.44
1:A:50:THR:HG21	1:A:239:PRO:HB2	2.00	0.43
1:B:175:MET:HE1	1:B:212:THR:HG21	1.98	0.43
1:C:180:ALA:HB1	1:C:238:VAL:O	2.18	0.43
1:B:10:PHE:CD2	1:B:15:ARG:HG3	2.53	0.43
1:A:283:ILE:O	1:A:286:ILE:HG12	2.18	0.43
1:C:85:TRP:NE1	1:C:109:HIS:HD2	2.14	0.43
1:C:325:VAL:HG22	2:C:414:HOH:O	2.17	0.43
1:D:80:PRO:HA	1:D:83:ILE:HD12	1.99	0.43
1:C:119:VAL:HG13	1:C:147:ILE:HD11	2.00	0.43
1:C:139:ILE:HD13	1:C:140:LEU:N	2.32	0.43
1:A:132:VAL:HG13	1:A:155:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ALA:O	1:D:218:ILE:HG22	2.18	0.43
1:A:5:VAL:HG12	1:A:6:GLY:N	2.33	0.43
1:A:12:ARG:O	1:A:16:LEU:HG	2.18	0.43
1:A:20:ARG:HD3	1:A:322:SER:HA	2.01	0.43
1:D:38:PRO:HG3	2:D:479:HOH:O	2.18	0.43
1:D:160:MET:HE2	1:D:292:PHE:HD1	1.83	0.43
1:A:313:TRP:O	1:A:314:TYR:HB3	2.19	0.43
1:C:85:TRP:HB3	1:C:90:VAL:CB	2.45	0.43
1:A:279:VAL:HG23	1:D:208:VAL:HA	2.01	0.43
1:B:206:ASN:CG	1:C:279:VAL:HG11	2.39	0.43
1:D:160:MET:HE2	1:D:292:PHE:CD1	2.53	0.43
1:D:160:MET:CE	1:D:310:VAL:HB	2.49	0.42
1:C:17:ALA:HA	1:C:321:THR:CG2	2.49	0.42
1:C:95:GLU:OE1	1:C:109:HIS:HE1	2.02	0.42
1:B:111:HIS:C	1:B:114:GLY:HA3	2.39	0.42
1:A:21:ILE:HD12	1:A:27:VAL:HG11	2.01	0.42
1:B:17:ALA:HA	1:B:321:THR:CG2	2.50	0.42
1:B:95:GLU:HG2	1:B:120:ILE:HD11	2.00	0.42
1:B:139:ILE:HD12	1:B:140:LEU:N	2.34	0.42
1:D:136:ASN:O	1:D:139:ILE:HG12	2.20	0.42
2:A:456:HOH:O	1:C:52:GLY:HA2	2.19	0.42
1:C:320:TYR:CE2	1:C:324:LEU:HD11	2.55	0.42
1:B:100:PHE:O	1:B:120:ILE:HD11	2.20	0.42
1:A:182:THR:C	1:A:184:ASP:H	2.23	0.42
1:B:238:VAL:HG21	1:C:207:ILE:HD12	2.01	0.42
1:B:257:GLU:H	1:B:257:GLU:CD	2.22	0.42
1:B:95:GLU:CG	1:B:120:ILE:HD13	2.50	0.41
1:C:16:LEU:HD22	1:C:318:MET:CE	2.50	0.41
1:D:156:CYS:HA	1:D:290:SER:HB2	2.02	0.41
1:B:118:VAL:O	1:B:147:ILE:HD13	2.20	0.41
1:B:184:ASP:OD2	1:B:199:ARG:HD3	2.20	0.41
1:B:199:ARG:HG3	1:B:210:ASN:HD21	1.84	0.41
1:B:128:VAL:HG13	1:B:147:ILE:HA	2.00	0.41
1:C:245:GLU:HG2	1:C:311:VAL:HG22	2.01	0.41
1:A:279:VAL:HG22	1:D:207:ILE:O	2.20	0.41
1:A:50:THR:CG2	1:A:239:PRO:HB2	2.51	0.41
1:A:207:ILE:O	1:D:279:VAL:HG22	2.20	0.41
1:A:160:MET:CE	1:A:292:PHE:HD1	2.34	0.41
1:B:13:ILE:H	1:B:13:ILE:CD1	2.32	0.41
1:B:95:GLU:CG	1:B:120:ILE:CD1	2.98	0.41
1:B:208:VAL:HG22	1:C:279:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LYS:CG	1:D:58:VAL:HB	2.47	0.41
1:A:279:VAL:HG22	1:D:206:ASN:HB3	2.02	0.41
1:D:160:MET:HE3	1:D:311:VAL:C	2.41	0.41
1:D:31:ARG:HD3	1:D:73:LYS:HD2	2.02	0.41
1:B:37:ASP:O	1:B:40:MET:HB3	2.20	0.41
1:C:278:ILE:HD12	1:C:283:ILE:CD1	2.49	0.41
1:C:321:THR:O	1:C:325:VAL:HG13	2.21	0.41
1:D:175:MET:HG2	1:D:176:THR:N	2.36	0.41
1:C:246:LEU:O	1:C:309:LYS:HA	2.21	0.41
1:D:149:GLY:O	1:D:150:ALA:HB3	2.21	0.40
1:B:46:LYS:HG3	1:B:58:VAL:HB	2.03	0.40
1:B:64:GLY:HA2	1:B:74:VAL:HB	2.03	0.40
1:D:264:LYS:HB2	1:D:273:TYR:CE2	2.55	0.40
1:B:130:THR:HG23	1:B:150:ALA:HB2	2.03	0.40
1:C:140:LEU:HA	1:C:144:GLU:OE2	2.22	0.40
1:C:160:MET:CE	1:C:292:PHE:HD1	2.34	0.40
1:D:122:ALA:HB1	1:D:123:PRO:CD	2.46	0.40
1:B:96:ALA:HA	1:B:121:THR:HG1	1.87	0.40
1:D:7:ILE:HD13	1:D:29:VAL:HG13	2.03	0.40
1:A:242:SER:HB2	1:A:314:TYR:CE1	2.57	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	331/344 (96%)	307 (93%)	23 (7%)	1 (0%)	41	64
1	B	328/344 (95%)	299 (91%)	28 (8%)	1 (0%)	41	64
1	C	331/344 (96%)	306 (92%)	24 (7%)	1 (0%)	41	64
1	D	335/344 (97%)	312 (93%)	22 (7%)	1 (0%)	41	64
All	All	1325/1376 (96%)	1224 (92%)	97 (7%)	4 (0%)	41	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	316	ASN
1	C	316	ASN
1	D	316	ASN
1	A	237	PRO

