Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:13 PM GMT

PDB ID	:	1EK9
Title	:	2.1A X-RAY STRUCTURE OF TOLC: AN INTEGRAL OUTER MEMBRANE PROTEIN AND EFFLUX PUMP COMPONENT FROM ESCHERICHIA COLI
Authors	:	Koronakis, V.; Sharff, A.J.; Koronakis, E.; Luisi, B.; Hughes, C.
Deposited on	:	2000-03-07
Resolution	:	2.10 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:

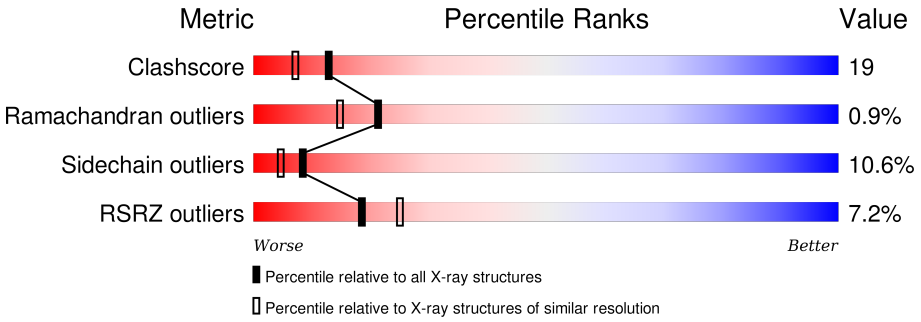
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	428	5% 67% 25% 7%
1	B	428	7% 71% 23% 5%
1	C	428	9% 68% 24% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11426 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	428	Total	C	N	O	Se	0	0	0
			3306	2038	586	677	5			
1	B	428	Total	C	N	O	Se	0	0	0
			3306	2038	586	677	5			
1	C	428	Total	C	N	O	Se	0	0	0
			3306	2038	586	677	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MSE	MET	MODIFIED RESIDUE	UNP P02930
A	78	MSE	MET	MODIFIED RESIDUE	UNP P02930
A	279	MSE	MET	MODIFIED RESIDUE	UNP P02930
A	297	MSE	MET	MODIFIED RESIDUE	UNP P02930
A	358	MSE	MET	MODIFIED RESIDUE	UNP P02930
B	4	MSE	MET	MODIFIED RESIDUE	UNP P02930
B	78	MSE	MET	MODIFIED RESIDUE	UNP P02930
B	279	MSE	MET	MODIFIED RESIDUE	UNP P02930
B	297	MSE	MET	MODIFIED RESIDUE	UNP P02930
B	358	MSE	MET	MODIFIED RESIDUE	UNP P02930
C	4	MSE	MET	MODIFIED RESIDUE	UNP P02930
C	78	MSE	MET	MODIFIED RESIDUE	UNP P02930
C	279	MSE	MET	MODIFIED RESIDUE	UNP P02930
C	297	MSE	MET	MODIFIED RESIDUE	UNP P02930
C	358	MSE	MET	MODIFIED RESIDUE	UNP P02930

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	442	Total	O	0	0
			442	442		
2	B	558	Total	O	0	0
			558	558		

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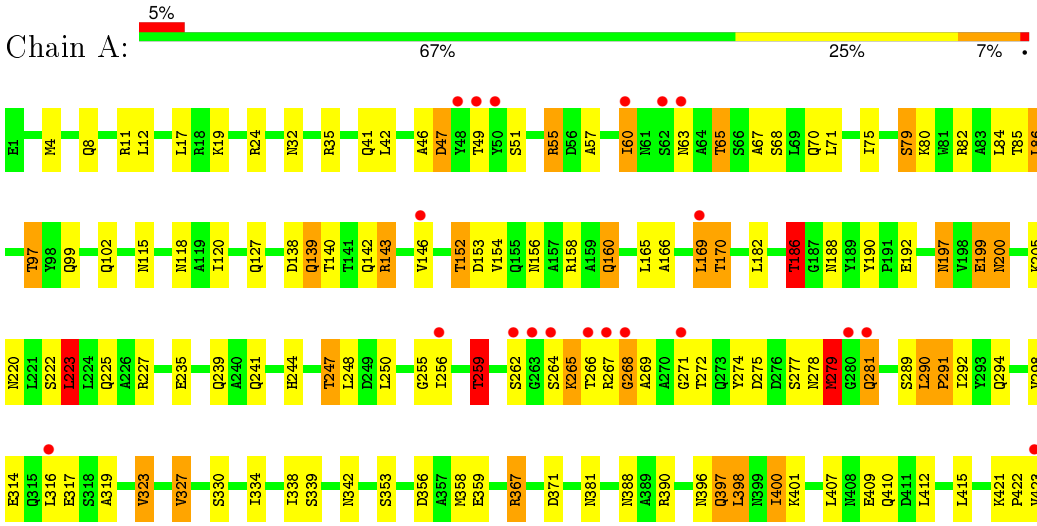
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	508	Total O 508 508	0	0

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.

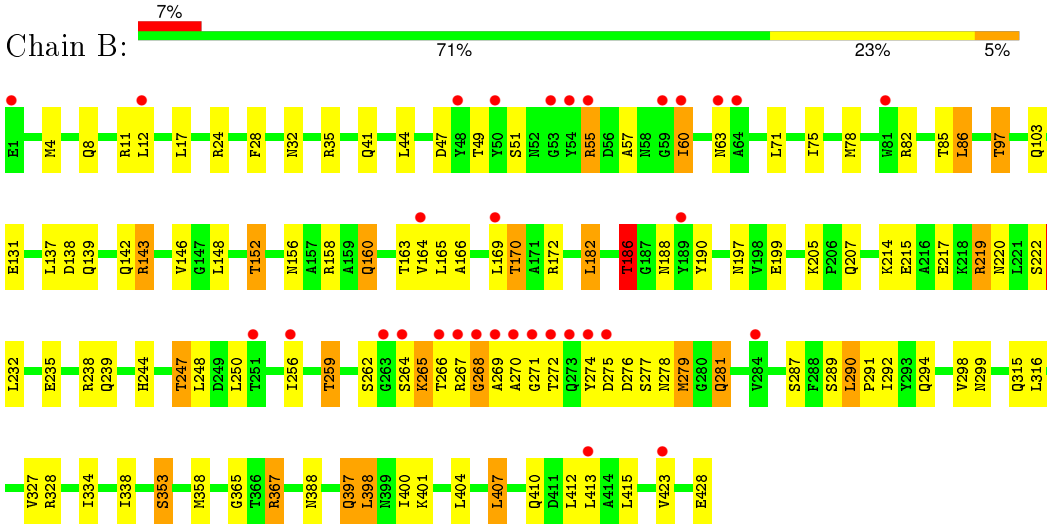
- Molecule 1: OUTER MEMBRANE PROTEIN TOLC

Chain A:



