



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:18 am GMT

PDB ID : 1OVM  
Title : Crystal structure of Indolepyruvate decarboxylase from *Enterobacter cloacae*  
Authors : Schutz, A.; Sandalova, T.; Ricagno, S.; Hubner, G.; Konig, S.; Schneider, G.  
Deposited on : 2003-03-27  
Resolution : 2.65 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

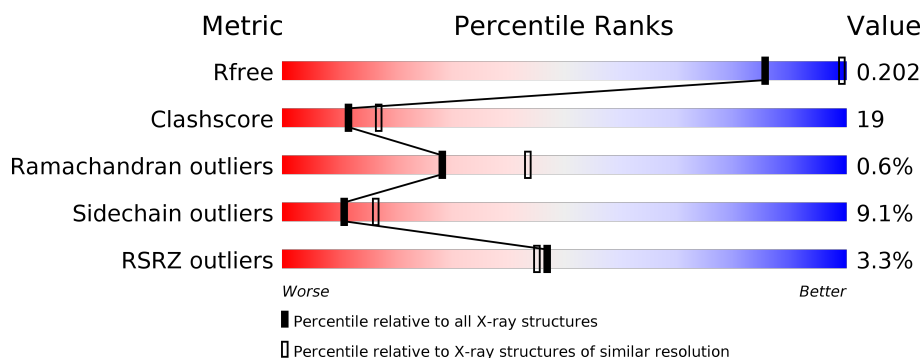
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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	552	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>5%</div> </div> </div>
1	B	552	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>28%</div> <div>5%</div> </div> </div>
1	C	552	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>29%</div> <div>5%</div> </div> </div>
1	D	552	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>5%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	D	601	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16859 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.

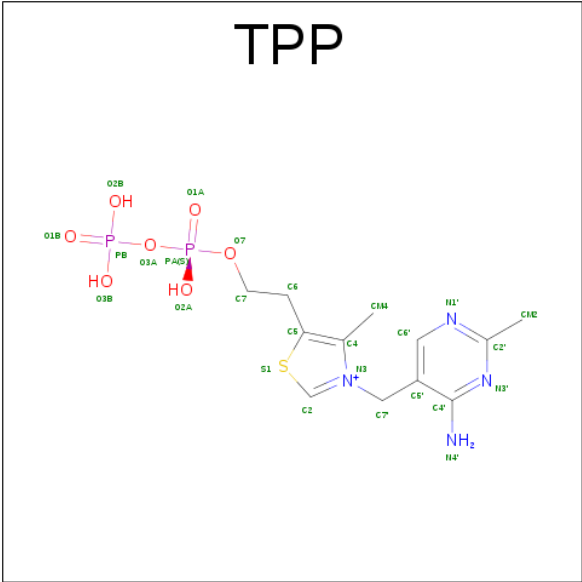
- Molecule 1 is a protein called Indole-3-pyruvate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4101	2596	718	764	23			
1	B	535	Total	C	N	O	S	0	0	0
			4101	2596	718	764	23			
1	C	535	Total	C	N	O	S	0	0	0
			4101	2596	718	764	23			
1	D	535	Total	C	N	O	S	0	0	0
			4101	2596	718	764	23			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

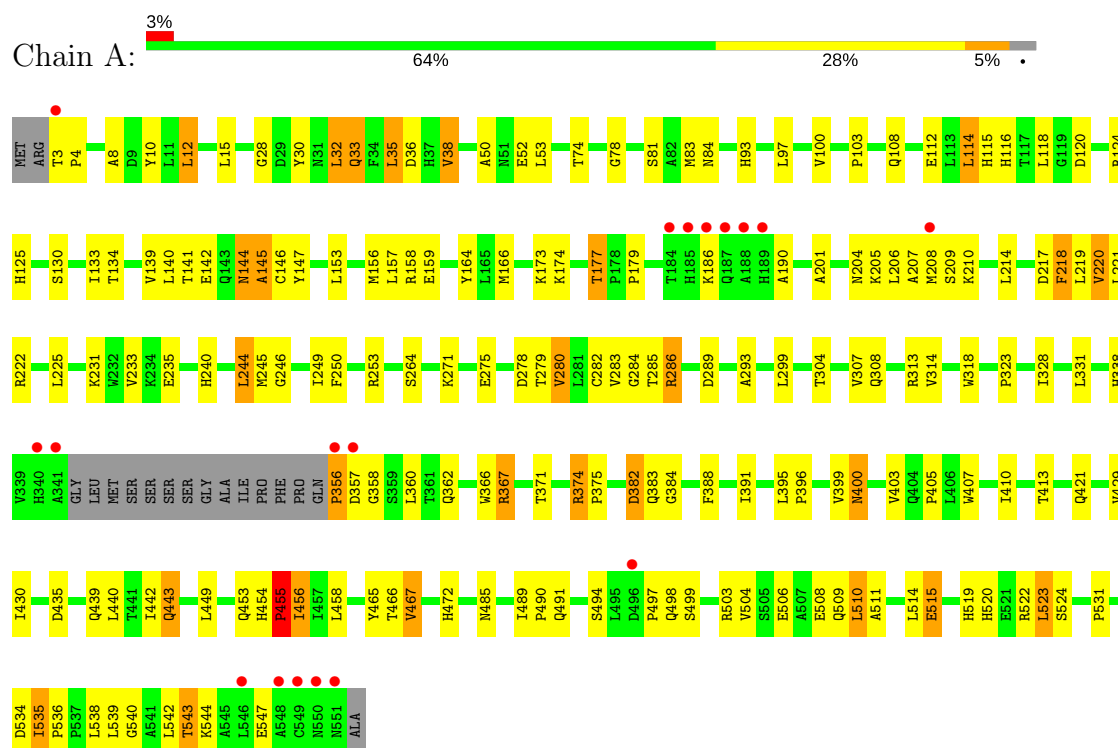
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	96	Total	O	0	0
			96	96		
4	C	86	Total	O	0	0
			86	86		
4	D	62	Total	O	0	0
			62	62		

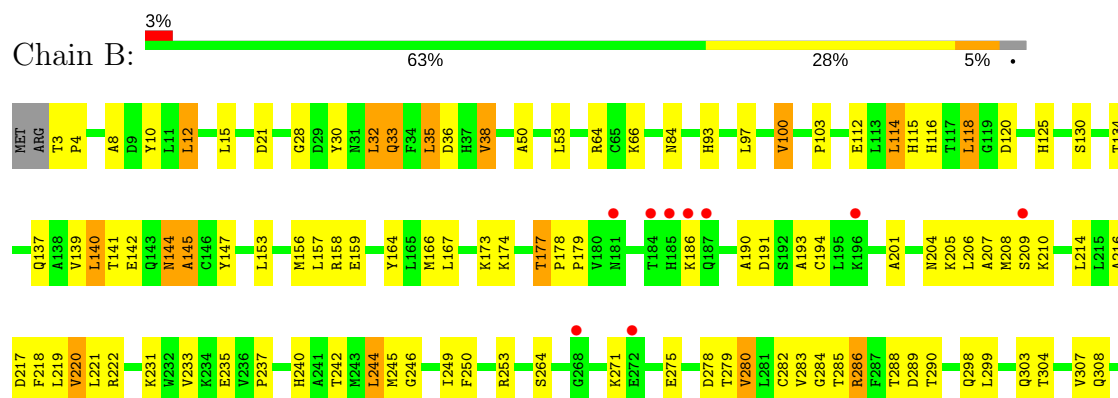
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

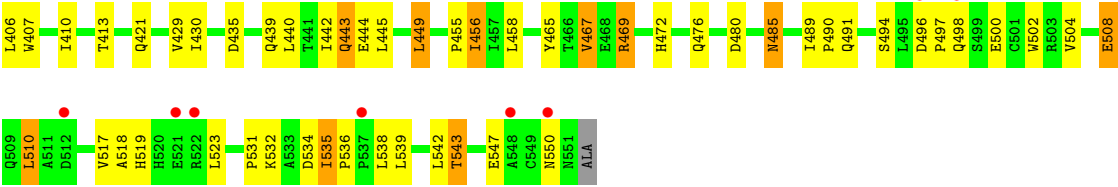
#### • Molecule 1: Indole-3-pyruvate decarboxylase



#### • Molecule 1: Indole-3-pyruvate decarboxylase









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.20Å 151.62Å 107.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.56 – 2.65 29.56 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.56-2.65) 100.0 (29.56-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.90 (at 2.64Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.236 0.208 , 0.202	Depositor DCC
$R_{free}$ test set	3198 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TPP

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	0.40	0/4194	0.64	1/5711 (0.0%)
1	B	0.40	0/4194	0.66	1/5711 (0.0%)
1	C	0.42	0/4194	0.65	1/5711 (0.0%)
1	D	0.41	0/4194	0.64	2/5711 (0.0%)
All	All	0.41	0/16776	0.65	5/22844 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	455	PRO	CA-N-CD	-11.09	95.98	111.50
1	C	396	PRO	CA-N-CD	-7.22	101.39	111.50
1	D	469	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	A	455	PRO	CA-N-CD	-6.09	102.97	111.50
1	D	469	ARG	NE-CZ-NH2	5.55	123.07	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4101	0	4037	159	0
1	B	4101	0	4037	151	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4101	0	4037	176	0
1	D	4101	0	4037	169	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	16	2	0
3	B	26	0	16	1	0
3	C	26	0	16	1	0
3	D	26	0	16	1	0
4	A	103	0	0	10	0
4	B	96	0	0	7	0
4	C	86	0	0	5	0
4	D	62	0	0	8	0
All	All	16859	0	16212	634	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 19.

