



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:03 PM UTC

PDB ID : 5L2Q / pdb_00005l2q
Title : Serine/threonine-protein kinase 40 (STK40) kinase homology domain
Authors : Durzynska, I.; Uljon, S.; Blacklow, S.C.
Deposited on : 2016-08-02
Resolution : 2.53 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

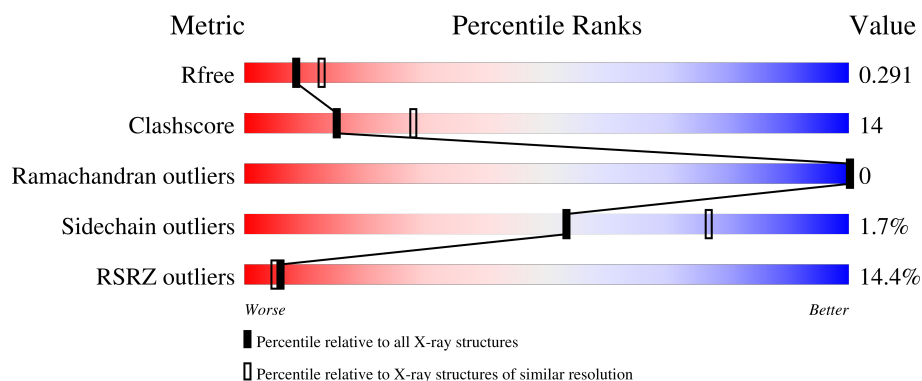
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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 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 $\leq 5\%$. 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	320	5% 64% 27% 8%
1	B	320	10% 66% 21% 12%
1	C	320	17% 66% 21% 12%
1	D	320	19% 67% 22% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8350 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 Serine/threonine-protein kinase 40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	282	Total	C	N	O	S	5	1	0
			2023	1298	352	362	11			
1	B	282	Total	C	N	O	S	0	0	0
			2072	1320	361	381	10			
1	A	293	Total	C	N	O	S	0	0	0
			2166	1394	376	386	10			
1	D	294	Total	C	N	O	S	0	0	0
			2023	1273	358	381	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	expression tag	UNP Q8N2I9
A	21	SER	-	expression tag	UNP Q8N2I9
B	20	GLY	-	expression tag	UNP Q8N2I9
B	21	SER	-	expression tag	UNP Q8N2I9
C	20	GLY	-	expression tag	UNP Q8N2I9
C	21	SER	-	expression tag	UNP Q8N2I9
D	20	GLY	-	expression tag	UNP Q8N2I9
D	21	SER	-	expression tag	UNP Q8N2I9

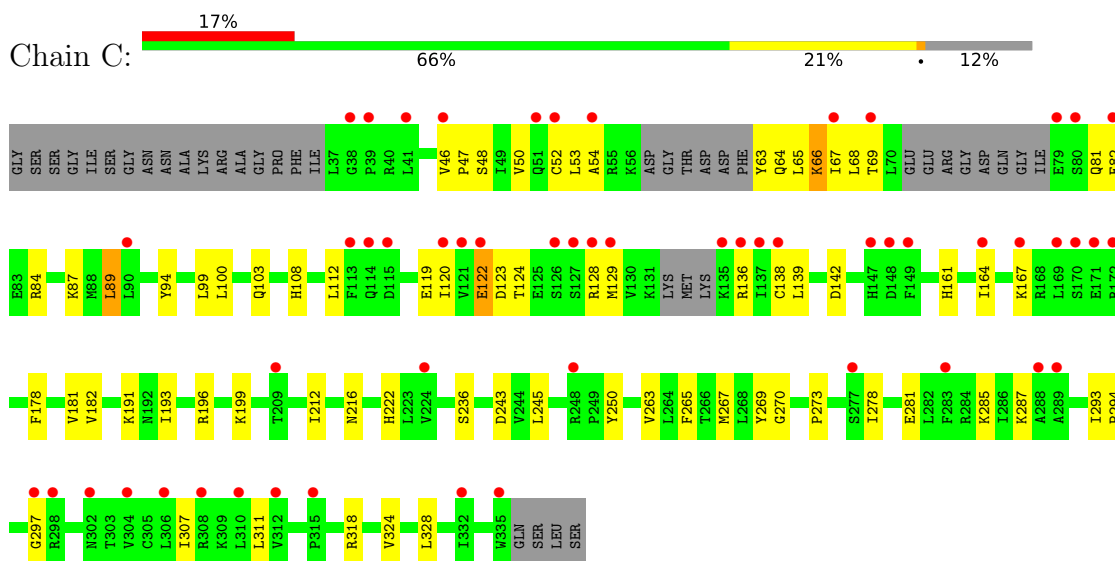
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	16	Total	O	0	0
			16	16		
2	B	17	Total	O	0	0
			17	17		
2	A	20	Total	O	0	0
			20	20		
2	D	13	Total	O	0	0
			13	13		