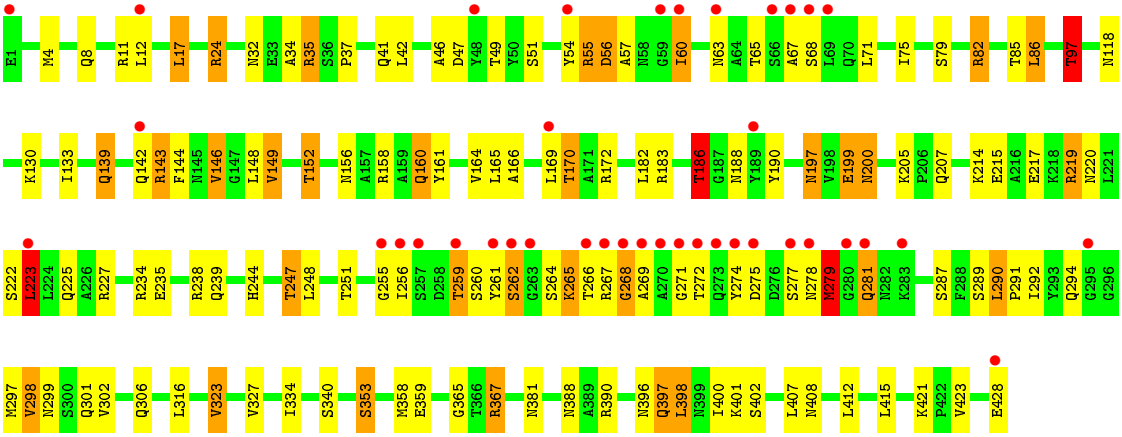
- Molecule 1: OUTER MEMBRANE PROTEIN TOLC

Chain B:



- Molecule 1: OUTER MEMBRANE PROTEIN TOLC

Chain C:


E1 M4 Q8 R11 L12 L17 R24 N32 E33 A34 R35 S36 P37 Q41 L42 A46 D47 Y48 T49 Y50 S51 Y54 R55 D56 A57 N58 G59 I60 N63 A64 T65 S66 A67 S68 L69 Q70 L71 I75 S79 R82 T85 L86 T97 N118
K130 I133 Q139 Q142 R143 F144 N145 V146 G147 L148 V149 T152 N156 A157 R158 A159 Q160 Y161 V164 L165 A166 L169 T170 A171 R172 L182 R183 T186 G187 N188 Y189 Y190 N197 V198 E199 N200 K205 P206 Q207 K214 E215 A216 E217 K218 R219 N220 L221
S222 L223 L224 Q225 A226 R227 R234 E235 R238 Q239 H244 T247 L248 T251 G255 I256 S257 D258 T259 S260 Y261 S262 G263 S264 K265 T266 R267 G268 A269 A270 G271 T272 Q273 Y274 D275 D276 S277 N278 M279 G280 Q281 N282 K283 S287 F288 S289 L290 P291 I292 Y293 Q294 G295 G296
M297 V298 N299 S300 Q301 V302 Q306 L316 V323 V327 I334 S340 S353 M358 E359 G365 T366 R367 N381 N388 A389 R390 N396 Q397 L398 N399 I400 K401 S402 L407 N408 L412 L415 K421 P422 V423 E428

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	265.05Å 265.05Å 95.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10 132.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.10) 99.6 (132.52-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.10Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.208 , 0.257 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 79.6	EDS
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 146143 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11426	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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

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	0.85	1/3342 (0.0%)	1.27	20/4530 (0.4%)
1	B	0.87	1/3342 (0.0%)	1.19	17/4530 (0.4%)
1	C	0.88	0/3342	1.26	28/4530 (0.6%)
All	All	0.86	2/10026 (0.0%)	1.24	65/13590 (0.5%)

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	2
1	C	0	5
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	SER	CB-OG	-5.97	1.34	1.42
1	B	353	SER	CB-OG	-5.54	1.35	1.42

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	367	ARG	NE-CZ-NH1	-21.04	109.78	120.30
1	A	367	ARG	NE-CZ-NH1	-19.04	110.78	120.30
1	B	143	ARG	NE-CZ-NH1	17.25	128.92	120.30
1	A	367	ARG	NE-CZ-NH2	17.23	128.91	120.30
1	B	367	ARG	NE-CZ-NH1	-14.76	112.92	120.30
1	A	143	ARG	NE-CZ-NH1	14.27	127.43	120.30
1	A	143	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	C	143	ARG	NE-CZ-NH1	13.03	126.82	120.30
1	C	143	ARG	NE-CZ-NH2	-11.90	114.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	367	ARG	NE-CZ-NH2	11.49	126.05	120.30
1	B	143	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	C	183	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	C	390	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	A	158	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	A	158	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	C	183	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	A	390	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	A	279	MSE	CA-CB-CG	7.94	126.79	113.30
1	A	259	THR	N-CA-CB	7.47	124.49	110.30
1	A	390	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	259	THR	N-CA-CB	7.11	123.81	110.30
1	C	143	ARG	CD-NE-CZ	7.10	133.53	123.60
1	C	367	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	B	223	LEU	CB-CA-C	6.95	123.40	110.20
1	B	428	GLU	N-CA-CB	6.71	122.68	110.60
1	C	259	THR	N-CA-CB	6.57	122.79	110.30
1	B	328	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	428	GLU	N-CA-CB	6.39	122.10	110.60
1	C	367	ARG	NH1-CZ-NH2	6.33	126.37	119.40
1	A	186	THR	N-CA-CB	-6.33	98.27	110.30
1	C	219	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	356	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	186	THR	N-CA-CB	-6.06	98.79	110.30
1	B	186	THR	N-CA-CB	-6.05	98.81	110.30
1	B	223	LEU	CA-CB-CG	5.98	129.06	115.30
1	C	24	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	C	428	GLU	N-CA-CB	5.82	121.08	110.60
1	A	143	ARG	CD-NE-CZ	5.81	131.74	123.60
1	A	223	LEU	CA-CB-CG	5.81	128.67	115.30
1	C	340	SER	N-CA-CB	5.79	119.18	110.50
1	C	223	LEU	CB-CA-C	5.76	121.14	110.20
1	C	35	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	C	367	ARG	CD-NE-CZ	5.75	131.65	123.60
1	A	223	LEU	CB-CA-C	5.72	121.07	110.20
1	B	172	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	298	VAL	CA-C-N	5.61	129.53	117.20
1	C	56	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	291	PRO	CA-C-N	5.55	129.41	117.20
1	C	149	VAL	N-CA-CB	-5.47	99.46	111.50
1	C	158	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	C	35	ARG	NE-CZ-NH1	-5.39	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	279	MSE	CA-CB-CG	5.38	122.44	113.30
1	B	164	VAL	CG1-CB-CG2	-5.35	102.34	110.90
1	B	232	LEU	CA-CB-CG	5.34	127.58	115.30
1	C	223	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	219	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	153	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	115	ASN	N-CA-CB	5.19	119.95	110.60
1	B	78	MSE	CG-SE-CE	-5.17	87.53	98.90
1	C	82	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	B	138	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	182	LEU	CA-CB-CG	5.10	127.04	115.30
1	C	17	LEU	CB-CG-CD2	5.08	119.64	111.00
1	C	158	ARG	CG-CD-NE	-5.06	101.17	111.80
1	A	153	ASP	CB-CG-OD2	-5.05	113.76	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	314	GLU	Mainchain
1	A	317	GLU	Mainchain
1	C	144	PHE	Mainchain
1	C	34	ALA	Mainchain
1	C	353	SER	Mainchain
1	C	402	SER	Mainchain
1	C	97	THR	Mainchain

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	3306	0	3256	135	0
1	B	3306	0	3256	131	0
1	C	3306	0	3256	145	0
2	A	442	0	0	40	2
2	B	558	0	0	45	1
2	C	508	0	0	54	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11426	0	9768	377	2

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 19.

