Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 12:48 am GMT

PDB ID	:	3N4X
Title	:	Structure of Csm1 full-length
Authors	:	Corbett, K.D.; Harrison, S.C.
Deposited on	:	2010-05-23
Resolution	:	3.41 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949
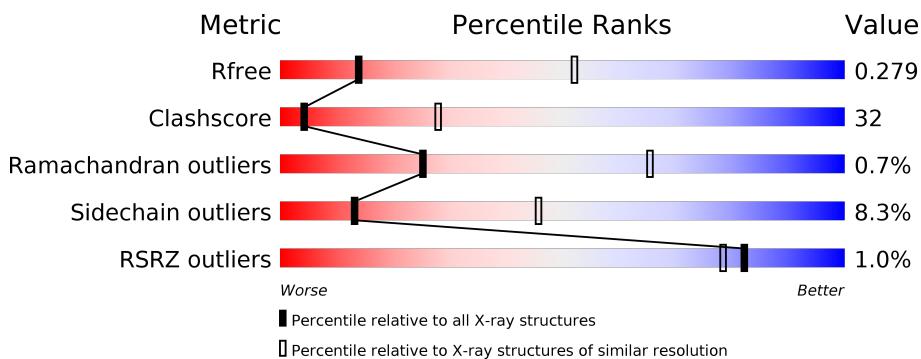
1　Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
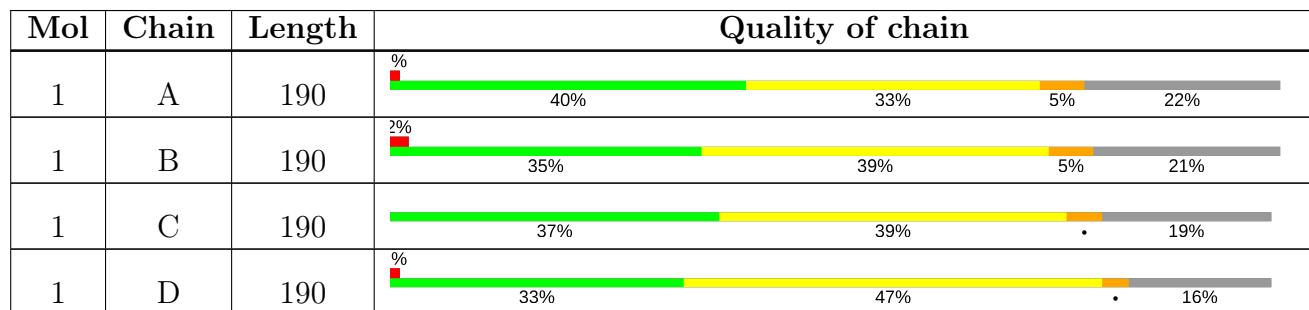
The reported resolution of this entry is 3.41 Å.

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	Percentile Ranks	Value
Rfree		0.279
Clashscore		32
Ramachandran outliers		0.7%
Sidechain outliers		8.3%
RSRZ outliers		1.0%

Worse ... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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	190	%　40%　33%　5%　22%
1	B	190	2%　35%　39%　5%　21%
1	C	190	37%　39%　•　19%
1	D	190	%　33%　47%　•　16%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 4949 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.
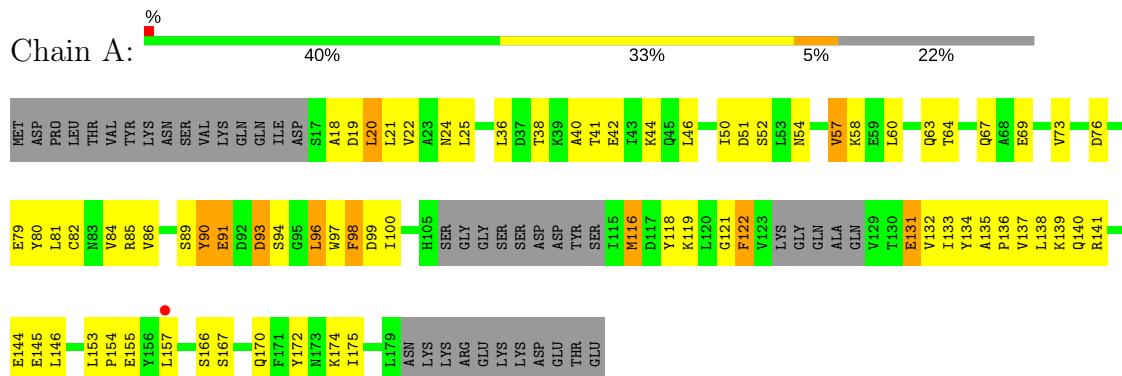
- Molecule 1 is a protein called Monopolin complex subunit CSM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1202	770	190	240	2			
1	B	151	Total	C	N	O	S	0	0	0
			1229	789	193	245	2			
1	C	153	Total	C	N	O	S	0	0	0
			1232	787	197	246	2			
1	D	159	Total	C	N	O	S	0	0	0
			1286	822	204	258	2			
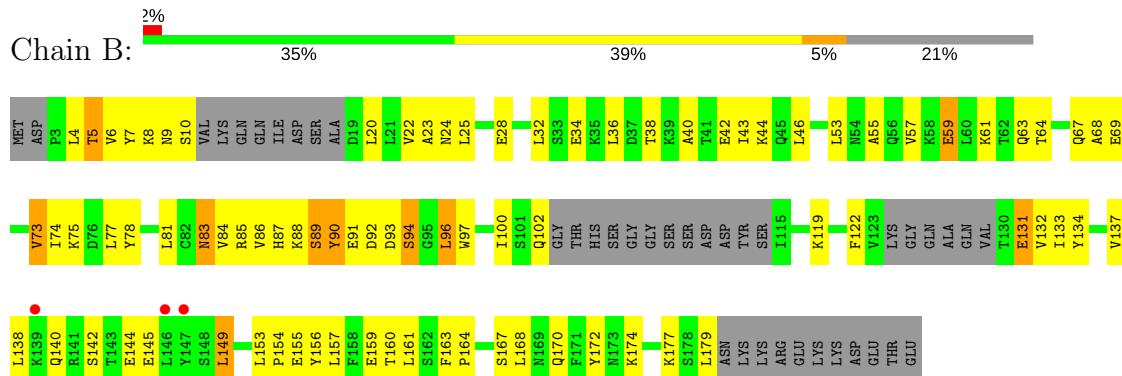
# 3 Residue-property plots ⓘ

