



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:27 PM GMT

PDB ID : 1TQQ  
Title : Structure of TolC in complex with hexamminecobalt  
Authors : Higgins, M.K.; Eswaran, J.; Edwards, P.C.; Schertler, G.F.; Hughes, C.; Koronakis, V.  
Deposited on : 2004-06-18  
Resolution : 2.75 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](mailto: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.

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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

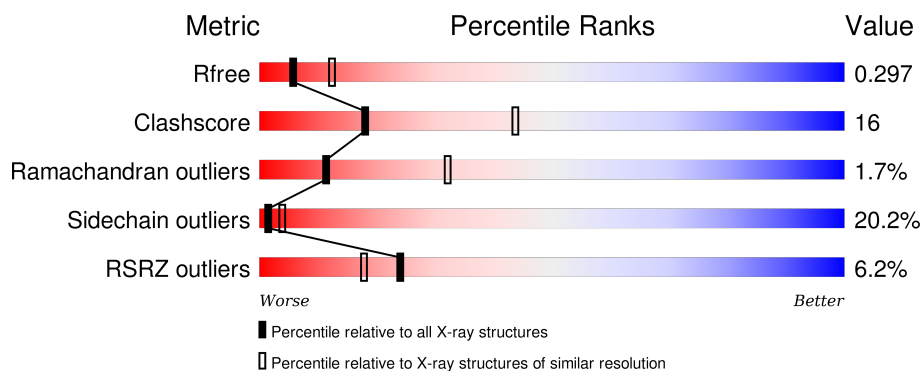
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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  $\geq 3$ , 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	471	<div> <div>4%</div> <div>55%</div> <div>28%</div> <div>7%</div> <div>9%</div> </div>
1	B	471	<div> <div>5%</div> <div>56%</div> <div>25%</div> <div>9%</div> <div>9%</div> </div>
1	C	471	<div> <div>7%</div> <div>58%</div> <div>24%</div> <div>9%</div> <div>9%</div> </div>

## 2 Entry composition [i](#)

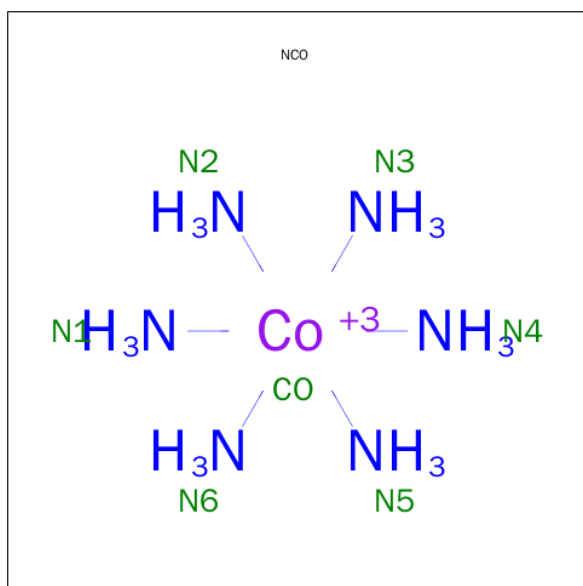
There are 3 unique types of molecules in this entry. The entry contains 10227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	S	0	0	0
			3305	2038	586	676	5			
1	B	428	Total	C	N	O	S	0	0	0
			3305	2038	586	676	5			
1	C	428	Total	C	N	O	S	0	0	0
			3305	2038	586	676	5			

- Molecule 2 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula:  $\text{CoH}_{18}\text{N}_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	Co	N	0	0
			7	1	6		

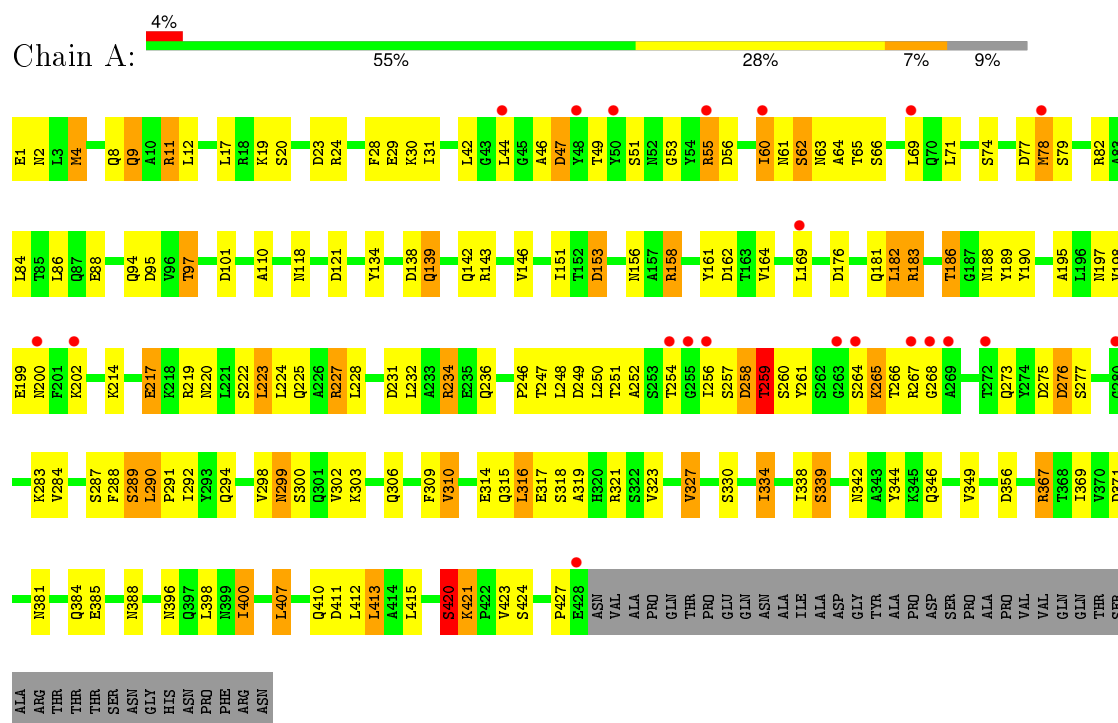
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total 97	O 97	0	0
3	B	101	Total 101	O 101	0	0
3	C	107	Total 107	O 107	0	0