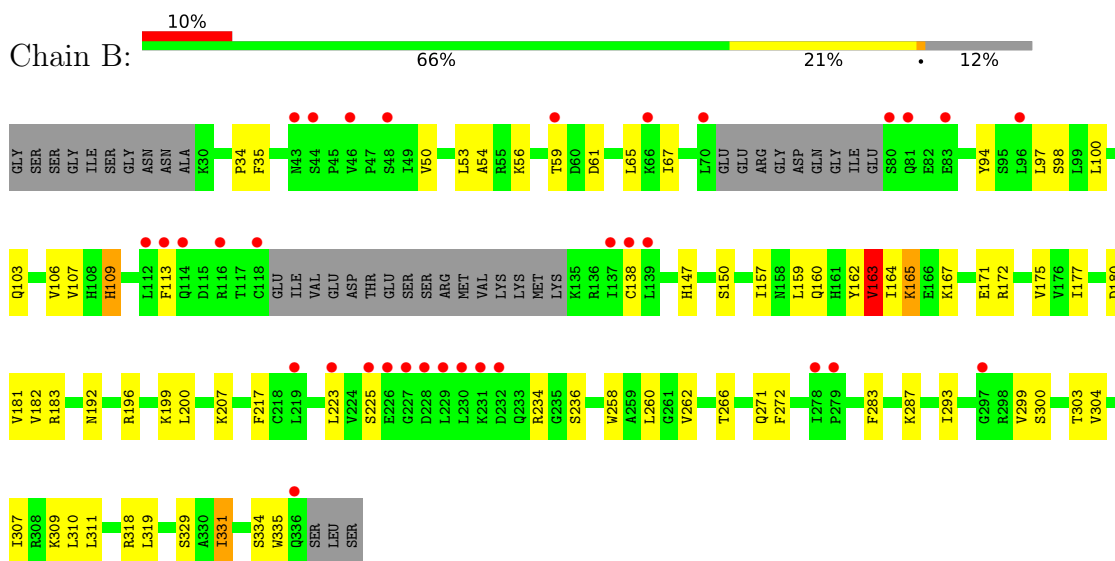
3 Residue-property plots

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.

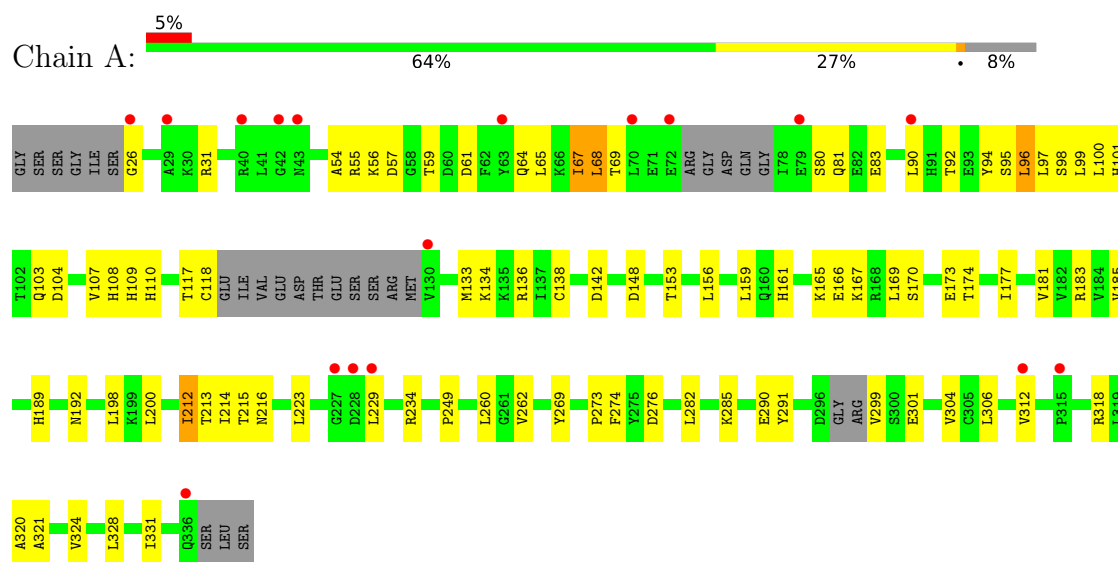
- Molecule 1: Serine/threonine-protein kinase 40