All (377) 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:156:ASN:HD21	1:C:367:ARG:NH1	1.34	1.23
1:B:423:VAL:HB	2:B:703:HOH:O	1.40	1.19
1:A:156:ASN:HD21	1:B:367:ARG:NH1	1.42	1.17
1:C:423:VAL:HB	2:C:624:HOH:O	1.42	1.16
1:A:367:ARG:NH1	1:C:156:ASN:HD21	1.46	1.14
1:B:146:VAL:HB	2:B:952:HOH:O	1.47	1.12
1:B:265:LYS:HG2	2:B:971:HOH:O	1.49	1.10
1:A:146:VAL:HB	2:A:750:HOH:O	1.55	1.03
1:C:388:ASN:HB2	2:C:525:HOH:O	1.61	0.99
1:A:426:ASN:HB2	2:A:803:HOH:O	1.65	0.97
1:B:156:ASN:ND2	1:C:367:ARG:NH1	2.11	0.96
1:B:156:ASN:HD21	1:C:367:ARG:HH12	1.05	0.94
1:B:97:THR:HG22	1:B:225:GLN:NE2	1.82	0.93
1:B:118:ASN:HD21	1:B:388:ASN:HD22	1.18	0.91
1:C:79:SER:HA	2:C:933:HOH:O	1.70	0.91
1:B:388:ASN:HB2	2:B:520:HOH:O	1.69	0.90
1:C:57:ALA:HB3	2:C:695:HOH:O	1.70	0.89
1:B:156:ASN:ND2	1:C:367:ARG:HH12	1.70	0.89
1:A:156:ASN:ND2	1:B:367:ARG:NH1	2.22	0.88
1:A:415:LEU:HD21	2:A:609:HOH:O	1.75	0.87
1:C:118:ASN:HD21	1:C:388:ASN:HD22	1.23	0.87
1:A:298:VAL:O	1:A:299:ASN:HB2	1.75	0.86
1:B:85:THR:HG22	2:B:581:HOH:O	1.75	0.86
1:A:118:ASN:HD21	1:A:388:ASN:HD22	1.22	0.85
1:A:156:ASN:HD21	1:B:367:ARG:HH12	1.20	0.84
1:A:227:ARG:HD3	2:A:721:HOH:O	1.75	0.84
1:A:421:LYS:HE3	2:A:787:HOH:O	1.78	0.84
1:A:97:THR:HG22	1:A:225:GLN:NE2	1.94	0.82
1:A:367:ARG:NH1	1:C:156:ASN:ND2	2.27	0.81
1:A:381:ASN:HB3	2:A:500:HOH:O	1.80	0.81
1:C:97:THR:HG22	1:C:225:GLN:NE2	1.96	0.81
1:C:160:GLN:HG3	2:C:875:HOH:O	1.81	0.81
1:A:186:THR:HG22	1:A:188:ASN:H	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLN:HG3	2:B:596:HOH:O	1.83	0.79
1:C:139:GLN:NE2	1:C:143:ARG:NH2	2.33	0.77
1:C:388:ASN:HB2	2:C:504:HOH:O	1.82	0.77
1:B:186:THR:HG22	1:B:188:ASN:H	1.48	0.77
1:B:130:LYS:CE	2:B:937:HOH:O	2.32	0.77
1:C:398:LEU:HD11	1:C:415:LEU:HD11	1.66	0.77
1:A:334:ILE:HD12	1:A:400:ILE:HD12	1.66	0.76
1:A:85:THR:HG22	2:A:736:HOH:O	1.85	0.76
1:B:97:THR:HG22	1:B:225:GLN:HE22	1.49	0.76
1:A:160:GLN:HG3	2:A:784:HOH:O	1.84	0.76
1:B:130:LYS:HE2	2:B:937:HOH:O	1.85	0.75
1:C:186:THR:HG22	1:C:188:ASN:H	1.52	0.75
1:C:139:GLN:NE2	1:C:143:ARG:HH22	1.84	0.74
1:B:367:ARG:NE	2:B:934:HOH:O	2.21	0.74
1:C:139:GLN:HE21	1:C:143:ARG:NH2	1.86	0.74
1:C:267:ARG:NE	2:C:925:HOH:O	2.20	0.74
1:B:139:GLN:NE2	1:B:143:ARG:NH2	2.35	0.74
1:C:85:THR:HG22	2:C:533:HOH:O	1.87	0.74
1:A:127:GLN:NE2	2:A:832:HOH:O	2.21	0.74
1:C:186:THR:HG21	1:C:190:TYR:HE1	1.53	0.73
1:A:139:GLN:NE2	1:A:143:ARG:NH2	2.36	0.73
1:A:165:LEU:O	1:A:169:LEU:HD22	1.89	0.73
1:B:298:VAL:O	1:B:299:ASN:HB2	1.88	0.73
1:A:358:MSE:SE	1:A:367:ARG:HD2	2.39	0.73
1:B:244:HIS:HE1	2:B:621:HOH:O	1.72	0.73
1:C:65:THR:HG21	2:C:921:HOH:O	1.89	0.72
1:B:367:ARG:NH2	2:B:934:HOH:O	2.22	0.72
1:C:133:ILE:HD11	2:C:850:HOH:O	1.89	0.72
1:B:367:ARG:CZ	2:B:934:HOH:O	2.36	0.72
1:A:65:THR:HG22	2:A:515:HOH:O	1.89	0.72
1:A:398:LEU:HD11	1:A:415:LEU:HD11	1.71	0.71
1:C:298:VAL:O	1:C:299:ASN:HB2	1.91	0.71
1:B:118:ASN:HD21	1:B:388:ASN:ND2	1.87	0.71
1:A:4:MSE:HG3	2:A:700:HOH:O	1.89	0.70
1:B:220:ASN:HD21	1:B:222:SER:HB2	1.56	0.70
1:C:220:ASN:HD22	1:C:223:LEU:H	1.40	0.70
1:B:410:GLN:HG2	2:B:627:HOH:O	1.91	0.70
1:C:146:VAL:CG2	2:C:629:HOH:O	2.39	0.70
1:C:146:VAL:HG23	2:C:629:HOH:O	1.92	0.69
1:C:398:LEU:CD1	1:C:415:LEU:HD11	2.23	0.68
1:B:169:LEU:HD13	2:B:648:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASN:HD22	1:A:223:LEU:H	1.38	0.68
1:A:219:ARG:HD2	2:A:571:HOH:O	1.94	0.68
1:B:413:LEU:CD2	2:B:823:HOH:O	2.41	0.68
1:A:220:ASN:HD21	1:A:222:SER:HB2	1.58	0.68
1:C:220:ASN:HD21	1:C:222:SER:HB2	1.59	0.68
1:A:186:THR:HG21	1:A:190:TYR:HE1	1.59	0.67
1:C:269:ALA:HB1	2:C:888:HOH:O	1.95	0.67
1:C:358:MSE:SE	1:C:367:ARG:HH11	2.28	0.67
1:C:265:LYS:HA	1:C:265:LYS:HE3	1.77	0.67
1:B:220:ASN:HD22	1:B:223:LEU:H	1.43	0.67
1:A:170:THR:HG21	2:B:508:HOH:O	1.94	0.66
1:C:32:ASN:HD22	1:C:35:ARG:HH22	1.41	0.66
1:C:397:GLN:HE21	1:C:397:GLN:HA	1.60	0.66
1:B:244:HIS:HD2	2:B:836:HOH:O	1.79	0.66
1:A:244:HIS:HE1	2:A:514:HOH:O	1.76	0.66
1:C:169:LEU:HD13	2:C:728:HOH:O	1.95	0.66
1:B:32:ASN:HD22	1:B:35:ARG:HH22	1.42	0.65
1:A:156:ASN:HD21	1:B:367:ARG:CZ	2.09	0.65
1:A:156:ASN:ND2	1:B:367:ARG:CZ	2.61	0.64