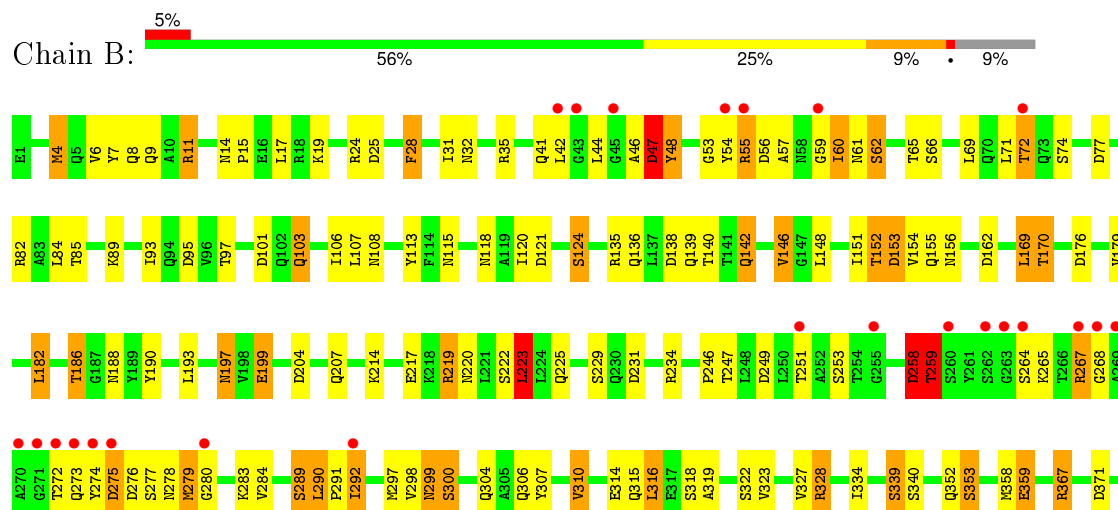
### 3 Residue-property plots [i](#)

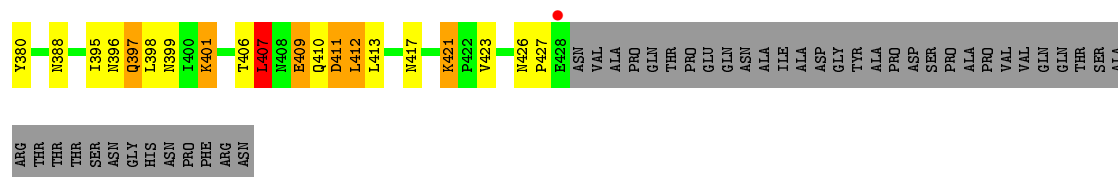
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

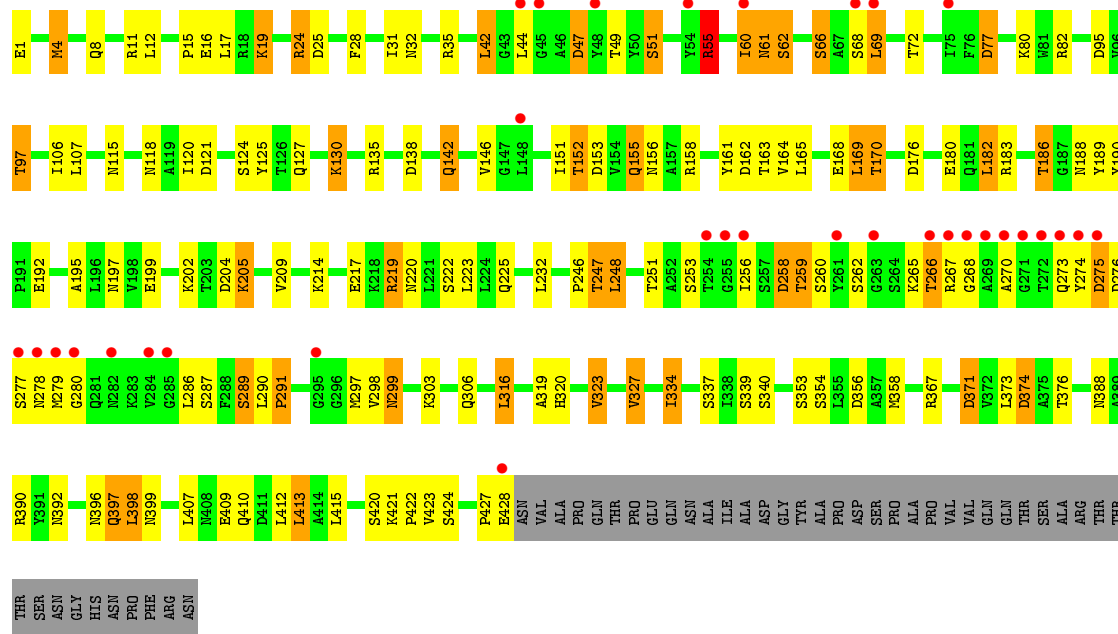


#### • Molecule 1: Outer membrane protein tolC





● Molecule 1: Outer membrane protein tolC



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	265.28 Å   265.28 Å   96.25 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	30.43 – 2.75 30.24 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.6 (30.43-2.75) 95.6 (30.24-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.76 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.264 , 0.305 0.253 , 0.297	Depositor DCC
$R_{free}$ test set	3174 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.7	EDS
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 62732 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	10227	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NCO

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	0.80	0/3346	1.06	18/4545 (0.4%)
1	B	0.85	1/3346 (0.0%)	1.08	28/4545 (0.6%)
1	C	0.84	0/3346	1.07	27/4545 (0.6%)
All	All	0.83	1/10038 (0.0%)	1.07	73/13635 (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	B	0	2
1	C	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	380	TYR	CD2-CE2	-5.00	1.31	1.39

