Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:56 AM GMT

PDB ID	:	2VDE
Title	:	CRYSTAL STRUCTURE OF THE OPEN STATE OF TOLC OUTER MEMBRANE COMPONENT OF MUTLIDRUG EFFLUX PUMPS
Authors	:	Bavro, V.N.; Pietras, Z.; Furnham, N.; Perez-Cano, L.; Fernandez-Recio, J.; Pei, X.Y.; Truer, R.; Misra, R.; Luisi, B.
Deposited on	:	2007-10-04
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

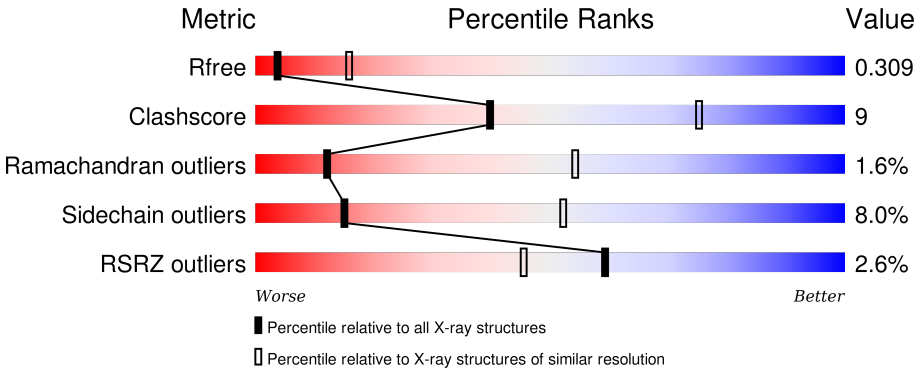
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 <=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	460	3%, 72%, 20%, 7%
1	B	460	2%, 64%, 27%, 7%
1	C	460	2%, 69%, 22%, 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	C	1453	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9921 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 OUTER MEMBRANE PROTEIN TOLC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	71	15	1
			3306	2039	584	678	5			
1	B	429	Total	C	N	O	S	51	10	1
			3303	2037	584	677	5			
1	C	429	Total	C	N	O	S	65	16	1
			3308	2040	584	679	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ARG	LYS	CONFLICT	UNP P02930
B	2	ARG	LYS	CONFLICT	UNP P02930
C	2	ARG	LYS	CONFLICT	UNP P02930
A	191	LEU	VAL	ENGINEERED MUTATION	UNP P02930
A	384	PHE	TYR	ENGINEERED MUTATION	UNP P02930
A	389	GLU	ARG	ENGINEERED MUTATION	UNP P02930
B	191	LEU	VAL	ENGINEERED MUTATION	UNP P02930
B	384	PHE	TYR	ENGINEERED MUTATION	UNP P02930
B	389	GLU	ARG	ENGINEERED MUTATION	UNP P02930
C	191	LEU	VAL	ENGINEERED MUTATION	UNP P02930
C	384	PHE	TYR	ENGINEERED MUTATION	UNP P02930
C	389	GLU	ARG	ENGINEERED MUTATION	UNP P02930

