



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:28 PM UTC

PDB ID : 3ND0 / pdb_00003nd0
Title : X-ray crystal structure of a slow cyanobacterial Cl⁻/H⁺ antiporter
Authors : Jayaram, H.; Robertson, J.; Wu, F.; Williams, C.; Miller, C.
Deposited on : 2010-06-06
Resolution : 3.20 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

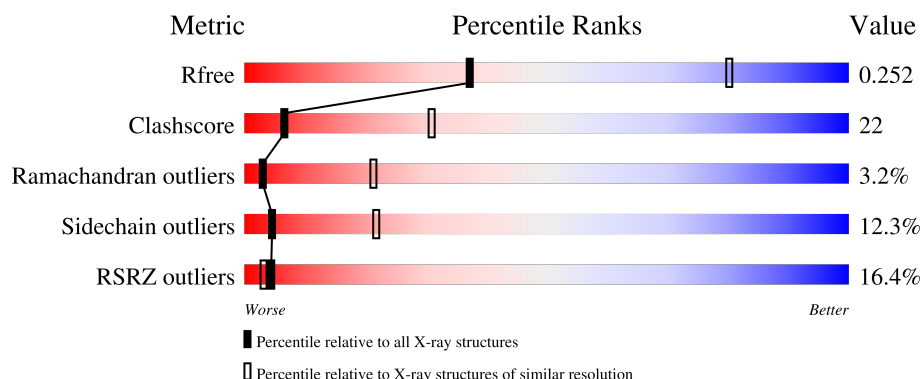
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	466	15% 50% 32% 9% 9%
1	B	466	15% 56% 28% 6% 9%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6400 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 Sll0855 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3199	2110	533	536	20			
1	B	425	Total	C	N	O	S	0	0	0
			3199	2110	533	536	20			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	SER	-	expression tag	UNP P73745
A	453	LEU	-	expression tag	UNP P73745
A	454	VAL	-	expression tag	UNP P73745
A	455	PRO	-	expression tag	UNP P73745
A	456	ARG	-	expression tag	UNP P73745
A	457	GLY	-	expression tag	UNP P73745
A	458	SER	-	expression tag	UNP P73745
A	459	GLY	-	expression tag	UNP P73745
A	460	GLY	-	expression tag	UNP P73745
A	461	HIS	-	expression tag	UNP P73745
A	462	HIS	-	expression tag	UNP P73745
A	463	HIS	-	expression tag	UNP P73745
A	464	HIS	-	expression tag	UNP P73745
A	465	HIS	-	expression tag	UNP P73745
A	466	HIS	-	expression tag	UNP P73745
B	452	SER	-	expression tag	UNP P73745
B	453	LEU	-	expression tag	UNP P73745
B	454	VAL	-	expression tag	UNP P73745
B	455	PRO	-	expression tag	UNP P73745
B	456	ARG	-	expression tag	UNP P73745
B	457	GLY	-	expression tag	UNP P73745
B	458	SER	-	expression tag	UNP P73745
B	459	GLY	-	expression tag	UNP P73745
B	460	GLY	-	expression tag	UNP P73745
B	461	HIS	-	expression tag	UNP P73745

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Chain	Residue	Modelled	Actual	Comment	Reference
B	462	HIS	-	expression tag	UNP P73745
B	463	HIS	-	expression tag	UNP P73745
B	464	HIS	-	expression tag	UNP P73745
B	465	HIS	-	expression tag	UNP P73745
B	466	HIS	-	expression tag	UNP P73745

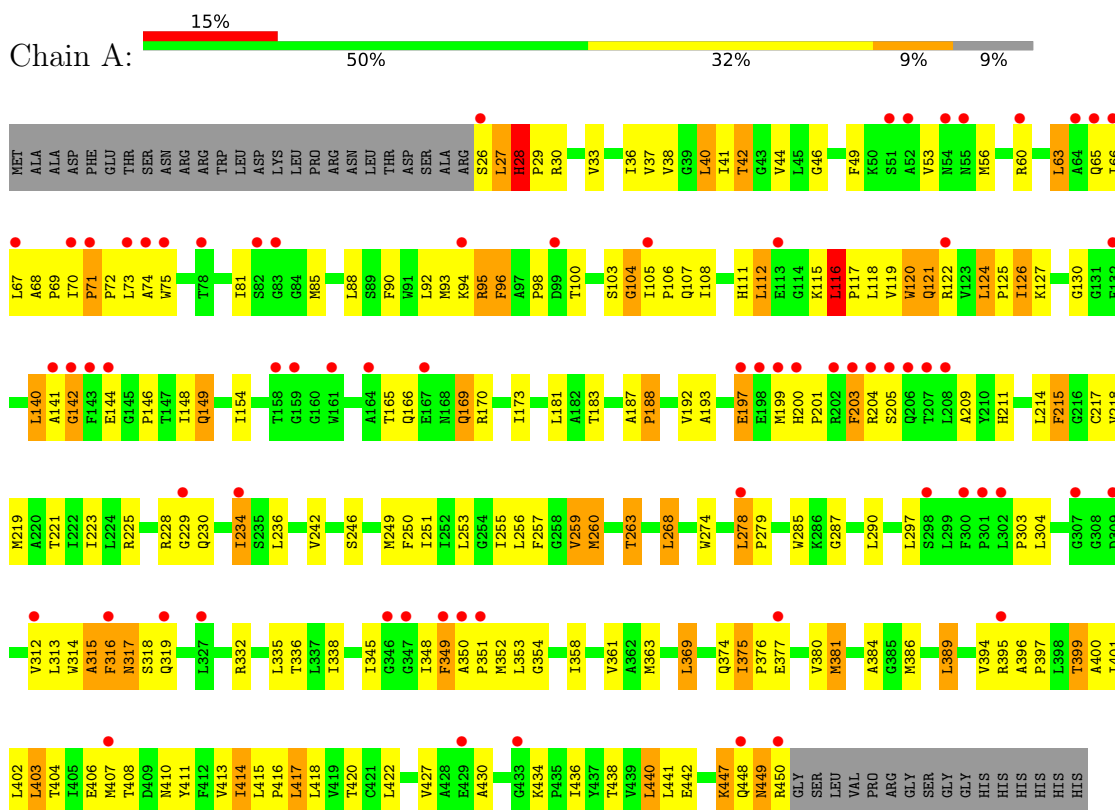
- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0