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	C	158	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	C	153	ASP	CB-CG-OD2	8.80	126.22	118.30
1	C	69	LEU	CA-CB-CG	8.77	135.48	115.30
1	A	356	ASP	CB-CG-OD2	8.45	125.90	118.30
1	B	276	ASP	CB-CG-OD2	8.43	125.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	LEU	CA-CB-CG	8.13	133.99	115.30
1	C	138	ASP	CB-CG-OD2	8.05	125.55	118.30
1	C	95	ASP	CB-CG-OD2	8.01	125.51	118.30
1	C	121	ASP	CB-CG-OD2	7.97	125.47	118.30
1	A	176	ASP	CB-CG-OD2	7.92	125.43	118.30
1	A	249	ASP	CB-CG-OD2	7.89	125.41	118.30
1	C	135	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	176	ASP	CB-CG-OD2	7.76	125.28	118.30
1	A	371	ASP	CB-CG-OD2	7.75	125.28	118.30
1	A	121	ASP	CB-CG-OD2	7.56	125.10	118.30
1	B	204	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	413	LEU	CA-CB-CG	7.48	132.51	115.30
1	A	77	ASP	CB-CG-OD2	7.43	124.99	118.30
1	B	138	ASP	CB-CG-OD2	7.39	124.95	118.30
1	B	182	LEU	CA-CB-CG	7.17	131.79	115.30
1	B	367	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	95	ASP	CB-CG-OD2	7.08	124.67	118.30
1	B	275	ASP	CB-CG-OD2	7.05	124.65	118.30
1	A	101	ASP	CB-CG-OD2	6.99	124.59	118.30
1	C	25	ASP	CB-CG-OD2	6.96	124.56	118.30
1	B	162	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	23	ASP	CB-CG-OD2	6.84	124.45	118.30
1	A	367	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	C	356	ASP	CB-CG-OD2	6.67	124.30	118.30
1	B	231	ASP	CB-CG-OD2	6.53	124.18	118.30
1	B	77	ASP	CB-CG-OD2	6.50	124.15	118.30
1	C	77	ASP	CB-CG-OD2	6.38	124.04	118.30
1	C	162	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	413	LEU	CA-CB-CG	6.33	129.85	115.30
1	C	42	LEU	CA-CB-CG	6.27	129.72	115.30
1	B	101	ASP	CB-CG-OD2	6.26	123.94	118.30
1	C	176	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	153	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	47	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	411	ASP	CB-CG-OD2	5.93	123.64	118.30
1	C	248	LEU	CA-CB-CG	5.90	128.86	115.30
1	C	275	ASP	CB-CG-OD2	5.85	123.56	118.30
1	C	276	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	232	LEU	CA-CB-CG	5.80	128.64	115.30
1	C	413	LEU	CA-CB-CG	5.76	128.56	115.30
1	C	374	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	316	LEU	CA-CB-CG	5.63	128.25	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	258	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	390	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	25	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	411	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	69	LEU	CA-CB-CG	5.44	127.80	115.30
1	B	153	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	367	ARG	CG-CD-NE	-5.38	100.50	111.80
1	A	407	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	353	SER	CB-CA-C	5.34	120.26	110.10
1	C	12	LEU	CA-CB-CG	5.30	127.48	115.30
1	C	371	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	135	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	47	ASP	CB-CG-OD2	5.28	123.06	118.30
1	B	121	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	316	LEU	CA-CB-CG	5.27	127.43	115.30
1	C	204	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	162	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	47	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	249	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	138	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	276	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	407	LEU	CA-CB-CG	5.11	127.06	115.30
1	C	334	ILE	CG1-CB-CG2	-5.09	100.20	111.40
1	C	286	LEU	CA-CB-CG	5.01	126.81	115.30
1	B	258	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	PRO	Peptide
1	A	62	SER	Peptide
1	B	427	PRO	Peptide
1	B	62	SER	Peptide
1	C	427	PRO	Peptide
1	C	62	SER	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	3305	0	3256	119	0
1	B	3305	0	3256	124	3
1	C	3305	0	3256	110	0
2	C	7	0	0	1	0
3	A	97	0	0	31	2
3	B	101	0	0	22	4
3	C	107	0	0	35	2
All	All	10227	0	9768	310	6

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 16.

