



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:46 AM UTC

PDB ID : 4QL6 / pdb_00004ql6
Title : Structure of C. trachomatis CT441
Authors : Kohlmann, F.; Hilgenfeld, R.; Hansen, G.
Deposited on : 2014-06-10
Resolution : 2.97 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

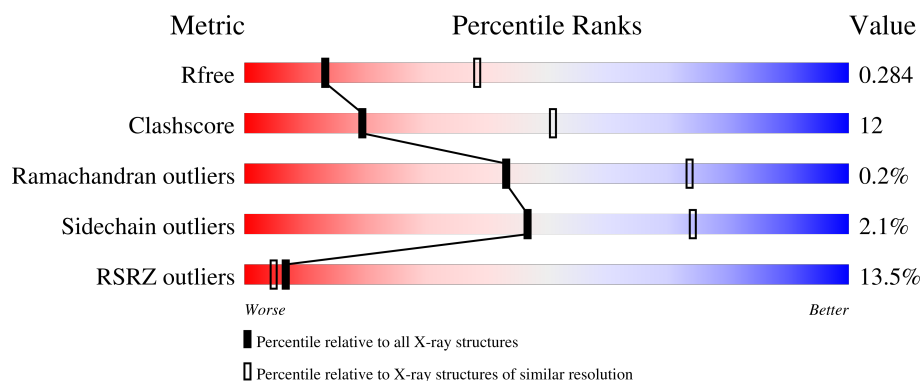
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	634	
1	B	634	
1	C	634	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12071 atoms, of which 0 are hydrogens and 0 are deuteriums.

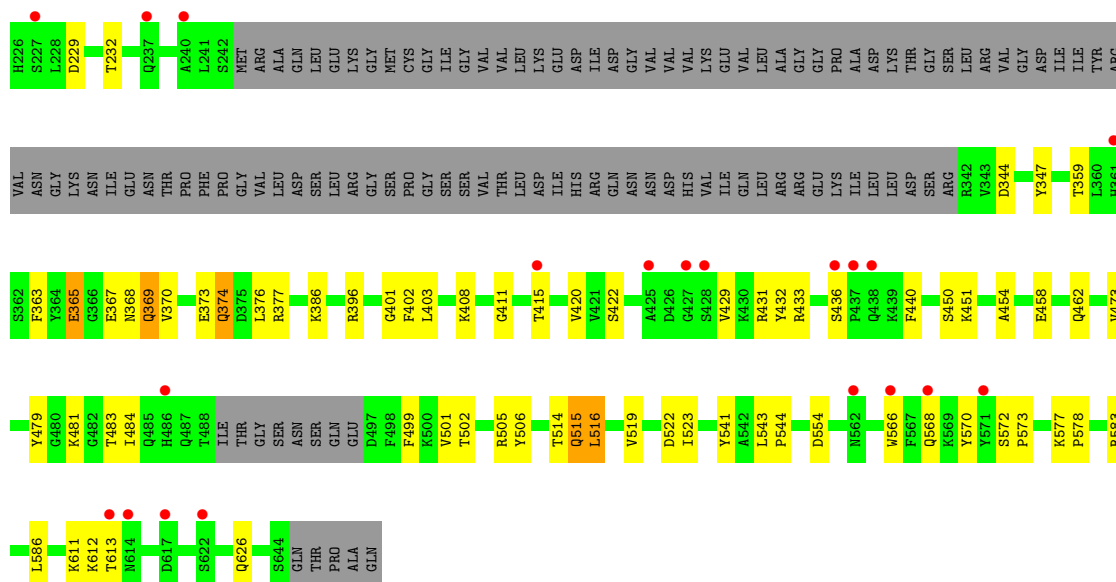
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Carboxy-terminal processing protease.

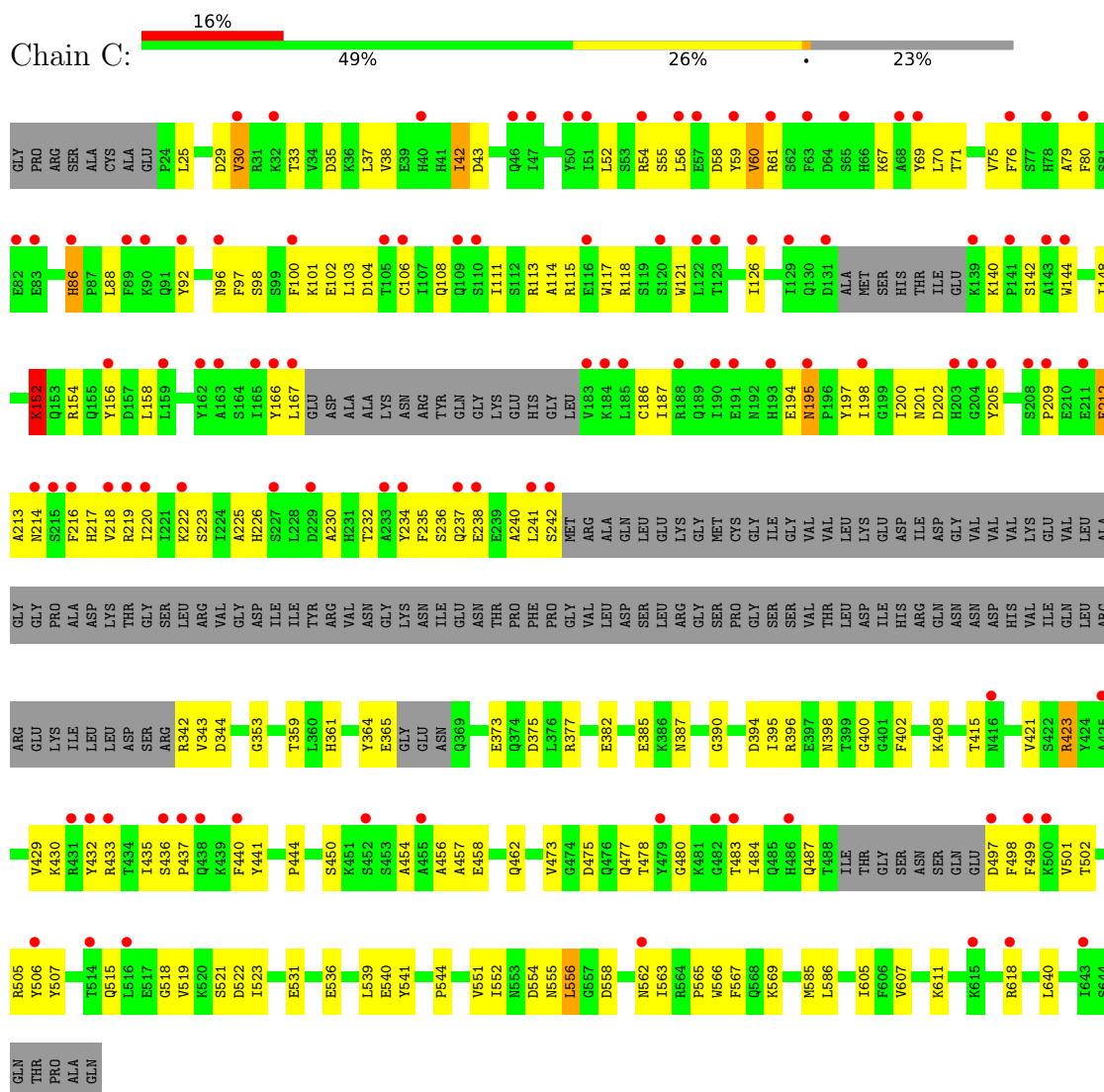
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3970	2510	687	767	6			
1	B	509	Total	C	N	O	S	0	0	0
			4127	2607	715	798	7			
1	C	489	Total	C	N	O	S	0	0	0
			3974	2515	688	765	6			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLY	-	expression tag	UNP B0B813
A	17	PRO	-	expression tag	UNP B0B813
A	18	ARG	-	expression tag	UNP B0B813
A	19	SER	-	expression tag	UNP B0B813
A	20	ALA	-	expression tag	UNP B0B813
A	21	CYS	-	expression tag	UNP B0B813
A	455	ALA	SER	engineered mutation	UNP B0B813
B	16	GLY	-	expression tag	UNP B0B813
B	17	PRO	-	expression tag	UNP B0B813
B	18	ARG	-	expression tag	UNP B0B813
B	19	SER	-	expression tag	UNP B0B813
B	20	ALA	-	expression tag	UNP B0B813
B	21	CYS	-	expression tag	UNP B0B813
B	455	ALA	SER	engineered mutation	UNP B0B813
C	16	GLY	-	expression tag	UNP B0B813
C	17	PRO	-	expression tag	UNP B0B813