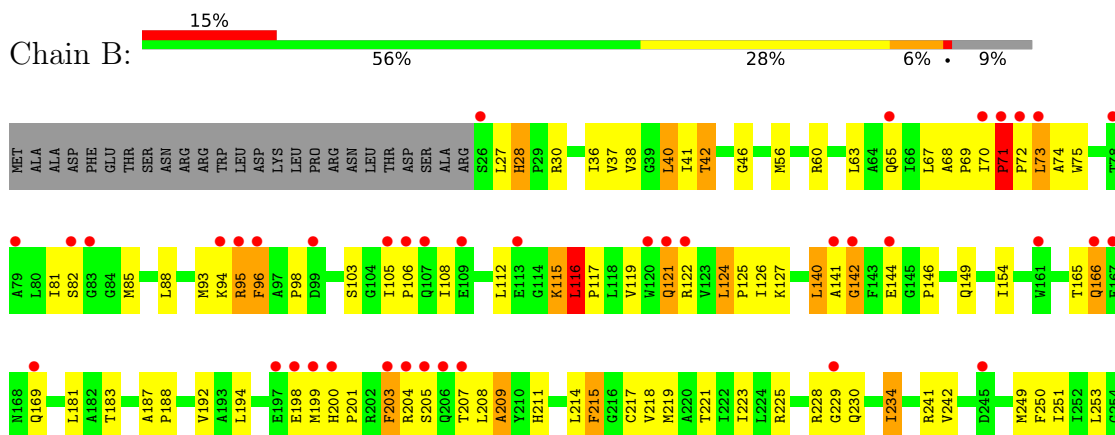
3 Residue-property plots

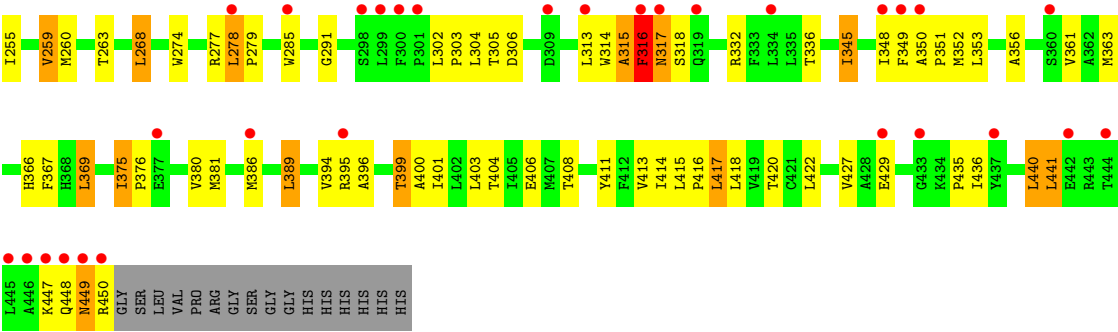
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sll0855 protein



• Molecule 1: Sll0855 protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.79Å 203.79Å 96.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.22 – 3.20 65.22 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.4 (65.22-3.20) 91.4 (65.22-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.26	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.6.1_357, REFMAC 5.5.0109	Depositor
R, R_{free}	0.243 , 0.269 0.233 , 0.252	Depositor DCC
R_{free} test set	1750 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	82.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.052 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6400	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

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

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	1/3276 (0.0%)	0.77	5/4457 (0.1%)
1	B	0.33	1/3276 (0.0%)	0.77	6/4457 (0.1%)
All	All	0.33	2/6552 (0.0%)	0.77	11/8914 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	GLN	CD-OE1	5.26	1.33	1.23
1	B	166	GLN	CD-OE1	5.14	1.33	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	HIS	CA-C-N	6.38	127.82	119.84
1	A	28	HIS	C-N-CA	6.38	127.82	119.84
1	B	28	HIS	CA-C-N	5.95	127.27	119.84
1	B	28	HIS	C-N-CA	5.95	127.27	119.84
1	A	209	ALA	N-CA-C	-5.81	106.15	113.18
1	B	316	PHE	N-CA-C	-5.53	101.47	110.20
1	A	414	ILE	N-CA-C	5.41	115.61	110.42
1	B	209	ALA	N-CA-C	-5.29	106.77	113.18
1	A	430	ALA	N-CA-C	-5.29	107.49	114.31
1	B	71	PRO	CA-C-N	-5.15	113.40	119.84
1	B	71	PRO	C-N-CA	-5.15	113.40	119.84

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	3199	0	3360	148	0
1	B	3199	0	3360	142	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	6400	0	6720	285	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 22.