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

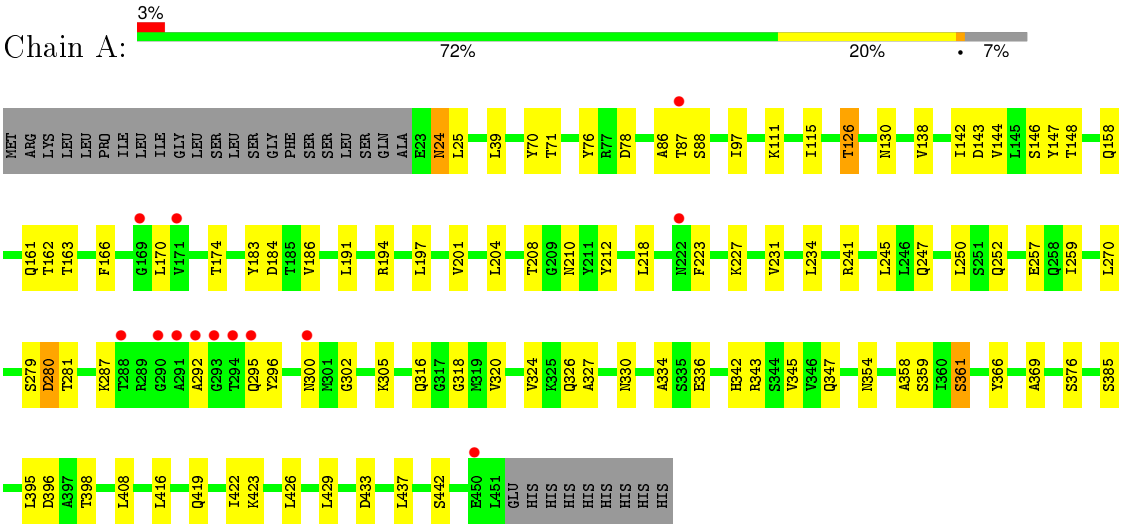
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	2	Total	Cl	0	0
			2	2		
2	C	1	Total	Cl	0	0
			1	1		

3 Residue-property plots (i)

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.

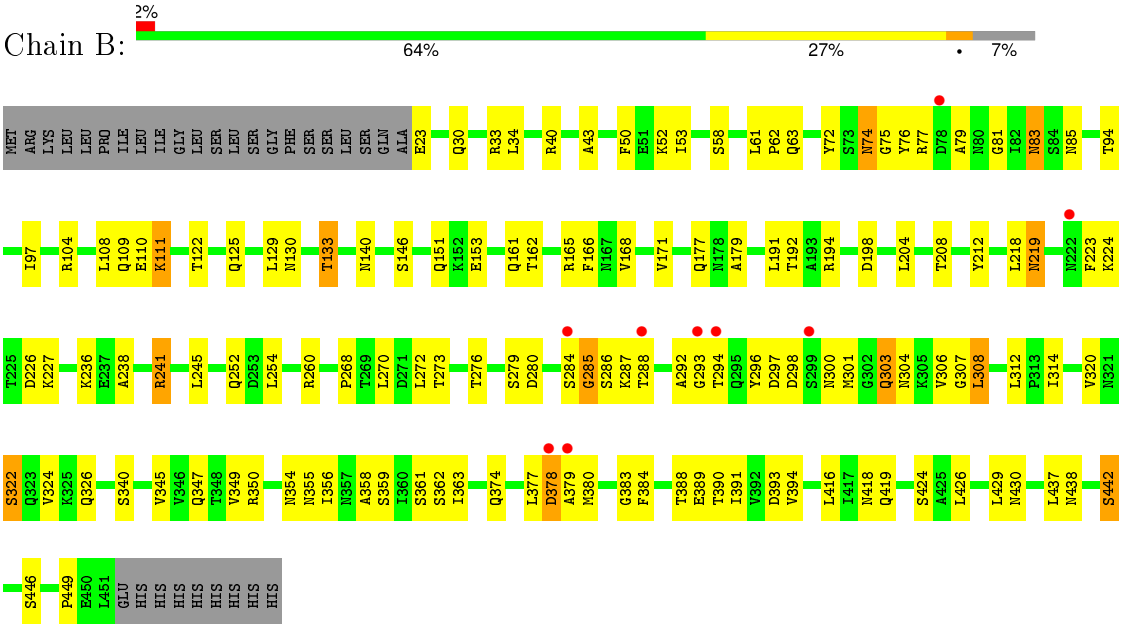
- Molecule 1: OUTER MEMBRANE PROTEIN TOLC

Chain A:



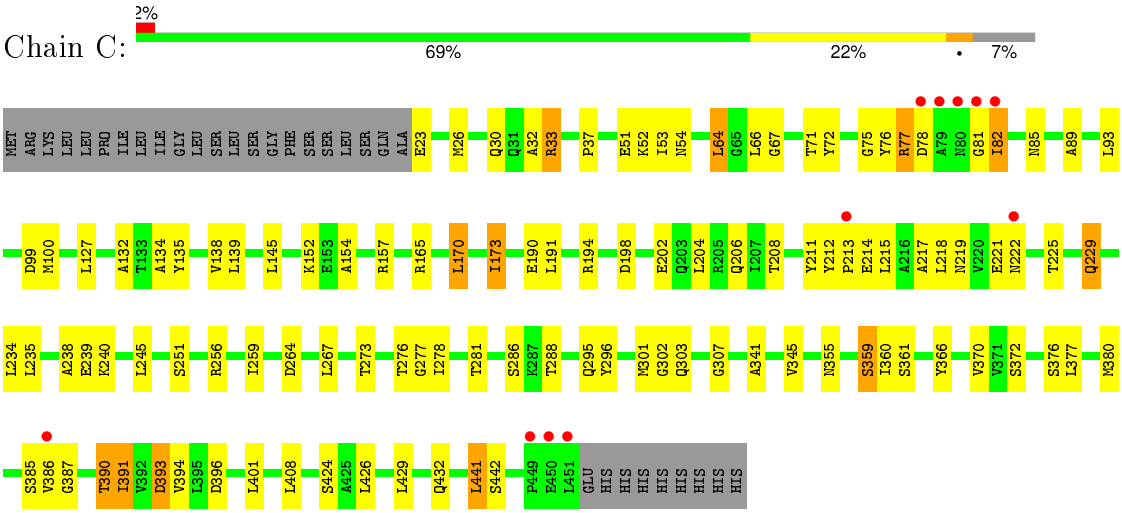
- Molecule 1: OUTER MEMBRANE PROTEIN TOLC

Chain B:



- Molecule 1: OUTER MEMBRANE PROTEIN TOLC

Chain C:


2%
69%
22%
7%
MET ARG LYS LEU LEU PRO ILE LEU ILE GLY LEU SER LEU SER GLY PHE SER SER LEU SER GLN ALA E23 M26 Q30 Q31 A32 R33 P37 E51 K52 I53 N54 L64 G65 L66 G67 T71 Y72 G75 Y76 R77 D78 A79 N80 G81 I82 N85 A89 L93
D99 M100 L127 A132 T133 A134 Y135 V138 L139 L145 K152 E153 A154 R157 R165 L170 I173 E190 L191 R194 D198 E202 Q203 L204 R205 Q206 I207 T208 Y211 Y212 P213 E214 L215 A216 A217 L218 N219 V220 E221 N222 T225 Q229
L234 L235 A238 E239 K240 L245 S251 R256 I259 D264 L267 T273 T276 G277 I278 T281 S286 K287 T288 Q295 Y296 M301 G302 Q303 G307 A341 V345 N355 S359 I360 S361 Y366 V370 Y371 S372 S376 L377 M380
S385 V386 G387 T390 I391 V392 D393 V394 L395 D396 L401 L408 S424 A425 L426 L429 Q432 L441 S442 P449 E450 L451 GLU HIS HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	128.28Å 136.18Å 136.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.08 – 3.20 22.08 – 3.22	Depositor EDS
% Data completeness (in resolution range)	96.7 (22.08-3.20) 96.7 (22.08-3.22)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 3.23Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.266 , 0.315 0.263 , 0.309	Depositor DCC
R_{free} test set	1906 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	70.2	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.1	EDS
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	3 of 37940 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9921	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.44	1/3350 (0.0%)	0.56	1/4551 (0.0%)
1	B	0.45	0/3344	0.57	1/4543 (0.0%)
1	C	0.45	2/3352 (0.1%)	0.57	1/4554 (0.0%)
All	All	0.44	3/10046 (0.0%)	0.56	3/13648 (0.0%)