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.
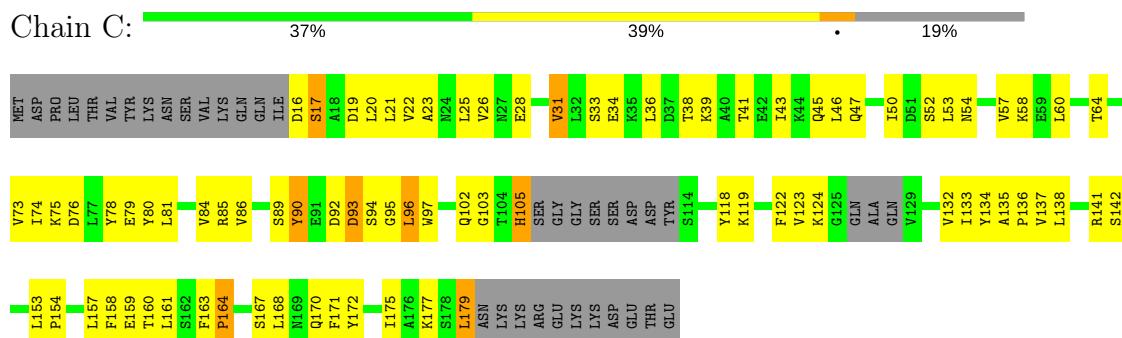
• Molecule 1: Monopolin complex subunit CSM1
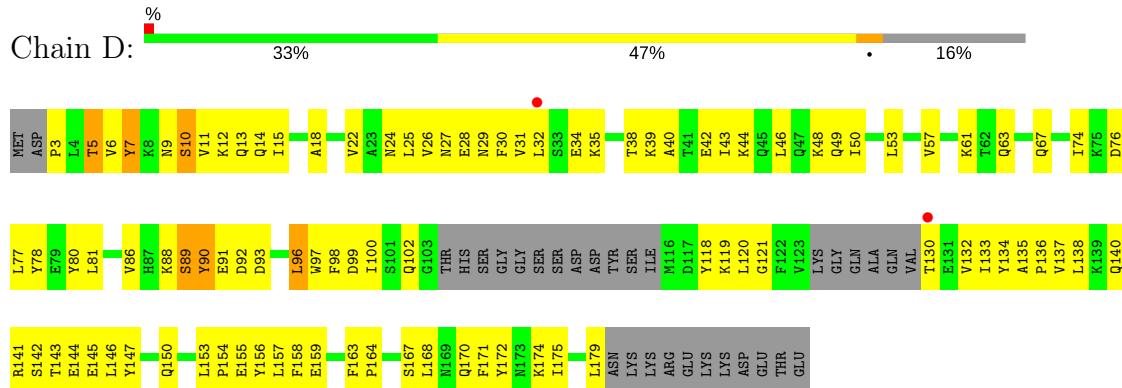
• Molecule 1: Monopolin complex subunit CSM1

• Molecule 1: Monopolin complex subunit CSM1

• Molecule 1: Monopolin complex subunit CSM1

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.27Å 105.27Å 234.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.04 – 3.41 49.35 – 3.41	Depositor EDS
% Data completeness (in resolution range)	78.6 (35.04-3.41) 78.5 (49.35-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.238 , 0.282 0.230 , 0.279	Depositor DCC
R_{free} test set	823 reflections (4.93%)	DCC
Wilson B-factor (Å^2)	125.8	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 83.6	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.086 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4949	wwPDB-VP
Average B, all atoms (Å^2)	164.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.59	0/1219	0.78	3/1646 (0.2%)
1	B	0.56	0/1247	0.71	2/1683 (0.1%)
1	C	0.49	0/1250	0.68	0/1686
1	D	0.46	0/1305	0.62	0/1762
All	All	0.53	0/5021	0.70	5/6777 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	LEU	CB-CG-CD1	-7.51	98.24	111.00
1	B	20	LEU	CB-CG-CD1	6.20	121.53	111.00
1	A	25	LEU	CA-CB-CG	6.07	129.26	115.30
1	B	149	LEU	CA-CB-CG	-5.67	102.26	115.30
1	A	20	LEU	CB-CG-CD1	-5.08	102.37	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	1202	0	1197	71	0
1	B	1229	0	1225	84	0
1	C	1232	0	1228	98	0
1	D	1286	0	1281	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4949	0	4931	318	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 32.