All (634) 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:D:141:THR:H	1:D:144:ASN:HD21	1.02	0.99
1:A:141:THR:H	1:A:144:ASN:HD21	1.07	0.98
1:D:282:CYS:HB3	1:D:285:THR:HG21	1.48	0.96
1:C:141:THR:H	1:C:144:ASN:HD21	1.15	0.94
1:B:282:CYS:HB3	1:B:285:THR:HG21	1.49	0.93
1:C:205:LYS:HE2	1:C:279:THR:HG22	1.50	0.93
1:A:535:ILE:HG13	1:A:539:LEU:HD23	1.52	0.92
1:A:144:ASN:HD22	1:A:145:ALA:N	1.68	0.92
1:C:210:LYS:HE2	1:C:210:LYS:HA	1.50	0.90
1:C:282:CYS:HB3	1:C:285:THR:HG21	1.53	0.90
1:B:210:LYS:HA	1:B:210:LYS:HE2	1.53	0.90
1:A:210:LYS:HA	1:A:210:LYS:HE2	1.53	0.90
1:B:144:ASN:HD22	1:B:145:ALA:N	1.71	0.89
1:B:535:ILE:HG13	1:B:539:LEU:HD23	1.51	0.89
1:B:141:THR:H	1:B:144:ASN:HD21	1.20	0.89
1:D:141:THR:H	1:D:144:ASN:ND2	1.71	0.88
1:D:210:LYS:HA	1:D:210:LYS:HE2	1.54	0.88
1:D:535:ILE:HG13	1:D:539:LEU:HD23	1.55	0.88
1:A:282:CYS:HB3	1:A:285:THR:HG21	1.56	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:ILE:HG13	1:C:539:LEU:HD23	1.55	0.87
1:C:511:ALA:O	1:C:515:GLU:HG2	1.75	0.87
1:C:504:VAL:HG13	1:C:509:GLN:HB2	1.54	0.87
1:C:205:LYS:HE2	1:C:279:THR:CG2	2.05	0.86
1:D:449:LEU:HD11	1:D:523:LEU:HD23	1.58	0.85
1:A:141:THR:H	1:A:144:ASN:ND2	1.74	0.84
1:D:201:ALA:HB1	1:D:314:VAL:HG21	1.58	0.84
1:C:141:THR:H	1:C:144:ASN:ND2	1.76	0.83
1:A:201:ALA:HB1	1:A:314:VAL:HG21	1.59	0.82
1:C:201:ALA:HB1	1:C:314:VAL:HG21	1.61	0.82
1:B:201:ALA:HB1	1:B:314:VAL:HG21	1.62	0.82
1:C:144:ASN:HD22	1:C:145:ALA:N	1.79	0.80
1:D:144:ASN:HD22	1:D:145:ALA:N	1.79	0.79
1:B:141:THR:H	1:B:144:ASN:ND2	1.80	0.78
1:D:384:GLY:HA2	1:D:467:VAL:HG11	1.64	0.77
1:C:244:LEU:HD22	1:C:403:VAL:HG11	1.66	0.76
1:A:511:ALA:O	1:A:515:GLU:HG2	1.85	0.76
1:C:384:GLY:HA2	1:C:467:VAL:HG11	1.67	0.76
1:D:97:LEU:HD13	1:D:156:MET:CE	2.15	0.76
1:B:253:ARG:HH21	1:B:396:PRO:HG3	1.51	0.76
1:C:36:ASP:OD2	1:D:472:HIS:HE1	1.69	0.75
1:A:421:GLN:HE21	1:A:455:PRO:HD3	1.51	0.75
1:B:244:LEU:HD22	1:B:403:VAL:HG11	1.68	0.75
1:C:217:ASP:O	1:C:220:VAL:HG13	1.87	0.74
1:D:449:LEU:CD1	1:D:523:LEU:HD23	2.17	0.74
1:A:293:ALA:HA	1:A:542:LEU:HD23	1.67	0.74
1:D:97:LEU:HD13	1:D:156:MET:HE1	1.69	0.74
1:A:205:LYS:HE3	1:A:279:THR:HG22	1.71	0.73
1:D:467:VAL:HG12	1:D:539:LEU:HD21	1.68	0.73
1:B:491:GLN:HA	1:B:497:PRO:HG2	1.71	0.73
1:A:491:GLN:HA	1:A:497:PRO:HG2	1.70	0.72
1:A:36:ASP:OD2	1:B:472:HIS:HE1	1.71	0.72
1:B:207:ALA:HA	1:B:338:HIS:CD2	2.25	0.72
1:C:456:ILE:HD11	1:C:458:LEU:HD11	1.72	0.72
1:C:362:GLN:NE2	1:C:366:TRP:HE1	1.88	0.71
1:D:246:GLY:O	1:D:249:ILE:HG23	1.90	0.71
1:D:205:LYS:HE3	1:D:279:THR:CG2	2.21	0.71
1:D:449:LEU:CD1	1:D:523:LEU:CD2	2.69	0.71
1:D:500:GLU:HB3	1:D:502:TRP:CH2	2.26	0.70
1:B:205:LYS:HE3	1:B:279:THR:CG2	2.21	0.70
1:A:384:GLY:HA2	1:A:467:VAL:HG11	1.72	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:PRO:HA	4:D:609:HOH:O	1.91	0.70
1:B:494:SER:HB3	1:B:497:PRO:HG3	1.74	0.69
1:D:290:THR:HA	1:D:542:LEU:HD11	1.75	0.69
1:C:491:GLN:HA	1:C:497:PRO:HG2	1.73	0.69
1:A:205:LYS:HE3	1:A:279:THR:CG2	2.21	0.69
1:B:144:ASN:HD22	1:B:144:ASN:C	1.96	0.69
1:B:467:VAL:HG12	1:B:539:LEU:HD21	1.74	0.68
1:B:217:ASP:O	1:B:220:VAL:HG13	1.93	0.68
1:C:356:PRO:HG3	1:C:367:ARG:NH1	2.09	0.68
1:A:293:ALA:HA	1:A:542:LEU:CD2	2.24	0.67
1:C:246:GLY:O	1:C:249:ILE:HG23	1.94	0.67
1:D:531:PRO:HB2	1:D:534:ASP:HB2	1.76	0.67
1:D:491:GLN:HA	1:D:497:PRO:HG2	1.77	0.67
1:A:456:ILE:HD11	1:A:458:LEU:HD11	1.74	0.67
1:C:455:PRO:HD2	1:C:523:LEU:HD22	1.75	0.67
1:A:217:ASP:O	1:A:220:VAL:HG13	1.95	0.67
1:B:246:GLY:O	1:B:249:ILE:HG23	1.94	0.67
1:A:246:GLY:O	1:A:249:ILE:HG23	1.94	0.67
1:A:494:SER:HB3	1:A:497:PRO:HG3	1.77	0.67
1:B:290:THR:HA	1:B:542:LEU:HD11	1.77	0.67
1:A:253:ARG:HH21	1:A:396:PRO:HG3	1.60	0.66
1:B:280:VAL:HG13	1:B:304:THR:HG22	1.77	0.66
1:B:384:GLY:HA2	1:B:467:VAL:HG11	1.77	0.66
1:A:531:PRO:HB2	1:A:534:ASP:HB2	1.78	0.66
1:C:290:THR:HA	1:C:542:LEU:HD11	1.77	0.66
1:C:467:VAL:HG12	1:C:539:LEU:HD21	1.77	0.66
1:D:500:GLU:HB3	1:D:502:TRP:CZ3	2.31	0.66
1:A:97:LEU:HD13	1:A:156:MET:CE	2.27	0.65
1:D:226:LYS:HE3	1:D:249:ILE:HA	1.77	0.65
1:A:358:GLY:HA2	1:A:508:GLU:OE2	1.97	0.65
1:D:205:LYS:HE3	1:D:279:THR:HG22	1.78	0.65
1:D:455:PRO:HD2	1:D:523:LEU:HD13	1.77	0.65
1:D:244:LEU:HD22	1:D:403:VAL:HG11	1.79	0.65
1:D:449:LEU:HD13	1:D:523:LEU:HD22	1.78	0.64
1:C:36:ASP:OD2	1:D:472:HIS:CE1	2.49	0.64
1:D:455:PRO:HG2	1:D:523:LEU:CD1	2.26	0.64
1:D:449:LEU:HD13	1:D:523:LEU:CD2	2.27	0.64
1:B:253:ARG:HD2	4:B:690:HOH:O	1.97	0.64
1:C:469:ARG:NH2	1:C:480:ASP:OD1	2.31	0.64
1:A:10:TYR:CE2	1:A:179:PRO:HG3	2.33	0.64
1:D:467:VAL:CG1	1:D:539:LEU:HD21	2.27	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LYS:HE3	1:B:279:THR:HG22	1.81	0.63
1:A:207:ALA:HA	1:A:338:HIS:CD2	2.33	0.63
1:D:141:THR:N	1:D:144:ASN:HD21	1.84	0.63
1:D:253:ARG:HH21	1:D:396:PRO:HG3	1.64	0.63
1:A:28:GLY:O	1:A:32:LEU:HD13	1.98	0.63
1:C:469:ARG:NH1	1:C:532:LYS:HG3	2.13	0.63
1:B:467:VAL:CG1	1:B:539:LEU:HD21	2.29	0.63
1:A:244:LEU:HD22	1:A:403:VAL:HG11	1.81	0.62
1:A:141:THR:N	1:A:144:ASN:HD21	1.89	0.62
1:A:144:ASN:C	1:A:144:ASN:HD22	1.99	0.62
1:A:472:HIS:HE1	1:B:36:ASP:OD2	1.82	0.62
1:D:456:ILE:HD11	1:D:458:LEU:HD11	1.82	0.62
1:A:421:GLN:NE2	1:A:455:PRO:HD3	2.15	0.62
1:A:467:VAL:HG12	1:A:539:LEU:HD21	1.82	0.62
1:C:446:GLY:HA3	4:D:604:HOH:O	2.00	0.62
1:C:472:HIS:HE1	1:D:36:ASP:OD2	1.82	0.61
1:D:217:ASP:O	1:D:220:VAL:HG13	1.99	0.61
1:D:108:GLN:HE22	1:D:166:MET:HE3	1.64	0.61
1:C:115:HIS:HD2	1:D:289:ASP:OD2	1.82	0.61
1:D:382:ASP:CA	1:D:413:THR:HG21	2.30	0.61
1:A:413:THR:HG22	4:A:628:HOH:O	1.99	0.61
1:B:139:VAL:HG13	1:B:166:MET:HE2	1.83	0.61
1:D:469:ARG:NH2	1:D:480:ASP:OD1	2.33	0.61
1:B:531:PRO:HB2	1:B:534:ASP:HB2	1.83	0.61
1:A:210:LYS:CA	1:A:210:LYS:HE2	2.30	0.60
1:D:280:VAL:HG13	1:D:304:THR:HG22	1.81	0.60
1:B:539:LEU:O	1:B:543:THR:HB	2.01	0.60
1:D:494:SER:HB3	1:D:497:PRO:HG3	1.82	0.60
1:A:139:VAL:HG13	1:A:166:MET:HE2	1.83	0.60
1:D:10:TYR:CE2	1:D:179:PRO:HG3	2.37	0.60
1:C:382:ASP:CA	1:C:413:THR:HG21	2.32	0.60
1:D:368:THR:HG21	1:D:510:LEU:HD13	1.83	0.60
1:C:28:GLY:O	1:C:32:LEU:HD13	2.02	0.60
1:C:144:ASN:C	1:C:144:ASN:HD22	2.03	0.60
1:A:52:GLU:HG2	1:A:81:SER:HB2	1.83	0.59
1:D:28:GLY:O	1:D:32:LEU:HD13	2.02	0.59
1:A:35:LEU:O	1:A:38:VAL:HG13	2.03	0.59
1:A:36:ASP:OD2	1:B:472:HIS:CE1	2.55	0.59
1:B:320:THR:OG1	1:D:146:CYS:SG	2.61	0.59
1:A:3:THR:N	1:A:4:PRO:HD3	2.18	0.59
1:B:153:LEU:HD23	1:B:156:MET:HE1	1.83	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:VAL:HG21	1:A:240:HIS:CE1	2.37	0.59
1:C:52:GLU:HG2	1:C:81:SER:HB2	1.84	0.59
1:C:190:ALA:HB2	1:C:323:PRO:HD2	1.85	0.59
1:B:500:GLU:HB3	1:B:502:TRP:CZ3	2.38	0.59
1:B:8:ALA:O	1:B:12:LEU:HD22	2.02	0.59
1:C:139:VAL:HG13	1:C:166:MET:HE2	1.85	0.59
1:D:360:LEU:HD11	1:D:504:VAL:HG12	1.84	0.59
1:D:3:THR:N	1:D:4:PRO:HD3	2.18	0.59
1:B:3:THR:N	1:B:4:PRO:HD3	2.18	0.58
1:D:282:CYS:HB3	1:D:285:THR:CG2	2.29	0.58
1:D:190:ALA:HB2	1:D:323:PRO:HD2	1.83	0.58
1:B:190:ALA:HB2	1:B:323:PRO:HD2	1.85	0.58
1:D:233:VAL:HG21	1:D:240:HIS:CE1	2.37	0.58
1:D:8:ALA:O	1:D:12:LEU:HD22	2.03	0.58
1:A:356:PRO:HB3	4:A:655:HOH:O	2.03	0.58
1:D:469:ARG:NH1	4:D:602:HOH:O	2.36	0.58
1:A:120:ASP:OD2	1:A:125:HIS:HE1	1.86	0.58