All (310) 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:78:MET:CE	1:A:78:MET:SD	2.03	1.46
1:B:423:VAL:HB	3:B:479:HOH:O	1.38	1.22
1:A:156:ASN:ND2	1:B:367:ARG:NH1	1.90	1.18
1:A:156:ASN:ND2	1:B:367:ARG:HH11	1.42	1.12
1:A:323:VAL:O	1:A:327:VAL:HG12	1.52	1.09
1:A:384:GLN:HB3	3:A:532:HOH:O	1.56	1.06
1:B:352:GLN:HB3	3:B:537:HOH:O	1.56	1.03
1:A:217:GLU:HG3	3:A:530:HOH:O	1.56	1.03
1:B:156:ASN:HD21	1:C:358:MET:HE1	1.24	1.02
1:A:186:THR:HG21	1:A:190:TYR:HE1	1.26	1.01
1:A:367:ARG:NH1	1:C:156:ASN:ND2	2.09	1.00
1:C:247:THR:HB	3:C:559:HOH:O	1.61	1.00
1:A:367:ARG:HH11	1:C:156:ASN:ND2	1.63	0.97
1:A:11:ARG:HD3	3:A:523:HOH:O	1.64	0.97
1:A:146:VAL:O	1:A:146:VAL:HG22	1.62	0.96
1:A:156:ASN:HD21	1:B:367:ARG:NH1	1.58	0.95
1:B:186:THR:HG21	1:B:190:TYR:HE1	1.29	0.93
1:A:367:ARG:HH11	1:C:156:ASN:HD21	1.14	0.92
1:A:156:ASN:HD21	1:B:367:ARG:HH11	0.91	0.91
1:C:219:ARG:HG3	1:C:219:ARG:HH11	1.34	0.91
1:A:156:ASN:HD21	1:B:358:MET:HE1	1.36	0.90
1:B:156:ASN:ND2	1:C:367:ARG:NH1	2.21	0.89
1:B:156:ASN:ND2	1:C:358:MET:HE1	1.87	0.88
1:A:60:ILE:HD11	1:A:261:TYR:HD2	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLN:HG2	3:A:493:HOH:O	1.73	0.88
1:B:169:LEU:HG	1:C:339:SER:HB3	1.55	0.87
1:A:298:VAL:O	1:A:299:ASN:HB2	1.73	0.86
1:A:156:ASN:HD22	1:B:367:ARG:NH1	1.73	0.85
1:B:186:THR:HG21	1:B:190:TYR:CE1	2.11	0.85
1:A:60:ILE:HD11	1:A:261:TYR:CD2	2.10	0.85
1:B:274:TYR:HE2	3:B:543:HOH:O	1.60	0.84
1:C:298:VAL:O	1:C:299:ASN:HB2	1.78	0.84
1:A:186:THR:HG22	1:A:188:ASN:H	1.40	0.84
1:B:59:GLY:HA2	3:B:539:HOH:O	1.77	0.83
1:B:298:VAL:O	1:B:299:ASN:HB2	1.77	0.83
1:C:60:ILE:C	1:C:61:ASN:HD22	1.82	0.83
1:A:186:THR:HG21	1:A:190:TYR:CE1	2.14	0.82
1:A:139:GLN:O	1:A:143:ARG:HG3	1.80	0.81
1:A:146:VAL:O	1:A:146:VAL:CG2	2.28	0.80
1:C:397:GLN:HE21	1:C:397:GLN:HA	1.43	0.80
1:A:97:THR:HG22	1:A:225:GLN:NE2	1.97	0.79
1:C:69:LEU:HD22	3:C:575:HOH:O	1.81	0.79
1:A:323:VAL:O	1:A:327:VAL:CG1	2.31	0.79
1:C:274:TYR:HB3	3:C:533:HOH:O	1.82	0.79
1:A:342:ASN:HB3	3:A:484:HOH:O	1.82	0.79
1:B:156:ASN:HD21	1:C:367:ARG:HH11	1.31	0.77
1:B:182:LEU:O	1:B:186:THR:HB	1.86	0.76
1:B:289:SER:HB2	3:B:515:HOH:O	1.84	0.76
1:C:274:TYR:CB	3:C:533:HOH:O	2.35	0.75
3:A:474:HOH:O	1:B:279:MET:SD	2.45	0.74
1:C:168:GLU:OE2	3:C:531:HOH:O	2.04	0.74
1:A:156:ASN:ND2	1:B:358:MET:HE1	2.03	0.74
1:B:60:ILE:HG21	3:B:516:HOH:O	1.88	0.73
1:C:182:LEU:O	1:C:186:THR:HB	1.88	0.73
1:B:48:TYR:O	1:B:48:TYR:HD1	1.71	0.73
1:A:195:ALA:HB2	1:A:423:VAL:CG2	2.19	0.72
1:B:156:ASN:HD21	1:C:367:ARG:NH1	1.86	0.71
1:A:228:LEU:HD11	3:A:508:HOH:O	1.89	0.71
1:A:367:ARG:NH1	1:C:156:ASN:HD22	1.86	0.70
1:C:219:ARG:NH1	1:C:219:ARG:HG3	1.96	0.70
1:B:334:ILE:HG13	1:B:396:ASN:HB3	1.73	0.70
1:B:136:GLN:NE2	1:B:359:GLU:OE2	2.21	0.70
1:C:260:SER:HB2	3:C:516:HOH:O	1.93	0.69
1:C:247:THR:HG23	1:C:289:SER:HB3	1.75	0.69
1:C:186:THR:HG21	1:C:190:TYR:HE1	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HD22	3:A:564:HOH:O	1.92	0.68
1:A:181:GLN:CG	3:A:493:HOH:O	2.34	0.68
1:A:346:GLN:NE2	1:A:346:GLN:HA	2.09	0.68
1:C:130:LYS:NZ	3:C:531:HOH:O	2.26	0.68
1:A:234:ARG:HG3	3:A:563:HOH:O	1.91	0.68
1:B:48:TYR:C	1:B:48:TYR:CD1	2.66	0.68
1:B:186:THR:HG22	1:B:188:ASN:H	1.58	0.68
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.58	0.67
1:C:256:ILE:O	3:C:534:HOH:O	2.11	0.67
1:C:16:GLU:CG	3:C:512:HOH:O	2.43	0.67
1:B:358:MET:CE	1:B:367:ARG:HD2	2.24	0.67
1:A:4:MET:O	1:A:8:GLN:HG2	1.95	0.67
1:C:55:ARG:HB3	3:C:527:HOH:O	1.93	0.67
1:A:195:ALA:HB2	1:A:423:VAL:HG21	1.75	0.67
1:A:9:GLN:HG3	3:A:552:HOH:O	1.95	0.67
1:A:319:ALA:O	1:A:323:VAL:HG13	1.94	0.66
1:B:323:VAL:O	1:B:327:VAL:HG13	1.96	0.66
1:B:97:THR:OG1	1:B:225:GLN:NE2	2.28	0.66
1:A:156:ASN:ND2	1:B:367:ARG:HH12	1.89	0.66
1:C:66:SER:HB3	3:C:534:HOH:O	1.96	0.66
1:A:349:VAL:HG13	3:A:498:HOH:O	1.96	0.65
1:B:32:ASN:HD22	1:B:35:ARG:HH22	1.45	0.65
1:A:42:LEU:O	1:B:291:PRO:O	2.16	0.64
1:C:4:MET:O	1:C:8:GLN:HG2	1.98	0.64
1:A:182:LEU:O	1:A:186:THR:HB	1.97	0.64
1:C:319:ALA:O	1:C:323:VAL:HG13	1.97	0.64
1:A:265:LYS:HG3	1:A:265:LYS:O	1.98	0.63
1:C:195:ALA:HB2	1:C:423:VAL:HG21	1.80	0.63
1:A:84:LEU:O	1:A:88:GLU:HG3	1.99	0.62
1:B:152:THR:HG21	3:C:482:HOH:O	1.99	0.62
1:B:153:ASP:OD1	1:C:367:ARG:NH2	2.30	0.62
1:C:28:PHE:O	1:C:31:ILE:HG13	1.99	0.62
1:A:71:LEU:HB3	1:A:252:ALA:HB3	1.82	0.62
1:C:44:LEU:HG	3:C:526:HOH:O	2.01	0.61
1:B:274:TYR:CE2	3:B:543:HOH:O	2.39	0.61
1:B:32:ASN:ND2	1:B:35:ARG:HH22	1.99	0.61
1:A:290:LEU:HD13	1:A:292:ILE:HG13	1.84	0.60
1:A:415:LEU:HD21	3:A:494:HOH:O	2.01	0.60
1:C:195:ALA:HB2	1:C:423:VAL:CG2	2.32	0.60
1:B:265:LYS:HD3	3:B:555:HOH:O	2.02	0.60