All (318) 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:A:81:LEU:HD11	1:B:172:TYR:HB2	1.29	1.11
1:C:172:TYR:HB2	1:D:81:LEU:HD11	1.42	1.01
1:C:81:LEU:HD11	1:D:172:TYR:HB2	1.45	0.95
1:C:54:ASN:O	1:C:58:LYS:HG2	1.71	0.89
1:B:96:LEU:H	1:B:96:LEU:HD12	1.34	0.88
1:B:9:ASN:HA	1:B:10:SER:HB2	1.54	0.87
1:C:79:GLU:OE2	1:C:85:ARG:HD2	1.75	0.86
1:C:57:VAL:HG22	1:D:57:VAL:HG22	1.58	0.85
1:C:90:TYR:CD2	1:C:97:TRP:HB2	2.13	0.84
1:D:88:LYS:HG2	1:D:89:SER:H	1.44	0.83
1:C:74:ILE:CG2	1:C:78:TYR:HE2	1.92	0.82
1:A:90:TYR:HB3	1:C:90:TYR:CE1	2.15	0.81
1:B:91:GLU:HG2	1:B:96:LEU:HB3	1.62	0.81
1:B:8:LYS:O	1:B:10:SER:HA	1.81	0.81
1:B:75:LYS:HG2	1:B:85:ARG:HE	1.46	0.81
1:A:97:TRP:C	1:A:98:PHE:HD2	1.85	0.79
1:B:69:GLU:OE1	1:B:69:GLU:HA	1.81	0.78
1:D:97:TRP:HB3	1:D:119:LYS:HE2	1.65	0.78
1:B:84:VAL:HG23	1:B:102:GLN:HB2	1.66	0.77
1:D:91:GLU:HG2	1:D:96:LEU:HB3	1.68	0.76
1:B:4:LEU:H	1:B:23:ALA:HB2	1.50	0.76
1:C:163:PHE:HB2	1:C:164:PRO:HD2	1.67	0.75
1:A:98:PHE:N	1:A:98:PHE:HD2	1.85	0.74
1:D:63:GLN:O	1:D:67:GLN:HG3	1.87	0.74
1:B:131:GLU:HG2	1:B:132:VAL:N	2.01	0.74
1:C:34:GLU:O	1:C:38:THR:HG23	1.87	0.74
1:D:99:ASP:O	1:D:100:ILE:HD13	1.87	0.73
1:A:81:LEU:HD11	1:B:172:TYR:CB	2.13	0.72
1:C:38:THR:O	1:C:41:THR:HG22	1.89	0.72
1:A:97:TRP:C	1:A:98:PHE:CD2	2.63	0.71
1:B:6:VAL:HG12	1:B:7:TYR:N	2.05	0.71
1:B:6:VAL:CG1	1:B:7:TYR:N	2.53	0.71
1:D:140:GLN:O	1:D:141:ARG:HG2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:VAL:O	1:D:15:ILE:HG13	1.89	0.71
1:B:42:GLU:O	1:B:46:LEU:HG	1.91	0.71
1:B:9:ASN:HA	1:B:10:SER:CB	2.20	0.71
1:C:172:TYR:HB2	1:D:81:LEU:CD1	2.20	0.70
1:A:172:TYR:HB2	1:B:81:LEU:HD11	1.72	0.70
1:D:88:LYS:HG2	1:D:89:SER:N	2.06	0.70
1:C:102:GLN:HE22	1:C:175:ILE:HG21	1.57	0.69
1:B:34:GLU:O	1:B:38:THR:HG23	1.92	0.69
1:D:89:SER:HB2	1:D:98:PHE:CE1	2.28	0.69
1:A:98:PHE:CD2	1:A:98:PHE:N	2.57	0.69
1:B:22:VAL:HA	1:B:25:LEU:HD12	1.75	0.69
1:D:96:LEU:HD13	1:D:98:PHE:CE2	2.28	0.69
1:B:81:LEU:O	1:B:81:LEU:HD12	1.94	0.68
1:D:26:VAL:HG12	1:D:30:PHE:HE2	1.58	0.68
1:C:76:ASP:O	1:C:80:TYR:HD2	1.78	0.67
1:D:7:TYR:C	1:D:7:TYR:CD2	2.68	0.67
1:D:27:ASN:O	1:D:31:VAL:HG23	1.95	0.67
1:B:6:VAL:O	1:B:7:TYR:CD1	2.49	0.66
1:D:34:GLU:O	1:D:38:THR:HG22	1.94	0.66
1:A:153:LEU:HD22	1:A:157:LEU:HD12	1.78	0.66
1:C:53:LEU:O	1:C:57:VAL:HG23	1.96	0.65
1:B:154:PRO:HD2	1:B:157:LEU:HD12	1.79	0.65
1:D:156:TYR:OH	1:D:174:LYS:CD	2.45	0.65
1:B:154:PRO:HD2	1:B:157:LEU:CD1	2.27	0.65
1:D:44:LYS:HE3	1:D:48:LYS:HE3	1.79	0.64
1:D:7:TYR:C	1:D:7:TYR:HD2	2.00	0.64
1:D:76:ASP:O	1:D:80:TYR:CD2	2.50	0.64
1:C:74:ILE:HG23	1:C:78:TYR:HE2	1.63	0.64
1:D:10:SER:OG	1:D:11:VAL:N	2.28	0.64
1:A:141:ARG:HD2	1:A:146:LEU:HG	1.79	0.64
1:A:38:THR:O	1:A:41:THR:HG22	1.98	0.64
1:D:3:PRO:O	1:D:6:VAL:HG12	1.98	0.63
