



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:41 PM GMT

PDB ID : 4FTP
Title : Structure of the E202Y mutant of the Cl⁻/H⁺ antiporter CLC-ec1 from E.Coli
Authors : Lim, H.H.; Shane, T.; Miller, C.
Deposited on : 2012-06-27
Resolution : 3.21 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

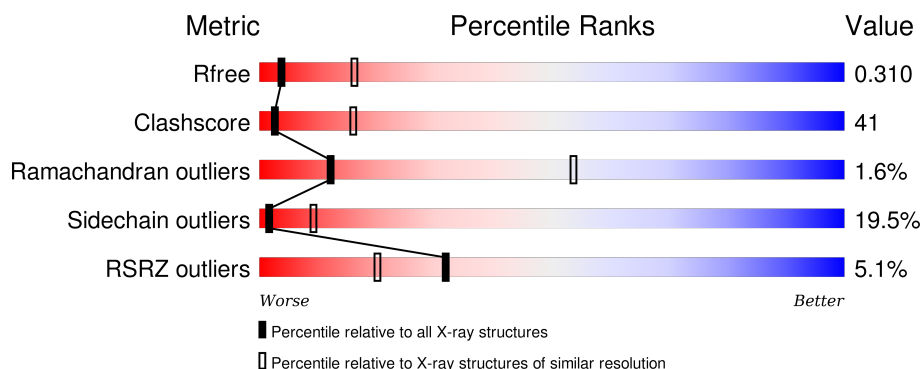
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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}	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	465	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3223 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 H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3222	2125	531	546	20			


There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	TYR	GLU	engineered mutation	UNP P37019

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- Chain A: 

Amino Acid	Percentage (%)
Met	5%
Lys	43%
Thr	43%
Asp	43%
Pro	43%
Ser	43%
Leu	43%
Glu	43%
Thr	43%
Pro	43%
Gln	43%
Ala	43%
Arg	43%
Leu	43%
Arg	43%
Arg	43%
Arg	43%
Gln	43%
Leu	43%
Glu	43%
Arg	43%
Asn	43%
Asp	43%
Thr	43%
Pro	43%
Ser	43%
Leu	43%
Glu	43%
Thr	43%
Pro	43%
Gln	43%
Ala	43%
Arg	43%
Leu	43%
Arg	43%
Arg	43%
Gln	43%
Leu	43%
Glu	43%
Arg	43%
Asn	43%
Asp	43%
Thr	43%
Pro	43%
Ser	43%
Leu	43%
Glu	43%
Thr	43%
Pro	43%
Gln	43%
Ala	43%
Arg	43%
Leu	43%
Arg	43%
Arg	43%
Gln	43%
Leu	43%
Glu	43%
Arg	43%
Asn	43%
Asp	43%
Thr	43%
Pro	43%
Ser	43%
Leu	43%
Glu	43%
Thr	43%
Pro	43%
Gln	43%
Ala	43%
Arg	43%
Leu	43%
Arg	43%
Arg	43%
Gln	43%
Leu	43%
Glu	43%
Arg	43%
Asn	43%
Asp	43%
Thr	43%
Pro	43%
Ser	43%
Leu	43%
Glu	43%
Thr	43%
Pro	43%
Gln	43%
Ala	43%
Arg	43%
Leu	43%
Arg	43%
Arg	43%
Gln	43%
Leu	43%
Glu	43%
Arg	43%
Asn	43%
Asp	43%
Thr	43%
Pro	43%
Ser	43%
Leu	43%
Glu	43%
Thr	43%
Pro	43%
Gln	43%
Ala	43%
Arg	43%
Leu	43%
Arg	43%
Arg	43%
Gln	43%
Leu	43%
Glu	43%
Arg	43%
Asn	43%
Asp	43%
Thr	43%
Pro	43%
Ser	43%
Leu	43%
Glu	43%
Thr	43%
Pro	43%
Gln	43%
Ala	43%
Arg	43%
Leu	43%
Arg	43%
Arg	43%
Gln	43%
Leu	43%
Glu	43%
Arg	43%
Asn	43%
Asp	43%
Thr	43%
Pro	43%
Ser	43%
Leu	43%
Glu	43%
Thr	43%
Pro	43%
Gln	43%
Ala	43%
Arg	43%
Leu	43%
Arg	43%
Arg	43%
Gln	43%
Leu	43%
Glu	43%
Arg	43%
Asn	43%
Asp	43%
