



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:16 AM UTC

PDB ID : 3Q17 / pdb_00003q17
Title : Structure of a slow CLC Cl⁻/H⁺ antiporter from a cyanobacterium in Bromide
Authors : Jayaram, H.; Robertson, J.L.; Fang, W.; Williams, C.; Miller, C.
Deposited on : 2010-12-16
Resolution : 3.60 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

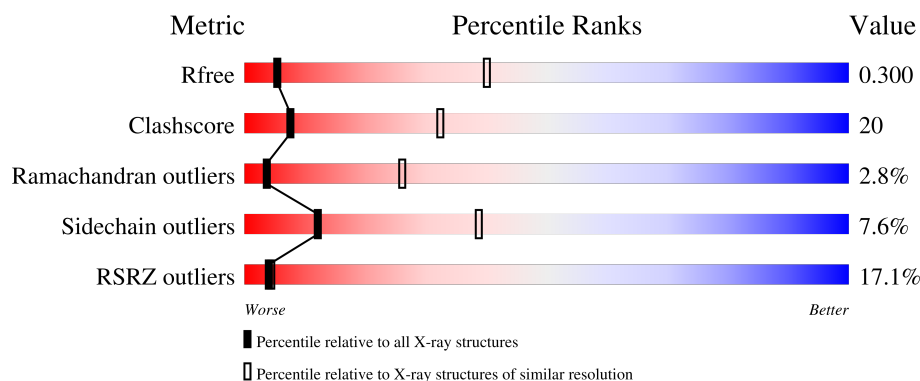
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	466	16% 50% 35% 6% 9%
1	B	466	15% 57% 30% • 9%

2 Entry composition

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 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	451	GLY	-	expression tag	UNP P73745
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	451	GLY	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	460	GLY	-	expression tag	UNP P73745
B	461	HIS	-	expression tag	UNP P73745
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

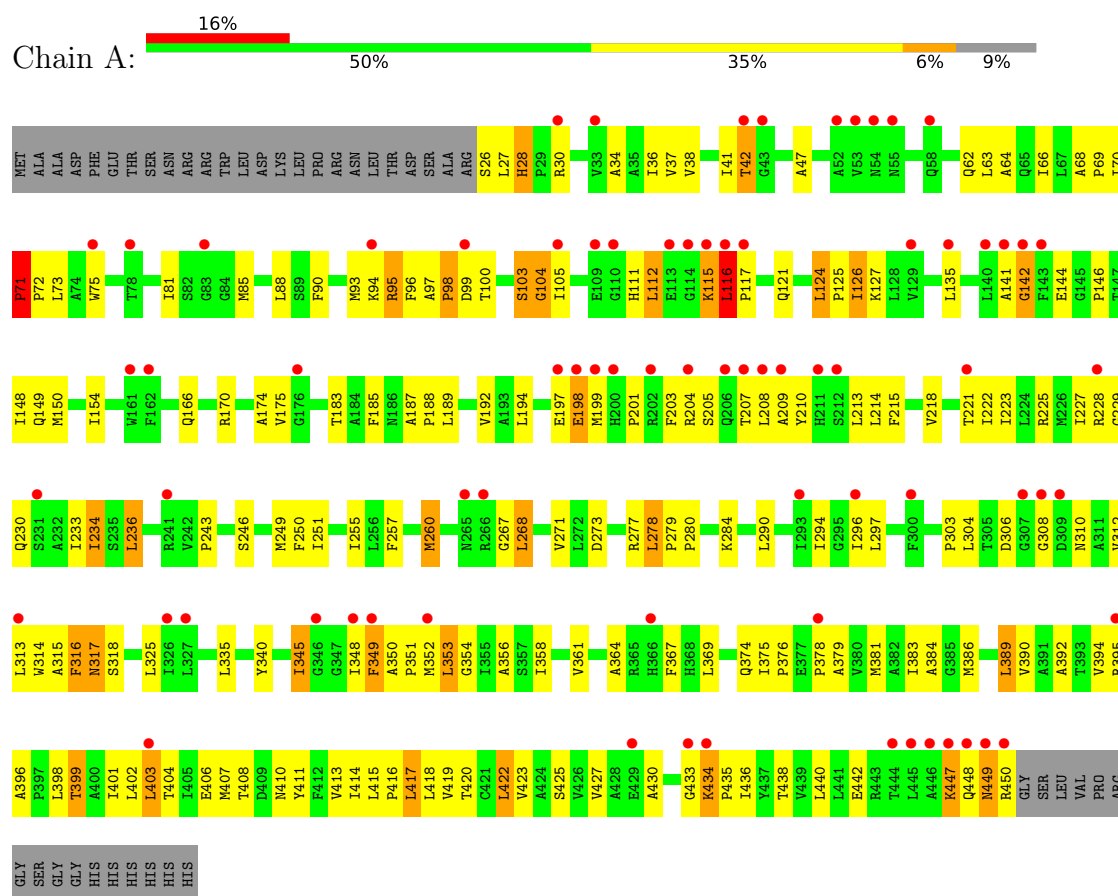
- Molecule 2 is BROMIDE ION (CCD ID: BR) (formula: Br).