1:D:24:ASN:O	1:D:28:GLU:HG3	1.99	0.63
1:B:96:LEU:N	1:B:96:LEU:HD12	2.08	0.62
1:A:122:PHE:CD2	1:A:122:PHE:N	2.67	0.62
1:D:153:LEU:HD22	1:D:157:LEU:HD13	1.82	0.62
1:D:49:GLN:O	1:D:53:LEU:HG	2.00	0.62
1:B:59:GLU:HB2	1:C:105:HIS:CE1	2.35	0.62
1:D:42:GLU:O	1:D:46:LEU:HG	2.00	0.61
1:D:147:TYR:HA	1:D:150:GLN:HG3	1.83	0.61
1:D:26:VAL:HG12	1:D:30:PHE:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:TYR:O	1:B:160:THR:HG23	2.01	0.61
1:B:40:ALA:O	1:B:43:ILE:HG22	2.01	0.61
1:D:147:TYR:O	1:D:150:GLN:HG3	2.01	0.61
1:B:4:LEU:HD23	1:B:5:THR:N	2.15	0.61
1:D:34:GLU:HG3	1:D:35:LYS:N	2.15	0.61
1:C:153:LEU:HD22	1:C:157:LEU:HD12	1.83	0.60
1:A:137:VAL:O	1:A:138:LEU:HD23	2.01	0.60
1:B:59:GLU:HA	1:C:105:HIS:CE1	2.37	0.60
1:A:69:GLU:O	1:A:73:VAL:HG23	2.01	0.60
1:C:39:LYS:NZ	1:D:40:ALA:HB2	2.17	0.60
1:A:20:LEU:HD23	1:A:24:ASN:HD21	1.66	0.59
1:C:167:SER:O	1:C:170:GLN:HG3	2.02	0.59
1:C:78:TYR:CD1	1:D:78:TYR:CE1	2.90	0.59
1:A:76:ASP:O	1:A:80:TYR:CD2	2.56	0.59
1:C:22:VAL:O	1:C:26:VAL:HG23	2.03	0.59
1:A:170:GLN:O	1:A:174:LYS:HG3	2.03	0.59
1:A:42:GLU:O	1:A:46:LEU:HG	2.03	0.59
1:A:131:GLU:HG2	1:A:132:VAL:N	2.17	0.59
1:D:31:VAL:O	1:D:34:GLU:HG2	2.03	0.59
1:A:91:GLU:CG	1:A:91:GLU:O	2.51	0.59
1:C:172:TYR:O	1:C:175:ILE:HG22	2.02	0.59
1:A:118:TYR:HA	1:A:137:VAL:HG23	1.85	0.58
1:A:79:GLU:OE2	1:A:85:ARG:NH2	2.35	0.58
1:C:54:ASN:O	1:C:58:LYS:CG	2.50	0.58
1:C:75:LYS:HG2	1:C:85:ARG:NH1	2.18	0.58
1:B:40:ALA:O	1:B:44:LYS:HG3	2.03	0.58
1:B:73:VAL:HG12	1:B:74:ILE:N	2.18	0.58
1:D:22:VAL:O	1:D:26:VAL:HG23	2.04	0.58
1:B:174:LYS:HD2	1:B:174:LYS:O	2.04	0.58
1:C:36:LEU:HD23	1:C:36:LEU:C	2.24	0.58
1:C:102:GLN:NE2	1:C:175:ILE:HD13	2.19	0.57
1:C:19:ASP:O	1:C:22:VAL:HG12	2.04	0.57
1:D:167:SER:O	1:D:170:GLN:HG3	2.05	0.57
1:D:3:PRO:N	1:D:5:THR:HG23	2.19	0.57
1:A:18:ALA:O	1:A:22:VAL:HG23	2.05	0.57
1:B:59:GLU:CA	1:C:105:HIS:CE1	2.89	0.56
1:C:90:TYR:CE2	1:C:97:TRP:HB2	2.41	0.56
1:B:132:VAL:HG12	1:B:133:ILE:N	2.21	0.56
1:B:6:VAL:O	1:B:7:TYR:HD1	1.89	0.56
1:D:44:LYS:O	1:D:48:LYS:HG3	2.06	0.56
1:D:76:ASP:O	1:D:80:TYR:HD2	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HB2	1:B:36:LEU:HD12	1.89	0.55
1:C:81:LEU:HD11	1:D:172:TYR:CB	2.30	0.55
1:A:144:GLU:HG3	1:A:145:GLU:HG3	1.89	0.55
1:D:156:TYR:OH	1:D:174:LYS:HD2	2.06	0.55
1:A:81:LEU:CD1	1:B:172:TYR:HB2	2.20	0.54
1:B:9:ASN:CA	1:B:10:SER:HB2	2.32	0.54
1:C:74:ILE:CG2	1:C:78:TYR:CE2	2.83	0.54
1:D:163:PHE:HB2	1:D:164:PRO:HD2	1.89	0.54
1:B:86:VAL:HG12	1:B:86:VAL:O	2.07	0.54
1:C:96:LEU:HD11	1:C:122:PHE:HB2	1.89	0.54
1:A:122:PHE:HD2	1:A:122:PHE:N	2.05	0.54
1:A:86:VAL:HG21	1:B:77:LEU:CD2	2.38	0.54
1:C:74:ILE:HG23	1:C:78:TYR:CE2	2.42	0.54
1:A:67:GLN:OE1	1:B:67:GLN:NE2	2.40	0.54
1:C:167:SER:HA	1:C:170:GLN:HE21	1.73	0.54
1:D:134:TYR:OH	1:D:157:LEU:O	2.18	0.54