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	B	1	1
1	C	0	1
All	All	1	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	214[A]	GLU	CB-CG	6.23	1.64	1.52
1	A	194[A]	ARG	CB-CG	-5.27	1.38	1.52
1	C	152[A]	LYS	CB-CG	5.08	1.66	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227[A]	LYS	CB-CG-CD	-5.95	96.13	111.60
1	C	152[A]	LYS	CA-CB-CG	-5.83	100.58	113.40
1	B	308	LEU	CA-CB-CG	5.61	128.20	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	288	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	292[A]	ALA	Peptide
1	C	77	ARG	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	3306	0	3221	53	0
1	B	3303	0	3233	74	0
1	C	3308	0	3215	71	0
2	A	2	0	0	1	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	9921	0	9669	167	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 9.

All (167) 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:191:LEU:HD11	1:C:361:SER:HB2	1.45	0.97
1:B:97:ILE:HD11	1:B:272:LEU:HB2	1.48	0.96
1:A:191:LEU:HD11	1:C:361:SER:CB	1.98	0.94
1:A:361:SER:HB3	1:B:191:LEU:HD11	1.48	0.93
1:C:82:ILE:HD12	1:C:288:THR:HG23	1.68	0.75
1:A:361:SER:HB3	1:B:191:LEU:CD1	2.16	0.74
1:A:24:ASN:HD22	1:A:24:ASN:H	1.36	0.74
1:C:366:TYR:O	1:C:370:VAL:HG23	1.87	0.73
1:C:219:ASN:HB3	1:C:222:ASN:HB3	1.71	0.72
1:C:23:GLU:N	1:C:215:LEU:HA	2.08	0.69
1:C:81:GLY:O	1:C:82:ILE:HB	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASN:ND2	1:A:24:ASN:H	1.93	0.66
1:C:225:THR:HB	1:C:360:ILE:HD12	1.76	0.66
1:A:280:ASP:HB3	1:A:300:ASN:HA	1.79	0.65
1:B:208:THR:HG21	1:B:212:TYR:OH	1.97	0.65
1:C:341:ALA:O	1:C:345:VAL:HG23	1.96	0.65
1:B:303:GLN:HA	1:C:75:GLY:HA3	1.79	0.64
1:B:326:GLN:CD	1:C:52:LYS:HB3	2.19	0.62
1:C:32:ALA:HB2	1:C:208:THR:HG23	1.80	0.62
1:A:191:LEU:HD11	1:C:361:SER:HB3	1.80	0.62
1:A:24:ASN:N	1:A:24:ASN:HD22	1.98	0.61
1:B:378:ASP:O	1:B:380:MET:N	2.33	0.61
1:C:380:MET:HB3	1:C:394:VAL:HG12	1.83	0.60
1:A:115:ILE:HG23	1:A:247:GLN:HG3	1.84	0.59
1:B:340:SER:OG	1:C:37:PRO:HB2	2.03	0.59
1:B:300:ASN:HB2	1:C:78:ASP:HB3	1.85	0.59
