



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:23 AM UTC

PDB ID : 2NXO / pdb_00002nxo
Title : Crystal structure of protein SCO4506 from Streptomyces coelicolor, Pfam DUF178
Authors : Tyagi, R.; Eswaramoorthy, S.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-11-17
Resolution : 2.04 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

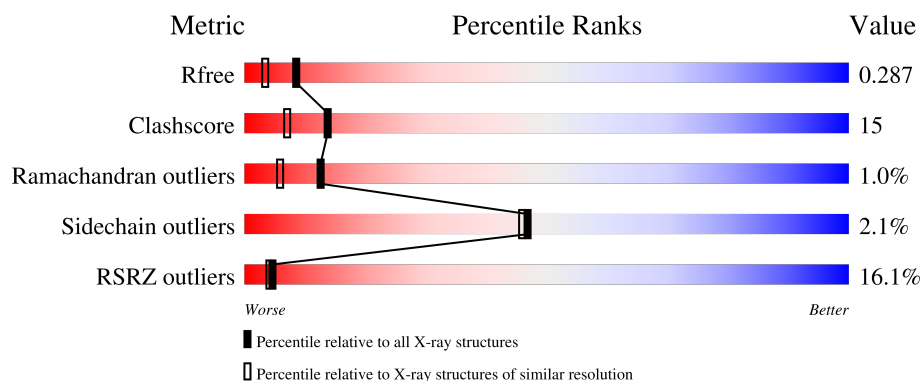
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	291	13% 67% 23% 7%
1	B	291	9% 69% 20% 9%
1	C	291	9% 70% 19% 8%
1	D	291	26% 56% 23% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8700 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 Hypothetical protein SCO4506.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2119	1360	359	393	7			
1	B	266	Total	C	N	O	S	0	0	0
			2082	1333	353	389	7			
1	C	269	Total	C	N	O	S	0	0	0
			2095	1341	356	391	7			
1	D	236	Total	C	N	O	S	0	0	0
			1854	1193	313	341	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	cloning artifact	UNP Q9L0T8
A	0	LEU	-	cloning artifact	UNP Q9L0T8
A	282	GLU	-	expression tag	UNP Q9L0T8
A	283	GLY	-	expression tag	UNP Q9L0T8
A	284	HIS	-	expression tag	UNP Q9L0T8
A	285	HIS	-	expression tag	UNP Q9L0T8
A	286	HIS	-	expression tag	UNP Q9L0T8
A	287	HIS	-	expression tag	UNP Q9L0T8
A	288	HIS	-	expression tag	UNP Q9L0T8
A	289	HIS	-	expression tag	UNP Q9L0T8
B	-1	SER	-	cloning artifact	UNP Q9L0T8
B	0	LEU	-	cloning artifact	UNP Q9L0T8
B	282	GLU	-	expression tag	UNP Q9L0T8
B	283	GLY	-	expression tag	UNP Q9L0T8
B	284	HIS	-	expression tag	UNP Q9L0T8
B	285	HIS	-	expression tag	UNP Q9L0T8
B	286	HIS	-	expression tag	UNP Q9L0T8
B	287	HIS	-	expression tag	UNP Q9L0T8
B	288	HIS	-	expression tag	UNP Q9L0T8
B	289	HIS	-	expression tag	UNP Q9L0T8
C	-1	SER	-	cloning artifact	UNP Q9L0T8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	LEU	-	cloning artifact	UNP Q9L0T8
C	282	GLU	-	expression tag	UNP Q9L0T8
C	283	GLY	-	expression tag	UNP Q9L0T8
C	284	HIS	-	expression tag	UNP Q9L0T8
C	285	HIS	-	expression tag	UNP Q9L0T8
C	286	HIS	-	expression tag	UNP Q9L0T8
C	287	HIS	-	expression tag	UNP Q9L0T8
C	288	HIS	-	expression tag	UNP Q9L0T8
C	289	HIS	-	expression tag	UNP Q9L0T8
D	-1	SER	-	cloning artifact	UNP Q9L0T8
D	0	LEU	-	cloning artifact	UNP Q9L0T8
D	282	GLU	-	expression tag	UNP Q9L0T8
D	283	GLY	-	expression tag	UNP Q9L0T8
D	284	HIS	-	expression tag	UNP Q9L0T8
D	285	HIS	-	expression tag	UNP Q9L0T8
D	286	HIS	-	expression tag	UNP Q9L0T8
D	287	HIS	-	expression tag	UNP Q9L0T8
D	288	HIS	-	expression tag	UNP Q9L0T8
D	289	HIS	-	expression tag	UNP Q9L0T8