1:B:53:GLY:HA2	1:C:280:GLY:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:THR:HG22	1:C:225:GLN:NE2	2.16	0.60
1:C:323:VAL:O	1:C:327:VAL:HG12	2.01	0.59
1:A:219:ARG:HG3	1:A:219:ARG:NH1	2.18	0.59
1:C:107:LEU:HD11	1:C:399:ASN:ND2	2.16	0.59
1:C:32:ASN:HD22	1:C:35:ARG:HH22	1.52	0.58
1:A:183:ARG:NH1	3:A:534:HOH:O	2.35	0.58
1:C:16:GLU:HG2	3:C:512:HOH:O	2.00	0.58
1:A:303:LYS:HD2	3:A:502:HOH:O	2.03	0.58
1:A:28:PHE:O	1:A:31:ILE:HB	2.03	0.58
1:B:32:ASN:HD22	1:B:35:ARG:NH2	2.02	0.58
1:A:330:SER:HB3	1:A:400:ILE:HG13	1.84	0.58
1:B:207:GLN:HG3	3:B:519:HOH:O	2.04	0.58
1:B:56:ASP:HB3	1:C:278:ASN:O	2.04	0.57
1:B:106:ILE:HG23	1:B:412:LEU:HD13	1.85	0.57
1:B:9:GLN:OE1	1:B:188:ASN:ND2	2.38	0.57
1:B:156:ASN:OD1	1:C:358:MET:CE	2.53	0.57
1:A:156:ASN:HD22	1:B:367:ARG:HH12	1.49	0.57
1:B:156:ASN:CG	1:C:358:MET:HE1	2.24	0.57
1:C:127:GLN:HG2	3:C:569:HOH:O	2.05	0.57
1:C:120:ILE:HG22	3:C:578:HOH:O	2.05	0.57
1:A:97:THR:HG22	1:A:225:GLN:HE22	1.70	0.56
1:A:183:ARG:NH1	1:A:189:TYR:HB2	2.20	0.56
1:A:219:ARG:HG3	1:A:219:ARG:HH11	1.71	0.56
1:B:156:ASN:ND2	1:C:367:ARG:HH12	2.01	0.56
1:B:28:PHE:O	1:B:31:ILE:HB	2.06	0.56
1:A:195:ALA:HB2	1:A:423:VAL:HG23	1.88	0.55
1:A:232:LEU:O	1:A:236:GLN:HG3	2.06	0.55
1:C:118:ASN:HD21	1:C:388:ASN:ND2	2.04	0.55
1:A:44:LEU:HD13	1:A:69:LEU:HD23	1.89	0.55
1:A:53:GLY:HA2	1:B:280:GLY:O	2.07	0.55
1:A:60:ILE:C	1:A:61:ASN:HD22	2.10	0.54
1:C:130:LYS:HD3	3:C:531:HOH:O	2.07	0.54
1:A:339:SER:HB3	1:C:169:LEU:HG	1.89	0.54
1:A:367:ARG:HH12	1:C:156:ASN:ND2	2.03	0.54
1:A:298:VAL:O	1:A:299:ASN:CB	2.50	0.54
1:C:16:GLU:HG3	3:C:512:HOH:O	2.05	0.54
1:B:93:ILE:HD13	3:B:542:HOH:O	2.06	0.54
1:A:220:ASN:ND2	1:A:323:VAL:HG11	2.22	0.54
1:B:409:GLU:HG2	3:B:501:HOH:O	2.08	0.54
1:A:220:ASN:O	1:A:223:LEU:HD12	2.08	0.54
1:A:11:ARG:HG2	3:A:548:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:MET:HA	1:B:358:MET:HE2	1.89	0.53
1:B:258:ASP:O	1:B:259:THR:OG1	2.20	0.53
1:B:156:ASN:OD1	1:C:358:MET:HE1	2.09	0.53
1:A:310:VAL:O	1:A:314:GLU:HG2	2.09	0.53
1:B:423:VAL:CB	3:B:479:HOH:O	2.20	0.52
1:C:32:ASN:ND2	1:C:35:ARG:HH22	2.06	0.52
1:C:189:TYR:HE2	3:C:555:HOH:O	1.91	0.52
1:C:323:VAL:O	1:C:327:VAL:CG1	2.57	0.52
1:A:346:GLN:HE21	1:A:346:GLN:HA	1.75	0.52
1:B:397:GLN:HA	1:B:397:GLN:HE21	1.73	0.52
1:A:315:GLN:NE2	1:C:19:LYS:HE2	2.25	0.52
1:B:169:LEU:CG	1:C:339:SER:HB3	2.36	0.51
1:A:334:ILE:HG12	1:A:396:ASN:HB3	1.92	0.51
1:C:266:THR:HA	3:C:533:HOH:O	2.11	0.51
1:B:358:MET:HE2	1:B:367:ARG:HG3	1.93	0.50
1:A:169:LEU:CD1	1:B:339:SER:HB3	2.42	0.50
1:B:103:GLN:HE21	1:B:407:LEU:H	1.58	0.50
1:B:59:GLY:CA	3:B:539:HOH:O	2.47	0.50
1:B:54:TYR:HD2	1:B:55:ARG:HB3	1.77	0.50
1:B:290:LEU:HD13	1:B:292:ILE:HG13	1.94	0.50
1:C:374:ASP:OD2	2:C:472:NCO:N2	2.45	0.49
1:B:151:ILE:O	1:B:155:GLN:HG3	2.12	0.49
1:B:220:ASN:ND2	1:B:223:LEU:H	2.10	0.49
1:C:220:ASN:ND2	1:C:323:VAL:HG11	2.27	0.49
1:A:19:LYS:HE2	1:B:315:GLN:NE2	2.27	0.49
1:B:358:MET:SD	1:B:367:ARG:HD2	2.53	0.49
1:A:56:ASP:OD1	1:A:56:ASP:O	2.30	0.49
1:C:421:LYS:HB2	3:C:517:HOH:O	2.11	0.49
1:A:258:ASP:O	1:A:259:THR:OG1	2.22	0.49
1:C:397:GLN:NE2	1:C:397:GLN:HA	2.20	0.49
1:B:42:LEU:O	1:C:291:PRO:O	2.30	0.49
1:C:398:LEU:HD11	1:C:415:LEU:HD11	1.95	0.49
1:C:183:ARG:NH1	1:C:189:TYR:HB2	2.27	0.49
1:A:410:GLN:NE2	1:A:410:GLN:HA	2.28	0.49
1:B:113:TYR:CE2	1:B:193:LEU:HD22	2.48	0.49
1:B:6:VAL:HG22	1:B:190:TYR:CZ	2.48	0.48
1:A:299:ASN:H	1:A:302:VAL:HG23	1.77	0.48
1:B:328:ARG:HH11	1:B:328:ARG:CG	2.24	0.48
1:A:265:LYS:CG	1:A:265:LYS:O	2.60	0.48
1:A:306:GLN:O	1:A:309:PHE:HB3	2.13	0.48
1:A:134:TYR:HB2	1:A:161:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:MET:SD	1:C:371:ASP:HB3	2.53	0.48
1:C:125:TYR:CE1	3:C:500:HOH:O	2.65	0.48
1:A:183:ARG:CZ	3:A:534:HOH:O	2.61	0.48
1:B:170:THR:HG22	3:C:485:HOH:O	2.14	0.48
1:B:4:MET:SD	1:B:412:LEU:HD23	2.54	0.48
3:A:486:HOH:O	1:C:169:LEU:HD12	2.13	0.48
1:A:29:GLU:OE1	1:B:300:SER:HB2	2.13	0.48
1:A:95:ASP:HB3	3:A:499:HOH:O	2.13	0.47
1:C:205:LYS:HA	1:C:205:LYS:HD3	1.75	0.47
1:B:48:TYR:O	1:B:48:TYR:CD1	2.55	0.47
1:A:169:LEU:HG	1:B:339:SER:HB3	1.97	0.47
1:A:294:GLN:NE2	3:A:568:HOH:O	2.47	0.47
1:A:161:TYR:O	1:A:164:VAL:HG12	2.14	0.47
1:B:47:ASP:HB3	3:B:524:HOH:O	2.14	0.47
1:B:103:GLN:NE2	1:B:407:LEU:H	2.13	0.47
1:A:64:ALA:HB1	3:A:514:HOH:O	2.14	0.47
1:B:41:GLN:HB2	1:B:72:THR:OG1	2.13	0.47
1:B:199:GLU:H	1:B:199:GLU:HG2	1.46	0.47
1:B:401:LYS:HG3	1:B:411:ASP:OD2	2.14	0.47
1:A:30:LYS:HE2	1:B:304:GLN:OE1	2.15	0.47
1:C:130:LYS:HE2	1:C:130:LYS:HB3	1.55	0.47
1:A:224:LEU:HD13	1:A:227:ARG:HH21	1.79	0.47