1:B:104:ARG:NH1	1:B:260:ARG:HB3	2.18	0.58
1:B:81:GLY:O	1:B:286:SER:N	2.32	0.58
1:B:279:SER:HB3	1:B:301:MET:HB2	1.83	0.58
1:A:208:THR:HG21	1:A:212:TYR:HE2	1.69	0.58
1:B:238:ALA:HB2	1:B:426:LEU:HD23	1.86	0.58
1:B:81:GLY:O	1:B:285:GLY:HA3	2.04	0.58
1:B:97:ILE:O	1:B:270:LEU:HB3	2.05	0.57
1:A:231:VAL:HA	1:A:234:LEU:HD12	1.87	0.57
1:A:302:GLY:C	1:B:76:TYR:HB3	2.26	0.56
1:C:288:THR:HB	1:C:296:TYR:HD2	1.70	0.56
1:A:342:HIS:HA	1:A:345:VAL:HG12	1.88	0.55
1:A:361:SER:CB	1:B:191:LEU:HD11	2.29	0.55
1:C:355:ASN:O	1:C:359:SER:HB2	2.07	0.55
1:C:377:LEU:HD22	1:C:401:LEU:HD22	1.89	0.55
1:B:53:ILE:HD13	1:B:109:GLN:HG3	1.88	0.55
1:B:345:VAL:O	1:B:349:VAL:HG22	2.07	0.55
1:B:111:LYS:HB3	1:B:254:LEU:HD12	1.89	0.54
1:A:86:ALA:HB2	1:A:281:THR:HG23	1.88	0.54
1:C:238:ALA:C	1:C:240:LYS:H	2.10	0.54
1:A:138:VAL:O	1:A:142:ILE:HG12	2.07	0.54
1:C:99:ASP:O	1:C:100:MET:HB2	2.07	0.53
1:A:191:LEU:CD1	1:C:361:SER:HB3	2.38	0.53
1:C:225:THR:HB	1:C:360:ILE:CD1	2.39	0.53
1:A:320:VAL:O	1:A:324:VAL:HG23	2.09	0.53
1:A:318:GLY:HA2	2:A:1454:CL:CL	2.46	0.53
1:A:204:LEU:O	1:A:208:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:THR:HB	1:C:296:TYR:CD2	2.44	0.52
1:B:374:GLN:HA	1:B:374:GLN:OE1	2.09	0.52
1:A:252:GLN:HA	1:A:334:ALA:HB1	1.92	0.52
1:A:115:ILE:HG12	1:A:250:LEU:HB3	1.92	0.52
1:B:326:GLN:OE1	1:C:52:LYS:HB3	2.10	0.52
1:C:286:SER:C	1:C:288:THR:H	2.12	0.51
1:C:165:ARG:HE	1:C:170:LEU:HD22	1.75	0.51
1:A:316:GLN:HB2	1:B:63:GLN:OE1	2.10	0.51
1:B:74:ASN:HA	1:B:83:ASN:HB3	1.91	0.51
1:C:424:SER:HB2	1:C:429:LEU:HD22	1.93	0.51
1:B:350:ARG:NE	1:C:211:TYR:OH	2.44	0.50
1:B:361:SER:C	1:C:191:LEU:HD11	2.31	0.50
1:B:194:ARG:NH2	1:B:449:PRO:O	2.44	0.50
1:B:383:GLY:O	1:B:388:THR:N	2.42	0.50
1:B:388:THR:HG22	1:B:389:GLU:HG2	1.93	0.50
1:A:183:TYR:O	1:A:186:VAL:HG12	2.12	0.49
1:A:184:ASP:OD2	1:C:372:SER:OG	2.28	0.49
1:C:139:LEU:HD11	1:C:217:ALA:HA	1.94	0.49
1:B:162:THR:OG1	1:B:391:ILE:HD12	2.11	0.49
1:B:94:THR:HG22	1:B:273:THR:HG23	1.94	0.49
1:B:286:SER:O	1:B:286:SER:OG	2.30	0.49