All (285) 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:225:ARG:HD3	1:B:230:GLN:HG3	1.33	1.08
1:A:225:ARG:HD3	1:A:230:GLN:HG3	1.36	1.04
1:A:71:PRO:HB2	1:A:72:PRO:CD	1.99	0.91
1:B:71:PRO:HB2	1:B:72:PRO:CD	2.03	0.88
1:B:95:ARG:HH22	1:B:450:ARG:HH22	1.18	0.88
1:A:218:VAL:HG22	1:B:418:LEU:HD13	1.57	0.86
1:A:71:PRO:HB2	1:A:72:PRO:HD2	1.58	0.84
1:A:278:LEU:HB3	1:A:279:PRO:HA	1.60	0.83
1:A:95:ARG:HH22	1:A:450:ARG:HH22	1.23	0.82
1:A:278:LEU:HB3	1:A:279:PRO:CA	2.09	0.82
1:B:386:MET:HE3	1:B:404:THR:HB	1.63	0.81
1:A:418:LEU:HD13	1:B:218:VAL:HG22	1.64	0.79
1:A:144:GLU:HG3	1:A:349:PHE:HB2	1.64	0.79
1:B:71:PRO:HB2	1:B:72:PRO:HD2	1.66	0.76
1:B:278:LEU:HB3	1:B:279:PRO:CA	2.16	0.76
1:B:144:GLU:HG3	1:B:349:PHE:HB2	1.70	0.74
1:B:375:ILE:HG22	1:B:375:ILE:O	1.88	0.73
1:A:395:ARG:HG2	1:A:395:ARG:O	1.89	0.73
1:A:188:PRO:HG3	1:A:221:THR:HG21	1.72	0.72
1:A:386:MET:HE3	1:A:404:THR:HB	1.72	0.72
1:B:188:PRO:HG3	1:B:221:THR:HG21	1.71	0.72
1:A:192:VAL:HG21	1:A:214:LEU:HD23	1.73	0.71
1:A:375:ILE:CG2	1:A:375:ILE:O	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ARG:O	1:B:395:ARG:HG2	1.91	0.70
1:B:116:LEU:HD23	1:B:117:PRO:HD2	1.74	0.70
1:A:375:ILE:O	1:A:375:ILE:HG22	1.92	0.69
1:B:303:PRO:HG3	1:B:314:TRP:CG	2.27	0.69
1:B:278:LEU:HB3	1:B:279:PRO:HA	1.74	0.69
1:B:268:LEU:HD12	1:B:436:ILE:HD11	1.74	0.68
1:B:259:VAL:O	1:B:263:THR:HG23	1.94	0.68
1:A:141:ALA:HB1	1:A:142:GLY:HA3	1.76	0.66
1:A:68:ALA:N	1:A:69:PRO:HD2	2.10	0.66
1:A:303:PRO:HG3	1:A:314:TRP:CG	2.30	0.66
1:B:278:LEU:HB3	1:B:279:PRO:C	2.21	0.66
1:A:127:LYS:HD2	1:A:146:PRO:HA	1.79	0.65
1:B:95:ARG:NH2	1:B:450:ARG:HH12	1.95	0.65
1:B:68:ALA:N	1:B:69:PRO:HD2	2.10	0.65
1:A:278:LEU:CB	1:A:279:PRO:HA	2.27	0.65
1:B:95:ARG:HH22	1:B:450:ARG:NH2	1.93	0.65
1:B:115:LYS:H	1:B:115:LYS:HD2	1.62	0.65
1:A:401:ILE:HG23	1:A:417:LEU:HD13	1.79	0.64
1:A:111:HIS:ND1	1:A:118:LEU:HB3	2.11	0.64
1:A:259:VAL:O	1:A:263:THR:HG23	1.96	0.64
1:B:94:LYS:HB3	1:B:98:PRO:HG3	1.79	0.64
1:B:375:ILE:O	1:B:375:ILE:CG2	2.46	0.64
1:A:411:TYR:CE1	1:A:414:ILE:HD12	2.32	0.64
1:B:367:PHE:CD2	1:B:381:MET:HE1	2.34	0.63
1:A:251:ILE:O	1:A:255:ILE:HG12	1.97	0.63
1:A:394:VAL:O	1:A:395:ARG:HB3	1.98	0.62
1:B:192:VAL:HG21	1:B:214:LEU:HD23	1.81	0.62
1:A:253:LEU:HD22	1:A:381:MET:HE3	1.82	0.62
1:A:422:LEU:HD11	1:B:215:PHE:CE1	2.33	0.62
1:A:363:MET:HB3	1:A:381:MET:HE2	1.82	0.61
1:B:141:ALA:HB1	1:B:142:GLY:HA3	1.82	0.61
1:A:28:HIS:NE2	1:A:30:ARG:HB2	2.15	0.61
1:B:278:LEU:CB	1:B:279:PRO:HA	2.30	0.61
1:A:413:VAL:HG12	1:A:413:VAL:O	2.00	0.60
1:A:278:LEU:CB	1:A:279:PRO:CA	2.80	0.60
1:B:71:PRO:CB	1:B:72:PRO:CD	2.79	0.60
1:A:225:ARG:HA	1:A:229:GLY:HA3	1.83	0.60
1:B:401:ILE:HD13	1:B:418:LEU:HD23	1.83	0.60
1:A:71:PRO:CB	1:A:72:PRO:HD2	2.31	0.60
1:B:127:LYS:HD2	1:B:146:PRO:HA	1.84	0.60
1:B:416:PRO:O	1:B:420:THR:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LEU:CB	1:B:279:PRO:CA	2.80	0.59
1:A:268:LEU:HD12	1:A:436:ILE:HD11	1.83	0.59
1:A:72:PRO:O	1:A:75:TRP:HB2	2.03	0.58
1:A:71:PRO:CB	1:A:72:PRO:CD	2.78	0.58
1:B:394:VAL:O	1:B:395:ARG:HB3	2.03	0.58
1:A:416:PRO:O	1:A:420:THR:HG22	2.02	0.58
1:B:396:ALA:HB1	1:B:399:THR:HG23	1.86	0.58