C	18	ARG	-	expression tag	UNP B0B813
C	19	SER	-	expression tag	UNP B0B813
C	20	ALA	-	expression tag	UNP B0B813
C	21	CYS	-	expression tag	UNP B0B813
C	455	ALA	SER	engineered mutation	UNP B0B813



• Molecule 1: Carboxy-terminal processing protease



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.73Å 183.99Å 209.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.44 – 2.97 33.44 – 2.97	Depositor EDS
% Data completeness (in resolution range)	91.5 (33.44-2.97) 91.4 (33.44-2.97)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.256 , 0.281 0.259 , 0.284	Depositor DCC
R_{free} test set	3232 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.9	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	0.90	EDS
Total number of atoms	12071	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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	0.33	0/4049	0.74	0/5469
1	B	0.32	0/4211	0.75	1/5687 (0.0%)
1	C	0.33	0/4053	0.81	6/5471 (0.1%)
All	All	0.33	0/12313	0.77	7/16627 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	HIS	CA-C-N	-7.34	112.61	120.47
1	C	86	HIS	C-N-CA	-7.34	112.61	120.47
1	C	515	GLN	N-CA-C	5.92	118.97	111.69
1	C	212	GLU	N-CA-C	-5.74	106.11	113.23
1	B	42	ILE	N-CA-C	5.33	115.54	110.53
1	C	42	ILE	N-CA-C	5.29	115.50	110.42
1	C	195	ASN	N-CA-C	5.16	121.21	109.81

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	3970	0	3884	69	0
1	B	4127	0	4040	75	0
1	C	3974	0	3903	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12071	0	11827	277	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 12.