1:C:380:MET:HE1	1:C:393:ASP:HB3	1.95	0.49
1:B:354:ASN:ND2	1:C:198:ASP:HB3	2.27	0.49
1:A:336:GLU:OE1	1:B:40:ARG:HB2	2.14	0.48
1:B:125:GLN:HG3	1:B:429:LEU:HB3	1.95	0.48
1:B:384:PHE:HB2	1:B:394:VAL:HG21	1.96	0.48
1:C:256:ARG:O	1:C:259:ILE:HG12	2.14	0.48
1:C:77:ARG:HB3	1:C:81:GLY:N	2.27	0.48
1:A:326:GLN:OE1	1:B:52:LYS:HG3	2.14	0.48
1:A:305:LYS:HA	1:B:72:TYR:O	2.13	0.48
1:C:278:ILE:HA	1:C:302:GLY:HA2	1.96	0.48
1:B:268:PRO:HB3	1:B:312:LEU:HD12	1.95	0.48
1:A:163:THR:HA	1:A:166:PHE:HB3	1.95	0.48
1:A:292:ALA:HB2	1:A:296:TYR:HD1	1.78	0.47
1:A:70:TYR:O	1:C:307:GLY:HA2	2.14	0.47
1:C:33:ARG:HA	1:C:127:LEU:HD21	1.96	0.47
1:C:218:LEU:HA	1:C:441:LEU:HA	1.96	0.47
1:B:30:GLN:HG2	1:B:33:ARG:HH12	1.79	0.47
1:A:144:VAL:O	1:A:148:THR:OG1	2.31	0.47
1:A:88:SER:HB3	1:A:279:SER:HB3	1.97	0.47
1:B:358:ALA:O	1:B:362:SER:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:SER:C	1:C:387:GLY:H	2.18	0.47
1:B:219:ASN:HB2	1:B:442:SER:OG	2.15	0.47
1:A:259:ILE:HA	1:A:327:ALA:HB1	1.96	0.47
1:B:161:GLN:O	1:B:165:ARG:HG3	2.14	0.47
1:A:416:LEU:HD22	1:A:437:LEU:HD22	1.96	0.46
1:A:78:ASP:HB2	1:C:301:MET:HB3	1.97	0.46
1:B:347:GLN:HG2	1:C:202:GLU:HB3	1.98	0.46
1:B:359:SER:O	1:B:363:ILE:HG12	2.16	0.46
1:C:67:GLY:O	1:C:89:ALA:HA	2.16	0.46
1:C:264:ASP:HA	1:C:267:LEU:HD13	1.97	0.45
1:C:64:LEU:HD12	1:C:93:LEU:HD12	1.98	0.45
1:C:229:GLN:CD	1:C:229:GLN:H	2.19	0.45
1:A:419:GLN:O	1:A:422:ILE:HG22	2.17	0.45
1:C:370:VAL:HG21	1:C:408:LEU:HD22	1.99	0.45
1:B:322:SER:OG	1:C:54:ASN:HB2	2.17	0.45
1:B:356:ILE:HD11	1:B:419:GLN:HG2	1.99	0.45
1:A:126:THR:HG22	1:A:130:ASN:ND2	2.32	0.45
1:B:424:SER:HB2	1:B:429:LEU:HD12	1.99	0.45
1:B:294:THR:C	1:B:296:TYR:H	2.20	0.45
1:B:314:ILE:HD11	1:C:66:LEU:HB2	1.98	0.45
1:C:82:ILE:HD12	1:C:288:THR:CG2	2.45	0.44
1:B:83:ASN:N	1:B:83:ASN:OD1	2.51	0.44
1:B:218:LEU:HD21	1:B:223:PHE:CD1	2.51	0.44
1:C:145:LEU:HD22	1:C:194:ARG:HA	2.00	0.44
1:C:154:ALA:HA	1:C:157:ARG:HH11	1.83	0.44
1:A:358:ALA:O	1:B:191:LEU:HD21	2.18	0.43
1:C:173:ILE:HG12	1:C:173:ILE:H	1.56	0.43
1:B:75:GLY:HA2	1:B:79:ALA:HB3	2.01	0.43