1:A:334:ILE:O	1:A:338:ILE:HD12	2.15	0.47
1:C:180:GLU:HA	1:C:180:GLU:OE1	2.15	0.47
1:A:153:ASP:HA	1:A:369:ILE:HG21	1.96	0.46
1:A:60:ILE:HD13	1:A:61:ASN:N	2.30	0.46
1:A:158:ARG:HE	1:A:158:ARG:HB2	1.54	0.46
1:C:51:SER:HB2	3:C:515:HOH:O	2.15	0.46
1:A:421:LYS:HB3	3:A:476:HOH:O	2.15	0.46
1:C:319:ALA:HA	3:C:579:HOH:O	2.15	0.46
1:A:227:ARG:NH1	3:A:550:HOH:O	2.24	0.46
1:C:320:HIS:HB2	3:C:479:HOH:O	2.15	0.46
1:B:156:ASN:OD1	1:C:358:MET:HE3	2.15	0.45
1:C:270:ALA:HB1	1:C:274:TYR:CD2	2.52	0.45
1:C:77:ASP:HA	3:C:559:HOH:O	2.15	0.45
1:B:283:LYS:O	1:B:284:VAL:HG13	2.16	0.45
1:C:24:ARG:HB3	1:C:24:ARG:HE	1.46	0.45
1:A:291:PRO:O	1:C:42:LEU:O	2.35	0.45
1:C:163:THR:HG23	3:C:492:HOH:O	2.15	0.45
1:C:165:LEU:O	1:C:169:LEU:HD22	2.17	0.45
1:B:358:MET:SD	1:B:371:ASP:HB3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:CZ	3:A:546:HOH:O	2.65	0.45
1:C:186:THR:CG2	1:C:188:ASN:H	2.29	0.45
1:C:170:THR:HG21	3:C:502:HOH:O	2.17	0.45
1:B:140:THR:HG22	1:B:154:VAL:HG22	1.99	0.45
1:B:7:TYR:CE1	1:B:106:ILE:HG13	2.52	0.45
1:B:421:LYS:HG2	3:B:490:HOH:O	2.17	0.45
1:B:265:LYS:O	1:B:265:LYS:CG	2.65	0.45
1:B:85:THR:HG22	1:B:89:LYS:HD2	1.99	0.44
1:A:234:ARG:CD	3:A:546:HOH:O	2.65	0.44
1:B:234:ARG:NE	3:B:541:HOH:O	2.48	0.44
3:A:496:HOH:O	1:B:297:MET:HG3	2.17	0.44
1:A:276:ASP:OD1	3:A:485:HOH:O	2.21	0.44
1:C:373:LEU:O	1:C:376:THR:HB	2.18	0.44
1:A:246:PRO:HA	1:A:289:SER:O	2.17	0.44
1:C:106:ILE:HG23	1:C:412:LEU:HD13	1.99	0.44
1:B:289:SER:CB	3:B:515:HOH:O	2.57	0.44
1:C:374:ASP:OD1	3:C:495:HOH:O	2.21	0.44
1:B:267:ARG:NH1	3:B:529:HOH:O	2.48	0.44
1:B:118:ASN:HD21	1:B:388:ASN:HD22	1.65	0.44
1:A:60:ILE:HD13	1:A:60:ILE:C	2.38	0.44
1:B:57:ALA:O	1:B:60:ILE:HG22	2.18	0.44
1:A:315:GLN:HE21	1:C:19:LYS:HE2	1.82	0.44
1:A:118:ASN:HD21	1:A:388:ASN:ND2	2.16	0.43
1:B:310:VAL:O	1:B:314:GLU:HG2	2.18	0.43
1:C:55:ARG:CG	1:C:55:ARG:O	2.66	0.43
1:B:220:ASN:HD22	1:B:223:LEU:H	1.67	0.43
1:B:401:LYS:HA	1:B:401:LYS:HD2	1.52	0.43
1:C:334:ILE:HG13	1:C:396:ASN:HB3	1.99	0.43
1:A:317:GLU:O	1:A:321:ARG:HG3	2.18	0.43
1:B:246:PRO:HA	1:B:289:SER:O	2.18	0.43
1:B:107:LEU:HD11	1:B:399:ASN:ND2	2.34	0.43
1:C:55:ARG:HG3	1:C:55:ARG:O	2.19	0.43
1:A:288:PHE:HE1	3:C:526:HOH:O	2.02	0.43
1:C:151:ILE:HG13	1:C:155:GLN:NE2	2.33	0.43
1:C:161:TYR:HA	1:C:164:VAL:HG12	2.01	0.43
1:C:192:GLU:OE1	1:C:422:PRO:HB3	2.19	0.43
1:C:306:GLN:HG2	3:C:556:HOH:O	2.18	0.42
1:B:14:ASN:HA	1:B:15:PRO:HD3	1.80	0.42
1:A:186:THR:HG22	1:A:188:ASN:N	2.20	0.42
1:C:186:THR:HG22	1:C:188:ASN:H	1.84	0.42
1:B:44:LEU:HG	3:B:558:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ASN:HD21	1:C:222:SER:HB2	1.84	0.42
1:B:120:ILE:O	1:B:124:SER:HB2	2.19	0.42
1:A:381:ASN:HB3	3:A:475:HOH:O	2.19	0.42
1:C:142:GLN:HB3	3:C:474:HOH:O	2.19	0.42
1:B:423:VAL:CG1	3:B:479:HOH:O	2.62	0.42
1:B:219:ARG:HD2	1:B:406:THR:CG2	2.48	0.42
1:B:358:MET:HE1	1:B:367:ARG:HH11	1.85	0.42
1:A:318:SER:OG	1:C:15:PRO:HB2	2.20	0.42
1:A:250:LEU:HG	3:A:527:HOH:O	2.19	0.42
1:C:61:ASN:N	1:C:61:ASN:HD22	2.15	0.42
1:A:110:ALA:HB3	1:A:398:LEU:HD23	2.01	0.42
1:B:115:ASN:HA	1:B:115:ASN:HD22	1.62	0.41
1:C:66:SER:CB	3:C:534:HOH:O	2.63	0.41
1:A:60:ILE:HD11	1:A:261:TYR:CE2	2.54	0.41
3:A:554:HOH:O	1:C:152:THR:HB	2.19	0.41
1:B:186:THR:HG22	1:B:188:ASN:N	2.32	0.41
1:B:417:ASN:ND2	3:B:567:HOH:O	2.52	0.41
1:B:41:GLN:O	1:B:71:LEU:HA	2.20	0.41
1:B:11:ARG:HB3	1:B:11:ARG:HE	1.82	0.41
1:C:316:LEU:HD13	3:C:537:HOH:O	2.20	0.41
1:C:354:SER:O	1:C:358:MET:HG2	2.21	0.41
1:B:197:ASN:C	1:B:197:ASN:HD22	2.23	0.41
1:B:55:ARG:O	1:C:278:ASN:O	2.39	0.41
1:A:60:ILE:CD1	1:A:261:TYR:HD2	2.22	0.40
1:B:220:ASN:ND2	1:B:323:VAL:HG11	2.36	0.40
1:A:169:LEU:HA	1:A:169:LEU:HD13	1.90	0.40
1:A:420:SER:OG	1:A:421:LYS:N	2.54	0.40
1:C:358:MET:HE2	1:C:367:ARG:HG3	2.03	0.40
1:A:346:GLN:CA	1:A:346:GLN:NE2	2.79	0.40
1:B:319:ALA:O	1:B:323:VAL:HG13	2.21	0.40
1:B:113:TYR:HE2	1:B:193:LEU:HD22	1.86	0.40
1:A:183:ARG:NH2	3:A:534:HOH:O	2.54	0.40
1:B:307:TYR:HA	1:B:310:VAL:HG13	2.02	0.40
1:C:334:ILE:HD11	1:C:396:ASN:O	2.21	0.40
1:B:426:ASN:ND2	3:B:553:HOH:O	2.54	0.40
1:A:258:ASP:O	1:A:259:THR:CB	2.69	0.40
1:B:146:VAL:CG1	1:B:148:LEU:HD12	2.51	0.40
1:A:344:TYR:CE2	1:A:385:GLU:HG3	2.57	0.40
1:C:246:PRO:HA	1:C:289:SER:O	2.22	0.40
1:C:279:MET:HG2	1:C:279:MET:H	1.77	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:CD1	3:B:535:HOH:O[9_654]	1.38	0.82
3:A:472:HOH:O	3:C:475:HOH:O[5_545]	1.47	0.73
3:B:483:HOH:O	3:B:484:HOH:O[5_545]	1.51	0.69
3:A:558:HOH:O	3:C:564:HOH:O[5_545]	1.55	0.65
1:B:148:LEU:CG	3:B:535:HOH:O[9_654]	1.96	0.24
1:B:142:GLN:NE2	3:B:534:HOH:O[9_654]	2.17	0.03