All (277) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LYS:HZ2	1:C:142:SER:H	1.23	0.86
1:C:235:PHE:HB2	1:C:498:PHE:HB3	1.58	0.85
1:A:111:ILE:HG22	1:A:115:ARG:HH12	1.48	0.78
1:C:42:ILE:HD11	1:C:505:ARG:HG3	1.69	0.75
1:C:423:ARG:HH11	1:C:423:ARG:CG	2.00	0.74
1:A:42:ILE:HD13	1:A:504:GLY:HA2	1.70	0.73
1:C:67:LYS:NZ	1:C:142:SER:H	1.86	0.72
1:B:129:ILE:HG13	1:B:179:GLU:HB3	1.71	0.72
1:C:423:ARG:HH11	1:C:423:ARG:HG3	1.55	0.71
1:B:363:PHE:HB2	1:B:401:GLY:HA3	1.72	0.71
1:A:41:HIS:O	1:A:45:GLN:NE2	2.24	0.70
1:C:195:ASN:HB3	1:C:200:ILE:HG13	1.75	0.69
1:C:121:TRP:HZ2	1:C:156:TYR:CD1	2.11	0.68
1:B:118:ARG:NH2	1:B:194:GLU:OE2	2.28	0.66
1:C:108:GLN:NE2	1:C:197:TYR:O	2.27	0.66
1:C:115:ARG:HD2	1:C:118:ARG:HH12	1.61	0.66
1:B:213:ALA:O	1:B:217:HIS:ND1	2.27	0.66
1:A:213:ALA:O	1:A:217:HIS:ND1	2.30	0.65
1:A:396:ARG:NH2	1:A:624:ASP:OD2	2.25	0.65
1:B:60:VAL:HG13	1:B:103:LEU:HD21	1.78	0.64
1:B:522:ASP:OD1	1:B:583:ARG:NH1	2.24	0.64
1:C:343:VAL:HG11	1:C:375:ASP:HB3	1.79	0.64
1:A:373:GLU:OE2	1:A:377:ARG:NH1	2.30	0.64
1:A:63:PHE:O	1:A:193:HIS:NE2	2.31	0.63
1:C:423:ARG:HH11	1:C:423:ARG:HB2	1.63	0.63
1:B:207:MET:HE3	1:B:212:GLU:HA	1.80	0.63
1:B:422:SER:HB2	1:B:429:VAL:HB	1.80	0.62
1:B:196:PRO:O	1:B:219:ARG:NH1	2.33	0.61
1:C:423:ARG:HH11	1:C:423:ARG:CB	2.14	0.60
1:A:210:GLU:O	1:A:214:ASN:N	2.33	0.60
1:C:536:GLU:HG3	1:C:539:LEU:HD12	1.82	0.60
1:B:422:SER:OG	1:B:431:ARG:NH1	2.35	0.59
1:B:91:GLN:HB3	1:B:96:ASN:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:GLN:HA	1:B:572:SER:HB2	1.84	0.59
1:A:238:GLU:OE1	1:A:238:GLU:N	2.36	0.59
1:C:556:LEU:HD13	1:C:567:PHE:HB2	1.85	0.59
1:C:69:TYR:O	1:C:113:ARG:NH2	2.36	0.59
1:C:225:ALA:HB1	1:C:232:THR:HG22	1.85	0.59
1:B:83:GLU:N	1:B:83:GLU:OE1	2.35	0.59
1:C:98:SER:HA	1:C:101:LYS:HG2	1.85	0.58
1:C:566:TRP:HE3	1:C:567:PHE:HD1	1.51	0.58
1:A:454:ALA:HA	1:A:458:GLU:HG3	1.86	0.58
1:B:454:ALA:HB2	1:B:479:TYR:HB3	1.86	0.57
1:C:423:ARG:HB2	1:C:423:ARG:NH1	2.18	0.57
1:A:396:ARG:NH1	1:A:626:GLN:HB2	2.19	0.57
1:A:432:TYR:HE1	1:A:554:ASP:OD2	1.87	0.57
1:C:67:LYS:HZ1	1:C:140:LYS:HB3	1.69	0.57
1:A:432:TYR:CE1	1:A:554:ASP:OD2	2.57	0.57
1:A:60:VAL:HG13	1:A:103:LEU:HD21	1.86	0.56
1:B:505:ARG:NH2	1:B:544:PRO:O	2.38	0.56
1:A:634:VAL:HA	1:A:637:MET:HE3	1.87	0.56
1:C:152:LYS:HG2	1:C:156:TYR:CE1	2.41	0.56
1:C:566:TRP:HE3	1:C:567:PHE:CD1	2.24	0.56
1:C:462:GLN:HB2	1:C:519:VAL:HG22	1.87	0.56
1:C:505:ARG:NH2	1:C:544:PRO:O	2.36	0.56
1:C:237:GLN:NE2	1:C:497:ASP:HB2	2.21	0.56
1:C:497:ASP:HB3	1:C:498:PHE:HB2	1.87	0.56
1:B:50:TYR:OH	1:B:54:ARG:NH1	2.38	0.55
1:C:396:ARG:O	1:C:450:SER:OG	2.24	0.55
1:B:577:LYS:HD2	1:B:578:PRO:HD2	1.89	0.55
1:B:566:TRP:CD2	1:C:566:TRP:HZ2	2.24	0.55
1:A:207:MET:HB2	1:A:211:GLU:HB3	1.88	0.55
1:B:111:ILE:HD13	1:B:194:GLU:HB3	1.88	0.55
1:C:230:ALA:N	1:C:541:TYR:O	2.40	0.55
1:C:483:THR:HB	1:C:502:THR:HG23	1.88	0.55