1:D:382:ASP:N	1:D:413:THR:HG21	2.19	0.58
1:A:124:ARG:NH2	4:A:693:HOH:O	2.36	0.58
1:C:382:ASP:N	1:C:413:THR:HG21	2.19	0.58
1:B:314:VAL:HG23	1:B:314:VAL:O	2.04	0.58
1:C:313:ARG:HD3	1:C:318:TRP:CE2	2.38	0.58
1:C:244:LEU:HD13	1:C:405:PRO:HG3	1.86	0.58
1:D:93:HIS:O	1:D:222:ARG:HD2	2.03	0.58
1:B:28:GLY:O	1:B:32:LEU:HD13	2.03	0.58
1:A:362:GLN:NE2	1:A:366:TRP:HE1	2.03	0.57
1:C:226:LYS:HE3	1:C:249:ILE:HA	1.85	0.57
1:C:531:PRO:HB2	1:C:534:ASP:HB2	1.86	0.57
1:D:209:SER:HB2	1:D:279:THR:HG21	1.85	0.57
1:D:413:THR:HG22	4:D:618:HOH:O	2.03	0.57
1:A:225:LEU:HD13	1:A:328:ILE:HD12	1.86	0.57
1:A:253:ARG:HG2	1:A:253:ARG:HH11	1.68	0.57
1:B:456:ILE:O	1:B:456:ILE:HG13	2.03	0.57
1:C:233:VAL:HG21	1:C:240:HIS:CE1	2.40	0.57
1:A:367:ARG:NH1	4:A:630:HOH:O	2.37	0.57
1:B:253:ARG:NH2	1:B:396:PRO:HG3	2.17	0.57
1:C:500:GLU:HG3	1:C:522:ARG:NH1	2.19	0.57
1:A:190:ALA:HB2	1:A:323:PRO:HD2	1.87	0.57
1:A:467:VAL:CG1	1:A:539:LEU:HD21	2.35	0.57
1:A:84:ASN:ND2	1:A:407:TRP:HE1	2.02	0.57
1:D:30:TYR:CZ	1:D:103:PRO:HG3	2.40	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HB2	4:B:617:HOH:O	2.03	0.57
1:B:207:ALA:HA	1:B:338:HIS:NE2	2.19	0.57
1:C:97:LEU:HD13	1:C:156:MET:CE	2.34	0.57
1:D:97:LEU:HD13	1:D:156:MET:HE2	1.86	0.57
1:C:539:LEU:O	1:C:543:THR:HB	2.04	0.56
1:C:368:THR:HG21	1:C:510:LEU:CD1	2.35	0.56
1:B:523:LEU:HD13	1:B:524:SER:N	2.20	0.56
1:D:469:ARG:NH1	1:D:532:LYS:HG3	2.21	0.56
1:C:494:SER:HB3	1:C:497:PRO:HG3	1.86	0.56
1:C:467:VAL:CG1	1:C:539:LEU:HD21	2.35	0.56
1:D:362:GLN:NE2	1:D:366:TRP:HE1	2.02	0.56
1:A:97:LEU:HD13	1:A:156:MET:HE1	1.88	0.56
1:A:201:ALA:CB	1:A:314:VAL:HG21	2.32	0.56
1:B:97:LEU:HD13	1:B:156:MET:CE	2.35	0.56
1:C:141:THR:N	1:C:144:ASN:HD21	1.94	0.56
1:B:190:ALA:HB2	1:B:323:PRO:CD	2.36	0.56
1:B:194:CYS:HA	1:D:177:THR:HG21	1.88	0.56
1:B:368:THR:HG21	1:B:510:LEU:HD13	1.88	0.55
1:B:201:ALA:CB	1:B:314:VAL:HG21	2.36	0.55
1:A:539:LEU:O	1:A:543:THR:HB	2.06	0.55
1:C:120:ASP:OD2	1:C:125:HIS:HE1	1.90	0.55
1:D:539:LEU:O	1:D:543:THR:HB	2.06	0.55
1:A:209:SER:HB2	1:A:279:THR:HG21	1.87	0.55
1:C:112:GLU:HB2	1:C:114:LEU:HD13	1.88	0.55
1:C:210:LYS:HE2	1:C:210:LYS:CA	2.31	0.55
1:A:144:ASN:C	1:A:144:ASN:ND2	2.60	0.55
1:B:357:ASP:HA	1:B:507:ALA:HB3	1.88	0.55
1:C:454:HIS:ND1	1:C:522:ARG:HA	2.20	0.55
1:D:190:ALA:HB2	1:D:323:PRO:CD	2.37	0.55
1:A:314:VAL:HG23	1:A:314:VAL:O	2.07	0.54
1:B:371:THR:O	1:B:374:ARG:NH2	2.41	0.54
1:D:280:VAL:HG11	1:D:299:LEU:HD22	1.89	0.54
1:A:97:LEU:HD13	1:A:156:MET:HE2	1.89	0.54
1:B:35:LEU:O	1:B:38:VAL:HG13	2.07	0.54
1:B:466:THR:HG22	4:B:603:HOH:O	2.05	0.54
1:C:253:ARG:NH2	1:C:396:PRO:HD3	2.22	0.54
1:C:440:LEU:HG	1:D:50:ALA:O	2.08	0.54
1:B:210:LYS:CA	1:B:210:LYS:HE2	2.31	0.54
1:C:93:HIS:O	1:C:222:ARG:HD2	2.07	0.54
1:C:84:ASN:ND2	1:C:407:TRP:HE1	2.06	0.54
1:B:421:GLN:HE21	1:B:455:PRO:HD3	1.72	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:VAL:HG11	1:B:299:LEU:HD22	1.88	0.54
1:C:158:ARG:HD2	1:C:159:GLU:OE2	2.07	0.54
1:D:517:VAL:O	1:D:519:HIS:N	2.41	0.54
1:B:388:PHE:CD2	1:B:539:LEU:HD13	2.42	0.54
1:C:30:TYR:CZ	1:C:103:PRO:HG3	2.42	0.54
1:D:245:MET:HG2	1:D:405:PRO:HD2	1.89	0.54
1:A:289:ASP:OD2	1:B:115:HIS:HD2	1.89	0.54
1:C:10:TYR:CE2	1:C:179:PRO:HG3	2.43	0.54
1:D:210:LYS:CA	1:D:210:LYS:HE2	2.32	0.54
1:A:158:ARG:HD2	1:A:159:GLU:OE2	2.08	0.54
1:A:456:ILE:HD11	1:A:458:LEU:CD1	2.37	0.54
1:A:190:ALA:HB2	1:A:323:PRO:CD	2.39	0.53
1:A:245:MET:HG2	1:A:405:PRO:HD2	1.91	0.53
1:C:371:THR:O	1:C:374:ARG:NH2	2.41	0.53
1:D:35:LEU:O	1:D:38:VAL:HG13	2.07	0.53
1:C:289:ASP:OD2	1:D:115:HIS:HD2	1.90	0.53
1:B:158:ARG:HD2	1:B:159:GLU:OE2	2.09	0.53
1:C:362:GLN:HE21	1:C:366:TRP:HE1	1.54	0.53
1:A:465:TYR:HB3	3:A:600:TPP:H62	1.90	0.53
1:C:356:PRO:HG3	1:C:367:ARG:HH12	1.73	0.53
1:C:456:ILE:O	1:C:456:ILE:HG13	2.07	0.53
1:C:50:ALA:O	1:D:440:LEU:HG	2.09	0.53
1:B:282:CYS:HB3	1:B:285:THR:CG2	2.30	0.53
1:B:382:ASP:CA	1:B:413:THR:HG21	2.39	0.53
1:B:144:ASN:ND2	1:B:144:ASN:C	2.61	0.53
1:A:367:ARG:HH11	1:A:367:ARG:HG2	1.74	0.52
1:A:440:LEU:HG	1:B:50:ALA:O	2.09	0.52
1:A:108:GLN:HE22	1:A:166:MET:HE3	1.75	0.52
1:B:233:VAL:HG21	1:B:240:HIS:CE1	2.44	0.52
1:C:97:LEU:HD13	1:C:156:MET:HE2	1.89	0.52
1:C:3:THR:N	1:C:4:PRO:HD3	2.23	0.52
1:C:314:VAL:HG23	1:C:314:VAL:O	2.07	0.52
1:A:50:ALA:O	1:B:440:LEU:HG	2.10	0.52
1:C:465:TYR:HB3	3:C:600:TPP:H62	1.90	0.52
1:D:120:ASP:OD2	1:D:125:HIS:HE1	1.92	0.52
1:D:357:ASP:HB2	1:D:508:GLU:HG3	1.91	0.52
1:A:371:THR:O	1:A:374:ARG:NH2	2.42	0.52
1:B:362:GLN:NE2	1:B:366:TRP:HE1	2.06	0.52
1:C:280:VAL:HG13	1:C:304:THR:HG22	1.92	0.52
1:D:144:ASN:HD22	1:D:144:ASN:C	2.08	0.52
1:C:201:ALA:CB	1:C:314:VAL:HG21	2.37	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:HIS:CE1	1:B:36:ASP:OD2	2.63	0.52
1:C:209:SER:HB2	1:C:279:THR:HG21	1.90	0.52
1:D:201:ALA:CB	1:D:314:VAL:HG21	2.33	0.52
1:A:221:LEU:HD21	1:A:249:ILE:HG22	1.92	0.52
1:B:465:TYR:HB3	3:B:600:TPP:H62	1.91	0.52
1:D:421:GLN:HG2	1:D:429:VAL:HG21	1.91	0.52
1:D:449:LEU:CD1	1:D:523:LEU:HD22	2.38	0.52
1:C:384:GLY:HA2	1:C:467:VAL:CG1	2.40	0.51
1:C:456:ILE:HD11	1:C:458:LEU:CD1	2.40	0.51
1:C:504:VAL:HG12	1:C:505:SER:N	2.25	0.51
1:C:506:GLU:HB2	1:C:509:GLN:HG3	1.93	0.51
1:C:455:PRO:HD2	1:C:523:LEU:CD2	2.38	0.51
1:D:217:ASP:OD2	1:D:245:MET:HB2	2.09	0.51
1:D:368:THR:HG21	1:D:510:LEU:CD1	2.38	0.51
1:C:280:VAL:HG11	1:C:299:LEU:HD22	1.91	0.51
1:D:84:ASN:ND2	1:D:407:TRP:HE1	2.08	0.51
1:A:374:ARG:HG3	1:A:375:PRO:HD2	1.92	0.51
1:B:141:THR:N	1:B:144:ASN:HD21	2.00	0.51
1:C:115:HIS:O	1:C:116:HIS:HB2	2.09	0.51
1:D:21:ASP:OD2	1:D:66:LYS:NZ	2.38	0.51
1:D:465:TYR:HB3	3:D:600:TPP:H62	1.92	0.51
1:D:445:LEU:HD11	1:D:523:LEU:HD21	1.91	0.51
1:C:504:VAL:HG13	1:C:509:GLN:CB	2.34	0.51
1:A:280:VAL:HG11	1:A:299:LEU:HD22	1.92	0.51
1:A:388:PHE:CD2	1:A:539:LEU:HD13	2.46	0.51
1:B:177:THR:HG21	1:D:194:CYS:HA	1.93	0.51
1:D:374:ARG:HG3	1:D:375:PRO:HD2	1.92	0.51
1:D:244:LEU:HD13	1:D:405:PRO:HG3	1.91	0.51
1:B:374:ARG:HG3	1:B:375:PRO:HD2	1.93	0.51
1:C:368:THR:HG21	1:C:510:LEU:HD12	1.93	0.51
1:C:190:ALA:HB2	1:C:323:PRO:CD	2.40	0.51
1:C:421:GLN:HG2	1:C:429:VAL:HG21	1.92	0.51
1:D:382:ASP:HA	1:D:413:THR:HG21	1.92	0.51
1:D:391:ILE:HG21	1:D:538:LEU:HD22	1.93	0.51
1:A:153:LEU:HD23	1:A:156:MET:HE1	1.92	0.51
1:C:8:ALA:O	1:C:12:LEU:HD22	2.11	0.51
1:B:506:GLU:HG2	1:B:509:GLN:OE1	2.10	0.51
1:A:115:HIS:HD2	1:B:289:ASP:OD2	1.94	0.50
1:D:374:ARG:HG3	1:D:375:PRO:CD	2.41	0.50
1:B:209:SER:HB2	1:B:279:THR:HG21	1.93	0.50
1:B:367:ARG:HG2	1:B:367:ARG:HH11	1.76	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:THR:O	1:D:374:ARG:NH2	2.44	0.50
1:A:382:ASP:CA	1:A:413:THR:HG21	2.41	0.50
1:A:456:ILE:HG13	1:A:456:ILE:O	2.12	0.50
1:C:245:MET:HG2	1:C:405:PRO:HD2	1.92	0.50
1:A:97:LEU:HD22	1:A:153:LEU:HD21	1.94	0.50
1:B:21:ASP:OD2	1:B:66:LYS:NZ	2.40	0.50
1:D:264:SER:HA	1:D:271:LYS:HE2	1.94	0.50
1:B:10:TYR:CE2	1:B:179:PRO:HG3	2.47	0.50
1:B:253:ARG:HH11	1:B:253:ARG:HG2	1.76	0.50
1:B:30:TYR:CZ	1:B:103:PRO:HG3	2.47	0.50
1:C:500:GLU:HB3	1:C:502:TRP:CH2	2.47	0.50
1:D:388:PHE:CD2	1:D:539:LEU:HD13	2.46	0.50
1:A:253:ARG:NH2	1:A:396:PRO:HG3	2.26	0.50
1:B:504:VAL:HG13	1:B:509:GLN:HB2	1.94	0.50