1:A:95:ARG:NH2	1:A:450:ARG:HH22	1.96	0.58
1:B:380:VAL:HG13	1:B:413:VAL:HG13	1.85	0.58
1:B:67:LEU:HB2	1:B:74:ALA:HB2	1.84	0.57
1:A:278:LEU:HB3	1:A:279:PRO:C	2.28	0.57
1:A:201:PRO:HG2	1:A:203:PHE:CE1	2.40	0.57
1:A:315:ALA:HB1	1:A:361:VAL:HG21	1.86	0.57
1:B:28:HIS:CE1	1:B:30:ARG:HB2	2.39	0.57
1:A:36:ILE:HD11	1:A:215:PHE:CD1	2.40	0.56
1:A:95:ARG:HH22	1:A:450:ARG:NH2	2.00	0.56
1:B:225:ARG:HA	1:B:229:GLY:HA3	1.85	0.56
1:B:71:PRO:CB	1:B:72:PRO:HD2	2.34	0.56
1:B:72:PRO:O	1:B:75:TRP:HB2	2.05	0.56
1:B:199:MET:O	1:B:199:MET:HG2	2.05	0.56
1:B:214:LEU:O	1:B:218:VAL:HG23	2.05	0.56
1:A:404:THR:OG1	1:A:417:LEU:HD11	2.05	0.56
1:B:187:ALA:HB1	1:B:406:GLU:OE1	2.05	0.56
1:A:37:VAL:O	1:A:41:ILE:HG12	2.04	0.56
1:A:348:ILE:HG23	1:A:352:MET:HE2	1.88	0.56
1:B:253:LEU:HD22	1:B:381:MET:HE3	1.87	0.56
1:B:93:MET:HE2	1:B:345:ILE:HG13	1.87	0.55
1:A:396:ALA:HB1	1:A:399:THR:CG2	2.37	0.55
1:B:242:VAL:HG11	1:B:416:PRO:HG2	1.88	0.55
1:B:386:MET:HE1	1:B:408:THR:HG21	1.87	0.55
1:A:400:ALA:O	1:A:404:THR:HG23	2.06	0.55
1:A:108:ILE:O	1:A:112:LEU:HB2	2.07	0.55
1:A:67:LEU:HB2	1:A:74:ALA:HB2	1.88	0.54
1:B:447:LYS:C	1:B:449:ASN:H	2.16	0.54
1:A:246:SER:HB2	1:A:249:MET:HE3	1.89	0.54
1:B:350:ALA:HB3	1:B:351:PRO:HD3	1.89	0.54
1:B:217:CYS:O	1:B:221:THR:HG23	2.07	0.54
1:B:41:ILE:HB	1:B:154:ILE:HG21	1.89	0.54
1:B:96:PHE:O	1:B:122:ARG:HD2	2.08	0.54
1:A:214:LEU:O	1:A:218:VAL:HG23	2.08	0.53
1:B:348:ILE:HG23	1:B:352:MET:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:VAL:HG12	1:B:413:VAL:O	2.08	0.53
1:B:251:ILE:O	1:B:255:ILE:HG12	2.08	0.53
1:B:255:ILE:HD13	1:B:427:VAL:HG21	1.88	0.53
1:B:56:MET:O	1:B:60:ARG:HG3	2.08	0.53
1:B:201:PRO:HG2	1:B:203:PHE:CE1	2.43	0.53
1:B:140:LEU:HD21	1:B:305:THR:HA	1.90	0.53
1:A:71:PRO:HD2	1:A:73:LEU:H	1.73	0.53
1:A:187:ALA:HB1	1:A:406:GLU:OE1	2.08	0.53
1:A:93:MET:HE2	1:A:345:ILE:HG13	1.89	0.53
1:B:285:TRP:HA	1:B:285:TRP:CE3	2.44	0.53
1:A:255:ILE:HD13	1:A:427:VAL:HG21	1.91	0.52
1:B:46:GLY:HA3	1:B:183:THR:HG21	1.91	0.52
1:A:369:LEU:C	1:A:369:LEU:HD13	2.34	0.52
1:A:40:LEU:HG	1:A:219:MET:HE2	1.91	0.52
1:B:395:ARG:HG3	1:B:429:GLU:OE2	2.10	0.52
1:B:386:MET:HE1	1:B:408:THR:CG2	2.39	0.52
1:A:96:PHE:O	1:A:122:ARG:HD2	2.10	0.51
1:A:312:VAL:C	1:A:314:TRP:H	2.19	0.51
1:A:350:ALA:HB3	1:A:351:PRO:HD3	1.93	0.51
1:B:366:HIS:O	1:B:369:LEU:HB3	2.11	0.51
1:B:40:LEU:HG	1:B:219:MET:HE2	1.93	0.51
1:B:400:ALA:O	1:B:404:THR:HG23	2.11	0.51
1:B:28:HIS:NE2	1:B:30:ARG:HB2	2.26	0.51
1:A:396:ALA:HB1	1:A:399:THR:HG23	1.93	0.50
1:A:38:VAL:O	1:A:42:THR:HG22	2.11	0.50
1:B:144:GLU:CG	1:B:349:PHE:HB2	2.40	0.50
1:B:37:VAL:O	1:B:41:ILE:HG12	2.12	0.50
1:B:316:PHE:CD2	1:B:316:PHE:N	2.77	0.50
1:B:208:LEU:HD12	1:B:211:HIS:CE1	2.46	0.50
1:B:140:LEU:N	1:B:140:LEU:HD23	2.26	0.49
1:B:303:PRO:O	1:B:332:ARG:HD2	2.12	0.49
1:A:46:GLY:HA3	1:A:183:THR:HG21	1.94	0.49
1:A:116:LEU:HD23	1:A:117:PRO:HD2	1.93	0.49
1:A:250:PHE:CZ	1:A:416:PRO:HB3	2.47	0.49
1:B:81:ILE:O	1:B:85:MET:HG3	2.12	0.49
1:A:242:VAL:HG22	1:A:380:VAL:HG21	1.95	0.49
1:B:140:LEU:CD2	1:B:305:THR:HA	2.43	0.49
1:A:40:LEU:HD23	1:A:223:ILE:HG13	1.94	0.49
1:B:121:GLN:H	1:B:121:GLN:CD	2.19	0.49