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	262/278 (94%)	247 (94%)	15 (6%)	20	41
1	B	260/278 (94%)	249 (96%)	11 (4%)	30	55
1	C	263/278 (95%)	252 (96%)	11 (4%)	30	55
1	D	263/278 (95%)	253 (96%)	10 (4%)	33	59
All	All	1048/1112 (94%)	1001 (96%)	47 (4%)	27	52

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	20	ARG
1	A	59	GLU
1	A	105	LYS
1	A	120	ILE
1	A	130	THR
1	A	175	MET
1	A	198	ARG
1	A	238	VAL
1	A	240	THR
1	A	243	VAL
1	A	274	THR
1	A	278	ILE
1	A	310	VAL
1	A	312	SER
1	B	10	PHE

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Mol	Chain	Res	Type
1	B	16	LEU
1	B	82	ASN
1	B	92	ILE
1	B	121	THR
1	B	147	ILE
1	B	184	ASP
1	B	216	LYS
1	B	238	VAL
1	B	250	LEU
1	B	274	THR
1	C	60	VAL
1	C	92	ILE
1	C	135	THR
1	C	139	ILE
1	C	210	ASN
1	C	229	LEU
1	C	238	VAL
1	C	279	VAL
1	C	283	ILE
1	C	316	ASN
1	C	325	VAL
1	D	10	PHE
1	D	19	ARG
1	D	79	GLU
1	D	92	ILE
1	D	136	ASN
1	D	175	MET
1	D	193	ARG
1	D	252	LYS
1	D	279	VAL
1	D	283	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	108	GLN
1	A	111	HIS
1	B	70	GLN
1	C	70	GLN
1	C	108	GLN
1	C	109	HIS

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Mol	Chain	Res	Type
1	D	108	GLN
1	D	136	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 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	333/344 (96%)	-0.41	6 (1%) 68 64	9, 21, 41, 50	0
1	B	332/344 (96%)	-0.05	6 (1%) 68 64	9, 31, 59, 72	0
1	C	333/344 (96%)	-0.27	7 (2%) 63 58	7, 26, 47, 56	0
1	D	337/344 (97%)	-0.36	0 100 100	8, 24, 42, 49	0
All	All	1335/1376 (97%)	-0.27	19 (1%) 75 71	7, 25, 49, 72	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	125	GLY	3.1
1	C	124	GLY	2.8
1	A	126	ASN	2.8
1	B	111	HIS	2.5
1	B	127	ASP	2.5
1	C	102	SER	2.4
1	B	62	GLU	2.4
1	A	124	GLY	2.4
1	C	99	PHE	2.4
1	C	193	ARG	2.3
1	C	126	ASN	2.3
1	B	120	ILE	2.2
1	B	124	GLY	2.2
1	A	125	GLY	2.2
1	C	101	ALA	2.2
1	B	125	GLY	2.1
1	A	115	ALA	2.1
1	A	123	PRO	2.0
1	A	79	GLU	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.