1:C:375:PRO:HG3	1:C:396:PRO:HB3	1.94	0.50
1:D:456:ILE:HG13	1:D:456:ILE:O	2.12	0.50
1:B:245:MET:HG2	1:B:405:PRO:HD2	1.93	0.49
1:C:498:GLN:O	1:C:522:ARG:HB2	2.12	0.49
1:B:120:ASP:OD2	1:B:125:HIS:HE1	1.95	0.49
1:B:430:ILE:HD12	1:B:430:ILE:N	2.28	0.49
1:C:253:ARG:HG2	1:C:253:ARG:HH11	1.77	0.49
1:C:253:ARG:HH21	1:C:396:PRO:HG3	1.76	0.49
1:D:253:ARG:HG2	1:D:253:ARG:HH11	1.78	0.49
1:A:286:ARG:NH1	1:A:308:GLN:OE1	2.45	0.49
1:A:8:ALA:O	1:A:12:LEU:HD22	2.13	0.49
1:C:314:VAL:O	1:C:314:VAL:CG2	2.61	0.49
1:C:367:ARG:HG2	1:C:367:ARG:HH11	1.78	0.49
1:D:314:VAL:HG23	1:D:314:VAL:O	2.12	0.49
1:A:523:LEU:HD13	1:A:524:SER:N	2.28	0.49
1:B:93:HIS:O	1:B:222:ARG:HD2	2.13	0.48
1:C:217:ASP:OD2	1:C:245:MET:HB2	2.13	0.48
1:C:360:LEU:HD12	1:C:505:SER:HA	1.95	0.48
1:C:52:GLU:CG	1:C:81:SER:HB2	2.43	0.48
1:C:391:ILE:HD13	1:C:538:LEU:HD22	1.95	0.48
1:C:523:LEU:HD13	1:C:524:SER:N	2.28	0.48
1:A:244:LEU:HD13	1:A:405:PRO:HG3	1.95	0.48
1:A:382:ASP:N	1:A:413:THR:HG21	2.28	0.48
1:B:142:GLU:OE2	1:B:174:LYS:HE2	2.12	0.48
1:B:410:ILE:HG13	1:B:440:LEU:HD22	1.95	0.48
1:B:522:ARG:HD3	4:B:686:HOH:O	2.12	0.48
1:A:33:GLN:NE2	1:A:173:LYS:HE2	2.28	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:VAL:HG22	3:A:600:TPP:O2B	2.12	0.48
1:B:15:LEU:HD11	1:B:97:LEU:HD23	1.95	0.48
1:B:204:ASN:O	1:B:208:MET:HG3	2.14	0.48
1:B:382:ASP:HA	1:B:413:THR:HG21	1.96	0.48
1:C:282:CYS:HB3	1:C:285:THR:CG2	2.35	0.48
1:B:314:VAL:CG2	1:B:314:VAL:O	2.62	0.48
1:C:382:ASP:HA	1:C:413:THR:HG21	1.94	0.48
1:D:489:ILE:HB	1:D:490:PRO:HD3	1.96	0.48
1:A:52:GLU:HG2	1:A:81:SER:CB	2.44	0.48
1:D:328:ILE:O	1:D:332:VAL:HG23	2.14	0.48
1:B:382:ASP:N	1:B:413:THR:HG21	2.29	0.48
1:C:153:LEU:HD23	1:C:156:MET:HE1	1.94	0.48
1:C:440:LEU:HD12	1:C:440:LEU:H	1.79	0.48
1:C:455:PRO:CD	1:C:523:LEU:HD22	2.42	0.48
1:A:217:ASP:OD2	1:A:245:MET:HB2	2.13	0.48
1:A:93:HIS:O	1:A:222:ARG:HD2	2.13	0.48
1:B:115:HIS:O	1:B:116:HIS:HB2	2.14	0.48
1:B:271:LYS:O	1:B:275:GLU:HB2	2.14	0.48
1:C:472:HIS:CE1	1:D:36:ASP:OD2	2.66	0.48
1:A:153:LEU:HD23	1:A:156:MET:CE	2.44	0.48
1:A:374:ARG:HG3	1:A:375:PRO:CD	2.43	0.48
1:C:231:LYS:HE2	1:C:235:GLU:OE2	2.14	0.48
1:D:225:LEU:HD13	1:D:328:ILE:HD12	1.95	0.48
1:D:504:VAL:HG11	1:D:510:LEU:HB2	1.96	0.48
1:B:382:ASP:CG	1:B:413:THR:HG23	2.35	0.47
1:C:33:GLN:NE2	1:C:173:LYS:HE2	2.28	0.47
1:C:509:GLN:O	1:C:513:VAL:HG23	2.14	0.47
1:C:221:LEU:HD21	1:C:249:ILE:HG22	1.96	0.47
1:C:35:LEU:O	1:C:38:VAL:HG13	2.15	0.47
1:C:477:ARG:NH2	4:D:613:HOH:O	2.47	0.47
1:D:178:PRO:HA	1:D:179:PRO:HD3	1.85	0.47
1:D:430:ILE:N	1:D:430:ILE:HD12	2.29	0.47
1:C:328:ILE:O	1:C:332:VAL:HG23	2.15	0.47
1:C:435:ASP:O	1:C:439:GLN:HG3	2.15	0.47
1:A:271:LYS:O	1:A:275:GLU:HB2	2.14	0.47
1:A:283:VAL:HG13	1:A:307:VAL:CG2	2.45	0.47
1:B:275:GLU:OE1	1:B:298:GLN:HB2	2.14	0.47
1:B:84:ASN:ND2	1:B:407:TRP:HE1	2.12	0.47
1:B:97:LEU:HD13	1:B:156:MET:HE1	1.96	0.47
1:D:244:LEU:HG	1:D:391:ILE:HD12	1.97	0.47
1:A:144:ASN:ND2	1:A:145:ALA:N	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:MET:HG2	4:A:704:HOH:O	2.14	0.47
1:B:97:LEU:HD13	1:B:156:MET:HE2	1.95	0.47
1:C:144:ASN:C	1:C:144:ASN:ND2	2.68	0.47
1:C:534:ASP:O	1:C:535:ILE:HD12	2.14	0.47
1:D:391:ILE:HG21	1:D:538:LEU:CD2	2.45	0.47
1:B:456:ILE:HD11	1:B:458:LEU:HD11	1.95	0.47
1:C:52:GLU:H	1:C:52:GLU:CD	2.13	0.47
1:D:442:ILE:HG23	1:D:443:GLN:N	2.29	0.47
1:B:178:PRO:HA	1:B:179:PRO:HD3	1.85	0.47
1:B:435:ASP:O	1:B:439:GLN:HG3	2.15	0.47
1:C:253:ARG:HE	1:C:396:PRO:HG3	1.80	0.47
1:D:360:LEU:CD1	1:D:504:VAL:HG12	2.45	0.47
1:B:547:GLU:O	1:B:547:GLU:HG3	2.14	0.46
1:A:382:ASP:CG	1:A:413:THR:HG23	2.36	0.46
1:C:369:LEU:HD21	1:C:432:LEU:HD21	1.96	0.46
1:C:52:GLU:HG2	1:C:81:SER:CB	2.45	0.46
1:A:410:ILE:HG13	1:A:440:LEU:HD22	1.97	0.46
1:A:83:MET:HE3	4:A:652:HOH:O	2.16	0.46
1:B:442:ILE:HG23	1:B:443:GLN:N	2.31	0.46
1:B:391:ILE:HG21	1:B:538:LEU:HD22	1.97	0.46
1:A:499:SER:HB3	1:A:523:LEU:HB3	1.96	0.46
1:C:375:PRO:HD3	1:C:396:PRO:CB	2.46	0.46
1:C:382:ASP:OD1	1:C:410:ILE:HA	2.16	0.46
1:D:35:LEU:HA	1:D:38:VAL:CG1	2.45	0.46
1:B:217:ASP:OD2	1:B:245:MET:HB2	2.15	0.46
1:C:504:VAL:HG11	1:C:510:LEU:N	2.30	0.46
1:C:6:CYS:HB2	1:C:174:LYS:O	2.16	0.46
1:D:226:LYS:HE3	1:D:248:GLY:O	2.16	0.46
1:D:279:THR:HA	1:D:303:GLN:O	2.16	0.46
1:A:280:VAL:HG13	1:A:304:THR:HG22	1.97	0.46
1:D:219:LEU:HB2	1:D:284:GLY:CA	2.46	0.46
1:A:146:CYS:HB2	1:C:320:THR:OG1	2.16	0.46
1:D:231:LYS:HE2	1:D:235:GLU:OE2	2.16	0.46
1:D:237:PRO:HD2	4:D:652:HOH:O	2.16	0.46
1:A:204:ASN:O	1:A:208:MET:HG3	2.16	0.46
1:C:395:LEU:HA	1:C:396:PRO:HD2	1.88	0.46
1:A:382:ASP:HA	1:A:413:THR:HG21	1.97	0.45
1:A:456:ILE:HD12	1:A:456:ILE:C	2.36	0.45
1:B:523:LEU:CD1	1:B:523:LEU:C	2.85	0.45
1:C:374:ARG:HG3	1:C:375:PRO:HD2	1.98	0.45
1:C:476:GLN:OE1	1:C:476:GLN:HA	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:GLN:NE2	1:A:536:PRO:HG3	2.32	0.45
1:D:476:GLN:HA	1:D:476:GLN:OE1	2.15	0.45
1:A:454:HIS:N	1:A:455:PRO:CD	2.80	0.45
1:A:391:ILE:HD13	1:A:538:LEU:HD22	1.99	0.45
1:C:303:GLN:O	1:C:303:GLN:HG2	2.17	0.45
1:D:288:THR:HG21	1:D:406:LEU:HD13	1.98	0.45
1:A:314:VAL:O	1:A:314:VAL:CG2	2.64	0.45
1:B:400:ASN:HD22	1:B:400:ASN:C	2.20	0.45
1:D:382:ASP:OD1	1:D:410:ILE:HA	2.17	0.45
1:A:264:SER:HA	1:A:271:LYS:HE2	1.97	0.45
1:A:52:GLU:CG	1:A:81:SER:HB2	2.46	0.45
1:C:498:GLN:OE1	1:C:498:GLN:HA	2.15	0.45
1:D:367:ARG:HG2	1:D:367:ARG:HH11	1.81	0.45
1:A:15:LEU:HD11	1:A:97:LEU:HD23	1.99	0.45
1:C:249:ILE:HD11	1:C:250:PHE:CE2	2.52	0.45
1:D:313:ARG:HD3	1:D:318:TRP:CE2	2.52	0.45
1:A:400:ASN:HD22	1:A:400:ASN:C	2.19	0.45
1:C:244:LEU:HD13	1:C:405:PRO:CG	2.46	0.45
1:C:410:ILE:HG13	1:C:440:LEU:HD22	1.99	0.45
1:D:547:GLU:HG3	1:D:547:GLU:O	2.16	0.45
1:C:540:GLY:O	1:C:543:THR:HG22	2.17	0.45
1:D:207:ALA:HA	1:D:338:HIS:CD2	2.52	0.45
1:A:35:LEU:HA	1:A:38:VAL:CG1	2.46	0.45
1:A:421:GLN:HG2	1:A:429:VAL:HG21	1.99	0.45
1:B:421:GLN:HG2	1:B:429:VAL:HG21	1.99	0.45
1:C:205:LYS:NZ	1:C:302:ALA:O	2.40	0.45
1:C:440:LEU:HD12	1:C:440:LEU:N	2.31	0.44
1:D:440:LEU:N	1:D:440:LEU:HD12	2.32	0.44
1:A:112:GLU:HB2	1:A:114:LEU:HD13	1.99	0.44
1:B:279:THR:HA	1:B:303:GLN:O	2.18	0.44
1:C:21:ASP:OD2	1:C:66:LYS:NZ	2.39	0.44
1:C:388:PHE:CD2	1:C:539:LEU:HD13	2.52	0.44
1:A:84:ASN:HD21	1:A:407:TRP:HE1	1.65	0.44
1:A:435:ASP:O	1:A:439:GLN:HG3	2.17	0.44
1:B:360:LEU:HD11	1:B:504:VAL:HG12	1.99	0.44
1:C:84:ASN:HD21	1:C:407:TRP:HE1	1.65	0.44
1:A:52:GLU:HG3	1:A:78:GLY:O	2.16	0.44
1:D:253:ARG:NH2	1:D:396:PRO:HG3	2.29	0.44
1:C:313:ARG:HB2	1:C:318:TRP:CD2	2.53	0.44
1:D:496:ASP:OD1	1:D:498:GLN:NE2	2.50	0.44
1:D:204:ASN:O	1:D:208:MET:HG3	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:ARG:HD2	1:D:159:GLU:OE2	2.17	0.44
1:A:313:ARG:HB2	1:A:318:TRP:CD2	2.53	0.44
1:A:177:THR:HG21	1:C:194:CYS:HA	2.00	0.44
1:B:35:LEU:HA	1:B:38:VAL:HG13	2.00	0.44
1:D:382:ASP:CG	1:D:413:THR:HG23	2.38	0.44
1:A:430:ILE:HD12	1:A:430:ILE:N	2.33	0.43
1:D:249:ILE:HD11	1:D:250:PHE:CE2	2.52	0.43
1:B:244:LEU:HG	1:B:391:ILE:HD12	2.00	0.43
1:C:400:ASN:HD22	1:C:400:ASN:C	2.19	0.43
1:D:5:TYR:CE1	1:D:178:PRO:HG3	2.52	0.43
1:D:382:ASP:HA	1:D:413:THR:CG2	2.48	0.43
1:B:33:GLN:NE2	1:B:173:LYS:HE2	2.33	0.43