1:B:363:MET:HB3	1:B:381:MET:HE2	1.95	0.49
1:B:404:THR:OG1	1:B:417:LEU:HD11	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:TYR:CE1	1:B:414:ILE:HD12	2.47	0.49
1:A:119:VAL:HG23	1:A:122:ARG:HB2	1.95	0.49
1:B:41:ILE:HG22	1:B:154:ILE:HD13	1.94	0.48
1:B:449:ASN:O	1:B:450:ARG:C	2.55	0.48
1:A:40:LEU:O	1:A:44:VAL:HG23	2.13	0.48
1:B:67:LEU:C	1:B:69:PRO:HD2	2.38	0.48
1:B:36:ILE:O	1:B:40:LEU:HB2	2.13	0.48
1:B:369:LEU:HD13	1:B:369:LEU:C	2.38	0.48
1:B:415:LEU:HB2	1:B:416:PRO:HD3	1.94	0.48
1:A:354:GLY:O	1:A:358:ILE:HG13	2.14	0.48
1:A:144:GLU:CG	1:A:349:PHE:HB2	2.38	0.48
1:B:124:LEU:HB3	1:B:125:PRO:HD3	1.96	0.48
1:A:204:ARG:HA	1:A:205:SER:HA	1.50	0.47
1:A:41:ILE:HG22	1:A:154:ILE:HD13	1.96	0.47
1:A:94:LYS:HB3	1:A:98:PRO:HG3	1.95	0.47
1:A:380:VAL:HG13	1:A:413:VAL:HG13	1.95	0.47
1:B:277:ARG:O	1:B:278:LEU:C	2.58	0.47
1:B:401:ILE:HG23	1:B:417:LEU:HD13	1.97	0.47
1:A:438:THR:O	1:A:442:GLU:HG3	2.15	0.47
1:A:111:HIS:C	1:A:111:HIS:CD2	2.92	0.46
1:A:303:PRO:O	1:A:332:ARG:HD2	2.15	0.46
1:B:249:MET:HG2	1:B:367:PHE:CE1	2.49	0.46
1:A:95:ARG:NH2	1:A:450:ARG:HH12	2.14	0.46
1:B:82:SER:HB3	1:B:291:GLY:O	2.16	0.46
1:A:304:LEU:HD23	1:A:304:LEU:H	1.80	0.46
1:B:250:PHE:CZ	1:B:416:PRO:HB3	2.50	0.46
1:A:199:MET:O	1:A:199:MET:HG2	2.15	0.46
1:B:204:ARG:HA	1:B:205:SER:HA	1.51	0.46
1:B:140:LEU:HB3	1:B:336:THR:HG22	1.97	0.46
1:B:441:LEU:O	1:B:441:LEU:HD22	2.15	0.46
1:A:81:ILE:O	1:A:85:MET:HG3	2.15	0.46
1:A:92:LEU:O	1:A:96:PHE:HB2	2.15	0.46
1:B:313:LEU:C	1:B:316:PHE:O	2.58	0.45
1:B:332:ARG:O	1:B:336:THR:HG23	2.16	0.45
1:A:140:LEU:HB3	1:A:336:THR:HG22	1.97	0.45
1:A:436:ILE:O	1:A:440:LEU:HB2	2.16	0.45
1:A:65:GLN:HA	1:A:68:ALA:HB2	1.98	0.45
1:B:40:LEU:HD23	1:B:223:ILE:HG13	1.99	0.45
1:B:447:LYS:HB3	1:B:450:ARG:HG2	1.99	0.45
1:A:384:ALA:HB1	1:A:420:THR:HG21	1.99	0.45
1:A:413:VAL:O	1:A:417:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:VAL:HG11	1:B:416:PRO:CG	2.46	0.45
1:B:395:ARG:HD3	1:B:435:PRO:HG3	2.00	0.44
1:A:313:LEU:C	1:A:316:PHE:O	2.59	0.44
1:B:71:PRO:HD2	1:B:73:LEU:H	1.83	0.44
1:A:119:VAL:HG23	1:A:119:VAL:O	2.18	0.44
1:A:225:ARG:HA	1:A:229:GLY:CA	2.47	0.44
1:B:234:ILE:HG23	1:B:234:ILE:O	2.17	0.44
1:A:107:GLN:CB	1:A:149:GLN:HE21	2.31	0.44
1:A:332:ARG:O	1:A:336:THR:HG23	2.18	0.44
1:B:356:ALA:HB2	1:B:389:LEU:HB2	2.00	0.44
1:A:130:GLY:C	1:A:345:ILE:HD12	2.42	0.44
1:A:105:ILE:HB	1:A:106:PRO:HD3	2.00	0.43
1:A:403:LEU:O	1:A:407:MET:HG2	2.18	0.43
1:B:285:TRP:HA	1:B:285:TRP:HE3	1.83	0.43
1:A:68:ALA:N	1:A:69:PRO:CD	2.80	0.43
1:B:303:PRO:HG3	1:B:314:TRP:CD2	2.52	0.43
1:A:63:LEU:O	1:A:63:LEU:HD22	2.19	0.43
1:A:140:LEU:HD12	1:A:336:THR:HG23	2.01	0.43
1:A:197:GLU:OE1	1:A:399:THR:HG22	2.18	0.43
1:A:297:LEU:HD13	1:A:335:LEU:HD11	2.01	0.43
1:B:68:ALA:N	1:B:69:PRO:CD	2.81	0.43
1:B:229:GLY:HA3	1:B:230:GLN:HA	1.78	0.43
1:A:250:PHE:CE1	1:A:416:PRO:HB3	2.54	0.43
1:B:71:PRO:HB2	1:B:72:PRO:HD3	1.97	0.43
1:B:316:PHE:HA	1:B:317:ASN:HA	1.74	0.43
1:B:369:LEU:HD13	1:B:369:LEU:O	2.19	0.43
1:A:148:ILE:HD11	1:A:181:LEU:HB2	2.01	0.43
1:A:253:LEU:HD13	1:A:381:MET:HE3	2.01	0.43
1:A:449:ASN:O	1:A:450:ARG:C	2.62	0.43
1:B:208:LEU:HD12	1:B:211:HIS:ND1	2.34	0.43