1:C:81:LEU:HD13	1:D:168:LEU:HG	1.89	0.54
1:A:19:ASP:C	1:A:19:ASP:OD1	2.47	0.53
1:A:90:TYR:HB3	1:C:90:TYR:CD1	2.43	0.53
1:D:86:VAL:HG22	1:D:100:ILE:CD1	2.38	0.53
1:B:164:PRO:HG2	1:B:167:SER:OG	2.07	0.53
1:A:137:VAL:C	1:A:138:LEU:HD23	2.29	0.53
1:A:144:GLU:HG3	1:A:145:GLU:N	2.24	0.53
1:C:57:VAL:HG22	1:D:57:VAL:CG2	2.36	0.53
1:B:59:GLU:HA	1:C:105:HIS:HE1	1.74	0.53
1:C:54:ASN:HB3	1:C:58:LYS:HE2	1.91	0.53
1:C:74:ILE:HG22	1:C:78:TYR:HE2	1.74	0.52
1:D:34:GLU:CG	1:D:35:LYS:N	2.72	0.52
1:A:167:SER:O	1:A:170:GLN:HG3	2.10	0.52
1:B:43:ILE:CG2	1:B:44:LYS:N	2.72	0.52
1:C:78:TYR:CD1	1:D:78:TYR:CD1	2.97	0.52
1:B:96:LEU:CD1	1:B:122:PHE:HB2	2.40	0.52
1:A:89:SER:HA	1:A:97:TRP:O	2.10	0.52
1:D:167:SER:HA	1:D:170:GLN:HG3	1.92	0.52
1:C:46:LEU:HD22	1:D:50:ILE:CD1	2.40	0.52
1:B:67:GLN:HG3	1:B:68:ALA:N	2.25	0.51
1:A:132:VAL:HG12	1:A:133:ILE:N	2.25	0.51
1:C:39:LYS:HZ3	1:D:40:ALA:HB2	1.74	0.51
1:C:96:LEU:O	1:C:96:LEU:HD12	2.10	0.51
1:A:116:MET:HE1	1:A:136:PRO:HB3	1.92	0.51
1:A:76:ASP:O	1:A:80:TYR:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:CYS:HB3	1:A:84:VAL:HG12	1.93	0.51
1:C:45:GLN:CG	1:C:46:LEU:N	2.74	0.51
1:D:35:LYS:O	1:D:39:LYS:HG2	2.10	0.51
1:D:40:ALA:O	1:D:43:ILE:HG22	2.10	0.51
1:A:40:ALA:O	1:A:44:LYS:HG3	2.09	0.51
1:C:96:LEU:CD1	1:C:122:PHE:HB2	2.41	0.51
1:A:63:GLN:O	1:A:67:GLN:HB2	2.11	0.51
1:D:167:SER:C	1:D:170:GLN:HG3	2.31	0.51
1:D:90:TYR:C	1:D:91:GLU:HG3	2.31	0.51
1:A:54:ASN:OD1	1:B:53:LEU:HD21	2.10	0.51
1:B:119:LYS:HG3	1:B:137:VAL:HG21	1.93	0.51
1:C:163:PHE:HB2	1:C:164:PRO:CD	2.38	0.51
1:D:88:LYS:HD3	1:D:90:TYR:CE1	2.46	0.51
1:A:172:TYR:HB2	1:B:81:LEU:CD1	2.39	0.51
1:B:57:VAL:O	1:B:61:LYS:HG3	2.11	0.51
1:A:81:LEU:O	1:A:81:LEU:HG	2.08	0.50
1:B:59:GLU:CB	1:C:105:HIS:CE1	2.94	0.50
1:C:154:PRO:HD2	1:C:157:LEU:HD12	1.94	0.50
1:C:103:GLY:HA2	1:C:179:LEU:HD23	1.93	0.50
1:D:97:TRP:CZ3	1:D:121:GLY:HA3	2.47	0.50
1:B:163:PHE:HB2	1:B:164:PRO:HD2	1.94	0.50
1:B:43:ILE:HG23	1:B:44:LYS:N	2.25	0.50
1:C:16:ASP:O	1:C:20:LEU:HG	2.12	0.50
1:A:121:GLY:C	1:A:122:PHE:CD2	2.86	0.50
1:D:88:LYS:CG	1:D:89:SER:H	2.19	0.50
1:B:137:VAL:O	1:B:138:LEU:HD23	2.12	0.49
1:C:102:GLN:NE2	1:C:175:ILE:HG21	2.24	0.49
1:C:28:GLU:O	1:C:31:VAL:HG12	2.12	0.49
1:C:54:ASN:O	1:C:58:LYS:HE2	2.12	0.49
1:B:6:VAL:CG1	1:B:7:TYR:H	2.25	0.49
1:B:90:TYR:HD2	1:B:97:TRP:HB2	1.77	0.49
1:B:90:TYR:CD2	1:B:97:TRP:HB2	2.46	0.49
1:C:118:TYR:HA	1:C:137:VAL:HG23	1.95	0.49
1:D:9:ASN:O	1:D:13:GLN:NE2	2.46	0.49
1:A:86:VAL:O	1:A:86:VAL:HG12	2.11	0.49
1:D:90:TYR:HE2	1:D:119:LYS:HE3	1.78	0.49
1:C:22:VAL:HG13	1:C:23:ALA:N	2.28	0.48
1:A:79:GLU:HB2	1:A:85:ARG:HG3	1.94	0.48
1:C:89:SER:HA	1:C:97:TRP:O	2.13	0.48
1:D:156:TYR:OH	1:D:174:LYS:HD3	2.14	0.48