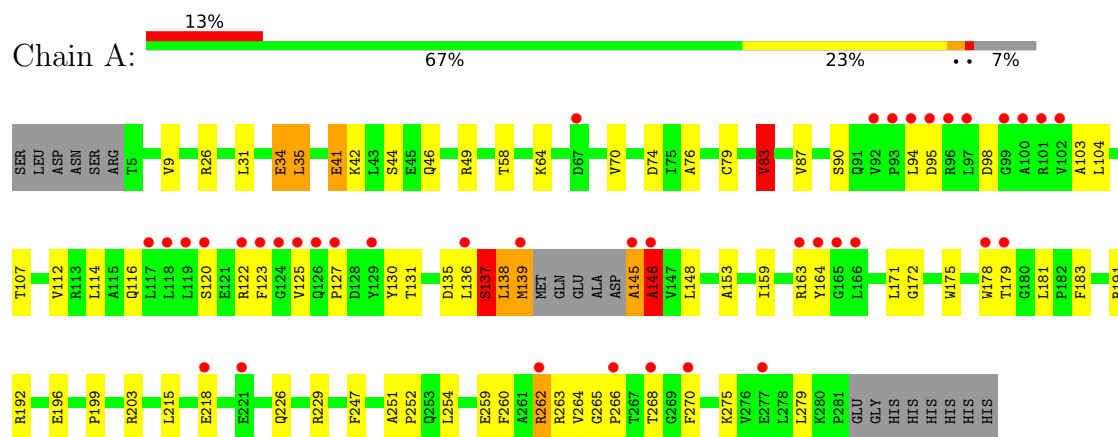
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	151	Total O 151 151	0	0
2	B	158	Total O 158 158	0	0
2	C	121	Total O 121 121	0	0
2	D	120	Total O 120 120	0	0

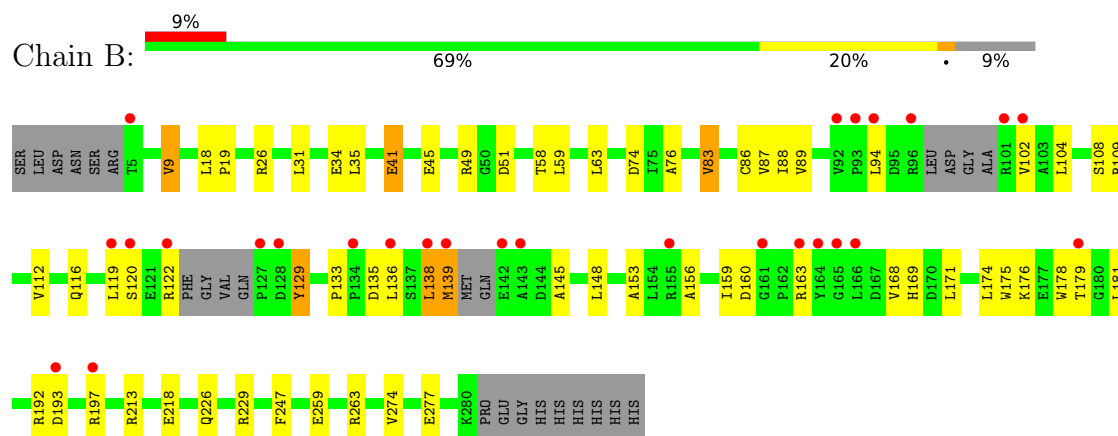
3 Residue-property plots

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.

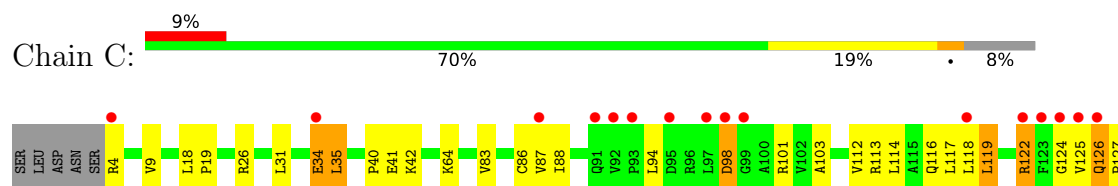
• Molecule 1: Hypothetical protein SCO4506