1:A:367:ARG:CZ	1:C:156:ASN:HD21	2.08	0.64
1:B:139:GLN:HE21	1:B:143:ARG:NH2	1.92	0.64
1:C:267:ARG:HG2	2:C:925:HOH:O	1.97	0.64
1:C:381:ASN:HB3	2:C:585:HOH:O	1.97	0.64
1:B:186:THR:CG2	1:B:188:ASN:H	2.11	0.64
1:B:413:LEU:HD22	2:B:823:HOH:O	1.98	0.64
1:C:281:GLN:HA	1:C:281:GLN:HE21	1.62	0.64
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.78	0.64
1:C:271:GLY:O	1:C:272:THR:HB	1.97	0.63
1:A:41:GLN:HE22	1:B:294:GLN:HB3	1.63	0.63
1:A:398:LEU:CD1	1:A:415:LEU:HD11	2.28	0.63
1:A:367:ARG:NH1	1:C:152:THR:OG1	2.32	0.63
1:C:267:ARG:CG	2:C:925:HOH:O	2.47	0.63
1:B:398:LEU:CD1	1:B:415:LEU:HD11	2.29	0.63
1:A:156:ASN:ND2	1:B:367:ARG:HH12	1.91	0.62
1:A:192:GLU:HB2	2:A:868:HOH:O	1.99	0.62
1:C:182:LEU:O	1:C:186:THR:HB	1.99	0.62
1:A:367:ARG:HH12	1:C:156:ASN:HD21	1.39	0.62
1:B:165:LEU:O	1:B:169:LEU:HD22	1.98	0.62
1:A:186:THR:CG2	1:A:188:ASN:H	2.11	0.62
1:A:244:HIS:HD2	2:A:845:HOH:O	1.83	0.61
1:C:172:ARG:HB2	2:C:720:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLN:HA	1:A:281:GLN:HE21	1.66	0.61
1:B:186:THR:HG21	1:B:190:TYR:HE1	1.64	0.60
1:B:268:GLY:O	1:B:269:ALA:HB3	2.01	0.60
1:B:281:GLN:HE21	1:B:281:GLN:HA	1.65	0.60
1:C:398:LEU:HD11	1:C:415:LEU:CD1	2.32	0.60
1:C:247:THR:HG23	1:C:289:SER:HB3	1.82	0.59
1:A:367:ARG:CZ	1:C:156:ASN:ND2	2.64	0.59
1:A:97:THR:HG22	1:A:225:GLN:HE22	1.64	0.59
1:C:165:LEU:O	1:C:169:LEU:HD22	2.03	0.59
1:B:205:LYS:HD2	2:B:655:HOH:O	2.02	0.59
1:A:397:GLN:HA	1:A:397:GLN:HE21	1.67	0.59
1:C:186:THR:HG21	1:C:190:TYR:CE1	2.37	0.59
1:A:290:LEU:HD13	1:A:292:ILE:HG13	1.85	0.58
1:A:118:ASN:HD21	1:A:388:ASN:ND2	1.96	0.58
1:A:32:ASN:HD22	1:A:35:ARG:HH22	1.51	0.58
1:B:130:LYS:NZ	2:B:937:HOH:O	2.20	0.58
1:B:290:LEU:HD13	1:B:292:ILE:HG13	1.85	0.58
1:B:57:ALA:O	1:B:60:ILE:HG22	2.04	0.58
1:A:118:ASN:ND2	1:A:388:ASN:HD22	1.99	0.58
1:A:79:SER:HA	2:A:811:HOH:O	2.04	0.57
1:C:207:GLN:NE2	2:C:927:HOH:O	2.37	0.57
1:B:410:GLN:NE2	2:B:728:HOH:O	2.36	0.57
1:B:320:HIS:HB2	2:B:681:HOH:O	2.04	0.57
1:A:4:MSE:O	1:A:8:GLN:HG2	2.05	0.57
1:B:247:THR:CG2	1:B:289:SER:HB3	2.35	0.57
1:B:244:HIS:O	2:B:966:HOH:O	2.17	0.56
1:C:290:LEU:HD13	1:C:292:ILE:HG13	1.87	0.56
1:A:265:LYS:HG3	2:A:775:HOH:O	2.05	0.56
1:A:268:GLY:O	1:A:269:ALA:HB3	2.06	0.56
1:C:160:GLN:NE2	2:C:509:HOH:O	2.39	0.56
1:B:397:GLN:HA	1:B:397:GLN:HE21	1.69	0.56
1:C:4:MSE:O	1:C:8:GLN:HG2	2.06	0.56
1:B:156:ASN:ND2	1:C:367:ARG:CZ	2.69	0.55
1:A:342:ASN:ND2	2:A:747:HOH:O	2.38	0.55
1:B:334:ILE:HD12	1:B:400:ILE:HD12	1.87	0.55
1:C:219:ARG:HD2	2:C:913:HOH:O	2.07	0.55
1:B:4:MSE:O	1:B:8:GLN:HG2	2.07	0.55
1:B:41:GLN:HE22	1:C:294:GLN:HB3	1.71	0.55
1:A:146:VAL:O	1:A:146:VAL:HG22	2.07	0.55
1:B:265:LYS:HA	1:B:265:LYS:HE3	1.88	0.55
1:A:120:ILE:HG21	1:A:423:VAL:HG11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:GLU:OE1	1:C:219:ARG:NH1	2.40	0.55
1:B:398:LEU:HD13	1:B:415:LEU:HD11	1.88	0.55
1:A:294:GLN:HB3	1:C:41:GLN:HE22	1.71	0.55
1:A:186:THR:HG21	1:A:190:TYR:CE1	2.40	0.54
1:B:247:THR:HG23	1:B:289:SER:HB3	1.88	0.54
1:B:170:THR:HG21	2:C:546:HOH:O	2.05	0.54
1:A:60:ILE:HD12	1:A:274:TYR:CE1	2.42	0.54
1:A:170:THR:CG2	2:B:508:HOH:O	2.55	0.54
1:C:8:GLN:NE2	2:C:908:HOH:O	2.38	0.54
1:C:170:THR:HG21	2:C:466:HOH:O	2.08	0.54
1:C:408:ASN:HB2	2:C:707:HOH:O	2.07	0.54
1:B:265:LYS:HD2	2:B:935:HOH:O	2.07	0.53
1:B:182:LEU:O	1:B:186:THR:HB	2.09	0.53
1:A:410:GLN:HG2	2:A:847:HOH:O	2.08	0.53
1:B:290:LEU:HD22	1:B:291:PRO:HD2	1.90	0.53
1:B:215:GLU:OE1	1:B:219:ARG:NH1	2.42	0.53
1:B:131:GLU:HB3	2:B:571:HOH:O	2.09	0.53
1:A:398:LEU:HD11	1:A:415:LEU:CD1	2.39	0.53
1:C:274:TYR:CD2	2:C:896:HOH:O	2.62	0.52
1:A:422:PRO:HB3	2:A:868:HOH:O	2.09	0.52
1:B:57:ALA:HB2	1:C:279:MSE:HE3	1.91	0.52
1:A:197:ASN:ND2	1:A:200:ASN:H	2.07	0.52
1:C:323:VAL:O	1:C:327:VAL:HG13	2.09	0.52
1:A:290:LEU:HD22	1:A:291:PRO:HD2	1.91	0.51
1:B:44:LEU:HB2	1:C:292:ILE:HD11	1.91	0.51
1:A:279:MSE:CE	2:A:661:HOH:O	2.58	0.51
1:A:247:THR:HG23	1:A:289:SER:HB3	1.92	0.51
1:C:65:THR:HG22	2:C:777:HOH:O	2.10	0.51
1:C:197:ASN:C	1:C:197:ASN:HD22	2.14	0.51
1:A:182:LEU:O	1:A:186:THR:HB	2.10	0.51
1:C:244:HIS:HE1	2:C:899:HOH:O	1.93	0.51
1:B:267:ARG:NH2	1:B:275:ASP:HA	2.26	0.51