1:A:197:GLU:OE2	1:A:397:PRO:HD2	2.19	0.42
1:B:144:GLU:H	1:B:144:GLU:CD	2.25	0.42
1:B:241:ARG:HD2	1:B:376:PRO:HG2	1.99	0.42
1:A:144:GLU:CD	1:A:144:GLU:H	2.26	0.42
1:A:200:HIS:HA	1:A:201:PRO:HD3	1.86	0.42
1:B:249:MET:HE1	1:B:375:ILE:HG12	2.01	0.42
1:B:436:ILE:O	1:B:440:LEU:HB2	2.19	0.42
1:A:374:GLN:C	1:A:376:PRO:HD3	2.44	0.42
1:A:415:LEU:HB2	1:A:416:PRO:HD3	2.00	0.42
1:B:119:VAL:HG23	1:B:119:VAL:O	2.19	0.42
1:B:200:HIS:HA	1:B:201:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:HA	1:B:229:GLY:CA	2.49	0.42
1:A:56:MET:O	1:A:60:ARG:HG3	2.20	0.42
1:A:169:GLN:O	1:A:173:ILE:HG13	2.19	0.42
1:B:108:ILE:O	1:B:112:LEU:HB2	2.19	0.42
1:B:413:VAL:O	1:B:417:LEU:HB2	2.20	0.42
1:A:28:HIS:CE1	1:A:30:ARG:HB2	2.55	0.42
1:B:65:GLN:HA	1:B:68:ALA:HB2	2.02	0.42
1:B:105:ILE:N	1:B:106:PRO:CD	2.82	0.42
1:B:116:LEU:HD23	1:B:117:PRO:CD	2.46	0.42
1:B:207:THR:C	1:B:209:ALA:H	2.27	0.42
1:A:410:ASN:OD1	1:A:413:VAL:HG23	2.19	0.42
1:B:198:GLU:O	1:B:199:MET:HB3	2.19	0.42
1:A:49:PHE:O	1:A:53:VAL:HG23	2.19	0.42
1:A:100:THR:HG21	1:A:126:ILE:HG22	2.01	0.42
1:A:94:LYS:HA	1:A:95:ARG:HA	1.75	0.42
1:A:121:GLN:CD	1:A:121:GLN:H	2.27	0.42
1:B:88:LEU:HD23	1:B:88:LEU:O	2.19	0.41
1:B:181:LEU:HD22	1:B:194:LEU:HD22	2.02	0.41
1:A:217:CYS:O	1:A:221:THR:HG23	2.19	0.41
1:B:105:ILE:HB	1:B:106:PRO:HD3	2.01	0.41
1:A:402:LEU:O	1:A:406:GLU:HG3	2.20	0.41
1:A:411:TYR:CE1	1:B:406:GLU:HG2	2.56	0.41
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.88	0.41
1:B:70:ILE:HA	1:B:71:PRO:HA	1.88	0.41
1:B:305:THR:O	1:B:306:ASP:HB2	2.20	0.41
1:B:242:VAL:HG13	1:B:380:VAL:HG11	2.02	0.41
1:A:285:TRP:HA	1:A:285:TRP:CE3	2.55	0.41
1:A:447:LYS:O	1:A:450:ARG:HG3	2.21	0.41
1:A:27:LEU:HD23	1:A:211:HIS:CG	2.56	0.41
1:A:104:GLY:HA2	1:A:149:GLN:HG3	2.01	0.41
1:A:127:LYS:CD	1:A:146:PRO:HA	2.50	0.41
1:B:422:LEU:C	1:B:422:LEU:HD12	2.45	0.41
1:A:70:ILE:O	1:A:70:ILE:HG23	2.21	0.41
1:B:119:VAL:HG23	1:B:122:ARG:HB2	2.03	0.41
1:A:28:HIS:HA	1:A:29:PRO:HD3	1.73	0.41
1:B:96:PHE:HB3	1:B:126:ILE:HG12	2.02	0.41
1:A:90:PHE:HD2	1:A:287:GLY:HA2	1.86	0.41
1:A:303:PRO:HG3	1:A:314:TRP:CD2	2.56	0.41
1:A:316:PHE:HA	1:A:317:ASN:HA	1.76	0.41
1:A:422:LEU:HD11	1:B:215:PHE:CZ	2.56	0.41
1:B:38:VAL:O	1:B:42:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LYS:CD	1:B:146:PRO:HA	2.51	0.41
1:A:88:LEU:HD23	1:A:88:LEU:O	2.21	0.41
1:A:193:ALA:HB2	1:A:402:LEU:HD12	2.03	0.41
1:A:260:MET:HE2	1:A:260:MET:HB3	1.96	0.41
1:A:386:MET:HE1	1:A:408:THR:HG21	2.02	0.41
1:B:315:ALA:HB1	1:B:361:VAL:HG21	2.02	0.41
1:A:124:LEU:HB3	1:A:125:PRO:HD3	2.04	0.40
1:A:234:ILE:HG23	1:A:234:ILE:O	2.21	0.40
1:A:250:PHE:HB3	1:A:420:THR:HB	2.03	0.40
1:B:94:LYS:HA	1:B:95:ARG:HA	1.80	0.40
1:A:41:ILE:HB	1:A:154:ILE:HG21	2.03	0.40
1:A:290:LEU:HD21	1:A:338:ILE:HG22	2.03	0.40
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.89	0.40
1:A:422:LEU:HD12	1:A:422:LEU:C	2.46	0.40
1:A:120:TRP:CD1	1:A:120:TRP:C	3.00	0.40
1:A:257:PHE:HA	1:A:260:MET:HB2	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	423/466 (91%)	365 (86%)	43 (10%)	15 (4%)	3	20
1	B	423/466 (91%)	375 (89%)	36 (8%)	12 (3%)	4	25
All	All	846/932 (91%)	740 (88%)	79 (9%)	27 (3%)	3	21