Thr	43%
Pro	43%
Ser	43%
Leu	43%
Glu	43%
Thr	43%
Pro	43%
Gln	43%
Ala	43%
Arg	43%
Leu	43%
Arg	43%
Arg	43%
Gln	43%
Leu	43%
Glu	43%
Arg	43%
Asn	43%
Asp	43%
Thr	43%
Pro	43%
Ser	43%
Leu	43%
Glu	43%
Thr	43%
Pro	43%
Gln	43%
Ala	43%
Arg	43%
Leu	43%
Arg	43%
Arg	43%
Gln	43%
Leu	43%
Glu	43%
Arg	43%
Asn	43%
Asp	43%
Thr	43%
Pro	43%
Ser	43%
Leu	43%
Glu	43%
Thr	43%
Pro	43%
Gln	43%
Ala	43%
Arg	43%
Leu	43%
Arg	43%
Arg	43%
Gln	43%
Leu	43%
Glu	43%
Arg	43%
Asn	43%
Asp	43%
Thr	43%
Pro	43%
Ser	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.70 Å 85.17 Å 100.09 Å 90.00° 102.61° 90.00°	Depositor
Resolution (Å)	25.00 – 3.21 24.42 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.8 (25.00-3.21) 99.2 (24.42-3.21)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.85 (at 3.23 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.233 , 0.311 0.229 , 0.310	Depositor DCC
R_{free} test set	638 reflections (5.55%)	DCC
Wilson B-factor (Å ²)	94.7	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 12137 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3223	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.51	0/3295	0.76	3/4477 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	238	LEU	CA-CB-CG	7.12	131.67	115.30
1	A	316	GLY	N-CA-C	-5.67	98.92	113.10
1	A	378	LEU	CB-CA-C	5.63	120.89	110.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	LYS	Peptide
1	A	200	ILE	Peptide
1	A	204	MET	Peptide
1	A	205	ARG	Peptide
1	A	316	GLY	Peptide
1	A	378	LEU	Peptide

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	3222	0	3356	271	0
2	A	1	0	0	1	0
All	All	3223	0	3356	271	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 41.

All (271) 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:30:LYS:HG2	1:A:31:THR:H	1.14	1.12
1:A:200:ILE:HG23	1:A:204:MET:HB3	1.13	1.11
1:A:38:MET:HA	1:A:41:VAL:HG13	1.31	1.04
1:A:29:ASP:CG	1:A:30:LYS:H	1.59	1.03
1:A:340:ARG:HG2	1:A:340:ARG:HH11	1.17	1.03
1:A:205:ARG:O	1:A:207:GLN:NE2	1.99	0.94
1:A:29:ASP:HA	1:A:213:ILE:O	1.69	0.92
1:A:198:LEU:O	1:A:201:ILE:HG22	1.70	0.91
1:A:378:LEU:O	1:A:381:GLN:HB2	1.70	0.90
1:A:202:TYR:HE1	1:A:406:LEU:HB2	1.36	0.89
1:A:44:THR:HG22	1:A:224:MET:HB3	1.53	0.89