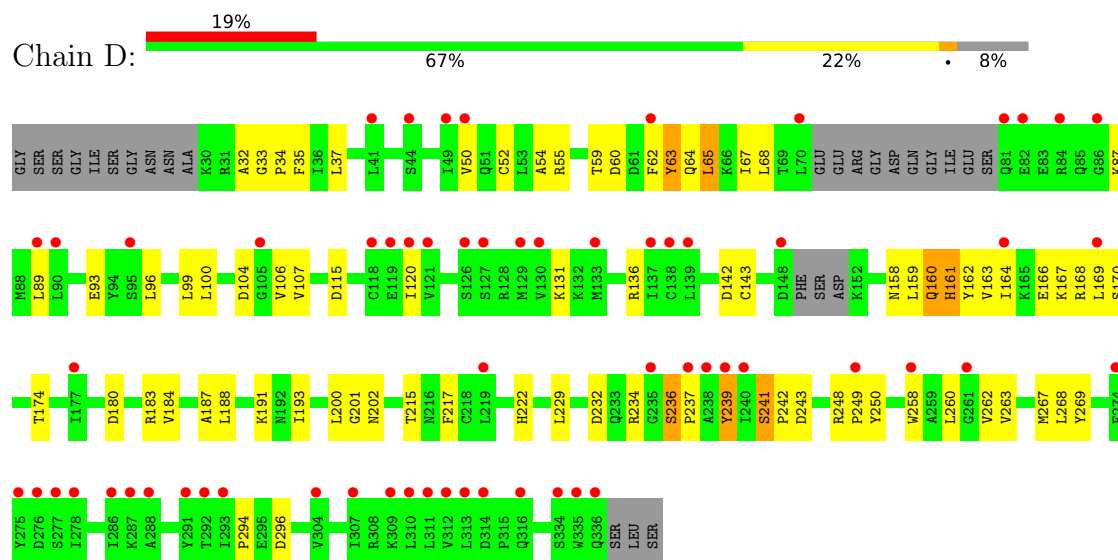
- Molecule 1: Serine/threonine-protein kinase 40



- Molecule 1: Serine/threonine-protein kinase 40



• Molecule 1: Serine/threonine-protein kinase 40



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.55Å 237.65Å 55.61Å 90.00° 106.32° 90.00°	Depositor
Resolution (Å)	59.41 – 2.53 59.41 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.6 (59.41-2.53) 98.6 (59.41-2.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	47.95 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.258 , 0.280 0.269 , 0.291	Depositor DCC
R_{free} test set	2383 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.043 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8350	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.76	8/2208 (0.4%)	0.55	3/3005 (0.1%)
1	B	0.67	4/2114 (0.2%)	0.49	1/2882 (0.0%)
1	C	0.43	3/2058 (0.1%)	0.54	4/2810 (0.1%)
1	D	0.52	0/2060	0.65	9/2828 (0.3%)
All	All	0.61	15/8440 (0.2%)	0.56	17/11525 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	TYR	C-O	-6.77	1.15	1.24
1	A	95	SER	C-O	-6.13	1.17	1.24
1	A	67	ILE	C-O	-6.12	1.17	1.24
1	A	214	ILE	C-O	-6.01	1.17	1.24
1	A	215	THR	C-O	-5.97	1.15	1.23
1	A	216	ASN	CA-C	-5.85	1.47	1.53
1	C	89	LEU	N-CA	-5.71	1.39	1.46
1	A	101	HIS	C-O	-5.68	1.16	1.24
1	A	98	SER	C-O	-5.34	1.17	1.24
1	A	67	ILE	CA-C	-5.17	1.46	1.52
1	C	87	LYS	C-O	-5.15	1.18	1.24
1	B	167	LYS	C-O	-5.09	1.17	1.24
1	B	165	LYS	C-O	-5.09	1.18	1.24
1	B	163	VAL	C-O	-5.06	1.17	1.24
1	C	89	LEU	C-O	-5.04	1.18	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	THR	N-CA-C	7.27	118.90	110.97
1	A	212	ILE	N-CA-C	6.22	118.70	108.99
1	A	101	HIS	N-CA-C	6.11	119.84	112.38
1	D	241	SER	CA-C-N	6.02	127.36	119.84
1	D	241	SER	C-N-CA	6.02	127.36	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	GLN	CA-C-N	-5.86	112.83	120.44
1	D	160	GLN	C-N-CA	-5.86	112.83	120.44
1	D	236	SER	CA-C-N	5.71	125.39	119.05
1	D	236	SER	C-N-CA	5.71	125.39	119.05
1	C	89	LEU	N-CA-C	-5.56	105.13	111.14
1	C	123	ASP	N-CA-C	-5.56	100.18	109.24
1	D	239	TYR	N-CA-C	5.50	118.20	111.82
1	D	241	SER	N-CA-C	5.46	121.87	109.81
1	C	122	GLU	N-CA-C	-5.16	99.81	110.80
1	D	161	HIS	N-CA-C	-5.16	105.55	111.07
1	A	100	LEU	N-CA-C	5.08	119.44	112.88
1	B	331	ILE	CB-CA-C	-5.01	105.31	112.22

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	2166	0	2083	56	0
1	B	2072	0	1932	54	0
1	C	2023	0	1873	46	0
1	D	2023	0	1718	61	0
2	A	20	0	0	3	0
2	B	17	0	0	2	0
2	C	16	0	0	0	0
2	D	13	0	0	1	0
All	All	8350	0	7606	216	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 14.