1:C:37:LEU:HD11	1:C:501:VAL:HB	1.88	0.55
1:A:567:PHE:HA	1:A:571:TYR:HB3	1.89	0.54
1:C:522:ASP:HB3	1:C:586:LEU:HD21	1.89	0.54
1:B:484:ILE:HG12	1:B:506:TYR:CE2	2.42	0.54
1:C:344:ASP:HB2	1:C:359:THR:HB	1.90	0.54
1:C:71:THR:O	1:C:75:VAL:HG23	2.08	0.54
1:C:115:ARG:CD	1:C:118:ARG:HH12	2.20	0.54
1:C:118:ARG:HD2	1:C:187:ILE:HD11	1.89	0.54
1:C:458:GLU:OE2	1:C:480:GLY:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:TYR:OH	1:C:104:ASP:OD2	2.25	0.54
1:C:114:ALA:O	1:C:118:ARG:HG3	2.07	0.54
1:B:225:ALA:HB1	1:B:232:THR:HG22	1.90	0.54
1:C:54:ARG:HD2	1:C:541:TYR:CE1	2.43	0.54
1:C:52:LEU:HD13	1:C:88:LEU:HB3	1.89	0.54
1:C:454:ALA:O	1:C:458:GLU:N	2.31	0.53
1:C:209:PRO:HA	1:C:212:GLU:HB3	1.89	0.53
1:B:232:THR:HG23	1:B:501:VAL:HG12	1.90	0.53
1:C:377:ARG:HA	1:C:440:PHE:HE2	1.73	0.53
1:C:166:TYR:HA	1:C:167:LEU:C	2.34	0.53
1:B:122:LEU:O	1:B:125:SER:OG	2.22	0.53
1:C:433:ARG:NH1	1:C:435:ILE:HD13	2.24	0.53
1:A:71:THR:HG23	1:A:74:GLU:OE2	2.08	0.53
1:A:201:ASN:OD1	1:A:203:HIS:N	2.38	0.53
1:C:121:TRP:CH2	1:C:156:TYR:HA	2.43	0.53
1:C:430:LYS:HD3	1:C:551:VAL:HG11	1.91	0.52
1:B:61:ARG:NH2	1:B:541:TYR:OH	2.43	0.52
1:C:111:ILE:HG23	1:C:194:GLU:OE2	2.10	0.52
1:C:421:VAL:O	1:C:507:TYR:N	2.43	0.52
1:C:121:TRP:HZ2	1:C:156:TYR:CE1	2.28	0.51
1:C:359:THR:HA	1:C:394:ASP:HB3	1.92	0.51
1:B:115:ARG:HH11	1:B:191:GLU:HG2	1.74	0.51
1:C:152:LYS:HG2	1:C:156:TYR:CZ	2.45	0.51
1:C:121:TRP:CZ2	1:C:156:TYR:CD1	2.98	0.51
1:C:531:GLU:OE2	1:C:611:LYS:HG2	2.11	0.51
1:C:104:ASP:OD2	1:C:216:PHE:HD1	1.93	0.51
1:B:207:MET:HB2	1:B:211:GLU:HB2	1.92	0.51
1:C:373:GLU:HG3	1:C:408:LYS:HB3	1.92	0.51
1:C:484:ILE:HG12	1:C:506:TYR:CZ	2.46	0.51
1:A:145:ALA:HB1	1:A:150:GLU:HB3	1.92	0.50
1:C:58:ASP:OD1	1:C:226:HIS:ND1	2.43	0.50
1:A:564:ARG:N	1:A:565:PRO:HD2	2.27	0.50
1:A:64:ASP:OD2	1:A:67:LYS:HA	2.12	0.50
1:C:55:SER:O	1:C:223:SER:OG	2.24	0.50
1:C:52:LEU:HB3	1:C:88:LEU:HD23	1.94	0.50
1:C:217:HIS:O	1:C:220:ILE:HG22	2.12	0.50
1:A:122:LEU:HD13	1:A:187:ILE:HD13	1.93	0.49
1:A:497:ASP:OD1	1:A:497:ASP:N	2.45	0.49
1:C:102:GLU:O	1:C:106:CYS:N	2.41	0.49
1:C:432:TYR:HE2	1:C:554:ASP:OD1	1.95	0.49
1:B:64:ASP:OD2	1:B:68:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:TRP:CZ3	1:B:570:TYR:HB2	2.47	0.49
1:B:568:GLN:O	1:B:573:PRO:HD3	2.11	0.49
1:C:565:PRO:O	1:C:569:LYS:HG3	2.12	0.49
1:A:111:ILE:CG2	1:A:115:ARG:HH12	2.21	0.49
1:C:201:ASN:N	1:C:205:TYR:O	2.37	0.49
1:A:435:ILE:HG23	1:A:436:SER:O	2.11	0.49
1:A:61:ARG:NH2	1:A:541:TYR:OH	2.45	0.49
1:C:353:GLY:HA2	1:C:387:ASN:HB3	1.95	0.49
1:A:515:GLN:NE2	1:A:543:LEU:O	2.37	0.49
1:C:61:ARG:NH1	1:C:540:GLU:HG2	2.28	0.49
1:B:200:ILE:HA	1:B:206:ARG:HA	1.94	0.48
1:C:395:ILE:HD12	1:C:457:ALA:HB1	1.95	0.48
1:A:415:THR:OG1	1:A:437:PRO:O	2.30	0.48
1:B:522:ASP:HB3	1:B:586:LEU:HD21	1.94	0.48
1:A:342:ARG:NH2	1:A:370:VAL:HG11	2.28	0.48
1:A:75:VAL:HG21	1:A:144:TRP:CD2	2.48	0.48