1:C:388:ASN:CB	2:C:504:HOH:O	2.50	0.51
1:A:334:ILE:HG13	1:A:396:ASN:HB3	1.93	0.51
1:C:234:ARG:NH1	2:C:667:HOH:O	2.32	0.51
1:A:166:ALA:HA	1:A:169:LEU:HD23	1.93	0.50
1:B:207:GLN:HG3	2:B:845:HOH:O	2.11	0.50
1:A:182:LEU:C	1:A:182:LEU:HD13	2.32	0.50
1:C:264:SER:OG	1:C:265:LYS:N	2.42	0.50
1:B:398:LEU:HD11	1:B:415:LEU:HD11	1.93	0.50
1:B:139:GLN:NE2	1:B:143:ARG:HH22	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:THR:O	1:C:63:ASN:HA	2.11	0.50
1:A:205:LYS:HD3	1:A:338:ILE:HD13	1.92	0.50
1:C:118:ASN:HD21	1:C:388:ASN:ND2	2.00	0.50
1:B:166:ALA:HA	1:B:169:LEU:HD23	1.94	0.50
1:C:260:SER:HB3	2:C:916:HOH:O	2.12	0.50
1:B:423:VAL:HG13	2:B:680:HOH:O	2.12	0.50
1:A:57:ALA:O	1:A:60:ILE:HG22	2.12	0.50
1:C:234:ARG:NH2	2:C:825:HOH:O	2.43	0.50
1:A:182:LEU:HD13	1:A:182:LEU:O	2.12	0.50
1:B:28:PHE:HD2	2:B:852:HOH:O	1.94	0.50
1:A:86:LEU:HD13	1:A:235:GLU:HG3	1.94	0.50
1:C:186:THR:CG2	1:C:188:ASN:H	2.21	0.49
1:A:139:GLN:NE2	1:A:143:ARG:HH22	2.09	0.49
1:A:49:THR:O	1:A:63:ASN:HA	2.12	0.49
1:A:138:ASP:OD2	2:A:818:HOH:O	2.20	0.49
1:B:276:ASP:HB3	2:B:956:HOH:O	2.12	0.49
1:C:397:GLN:HE21	1:C:397:GLN:CA	2.24	0.49
1:B:223:LEU:CD1	2:B:663:HOH:O	2.59	0.49
1:A:400:ILE:HG22	2:A:602:HOH:O	2.11	0.49
1:A:247:THR:CG2	1:A:289:SER:HB3	2.42	0.49
1:A:4:MSE:CG	2:A:700:HOH:O	2.55	0.49
1:B:186:THR:HG21	1:B:190:TYR:CE1	2.47	0.48
1:B:358:MSE:SE	1:B:367:ARG:HH11	2.46	0.48
1:A:241:GLN:HG2	2:A:776:HOH:O	2.13	0.48
1:A:82:ARG:HG2	1:A:239:GLN:HB2	1.95	0.48
1:B:82:ARG:HG2	1:B:239:GLN:HB2	1.95	0.48
2:A:474:HOH:O	1:C:152:THR:HB	2.13	0.48
1:B:165:LEU:HD12	2:B:633:HOH:O	2.13	0.48
1:A:223:LEU:HD11	2:A:801:HOH:O	2.14	0.48
1:B:55:ARG:O	1:C:278:ASN:O	2.32	0.48
1:C:37:PRO:HG2	2:C:688:HOH:O	2.12	0.48
1:A:152:THR:HG21	2:B:432:HOH:O	2.13	0.48
1:B:223:LEU:HD12	2:B:663:HOH:O	2.14	0.48
1:A:334:ILE:HD12	1:A:400:ILE:CD1	2.41	0.48
1:B:388:ASN:HB2	2:B:597:HOH:O	2.12	0.48
1:C:269:ALA:CB	2:C:888:HOH:O	2.58	0.48
1:A:99:GLN:NE2	2:A:668:HOH:O	2.46	0.48
1:C:60:ILE:HD12	1:C:274:TYR:CE1	2.48	0.47
1:C:275:ASP:N	2:C:797:HOH:O	2.47	0.47
1:A:223:LEU:CD1	2:A:801:HOH:O	2.61	0.47
1:C:247:THR:CG2	1:C:289:SER:HB3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLY:O	1:B:272:THR:HB	2.13	0.47
1:C:75:ILE:HG21	1:C:248:LEU:HD12	1.97	0.47
1:A:323:VAL:O	1:A:327:VAL:HG13	2.15	0.47
1:A:140:THR:HG22	1:A:154:VAL:HG22	1.96	0.47
1:B:152:THR:HG21	2:C:431:HOH:O	2.14	0.47
1:A:19:LYS:HE3	1:B:315:GLN:NE2	2.29	0.47
1:C:79:SER:CB	2:C:933:HOH:O	2.62	0.47
1:A:267:ARG:NH2	1:A:275:ASP:HA	2.29	0.47
1:C:323:VAL:HG12	2:C:807:HOH:O	2.15	0.47
1:B:250:LEU:C	1:B:250:LEU:HD23	2.35	0.47
1:A:264:SER:OG	1:A:265:LYS:N	2.49	0.46
1:A:197:ASN:ND2	1:A:199:GLU:HG2	2.31	0.46
1:C:267:ARG:HB3	1:C:268:GLY:H	1.61	0.46
1:C:161:TYR:O	1:C:164:VAL:HG12	2.15	0.46
1:C:397:GLN:NE2	1:C:397:GLN:HA	2.30	0.46
1:C:8:GLN:OE1	1:C:11:ARG:NH2	2.49	0.46
1:C:97:THR:HG22	1:C:225:GLN:HE22	1.75	0.46
1:C:334:ILE:HG13	1:C:396:ASN:HB3	1.97	0.46
1:C:261:TYR:O	1:C:262:SER:HB3	2.15	0.46
1:B:235:GLU:OE2	1:B:238:ARG:NH1	2.49	0.46
1:B:49:THR:O	1:B:63:ASN:HA	2.15	0.45
1:B:146:VAL:HG22	1:B:146:VAL:O	2.16	0.45
1:B:265:LYS:O	1:B:265:LYS:HG3	2.17	0.45
1:A:267:ARG:HB3	1:A:268:GLY:H	1.68	0.45
1:A:381:ASN:ND2	2:A:722:HOH:O	2.44	0.45
1:C:199:GLU:H	1:C:199:GLU:HG2	1.50	0.45
1:C:334:ILE:HD12	1:C:400:ILE:HD12	1.97	0.45
1:B:265:LYS:CD	2:B:935:HOH:O	2.64	0.45
1:A:279:MSE:HE2	2:A:661:HOH:O	2.16	0.45
1:A:139:GLN:HE21	1:A:143:ARG:NH2	2.13	0.45
1:A:94:GLN:NE2	2:A:731:HOH:O	2.50	0.45
1:C:301:GLN:NE2	2:C:730:HOH:O	2.49	0.45
1:A:152:THR:OG1	1:B:367:ARG:NH1	2.50	0.45
1:C:160:GLN:HB2	1:C:160:GLN:HE21	1.35	0.45
1:C:223:LEU:HD13	1:C:227:ARG:NH1	2.32	0.45
1:C:265:LYS:HG3	1:C:265:LYS:O	2.16	0.45
1:C:146:VAL:HG13	1:C:148:LEU:HG	1.99	0.45
1:C:199:GLU:CD	2:C:574:HOH:O	2.56	0.44
1:C:223:LEU:CD1	1:C:227:ARG:NH1	2.80	0.44
1:A:102:GLN:HG2	2:A:598:HOH:O	2.17	0.44
1:C:182:LEU:HD13	1:C:182:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:LEU:CD1	2:C:873:HOH:O	2.66	0.44
1:A:55:ARG:O	1:B:278:ASN:O	2.35	0.44
1:A:339:SER:HB3	1:C:169:LEU:CD1	2.47	0.44
1:B:267:ARG:HB3	1:B:268:GLY:H	1.72	0.44
