



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 01:50 PM UTC

PDB ID : 6QB5 / pdb_00006qb5
Title : Crystal structure of the N-terminal region of human cohesin subunit STAG1
Authors : Newman, J.A.; Katis, V.L.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Gileadi, O.
Deposited on : 2018-12-20
Resolution : 2.02 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

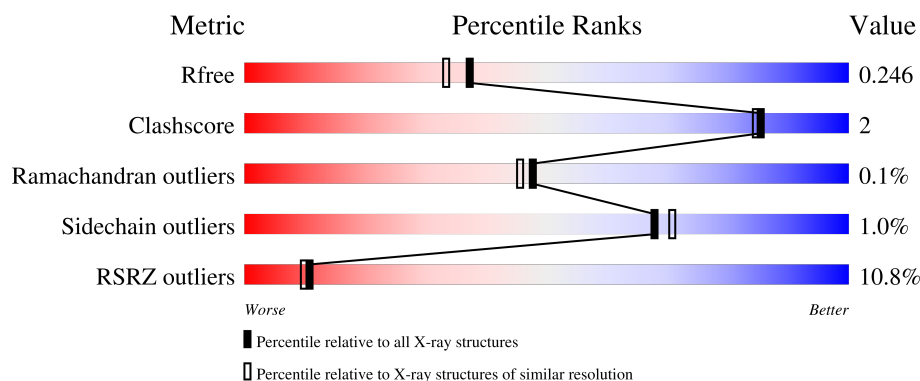
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	339	11% 84% 5% 11%
1	B	339	12% 84% 9% 7%
1	C	339	8% 86% 7% 7%
1	D	339	9% 83% 6% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10628 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 Cohesin subunit SA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	315	Total	C	N	O	S	0	1	0
			2571	1637	434	480	20			
1	A	303	Total	C	N	O	S	0	0	0
			2414	1540	404	450	20			
1	B	316	Total	C	N	O	S	0	0	0
			2549	1623	432	474	20			
1	D	305	Total	C	N	O	S	0	0	0
			2466	1569	416	461	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	82	SER	-	expression tag	UNP Q8WVM7
C	83	MET	-	expression tag	UNP Q8WVM7
C	84	GLY	-	expression tag	UNP Q8WVM7
C	85	GLY	-	expression tag	UNP Q8WVM7
A	82	SER	-	expression tag	UNP Q8WVM7
A	83	MET	-	expression tag	UNP Q8WVM7
A	84	GLY	-	expression tag	UNP Q8WVM7
A	85	GLY	-	expression tag	UNP Q8WVM7
B	82	SER	-	expression tag	UNP Q8WVM7
B	83	MET	-	expression tag	UNP Q8WVM7
B	84	GLY	-	expression tag	UNP Q8WVM7
B	85	GLY	-	expression tag	UNP Q8WVM7
D	82	SER	-	expression tag	UNP Q8WVM7
D	83	MET	-	expression tag	UNP Q8WVM7
D	84	GLY	-	expression tag	UNP Q8WVM7
D	85	GLY	-	expression tag	UNP Q8WVM7

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Na 1	0	0

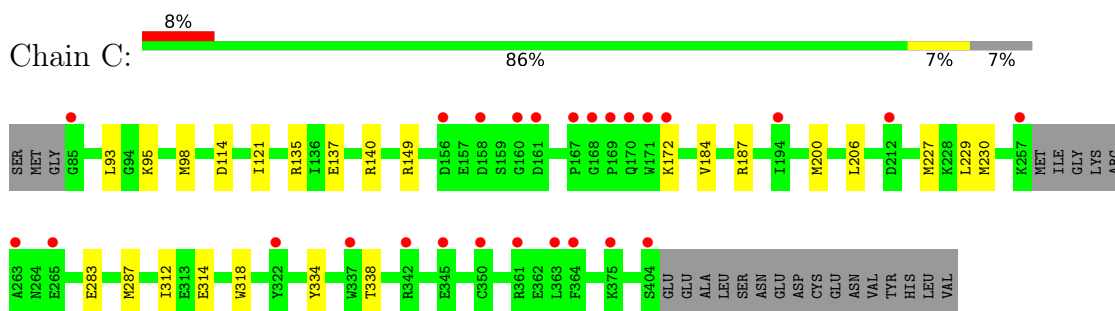
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	169	Total 169	O 169	0	0
3	A	152	Total 152	O 152	0	0
3	B	148	Total 148	O 148	0	0
3	D	158	Total 158	O 158	0	0