1:A:26:ARG:HH21	1:A:27:ARG:HH21	1.60	0.48
1:C:115:ARG:HA	1:C:118:ARG:NH1	2.28	0.48
1:C:117:TRP:CZ2	1:C:152:LYS:HG3	2.49	0.48
1:B:43:ASP:OD1	1:B:505:ARG:NH1	2.46	0.47
1:C:197:TYR:CE2	1:C:219:ARG:NH1	2.83	0.47
1:B:411:GLY:HA3	1:B:433:ARG:HE	1.79	0.47
1:A:540:GLU:OE2	1:A:540:GLU:N	2.45	0.47
1:B:368:ASN:HA	1:B:369:GLN:HA	1.50	0.47
1:C:200:ILE:HG22	1:C:201:ASN:O	2.14	0.47
1:C:30:VAL:HG21	1:C:97:PHE:CZ	2.49	0.47
1:C:37:LEU:HD13	1:C:499:PHE:CG	2.49	0.47
1:A:473:VAL:HG12	1:A:523:ILE:HB	1.97	0.47
1:B:34:VAL:O	1:B:37:LEU:HB3	2.15	0.47
1:A:165:ILE:O	1:A:167:LEU:HB2	2.14	0.47
1:B:347:TYR:OH	1:B:386:LYS:HE2	2.14	0.47
1:B:462:GLN:HB2	1:B:519:VAL:HG22	1.96	0.47
1:B:516:LEU:HD12	1:B:516:LEU:H	1.79	0.47
1:C:30:VAL:HG21	1:C:97:PHE:HZ	1.79	0.47
1:C:76:PHE:CD1	1:C:80:PHE:HB2	2.50	0.47
1:C:361:HIS:O	1:C:398:ASN:HA	2.15	0.47
1:B:450:SER:OG	1:B:451:LYS:N	2.48	0.47
1:A:198:ILE:HG13	1:A:200:ILE:HG12	1.97	0.47
1:C:556:LEU:HD13	1:C:567:PHE:CB	2.45	0.47
1:C:400:GLY:HA2	1:C:456:ALA:HB3	1.97	0.46
1:B:369:GLN:HB2	1:B:374:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:LEU:HA	1:C:29:ASP:OD2	2.15	0.46
1:C:487:GLN:HB3	1:C:498:PHE:CZ	2.51	0.46
1:C:98:SER:HA	1:C:101:LYS:NZ	2.30	0.46
1:C:222:LYS:HG2	1:C:234:TYR:HB3	1.97	0.46
1:C:423:ARG:HG3	1:C:423:ARG:NH1	2.26	0.46
1:C:555:ASN:C	1:C:556:LEU:HG	2.41	0.46
1:A:124:ASP:OD2	1:A:127:ARG:HB3	2.16	0.46
1:B:566:TRP:CE3	1:C:566:TRP:HZ2	2.34	0.46
1:B:166:TYR:HD2	1:B:182:LEU:HD11	1.81	0.46
1:B:611:LYS:O	1:B:612:LYS:HB3	2.15	0.46
1:B:69:TYR:OH	1:B:194:GLU:OE2	2.29	0.46
1:B:199:GLY:HA2	1:B:207:MET:HE2	1.98	0.46
1:C:35:ASP:HA	1:C:38:VAL:HG22	1.97	0.46
1:C:56:LEU:HD21	1:C:79:ALA:HA	1.97	0.45
1:C:365:GLU:HB3	1:C:402:PHE:CD2	2.51	0.45
1:B:33:THR:HG22	1:B:499:PHE:HE2	1.81	0.45
1:B:229:ASP:OD2	1:B:502:THR:OG1	2.33	0.45
1:C:214:ASN:O	1:C:218:VAL:N	2.37	0.45
1:C:96:ASN:OD1	1:C:98:SER:N	2.36	0.45
1:C:75:VAL:HG21	1:C:144:TRP:CD2	2.52	0.45
1:A:342:ARG:HB3	1:A:343:VAL:H	1.48	0.45
1:B:367:GLU:O	1:B:370:VAL:N	2.50	0.45
1:A:56:LEU:HD23	1:A:85:THR:HG22	1.98	0.44
1:A:381:ARG:HG3	1:A:440:PHE:HZ	1.82	0.44
1:B:611:LYS:HB2	1:B:613:THR:HG22	1.98	0.44
1:B:365:GLU:HB2	1:B:402:PHE:CD2	2.53	0.44
1:C:113:ARG:NH1	1:C:148:ILE:HD11	2.32	0.44
1:B:522:ASP:HB3	1:B:586:LEU:HD11	1.99	0.44
1:A:359:THR:HA	1:A:394:ASP:HB3	1.99	0.44
1:C:69:TYR:HB2	1:C:70:LEU:HD12	2.00	0.44
1:A:229:ASP:OD2	1:A:502:THR:HB	2.18	0.44
1:A:201:ASN:OD1	1:A:202:ASP:N	2.51	0.44
1:B:515:GLN:HA	1:B:516:LEU:HA	1.60	0.44
1:B:612:LYS:O	1:B:612:LYS:HG2	2.18	0.44
1:C:605:ILE:HD13	1:C:618:ARG:HB3	2.00	0.44
1:A:415:THR:O	1:A:435:ILE:HG22	2.18	0.44
1:C:241:LEU:HD12	1:C:242:SER:N	2.32	0.44
1:C:342:ARG:HB3	1:C:364:TYR:OH	2.18	0.44
1:C:58:ASP:CG	1:C:226:HIS:HD1	2.26	0.44
1:A:166:TYR:HA	1:A:167:LEU:C	2.43	0.43
1:A:239:GLU:HA	1:A:240:ALA:HA	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:TYR:O	1:A:165:ILE:HG22	2.18	0.43