All (216) 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:D:241:SER:CB	1:D:242:PRO:CD	2.19	1.16
1:B:303:THR:HG22	1:B:331:ILE:HD13	1.38	1.06
1:B:94:TYR:CE1	1:B:109:HIS:HE1	1.78	1.01
1:D:241:SER:CB	1:D:242:PRO:HD2	1.91	1.00
1:D:241:SER:CB	1:D:242:PRO:HD3	1.94	0.97
1:A:177:ILE:CG2	1:A:212:ILE:HD11	1.98	0.94
1:A:177:ILE:HG23	1:A:212:ILE:HD11	1.52	0.91
1:B:192:ASN:HB3	1:B:223:LEU:HB2	1.52	0.91
1:D:239:TYR:HD1	1:D:262:VAL:CG2	1.85	0.89
1:D:63:TYR:HA	1:D:143:CYS:HB2	1.55	0.87
1:A:229:LEU:HD21	1:A:249:PRO:HB3	1.55	0.86
1:B:331:ILE:O	1:B:334:SER:OG	1.94	0.84
1:B:67:ILE:HD12	1:B:138:CYS:SG	2.18	0.84
1:B:175:VAL:CG2	1:B:335:TRP:HH2	1.91	0.83
1:D:100:LEU:HD23	1:D:106:VAL:HG11	1.60	0.82
1:B:94:TYR:CE1	1:B:109:HIS:CE1	2.67	0.81
1:B:94:TYR:CD1	1:B:109:HIS:CE1	2.68	0.80
1:D:166:GLU:HB2	1:D:169:LEU:HD21	1.63	0.78
1:D:239:TYR:HD1	1:D:262:VAL:HG23	1.47	0.78
1:B:165:LYS:HD2	1:A:148:ASP:O	1.84	0.77
1:A:92:THR:O	1:A:96:LEU:HD12	1.84	0.77
1:B:303:THR:HG22	1:B:331:ILE:CD1	2.13	0.77
1:B:59:THR:HG23	1:B:61:ASP:H	1.51	0.76
1:B:94:TYR:CD1	1:B:109:HIS:HE1	2.05	0.75
1:C:53:LEU:HA	1:C:64:GLN:HA	1.69	0.74
1:A:67:ILE:HG12	1:A:138:CYS:HB3	1.70	0.74
1:B:309:LYS:HB3	1:B:319:LEU:HD13	1.70	0.73
1:D:239:TYR:CD1	1:D:262:VAL:CG2	2.72	0.73
1:B:225:SER:O	2:B:401:HOH:O	2.06	0.72
1:D:168:ARG:HG3	1:D:269:TYR:HA	1.70	0.72
1:B:175:VAL:HG21	1:B:335:TRP:CH2	2.24	0.71
1:B:266:THR:HG22	1:B:272:PHE:HA	1.72	0.71
1:D:239:TYR:CD1	1:D:262:VAL:HG23	2.26	0.71
1:C:81:GLN:O	1:C:82:GLU:C	2.34	0.70
1:D:232:ASP:O	1:D:250:TYR:OH	2.07	0.70
1:B:175:VAL:CG2	1:B:335:TRP:CH2	2.74	0.69
1:C:245:LEU:HB3	1:C:287:LYS:HE2	1.73	0.69
1:C:52:CYS:O	1:C:65:LEU:N	2.24	0.68
1:C:243:ASP:OD2	1:C:318:ARG:NH2	2.26	0.68
1:A:177:ILE:HG23	1:A:212:ILE:CD1	2.23	0.67
1:C:167:LYS:O	1:C:270:GLY:HA3	1.95	0.67
1:A:159:LEU:HG	1:A:200:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:THR:HG23	1:A:61:ASP:H	1.61	0.66
1:C:112:LEU:HD13	1:C:139:LEU:HD13	1.77	0.66
1:D:239:TYR:HD1	1:D:262:VAL:HG21	1.61	0.66
1:D:260:LEU:HA	1:D:263:VAL:HG12	1.80	0.64
1:A:285:LYS:HG3	1:A:290:GLU:HB3	1.79	0.63
1:D:55:ARG:NH2	2:D:401:HOH:O	2.30	0.63
1:C:122:GLU:HA	1:C:129:MET:HE1	1.78	0.63
1:B:147:HIS:HE1	1:B:150:SER:HB3	1.62	0.63
1:D:239:TYR:CD1	1:D:262:VAL:HG21	2.34	0.63
1:A:117:THR:O	1:A:134:LYS:N	2.29	0.62
1:C:66:LYS:NZ	1:C:216:ASN:ND2	2.47	0.62
1:A:312:VAL:O	1:A:318:ARG:NH2	2.30	0.62
1:D:115:ASP:OD2	1:D:136:ARG:NH2	2.32	0.62
1:D:50:VAL:HG13	1:D:67:ILE:HB	1.81	0.62