1:A:379:PHE:HB3	1:A:380:PRO:HD3	1.56	0.86
1:A:284:HIS:HD2	1:A:291:TRP:HA	1.42	0.85
1:A:122:VAL:HG13	1:A:157:ASN:ND2	1.91	0.85
1:A:200:ILE:HG23	1:A:204:MET:CB	2.03	0.85
1:A:340:ARG:CG	1:A:340:ARG:HH11	1.88	0.84
1:A:364:GLY:HA3	1:A:394:MET:HA	1.60	0.83
1:A:231:ILE:HG22	1:A:232:PHE:CD1	2.14	0.83
1:A:29:ASP:CG	1:A:30:LYS:N	2.34	0.81
1:A:264:ILE:HG13	1:A:435:LEU:HD12	1.62	0.81
1:A:168:LEU:O	1:A:174:ARG:NH2	2.14	0.80
1:A:317:PHE:H	1:A:320:ILE:HD13	1.46	0.80
1:A:30:LYS:HG2	1:A:31:THR:N	1.97	0.79
1:A:165:ILE:HG22	1:A:166:PHE:CD2	2.16	0.79
1:A:206:PRO:HA	1:A:208:PHE:N	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ILE:CG2	1:A:204:MET:HB3	2.05	0.79
1:A:205:ARG:O	1:A:207:GLN:HB2	1.84	0.78
1:A:333:LEU:HD11	1:A:369:THR:HG22	1.63	0.78
1:A:298:ILE:HD13	1:A:346:LEU:HG	1.65	0.78
1:A:284:HIS:CD2	1:A:291:TRP:HA	2.21	0.76
1:A:148:GLU:HG2	1:A:357:PHE:HB3	1.68	0.75
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.68	0.74
1:A:263:GLY:HA3	1:A:435:LEU:HB3	1.70	0.74
1:A:340:ARG:HG2	1:A:340:ARG:NH1	1.99	0.74
1:A:30:LYS:O	1:A:31:THR:OG1	2.06	0.73
1:A:413:LEU:HD11	1:A:422:ILE:CG1	2.18	0.73
1:A:148:GLU:OE2	1:A:149:GLY:N	2.21	0.73
1:A:35:ILE:HG21	1:A:176:THR:HG21	1.69	0.73
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.19	0.72
1:A:378:LEU:HB3	1:A:382:TYR:HB2	1.71	0.72
1:A:239:ILE:HG21	1:A:416:THR:HG22	1.71	0.72
1:A:375:ALA:HB1	1:A:384:LEU:CD1	2.21	0.71
1:A:234:HIS:CD2	1:A:235:GLU:HG3	2.25	0.71
1:A:289:THR:O	1:A:293:LEU:HG	1.91	0.70
1:A:200:ILE:HA	1:A:204:MET:O	1.92	0.70
1:A:379:PHE:CB	1:A:380:PRO:HD3	2.22	0.70
1:A:288:ILE:O	1:A:292:VAL:N	2.24	0.69
1:A:202:TYR:CE2	1:A:405:PRO:HD2	2.27	0.69
1:A:53:PHE:O	1:A:57:VAL:HG23	1.91	0.69
1:A:30:LYS:CG	1:A:31:THR:H	1.95	0.69
1:A:38:MET:O	1:A:42:VAL:HG23	1.93	0.69
1:A:38:MET:HA	1:A:41:VAL:CG1	2.18	0.68
1:A:317:PHE:H	1:A:320:ILE:CD1	2.06	0.68
1:A:99:LYS:HG2	1:A:100:TYR:CE1	2.28	0.68
1:A:377:GLU:C	1:A:378:LEU:HD22	2.14	0.67
1:A:416:THR:OG1	1:A:416:THR:O	2.06	0.67
1:A:263:GLY:HA2	1:A:432:ALA:O	1.96	0.66
1:A:406:LEU:O	1:A:410:ILE:HG12	1.96	0.66
1:A:312:THR:HG22	1:A:339:ALA:HB1	1.77	0.66
1:A:42:VAL:O	1:A:46:VAL:HG23	1.96	0.65
1:A:333:LEU:HD11	1:A:369:THR:CG2	2.26	0.65
1:A:239:ILE:CG2	1:A:416:THR:HG22	2.26	0.65