1:A:420:VAL:HG13	1:A:431:ARG:HG3	2.00	0.43
1:C:201:ASN:OD1	1:C:202:ASP:N	2.51	0.43
1:C:566:TRP:CE3	1:C:567:PHE:CD1	3.06	0.43
1:A:605:ILE:HD13	1:A:618:ARG:HB3	2.00	0.43
1:B:373:GLU:O	1:B:377:ARG:HB2	2.17	0.43
1:C:441:TYR:OH	1:C:444:PRO:O	2.32	0.43
1:A:445:LEU:HD23	1:A:470:ALA:HB2	2.00	0.43
1:B:403:LEU:HD11	1:B:420:VAL:HG11	2.01	0.43
1:C:115:ARG:NE	1:C:118:ARG:HH12	2.16	0.43
1:A:436:SER:OG	1:A:437:PRO:HD2	2.19	0.43
1:C:29:ASP:O	1:C:33:THR:OG1	2.33	0.43
1:A:454:ALA:HB2	1:A:479:TYR:HB3	2.00	0.43
1:C:377:ARG:HA	1:C:440:PHE:CE2	2.54	0.43
1:C:43:ASP:CG	1:C:505:ARG:HH12	2.27	0.42
1:C:585:MET:HB2	1:C:640:LEU:HD13	2.01	0.42
1:A:462:GLN:NE2	1:A:512:LYS:HG3	2.34	0.42
1:B:473:VAL:HG12	1:B:523:ILE:HB	2.01	0.42
1:C:60:VAL:HG22	1:C:103:LEU:HD21	2.01	0.42
1:C:118:ARG:HG2	1:C:121:TRP:CZ3	2.54	0.42
1:C:458:GLU:CD	1:C:480:GLY:H	2.27	0.42
1:A:376:LEU:HD23	1:A:412:LEU:HD12	2.02	0.42
1:C:236:SER:O	1:C:240:ALA:N	2.53	0.42
1:A:480:GLY:HA2	1:A:514:THR:O	2.19	0.42
1:A:63:PHE:HB2	1:A:197:TYR:CZ	2.55	0.42
1:B:28:GLN:HA	1:B:95:ASP:OD2	2.18	0.42
1:B:105:THR:O	1:B:109:GLN:HG3	2.19	0.42
1:B:115:ARG:CD	1:B:118:ARG:HH12	2.33	0.42
1:C:154:ARG:O	1:C:158:LEU:N	2.53	0.42
1:C:458:GLU:OE2	1:C:478:THR:OG1	2.33	0.42
1:C:562:ASN:OD1	1:C:563:ILE:N	2.52	0.42
1:B:481:LYS:O	1:B:514:THR:OG1	2.37	0.42
1:A:455:ALA:HB2	1:A:481:LYS:HD3	2.02	0.42
1:C:436:SER:OG	1:C:437:PRO:HD2	2.20	0.42
1:B:483:THR:HB	1:B:502:THR:HG23	2.02	0.42
1:C:118:ARG:HA	1:C:121:TRP:CE3	2.55	0.42
1:C:195:ASN:HA	1:C:198:ILE:HD13	2.02	0.42
1:A:90:LYS:HD3	1:A:90:LYS:HA	1.88	0.42
1:A:525:ILE:HG22	1:A:626:GLN:HG3	2.03	0.41
1:B:408:LYS:HD3	1:B:433:ARG:HH22	1.85	0.41
1:C:61:ARG:NH2	1:C:541:TYR:OH	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:GLN:HG3	1:C:518:GLY:H	1.85	0.41
1:A:92:TYR:HD1	1:A:97:PHE:HE1	1.68	0.41
1:B:140:LYS:H	1:B:140:LYS:HG2	1.64	0.41
1:B:124:ASP:OD2	1:B:127:ARG:HB3	2.21	0.41
1:A:37:LEU:HD12	1:A:501:VAL:HG22	2.03	0.41
1:C:56:LEU:HA	1:C:100:PHE:HE1	1.86	0.41
1:C:382:GLU:OE2	1:C:385:GLU:OE2	2.39	0.41
1:C:432:TYR:OH	1:C:558:ASP:OD1	2.36	0.41
1:A:229:ASP:OD1	1:A:232:THR:OG1	2.31	0.41
1:B:63:PHE:CZ	1:B:107:ILE:HG23	2.56	0.41
1:B:432:TYR:CE1	1:B:554:ASP:OD2	2.74	0.41
1:C:390:GLY:HA2	1:C:444:PRO:HG2	2.02	0.41
1:C:415:THR:O	1:C:435:ILE:HG22	2.21	0.41
1:C:475:ASP:O	1:C:521:SER:OG	2.25	0.41
1:B:454:ALA:HB2	1:B:479:TYR:CB	2.51	0.41
1:C:226:HIS:HD2	1:C:232:THR:O	2.03	0.41
1:C:238:GLU:OE1	1:C:238:GLU:N	2.43	0.41
1:A:57:GLU:HG2	1:A:61:ARG:HE	1.86	0.41
1:A:411:GLY:HA3	1:A:433:ARG:HG2	2.03	0.41
1:A:550:ASN:OD1	1:A:551:VAL:N	2.54	0.41
1:B:161:SER:O	1:B:165:ILE:HG12	2.21	0.41
1:A:75:VAL:HG21	1:A:144:TRP:CG	2.56	0.40
1:B:63:PHE:CE2	1:B:107:ILE:HG23	2.57	0.40
1:B:344:ASP:HB2	1:B:359:THR:HB	2.04	0.40
1:B:543:LEU:HA	1:B:544:PRO:HD3	1.93	0.40
1:C:121:TRP:CZ2	1:C:156:TYR:CG	3.09	0.40