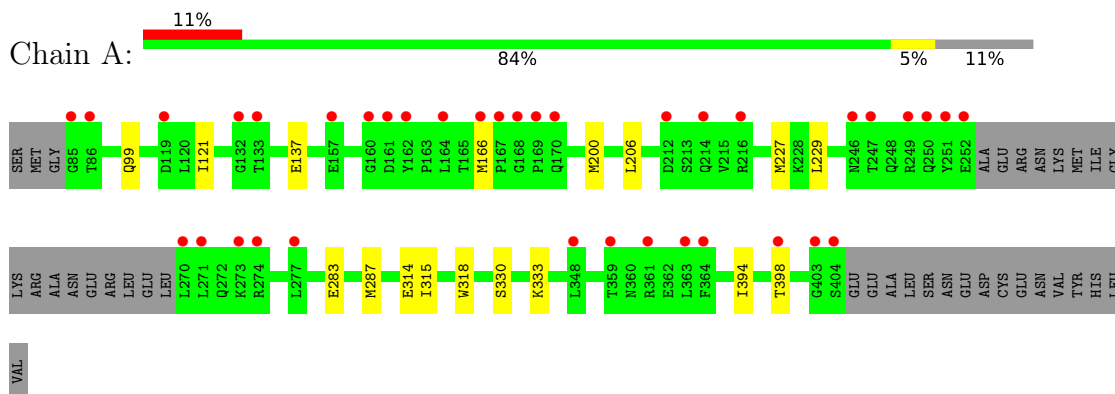
3 Residue-property plots [i](#)

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.