1:B:271:GLN:NE2	2:B:404:HOH:O	2.32	0.61
1:C:128:ARG:H	1:C:128:ARG:HD3	1.65	0.61
1:B:157:ILE:HB	1:B:207:LYS:HE2	1.82	0.61
1:A:31:ARG:NH2	1:A:57:ASP:OD2	2.34	0.60
1:D:166:GLU:CB	1:D:169:LEU:HD21	2.30	0.60
1:C:196:ARG:NH2	1:C:250:TYR:OH	2.34	0.60
1:A:328:LEU:HA	1:A:331:ILE:HD12	1.83	0.60
1:A:177:ILE:CG2	1:A:212:ILE:CD1	2.76	0.59
1:B:160:GLN:O	1:B:164:ILE:HG13	2.02	0.59
1:D:200:LEU:HG	1:D:263:VAL:HG23	1.83	0.59
1:D:35:PHE:HD2	1:D:65:LEU:HD11	1.68	0.59
1:C:69:THR:HA	1:C:136:ARG:HG2	1.85	0.58
1:C:112:LEU:HD12	1:C:138:CYS:O	2.04	0.58
1:C:263:VAL:O	1:C:267:MET:HG3	2.04	0.58
1:B:59:THR:HG23	1:B:61:ASP:N	2.19	0.58
1:D:161:HIS:O	1:D:164:ILE:HG12	2.04	0.57
1:A:169:LEU:HD22	1:A:173:GLU:OE2	2.05	0.56
1:C:81:GLN:O	1:C:84:ARG:N	2.38	0.56
1:D:55:ARG:NH1	1:D:59:THR:O	2.38	0.56
1:D:229:LEU:HA	1:D:250:TYR:O	2.04	0.56
1:C:199:LYS:NZ	1:C:236:SER:OG	2.37	0.56
1:B:307:ILE:HG23	1:B:311:LEU:HD12	1.87	0.56
1:C:99:LEU:HD23	1:C:193:ILE:HD11	1.89	0.55
1:A:165:LYS:O	1:A:165:LYS:HG2	2.07	0.55
1:C:178:PHE:O	1:C:181:VAL:HG22	2.07	0.55
1:A:212:ILE:CG2	1:A:213:THR:N	2.70	0.55
1:B:53:LEU:HD12	1:B:54:ALA:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:HB2	1:A:90:LEU:HD11	1.89	0.54
1:A:64:GLN:NE2	2:A:401:HOH:O	2.28	0.54
1:C:269:TYR:CE2	1:C:293:ILE:HG23	2.42	0.54
1:D:239:TYR:O	1:D:258:TRP:CD1	2.60	0.54
1:B:310:LEU:O	1:B:318:ARG:HD3	2.08	0.54
1:C:281:GLU:O	1:C:285:LYS:HG3	2.08	0.54
1:B:54:ALA:HB3	1:B:65:LEU:HD13	1.90	0.54
1:B:171:GLU:HG3	1:B:299:VAL:HG23	1.90	0.54
1:A:69:THR:HA	1:A:136:ARG:HA	1.90	0.53
1:A:166:GLU:O	1:A:167:LYS:HB2	2.07	0.53
1:D:184:VAL:O	1:D:188:LEU:HD12	2.08	0.53
1:A:276:ASP:H	1:A:282:LEU:HD23	1.74	0.53
1:D:248:ARG:CB	1:D:249:PRO:CD	2.87	0.53
1:B:94:TYR:O	1:B:98:SER:OG	2.23	0.53
1:B:180:ASP:HA	1:B:183:ARG:HB3	1.90	0.52
1:D:93:GLU:OE2	1:D:217:PHE:N	2.42	0.52
1:D:187:ALA:O	1:D:191:LYS:HG3	2.09	0.52
1:A:118:CYS:HA	1:A:133:MET:HA	1.90	0.51
1:A:269:TYR:OH	1:A:299:VAL:HG11	2.11	0.51
1:A:68:LEU:HB2	1:A:90:LEU:CD1	2.41	0.51
1:C:64:GLN:HG2	1:C:142:ASP:O	2.10	0.51
1:C:100:LEU:O	1:C:108:HIS:ND1	2.42	0.51
1:C:181:VAL:HG12	1:C:212:ILE:HG12	1.92	0.51
1:C:178:PHE:O	1:C:182:VAL:HG23	2.11	0.51
1:B:196:ARG:NH2	1:B:234:ARG:O	2.43	0.50
1:C:100:LEU:HB3	1:C:103:GLN:HB3	1.94	0.50
1:B:100:LEU:HB3	1:B:103:GLN:HB3	1.92	0.50
1:A:68:LEU:C	1:A:68:LEU:CD2	2.85	0.50
1:A:80:SER:OG	1:A:81:GLN:N	2.44	0.50
1:A:97:LEU:HD22	1:A:107:VAL:O	2.12	0.50
1:A:189:HIS:HD2	1:A:321:ALA:HB2	1.76	0.50