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

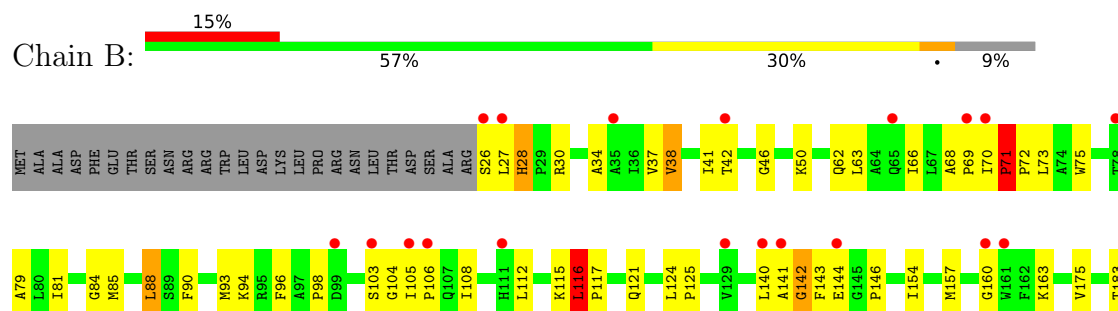
3 Residue-property plots

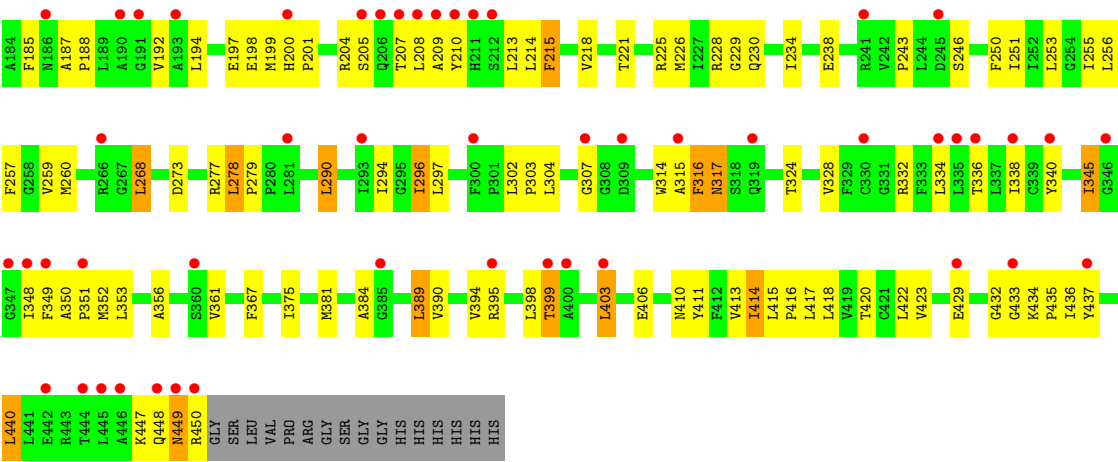
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	207.21Å 207.21Å 105.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.48 – 3.60 68.48 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (68.48-3.60) 97.4 (68.48-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.26	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.6.1_357, REFMAC 5.5.0109	Depositor
R, R_{free}	0.281 , 0.310 0.271 , 0.300	Depositor DCC
R_{free} test set	1497 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 94.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	6400	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: BR

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	0.30	0/3276	0.79	6/4457 (0.1%)
1	B	0.28	0/3276	0.78	6/4457 (0.1%)
All	All	0.29	0/6552	0.79	12/8914 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	PRO	CA-C-N	-8.98	112.58	121.65
1	A	71	PRO	C-N-CA	-8.98	112.58	121.65
1	B	71	PRO	CA-C-N	-7.80	113.77	121.65
1	B	71	PRO	C-N-CA	-7.80	113.77	121.65
1	B	209	ALA	N-CA-C	-5.70	106.33	113.28
1	A	28	HIS	CA-C-N	5.56	126.80	119.84
1	A	28	HIS	C-N-CA	5.56	126.80	119.84
1	A	209	ALA	N-CA-C	-5.45	106.63	113.28
1	B	414	ILE	N-CA-C	5.24	115.39	110.30
1	B	28	HIS	CA-C-N	5.09	126.21	119.84
1	B	28	HIS	C-N-CA	5.09	126.21	119.84
1	A	430	ALA	N-CA-C	-5.05	107.28	113.50

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	3199	0	3360	154	0
1	B	3199	0	3360	126	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
All	All	6400	0	6720	265	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 20.