1:D:89:SER:HA	1:D:97:TRP:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:TYR:CG	1:A:135:ALA:N	2.82	0.48
1:A:60:LEU:O	1:A:64:THR:HG23	2.14	0.48
1:C:134:TYR:O	1:C:160:THR:HG23	2.13	0.48
1:C:167:SER:HA	1:C:170:GLN:HG3	1.94	0.48
1:C:43:ILE:O	1:C:47:GLN:HG3	2.14	0.48
1:D:88:LYS:CG	1:D:89:SER:N	2.75	0.48
1:C:81:LEU:HD12	1:C:81:LEU:O	2.13	0.48
1:C:132:VAL:HG12	1:C:133:ILE:N	2.28	0.48
1:C:158:PHE:C	1:C:159:GLU:HG3	2.33	0.47
1:D:147:TYR:HA	1:D:150:GLN:CG	2.43	0.47
1:C:57:VAL:CG2	1:D:57:VAL:HG22	2.39	0.47
1:A:91:GLU:HB2	1:A:96:LEU:HD23	1.95	0.47
1:B:153:LEU:HD22	1:B:157:LEU:HD13	1.97	0.47
1:B:154:PRO:O	1:B:155:GLU:C	2.53	0.47
1:B:132:VAL:CG1	1:B:133:ILE:N	2.76	0.47
1:B:77:LEU:HG	1:B:78:TYR:N	2.29	0.47
1:C:168:LEU:O	1:C:171:PHE:HB3	2.14	0.46
1:D:134:TYR:CG	1:D:135:ALA:N	2.83	0.46
1:A:90:TYR:OH	1:A:119:LYS:NZ	2.41	0.46
1:D:136:PRO:HG2	1:D:158:PHE:C	2.36	0.46
1:D:92:ASP:OD1	1:D:97:TRP:NE1	2.47	0.46
1:C:137:VAL:O	1:C:138:LEU:HD23	2.16	0.46
1:C:167:SER:C	1:C:170:GLN:HG3	2.35	0.46
1:C:17:SER:O	1:C:21:LEU:HD23	2.15	0.46
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.61	0.46
1:A:167:SER:HA	1:A:170:GLN:HG3	1.98	0.46
1:D:9:ASN:HB3	1:D:13:GLN:NE2	2.31	0.46
1:A:91:GLU:HG3	1:A:91:GLU:O	2.15	0.46
1:C:103:GLY:CA	1:C:179:LEU:HD23	2.46	0.46
1:D:44:LYS:HE3	1:D:48:LYS:CE	2.43	0.46
1:B:137:VAL:C	1:B:138:LEU:HD23	2.37	0.45
1:A:119:LYS:HG3	1:A:137:VAL:HG21	1.98	0.45
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.75	0.45
1:A:57:VAL:HG12	1:A:58:LYS:N	2.31	0.45
1:B:144:GLU:HG3	1:B:145:GLU:N	2.30	0.45
1:A:154:PRO:O	1:A:155:GLU:C	2.54	0.45
1:B:86:VAL:HG22	1:B:100:ILE:HD13	1.98	0.45
1:D:3:PRO:C	1:D:5:THR:N	2.69	0.45
1:C:123:VAL:C	1:C:124:LYS:HG3	2.37	0.45
1:C:60:LEU:O	1:C:64:THR:HG22	2.17	0.45
1:C:78:TYR:HD1	1:D:78:TYR:CE1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLU:O	1:B:32:LEU:HD13	2.17	0.45
1:D:28:GLU:O	1:D:32:LEU:HG	2.16	0.45
1:A:140:GLN:HG2	1:A:140:GLN:O	2.16	0.45
1:D:44:LYS:HD2	1:D:44:LYS:HA	1.61	0.45
1:C:54:ASN:C	1:C:58:LYS:HE2	2.37	0.45
1:D:57:VAL:HG12	1:D:61:LYS:HE3	1.99	0.45
1:A:36:LEU:HD12	1:B:36:LEU:HB2	1.98	0.45
1:C:84:VAL:O	1:C:84:VAL:HG13	2.17	0.45
1:B:89:SER:HA	1:B:97:TRP:O	2.16	0.44
1:D:86:VAL:HG22	1:D:100:ILE:HD12	1.99	0.44
1:B:168:LEU:HD12	1:B:168:LEU:HA	1.71	0.44
1:A:19:ASP:O	1:A:19:ASP:OD1	2.35	0.44
1:C:153:LEU:HA	1:C:154:PRO:HD3	1.84	0.44
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.70	0.44
1:A:93:ASP:HB2	1:A:94:SER:H	1.59	0.44
1:C:119:LYS:HG3	1:C:135:ALA:HB3	2.00	0.44
1:D:96:LEU:HD13	1:D:98:PHE:HE2	1.76	0.44
1:D:97:TRP:CB	1:D:119:LYS:HE2	2.41	0.44
1:A:90:TYR:CD2	1:A:90:TYR:N	2.85	0.44
1:D:137:VAL:O	1:D:138:LEU:HD23	2.18	0.44
1:C:93:ASP:HB3	1:C:94:SER:H	1.59	0.44
1:B:177:LYS:HA	1:B:177:LYS:HD3	1.65	0.43
1:C:75:LYS:HG2	1:C:85:ARG:HH12	1.83	0.43