1:A:88:VAL:HG12	1:A:89:LEU:HD23	1.79	0.65
1:A:429:GLY:O	1:A:433:THR:HB	1.97	0.65
1:A:379:PHE:HB3	1:A:380:PRO:CD	2.26	0.65
1:A:312:THR:CG2	1:A:339:ALA:HB1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:TYR:O	1:A:383:HIS:HB2	1.97	0.64
1:A:148:GLU:OE2	1:A:355:GLY:HA3	1.97	0.64
1:A:29:ASP:OD2	1:A:30:LYS:N	2.26	0.64
1:A:376:VAL:HA	1:A:379:PHE:HB2	1.80	0.64
1:A:206:PRO:CG	1:A:211:THR:HB	2.28	0.63
1:A:206:PRO:HA	1:A:208:PHE:H	1.61	0.63
1:A:312:THR:HG22	1:A:339:ALA:CB	2.28	0.63
1:A:202:TYR:OH	1:A:405:PRO:HB2	1.98	0.62
1:A:40:ALA:O	1:A:44:THR:HG23	2.00	0.62
1:A:206:PRO:HG2	1:A:211:THR:HB	1.80	0.62
1:A:229:TYR:O	1:A:233:ASN:HB2	2.00	0.62
1:A:218:VAL:O	1:A:222:VAL:HG23	2.01	0.60
1:A:206:PRO:HG3	1:A:211:THR:OG1	2.00	0.60
1:A:53:PHE:CE1	1:A:136:LEU:HD12	2.36	0.60
1:A:170:GLY:H	1:A:174:ARG:NH2	1.98	0.60
1:A:376:VAL:HA	1:A:379:PHE:CG	2.36	0.60
1:A:35:ILE:HG21	1:A:176:THR:CG2	2.32	0.60
1:A:251:THR:O	1:A:254:LEU:HB2	2.01	0.59
1:A:233:ASN:HD21	1:A:236:VAL:CG2	2.15	0.59
1:A:304:LEU:HD12	1:A:305:LEU:H	1.67	0.59
1:A:213:ILE:O	1:A:213:ILE:CG2	2.51	0.59
1:A:378:LEU:N	1:A:378:LEU:HD22	2.16	0.59
1:A:38:MET:CA	1:A:41:VAL:HG13	2.21	0.59
1:A:376:VAL:HA	1:A:379:PHE:CD1	2.37	0.58
1:A:213:ILE:O	1:A:213:ILE:HG22	2.02	0.58
1:A:421:LEU:O	1:A:425:MET:HG3	2.04	0.58
1:A:376:VAL:CA	1:A:379:PHE:HB2	2.33	0.58
1:A:216:LYS:HD3	1:A:216:LYS:H	1.69	0.58
1:A:146:GLY:HA3	1:A:148:GLU:OE1	2.04	0.58
1:A:322:ILE:HG22	1:A:328:PHE:CE2	2.39	0.57
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.86	0.57
1:A:375:ALA:HB3	1:A:379:PHE:CE2	2.39	0.57
1:A:346:LEU:O	1:A:350:SER:HB3	2.04	0.57
1:A:216:LYS:HD3	1:A:216:LYS:N	2.18	0.57
1:A:336:ILE:O	1:A:340:ARG:HB2	2.05	0.56
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.40	0.56
1:A:233:ASN:ND2	1:A:236:VAL:HG23	2.20	0.56
1:A:376:VAL:HA	1:A:379:PHE:CB	2.36	0.56
1:A:358:ALA:HB3	1:A:359:PRO:CD	2.36	0.56
1:A:180:THR:CG2	1:A:221:GLY:HA3	2.36	0.56
1:A:317:PHE:N	1:A:320:ILE:HD13	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD13	1:A:33:LEU:H	1.70	0.56
1:A:175:HIS:HA	1:A:178:LEU:HD23	1.87	0.55
1:A:264:ILE:HG13	1:A:435:LEU:CD1	2.34	0.55
1:A:163:LEU:HD22	1:A:174:ARG:HA	1.89	0.55
1:A:172:GLU:HG3	1:A:212:LEU:HD22	1.89	0.55