All (265) 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:225:ARG:HD3	1:A:230:GLN:HG3	1.27	1.10
1:B:225:ARG:HD3	1:B:230:GLN:HG3	1.35	1.09
1:B:71:PRO:HB2	1:B:72:PRO:HD2	1.34	1.08
1:A:278:LEU:HB3	1:A:279:PRO:HA	1.38	1.01
1:B:278:LEU:HB3	1:B:279:PRO:HA	1.41	1.00
1:A:36:ILE:HD11	1:A:215:PHE:HD1	1.28	0.98
1:B:71:PRO:HB2	1:B:72:PRO:CD	1.96	0.95
1:A:71:PRO:HB2	1:A:72:PRO:HD2	1.47	0.94
1:A:278:LEU:HB3	1:A:279:PRO:CA	2.01	0.90
1:A:71:PRO:HB2	1:A:72:PRO:CD	2.04	0.88
1:B:278:LEU:HB3	1:B:279:PRO:CA	2.04	0.87
1:A:36:ILE:HD11	1:A:215:PHE:CD1	2.13	0.83
1:B:144:GLU:HG3	1:B:349:PHE:HB2	1.60	0.82
1:A:218:VAL:HG22	1:B:418:LEU:HD13	1.64	0.80
1:A:418:LEU:HD13	1:B:218:VAL:HG22	1.64	0.78
1:A:188:PRO:HG3	1:A:221:THR:HG21	1.64	0.77
1:A:144:GLU:HG3	1:A:349:PHE:HB2	1.65	0.77
1:B:71:PRO:HD2	1:B:73:LEU:HB2	1.67	0.76
1:A:436:ILE:O	1:A:440:LEU:HB2	1.86	0.76
1:B:116:LEU:HD23	1:B:117:PRO:HD2	1.69	0.75
1:B:243:PRO:HG2	1:B:246:SER:HB3	1.71	0.72
1:B:68:ALA:N	1:B:69:PRO:HD2	2.05	0.71
1:B:348:ILE:HG23	1:B:352:MET:HE2	1.74	0.70
1:B:411:TYR:CE1	1:B:414:ILE:HD12	2.27	0.70
1:A:71:PRO:HD2	1:A:73:LEU:HB2	1.73	0.69
1:B:268:LEU:HD12	1:B:436:ILE:HD11	1.73	0.69
1:A:37:VAL:O	1:A:41:ILE:HG12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ILE:O	1:A:255:ILE:HG12	1.94	0.68
1:B:356:ALA:HB2	1:B:389:LEU:HB2	1.75	0.68
1:A:395:ARG:HG2	1:A:395:ARG:O	1.93	0.68
1:A:225:ARG:HA	1:A:229:GLY:HA3	1.75	0.67
1:A:303:PRO:HG3	1:A:314:TRP:CG	2.30	0.67
1:A:68:ALA:N	1:A:69:PRO:HD2	2.10	0.67
1:B:251:ILE:O	1:B:255:ILE:HG12	1.95	0.67
1:B:192:VAL:HG21	1:B:214:LEU:HD23	1.78	0.65
1:A:268:LEU:HD12	1:A:436:ILE:HD11	1.80	0.64
1:A:95:ARG:HH22	1:A:450:ARG:HH22	1.44	0.64
1:B:28:HIS:CE1	1:B:30:ARG:HB2	2.33	0.64
1:B:395:ARG:O	1:B:395:ARG:HG2	1.97	0.63
1:B:41:ILE:HG22	1:B:154:ILE:HD13	1.81	0.63
1:B:303:PRO:HG3	1:B:314:TRP:CG	2.34	0.62
1:B:175:VAL:HA	1:B:213:LEU:HD23	1.80	0.62
1:A:135:LEU:HG	1:A:141:ALA:O	1.99	0.62
1:A:411:TYR:CE1	1:A:414:ILE:HD12	2.35	0.62
1:B:225:ARG:HA	1:B:229:GLY:HA3	1.81	0.62
1:A:422:LEU:HD11	1:B:215:PHE:CZ	2.35	0.61
1:B:315:ALA:HB1	1:B:361:VAL:HG21	1.82	0.61
1:A:112:LEU:HD11	1:A:174:ALA:HB2	1.82	0.61
1:A:348:ILE:HG23	1:A:352:MET:HE2	1.84	0.60
1:A:396:ALA:HB1	1:A:399:THR:CG2	2.32	0.60
1:A:94:LYS:HB3	1:A:98:PRO:HG3	1.84	0.59
1:A:384:ALA:HB1	1:A:420:THR:HG21	1.84	0.59
1:A:315:ALA:HB1	1:A:361:VAL:HG21	1.84	0.59
1:B:367:PHE:CD2	1:B:381:MET:HE1	2.36	0.59
1:B:395:ARG:HD3	1:B:435:PRO:HG3	1.84	0.59
1:A:215:PHE:CZ	1:B:422:LEU:HD13	2.38	0.59
1:A:234:ILE:HD12	1:A:313:LEU:HD23	1.85	0.59
1:B:90:PHE:HA	1:B:93:MET:HE3	1.84	0.59
1:A:116:LEU:HD23	1:A:117:PRO:HD2	1.84	0.58
1:A:340:TYR:OH	1:A:440:LEU:HD21	2.03	0.58
1:B:94:LYS:HB3	1:B:98:PRO:HG3	1.86	0.58
1:A:394:VAL:O	1:A:395:ARG:HB3	2.03	0.58
1:A:38:VAL:O	1:A:42:THR:HG22	2.03	0.58
1:A:243:PRO:HG2	1:A:246:SER:HB3	1.86	0.57
1:A:306:ASP:HB2	1:A:310:ASN:HD21	1.69	0.57
1:B:394:VAL:O	1:B:395:ARG:HB3	2.03	0.57