1:A:278:ASN:HB3	1:C:55:ARG:CZ	2.48	0.44
1:C:46:ALA:HA	1:C:67:ALA:HA	2.00	0.44
1:C:166:ALA:HA	1:C:169:LEU:HD23	1.99	0.44
1:A:265:LYS:HG3	1:A:265:LYS:O	2.18	0.44
1:B:205:LYS:HD3	1:B:338:ILE:HD13	1.99	0.44
1:B:143:ARG:HA	1:B:146:VAL:HG12	1.99	0.43
1:C:268:GLY:O	1:C:269:ALA:HB3	2.18	0.43
1:A:24:ARG:HA	1:A:94:GLN:HG3	1.99	0.43
1:C:359:GLU:OE2	2:C:706:HOH:O	2.21	0.43
1:C:290:LEU:HD22	1:C:291:PRO:HD2	2.01	0.43
1:C:358:MSE:SE	1:C:367:ARG:HD2	2.68	0.43
1:B:11:ARG:NE	2:B:692:HOH:O	2.52	0.43
1:B:146:VAL:HG13	1:B:148:LEU:HG	1.99	0.43
1:C:291:PRO:O	1:C:292:ILE:HB	2.18	0.43
1:B:24:ARG:HE	1:B:24:ARG:HB3	1.58	0.43
1:C:75:ILE:HB	1:C:248:LEU:O	2.18	0.43
1:B:214:LYS:HB3	1:B:214:LYS:HE3	1.84	0.43
1:B:103:GLN:HG3	1:B:407:LEU:HB3	2.00	0.43
1:B:264:SER:OG	1:B:265:LYS:N	2.52	0.43
1:A:421:LYS:HA	1:A:422:PRO:HD3	1.93	0.43
1:A:8:GLN:OE1	1:A:11:ARG:NH2	2.52	0.43
1:A:319:ALA:O	1:A:323:VAL:HG13	2.19	0.43
1:C:235:GLU:OE2	1:C:238:ARG:NH1	2.52	0.43
1:B:358:MSE:SE	1:B:367:ARG:HD2	2.69	0.43
1:A:75:ILE:HB	1:A:248:LEU:O	2.19	0.43
1:C:24:ARG:NH1	2:C:764:HOH:O	2.52	0.42
1:C:197:ASN:ND2	1:C:200:ASN:H	2.17	0.42
1:A:358:MSE:SE	1:A:371:ASP:HB3	2.70	0.42
1:B:323:VAL:O	1:B:327:VAL:HG13	2.18	0.42
1:A:152:THR:CG2	2:B:432:HOH:O	2.67	0.42
1:A:47:ASP:HB3	1:B:287:SER:HA	2.00	0.42
1:C:55:ARG:O	1:C:56:ASP:HB3	2.20	0.42
1:A:421:LYS:HG3	2:A:787:HOH:O	2.20	0.42
1:A:330:SER:HB2	1:A:400:ILE:HG13	2.01	0.42
1:B:223:LEU:C	1:B:223:LEU:HD12	2.40	0.42
1:B:289:SER:HB2	2:B:775:HOH:O	2.20	0.42
1:C:365:GLY:HA2	2:C:543:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:HD21	1:B:158:ARG:CZ	2.49	0.42
1:B:160:GLN:HE21	1:B:160:GLN:HB2	1.42	0.42
1:B:320:HIS:CG	2:B:681:HOH:O	2.73	0.42
1:C:205:LYS:HD2	2:C:673:HOH:O	2.20	0.42
1:C:54:TYR:O	2:C:695:HOH:O	2.22	0.42
1:A:42:LEU:HD12	1:A:70:GLN:O	2.19	0.42
1:B:270:ALA:HB1	1:B:274:TYR:CD2	2.55	0.42
1:B:152:THR:CG2	2:C:431:HOH:O	2.67	0.42
1:B:86:LEU:HD13	1:B:235:GLU:CG	2.50	0.42
1:C:86:LEU:HD13	1:C:235:GLU:CG	2.50	0.42
1:A:46:ALA:HA	1:A:67:ALA:HA	2.01	0.42
1:B:170:THR:CG2	2:C:546:HOH:O	2.66	0.41
1:B:207:GLN:NE2	2:B:815:HOH:O	2.51	0.41
1:C:86:LEU:HD13	1:C:235:GLU:HG3	2.02	0.41
1:A:8:GLN:HG3	2:A:778:HOH:O	2.19	0.41
1:C:68:SER:HB3	1:C:255:GLY:HA3	2.02	0.41
1:C:130:LYS:NZ	2:C:755:HOH:O	2.53	0.41
1:B:75:ILE:HG21	1:B:248:LEU:HD12	2.02	0.41
1:A:367:ARG:HH12	1:C:156:ASN:ND2	2.05	0.41
1:A:166:ALA:HA	1:A:169:LEU:CD2	2.49	0.41
1:B:4:MSE:SE	2:B:704:HOH:O	2.88	0.41
1:A:80:LYS:HE2	2:A:570:HOH:O	2.20	0.41
1:A:271:GLY:O	1:A:272:THR:HB	2.19	0.41
1:C:79:SER:CA	2:C:933:HOH:O	2.47	0.41
1:B:365:GLY:HA2	2:B:647:HOH:O	2.20	0.41
1:B:47:ASP:HB3	1:C:287:SER:HA	2.02	0.41
1:C:79:SER:HB2	2:C:933:HOH:O	2.21	0.41
1:C:223:LEU:HD11	2:C:873:HOH:O	2.20	0.41
1:A:42:LEU:O	1:B:291:PRO:O	2.38	0.41
1:B:270:ALA:HB1	1:B:274:TYR:HD2	1.86	0.41
1:C:274:TYR:CE2	2:C:896:HOH:O	2.57	0.41
1:C:82:ARG:HG2	1:C:239:GLN:HA	2.02	0.41
1:B:8:GLN:OE1	1:B:11:ARG:NH2	2.54	0.41
1:C:421:LYS:NZ	2:C:663:HOH:O	2.53	0.41
1:C:302:VAL:O	1:C:306:GLN:HG3	2.21	0.41
1:A:219:ARG:CD	2:A:571:HOH:O	2.60	0.41
1:B:60:ILE:HD12	1:B:274:TYR:CE1	2.56	0.41
1:C:214:LYS:HB3	1:C:214:LYS:HE3	1.88	0.41
1:A:68:SER:HB3	1:A:255:GLY:HA3	2.02	0.41
1:A:11:ARG:NH1	1:A:409:GLU:OE2	2.54	0.41
1:A:291:PRO:O	1:C:42:LEU:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLN:HB3	1:C:41:GLN:NE2	2.36	0.41
2:A:547:HOH:O	1:C:170:THR:HG22	2.20	0.41
1:A:24:ARG:HE	1:A:24:ARG:HB3	1.61	0.41
1:A:250:LEU:HD23	1:A:250:LEU:C	2.41	0.41
1:A:160:GLN:NE2	2:A:525:HOH:O	2.53	0.40
1:B:219:ARG:HB2	1:B:404:LEU:O	2.22	0.40
1:C:358:MSE:SE	1:C:367:ARG:NH1	2.99	0.40
1:B:398:LEU:HD11	1:B:415:LEU:CD1	2.51	0.40
1:A:359:GLU:HB3	2:A:622:HOH:O	2.22	0.40
1:C:223:LEU:C	1:C:223:LEU:HD12	2.41	0.40
1:C:32:ASN:ND2	1:C:35:ARG:HH22	2.15	0.40
1:B:75:ILE:HB	1:B:248:LEU:O	2.20	0.40
1:B:163:THR:HG23	2:B:803:HOH:O	2.20	0.40
1:B:388:ASN:CB	2:B:597:HOH:O	2.69	0.40
1:A:84:LEU:O	1:A:88:GLU:HG3	2.22	0.40
1:C:297:MSE:C	1:C:298:VAL:O	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:773:HOH:O	2:C:709:HOH:O[9_554]	2.11	0.09
2:A:683:HOH:O	2:B:797:HOH:O[9_554]	2.15	0.05