1:A:421:LEU:C	1:A:424:PRO:HD2	2.27	0.55
1:A:267:PRO:HG2	1:A:439:THR:HB	1.88	0.55
1:A:206:PRO:HG3	1:A:211:THR:CB	2.37	0.54
1:A:263:GLY:CA	1:A:435:LEU:HB3	2.38	0.54
1:A:90:ALA:O	1:A:94:TYR:HD1	1.91	0.54
1:A:30:LYS:O	1:A:214:SER:HB2	2.07	0.54
1:A:34:ALA:O	1:A:38:MET:SD	2.65	0.54
1:A:375:ALA:HB1	1:A:384:LEU:HD12	1.88	0.54
1:A:175:HIS:HA	1:A:178:LEU:CD2	2.37	0.54
1:A:202:TYR:CE1	1:A:406:LEU:HB2	2.29	0.54
1:A:130:VAL:O	1:A:134:GLY:N	2.36	0.54
1:A:238:LEU:HG	1:A:317:PHE:HE1	1.72	0.54
1:A:304:LEU:HD12	1:A:305:LEU:N	2.22	0.54
1:A:206:PRO:HA	1:A:207:GLN:HB2	1.90	0.54
1:A:144:VAL:HG13	1:A:314:GLY:O	2.08	0.53
1:A:378:LEU:HG	1:A:382:TYR:HD1	1.74	0.53
1:A:301:LEU:O	1:A:305:LEU:N	2.41	0.53
1:A:215:ILE:HD13	1:A:215:ILE:N	2.23	0.53
1:A:288:ILE:O	1:A:289:THR:C	2.47	0.53
1:A:364:GLY:CA	1:A:394:MET:HA	2.35	0.53
1:A:262:PHE:HD1	1:A:397:LEU:HD13	1.74	0.53
1:A:233:ASN:HD21	1:A:236:VAL:HG23	1.73	0.53
1:A:64:ARG:HH11	1:A:86:SER:HB2	1.74	0.53
1:A:452:THR:HA	1:A:455:LYS:HG2	1.92	0.52
1:A:86:SER:CB	1:A:303:GLY:HA3	2.40	0.52
1:A:163:LEU:CD2	1:A:174:ARG:HA	2.38	0.52
1:A:394:MET:CE	1:A:412:VAL:HG13	2.39	0.52
1:A:382:TYR:HB3	1:A:384:LEU:HG	1.92	0.52
1:A:287:ASN:HB3	1:A:290:LYS:HB2	1.92	0.52
1:A:413:LEU:HD11	1:A:422:ILE:HG13	1.90	0.52
1:A:110:PRO:HG2	1:A:448:ILE:HG21	1.92	0.52
1:A:264:ILE:O	1:A:267:PRO:HD2	2.10	0.52
1:A:378:LEU:N	1:A:378:LEU:CD2	2.73	0.51
1:A:376:VAL:C	1:A:379:PHE:HB2	2.31	0.51
1:A:205:ARG:HG2	1:A:207:GLN:HG3	1.91	0.51
1:A:340:ARG:CG	1:A:340:ARG:NH1	2.55	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:HD12	1:A:382:TYR:CD1	2.45	0.51
1:A:206:PRO:HA	1:A:207:GLN:C	2.26	0.51
1:A:143:MET:HE3	1:A:298:ILE:HG22	1.93	0.51
1:A:272:TRP:O	1:A:276:MET:HB2	2.11	0.51
1:A:250:ASN:HB2	1:A:382:TYR:HE2	1.76	0.51
1:A:47:GLY:O	1:A:51:VAL:HG23	2.11	0.51
1:A:248:PRO:HB2	1:A:250:ASN:OD1	2.11	0.50
1:A:433:THR:HG22	1:A:434:LEU:N	2.27	0.50
1:A:38:MET:CE	1:A:177:LEU:HD11	2.41	0.50
1:A:316:GLY:HA3	1:A:362:ALA:HB2	1.94	0.50
1:A:64:ARG:NH1	1:A:86:SER:HB2	2.27	0.49
1:A:33:LEU:H	1:A:33:LEU:CD1	2.24	0.49
1:A:33:LEU:N	1:A:33:LEU:CD1	2.75	0.49
1:A:160:ARG:NH1	1:A:164:ASP:OD2	2.46	0.49
1:A:147:ARG:NH2	1:A:189:ALA:O	2.45	0.49