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	103	SER

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Mol	Chain	Res	Type
1	A	449	ASN
1	B	71	PRO
1	B	96	PHE
1	B	103	SER
1	B	278	LEU
1	A	96	PHE
1	A	278	LEU
1	A	318	SER
1	B	449	ASN
1	A	104	GLY
1	A	142	GLY
1	B	318	SER
1	A	116	LEU
1	A	197	GLU
1	A	203	PHE
1	A	315	ALA
1	B	116	LEU
1	B	142	GLY
1	B	315	ALA
1	A	434	LYS
1	B	203	PHE
1	B	234	ILE
1	A	188	PRO
1	A	234	ILE
1	B	345	ILE

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	334/368 (91%)	287 (86%)	47 (14%)	3	17
1	B	334/368 (91%)	299 (90%)	35 (10%)	6	28
All	All	668/736 (91%)	586 (88%)	82 (12%)	4	22

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	27	LEU
1	A	28	HIS
1	A	33	VAL
1	A	40	LEU
1	A	42	THR
1	A	63	LEU
1	A	66	ILE
1	A	95	ARG
1	A	112	LEU
1	A	115	LYS
1	A	116	LEU
1	A	120	TRP
1	A	121	GLN
1	A	124	LEU
1	A	126	ILE
1	A	140	LEU
1	A	149	GLN
1	A	165	THR
1	A	166	GLN
1	A	169	GLN
1	A	170	ARG
1	A	215	PHE
1	A	228	ARG
1	A	236	LEU
1	A	256	LEU
1	A	259	VAL
1	A	260	MET
1	A	263	THR
1	A	268	LEU
1	A	274	TRP
1	A	316	PHE
1	A	317	ASN
1	A	349	PHE
1	A	353	LEU
1	A	369	LEU
1	A	375	ILE
1	A	377	GLU
1	A	381	MET
1	A	389	LEU
1	A	399	THR
1	A	403	LEU
1	A	417	LEU

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Mol	Chain	Res	Type
1	A	440	LEU
1	A	441	LEU
1	A	447	LYS
1	A	448	GLN
1	B	27	LEU
1	B	40	LEU
1	B	42	THR
1	B	63	LEU
1	B	73	LEU
1	B	95	ARG
1	B	115	LYS
1	B	116	LEU
1	B	121	GLN
1	B	124	LEU
1	B	140	LEU
1	B	149	GLN
1	B	165	THR
1	B	166	GLN
1	B	169	GLN
1	B	215	PHE
1	B	228	ARG
1	B	259	VAL
1	B	260	MET
1	B	268	LEU
1	B	274	TRP
1	B	302	LEU
1	B	304	LEU
1	B	316	PHE
1	B	317	ASN
1	B	353	LEU
1	B	369	LEU
1	B	375	ILE
1	B	389	LEU
1	B	399	THR
1	B	403	LEU
1	B	417	LEU
1	B	440	LEU
1	B	441	LEU
1	B	448	GLN