## 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	426/471 (90%)	402 (94%)	16 (4%)	8 (2%)	10	28
1	B	426/471 (90%)	397 (93%)	22 (5%)	7 (2%)	12	34
1	C	426/471 (90%)	400 (94%)	19 (4%)	7 (2%)	12	34
All	All	1278/1413 (90%)	1199 (94%)	57 (4%)	22 (2%)	11	32

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	ASP
1	A	299	ASN
1	B	258	ASP
1	B	299	ASN
1	C	299	ASN
1	A	259	THR
1	A	268	GLY
1	A	275	ASP
1	B	55	ARG
1	B	268	GLY
1	C	55	ARG
1	C	258	ASP

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Mol	Chain	Res	Type
1	C	268	GLY
1	A	55	ARG
1	A	420	SER
1	B	259	THR
1	C	259	THR
1	C	420	SER
1	A	46	ALA
1	C	275	ASP
1	B	46	ALA
1	B	275	ASP

### 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	358/393 (91%)	283 (79%)	75 (21%)	1	3
1	B	358/393 (91%)	287 (80%)	71 (20%)	1	4
1	C	358/393 (91%)	287 (80%)	71 (20%)	1	4
All	All	1074/1179 (91%)	857 (80%)	217 (20%)	1	4

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	2	ASN
1	A	4	MET
1	A	9	GLN
1	A	11	ARG
1	A	12	LEU
1	A	17	LEU
1	A	20	SER
1	A	24	ARG
1	A	47	ASP
1	A	49	THR
1	A	51	SER

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Mol	Chain	Res	Type
1	A	55	ARG
1	A	60	ILE
1	A	62	SER
1	A	63	ASN
1	A	65	THR
1	A	66	SER
1	A	74	SER
1	A	78	MET
1	A	79	SER
1	A	82	ARG
1	A	86	LEU
1	A	94	GLN
1	A	97	THR
1	A	139	GLN
1	A	142	GLN
1	A	151	ILE
1	A	158	ARG
1	A	182	LEU
1	A	183	ARG
1	A	186	THR
1	A	197	ASN
1	A	198	VAL
1	A	199	GLU
1	A	200	ASN
1	A	202	LYS
1	A	214	LYS
1	A	217	GLU
1	A	222	SER
1	A	223	LEU
1	A	227	ARG
1	A	231	ASP
1	A	234	ARG
1	A	247	THR
1	A	248	LEU
1	A	251	THR
1	A	254	THR
1	A	256	ILE
1	A	257	SER
1	A	259	THR
1	A	260	SER
1	A	264	SER
1	A	265	LYS

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Mol	Chain	Res	Type
1	A	266	THR
1	A	267	ARG
1	A	273	GLN
1	A	277	SER
1	A	283	LYS
1	A	284	VAL
1	A	287	SER
1	A	289	SER
1	A	290	LEU
1	A	300	SER
1	A	310	VAL
1	A	316	LEU
1	A	327	VAL
1	A	334	ILE
1	A	339	SER
1	A	400	ILE
1	A	407	LEU
1	A	412	LEU
1	A	420	SER
1	A	421	LYS
1	A	424	SER
1	B	4	MET
1	B	8	GLN
1	B	11	ARG
1	B	17	LEU
1	B	19	LYS
1	B	24	ARG
1	B	28	PHE
1	B	47	ASP
1	B	48	TYR
1	B	60	ILE
1	B	61	ASN
1	B	62	SER
1	B	65	THR
1	B	66	SER
1	B	72	THR
1	B	74	SER
1	B	82	ARG
1	B	84	LEU
1	B	103	GLN
1	B	108	ASN
1	B	124	SER

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Mol	Chain	Res	Type
1	B	139	GLN
1	B	142	GLN
1	B	146	VAL
1	B	152	THR
1	B	169	LEU
1	B	170	THR
1	B	179	VAL
1	B	186	THR
1	B	197	ASN
1	B	199	GLU
1	B	214	LYS
1	B	217	GLU
1	B	219	ARG
1	B	222	SER
1	B	223	LEU
1	B	229	SER
1	B	247	THR
1	B	251	THR
1	B	253	SER
1	B	259	THR
1	B	264	SER
1	B	267	ARG
1	B	272	THR
1	B	273	GLN
1	B	277	SER
1	B	278	ASN
1	B	279	MET
1	B	289	SER
1	B	290	LEU
1	B	292	ILE
1	B	300	SER
1	B	306	GLN
1	B	310	VAL
1	B	316	LEU
1	B	318	SER
1	B	322	SER
1	B	328	ARG
1	B	339	SER
1	B	340	SER
1	B	353	SER
1	B	359	GLU
1	B	395	ILE