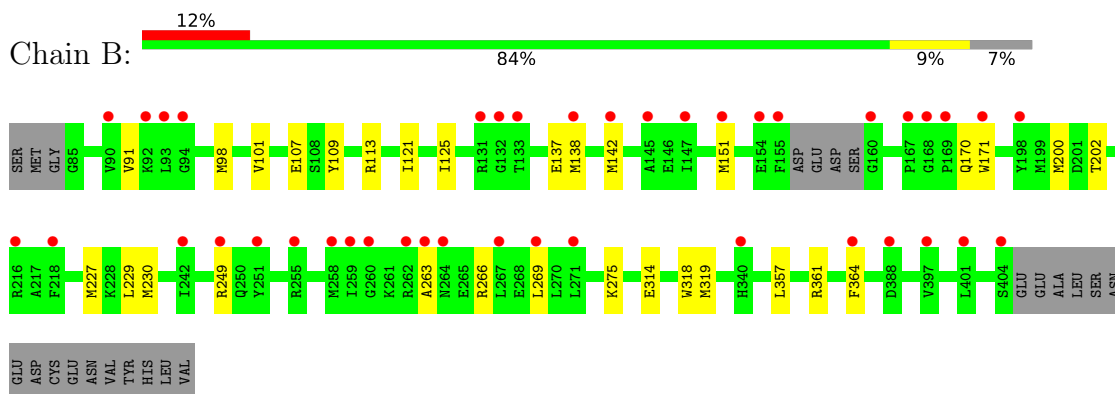
- Molecule 1: Cohesin subunit SA-1



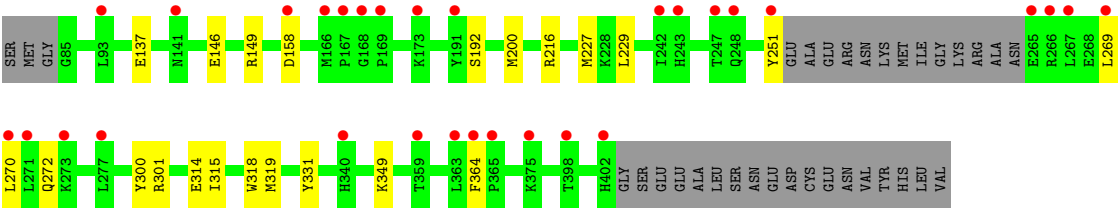
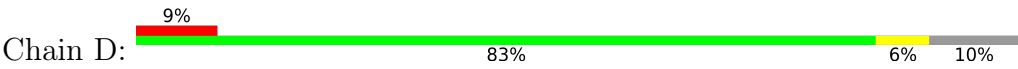
- Molecule 1: Cohesin subunit SA-1



- Molecule 1: Cohesin subunit SA-1



- Molecule 1: Cohesin subunit SA-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.61Å 124.98Å 231.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.00 – 2.02 85.00 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.5 (85.00-2.02) 99.7 (85.00-2.02)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.02Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.218 , 0.245 0.221 , 0.246	Depositor DCC
R_{free} test set	6246 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10628	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.08	0/2455	0.23	0/3313
1	B	0.08	0/2591	0.23	0/3492
1	C	0.09	0/2615	0.24	0/3523
1	D	0.08	0/2507	0.24	0/3381
All	All	0.08	0/10168	0.24	0/13709

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2414	0	2369	8	0
1	B	2549	0	2522	14	0
1	C	2571	0	2550	13	0
1	D	2466	0	2433	10	0
2	D	1	0	0	0	0
3	A	152	0	0	0	0
3	B	148	0	0	1	0
3	C	169	0	0	1	0
3	D	158	0	0	1	0
All	All	10628	0	9874	44	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 2.

All (44) 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:B:138:MET:HB3	1:B:142:MET:HE2	1.76	0.67
1:D:300:TYR:OH	1:D:301:ARG:NH2	2.31	0.63
1:A:121:ILE:HG12	1:A:206:LEU:HD22	1.81	0.62
1:C:227:MET:HB3	1:C:314:GLU:HG2	1.83	0.61
1:D:227:MET:HB3	1:D:314:GLU:HG2	1.83	0.60
1:D:200:MET:HE1	1:D:229:LEU:HD11	1.84	0.60
1:B:227:MET:HB3	1:B:314:GLU:HG2	1.83	0.59
1:C:135:ARG:NH1	1:C:137:GLU:OE2	2.38	0.57
1:A:227:MET:HB3	1:A:314:GLU:HG2	1.87	0.57
1:D:319:MET:HE2	1:D:331:TYR:HB3	1.86	0.57
1:C:98:MET:HE1	1:B:91:VAL:HA	1.86	0.57