1:B:93:MET:HE2	1:B:345:ILE:HG13	1.87	0.57
1:A:304:LEU:HD23	1:A:304:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ILE:O	1:B:440:LEU:HB2	2.05	0.57
1:B:188:PRO:HG3	1:B:221:THR:HG21	1.86	0.57
1:A:175:VAL:HA	1:A:213:LEU:HD23	1.86	0.56
1:B:207:THR:HG23	1:B:208:LEU:HD22	1.87	0.56
1:B:37:VAL:O	1:B:41:ILE:HG12	2.05	0.56
1:A:187:ALA:HB1	1:A:406:GLU:OE1	2.06	0.56
1:A:257:PHE:HA	1:A:260:MET:HB2	1.88	0.56
1:A:413:VAL:HG12	1:A:413:VAL:O	2.06	0.56
1:A:308:GLY:O	1:A:312:VAL:HG23	2.06	0.55
1:A:416:PRO:O	1:A:420:THR:HG22	2.05	0.55
1:B:26:SER:HB2	1:B:208:LEU:HD23	1.88	0.55
1:B:422:LEU:HD12	1:B:423:VAL:N	2.21	0.55
1:A:192:VAL:HG21	1:A:214:LEU:HD23	1.88	0.55
1:B:384:ALA:HB1	1:B:420:THR:HG21	1.88	0.55
1:A:278:LEU:CB	1:A:279:PRO:HA	2.26	0.55
1:A:71:PRO:CB	1:A:72:PRO:CD	2.83	0.55
1:B:413:VAL:HG12	1:B:413:VAL:O	2.07	0.54
1:A:352:MET:HE3	1:A:390:VAL:HG22	1.88	0.54
1:A:41:ILE:HB	1:A:154:ILE:HG21	1.90	0.54
1:B:414:ILE:HG23	1:B:415:LEU:N	2.23	0.54
1:A:197:GLU:HG3	1:B:210:TYR:HD2	1.73	0.54
1:A:185:PHE:CD2	1:A:403:LEU:HD21	2.43	0.53
1:B:141:ALA:HB1	1:B:142:GLY:HA3	1.90	0.53
1:A:97:ALA:C	1:A:99:ASP:H	2.17	0.53
1:B:410:ASN:OD1	1:B:413:VAL:HG23	2.09	0.53
1:A:225:ARG:HA	1:A:229:GLY:CA	2.37	0.53
1:A:215:PHE:CE2	1:B:422:LEU:HD13	2.43	0.53
1:A:398:LEU:HD23	1:B:214:LEU:HD21	1.90	0.53
1:A:267:GLY:O	1:A:271:VAL:HG23	2.08	0.53
1:A:414:ILE:HG23	1:A:415:LEU:N	2.24	0.53
1:A:210:TYR:HD2	1:B:197:GLU:HG3	1.74	0.53
1:A:356:ALA:HB2	1:A:389:LEU:HB2	1.91	0.53
1:B:350:ALA:HB3	1:B:351:PRO:HD3	1.90	0.52
1:A:201:PRO:HG2	1:A:203:PHE:CE1	2.44	0.52
1:A:214:LEU:HD21	1:B:398:LEU:HD23	1.91	0.52
1:B:62:GLN:O	1:B:66:ILE:HG13	2.09	0.52
1:A:234:ILE:HG23	1:A:234:ILE:O	2.10	0.52
1:A:395:ARG:HD3	1:A:435:PRO:HG3	1.91	0.52
1:B:185:PHE:CD2	1:B:403:LEU:HD21	2.45	0.52
1:A:375:ILE:HG22	1:A:375:ILE:O	2.10	0.52
1:A:124:LEU:HB3	1:A:125:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:HIS:CE1	1:A:30:ARG:HB2	2.45	0.51
1:B:72:PRO:O	1:B:75:TRP:HB2	2.11	0.51
1:A:197:GLU:HA	1:B:210:TYR:HE2	1.75	0.51
1:B:187:ALA:HB1	1:B:406:GLU:OE1	2.10	0.51
1:B:268:LEU:HD21	1:B:340:TYR:HD2	1.76	0.51
1:B:375:ILE:HG22	1:B:375:ILE:O	2.09	0.51
1:A:197:GLU:OE1	1:A:399:THR:HG22	2.11	0.51
1:B:278:LEU:CB	1:B:279:PRO:HA	2.28	0.50
1:A:71:PRO:CB	1:A:72:PRO:HD2	2.31	0.50
1:B:250:PHE:HB3	1:B:420:THR:HB	1.93	0.50
1:B:225:ARG:HA	1:B:229:GLY:CA	2.41	0.50
1:A:36:ILE:CD1	1:A:215:PHE:HD1	2.14	0.50
1:A:189:LEU:HB3	1:A:402:LEU:HD13	1.94	0.50
1:A:222:ILE:HG12	1:B:415:LEU:HD13	1.92	0.50
1:B:46:GLY:HA3	1:B:183:THR:HG21	1.93	0.49
1:B:449:ASN:O	1:B:450:ARG:C	2.54	0.49
1:A:199:MET:O	1:A:199:MET:HG2	2.12	0.49
1:A:104:GLY:CA	1:A:149:GLN:HG3	2.43	0.48
1:A:141:ALA:HB1	1:A:142:GLY:HA3	1.94	0.48
1:A:194:LEU:O	1:A:198:GLU:O	2.31	0.48
1:A:144:GLU:HG3	1:A:349:PHE:CB	2.41	0.48
1:B:257:PHE:HA	1:B:260:MET:HB2	1.94	0.48
1:A:104:GLY:HA2	1:A:149:GLN:HG3	1.96	0.48
1:B:144:GLU:CG	1:B:349:PHE:HB2	2.40	0.48