1:A:110:SER:HA	1:A:113:ARG:HB3	2.03	0.40
1:B:37:LEU:HD13	1:B:499:PHE:CG	2.56	0.40
1:B:377:ARG:HG2	1:B:440:PHE:CZ	2.56	0.40
1:B:396:ARG:NH1	1:B:626:GLN:HB2	2.36	0.40
1:B:454:ALA:HA	1:B:458:GLU:HG3	2.03	0.40
1:C:88:LEU:O	1:C:92:TYR:N	2.46	0.40
1:C:121:TRP:HZ2	1:C:156:TYR:CG	2.39	0.40
1:A:41:HIS:HB3	1:A:44:THR:O	2.22	0.40
1:A:344:ASP:HB2	1:A:359:THR:HB	2.03	0.40
1:C:42:ILE:HG23	1:C:43:ASP:N	2.37	0.40
1:C:607:VAL:O	1:C:611:LYS:HG3	2.22	0.40
1:C:209:PRO:O	1:C:213:ALA:N	2.55	0.40
1:C:473:VAL:HG12	1:C:523:ILE:HB	2.03	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	477/634 (75%)	467 (98%)	9 (2%)	1 (0%)	43	73
1	B	501/634 (79%)	490 (98%)	11 (2%)	0	100	100
1	C	477/634 (75%)	463 (97%)	12 (2%)	2 (0%)	30	62
All	All	1455/1902 (76%)	1420 (98%)	32 (2%)	3 (0%)	43	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	PHE
1	C	152	LYS
1	C	86	HIS

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	439/560 (78%)	431 (98%)	8 (2%)	51	76
1	B	456/560 (81%)	445 (98%)	11 (2%)	43	72
1	C	441/560 (79%)	432 (98%)	9 (2%)	48	75
All	All	1336/1680 (80%)	1308 (98%)	28 (2%)	47	74

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ILE
1	A	201	ASN
1	A	415	THR
1	A	515	GLN
1	A	552	ILE
1	A	569	LYS
1	A	615	LYS
1	A	616	GLN
1	B	115	ARG
1	B	126	ILE
1	B	135	HIS
1	B	365	GLU
1	B	369	GLN
1	B	374	GLN
1	B	376	LEU
1	B	415	THR
1	B	436	SER
1	B	515	GLN
1	B	516	LEU
1	C	30	VAL
1	C	60	VAL
1	C	126	ILE
1	C	152	LYS
1	C	186	CYS
1	C	423	ARG
1	C	429	VAL
1	C	552	ILE
1	C	556	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	374	GLN
1	A	462	GLN
1	A	485	GLN
1	A	486	HIS
1	A	591	HIS
1	A	592	ASN
1	B	66	HIS
1	B	226	HIS
1	B	231	HIS
1	B	374	GLN

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Mol	Chain	Res	Type
1	B	477	GLN
1	B	553	ASN
1	B	568	GLN
1	B	588	GLN
1	B	591	HIS
1	B	600	ASN
1	C	462	GLN
1	C	465	GLN

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	489/634 (77%)	0.69	56 (11%) 9 6	50, 83, 156, 199	0
1	B	509/634 (80%)	0.50	41 (8%) 18 11	56, 76, 107, 126	0
1	C	489/634 (77%)	1.09	104 (21%) 2 2	58, 108, 205, 238	0
All	All	1487/1902 (78%)	0.76	201 (13%) 7 5	50, 86, 180, 238	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	VAL	7.3
1	C	123	THR	7.2
1	B	142	SER	7.0
1	B	436	SER	6.9
1	C	184	LYS	6.7
1	A	129	ILE	6.6
1	C	205	TYR	6.4
1	C	193	HIS	5.5
1	B	437	PRO	5.4
1	B	22	ALA	5.3
1	C	437	PRO	4.8
1	C	59	TYR	4.5
1	B	133	MET	4.5
1	A	36	LYS	4.3
1	B	175	TYR	4.3
1	A	204	GLY	4.3
1	C	241	LEU	4.3
1	C	183	VAL	4.2
1	C	57	GLU	4.2
1	A	162	TYR	4.0
1	B	562	ASN	4.0
1	B	614	ASN	4.0
1	C	190	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	163	ALA	3.8
1	C	209	PRO	3.8
1	B	415	THR	3.8
1	C	110	SER	3.7
1	C	56	LEU	3.6
1	C	69	TYR	3.6
1	C	506	TYR	3.5
1	B	135	HIS	3.5
1	C	47	ILE	3.4
1	C	126	ILE	3.4
1	C	68	ALA	3.4
1	A	497	ASP	3.4
1	A	370	VAL	3.4
1	A	427	GLY	3.3
1	B	613	THR	3.3
1	C	499	PHE	3.3