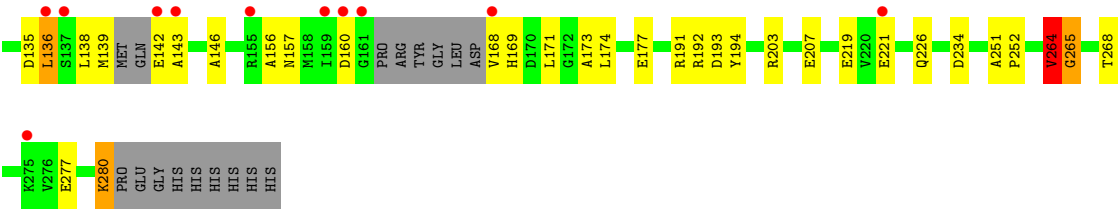


• Molecule 1: Hypothetical protein SCO4506

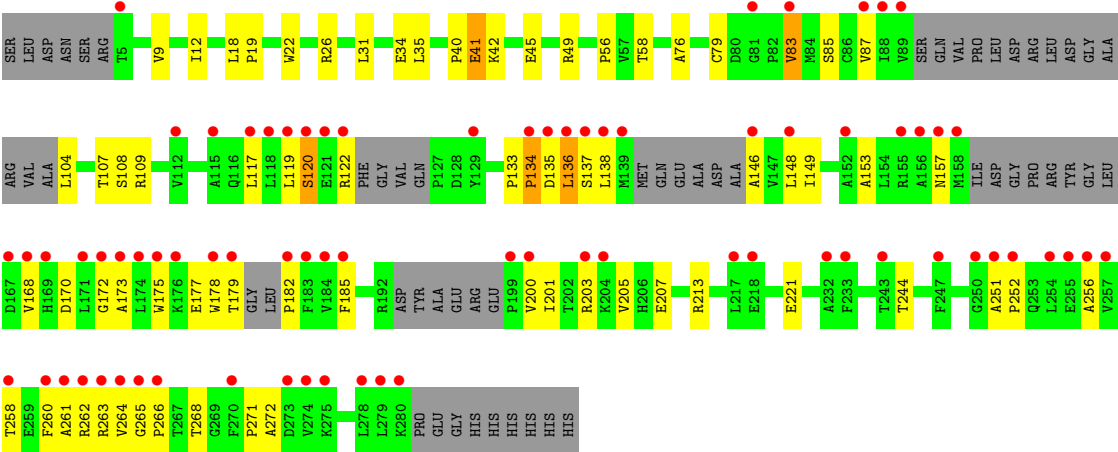


• Molecule 1: Hypothetical protein SCO4506





● Molecule 1: Hypothetical protein SCO4506



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.79Å 97.37Å 86.57Å 90.00° 106.48° 90.00°	Depositor
Resolution (Å)	30.28 – 2.04 30.28 – 2.04	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.28-2.04) 97.0 (30.28-2.04)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.280 0.250 , 0.287	Depositor DCC
R_{free} test set	2264 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8700	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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

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	0.45	0/2167	0.96	13/2953 (0.4%)
1	B	0.43	0/2126	0.92	9/2892 (0.3%)
1	C	0.41	0/2139	0.91	11/2911 (0.4%)
1	D	0.38	0/1891	0.89	8/2565 (0.3%)
All	All	0.42	0/8323	0.92	41/11321 (0.4%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	VAL	N-CA-C	7.61	118.10	108.82
1	A	138	LEU	N-CA-C	-7.54	102.42	111.69
1	D	87	VAL	N-CA-C	7.49	117.96	108.82
1	A	146	ALA	N-CA-C	6.93	125.56	110.80
1	C	264	VAL	N-CA-C	6.91	117.75	111.81
1	B	34	GLU	N-CA-C	-6.87	94.66	107.71
1	B	74	ASP	N-CA-C	6.69	122.85	113.56
1	D	34	GLU	N-CA-C	-6.40	93.66	107.49
1	B	59	LEU	N-CA-C	6.35	118.73	111.11
1	B	83	VAL	N-CA-C	-6.06	107.35	113.47
1	B	87	VAL	N-CA-C	5.95	117.28	108.65
1	A	137	SER	N-CA-C	-5.91	98.21	110.80
1	A	35	LEU	N-CA-C	5.84	119.42	110.20
1	D	9	VAL	N-CA-C	5.81	116.31	108.17
1	A	191	ARG	N-CA-C	-5.76	101.87	110.23
1	C	40	PRO	N-CA-C	5.76	122.33	113.75
1	D	200	VAL	N-CA-C	-5.74	105.50	111.58
1	C	34	GLU	N-CA-C	-5.70	95.89	107.41
1	C	9	VAL	N-CA-C	5.68	116.12	108.17
1	B	133	PRO	CA-C-N	5.60	126.84	119.84
1	B	133	PRO	C-N-CA	5.60	126.84	119.84
1	A	9	VAL	N-CA-C	5.59	116.00	108.17
1	A	83	VAL	N-CA-C	-5.53	106.95	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ALA	CA-C-N	5.47	132.00	121.54
1	A	145	ALA	C-N-CA	5.47	132.00	121.54
1	C	87	VAL	N-CA-C	5.47	116.79	108.80
1	A	34	GLU	N-CA-C	-5.44	95.73	107.49
1	A	74	ASP	N-CA-C	5.43	121.11	113.56
1	D	83	VAL	N-CA-C	-5.36	107.14	113.42
1	A	83	VAL	CB-CA-C	-5.31	105.09	110.88
1	D	35	LEU	N-CA-C	5.30	118.87	109.96
1	D	260	PHE	N-CA-C	-5.29	105.60	111.36
1	B	129	TYR	N-CA-C	5.28	118.61	110.42
1	C	35	LEU	N-CA-C	5.25	118.67	110.32
1	C	126	GLN	CA-C-N	5.19	125.66	120.52
1	C	126	GLN	C-N-CA	5.19	125.66	120.52
1	C	265	GLY	CA-C-N	5.08	126.19	119.84
1	C	265	GLY	C-N-CA	5.08	126.19	119.84
1	B	9	VAL	N-CA-C	5.08	115.28	108.17
1	C	191	ARG	N-CA-C	-5.07	102.88	110.23
1	D	177	GLU	N-CA-C	-5.03	106.89	112.57