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Mol	Chain	Res	Type
1	B	397	GLN
1	B	398	LEU
1	B	401	LYS
1	B	407	LEU
1	B	409	GLU
1	B	410	GLN
1	B	412	LEU
1	B	421	LYS
1	C	1	GLU
1	C	4	MET
1	C	11	ARG
1	C	17	LEU
1	C	19	LYS
1	C	24	ARG
1	C	47	ASP
1	C	49	THR
1	C	51	SER
1	C	55	ARG
1	C	60	ILE
1	C	61	ASN
1	C	62	SER
1	C	66	SER
1	C	68	SER
1	C	72	THR
1	C	80	LYS
1	C	82	ARG
1	C	97	THR
1	C	115	ASN
1	C	124	SER
1	C	130	LYS
1	C	142	GLN
1	C	146	VAL
1	C	152	THR
1	C	155	GLN
1	C	169	LEU
1	C	170	THR
1	C	182	LEU
1	C	186	THR
1	C	197	ASN
1	C	199	GLU
1	C	202	LYS
1	C	205	LYS

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Mol	Chain	Res	Type
1	C	209	VAL
1	C	214	LYS
1	C	217	GLU
1	C	219	ARG
1	C	223	LEU
1	C	247	THR
1	C	248	LEU
1	C	251	THR
1	C	253	SER
1	C	259	THR
1	C	262	SER
1	C	265	LYS
1	C	266	THR
1	C	267	ARG
1	C	273	GLN
1	C	277	SER
1	C	287	SER
1	C	289	SER
1	C	290	LEU
1	C	291	PRO
1	C	297	MET
1	C	303	LYS
1	C	316	LEU
1	C	323	VAL
1	C	327	VAL
1	C	337	SER
1	C	340	SER
1	C	353	SER
1	C	392	ASN
1	C	397	GLN
1	C	398	LEU
1	C	407	LEU
1	C	409	GLU
1	C	410	GLN
1	C	413	LEU
1	C	424	SER
1	C	428	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN

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Mol	Chain	Res	Type
1	A	41	GLN
1	A	61	ASN
1	A	63	ASN
1	A	103	GLN
1	A	108	ASN
1	A	115	ASN
1	A	127	GLN
1	A	139	GLN
1	A	155	GLN
1	A	156	ASN
1	A	174	ASN
1	A	197	ASN
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	332	ASN
1	A	346	GLN
1	A	381	ASN
1	A	388	ASN
1	A	392	ASN
1	A	399	ASN
1	A	410	GLN
1	B	8	GLN
1	B	9	GLN
1	B	32	ASN
1	B	41	GLN
1	B	52	ASN
1	B	103	GLN
1	B	108	ASN
1	B	115	ASN
1	B	127	GLN
1	B	155	GLN
1	B	156	ASN
1	B	160	GLN
1	B	174	ASN
1	B	188	ASN
1	B	197	ASN
1	B	200	ASN
1	B	207	GLN

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Mol	Chain	Res	Type
1	B	220	ASN
1	B	225	GLN
1	B	236	GLN
1	B	301	GLN
1	B	315	GLN
1	B	332	ASN
1	B	342	ASN
1	B	346	GLN
1	B	381	ASN
1	B	388	ASN
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	52	ASN
1	C	61	ASN
1	C	108	ASN
1	C	127	GLN
1	C	139	GLN
1	C	155	GLN
1	C	156	ASN
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	301	GLN
1	C	332	ASN
1	C	342	ASN
1	C	381	ASN
1	C	388	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 [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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NCO	C	472	-	6,6,6	0.63	0	0,15,15	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NCO	C	472	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	472	NCO	1	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	428/471 (90%)	0.31	21 (4%) 33 26	15, 50, 72, 83	0
1	B	428/471 (90%)	0.44	25 (5%) 26 20	13, 50, 72, 85	0
1	C	428/471 (90%)	0.49	33 (7%) 16 11	14, 50, 72, 82	0
All	All	1284/1413 (90%)	0.41	79 (6%) 24 18	13, 50, 72, 85	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	268	GLY	10.4
1	C	269	ALA	8.9
1	C	271	GLY	8.4
1	C	272	THR	7.8
1	C	270	ALA	7.5
1	B	270	ALA	6.2
1	A	269	ALA	6.1
1	B	268	GLY	6.0
1	B	272	THR	5.7
1	B	59	GLY	5.6
1	C	273	GLN	5.5
1	B	269	ALA	5.2
1	B	264	SER	4.9
1	C	263	GLY	4.9
1	A	267	ARG	4.8
1	C	274	TYR	4.7
1	B	273	GLN	4.6
1	B	267	ARG	4.4
1	B	271	GLY	4.2
1	C	69	LEU	4.1
1	C	275	ASP	4.0
1	B	292	ILE	3.7
1	A	44	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	268	GLY	3.6
1	A	48	TYR	3.6
1	B	274	TYR	3.6
1	A	55	ARG	3.6
1	C	266	THR	3.5
1	A	428	GLU	3.4
1	B	263	GLY	3.4
1	C	45	GLY	3.4
1	C	48	TYR	3.3
1	C	254	THR	3.3
1	B	54	TYR	3.2
1	C	278	ASN	3.2
1	B	260	SER	3.2
1	C	256	ILE	3.2
1	B	280	GLY	3.2
1	C	255	GLY	3.2
1	B	255	GLY	3.1
1	C	60	ILE	3.1
1	C	277	SER	3.1
1	A	256	ILE	3.1
1	A	263	GLY	3.0
1	A	200	ASN	3.0
1	B	275	ASP	3.0
1	C	280	GLY	2.9
1	C	279	MET	2.9
1	C	44	LEU	2.9
1	B	43	GLY	2.9
1	C	428	GLU	2.8
1	C	295	GLY	2.6
1	A	202	LYS	2.6
1	A	50	TYR	2.6
1	A	254	THR	2.6
1	C	267	ARG	2.6
1	C	284	VAL	2.6
1	C	148	LEU	2.5
1	B	72	THR	2.4
1	A	280	GLY	2.4
1	C	261	TYR	2.4
1	A	78	MET	2.4
1	C	54	TYR	2.4
1	A	264	SER	2.3
1	C	282	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	285	GLY	2.2
1	C	68	SER	2.2
1	A	272	THR	2.2
1	B	42	LEU	2.2
1	B	428	GLU	2.2
1	C	75	ILE	2.1
1	A	169	LEU	2.1
1	B	251	THR	2.1
1	B	262	SER	2.1
1	B	45	GLY	2.1
1	A	60	ILE	2.0
1	A	255	GLY	2.0
1	B	55	ARG	2.0
1	A	69	LEU	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NCO	C	472	7/7	0.98	0.23	0.51	25,27,28,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.