1:A:143:ASP:O	1:A:147:TYR:HD2	2.01	0.43
1:C:72:TYR:HD1	1:C:85:ASN:ND2	2.16	0.43
1:C:208:THR:HG21	1:C:212:TYR:HE1	1.84	0.43
1:C:81:GLY:O	1:C:82:ILE:CB	2.66	0.43
1:B:53:ILE:HD11	1:B:110:GLU:HA	2.01	0.43
1:B:50:PHE:O	1:B:53:ILE:HG12	2.19	0.43
1:B:166:PHE:HD1	1:B:171:VAL:O	2.02	0.43
1:A:376:SER:HA	1:B:177:GLN:HB3	2.01	0.42
1:A:70:TYR:HD1	1:A:87:THR:HG22	1.84	0.42
1:A:97:ILE:HD12	1:A:270:LEU:HD22	2.02	0.42
1:B:307:GLY:HA3	1:C:71:THR:HA	2.01	0.42
1:A:24:ASN:ND2	1:A:24:ASN:N	2.58	0.42
1:B:416:LEU:HD22	1:B:437:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLY:HA3	1:B:286:SER:HB3	2.02	0.42
1:A:197:LEU:O	1:A:201:VAL:HG23	2.20	0.42
1:C:132:ALA:O	1:C:135:TYR:HB3	2.20	0.42
1:B:61:LEU:HB3	1:B:62:PRO:HD2	2.02	0.41
1:C:390:THR:HG22	1:C:391:ILE:H	1.85	0.41
1:B:320:VAL:O	1:B:324:VAL:HG23	2.20	0.41
1:B:130:ASN:O	1:B:133:THR:HG22	2.20	0.41
1:A:366:TYR:HA	1:A:369:ALA:HB3	2.02	0.41
1:A:218:LEU:HD11	1:A:223:PHE:HD1	1.85	0.41
1:B:355:ASN:HB3	1:B:418:ASN:ND2	2.36	0.41
1:C:208:THR:HG21	1:C:212:TYR:CE1	2.56	0.41
1:C:277:GLY:O	1:C:303:GLN:N	2.54	0.41
1:C:376:SER:O	1:C:380:MET:HG2	2.21	0.41
1:A:208:THR:HG23	1:A:210:ASN:H	1.85	0.41
1:C:204:LEU:C	1:C:206:GLN:H	2.24	0.41
1:A:423:LYS:HG2	1:A:433:ASP:OD2	2.21	0.41
1:C:212:TYR:HA	1:C:213:PRO:HD3	1.87	0.41
1:C:26:MET:O	1:C:30:GLN:HB2	2.21	0.40
1:B:77:ARG:HA	1:B:77:ARG:HD2	1.86	0.40
1:A:354:ASN:ND2	1:B:198:ASP:HB3	2.36	0.40
1:B:194:ARG:O	1:B:194:ARG:HD3	2.20	0.40
1:B:179:ALA:HB2	1:B:391:ILE:HD13	2.03	0.40
1:B:354:ASN:HD22	1:C:198:ASP:HB3	1.85	0.40
1:C:234:LEU:HD22	1:C:426:LEU:HD21	2.03	0.40
1:A:111:LYS:HE3	1:A:257:GLU:HG3	2.02	0.40
1:B:241:ARG:HB3	1:B:426:LEU:O	2.22	0.40
1:B:40:ARG:O	1:B:43:ALA:HB3	2.22	0.40
1:C:134:ALA:O	1:C:138:VAL:HG23	2.21	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	428/460 (93%)	400 (94%)	24 (6%)	4 (1%)	21 67
1	B	427/460 (93%)	388 (91%)	28 (7%)	11 (3%)	7 40
1	C	428/460 (93%)	397 (93%)	26 (6%)	5 (1%)	16 60
All	All	1283/1380 (93%)	1185 (92%)	78 (6%)	20 (2%)	12 54