1:A:26:SER:HB2	1:A:208:LEU:HD23	1.95	0.47
1:A:207:THR:HG23	1:A:208:LEU:HD22	1.96	0.47
1:B:68:ALA:N	1:B:69:PRO:CD	2.76	0.47
1:A:198:GLU:HG3	1:A:394:VAL:HG12	1.97	0.47
1:A:214:LEU:O	1:A:218:VAL:HG23	2.15	0.47
1:A:386:MET:HE1	1:A:408:THR:HG21	1.96	0.47
1:B:34:ALA:O	1:B:38:VAL:HG23	2.15	0.47
1:A:72:PRO:O	1:A:75:TRP:HB2	2.14	0.47
1:A:111:HIS:O	1:A:170:ARG:NH2	2.48	0.47
1:A:304:LEU:H	1:A:304:LEU:CD2	2.28	0.47
1:A:367:PHE:CD2	1:A:381:MET:HE1	2.49	0.47
1:A:374:GLN:C	1:A:376:PRO:HD3	2.40	0.47
1:A:410:ASN:OD1	1:A:413:VAL:HG23	2.15	0.47
1:B:124:LEU:HB3	1:B:125:PRO:HD3	1.97	0.47
1:A:127:LYS:HD2	1:A:146:PRO:HA	1.97	0.46
1:A:278:LEU:CB	1:A:279:PRO:CA	2.84	0.46
1:A:350:ALA:HB3	1:A:351:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:VAL:O	1:B:394:VAL:HG12	2.15	0.46
1:B:394:VAL:HG13	1:B:437:TYR:HD2	1.79	0.46
1:A:105:ILE:HG23	1:A:199:MET:HE3	1.98	0.46
1:A:447:LYS:C	1:A:449:ASN:H	2.23	0.46
1:A:233:ILE:HB	1:A:407:MET:HB2	1.97	0.46
1:B:81:ILE:O	1:B:85:MET:HG3	2.15	0.46
1:B:144:GLU:H	1:B:144:GLU:CD	2.24	0.46
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.75	0.46
1:B:108:ILE:O	1:B:112:LEU:HB2	2.16	0.46
1:B:278:LEU:CB	1:B:279:PRO:CA	2.85	0.46
1:A:93:MET:HE2	1:A:345:ILE:HG13	1.97	0.46
1:A:71:PRO:HD2	1:A:73:LEU:CB	2.43	0.46
1:B:41:ILE:HB	1:B:154:ILE:HG21	1.98	0.46
1:B:429:GLU:OE1	1:B:435:PRO:HD3	2.16	0.46
1:A:250:PHE:CZ	1:A:416:PRO:HB3	2.51	0.46
1:A:280:PRO:O	1:A:284:LYS:HG2	2.16	0.46
1:A:438:THR:O	1:A:442:GLU:HG3	2.16	0.46
1:A:314:TRP:CZ3	1:A:325:LEU:HD23	2.51	0.45
1:A:369:LEU:C	1:A:369:LEU:HD13	2.42	0.45
1:B:71:PRO:CD	1:B:73:LEU:HB2	2.42	0.45
1:A:95:ARG:HH22	1:A:450:ARG:NH2	2.14	0.45
1:B:198:GLU:O	1:B:199:MET:HB3	2.16	0.45
1:A:175:VAL:HG22	1:A:213:LEU:HA	1.98	0.45
1:A:303:PRO:HG3	1:A:314:TRP:CD2	2.52	0.45
1:B:73:LEU:HD23	1:B:73:LEU:O	2.16	0.45
1:B:221:THR:O	1:B:225:ARG:HG3	2.17	0.45
1:B:234:ILE:HG23	1:B:234:ILE:O	2.17	0.45
1:A:103:SER:OG	1:A:104:GLY:N	2.50	0.45
1:A:273:ASP:O	1:A:277:ARG:HD3	2.16	0.45
1:A:413:VAL:O	1:A:417:LEU:HB2	2.17	0.45
1:B:332:ARG:O	1:B:336:THR:HG23	2.17	0.45
1:B:416:PRO:O	1:B:420:THR:HG22	2.17	0.45
1:A:103:SER:OG	2:A:1:BR:BR	2.84	0.45
1:B:229:GLY:HA3	1:B:230:GLN:HA	1.77	0.45
1:B:273:ASP:O	1:B:277:ARG:HD3	2.16	0.45
1:B:422:LEU:HD12	1:B:423:VAL:HG23	1.98	0.44
1:B:315:ALA:HB1	1:B:361:VAL:CG2	2.45	0.44
1:A:297:LEU:O	1:A:304:LEU:HD21	2.18	0.44
1:A:90:PHE:HA	1:A:93:MET:HE3	1.99	0.44
1:B:105:ILE:HG23	1:B:199:MET:HE3	1.99	0.44
1:A:419:VAL:O	1:A:423:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLY:O	1:A:434:LYS:HB2	2.18	0.44
1:A:404:THR:OG1	1:A:417:LEU:HD11	2.18	0.44
1:B:121:GLN:H	1:B:121:GLN:CD	2.25	0.44
1:B:290:LEU:HD21	1:B:338:ILE:CG2	2.47	0.44
1:A:354:GLY:O	1:A:358:ILE:HG13	2.18	0.44
1:B:294:ILE:HD13	1:B:297:LEU:HD12	1.99	0.44
1:A:197:GLU:HG3	1:B:210:TYR:CD2	2.52	0.43
1:B:84:GLY:O	1:B:88:LEU:HB2	2.17	0.43
1:A:105:ILE:N	1:A:105:ILE:HD12	2.33	0.43