1:A:234:ARG:NE	2:A:405:HOH:O	2.38	0.49
1:A:192:ASN:HB3	1:A:223:LEU:HB2	1.93	0.49
1:A:276:ASP:N	1:A:282:LEU:HD23	2.28	0.49
1:B:200:LEU:HD11	1:B:266:THR:OG1	2.13	0.48
1:A:153:THR:HB	1:A:156:LEU:HD12	1.95	0.48
1:A:55:ARG:NH1	1:A:59:THR:O	2.36	0.48
1:B:113:PHE:O	1:B:138:CYS:N	2.41	0.48
1:A:104:ASP:CG	1:A:183:ARG:HH22	2.22	0.48
1:C:66:LYS:HZ3	1:C:216:ASN:ND2	2.09	0.48
1:D:59:THR:OG1	1:D:60:ASP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LYS:O	1:B:59:THR:HG22	2.14	0.48
1:D:269:TYR:CE1	1:D:294:PRO:HG2	2.48	0.48
1:B:262:VAL:O	1:B:266:THR:HG23	2.14	0.48
1:D:161:HIS:O	1:D:162:TYR:C	2.57	0.48
1:D:184:VAL:HG12	1:D:188:LEU:HD11	1.95	0.47
1:B:182:VAL:HG22	1:B:260:LEU:HD13	1.95	0.47
1:B:283:PHE:HB3	1:B:287:LYS:HE2	1.95	0.47
1:A:212:ILE:HG22	1:A:213:THR:N	2.28	0.47
1:D:100:LEU:HD11	1:D:193:ILE:HD12	1.96	0.47
1:D:168:ARG:NH2	1:D:296:ASP:OD2	2.47	0.47
1:A:103:GLN:O	1:A:108:HIS:NE2	2.46	0.47
1:D:120:ILE:HA	1:D:131:LYS:HA	1.96	0.47
1:A:301:GLU:HA	1:A:304:VAL:HG22	1.94	0.47
1:A:306:LEU:HD13	1:A:324:VAL:HG23	1.96	0.47
1:D:104:ASP:OD1	1:D:183:ARG:NH1	2.48	0.47
1:D:163:VAL:O	1:D:167:LYS:N	2.48	0.46
1:D:170:SER:O	1:D:174:THR:HG23	2.15	0.46
1:D:158:ASN:OD1	1:D:160:GLN:N	2.47	0.46
1:C:99:LEU:HD21	1:C:222:HIS:ND1	2.31	0.46
1:A:94:TYR:HE1	1:A:109:HIS:CE1	2.34	0.46
1:B:159:LEU:O	1:B:163:VAL:HG13	2.16	0.46
1:A:54:ALA:HB3	1:A:65:LEU:HD13	1.97	0.46
1:B:97:LEU:HD22	1:B:107:VAL:O	2.15	0.46
1:A:161:HIS:NE2	2:A:404:HOH:O	2.36	0.46
1:D:250:TYR:CD1	1:D:250:TYR:N	2.84	0.46
1:A:80:SER:HB3	1:A:83:GLU:HG2	1.98	0.46
1:C:324:VAL:O	1:C:328:LEU:HD12	2.17	0.45
1:B:97:LEU:HD21	1:B:217:PHE:CD1	2.51	0.45
1:B:106:VAL:HG12	1:B:107:VAL:O	2.16	0.45
1:A:110:HIS:NE2	1:A:142:ASP:OD1	2.45	0.45
1:A:274:PHE:CE1	1:A:291:TYR:HB3	2.51	0.45
1:A:320:ALA:O	1:A:324:VAL:HG12	2.16	0.45
1:D:202:ASN:HB3	1:D:215:THR:O	2.17	0.45
1:C:243:ASP:HB3	1:C:250:TYR:HB2	1.99	0.45
1:A:185:VAL:HG11	1:A:260:LEU:HD11	1.97	0.44
1:B:50:VAL:HG23	1:B:67:ILE:HG23	1.99	0.44
1:D:168:ARG:HH22	1:D:296:ASP:CG	2.25	0.44
1:D:35:PHE:CD2	1:D:65:LEU:HD11	2.48	0.44
1:D:158:ASN:HD21	1:D:201:GLY:HA2	1.82	0.44
1:D:168:ARG:HG3	1:D:268:LEU:O	2.18	0.44
1:C:54:ALA:O	1:C:63:TYR:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ILE:O	1:B:293:ILE:HG13	2.17	0.44
1:B:175:VAL:HG21	1:B:335:TRP:CZ2	2.53	0.44
1:D:54:ALA:HB3	1:D:65:LEU:HD12	1.99	0.44
1:A:26:GLY:N	1:A:55:ARG:HH21	2.16	0.43
1:A:177:ILE:O	1:A:181:VAL:HG23	2.18	0.43
1:D:55:ARG:HA	1:D:62:PHE:HA	2.00	0.43