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	2119	0	2108	76	0
1	B	2082	0	2069	51	0
1	C	2095	0	2081	45	0
1	D	1854	0	1857	67	0
2	A	151	0	0	11	0
2	B	158	0	0	12	0
2	C	121	0	0	7	0
2	D	120	0	0	18	0
All	All	8700	0	8115	236	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 (236) 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:139:MET:SD	1:A:146:ALA:HB2	1.98	1.02
1:C:139:MET:HE2	1:C:146:ALA:HB1	1.46	0.94
1:B:138:LEU:HD22	2:B:441:HOH:O	1.71	0.90
1:A:98:ASP:HA	1:A:125:VAL:HG13	1.51	0.90
1:A:262:ARG:HH11	1:A:262:ARG:HB3	1.38	0.86
1:A:179:THR:HB	2:A:388:HOH:O	1.78	0.84
1:A:138:LEU:O	1:A:139:MET:HB2	1.79	0.83
1:C:42:LYS:HB2	2:C:374:HOH:O	1.81	0.80
1:A:44:SER:HB2	2:A:317:HOH:O	1.82	0.79
1:A:103:ALA:HB3	1:A:139:MET:SD	2.23	0.77
1:A:90:SER:HA	1:A:145:ALA:HB1	1.67	0.77
1:B:109:ARG:HG2	2:B:411:HOH:O	1.86	0.74
1:B:94:LEU:HD11	1:B:169:HIS:NE2	2.02	0.73
1:A:79:CYS:SG	1:A:83:VAL:HG22	2.28	0.73
1:C:156:ALA:HA	1:C:160:ASP:HB2	1.70	0.73
1:B:175:TRP:O	1:B:179:THR:HG22	1.89	0.72
1:A:122:ARG:HD2	1:A:178:TRP:HB2	1.70	0.72
1:A:179:THR:HG23	1:A:181:LEU:H	1.54	0.71
1:C:264:VAL:HG13	1:C:268:THR:OG1	1.89	0.71
1:D:263:ARG:HG3	2:D:353:HOH:O	1.89	0.71
1:C:113:ARG:NH1	1:C:264:VAL:HG22	2.06	0.70
1:D:136:LEU:HG	1:D:137:SER:H	1.56	0.70
1:D:109:ARG:HG2	2:D:335:HOH:O	1.91	0.69
1:D:41:GLU:HB3	2:D:335:HOH:O	1.92	0.68
1:B:274:VAL:O	2:B:443:HOH:O	2.10	0.68
1:C:101:ARG:O	1:C:143:ALA:HB1	1.94	0.68
1:A:175:TRP:O	1:A:179:THR:HG22	1.94	0.67
2:B:428:HOH:O	1:C:226:GLN:HG3	1.95	0.67
1:B:41:GLU:HB2	2:B:411:HOH:O	1.95	0.66
1:B:41:GLU:HB3	2:B:412:HOH:O	1.94	0.66
1:D:133:PRO:C	1:D:135:ASP:H	2.04	0.66
2:B:323:HOH:O	1:C:226:GLN:HG2	1.97	0.65
1:B:139:MET:HE1	1:B:148:LEU:HD21	1.77	0.65
1:D:136:LEU:CG	1:D:137:SER:H	2.09	0.65
1:A:41:GLU:HG3	1:A:42:LYS:H	1.61	0.64
1:A:98:ASP:CA	1:A:125:VAL:HG13	2.26	0.64
1:D:251:ALA:HB3	1:D:252:PRO:HD3	1.79	0.63
1:C:34:GLU:HG3	2:C:400:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:VAL:HG23	1:D:172:GLY:HA3	1.80	0.63
1:A:262:ARG:HB3	1:A:262:ARG:NH1	2.12	0.62
1:C:157:ASN:HA	1:C:168:VAL:HG11	1.81	0.61
1:C:98:ASP:O	1:C:127:PRO:HA	1.99	0.61
1:A:90:SER:HB3	2:A:391:HOH:O	2.00	0.61
1:A:90:SER:HA	1:A:145:ALA:CB	2.30	0.61
1:B:94:LEU:HD12	1:B:94:LEU:H	1.65	0.61
1:C:280:LYS:HD2	1:C:280:LYS:O	2.01	0.60
1:C:122:ARG:HD3	1:C:122:ARG:O	2.02	0.60
1:D:170:ASP:HB3	1:D:173:ALA:HB3	1.84	0.60
1:A:139:MET:SD	1:A:146:ALA:CB	2.81	0.60
1:B:41:GLU:O	1:B:45:GLU:HG3	2.01	0.60
1:C:139:MET:O	1:C:142:GLU:HB3	2.01	0.60
1:B:122:ARG:HD2	1:B:178:TRP:HB2	1.85	0.59
1:B:135:ASP:OD2	1:B:138:LEU:HB2	2.03	0.59
1:C:135:ASP:O	1:C:136:LEU:HB2	2.02	0.58
1:D:79:CYS:CB	1:D:83:VAL:HG22	2.33	0.58