1:B:250:PHE:HA	1:B:253:LEU:HB3	1.99	0.43
1:A:94:LYS:HA	1:A:95:ARG:HA	1.64	0.43
1:A:401:ILE:HD13	1:A:418:LEU:HD23	2.00	0.43
1:B:197:GLU:OE1	1:B:399:THR:HG23	2.18	0.43
1:A:411:TYR:CE1	1:B:406:GLU:HG2	2.53	0.43
1:A:221:THR:O	1:A:225:ARG:HG3	2.18	0.43
1:B:334:LEU:O	1:B:338:ILE:HD13	2.19	0.43
1:A:100:THR:HG21	1:A:126:ILE:HG22	2.00	0.43
1:B:70:ILE:HA	1:B:71:PRO:HA	1.78	0.43
1:A:255:ILE:HD13	1:A:427:VAL:HG21	2.01	0.43
1:A:68:ALA:N	1:A:69:PRO:CD	2.80	0.43
1:B:105:ILE:N	1:B:106:PRO:CD	2.82	0.43
1:B:447:LYS:C	1:B:449:ASN:H	2.27	0.43
1:A:144:GLU:CG	1:A:349:PHE:HB2	2.42	0.42
1:A:294:ILE:HD11	1:A:335:LEU:HD22	2.00	0.42
1:A:62:GLN:O	1:A:66:ILE:HG13	2.19	0.42
1:A:204:ARG:HA	1:A:205:SER:HA	1.47	0.42
1:A:379:ALA:O	1:A:383:ILE:HG13	2.18	0.42
1:A:95:ARG:NH2	1:A:450:ARG:HH12	2.18	0.42
1:A:225:ARG:CA	1:A:229:GLY:HA3	2.47	0.42
1:A:183:THR:O	1:A:183:THR:HG22	2.19	0.42
1:B:199:MET:O	1:B:199:MET:HG2	2.18	0.42
1:B:324:THR:O	1:B:328:VAL:HG23	2.20	0.42
1:B:256:LEU:HD13	1:B:256:LEU:C	2.45	0.42
1:B:256:LEU:O	1:B:259:VAL:HG22	2.20	0.42
1:A:34:ALA:O	1:A:38:VAL:HG23	2.19	0.42
1:A:315:ALA:HB1	1:A:361:VAL:CG2	2.49	0.42
1:A:392:ALA:HA	1:A:425:SER:HA	2.02	0.42
1:B:200:HIS:HA	1:B:201:PRO:HD3	1.81	0.42
1:B:302:LEU:HD12	1:B:302:LEU:HA	1.94	0.42
1:B:316:PHE:HA	1:B:317:ASN:HA	1.67	0.42
1:B:140:LEU:HD12	1:B:336:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:O	1:B:198:GLU:O	2.38	0.41
1:A:47:ALA:HB3	1:A:227:ILE:HD12	2.01	0.41
1:A:64:ALA:O	1:A:68:ALA:HB2	2.19	0.41
1:A:105:ILE:HD11	1:A:148:ILE:HD12	2.02	0.41
1:A:250:PHE:HB3	1:A:420:THR:HB	2.02	0.41
1:B:79:ALA:HB2	1:B:296:ILE:CD1	2.50	0.41
1:B:433:GLY:O	1:B:434:LYS:HB2	2.20	0.41
1:B:143:PHE:O	1:B:146:PRO:HD2	2.21	0.41
1:A:234:ILE:HG12	1:A:236:LEU:CD1	2.50	0.41
1:A:415:LEU:HD11	1:B:225:ARG:HD2	2.02	0.41
1:B:238:GLU:CD	1:B:238:GLU:H	2.28	0.41
1:B:260:MET:HE2	1:B:260:MET:HB3	1.97	0.41
1:B:141:ALA:C	1:B:307:GLY:HA2	2.45	0.41
1:A:81:ILE:O	1:A:85:MET:HG3	2.21	0.41
1:A:150:MET:O	1:A:154:ILE:HG13	2.21	0.41
1:A:223:ILE:O	1:A:227:ILE:HG13	2.20	0.41
1:B:105:ILE:N	1:B:105:ILE:HD12	2.36	0.41
1:B:204:ARG:HA	1:B:205:SER:HA	1.48	0.41
1:A:121:GLN:CD	1:A:121:GLN:H	2.28	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:CE1	2.55	0.41
1:B:50:LYS:HG2	1:B:143:PHE:CD1	2.56	0.41
1:B:70:ILE:HG23	1:B:70:ILE:O	2.20	0.41
1:B:226:MET:HE2	1:B:226:MET:HB3	1.96	0.41
1:B:340:TYR:OH	1:B:440:LEU:HD21	2.21	0.41
1:B:440:LEU:HD12	1:B:440:LEU:HA	1.86	0.41
1:A:115:LYS:HD2	1:A:115:LYS:H	1.86	0.41
1:A:364:ALA:HB1	1:A:378:PRO:O	2.21	0.40
1:A:70:ILE:O	1:A:70:ILE:HG23	2.21	0.40
1:A:144:GLU:H	1:A:144:GLU:CD	2.28	0.40
1:B:352:MET:HE3	1:B:390:VAL:HG22	2.03	0.40
1:B:160:GLY:O	1:B:163:LYS:HD2	2.21	0.40
1:A:249:MET:HG2	1:A:367:PHE:CE1	2.56	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%)	367 (87%)	43 (10%)	13 (3%)	3	25
1	B	423/466 (91%)	374 (88%)	38 (9%)	11 (3%)	4	27
All	All	846/932 (91%)	741 (88%)	81 (10%)	24 (3%)	4	26