1:A:234:HIS:HD2	1:A:235:GLU:HG3	1.74	0.49
1:A:38:MET:HE3	1:A:177:LEU:HD11	1.94	0.49
1:A:206:PRO:HG3	1:A:211:THR:HB	1.95	0.49
1:A:288:ILE:HG22	1:A:289:THR:N	2.28	0.48
1:A:269:PHE:O	1:A:273:VAL:HG12	2.13	0.48
1:A:83:PHE:C	1:A:83:PHE:CD1	2.87	0.48
1:A:277:GLN:OE1	1:A:448:ILE:HD11	2.13	0.48
1:A:30:LYS:C	1:A:31:THR:OG1	2.52	0.48
1:A:288:ILE:O	1:A:291:TRP:N	2.46	0.48
1:A:86:SER:HB3	1:A:303:GLY:HA3	1.95	0.48
1:A:379:PHE:HD2	1:A:384:LEU:HD12	1.79	0.48
1:A:312:THR:CG2	1:A:339:ALA:CB	2.90	0.48
1:A:309:ALA:O	1:A:312:THR:OG1	2.32	0.48
1:A:375:ALA:C	1:A:377:GLU:N	2.66	0.48
1:A:330:MET:O	1:A:330:MET:HG3	2.12	0.47
1:A:322:ILE:CG2	1:A:328:PHE:CE2	2.98	0.47
1:A:139:LEU:CD2	1:A:145:LEU:HB2	2.44	0.47
1:A:199:PHE:HA	1:A:202:TYR:HB2	1.95	0.47
1:A:110:PRO:HG2	1:A:448:ILE:CG2	2.45	0.47
1:A:202:TYR:HE2	1:A:405:PRO:HD2	1.79	0.47
1:A:379:PHE:CB	1:A:380:PRO:CD	2.89	0.47
1:A:304:LEU:O	1:A:308:VAL:HG13	2.15	0.46
1:A:341:VAL:O	1:A:344:THR:HB	2.14	0.46
1:A:44:THR:HG22	1:A:224:MET:CB	2.36	0.46
1:A:53:PHE:CD1	1:A:136:LEU:HD12	2.50	0.46
1:A:378:LEU:HB2	1:A:379:PHE:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:CB	1:A:382:TYR:HB2	2.43	0.46
1:A:171:ASP:H	1:A:174:ARG:HD2	1.81	0.46
1:A:283:VAL:O	1:A:283:VAL:HG12	2.15	0.46
1:A:31:THR:HG22	1:A:32:PRO:HD2	1.97	0.46
1:A:320:ILE:HD11	1:A:362:ALA:HA	1.98	0.46
1:A:413:LEU:HD12	1:A:425:MET:CE	2.46	0.46
1:A:202:TYR:CZ	1:A:405:PRO:HD2	2.50	0.46
1:A:375:ALA:O	1:A:379:PHE:CD2	2.69	0.45
1:A:445:TYR:OH	2:A:501:CL:CL	2.62	0.45
1:A:175:HIS:O	1:A:176:THR:C	2.55	0.45
1:A:423:LEU:O	1:A:424:PRO:C	2.54	0.45
1:A:37:PHE:CD2	1:A:38:MET:HG3	2.52	0.45
1:A:51:VAL:O	1:A:54:ASP:HB2	2.16	0.45
1:A:139:LEU:HD21	1:A:145:LEU:HB2	1.97	0.45
1:A:103:GLU:OE1	1:A:123:ARG:HB2	2.16	0.45
1:A:193:PRO:O	1:A:197:ILE:HD12	2.17	0.45
1:A:171:ASP:N	1:A:174:ARG:HD2	2.32	0.45
1:A:402:ILE:O	1:A:402:ILE:HG13	2.15	0.45
1:A:438:PHE:N	1:A:438:PHE:CD1	2.83	0.45
1:A:31:THR:HG21	1:A:35:ILE:HG13	1.98	0.45
1:A:250:ASN:HB2	1:A:382:TYR:CE2	2.52	0.45
1:A:239:ILE:HG21	1:A:416:THR:CG2	2.45	0.45
1:A:172:GLU:O	1:A:176:THR:HB	2.16	0.45
1:A:413:LEU:CD1	1:A:422:ILE:HG12	2.47	0.45
1:A:415:MET:HE2	1:A:415:MET:HB2	1.78	0.45
1:A:315:GLY:C	1:A:340:ARG:HH22	2.21	0.44