1:B:192:ARG:HH12	1:B:277:GLU:HG2	1.68	0.58
1:A:199:PRO:O	1:A:203:ARG:HG3	2.04	0.57
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.69	0.57
1:B:108:SER:HA	2:B:332:HOH:O	2.04	0.57
1:B:193:ASP:O	1:B:197:ARG:HD3	2.04	0.57
1:A:94:LEU:HB2	1:A:123:PHE:CD2	2.39	0.57
1:D:79:CYS:SG	1:D:83:VAL:HG22	2.44	0.56
1:D:122:ARG:HD2	1:D:178:TRP:CG	2.40	0.56
1:C:251:ALA:HB3	1:C:252:PRO:HD3	1.86	0.56
1:B:159:ILE:HG22	1:B:163:ARG:HD3	1.86	0.56
1:A:26:ARG:NH2	2:A:336:HOH:O	2.39	0.56
1:C:41:GLU:CD	2:C:293:HOH:O	2.49	0.56
1:D:264:VAL:HG13	2:D:332:HOH:O	2.05	0.56
1:B:226:GLN:HG3	1:B:229:ARG:NH2	2.21	0.56
1:B:88:ILE:HG13	1:B:171:LEU:HD21	1.88	0.55
1:D:258:THR:HG22	2:D:333:HOH:O	2.06	0.55
1:A:120:SER:HA	1:A:125:VAL:H	1.70	0.55
1:A:114:LEU:HG	2:A:408:HOH:O	2.07	0.55
1:D:157:ASN:HA	1:D:168:VAL:HG11	1.89	0.55
1:B:89:VAL:HG22	1:B:168:VAL:HG22	1.89	0.54
1:A:70:VAL:O	1:A:70:VAL:HG13	2.07	0.54
1:B:83:VAL:HG11	1:B:86:CYS:HB2	1.88	0.54
1:D:107:THR:HG23	1:D:134:PRO:HG3	1.90	0.54
1:A:226:GLN:HG3	1:A:229:ARG:NH2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ALA:HB1	2:D:298:HOH:O	2.06	0.54
1:B:49:ARG:NE	1:B:51:ASP:OD2	2.36	0.54
1:A:103:ALA:HB2	1:A:139:MET:HG3	1.90	0.53
1:D:136:LEU:O	1:D:137:SER:HB3	2.08	0.53
1:A:103:ALA:HB2	1:A:130:TYR:CZ	2.44	0.53
1:D:83:VAL:HG21	1:D:185:PHE:CE2	2.44	0.53
1:A:58:THR:HG22	2:A:317:HOH:O	2.09	0.53
1:C:221:GLU:CD	1:C:221:GLU:H	2.17	0.53
1:A:171:LEU:HB3	2:A:408:HOH:O	2.08	0.52
1:C:64:LYS:HE2	1:C:268:THR:O	2.09	0.52
1:A:103:ALA:O	1:A:146:ALA:HA	2.10	0.52
1:C:135:ASP:O	1:C:136:LEU:CB	2.58	0.52
1:A:275:LYS:HE3	2:A:405:HOH:O	2.09	0.52
1:B:193:ASP:HB2	2:B:393:HOH:O	2.10	0.52
1:D:179:THR:C	2:D:373:HOH:O	2.53	0.52
1:D:268:THR:HG22	1:D:268:THR:O	2.09	0.52
1:B:169:HIS:HB3	1:B:174:LEU:HD11	1.92	0.52
1:C:31:LEU:HD12	1:C:31:LEU:N	2.26	0.51
1:A:125:VAL:O	1:A:127:PRO:HD3	2.10	0.51
1:D:40:PRO:HB2	2:D:316:HOH:O	2.11	0.51
1:D:182:PRO:HG2	1:D:256:ALA:HB2	1.93	0.51
1:B:94:LEU:HD23	1:B:119:LEU:HD21	1.93	0.51
1:D:31:LEU:N	1:D:31:LEU:HD12	2.26	0.51
1:A:262:ARG:HD2	1:A:262:ARG:C	2.36	0.50
1:D:22:TRP:O	1:D:26:ARG:HG2	2.11	0.50
1:A:103:ALA:CB	1:A:139:MET:HG3	2.41	0.50
1:D:262:ARG:HD2	2:D:391:HOH:O	2.12	0.50
1:A:125:VAL:HG12	1:A:127:PRO:HG3	1.93	0.50
1:A:215:LEU:HA	1:A:218:GLU:CG	2.42	0.49
1:C:122:ARG:HD3	1:C:122:ARG:C	2.37	0.49
1:D:136:LEU:HG	1:D:137:SER:N	2.25	0.49
1:A:135:ASP:OD2	1:A:137:SER:HB3	2.12	0.49
1:D:263:ARG:HB2	2:D:332:HOH:O	2.12	0.49
1:D:41:GLU:HG3	1:D:42:LYS:H	1.77	0.49
1:A:94:LEU:HD12	1:A:123:PHE:CZ	2.47	0.49
1:D:203:ARG:O	1:D:207:GLU:HG3	2.13	0.49
1:A:34:GLU:HG2	2:A:398:HOH:O	2.13	0.49
1:D:201:ILE:O	1:D:205:VAL:HG23	2.12	0.49
1:C:138:LEU:HD11	1:D:271:PRO:HD3	1.95	0.49