1:A:50:ILE:HG22	1:A:51:ASP:N	2.33	0.43
1:C:74:ILE:O	1:C:78:TYR:HD2	2.01	0.43
1:D:92:ASP:O	1:D:92:ASP:CG	2.56	0.43
1:C:75:LYS:HG2	1:C:85:ARG:CZ	2.48	0.43
1:B:179:LEU:HD12	1:B:179:LEU:HA	1.78	0.43
1:C:76:ASP:O	1:C:80:TYR:CD2	2.65	0.43
1:C:132:VAL:CG1	1:C:133:ILE:N	2.82	0.43
1:C:90:TYR:CE2	1:C:97:TRP:CB	3.01	0.43
1:C:90:TYR:HD2	1:C:97:TRP:HB2	1.74	0.43
1:C:86:VAL:HG21	1:D:77:LEU:HD23	2.00	0.43
1:A:90:TYR:OH	1:A:119:LYS:HD3	2.19	0.42
1:A:139:LYS:HB3	1:A:140:GLN:OE1	2.18	0.42
1:A:60:LEU:HA	1:A:60:LEU:HD12	1.62	0.42
1:B:149:LEU:HD23	1:B:149:LEU:HA	1.69	0.42
1:D:143:THR:O	1:D:147:TYR:HD2	2.02	0.42
1:B:64:THR:HA	1:B:67:GLN:HG2	2.00	0.42
1:B:144:GLU:HG3	1:B:145:GLU:HG3	2.00	0.42
1:B:83:ASN:HD22	1:B:83:ASN:HA	1.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:TYR:O	1:B:161:LEU:HD11	2.20	0.42
1:D:144:GLU:HG3	1:D:145:GLU:N	2.33	0.42
1:B:91:GLU:CG	1:B:96:LEU:HB3	2.42	0.42
1:A:99:ASP:C	1:A:100:ILE:HG12	2.40	0.42
1:C:17:SER:O	1:C:21:LEU:CD2	2.68	0.42
1:C:92:ASP:O	1:C:94:SER:N	2.53	0.42
1:D:154:PRO:O	1:D:155:GLU:C	2.57	0.42
1:B:87:HIS:C	1:B:88:LYS:HD2	2.41	0.42
1:B:69:GLU:OE1	1:B:69:GLU:CA	2.57	0.42
1:B:92:ASP:O	1:B:94:SER:N	2.53	0.42
1:D:132:VAL:HG12	1:D:133:ILE:N	2.34	0.42
1:D:29:ASN:OD1	1:D:29:ASN:O	2.38	0.42
1:C:159:GLU:O	1:C:161:LEU:HG	2.20	0.41
1:D:40:ALA:C	1:D:43:ILE:HG22	2.40	0.41
1:A:82:CYS:CB	1:A:84:VAL:HG12	2.50	0.41
1:C:136:PRO:HG2	1:C:158:PHE:C	2.41	0.41
1:D:167:SER:CA	1:D:170:GLN:HG3	2.50	0.41
1:D:118:TYR:HA	1:D:137:VAL:HG23	2.02	0.41
1:D:14:GLN:O	1:D:18:ALA:CB	2.68	0.41
1:D:25:LEU:HD23	1:D:25:LEU:HA	1.77	0.41
1:D:43:ILE:HG23	1:D:44:LYS:N	2.36	0.41
1:A:141:ARG:HD2	1:A:146:LEU:CG	2.49	0.41
1:A:99:ASP:OD1	1:A:119:LYS:HE2	2.20	0.41
1:B:142:SER:N	1:B:145:GLU:OE1	2.53	0.41
1:C:46:LEU:O	1:C:50:ILE:HG13	2.21	0.41
1:D:120:LEU:HD23	1:D:120:LEU:HA	1.87	0.41
1:B:6:VAL:HG13	1:B:7:TYR:H	1.85	0.41
1:D:171:PHE:CE2	1:D:175:ILE:HD11	2.56	0.41
1:D:86:VAL:HG12	1:D:86:VAL:O	2.20	0.41
1:B:167:SER:HA	1:B:170:GLN:HG3	2.03	0.41
1:B:24:ASN:O	1:B:28:GLU:CB	2.69	0.41
1:C:177:LYS:HA	1:C:177:LYS:HD3	1.74	0.40
1:C:95:GLY:HA2	1:C:122:PHE:O	2.22	0.40
1:D:74:ILE:O	1:D:77:LEU:HB3	2.21	0.40
1:B:55:ALA:HB1	1:C:105:HIS:HB3	2.03	0.40
1:C:31:VAL:O	1:C:34:GLU:HG2	2.22	0.40
1:D:102:GLN:NE2	1:D:118:TYR:OH	2.54	0.40
1:B:90:TYR:O	1:B:96:LEU:HA	2.21	0.40
1:C:73:VAL:HG12	1:C:74:ILE:N	2.35	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	143/190 (75%)	134 (94%)	8 (6%)	1 (1%)	25	65
1	B	143/190 (75%)	129 (90%)	13 (9%)	1 (1%)	25	65
1	C	147/190 (77%)	136 (92%)	10 (7%)	1 (1%)	25	65
1	D	153/190 (80%)	141 (92%)	11 (7%)	1 (1%)	25	65
All	All	586/760 (77%)	540 (92%)	42 (7%)	4 (1%)	25	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	93	ASP
1	A	93	ASP
1	D	93	ASP
1	C	93	ASP