1:C:94:TYR:CE2	1:C:112:LEU:HD22	2.53	0.43
1:B:34:PRO:O	1:B:56:LYS:HA	2.19	0.43
1:A:56:LYS:O	1:A:59:THR:HG22	2.19	0.43
1:C:122:GLU:CA	1:C:129:MET:HE1	2.46	0.43
1:B:177:ILE:O	1:B:181:VAL:HG23	2.18	0.43
1:C:119:GLU:HG2	1:C:120:ILE:H	1.83	0.43
1:C:265:PHE:CG	1:C:273:PRO:HG3	2.53	0.43
1:B:94:TYR:HE1	1:B:109:HIS:HE1	1.55	0.43
1:A:198:LEU:HD13	1:A:260:LEU:HD21	2.00	0.43
1:D:32:ALA:H	1:D:37:LEU:HD13	1.84	0.43
1:C:48:SER:HB2	1:C:68:LEU:CD1	2.49	0.43
1:C:100:LEU:HD23	1:C:191:LYS:NZ	2.34	0.42
1:C:269:TYR:HE1	1:C:297:GLY:H	1.66	0.42
1:C:99:LEU:CD2	1:C:193:ILE:HD11	2.49	0.42
1:A:170:SER:O	1:A:174:THR:OG1	2.14	0.42
1:D:33:GLY:HA3	1:D:34:PRO:HD3	1.88	0.42
1:A:262:VAL:HG13	1:A:273:PRO:HD2	2.01	0.42
1:D:68:LEU:HD21	1:D:87:LYS:HA	2.00	0.42
1:B:147:HIS:CE1	1:B:150:SER:HB3	2.49	0.42
1:D:37:LEU:HG	1:D:52:CYS:SG	2.60	0.42
1:C:307:ILE:O	1:C:311:LEU:HG	2.20	0.42
1:D:96:LEU:HD22	1:D:222:HIS:HB2	2.02	0.42
1:C:50:VAL:O	1:C:67:ILE:HG22	2.18	0.41
1:D:159:LEU:HD11	1:D:267:MET:HE3	2.00	0.41
1:D:107:VAL:HG23	1:D:142:ASP:HB2	2.02	0.41
1:C:278:ILE:CG2	1:C:281:GLU:HB3	2.50	0.41
1:D:99:LEU:HD11	1:D:222:HIS:CD2	2.54	0.41
1:D:236:SER:HA	1:D:237:PRO:HD3	1.72	0.41
1:A:56:LYS:HB3	1:A:59:THR:CG2	2.51	0.41
1:C:46:VAL:HG12	1:C:47:PRO:HD2	2.03	0.41
1:C:81:GLN:HA	1:C:84:ARG:HB2	2.02	0.41
1:B:199:LYS:HE2	1:B:236:SER:OG	2.21	0.41
1:B:300:SER:O	1:B:304:VAL:HG23	2.21	0.41
1:D:174:THR:HG21	1:D:268:LEU:HD23	2.03	0.41
1:B:258:TRP:HB2	1:B:318:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:HIS:HA	1:C:164:ILE:HG12	2.03	0.41
1:D:180:ASP:O	1:D:184:VAL:HG23	2.21	0.41
1:C:89:LEU:HD23	1:C:89:LEU:HA	1.89	0.40
1:C:293:ILE:HA	1:C:294:PRO:HD3	1.83	0.40
1:D:50:VAL:O	1:D:67:ILE:N	2.50	0.40
1:B:35:PHE:HB3	1:B:54:ALA:HB1	2.03	0.40
1:B:94:TYR:HE1	1:B:109:HIS:CE1	2.34	0.40
1:B:172:ARG:HH11	1:B:172:ARG:HD3	1.74	0.40
1:D:263:VAL:O	1:D:267:MET:HG3	2.22	0.40
1:A:104:ASP:OD1	1:A:183:ARG:NH2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	285/320 (89%)	271 (95%)	14 (5%)	0	100	100
1	B	276/320 (86%)	264 (96%)	12 (4%)	0	100	100
1	C	275/320 (86%)	259 (94%)	16 (6%)	0	100	100
1	D	288/320 (90%)	260 (90%)	28 (10%)	0	100	100
All	All	1124/1280 (88%)	1054 (94%)	70 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	215/283 (76%)	212 (99%)	3 (1%)	59	80
1	B	204/283 (72%)	201 (98%)	3 (2%)	57	79
1	C	188/283 (66%)	187 (100%)	1 (0%)	81	91
1	D	172/283 (61%)	166 (96%)	6 (4%)	32	56
All	All	779/1132 (69%)	766 (98%)	13 (2%)	53	77