1:A:114:LEU:HD22	1:A:183:PHE:CZ	2.48	0.48
1:A:262:ARG:HD2	1:A:262:ARG:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LYS:NZ	2:B:424:HOH:O	2.45	0.48
1:C:18:LEU:HB3	1:C:19:PRO:HD3	1.95	0.48
1:A:76:ALA:O	1:A:247:PHE:HA	2.13	0.48
1:B:112:VAL:O	1:B:116:GLN:HG3	2.13	0.48
1:C:119:LEU:O	1:C:125:VAL:HG22	2.13	0.48
1:B:94:LEU:HD11	1:B:169:HIS:CE1	2.48	0.48
1:C:169:HIS:HB3	1:C:174:LEU:HD11	1.95	0.48
1:D:122:ARG:HH11	1:D:122:ARG:HG2	1.79	0.48
1:A:125:VAL:C	1:A:127:PRO:HD3	2.38	0.48
1:D:18:LEU:HB3	1:D:19:PRO:HD3	1.96	0.48
1:D:41:GLU:HG2	1:D:107:THR:HA	1.95	0.47
1:D:104:LEU:N	2:D:371:HOH:O	2.46	0.47
1:A:41:GLU:HG3	1:A:42:LYS:N	2.28	0.47
1:D:137:SER:C	1:D:138:LEU:HD12	2.38	0.47
1:B:9:VAL:O	1:B:35:LEU:HA	2.15	0.47
1:C:94:LEU:HD22	1:C:119:LEU:HD11	1.96	0.47
1:A:123:PHE:O	1:A:125:VAL:HG23	2.15	0.47
1:B:192:ARG:NH1	1:B:277:GLU:HG2	2.30	0.47
1:A:265:GLY:N	1:A:266:PRO:HD2	2.29	0.47
1:B:179:THR:HG23	1:B:181:LEU:H	1.79	0.47
1:B:31:LEU:N	1:B:31:LEU:HD12	2.30	0.47
1:C:103:ALA:CB	1:C:139:MET:HB2	2.45	0.46
1:A:251:ALA:HB3	1:A:252:PRO:HD3	1.96	0.46
1:B:213:ARG:HD2	1:B:213:ARG:C	2.40	0.46
1:B:259:GLU:O	1:B:263:ARG:HG3	2.14	0.46
1:C:26:ARG:HD3	1:C:219:GLU:OE1	2.15	0.46
1:A:94:LEU:HB2	1:A:123:PHE:CE2	2.51	0.46
1:B:88:ILE:HG23	2:B:353:HOH:O	2.14	0.46
1:C:41:GLU:HG3	2:C:293:HOH:O	2.14	0.46
1:B:94:LEU:HD12	1:B:94:LEU:N	2.31	0.46
1:D:83:VAL:HG21	1:D:185:PHE:HE2	1.79	0.46
1:A:31:LEU:HD12	1:A:31:LEU:N	2.30	0.46
1:D:175:TRP:O	1:D:179:THR:HG22	2.16	0.46
1:D:157:ASN:OD1	1:D:157:ASN:O	2.35	0.45
1:B:102:VAL:HG12	1:B:145:ALA:HB3	1.97	0.45
1:D:41:GLU:O	1:D:45:GLU:HG3	2.16	0.45
1:D:133:PRO:C	1:D:135:ASP:N	2.73	0.45
1:D:136:LEU:CG	1:D:137:SER:N	2.77	0.45
1:D:251:ALA:HA	2:D:344:HOH:O	2.16	0.45
1:D:122:ARG:HD2	1:D:178:TRP:CD1	2.51	0.45
1:D:45:GLU:O	1:D:49:ARG:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:LEU:N	1:D:19:PRO:CD	2.80	0.45
1:D:85:SER:O	1:D:149:ILE:HA	2.16	0.45
1:A:41:GLU:HB2	2:A:417:HOH:O	2.17	0.45
1:B:41:GLU:HG3	1:B:109:ARG:NH2	2.33	0.44
1:D:244:THR:HB	2:D:355:HOH:O	2.16	0.44
1:A:203:ARG:HD3	2:A:392:HOH:O	2.17	0.44
1:C:88:ILE:HD11	1:C:171:LEU:HD21	1.98	0.44
1:D:12:ILE:HG13	1:D:56:PRO:HG3	2.00	0.44
1:D:133:PRO:O	1:D:135:ASP:N	2.49	0.44
1:B:148:LEU:C	1:B:153:ALA:HB2	2.43	0.44
1:B:229:ARG:HB3	1:C:4:ARG:NH2	2.32	0.44
1:C:113:ARG:HH11	1:C:264:VAL:HG13	1.83	0.44
1:C:192:ARG:NH2	1:C:277:GLU:OE1	2.51	0.44
1:A:163:ARG:HD2	1:A:164:TYR:CZ	2.53	0.44
1:A:215:LEU:HD12	1:A:218:GLU:HG3	1.99	0.44
1:C:203:ARG:HD3	1:C:207:GLU:OE1	2.18	0.44
1:A:148:LEU:C	1:A:153:ALA:HB2	2.43	0.44
1:A:64:LYS:HE2	1:A:268:THR:O	2.18	0.43
1:D:31:LEU:HD12	1:D:31:LEU:H	1.83	0.43
1:B:104:LEU:HD11	1:B:129:TYR:HB3	2.01	0.43