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

Mol	Chain	Res	Type
1	A	156	GLN
1	A	168	ASN
1	A	206	GLN
1	A	230	GLN
1	B	156	GLN
1	B	168	ASN
1	B	206	GLN
1	B	230	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	425/466 (91%)	0.87	69 (16%) 4 3	39, 67, 108, 198	0
1	B	425/466 (91%)	0.92	70 (16%) 4 3	37, 69, 115, 253	0
All	All	850/932 (91%)	0.89	139 (16%) 4 3	37, 69, 112, 253	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	SER	9.1
1	B	205	SER	7.9
1	A	309	ASP	7.0
1	B	301	PRO	6.8
1	B	450	ARG	6.8
1	B	449	ASN	6.4
1	A	70	ILE	6.3
1	A	204	ARG	6.3
1	B	109	GLU	5.7
1	A	144	GLU	5.6
1	B	444	THR	5.4
1	A	99	ASP	5.3
1	B	442	GLU	5.2
1	B	94	LYS	5.1
1	B	204	ARG	5.1
1	A	141	ALA	5.0
1	A	71	PRO	4.9
1	B	300	PHE	4.7
1	B	26	SER	4.7
1	B	99	ASP	4.6
1	B	448	GLN	4.6
1	A	142	GLY	4.5
1	A	202	ARG	4.3
1	B	95	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	278	LEU	4.2
1	B	299	LEU	4.1
1	B	395	ARG	4.0
1	A	26	SER	4.0
1	B	169	GLN	3.9
1	B	200	HIS	3.9
1	A	54	ASN	3.9
1	A	307	GLY	3.8
1	B	105	ILE	3.8
1	B	113	GLU	3.7
1	A	78	THR	3.7
1	A	64	ALA	3.7
1	B	73	LEU	3.7
1	A	300	PHE	3.7
1	A	347	GLY	3.7
1	B	142	GLY	3.6
1	B	447	LYS	3.6
1	A	203	PHE	3.6
1	B	206	GLN	3.5
1	A	350	ALA	3.5
1	B	207	THR	3.5
1	A	74	ALA	3.5
1	B	161	TRP	3.5
1	A	395	ARG	3.5
1	A	319	GLN	3.5
1	A	349	PHE	3.4
1	B	317	ASN	3.4
1	B	121	GLN	3.4
1	A	301	PRO	3.4
1	A	94	LYS	3.3
1	B	229	GLY	3.3
1	B	78	THR	3.3
1	B	360	SER	3.3
1	B	141	ALA	3.3
1	A	450	ARG	3.3
1	A	52	ALA	3.3
1	B	313	LEU	3.3
1	A	229	GLY	3.3
1	A	433	GLY	3.3
1	B	349	PHE	3.3
1	B	197	GLU	3.3
1	A	346	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	164	ALA	3.2
1	A	167	GLU	3.2
1	A	83	GLY	3.2
1	A	65	GLN	3.2
1	B	70	ILE	3.1
1	A	161	TRP	3.1
1	A	206	GLN	3.0
1	B	433	GLY	3.0
1	A	105	ILE	3.0
1	B	245	ASP	3.0
1	A	200	HIS	2.9
1	B	445	LEU	2.9
1	B	82	SER	2.9
1	B	166	GLN	2.8
1	B	309	ASP	2.8
1	B	144	GLU	2.8
1	A	73	LEU	2.8
1	A	159	GLY	2.8
1	A	278	LEU	2.8
1	A	208	LEU	2.8
1	A	207	THR	2.8
1	A	113	GLU	2.7
1	B	71	PRO	2.7
1	A	132	PHE	2.7
1	A	67	LEU	2.7
1	A	448	GLN	2.6
1	B	350	ALA	2.6
1	B	83	GLY	2.6
1	B	285	TRP	2.5
1	A	122	ARG	2.5
1	B	429	GLU	2.5
1	B	72	PRO	2.5
1	B	298	SER	2.5
1	A	197	GLU	2.5
1	B	167	GLU	2.5
1	B	446	ALA	2.5
1	A	199	MET	2.5
1	B	65	GLN	2.5
1	B	198	GLU	2.5
1	A	55	ASN	2.5
1	B	437	TYR	2.5
1	B	334	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	66	ILE	2.4
1	A	158	THR	2.4
1	B	316	PHE	2.4
1	A	377	GLU	2.4
1	B	377	GLU	2.4
1	A	75	TRP	2.4
1	B	106	PRO	2.4
1	B	79	ALA	2.3
1	A	316	PHE	2.3
1	A	51	SER	2.3
1	A	298	SER	2.3
1	A	429	GLU	2.3
1	B	319	GLN	2.3
1	A	143	PHE	2.3
1	B	348	ILE	2.2
1	A	198	GLU	2.2
1	A	302	LEU	2.2
1	B	199	MET	2.2
1	A	234	ILE	2.2
1	A	407	MET	2.2
1	B	96	PHE	2.2
1	B	120	TRP	2.2
1	B	122	ARG	2.1
1	A	327	LEU	2.1
1	B	107	GLN	2.1
1	B	203	PHE	2.1
1	A	82	SER	2.1
1	A	312	VAL	2.1
1	A	60	ARG	2.0
1	B	386	MET	2.0
1	A	351	PRO	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](#)

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(Å ²)	Q<0.9
2	CL	A	467	1/1	0.92	0.47	79,79,79,79	0
2	CL	B	467	1/1	0.94	0.37	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.