1:C:114:ASP:OD2	1:C:140:ARG:NH1	2.41	0.53
1:C:200:MET:HE1	1:C:229:LEU:HD11	1.92	0.52
1:A:330:SER:O	1:A:333:LYS:NZ	2.39	0.52
1:B:121:ILE:HD11	1:B:202:THR:HG22	1.92	0.52
1:A:200:MET:HE1	1:A:229:LEU:HD11	1.92	0.51
1:A:394:ILE:O	1:A:398:THR:HG23	2.11	0.51
1:C:312:ILE:HG13	1:C:338:THR:HG21	1.92	0.51
1:D:146:GLU:HG3	1:D:149:ARG:HH22	1.78	0.49
1:C:149:ARG:NH2	3:C:503:HOH:O	2.35	0.49
1:C:121:ILE:HG12	1:C:206:LEU:HD22	1.95	0.48
1:B:275:LYS:NZ	3:B:513:HOH:O	2.45	0.48
1:C:93:LEU:HD21	1:C:95:LYS:HE3	1.95	0.48
1:D:158:ASP:OD1	1:D:216:ARG:NE	2.47	0.47
1:B:200:MET:HE1	1:B:229:LEU:HD11	1.96	0.46
1:B:109:TYR:CZ	1:B:113:ARG:HG2	2.51	0.46
1:D:251:TYR:HA	1:D:270:LEU:HD13	1.97	0.45
1:C:184:VAL:HG22	1:C:187:ARG:HH22	1.81	0.45
1:D:349:LYS:NZ	3:D:602:HOH:O	2.32	0.45
1:A:283:GLU:HG3	1:A:287:MET:HE3	1.99	0.45
1:C:283:GLU:HG2	1:C:287:MET:HE3	1.98	0.44
1:C:334:TYR:O	1:C:338:THR:OG1	2.31	0.43
1:D:315:ILE:HG12	1:D:319:MET:HE3	2.00	0.43
1:C:230:MET:HG2	1:C:318:TRP:CE2	2.55	0.42
1:B:263:ALA:HB3	1:B:266:ARG:HB3	2.02	0.42
1:D:315:ILE:HA	1:D:318:TRP:CE3	2.55	0.42
1:B:319:MET:HE3	1:B:357:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:MET:HA	1:B:101:VAL:HG12	2.02	0.41
1:A:166:MET:HE2	1:A:166:MET:HB3	1.99	0.41
1:B:125:ILE:HG21	1:B:151:MET:HE3	2.02	0.41
1:B:170:GLN:HG2	1:B:171:TRP:CD1	2.56	0.41
1:B:361:ARG:HA	1:B:364:PHE:CD1	2.56	0.41
1:B:230:MET:HG2	1:B:318:TRP:CZ2	2.56	0.40
1:A:315:ILE:HA	1:A:318:TRP:CE3	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	299/339 (88%)	293 (98%)	6 (2%)	0	100	100
1	B	312/339 (92%)	307 (98%)	5 (2%)	0	100	100
1	C	312/339 (92%)	307 (98%)	5 (2%)	0	100	100
1	D	301/339 (89%)	296 (98%)	4 (1%)	1 (0%)	36	31
All	All	1224/1356 (90%)	1203 (98%)	20 (2%)	1 (0%)	48	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	192	SER