1:B:156:ALA:HA	1:B:160:ASP:HB2	2.00	0.43
1:A:41:GLU:OE2	1:A:107:THR:HA	2.19	0.43
1:B:18:LEU:N	1:B:19:PRO:CD	2.81	0.43
1:A:259:GLU:O	1:A:263:ARG:HG3	2.18	0.43
1:C:112:VAL:O	1:C:116:GLN:HG3	2.17	0.43
1:D:272:ALA:HA	2:D:298:HOH:O	2.18	0.43
1:D:76:ALA:HB3	2:D:347:HOH:O	2.17	0.43
1:D:79:CYS:HB3	1:D:83:VAL:HG22	2.00	0.43
1:D:265:GLY:N	1:D:266:PRO:HD2	2.33	0.43
1:A:135:ASP:O	1:A:136:LEU:C	2.61	0.43
1:A:136:LEU:HB2	1:A:148:LEU:HD11	2.00	0.43
1:A:192:ARG:O	1:A:196:GLU:HG3	2.19	0.43
1:A:159:ILE:CG2	1:A:163:ARG:HH21	2.32	0.42
1:B:94:LEU:HD11	1:B:169:HIS:CD2	2.53	0.42
1:A:122:ARG:HD2	1:A:178:TRP:CG	2.54	0.42
1:A:122:ARG:HH11	1:A:178:TRP:CD1	2.38	0.42
1:B:58:THR:HG21	1:B:109:ARG:HB2	2.02	0.42
1:A:46:GLN:HA	1:A:49:ARG:HE	1.85	0.42
1:A:112:VAL:O	1:A:116:GLN:HG3	2.19	0.42
1:A:130:TYR:OH	1:A:139:MET:HG3	2.18	0.42
1:C:122:ARG:NH1	2:C:384:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PHE:O	1:A:264:VAL:HG22	2.20	0.42
1:A:265:GLY:HA2	1:A:270:PHE:CE1	2.55	0.42
1:B:76:ALA:O	1:B:247:PHE:HA	2.19	0.42
1:A:125:VAL:HG12	1:A:127:PRO:CD	2.50	0.42
1:B:197:ARG:N	1:B:197:ARG:HD2	2.35	0.41
1:B:259:GLU:OE2	1:B:263:ARG:NE	2.53	0.41
1:C:83:VAL:HG11	1:C:86:CYS:HB2	2.02	0.41
1:D:58:THR:HG21	1:D:109:ARG:HB2	2.03	0.41
1:A:163:ARG:HD2	1:A:164:TYR:CE2	2.55	0.41
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.94	0.41
1:D:117:LEU:HD22	2:D:332:HOH:O	2.19	0.41
1:D:221:GLU:CD	1:D:221:GLU:H	2.28	0.41
1:B:63:LEU:HD22	1:B:274:VAL:HG11	2.02	0.41
1:B:218:GLU:CB	2:B:447:HOH:O	2.68	0.41
1:A:122:ARG:HD2	1:A:178:TRP:CB	2.44	0.41
1:D:119:LEU:O	1:D:120:SER:HB3	2.19	0.41
1:B:175:TRP:CE2	1:B:179:THR:HG21	2.56	0.41
1:C:41:GLU:CG	2:C:293:HOH:O	2.69	0.41
1:D:213:ARG:HD2	1:D:213:ARG:C	2.46	0.41
1:A:83:VAL:HG23	1:A:172:GLY:HA3	2.01	0.41
1:C:114:LEU:O	1:C:118:LEU:HD23	2.21	0.41
1:D:108:SER:HB2	1:D:149:ILE:HD13	2.03	0.41
1:D:148:LEU:C	1:D:153:ALA:HB2	2.46	0.41
1:A:104:LEU:O	1:A:131:THR:HG23	2.21	0.40
1:C:173:ALA:O	1:C:177:GLU:HG3	2.21	0.40
1:D:26:ARG:NH2	2:D:310:HOH:O	2.53	0.40
1:D:182:PRO:O	1:D:256:ALA:HB1	2.21	0.40
1:A:125:VAL:HG12	1:A:127:PRO:HD3	2.03	0.40
1:B:26:ARG:HD2	1:C:26:ARG:O	2.21	0.40
1:D:136:LEU:CD1	1:D:137:SER:H	2.33	0.40
1:C:125:VAL:HG23	1:C:126:GLN:N	2.36	0.40
1:D:146:ALA:HA	2:D:371:HOH:O	2.21	0.40
1:C:193:ASP:OD1	1:C:194:TYR:N	2.55	0.40
1:C:234:ASP:HB2	2:C:347:HOH:O	2.21	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	268/291 (92%)	255 (95%)	11 (4%)	2 (1%)	18	10
1	B	258/291 (89%)	247 (96%)	10 (4%)	1 (0%)	30	22
1	C	263/291 (90%)	248 (94%)	11 (4%)	4 (2%)	8	2
1	D	222/291 (76%)	211 (95%)	8 (4%)	3 (1%)	9	3
All	All	1011/1164 (87%)	961 (95%)	40 (4%)	10 (1%)	12	6