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	B	71	PRO
1	A	142	GLY
1	A	278	LEU
1	A	449	ASN
1	B	103	SER
1	B	278	LEU
1	A	96	PHE
1	A	103	SER
1	B	104	GLY
1	B	142	GLY
1	A	116	LEU
1	A	318	SER
1	B	96	PHE
1	B	116	LEU
1	B	345	ILE
1	A	434	LYS
1	B	449	ASN
1	A	234	ILE
1	A	345	ILE
1	B	38	VAL
1	A	104	GLY
1	A	98	PRO
1	B	432	GLY

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%)	305 (91%)	29 (9%)	9	34
1	B	334/368 (91%)	312 (93%)	22 (7%)	15	43
All	All	668/736 (91%)	617 (92%)	51 (8%)	12	39

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	42	THR
1	A	63	LEU
1	A	88	LEU
1	A	95	ARG
1	A	112	LEU
1	A	115	LYS
1	A	116	LEU
1	A	124	LEU
1	A	126	ILE
1	A	166	GLN
1	A	198	GLU
1	A	228	ARG
1	A	236	LEU
1	A	260	MET
1	A	268	LEU
1	A	290	LEU
1	A	296	ILE
1	A	316	PHE
1	A	317	ASN
1	A	349	PHE
1	A	353	LEU
1	A	389	LEU
1	A	399	THR
1	A	403	LEU
1	A	417	LEU
1	A	422	LEU