1:B:381:ALA:HA	1:B:432:LEU:O	2.18	0.43
1:C:29:ASP:HB2	4:C:681:HOH:O	2.18	0.43
1:D:314:VAL:O	1:D:314:VAL:CG2	2.66	0.43
1:D:362:GLN:NE2	1:D:536:PRO:HG3	2.33	0.43
1:D:35:LEU:HA	1:D:38:VAL:HG13	2.00	0.43
1:D:435:ASP:O	1:D:439:GLN:HG3	2.18	0.43
1:B:249:ILE:HD11	1:B:250:PHE:CE2	2.53	0.43
1:B:283:VAL:HG13	1:B:307:VAL:CG2	2.48	0.43
1:D:29:ASP:C	1:D:29:ASP:OD1	2.56	0.43
1:D:485:ASN:ND2	4:D:629:HOH:O	2.46	0.43
1:D:455:PRO:CD	1:D:523:LEU:HD13	2.46	0.43
1:A:547:GLU:HG3	1:A:547:GLU:O	2.18	0.43
1:B:374:ARG:HG3	1:B:375:PRO:CD	2.48	0.43
1:B:395:LEU:HA	1:B:396:PRO:HD3	1.76	0.43
1:D:144:ASN:ND2	1:D:144:ASN:C	2.71	0.43
1:A:225:LEU:HD13	1:A:328:ILE:CD1	2.49	0.43
1:A:506:GLU:HB2	1:A:509:GLN:HG3	2.01	0.43
1:A:540:GLY:O	1:A:543:THR:HG22	2.19	0.43
1:B:112:GLU:HB2	1:B:114:LEU:HD13	2.00	0.43
1:C:308:GLN:HB3	1:C:309:PRO:CD	2.48	0.43
1:C:35:LEU:HA	1:C:38:VAL:HG13	2.01	0.43
1:C:442:ILE:HG23	1:C:443:GLN:N	2.33	0.43
1:C:508:GLU:H	1:C:508:GLU:CD	2.22	0.43
1:D:139:VAL:HG13	1:D:166:MET:HE2	2.00	0.43
1:D:33:GLN:NE2	1:D:173:LYS:HE2	2.33	0.43
1:B:177:THR:HA	1:B:178:PRO:HD3	1.91	0.43
1:B:510:LEU:HD22	1:B:514:LEU:HG	2.00	0.43
1:B:313:ARG:HD3	1:B:318:TRP:CE2	2.53	0.43
1:B:360:LEU:HD12	1:B:505:SER:HA	2.01	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ARG:HD2	1:C:222:ARG:O	2.18	0.43
1:A:498:GLN:HA	1:A:498:GLN:OE1	2.19	0.43
1:C:500:GLU:HB3	1:C:502:TRP:CZ3	2.54	0.43
1:D:115:HIS:O	1:D:116:HIS:HB2	2.19	0.43
1:D:72:LEU:HD12	1:D:99:ILE:O	2.19	0.43
1:A:115:HIS:O	1:A:116:HIS:HB2	2.18	0.42
1:A:403:VAL:HG13	1:A:405:PRO:HD3	1.99	0.42
1:A:522:ARG:HD3	4:A:677:HOH:O	2.18	0.42
1:B:137:GLN:HA	1:B:164:TYR:O	2.18	0.42
1:B:476:GLN:OE1	1:B:476:GLN:HA	2.18	0.42
1:C:308:GLN:HB3	1:C:309:PRO:HD2	2.01	0.42
1:D:134:THR:HG21	1:D:164:TYR:HB2	2.00	0.42
1:B:449:LEU:HD12	1:B:449:LEU:HA	1.92	0.42
1:D:153:LEU:HD23	1:D:156:MET:HE1	2.01	0.42
1:A:382:ASP:OD1	1:A:410:ILE:HA	2.19	0.42
1:A:489:ILE:HB	1:A:490:PRO:HD3	2.00	0.42
1:B:219:LEU:HB2	1:B:284:GLY:CA	2.49	0.42
1:B:519:HIS:O	1:B:520:HIS:C	2.57	0.42
1:C:504:VAL:CG1	1:C:505:SER:N	2.82	0.42
1:D:52:GLU:CG	1:D:81:SER:HB2	2.49	0.42
1:A:83:MET:HE2	1:A:133:ILE:HD11	2.01	0.42
1:A:510:LEU:HD22	1:A:514:LEU:HG	2.00	0.42
1:B:100:VAL:HG11	1:B:164:TYR:CZ	2.54	0.42
1:B:144:ASN:HA	1:B:147:TYR:CE2	2.55	0.42
1:C:303:GLN:O	1:C:303:GLN:CG	2.67	0.42
1:D:384:GLY:HA2	1:D:467:VAL:CG1	2.42	0.42
1:D:391:ILE:HD13	1:D:538:LEU:HD22	2.02	0.42
1:A:125:HIS:HB2	4:A:637:HOH:O	2.19	0.42
1:B:35:LEU:HA	1:B:38:VAL:CG1	2.50	0.42
1:A:231:LYS:HE2	1:A:235:GLU:OE2	2.18	0.42
1:B:288:THR:HG21	1:B:406:LEU:HD13	2.01	0.42
1:C:403:VAL:HG13	1:C:405:PRO:HD3	2.01	0.42
1:D:400:ASN:HD22	1:D:400:ASN:C	2.21	0.42
1:C:226:LYS:HE3	1:C:248:GLY:O	2.20	0.42
1:C:331:LEU:HD12	1:C:331:LEU:HA	1.85	0.42
1:D:455:PRO:CG	1:D:523:LEU:CD1	2.97	0.42
1:A:134:THR:HG21	1:A:164:TYR:HB2	2.02	0.42
1:A:283:VAL:HA	1:A:307:VAL:HG22	2.02	0.42
1:A:440:LEU:HD12	1:A:440:LEU:N	2.35	0.42
1:B:264:SER:HA	1:B:271:LYS:HE2	2.02	0.42
1:B:286:ARG:NH1	1:B:308:GLN:OE1	2.53	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:HIS:HD2	4:C:680:HOH:O	2.02	0.42
1:D:52:GLU:HG2	1:D:81:SER:HB2	2.02	0.42
1:A:108:GLN:HE22	1:A:166:MET:CE	2.33	0.42
1:A:282:CYS:HB3	1:A:285:THR:CG2	2.38	0.42
1:A:384:GLY:HA2	1:A:467:VAL:CG1	2.44	0.42
1:B:191:ASP:OD2	1:B:193:ALA:HB3	2.20	0.42
1:A:144:ASN:HA	1:A:147:TYR:CE2	2.55	0.41
1:A:142:GLU:OE2	1:A:174:LYS:HE2	2.19	0.41
1:A:360:LEU:HD11	1:A:504:VAL:CG1	2.50	0.41
1:B:235:GLU:O	1:B:237:PRO:HD3	2.20	0.41
1:B:384:GLY:HA2	1:B:467:VAL:CG1	2.48	0.41
1:C:469:ARG:HH11	1:C:532:LYS:HG3	1.83	0.41
1:D:33:GLN:HB3	1:D:33:GLN:HE21	1.51	0.41
1:D:381:ALA:C	1:D:413:THR:HG21	2.39	0.41
1:A:244:LEU:HG	1:A:391:ILE:HD12	2.02	0.41
1:B:216:ALA:O	1:B:242:THR:HA	2.19	0.41
1:B:340:HIS:O	1:B:341:ALA:C	2.58	0.41
1:C:382:ASP:CG	1:C:413:THR:HG23	2.40	0.41
1:C:253:ARG:CZ	1:C:396:PRO:HD3	2.50	0.41
1:A:218:PHE:HB3	1:A:245:MET:HB3	2.02	0.41
1:C:381:ALA:C	1:C:413:THR:HG21	2.40	0.41
1:C:504:VAL:HG11	1:C:510:LEU:HB2	2.01	0.41
1:C:455:PRO:HG2	1:C:523:LEU:HD22	2.02	0.41
1:A:442:ILE:HG23	1:A:443:GLN:N	2.34	0.41
1:A:466:THR:HG22	4:A:603:HOH:O	2.21	0.41
1:D:3:THR:N	4:D:657:HOH:O	2.53	0.41
1:C:385:THR:HG22	1:C:536:PRO:HD3	2.02	0.41
1:D:331:LEU:HD12	1:D:331:LEU:HA	1.84	0.41
1:D:52:GLU:H	1:D:52:GLU:CD	2.23	0.41
1:B:231:LYS:HE2	1:B:235:GLU:OE2	2.20	0.41
1:D:140:LEU:HD23	1:D:167:LEU:HD13	2.01	0.41
1:D:275:GLU:OE1	1:D:298:GLN:HB2	2.21	0.41
1:B:142:GLU:CD	1:B:174:LYS:HE2	2.41	0.41
1:B:221:LEU:HD21	1:B:249:ILE:HG22	2.02	0.41
1:C:52:GLU:HG3	1:C:78:GLY:O	2.21	0.41
1:C:93:HIS:CD2	4:C:680:HOH:O	2.73	0.41
1:C:97:LEU:HD13	1:C:156:MET:HE1	2.01	0.41
1:D:35:LEU:HD12	1:D:35:LEU:HA	1.89	0.41
1:D:547:GLU:HA	1:D:550:ASN:HD22	1.85	0.41
1:A:74:THR:HG22	4:A:607:HOH:O	2.19	0.41
1:A:395:LEU:HA	1:A:396:PRO:HD3	1.75	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ARG:HD3	4:B:681:HOH:O	2.20	0.41
1:C:410:ILE:HG13	1:C:410:ILE:O	2.19	0.41
1:D:455:PRO:O	1:D:523:LEU:HD12	2.21	0.41
1:D:14:ARG:HB3	1:D:153:LEU:CD1	2.51	0.41
1:A:453:GLN:C	1:A:455:PRO:HD2	2.40	0.41
1:A:519:HIS:O	1:A:520:HIS:C	2.60	0.41
1:A:543:THR:CG2	1:A:544:LYS:N	2.84	0.41
1:B:134:THR:HG21	1:B:164:TYR:HB2	2.02	0.41
1:C:199:ARG:HG3	1:C:330:THR:HG23	2.03	0.41
1:C:455:PRO:CG	1:C:523:LEU:HD22	2.51	0.41
1:D:185:HIS:O	1:D:186:LYS:C	2.59	0.41
1:D:219:LEU:HB2	1:D:284:GLY:HA3	2.03	0.41
1:A:249:ILE:HD11	1:A:250:PHE:CE2	2.56	0.40
1:B:140:LEU:HD23	1:B:167:LEU:HD13	2.03	0.40
1:B:498:GLN:HA	1:B:498:GLN:OE1	2.20	0.40
1:C:159:GLU:O	1:C:160:ARG:HB2	2.21	0.40
1:D:159:GLU:O	1:D:160:ARG:HB2	2.20	0.40
1:D:166:MET:O	1:D:168:PRO:HD3	2.22	0.40
1:A:360:LEU:CD1	1:A:504:VAL:HG12	2.52	0.40
1:C:520:HIS:CD2	1:C:520:HIS:O	2.74	0.40
1:C:547:GLU:HG3	1:C:547:GLU:O	2.19	0.40
1:B:218:PHE:HB3	1:B:245:MET:HB3	2.04	0.40
1:B:485:ASN:ND2	4:B:606:HOH:O	2.53	0.40
1:B:540:GLY:O	1:B:543:THR:HG22	2.22	0.40
1:C:108:GLN:HE22	1:C:166:MET:HE3	1.86	0.40
1:C:35:LEU:HA	1:C:38:VAL:CG1	2.52	0.40
1:C:62:TYR:CZ	1:C:66:LYS:HD3	2.56	0.40
1:D:209:SER:HB2	1:D:279:THR:CG2	2.51	0.40
1:D:440:LEU:HD12	1:D:440:LEU:H	1.87	0.40
1:C:140:LEU:HD23	1:C:167:LEU:HD13	2.04	0.40
1:D:282:CYS:CB	1:D:285:THR:HG21	2.35	0.40
1:A:219:LEU:HB2	1:A:284:GLY:CA	2.52	0.40
1:A:233:VAL:HG21	1:A:240:HIS:ND1	2.36	0.40
1:A:30:TYR:CZ	1:A:103:PRO:HG3	2.57	0.40
1:B:328:ILE:O	1:B:332:VAL:HG23	2.22	0.40
1:B:382:ASP:HB3	4:B:616:HOH:O	2.22	0.40
1:B:391:ILE:HG21	1:B:538:LEU:CD2	2.51	0.40
1:C:113:LEU:HA	4:C:650:HOH:O	2.20	0.40
1:C:430:ILE:HD12	1:C:430:ILE:N	2.35	0.40
1:C:450:ARG:NH1	4:C:616:HOH:O	2.52	0.40
1:D:52:GLU:HG3	1:D:78:GLY:O	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	531/552 (96%)	511 (96%)	17 (3%)	3 (1%)	28	43
1	B	531/552 (96%)	507 (96%)	21 (4%)	3 (1%)	28	43
1	C	531/552 (96%)	506 (95%)	22 (4%)	3 (1%)	28	43
1	D	531/552 (96%)	505 (95%)	23 (4%)	3 (1%)	28	43
All	All	2124/2208 (96%)	2029 (96%)	83 (4%)	12 (1%)	28	43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ALA
1	B	145	ALA
1	C	145	ALA
1	D	145	ALA
1	D	518	ALA
1	A	218	PHE
1	D	186	LYS
1	B	186	LYS
1	C	186	LYS
1	A	186	LYS
1	B	520	HIS
1	C	520	HIS