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	426/428 (100%)	403 (95%)	19 (4%)	4 (1%)	21	15
1	B	426/428 (100%)	403 (95%)	19 (4%)	4 (1%)	21	15
1	C	426/428 (100%)	397 (93%)	25 (6%)	4 (1%)	21	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1278/1284 (100%)	1203 (94%)	63 (5%)	12 (1%)	21 15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	THR
1	B	279	MSE
1	A	259	THR
1	C	259	THR
1	C	279	MSE
1	A	55	ARG
1	A	279	MSE
1	B	55	ARG
1	C	268	GLY
1	C	55	ARG
1	B	268	GLY
1	A	268	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	358/353 (101%)	316 (88%)	42 (12%)	7 3
1	B	358/353 (101%)	325 (91%)	33 (9%)	11 7
1	C	358/353 (101%)	319 (89%)	39 (11%)	8 4
All	All	1074/1059 (101%)	960 (89%)	114 (11%)	8 5

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	17	LEU
1	A	47	ASP
1	A	51	SER

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Mol	Chain	Res	Type
1	A	60	ILE
1	A	65	THR
1	A	71	LEU
1	A	79	SER
1	A	86	LEU
1	A	97	THR
1	A	139	GLN
1	A	142	GLN
1	A	152	THR
1	A	160	GLN
1	A	169	LEU
1	A	170	THR
1	A	186	THR
1	A	197	ASN
1	A	199	GLU
1	A	200	ASN
1	A	217	GLU
1	A	223	LEU
1	A	247	THR
1	A	256	ILE
1	A	259	THR
1	A	262	SER
1	A	265	LYS
1	A	266	THR
1	A	277	SER
1	A	279	MSE
1	A	281	GLN
1	A	290	LEU
1	A	310	VAL
1	A	316	LEU
1	A	323	VAL
1	A	327	VAL
1	A	397	GLN
1	A	398	LEU
1	A	400	ILE
1	A	401	LYS
1	A	407	LEU
1	A	412	LEU
1	B	12	LEU
1	B	17	LEU
1	B	51	SER
1	B	60	ILE