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	260/306 (85%)	258 (99%)	2 (1%)	73	75
1	B	275/306 (90%)	271 (98%)	4 (2%)	57	59
1	C	281/306 (92%)	280 (100%)	1 (0%)	84	84
1	D	269/306 (88%)	265 (98%)	4 (2%)	57	59
All	All	1085/1224 (89%)	1074 (99%)	11 (1%)	68	71

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	172	LYS
1	A	99	GLN
1	A	137	GLU
1	B	107	GLU
1	B	137	GLU
1	B	249	ARG
1	B	269	LEU
1	D	137	GLU
1	D	269	LEU
1	D	272	GLN
1	D	364	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	188	GLN
1	C	278	GLN
1	C	360	ASN
1	A	141	ASN
1	A	286	ASN
1	B	188	GLN
1	D	243	HIS
1	D	289	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	303/339 (89%)	0.76	37 (12%) 8 7	28, 43, 80, 94	0
1	B	316/339 (93%)	0.89	41 (12%) 7 6	28, 47, 74, 86	0
1	C	315/339 (92%)	0.73	26 (8%) 17 16	25, 42, 74, 100	1 (0%)
1	D	305/339 (89%)	0.79	30 (9%) 13 12	29, 43, 81, 104	0
All	All	1239/1356 (91%)	0.79	134 (10%) 11 10	25, 44, 77, 104	1 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337[A]	TRP	10.8
1	D	267	LEU	6.7
1	D	269	LEU	6.5
1	A	270	LEU	6.2
1	D	270	LEU	5.8
1	D	251	TYR	5.2
1	A	251	TYR	5.2
1	A	162	TYR	5.1
1	A	85	GLY	4.7
1	A	271	LEU	4.3
1	C	364	PHE	4.1
1	A	364	PHE	4.1
1	D	266	ARG	4.0
1	D	191	TYR	4.0
1	A	403	GLY	3.8
1	A	168	GLY	3.8
1	B	93	LEU	3.6
1	B	267	LEU	3.6
1	C	168	GLY	3.6
1	B	160	GLY	3.6
1	B	242	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	271	LEU	3.4
1	B	258	MET	3.4
1	C	170	GLN	3.4
1	A	246	ASN	3.3
1	A	160	GLY	3.3
1	D	141	ASN	3.3
1	A	86	THR	3.2
1	D	265	GLU	3.2
1	B	263	ALA	3.2
1	C	171	TRP	3.2
1	C	167	PRO	3.2
1	C	404	SER	3.1
1	A	161	ASP	3.1
1	A	247	THR	3.1
1	D	364	PHE	3.1
1	A	212	ASP	3.1
1	B	260	GLY	3.0
1	C	169	PRO	3.0
1	B	155	PHE	3.0
1	B	131	ARG	3.0
1	D	247	THR	3.0
1	B	264	ASN	3.0
1	B	340	HIS	2.9
1	A	170	GLN	2.9
1	B	198	TYR	2.9
1	B	151	MET	2.9
1	A	169	PRO	2.9
1	B	154	GLU	2.9
1	C	263	ALA	2.9
1	C	160	GLY	2.9
1	C	361	ARG	2.8
1	D	167	PRO	2.8
1	B	364	PHE	2.8
1	A	404	SER	2.8
1	C	158	ASP	2.8
1	B	138	MET	2.7
1	D	273	LYS	2.7
1	B	249	ARG	2.7
1	D	93	LEU	2.7
1	B	90	VAL	2.7
1	A	157	GLU	2.7
1	C	212	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	363	LEU	2.6
1	D	398	THR	2.6
1	D	243	HIS	2.6
1	A	273	LYS	2.6
1	D	242	ILE	2.6
1	B	218	PHE	2.6
1	D	173	LYS	2.6
1	A	167	PRO	2.6
1	B	167	PRO	2.6
1	A	249	ARG	2.5
1	C	172	LYS	2.5
1	B	169	PRO	2.5
1	A	359	THR	2.4
1	D	169	PRO	2.4
1	A	274	ARG	2.4
1	B	255	ARG	2.4
1	A	166	MET	2.4
1	B	142	MET	2.4
1	A	214	GLN	2.4
1	B	397	VAL	2.4
1	A	398	THR	2.4
1	D	365	PRO	2.4
1	D	363	LEU	2.4
1	D	168	GLY	2.4
1	B	404	SER	2.4
1	B	133	THR	2.4
1	D	402	HIS	2.4
1	B	94	GLY	2.3
1	B	147	ILE	2.3
1	C	345	GLU	2.3
1	B	269	LEU	2.3
1	A	216	ARG	2.3
1	D	166	MET	2.3
1	B	259	ILE	2.3
1	C	350	CYS	2.3
1	C	85	GLY	2.3
1	C	161	ASP	2.3
1	A	164	LEU	2.3
1	D	248	GLN	2.3
1	D	359	THR	2.3
1	B	262	ARG	2.3
1	B	271	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	342	ARG	2.2
1	A	363	LEU	2.2
1	B	168	GLY	2.2
1	B	145	ALA	2.2
1	C	257	LYS	2.2
1	A	119	ASP	2.2
1	D	158	ASP	2.2
1	B	92	LYS	2.2
1	A	252	GLU	2.1
1	B	132	GLY	2.1
1	A	133	THR	2.1
1	A	250	GLN	2.1
1	A	361	ARG	2.1
1	A	277	LEU	2.1
1	B	171	TRP	2.1
1	B	401	LEU	2.1
1	D	277	LEU	2.1
1	C	265	GLU	2.1
1	C	156	ASP	2.1
1	B	251	TYR	2.1
1	D	340	HIS	2.1
1	C	194	ILE	2.1
1	C	375	LYS	2.1
1	A	348	LEU	2.0
1	B	388	ASP	2.0
1	B	216	ARG	2.0
1	D	375	LYS	2.0
1	A	132	GLY	2.0
1	C	322	TYR	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 oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	D	501	1/1	0.93	0.12	45,45,45,45	0

6.5 Other polymers

There are no such residues in this entry.