### 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	426/439 (97%)	384 (90%)	42 (10%)	9	13
1	B	426/439 (97%)	388 (91%)	38 (9%)	11	17
1	C	426/439 (97%)	387 (91%)	39 (9%)	11	16
1	D	426/439 (97%)	390 (92%)	36 (8%)	12	19
All	All	1704/1756 (97%)	1549 (91%)	155 (9%)	11	16

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	32	LEU
1	A	33	GLN
1	A	35	LEU
1	A	38	VAL
1	A	53	LEU
1	A	100	VAL
1	A	114	LEU
1	A	118	LEU
1	A	130	SER
1	A	140	LEU
1	A	144	ASN
1	A	157	LEU
1	A	177	THR
1	A	206	LEU
1	A	214	LEU
1	A	220	VAL
1	A	244	LEU
1	A	278	ASP
1	A	280	VAL
1	A	286	ARG
1	A	331	LEU
1	A	356	PRO
1	A	357	ASP
1	A	367	ARG
1	A	374	ARG
1	A	382	ASP
1	A	383	GLN
1	A	399	VAL
1	A	400	ASN
1	A	443	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	449	LEU
1	A	455	PRO
1	A	456	ILE
1	A	467	VAL
1	A	485	ASN
1	A	503	ARG
1	A	510	LEU
1	A	515	GLU
1	A	523	LEU
1	A	535	ILE
1	A	543	THR
1	B	12	LEU
1	B	32	LEU
1	B	33	GLN
1	B	35	LEU
1	B	38	VAL
1	B	53	LEU
1	B	100	VAL
1	B	114	LEU
1	B	118	LEU
1	B	130	SER
1	B	140	LEU
1	B	144	ASN
1	B	157	LEU
1	B	177	THR
1	B	206	LEU
1	B	214	LEU
1	B	220	VAL
1	B	244	LEU
1	B	278	ASP
1	B	280	VAL
1	B	286	ARG
1	B	331	LEU
1	B	367	ARG
1	B	374	ARG
1	B	382	ASP
1	B	383	GLN
1	B	399	VAL
1	B	400	ASN
1	B	449	LEU
1	B	455	PRO
1	B	456	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	467	VAL
1	B	485	ASN
1	B	500	GLU
1	B	510	LEU
1	B	523	LEU
1	B	535	ILE
1	B	543	THR
1	C	12	LEU
1	C	32	LEU
1	C	33	GLN
1	C	35	LEU
1	C	38	VAL
1	C	53	LEU
1	C	100	VAL
1	C	114	LEU
1	C	118	LEU
1	C	130	SER
1	C	140	LEU
1	C	144	ASN
1	C	157	LEU
1	C	177	THR
1	C	205	LYS
1	C	206	LEU
1	C	208	MET
1	C	214	LEU
1	C	244	LEU
1	C	278	ASP
1	C	280	VAL
1	C	286	ARG
1	C	331	LEU
1	C	367	ARG
1	C	383	GLN
1	C	396	PRO
1	C	399	VAL
1	C	400	ASN
1	C	449	LEU
1	C	456	ILE
1	C	467	VAL
1	C	485	ASN
1	C	500	GLU
1	C	503	ARG
1	C	508	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	522	ARG
1	C	523	LEU
1	C	535	ILE
1	C	543	THR
1	D	12	LEU
1	D	32	LEU
1	D	33	GLN
1	D	35	LEU
1	D	38	VAL
1	D	53	LEU
1	D	100	VAL
1	D	114	LEU
1	D	118	LEU
1	D	130	SER
1	D	140	LEU
1	D	144	ASN
1	D	157	LEU
1	D	177	THR
1	D	208	MET
1	D	214	LEU
1	D	244	LEU
1	D	278	ASP
1	D	280	VAL
1	D	331	LEU
1	D	367	ARG
1	D	374	ARG
1	D	382	ASP
1	D	383	GLN
1	D	399	VAL
1	D	400	ASN
1	D	443	GLN
1	D	444	GLU
1	D	449	LEU
1	D	456	ILE
1	D	467	VAL
1	D	485	ASN
1	D	508	GLU
1	D	510	LEU
1	D	535	ILE
1	D	543	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	54	ASN
1	A	84	ASN
1	A	108	GLN
1	A	115	HIS
1	A	125	HIS
1	A	137	GLN
1	A	144	ASN
1	A	181	ASN
1	A	362	GLN
1	A	383	GLN
1	A	400	ASN
1	A	472	HIS
1	A	485	ASN
1	B	33	GLN
1	B	54	ASN
1	B	84	ASN
1	B	108	GLN
1	B	115	HIS
1	B	125	HIS
1	B	137	GLN
1	B	144	ASN
1	B	181	ASN
1	B	362	GLN
1	B	400	ASN
1	B	472	HIS
1	B	485	ASN
1	C	33	GLN
1	C	54	ASN
1	C	84	ASN
1	C	93	HIS
1	C	115	HIS
1	C	125	HIS
1	C	137	GLN
1	C	144	ASN
1	C	181	ASN
1	C	340	HIS
1	C	362	GLN
1	C	383	GLN
1	C	400	ASN
1	C	472	HIS
1	C	485	ASN
1	C	550	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	33	GLN
1	D	54	ASN
1	D	84	ASN
1	D	108	GLN
1	D	125	HIS
1	D	137	GLN
1	D	144	ASN
1	D	181	ASN
1	D	337	GLN
1	D	338	HIS
1	D	340	HIS
1	D	362	GLN
1	D	400	ASN
1	D	472	HIS
1	D	485	ASN
1	D	550	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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
3	TPP	A	600	2	21,27,27	3.04	7 (33%)	25,40,40	1.92	9 (36%)
3	TPP	B	600	2	21,27,27	2.92	8 (38%)	25,40,40	1.87	9 (36%)
3	TPP	C	600	2	21,27,27	2.96	7 (33%)	25,40,40	1.94	9 (36%)
3	TPP	D	600	2	21,27,27	2.90	6 (28%)	25,40,40	1.87	9 (36%)