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Mol	Chain	Res	Type
1	B	71	LEU
1	B	86	LEU
1	B	97	THR
1	B	142	GLN
1	B	152	THR
1	B	160	GLN
1	B	170	THR
1	B	186	THR
1	B	197	ASN
1	B	199	GLU
1	B	217	GLU
1	B	223	LEU
1	B	247	THR
1	B	256	ILE
1	B	262	SER
1	B	265	LYS
1	B	266	THR
1	B	277	SER
1	B	279	MSE
1	B	281	GLN
1	B	290	LEU
1	B	316	LEU
1	B	323	VAL
1	B	353	SER
1	B	397	GLN
1	B	398	LEU
1	B	401	LYS
1	B	407	LEU
1	B	412	LEU
1	C	12	LEU
1	C	17	LEU
1	C	47	ASP
1	C	51	SER
1	C	60	ILE
1	C	71	LEU
1	C	86	LEU
1	C	97	THR
1	C	139	GLN
1	C	142	GLN
1	C	146	VAL
1	C	149	VAL
1	C	152	THR

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Mol	Chain	Res	Type
1	C	160	GLN
1	C	170	THR
1	C	186	THR
1	C	197	ASN
1	C	199	GLU
1	C	200	ASN
1	C	217	GLU
1	C	223	LEU
1	C	247	THR
1	C	251	THR
1	C	256	ILE
1	C	262	SER
1	C	265	LYS
1	C	266	THR
1	C	277	SER
1	C	279	MSE
1	C	281	GLN
1	C	290	LEU
1	C	316	LEU
1	C	323	VAL
1	C	353	SER
1	C	397	GLN
1	C	398	LEU
1	C	401	LYS
1	C	407	LEU
1	C	412	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	41	GLN
1	A	61	ASN
1	A	103	GLN
1	A	108	ASN
1	A	115	ASN
1	A	127	GLN
1	A	139	GLN
1	A	142	GLN
1	A	155	GLN
1	A	156	ASN
1	A	160	GLN

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Mol	Chain	Res	Type
1	A	174	ASN
1	A	197	ASN
1	A	207	GLN
1	A	210	ASN
1	A	220	ASN
1	A	225	GLN
1	A	281	GLN
1	A	301	GLN
1	A	315	GLN
1	A	320	HIS
1	A	332	ASN
1	A	342	ASN
1	A	346	GLN
1	A	381	ASN
1	A	388	ASN
1	A	392	ASN
1	A	397	GLN
1	A	399	ASN
1	A	417	ASN
1	B	32	ASN
1	B	41	GLN
1	B	61	ASN
1	B	103	GLN
1	B	108	ASN
1	B	127	GLN
1	B	139	GLN
1	B	142	GLN
1	B	155	GLN
1	B	156	ASN
1	B	160	GLN
1	B	174	ASN
1	B	197	ASN
1	B	207	GLN
1	B	210	ASN
1	B	220	ASN
1	B	225	GLN
1	B	281	GLN
1	B	301	GLN
1	B	342	ASN
1	B	346	GLN
1	B	381	ASN
1	B	388	ASN

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Mol	Chain	Res	Type
1	B	392	ASN
1	B	397	GLN
1	B	399	ASN
1	B	417	ASN
1	C	32	ASN
1	C	41	GLN
1	C	61	ASN
1	C	103	GLN
1	C	108	ASN
1	C	115	ASN
1	C	127	GLN
1	C	139	GLN
1	C	142	GLN
1	C	155	GLN
1	C	156	ASN
1	C	160	GLN
1	C	174	ASN
1	C	197	ASN
1	C	207	GLN
1	C	210	ASN
1	C	220	ASN
1	C	225	GLN
1	C	281	GLN
1	C	301	GLN
1	C	320	HIS
1	C	332	ASN
1	C	342	ASN
1	C	381	ASN
1	C	388	ASN
1	C	392	ASN
1	C	397	GLN
1	C	399	ASN
1	C	417	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

There are no ligands in this entry.

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	423/428 (98%)	0.51	20 (4%)	35	44	25, 48, 81, 84	0
1	B	423/428 (98%)	0.83	32 (7%)	17	23	24, 47, 81, 84	0
1	C	423/428 (98%)	0.83	39 (9%)	11	15	24, 47, 81, 84	0
All	All	1269/1284 (98%)	0.72	91 (7%)	18	25	24, 47, 81, 84	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	269	ALA	11.6
1	B	270	ALA	11.3
1	C	270	ALA	10.8
1	B	269	ALA	10.7
1	C	268	GLY	10.0
1	C	274	TYR	9.2
1	C	273	GLN	9.1
1	B	268	GLY	8.9
1	B	272	THR	7.8
1	C	255	GLY	7.5
1	B	271	GLY	6.8
1	B	273	GLN	6.7
1	B	264	SER	6.4
1	A	267	ARG	5.7
1	C	60	ILE	5.6
1	B	50	TYR	5.5
1	B	267	ARG	5.3
1	C	281	GLN	5.3
1	B	54	TYR	5.2
1	C	271	GLY	5.2
1	C	256	ILE	5.1
1	A	263	GLY	5.0
1	C	280	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	263	GLY	4.8
1	C	267	ARG	4.8
1	C	266	THR	4.7
1	C	272	THR	4.7
1	A	60	ILE	4.5
1	C	263	GLY	4.4
1	C	275	ASP	4.4
1	B	59	GLY	4.3
1	B	274	TYR	4.3
1	C	278	ASN	4.1
1	C	66	SER	4.1
1	A	281	GLN	4.1
1	C	48	TYR	3.9
1	B	275	ASP	3.9
1	A	48	TYR	3.9
1	B	60	ILE	3.8
1	C	277	SER	3.7
1	A	63	ASN	3.6
1	C	283	LYS	3.4
1	A	50	TYR	3.4
1	C	262	SER	3.4
1	C	169	LEU	3.4
1	A	264	SER	3.3
1	B	48	TYR	3.3
1	A	169	LEU	3.2
1	C	295	GLY	3.2
1	B	284	VAL	3.2
1	B	53	GLY	3.2
1	B	12	LEU	3.1
1	A	271	GLY	3.1
1	B	55	ARG	3.0
1	B	169	LEU	3.0
1	A	146	VAL	2.9
1	A	266	THR	2.9
1	B	63	ASN	2.8
1	B	81	TRP	2.8
1	A	49	THR	2.8
1	C	69	LEU	2.7
1	C	54	TYR	2.7
1	C	68	SER	2.7
1	C	257	SER	2.7
1	C	259	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	12	LEU	2.6
1	B	164	VAL	2.6
1	C	142	GLN	2.6
1	C	428	GLU	2.6
1	C	223	LEU	2.5
1	B	256	ILE	2.5
1	A	268	GLY	2.5
1	C	67	ALA	2.4
1	B	413	LEU	2.4
1	C	261	TYR	2.4
1	A	256	ILE	2.3
1	A	316	LEU	2.3
1	B	266	THR	2.2
1	B	64	ALA	2.2
1	A	262	SER	2.2
1	C	63	ASN	2.2
1	C	189	TYR	2.2
1	B	1	GLU	2.1
1	C	59	GLY	2.1
1	C	1	GLU	2.1
1	B	189	TYR	2.1
1	B	251	THR	2.0
1	B	423	VAL	2.0
1	A	62	SER	2.0
1	A	423	VAL	2.0
1	A	280	GLY	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.