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	137/176 (78%)	125 (91%)	12 (9%)	12	42
1	B	142/176 (81%)	130 (92%)	12 (8%)	12	45
1	C	141/176 (80%)	130 (92%)	11 (8%)	15	49
1	D	148/176 (84%)	136 (92%)	12 (8%)	14	47
All	All	568/704 (81%)	521 (92%)	47 (8%)	13	46

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

Mol	Chain	Res	Type
1	A	21	LEU
1	A	52	SER
1	A	57	VAL
1	A	90	TYR
1	A	91	GLU
1	A	96	LEU
1	A	98	PHE
1	A	116	MET
1	A	122	PHE
1	A	131	GLU
1	A	166	SER
1	A	175	ILE
1	B	5	THR
1	B	59	GLU
1	B	63	GLN
1	B	73	VAL
1	B	83	ASN
1	B	89	SER
1	B	90	TYR
1	B	94	SER
1	B	96	LEU
1	B	131	GLU
1	B	140	GLN
1	B	159	GLU
1	C	17	SER
1	C	31	VAL
1	C	33	SER
1	C	52	SER
1	C	90	TYR
1	C	96	LEU
1	C	105	HIS
1	C	141	ARG
1	C	142	SER
1	C	164	PRO
1	C	179	LEU
1	D	5	THR
1	D	7	TYR
1	D	10	SER
1	D	12	LYS
1	D	89	SER
1	D	90	TYR
1	D	96	LEU

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Mol	Chain	Res	Type
1	D	130	THR
1	D	142	SER
1	D	146	LEU
1	D	159	GLU
1	D	179	LEU

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

Mol	Chain	Res	Type
1	A	24	ASN
1	A	83	ASN
1	A	102	GLN
1	B	67	GLN
1	B	83	ASN
1	C	102	GLN
1	C	105	HIS
1	D	13	GLN
1	D	83	ASN
1	D	102	GLN
1	D	169	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	149/190 (78%)	-0.09	1 (0%)	87	85	106, 152, 220, 262	0
1	B	151/190 (79%)	-0.06	3 (1%)	65	61	97, 161, 222, 268	0
1	C	153/190 (80%)	-0.18	0	100	100	98, 161, 217, 248	0
1	D	159/190 (83%)	-0.15	2 (1%)	77	73	108, 169, 227, 267	0
All	All	612/760 (80%)	-0.12	6 (0%)	82	78	97, 162, 222, 268	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	LYS	3.0
1	D	130	THR	2.6
1	B	146	LEU	2.5
1	A	157	LEU	2.5
1	B	147	TYR	2.4
1	D	32	LEU	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 (i)

There are no such residues in this entry.