1:A:403:ARG:C	1:A:405:PRO:HD3	2.36	0.44
1:A:248:PRO:HG2	1:A:251:THR:HG23	1.98	0.44
1:A:375:ALA:C	1:A:377:GLU:H	2.20	0.44
1:A:65:MET:HG3	1:A:66:GLY:N	2.32	0.44
1:A:399:ALA:O	1:A:403:ARG:HA	2.17	0.44
1:A:320:ILE:N	1:A:321:PRO:HD2	2.33	0.44
1:A:38:MET:SD	1:A:168:LEU:HD21	2.57	0.44
1:A:143:MET:HE2	1:A:347:CYS:HB3	2.00	0.44
1:A:124:TRP:CE3	1:A:161:MET:HG3	2.52	0.44
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.53	0.44
1:A:374:VAL:O	1:A:377:GLU:OE1	2.36	0.43
1:A:394:MET:HE3	1:A:412:VAL:HG13	2.00	0.43
1:A:263:GLY:HA3	1:A:435:LEU:CB	2.43	0.43
1:A:413:LEU:HD11	1:A:422:ILE:HD11	1.99	0.43
1:A:258:LEU:HD13	1:A:371:PHE:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:HG2	1:A:100:TYR:CZ	2.54	0.43
1:A:47:GLY:HA3	1:A:228:MET:HB2	1.99	0.43
1:A:30:LYS:O	1:A:214:SER:CB	2.66	0.43
1:A:435:LEU:HD22	1:A:435:LEU:HA	1.79	0.43
1:A:455:LYS:O	1:A:459:GLU:HG2	2.18	0.43
1:A:31:THR:CG2	1:A:35:ILE:HG13	2.49	0.43
1:A:377:GLU:HG3	1:A:377:GLU:H	1.68	0.43
1:A:431:GLY:O	1:A:435:LEU:HB2	2.18	0.43
1:A:413:LEU:HD11	1:A:422:ILE:CD1	2.48	0.43
1:A:251:THR:HG21	1:A:384:LEU:HD23	2.01	0.43
1:A:95:PHE:O	1:A:98:ARG:N	2.52	0.42
1:A:197:ILE:HG22	1:A:198:LEU:N	2.34	0.42
1:A:456:GLN:O	1:A:459:GLU:HB2	2.19	0.42
1:A:170:GLY:H	1:A:174:ARG:CZ	2.32	0.42
1:A:284:HIS:CD2	1:A:291:TRP:CA	2.97	0.42
1:A:209:ARG:HB3	1:A:210:TYR:H	1.59	0.42
1:A:248:PRO:HG2	1:A:251:THR:CG2	2.49	0.42
1:A:206:PRO:HB3	1:A:209:ARG:H	1.85	0.42
1:A:284:HIS:HB3	1:A:290:LYS:HB3	2.02	0.42
1:A:424:PRO:O	1:A:427:ILE:HB	2.20	0.42
1:A:88:VAL:O	1:A:91:MET:HB2	2.20	0.42
1:A:448:ILE:HA	1:A:448:ILE:HD13	1.70	0.42
1:A:30:LYS:HB3	1:A:30:LYS:HE2	1.51	0.42
1:A:206:PRO:CG	1:A:211:THR:CB	2.97	0.42
1:A:438:PHE:C	1:A:440:GLY:N	2.73	0.42
1:A:333:LEU:HA	1:A:333:LEU:HD23	1.82	0.41
1:A:173:ALA:O	1:A:174:ARG:C	2.58	0.41
1:A:357:PHE:CE1	1:A:402:ILE:HD13	2.55	0.41
1:A:278:ASP:OD1	1:A:278:ASP:N	2.54	0.41
1:A:218:VAL:O	1:A:222:VAL:CG2	2.67	0.41
1:A:174:ARG:O	1:A:178:LEU:HD23	2.21	0.41
1:A:51:VAL:O	1:A:54:ASP:N	2.53	0.41
1:A:413:LEU:CD1	1:A:422:ILE:CG1	2.94	0.41
1:A:223:ILE:O	1:A:227:ILE:HG13	2.21	0.41
1:A:109:ILE:N	1:A:110:PRO:CD	2.84	0.41
1:A:301:LEU:O	1:A:305:LEU:HB3	2.22	0.40
1:A:356:ILE:HD12	1:A:356:ILE:HA	1.61	0.40