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	98	ASP
1	C	136	LEU
1	D	120	SER
1	A	137	SER
1	A	146	ALA
1	B	120	SER
1	C	124	GLY
1	D	136	LEU
1	C	265	GLY
1	D	134	PRO

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	224/243 (92%)	217 (97%)	7 (3%)	35	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	221/243 (91%)	217 (98%)	4 (2%)	51	51
1	C	221/243 (91%)	215 (97%)	6 (3%)	39	36
1	D	199/243 (82%)	198 (100%)	1 (0%)	81	85
All	All	865/972 (89%)	847 (98%)	18 (2%)	47	46

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	41	GLU
1	A	83	VAL
1	A	95	ASP
1	A	139	MET
1	A	262	ARG
1	A	279	LEU
1	B	41	GLU
1	B	136	LEU
1	B	138	LEU
1	B	139	MET
1	C	35	LEU
1	C	117	LEU
1	C	119	LEU
1	C	122	ARG
1	C	264	VAL
1	C	280	LYS
1	D	41	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	B	46	GLN
1	C	65	ASN
1	D	46	GLN

5.3.3 RNA ⓘ

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	272/291 (93%)	0.77	39 (14%) 6 5	13, 28, 52, 68	0
1	B	266/291 (91%)	0.39	27 (10%) 12 12	14, 24, 51, 66	0
1	C	269/291 (92%)	0.60	27 (10%) 12 12	17, 29, 49, 63	0
1	D	236/291 (81%)	1.37	75 (31%) 1 0	16, 38, 55, 64	0
All	All	1043/1164 (89%)	0.77	168 (16%) 4 4	13, 29, 52, 68	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	PRO	8.9
1	A	139	MET	7.3
1	B	96	ARG	6.2
1	A	145	ALA	6.2
1	D	119	LEU	5.6
1	C	125	VAL	5.2
1	B	94	LEU	5.0
1	A	136	LEU	4.9
1	D	179	THR	4.9
1	A	124	GLY	4.9
1	B	139	MET	4.7
1	C	161	GLY	4.6
1	D	139	MET	4.6
1	D	178	TRP	4.3
1	C	123	PHE	4.2
1	D	136	LEU	4.2
1	D	89	VAL	4.2
1	D	135	ASP	4.1
1	D	174	LEU	4.1
1	D	120	SER	4.1
1	B	165	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	169	HIS	4.0
1	A	125	VAL	4.0
1	D	118	LEU	3.9
1	B	119	LEU	3.8
1	A	129	TYR	3.8
1	A	163	ARG	3.8
1	D	117	LEU	3.7
1	B	164	TYR	3.7
1	A	123	PHE	3.7
1	A	122	ARG	3.7
1	A	164	TYR	3.6
1	D	175	TRP	3.6
1	B	122	ARG	3.6
1	A	96	ARG	3.6
1	D	168	VAL	3.6
1	D	254	LEU	3.6
1	D	167	ASP	3.5
1	D	83	VAL	3.5
1	D	134	PRO	3.5
1	D	137	SER	3.5
1	B	193	ASP	3.5
1	D	233	PHE	3.4
1	D	258	THR	3.4
1	D	261	ALA	3.3
1	D	155	ARG	3.3
1	D	199	PRO	3.2
1	A	119	LEU	3.2
1	B	138	LEU	3.2
1	B	197	ARG	3.2
1	D	257	VAL	3.2
1	D	280	LYS	3.1
1	A	118	LEU	3.1
1	D	171	LEU	3.1
1	D	156	ALA	3.1
1	D	275	LYS	3.1
1	D	274	VAL	3.0
1	A	165	GLY	3.0
1	C	159	ILE	3.0
1	C	124	GLY	3.0
1	D	122	ARG	3.0
1	C	97	LEU	3.0
1	D	256	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	179	THR	2.9
1	D	270	PHE	2.9
1	D	203	ARG	2.8
1	B	128	ASP	2.8
1	C	136	LEU	2.8
1	C	91	GLN	2.8
1	A	93	PRO	2.8
1	A	102	VAL	2.7
1	C	168	VAL	2.7
1	A	146	ALA	2.7
1	A	179	THR	2.7
1	C	118	LEU	2.7
1	C	126	GLN	2.7
1	D	252	PRO	2.7
1	C	92	VAL	2.7
1	A	268	THR	2.7
1	B	5	THR	2.7
1	B	134	PRO	2.7
1	C	34	GLU	2.6
1	D	115	ALA	2.6
1	D	232	ALA	2.6
1	A	67	ASP	2.6
1	A	92	VAL	2.6
1	B	102	VAL	2.6
1	C	275	LYS	2.6
1	D	176	LYS	2.6
1	D	266	PRO	2.6
1	D	265	GLY	2.6
1	D	255	GLU	2.6
1	A	166	LEU	2.6
1	D	263	ARG	2.6
1	A	266	PRO	2.6
1	A	94	LEU	2.6
1	A	97	LEU	2.6
1	B	166	LEU	2.6
1	D	278	LEU	2.6
1	D	81	GLY	2.5
1	C	221	GLU	2.5
1	A	178	TRP	2.5
1	D	158	MET	2.5
1	D	247	PHE	2.5
1	A	100	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	143	ALA	2.5
1	C	4	ARG	2.5
1	C	87	VAL	2.4
1	D	264	VAL	2.4
1	D	129	TYR	2.4
1	D	182	PRO	2.4
1	D	146	ALA	2.4
1	B	163	ARG	2.4
1	D	138	LEU	2.4
1	D	112	VAL	2.4
1	A	101	ARG	2.4
1	C	122	ARG	2.4
1	D	5	THR	2.4
1	D	218	GLU	2.4
1	A	99	GLY	2.4
1	A	262	ARG	2.4
1	B	92	VAL	2.4
1	D	250	GLY	2.3
1	C	95	ASP	2.3
1	D	260	PHE	2.3
1	C	93	PRO	2.3
1	D	251	ALA	2.3
1	B	101	ARG	2.3
1	D	204	LYS	2.3
1	D	183	PHE	2.3
1	D	152	ALA	2.3
1	A	95	ASP	2.3
1	A	117	LEU	2.3
1	C	99	GLY	2.3
1	D	87	VAL	2.3
1	C	155	ARG	2.3
1	A	120	SER	2.2
1	D	217	LEU	2.2
1	A	127	PRO	2.2
1	D	157	ASN	2.2
1	D	184	VAL	2.2
1	A	221	GLU	2.2
1	A	126	GLN	2.2
1	C	160	ASP	2.2
1	B	142	GLU	2.2
1	C	143	ALA	2.2
1	B	136	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	279	LEU	2.2
1	D	262	ARG	2.2
1	D	243	THR	2.2
1	D	88	ILE	2.1
1	D	173	ALA	2.1
1	C	98	ASP	2.1
1	A	270	PHE	2.1
1	D	185	PHE	2.1
1	D	172	GLY	2.1
1	D	200	VAL	2.1
1	D	148	LEU	2.1
1	C	142	GLU	2.1
1	D	121	GLU	2.1
1	D	273	ASP	2.0
1	B	93	PRO	2.0
1	B	161	GLY	2.0
1	A	218	GLU	2.0
1	A	277	GLU	2.0
1	B	120	SER	2.0
1	C	137	SER	2.0
1	B	155	ARG	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.