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

Mol	Chain	Res	Type
1	C	66	LYS
1	B	109	HIS
1	B	163	VAL
1	B	329	SER
1	A	68	LEU
1	A	96	LEU
1	A	99	LEU
1	D	63	TYR
1	D	64	GLN
1	D	65	LEU
1	D	89	LEU
1	D	234	ARG
1	D	243	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	160	GLN
1	C	190	GLN
1	C	216	ASN
1	B	101	HIS
1	B	109	HIS
1	B	147	HIS
1	B	190	GLN
1	A	161	HIS
1	A	189	HIS
1	A	190	GLN
1	D	161	HIS
1	D	189	HIS

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Mol	Chain	Res	Type
1	D	192	ASN
1	D	222	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	293/320 (91%)	0.59	17 (5%) 29 26	39, 68, 107, 145	0
1	B	282/320 (88%)	0.86	33 (11%) 9 7	39, 71, 125, 171	0
1	C	281/320 (87%)	1.21	54 (19%) 3 2	39, 86, 144, 189	0
1	D	294/320 (91%)	1.32	62 (21%) 2 2	64, 102, 137, 166	0
All	All	1150/1280 (89%)	0.99	166 (14%) 6 5	39, 83, 134, 189	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	310	LEU	5.6
1	B	229	LEU	5.1
1	C	137	ILE	4.9
1	C	114	GLN	4.7
1	D	126	SER	4.7
1	B	228	ASP	4.6
1	C	113	PHE	4.2
1	D	127	SER	4.2
1	D	137	ILE	4.0
1	C	126	SER	3.9
1	C	115	ASP	3.8
1	D	49	ILE	3.8
1	A	336	GLN	3.8
1	D	235	GLY	3.7
1	D	120	ILE	3.7
1	A	228	ASP	3.6
1	D	121	VAL	3.6
1	C	288	ALA	3.5
1	D	291	TYR	3.5
1	C	52	CYS	3.5
1	D	276	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	139	LEU	3.4
1	D	277	SER	3.3
1	D	336	GLN	3.3
1	B	223	LEU	3.3
1	C	120	ILE	3.3
1	C	41	LEU	3.3
1	B	231	LYS	3.3
1	B	279	PRO	3.2
1	D	311	LEU	3.2
1	C	306	LEU	3.2
1	D	335	TRP	3.1
1	A	229	LEU	3.1
1	D	41	LEU	3.1
1	B	43	ASN	3.1
1	C	149	PHE	3.0
1	C	135	LYS	3.0
1	C	332	ILE	3.0
1	D	313	LEU	3.0
1	D	130	VAL	3.0
1	C	298	ARG	3.0
1	B	297	GLY	3.0
1	C	308	ARG	3.0
1	C	54	ALA	2.9
1	A	26	GLY	2.9
1	D	293	ILE	2.9
1	B	70	LEU	2.9
1	C	67	ILE	2.9
1	C	315	PRO	2.9
1	D	139	LEU	2.9
1	D	275	TYR	2.9
1	D	119	GLU	2.9
1	C	164	ILE	2.8
1	A	90	LEU	2.8
1	C	129	MET	2.8
1	C	39	PRO	2.8
1	C	69	THR	2.8
1	C	128	ARG	2.8
1	D	258	TRP	2.8
1	D	292	THR	2.8
1	D	95	SER	2.8
1	C	312	VAL	2.7
1	C	289	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	137	ILE	2.7
1	A	315	PRO	2.7
1	B	96	LEU	2.7
1	D	129	MET	2.7
1	D	316	GLN	2.7
1	B	48	SER	2.7
1	C	79	GLU	2.7
1	D	81	GLN	2.7
1	B	138	CYS	2.6
1	A	42	GLY	2.6
1	C	310	LEU	2.6
1	A	79	GLU	2.6
1	A	227	GLY	2.6
1	C	172	ARG	2.6
1	C	80	SER	2.6
1	B	114	GLN	2.6
1	D	148	ASP	2.5
1	B	83	GLU	2.5
1	D	304	VAL	2.5
1	C	170	SER	2.5
1	C	169	LEU	2.5
1	C	51	GLN	2.5
1	B	336	GLN	2.5
1	B	46	VAL	2.5
1	A	43	ASN	2.5
1	C	122	GLU	2.5
1	D	70	LEU	2.5
1	D	274	PHE	2.5
1	D	177	ILE	2.5
1	D	62	PHE	2.5
1	B	80	SER	2.5
1	C	297	GLY	2.4
1	D	82	GLU	2.4
1	D	286	ILE	2.4
1	B	225	SER	2.4
1	D	237	PRO	2.4
1	C	138	CYS	2.4
1	B	81	GLN	2.4
1	B	219	LEU	2.4
1	A	40	ARG	2.4
1	C	302	ASN	2.4
1	A	29	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	314	ASP	2.4
1	C	171	GLU	2.4
1	B	230	LEU	2.4
1	A	130	VAL	2.4
1	B	226	GLU	2.4
1	C	38	GLY	2.3
1	D	138	CYS	2.3
1	C	283	PHE	2.3
1	C	224	VAL	2.3
1	D	44	SER	2.3
1	D	118	CYS	2.3
1	D	288	ALA	2.3
1	D	261	GLY	2.3
1	C	148	ASP	2.3
1	B	113	PHE	2.3
1	B	118	CYS	2.3
1	D	239	TYR	2.3
1	C	147	HIS	2.2
1	D	105	GLY	2.2
1	B	278	ILE	2.2
1	C	121	VAL	2.2
1	C	209	THR	2.2
1	D	90	LEU	2.2
1	D	240	ILE	2.2
1	C	46	VAL	2.2
1	A	312	VAL	2.2
1	D	312	VAL	2.2
1	B	59	THR	2.2
1	C	136	ARG	2.2
1	D	50	VAL	2.2
1	C	167	LYS	2.2
1	C	90	LEU	2.2
1	B	44	SER	2.2
1	C	335	TRP	2.2
1	D	133	MET	2.1
1	B	227	GLY	2.1
1	D	278	ILE	2.1
1	C	248	ARG	2.1
1	A	72	GLU	2.1
1	D	249	PRO	2.1
1	D	169	LEU	2.1
1	D	307	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	84	ARG	2.1
1	C	277	SER	2.1
1	C	304	VAL	2.1
1	D	89	LEU	2.1
1	D	287	LYS	2.1
1	D	309	LYS	2.1
1	B	112	LEU	2.1
1	D	164	ILE	2.1
1	B	66	LYS	2.1
1	B	232	ASP	2.1
1	C	127	SER	2.1
1	B	116	ARG	2.0
1	D	238	ALA	2.0
1	A	70	LEU	2.0
1	D	219	LEU	2.0
1	A	63	TYR	2.0
1	D	334	SER	2.0
1	C	82	GLU	2.0
1	D	86	GLY	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 oligosaccharides 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.