1:A:259:GLY:O	1:A:432:ALA:HA	2.22	0.40
1:A:289:THR:O	1:A:293:LEU:CG	2.66	0.40
1:A:453:LEU:O	1:A:456:GLN:N	2.47	0.40
1:A:148:GLU:CG	1:A:357:PHE:HB3	2.46	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	430/465 (92%)	364 (85%)	59 (14%)	7 (2%)	12 54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ILE
1	A	288	ILE
1	A	235	GLU
1	A	72	ALA
1	A	197	ILE
1	A	379	PHE
1	A	31	THR

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	323/353 (92%)	260 (80%)	63 (20%)	2 9

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP

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Mol	Chain	Res	Type
1	A	31	THR
1	A	33	LEU
1	A	38	MET
1	A	44	THR
1	A	54	ASP
1	A	60	LEU
1	A	77	LEU
1	A	99	LYS
1	A	123	ARG
1	A	126	ARG
1	A	148	GLU
1	A	151	THR
1	A	157	ASN
1	A	160	ARG
1	A	169	LYS
1	A	174	ARG
1	A	176	THR
1	A	177	LEU
1	A	198	LEU
1	A	200	ILE
1	A	202	TYR
1	A	203	GLU
1	A	204	MET
1	A	209	ARG
1	A	210	TYR
1	A	213	ILE
1	A	216	LYS
1	A	226	THR
1	A	230	ARG
1	A	233	ASN
1	A	234	HIS
1	A	235	GLU
1	A	238	LEU
1	A	281	HIS
1	A	284	HIS
1	A	301	LEU
1	A	308	VAL
1	A	319	LEU
1	A	327	ASN
1	A	340	ARG
1	A	356	ILE
1	A	357	PHE

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Mol	Chain	Res	Type
1	A	359	PRO
1	A	365	THR
1	A	376	VAL
1	A	377	GLU
1	A	378	LEU
1	A	382	TYR
1	A	383	HIS
1	A	385	GLU
1	A	402	ILE
1	A	413	LEU
1	A	419	TYR
1	A	420	GLN
1	A	423	LEU
1	A	430	LEU
1	A	433	THR
1	A	435	LEU
1	A	444	LEU
1	A	448	ILE
1	A	449	LEU
1	A	455	LYS

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

Mol	Chain	Res	Type
1	A	233	ASN
1	A	234	HIS
1	A	284	HIS
1	A	418	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	432/465 (92%)	-0.03	22 (5%) 32 20	43, 85, 150, 211	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	THR	7.7
1	A	210	TYR	4.3
1	A	75	TYR	4.3
1	A	283	VAL	4.1
1	A	209	ARG	4.0
1	A	237	ALA	3.9
1	A	211	THR	3.7
1	A	212	LEU	3.7
1	A	70	HIS	3.3
1	A	30	LYS	3.3
1	A	284	HIS	2.8
1	A	72	ALA	2.7
1	A	459	GLU	2.7
1	A	119	GLN	2.6
1	A	73	ASP	2.6
1	A	74	ASN	2.4
1	A	71	THR	2.4
1	A	236	VAL	2.3
1	A	208	PHE	2.3
1	A	118	ASP	2.2
1	A	328	PHE	2.0
1	A	59	TRP	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CL	A	501	1/1	0.70	0.18	-0.81	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.