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Mol	Chain	Res	Type
1	A	447	LYS
1	A	448	GLN
1	B	27	LEU
1	B	42	THR
1	B	63	LEU
1	B	88	LEU
1	B	115	LYS
1	B	116	LEU
1	B	157	MET
1	B	215	PHE
1	B	228	ARG
1	B	268	LEU
1	B	290	LEU
1	B	296	ILE
1	B	304	LEU
1	B	316	PHE
1	B	317	ASN
1	B	353	LEU
1	B	389	LEU
1	B	399	THR
1	B	403	LEU
1	B	417	LEU
1	B	440	LEU
1	B	448	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	206	GLN
1	A	230	GLN
1	A	448	GLN
1	B	206	GLN
1	B	230	GLN
1	B	319	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](#)

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 [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	425/466 (91%)	1.05	76 (17%) 3 4	68, 106, 159, 262	0
1	B	425/466 (91%)	1.01	69 (16%) 4 5	66, 126, 186, 252	0
All	All	850/932 (91%)	1.03	145 (17%) 4 4	66, 114, 180, 262	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	449	ASN	7.0
1	A	115	LYS	7.0
1	A	113	GLU	6.9
1	A	449	ASN	6.1
1	B	319	GLN	6.1
1	A	141	ALA	6.1
1	A	30	ARG	6.0
1	B	209	ALA	5.6
1	A	114	GLY	5.4
1	B	70	ILE	5.4
1	B	348	ILE	5.3
1	B	399	THR	5.3
1	B	446	ALA	5.0
1	A	446	ALA	5.0
1	A	433	GLY	4.9
1	B	349	PHE	4.8
1	A	55	ASN	4.8
1	B	400	ALA	4.7
1	A	378	PRO	4.7
1	A	109	GLU	4.7
1	B	129	VAL	4.2
1	B	450	ARG	4.0
1	A	204	ARG	3.9
1	A	300	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	307	GLY	3.9
1	A	94	LYS	3.9
1	A	448	GLN	3.9
1	B	346	GLY	3.9
1	A	33	VAL	3.8
1	A	129	VAL	3.8
1	A	434	LYS	3.8
1	A	202	ARG	3.8
1	B	69	PRO	3.8
1	B	193	ALA	3.8
1	A	54	ASN	3.7
1	A	116	LEU	3.7
1	B	27	LEU	3.6
1	A	52	ALA	3.6
1	A	313	LEU	3.6
1	A	58	GLN	3.6
1	A	348	ILE	3.6
1	A	308	GLY	3.5
1	A	450	ARG	3.5
1	A	231	SER	3.5
1	B	340	TYR	3.5
1	A	327	LEU	3.3
1	A	99	ASP	3.3
1	B	141	ALA	3.2
1	A	110	GLY	3.2
1	A	75	TRP	3.2
1	B	266	ARG	3.2
1	A	199	MET	3.2
1	B	347	GLY	3.2
1	A	395	ARG	3.2
1	B	445	LEU	3.1
1	B	99	ASP	3.1
1	A	211	HIS	3.1
1	B	429	GLU	3.1
1	B	161	TRP	3.1
1	A	53	VAL	3.0
1	A	293	ILE	3.0
1	A	309	ASP	3.0
1	A	349	PHE	3.0
1	B	309	ASP	3.0
1	A	208	LEU	2.9
1	B	160	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	208	LEU	2.9
1	B	334	LEU	2.9
1	B	315	ALA	2.9
1	A	366	HIS	2.9
1	A	266	ARG	2.9
1	B	42	THR	2.8
1	A	161	TRP	2.8
1	B	395	ARG	2.8
1	A	200	HIS	2.8
1	B	437	TYR	2.8
1	A	429	GLU	2.8
1	B	293	ILE	2.8
1	B	212	SER	2.8
1	B	211	HIS	2.8
1	B	140	LEU	2.8
1	A	228	ARG	2.8
1	B	111	HIS	2.7
1	A	176	GLY	2.7
1	A	346	GLY	2.7
1	A	142	GLY	2.7
1	B	105	ILE	2.7
1	B	336	THR	2.6
1	A	444	THR	2.6
1	A	143	PHE	2.6
1	B	78	THR	2.6
1	A	209	ALA	2.6
1	B	35	ALA	2.6
1	B	403	LEU	2.6
1	A	43	GLY	2.6
1	A	296	ILE	2.5
1	B	335	LEU	2.5
1	A	207	THR	2.5
1	A	445	LEU	2.5
1	B	200	HIS	2.5
1	B	144	GLU	2.5
1	B	191	GLY	2.5
1	B	210	TYR	2.5
1	A	105	ILE	2.4
1	B	330	CYS	2.4
1	A	78	THR	2.4
1	B	26	SER	2.4
1	B	103	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	2.4
1	A	140	LEU	2.4
1	A	197	GLU	2.4
1	B	65	GLN	2.4
1	B	106	PRO	2.4
1	B	433	GLY	2.4
1	B	205	SER	2.3
1	A	326	ILE	2.3
1	B	338	ILE	2.3
1	A	265	ASN	2.3
1	B	241	ARG	2.3
1	B	245	ASP	2.3
1	A	221	THR	2.2
1	B	207	THR	2.2
1	B	190	ALA	2.2
1	A	206	GLN	2.2
1	A	212	SER	2.2
1	B	360	SER	2.2
1	B	307	GLY	2.2
1	B	385	GLY	2.2
1	B	206	GLN	2.2
1	B	444	THR	2.2
1	A	241	ARG	2.1
1	B	442	GLU	2.1
1	A	403	LEU	2.1
1	B	448	GLN	2.1
1	A	162	PHE	2.1
1	A	198	GLU	2.1
1	B	281	LEU	2.1
1	A	83	GLY	2.1
1	B	351	PRO	2.1
1	A	135	LEU	2.1
1	A	117	PRO	2.1
1	B	186	ASN	2.1
1	A	447	LYS	2.0
1	A	42	THR	2.0
1	A	352	MET	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 [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($\text{\AA}^2$)	Q<0.9
2	BR	B	1	1/1	0.90	0.45	176,176,176,176	0
2	BR	A	1	1/1	0.93	0.30	147,147,147,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.