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
3	TPP	A	600	2	-	0/16/17/17	0/2/2/2
3	TPP	B	600	2	-	0/16/17/17	0/2/2/2
3	TPP	C	600	2	-	0/16/17/17	0/2/2/2
3	TPP	D	600	2	-	0/16/17/17	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	TPP	C4-N3	-5.88	1.34	1.39
3	D	600	TPP	C4-N3	-5.78	1.34	1.39
3	C	600	TPP	C4-N3	-5.29	1.35	1.39
3	B	600	TPP	C4-N3	-4.48	1.35	1.39
3	B	600	TPP	PB-O2B	-2.24	1.45	1.54
3	A	600	TPP	PA-O2A	-2.11	1.44	1.55
3	C	600	TPP	PA-O2A	-2.06	1.44	1.55
3	B	600	TPP	PA-O2A	-2.04	1.44	1.55
3	D	600	TPP	C6'-N1'	2.13	1.39	1.34
3	B	600	TPP	C6'-N1'	2.29	1.39	1.34
3	C	600	TPP	C6'-N1'	2.34	1.39	1.34
3	A	600	TPP	C6'-N1'	2.37	1.39	1.34
3	D	600	TPP	C7'-N3	3.27	1.54	1.48
3	A	600	TPP	C7'-N3	3.44	1.55	1.48
3	C	600	TPP	C4'-N3'	3.55	1.40	1.35
3	B	600	TPP	C7'-N3	3.67	1.55	1.48
3	D	600	TPP	C4'-N3'	3.73	1.40	1.35
3	B	600	TPP	C4'-N3'	3.96	1.41	1.35
3	C	600	TPP	C7'-N3	3.97	1.56	1.48
3	A	600	TPP	C4'-N3'	4.28	1.41	1.35
3	D	600	TPP	C5'-C4'	6.43	1.57	1.42
3	B	600	TPP	C5'-C4'	6.56	1.58	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	600	TPP	C5'-C4'	6.92	1.59	1.42
3	A	600	TPP	C5'-C4'	6.96	1.59	1.42
3	A	600	TPP	C6'-C5'	7.46	1.53	1.37
3	C	600	TPP	C6'-C5'	7.66	1.54	1.37
3	D	600	TPP	C6'-C5'	7.70	1.54	1.37
3	B	600	TPP	C6'-C5'	7.81	1.54	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	TPP	C6'-C5'-C4'	-3.24	111.37	115.68
3	D	600	TPP	C6'-C5'-C4'	-3.24	111.37	115.68
3	B	600	TPP	C6'-C5'-C4'	-3.18	111.46	115.68
3	C	600	TPP	C6'-C5'-C4'	-3.05	111.62	115.68
3	B	600	TPP	O3A-PB-O1B	-2.98	93.14	111.44
3	A	600	TPP	O3A-PB-O1B	-2.93	93.39	111.44
3	D	600	TPP	O3A-PB-O1B	-2.88	93.71	111.44
3	C	600	TPP	O3A-PB-O1B	-2.78	94.35	111.44
3	C	600	TPP	C5'-C7'-N3	-2.75	108.73	113.33
3	C	600	TPP	O2A-PA-O7	-2.69	95.43	108.14
3	B	600	TPP	O2A-PA-O7	-2.55	96.12	108.14
3	D	600	TPP	O2A-PA-O7	-2.40	96.81	108.14
3	A	600	TPP	O2A-PA-O7	-2.37	96.93	108.14
3	D	600	TPP	C5'-C7'-N3	-2.18	109.68	113.33
3	B	600	TPP	C5'-C7'-N3	-2.11	109.80	113.33
3	A	600	TPP	C5'-C7'-N3	-2.09	109.84	113.33
3	B	600	TPP	O7-PA-O1A	2.04	117.49	109.25
3	C	600	TPP	O7-PA-O1A	2.05	117.51	109.25
3	A	600	TPP	O7-PA-O1A	2.11	117.75	109.25
3	D	600	TPP	O7-PA-O1A	2.12	117.80	109.25
3	A	600	TPP	O3B-PB-O1B	2.47	120.17	110.50
3	B	600	TPP	C2'-N3'-C4'	2.55	122.55	118.16
3	A	600	TPP	C2'-N3'-C4'	2.56	122.57	118.16
3	D	600	TPP	O3B-PB-O1B	2.58	120.60	110.50
3	D	600	TPP	C2'-N3'-C4'	2.62	122.68	118.16
3	C	600	TPP	C2'-N3'-C4'	2.65	122.73	118.16
3	B	600	TPP	O3B-PB-O1B	2.65	120.88	110.50
3	C	600	TPP	O3B-PB-O1B	2.70	121.07	110.50
3	A	600	TPP	C5-C4-N3	3.01	113.60	107.57
3	B	600	TPP	C5-C4-N3	3.02	113.61	107.57
3	D	600	TPP	C5-C4-N3	3.03	113.64	107.57
3	C	600	TPP	C5-C4-N3	3.18	113.93	107.57