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287[A]	LYS
1	B	293	GLY
1	B	379	ALA
1	B	298	ASP
1	C	82	ILE
1	C	386	VAL
1	A	161[A]	GLN
1	A	442	SER
1	B	276	THR
1	B	377	LEU
1	B	378	ASP
1	B	442	SER
1	C	239	GLU
1	C	442	SER
1	A	170	LEU
1	A	287[A]	LYS
1	C	295[A]	GLN
1	B	306	VAL
1	B	227[A]	LYS
1	B	285	GLY

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	359/387 (93%)	334 (93%)	25 (7%)	19 58
1	B	358/387 (92%)	320 (89%)	38 (11%)	8 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	359/387 (93%)	336 (94%)	23 (6%)	22 62
All	All	1076/1161 (93%)	990 (92%)	86 (8%)	15 52

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	25	LEU
1	A	39	LEU
1	A	71	THR
1	A	76	TYR
1	A	126	THR
1	A	146	SER
1	A	158[A]	GLN
1	A	174	THR
1	A	241	ARG
1	A	245	LEU
1	A	280	ASP
1	A	295[A]	GLN
1	A	330	ASN
1	A	343	ARG
1	A	347	GLN
1	A	359	SER
1	A	361	SER
1	A	385	SER
1	A	395	LEU
1	A	396	ASP
1	A	398	THR
1	A	408	LEU
1	A	426	LEU
1	A	429	LEU
1	B	23	GLU
1	B	34	LEU
1	B	58	SER
1	B	74	ASN
1	B	83	ASN
1	B	85	ASN
1	B	108	LEU
1	B	111	LYS
1	B	122	THR
1	B	129	LEU
1	B	133	THR

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Mol	Chain	Res	Type
1	B	140	ASN
1	B	146	SER
1	B	151	GLN
1	B	153	GLU
1	B	168	VAL
1	B	192	THR
1	B	204	LEU
1	B	219	ASN
1	B	224[A]	LYS
1	B	226	ASP
1	B	236[A]	LYS
1	B	241	ARG
1	B	245	LEU
1	B	252	GLN
1	B	280	ASP
1	B	284	SER
1	B	288	THR
1	B	297	ASP
1	B	303	GLN
1	B	304	ASN
1	B	308	LEU
1	B	322	SER
1	B	390	THR
1	B	393	ASP
1	B	430	ASN
1	B	438	ASN
1	B	446	SER
1	C	33	ARG
1	C	51	GLU
1	C	53	ILE
1	C	64	LEU
1	C	76	TYR
1	C	170	LEU
1	C	173	ILE
1	C	190	GLU
1	C	221	GLU
1	C	229	GLN
1	C	235	LEU
1	C	245	LEU
1	C	251	SER
1	C	273	THR
1	C	276	THR

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Mol	Chain	Res	Type
1	C	281	THR
1	C	359	SER
1	C	390	THR
1	C	391	ILE
1	C	393	ASP
1	C	396	ASP
1	C	432	GLN
1	C	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	B	219	ASN
1	C	130	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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, 95^{th} 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	429/460 (93%)	-0.25	13 (3%) 54 39	40, 61, 98, 106	14 (3%)
1	B	425/460 (92%)	-0.23	9 (2%) 67 52	44, 64, 83, 100	6 (1%)
1	C	429/460 (93%)	-0.12	11 (2%) 59 45	52, 79, 98, 103	15 (3%)
All	All	1283/1380 (92%)	-0.20	33 (2%) 59 45	40, 69, 97, 106	35 (2%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	THR	6.5
1	C	81	GLY	4.4
1	C	80[A]	ASN	4.4
1	C	450	GLU	4.2
1	A	293	GLY	4.1
1	A	292	ALA	4.1
1	A	291	ALA	3.6
1	A	171	VAL	3.5
1	C	449	PRO	3.3
1	A	288	THR	3.1
1	B	294	THR	3.0
1	C	78	ASP	2.9
1	B	378	ASP	2.8
1	B	293	GLY	2.8
1	B	284	SER	2.7
1	B	78	ASP	2.7
1	A	295[A]	GLN	2.7
1	B	222	ASN	2.5
1	B	299	SER	2.3
1	C	213	PRO	2.3
1	C	222	ASN	2.3
1	A	290	GLY	2.3
1	C	451	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	288	THR	2.2
1	A	222	ASN	2.2
1	A	300	ASN	2.2
1	C	79	ALA	2.1
1	A	87	THR	2.1
1	C	386	VAL	2.1
1	B	379	ALA	2.1
1	C	82	ILE	2.1
1	A	169	GLY	2.1
1	A	450	GLU	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, 95^{th} 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(Å^2)	Q<0.9
2	CL	C	1453	1/1	0.97	0.29	2.08	45,45,45,45	0
2	CL	A	1454	1/1	0.97	0.29	1.02	28,28,28,28	0
2	CL	B	1453	1/1	0.98	0.21	-0.63	48,48,48,48	0
2	CL	A	1453	1/1	0.93	0.18	-	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.