1	C	204	GLY	3.3
1	A	126	ILE	3.3
1	C	122	LEU	3.3
1	A	206	ARG	3.3
1	A	160	LEU	3.3
1	C	61	ARG	3.3
1	A	156	TYR	3.2
1	C	242	SER	3.2
1	B	128	VAL	3.2
1	C	500	LYS	3.2
1	A	437	PRO	3.2
1	C	486	HIS	3.2
1	B	167	LEU	3.1
1	C	233	ALA	3.1
1	A	499	PHE	3.1
1	C	89	PHE	3.1
1	A	69	TYR	3.1
1	A	486	HIS	3.1
1	A	488	THR	3.1
1	A	84	ALA	3.1
1	A	425	ALA	3.1
1	A	190	ILE	3.1
1	A	118	ARG	3.1
1	A	85	THR	3.1
1	B	139	LYS	3.1
1	C	78	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	428	SER	3.0
1	C	452	SER	3.0
1	C	165	ILE	3.0
1	C	219	ARG	3.0
1	B	132	ALA	3.0
1	A	145	ALA	3.0
1	A	66	HIS	3.0
1	C	139	LYS	2.9
1	C	106	CYS	2.9
1	C	438	GLN	2.9
1	A	132	ALA	2.9
1	C	185	LEU	2.9
1	B	617	ASP	2.9
1	C	425	ALA	2.9
1	C	90	LYS	2.9
1	C	497	ASP	2.8
1	A	107	ILE	2.8
1	C	514	THR	2.8
1	A	122	LEU	2.8
1	C	482	GLY	2.8
1	A	212	GLU	2.8
1	C	116	GLU	2.8
1	C	191	GLU	2.8
1	C	234	TYR	2.8
1	C	54	ARG	2.7
1	C	229	ASP	2.7
1	B	126	ILE	2.7
1	B	622	SER	2.7
1	C	86	HIS	2.7
1	B	160	LEU	2.7
1	A	121	TRP	2.6
1	A	164	SER	2.6
1	A	422	SER	2.6
1	B	177	GLY	2.6
1	C	141	PRO	2.6
1	A	434	THR	2.6
1	C	216	PHE	2.6
1	C	166	TYR	2.6
1	C	218	VAL	2.6
1	C	143	ALA	2.6
1	A	88	LEU	2.6
1	C	51	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	433	ARG	2.5
1	B	227	SER	2.5
1	C	220	ILE	2.5
1	C	167	LEU	2.5
1	C	50	TYR	2.5
1	C	432	TYR	2.5
1	B	66	HIS	2.5
1	C	120	SER	2.5
1	A	200	ILE	2.5
1	B	571	TYR	2.5
1	A	152	LYS	2.5
1	C	198	ILE	2.5
1	C	238	GLU	2.4
1	C	615	LYS	2.4
1	C	214	ASN	2.4
1	C	516	LEU	2.4
1	A	148	ILE	2.4
1	C	131	ASP	2.4
1	A	117	TRP	2.4
1	C	80	PHE	2.4
1	B	166	TYR	2.4
1	B	361	HIS	2.4
1	A	622	SER	2.4
1	C	203	HIS	2.4
1	C	208	SER	2.4
1	C	159	LEU	2.4
1	C	30	VAL	2.3
1	B	427	GLY	2.3
1	C	433	ARG	2.3
1	A	240	ALA	2.3
1	C	156	TYR	2.3
1	C	109	GLN	2.3
1	B	566	TRP	2.3
1	C	129	ILE	2.3
1	C	83	GLU	2.3
1	B	438	GLN	2.3
1	C	46	GLN	2.3
1	A	90	LYS	2.3
1	A	452	SER	2.3
1	C	63	PHE	2.3
1	C	416	ASN	2.3
1	B	568	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	144	TRP	2.3
1	C	483	THR	2.3
1	A	22	ALA	2.2
1	B	179	GLU	2.2
1	C	562	ASN	2.2
1	A	159	LEU	2.2
1	B	237	GLN	2.2
1	C	431	ARG	2.2
1	A	123	THR	2.2
1	C	105	THR	2.2
1	C	82	GLU	2.2
1	C	455	ALA	2.2
1	A	198	ILE	2.2
1	C	40	HIS	2.2
1	A	202	ASP	2.2
1	A	234	TYR	2.2
1	C	215	SER	2.2
1	C	227	SER	2.2
1	C	100	PHE	2.2
1	C	163	ALA	2.2
1	C	96	ASN	2.2
1	C	479	TYR	2.2
1	C	436	SER	2.2
1	C	188	ARG	2.1
1	C	237	GLN	2.1
1	C	162	TYR	2.1
1	C	65	SER	2.1
1	C	618	ARG	2.1
1	B	60	VAL	2.1
1	C	32	LYS	2.1
1	C	195	ASN	2.1
1	A	205	TYR	2.1
1	C	92	TYR	2.1
1	B	65	SER	2.1
1	C	440	PHE	2.1
1	A	415	THR	2.1
1	C	211	GLU	2.1
1	B	223	SER	2.0
1	A	130	GLN	2.0
1	C	222	LYS	2.0
1	B	486	HIS	2.0
1	A	187	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	240	ALA	2.0
1	B	162	TYR	2.0
1	A	103	LEU	2.0
1	A	185	LEU	2.0
1	C	76	PHE	2.0
1	B	200	ILE	2.0
1	C	643	ILE	2.0
1	B	425	ALA	2.0
1	A	131	ASP	2.0
1	B	202	ASP	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.