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	600	TPP	C6'-N1'-C2'	3.54	122.00	115.88
3	B	600	TPP	C6'-N1'-C2'	3.58	122.06	115.88
3	C	600	TPP	C6'-N1'-C2'	3.63	122.15	115.88
3	A	600	TPP	C6'-N1'-C2'	3.97	122.74	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	TPP	2	0
3	B	600	TPP	1	0
3	C	600	TPP	1	0
3	D	600	TPP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	535/552 (96%)	-0.04	18 (3%)	46 44	14, 30, 54, 82	0
1	B	535/552 (96%)	-0.05	15 (2%)	53 52	16, 31, 54, 87	0
1	C	535/552 (96%)	-0.08	18 (3%)	46 44	16, 31, 55, 84	0
1	D	535/552 (96%)	0.04	19 (3%)	43 41	17, 33, 58, 84	0
All	All	2140/2208 (96%)	-0.03	70 (3%)	47 45	14, 31, 57, 87	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	HIS	5.7
1	C	3	THR	5.6
1	A	340	HIS	4.7
1	A	341	ALA	4.5
1	A	356	PRO	4.5
1	D	341	ALA	4.5
1	C	187	GLN	4.4
1	B	340	HIS	4.4
1	C	185	HIS	4.3
1	D	357	ASP	4.2
1	A	548	ALA	3.9
1	B	186	LYS	3.9
1	B	341	ALA	3.8
1	A	185	HIS	3.8
1	B	187	GLN	3.7
1	B	357	ASP	3.7
1	A	3	THR	3.6
1	C	186	LYS	3.4
1	C	184	THR	3.3
1	C	498	GLN	3.2
1	C	341	ALA	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	357	ASP	3.1
1	A	187	GLN	3.1
1	A	188	ALA	3.0
1	C	356	PRO	3.0
1	B	496	ASP	2.9
1	C	208	MET	2.9
1	B	356	PRO	2.9
1	D	398	ASP	2.9
1	B	339	VAL	2.9
1	C	548	ALA	2.8
1	D	356	PRO	2.8
1	B	184	THR	2.8
1	C	340	HIS	2.7
1	B	209	SER	2.7
1	D	512	ASP	2.6
1	A	186	LYS	2.6
1	A	189	HIS	2.6
1	A	550	ASN	2.5
1	D	180	VAL	2.5
1	B	272	GLU	2.5
1	C	551	ASN	2.5
1	D	209	SER	2.5
1	C	339	VAL	2.4
1	A	551	ASN	2.4
1	B	268	GLY	2.4
1	C	544	LYS	2.4
1	D	522	ARG	2.4
1	D	359	SER	2.4
1	A	184	THR	2.4
1	D	550	ASN	2.4
1	D	537	PRO	2.4
1	A	546	LEU	2.4
1	A	496	ASP	2.4
1	A	357	ASP	2.3
1	A	208	MET	2.3
1	D	340	HIS	2.3
1	B	181	ASN	2.3
1	A	549	CYS	2.3
1	D	265	ALA	2.2
1	D	187	GLN	2.2
1	B	196	LYS	2.2
1	C	549	CYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	183	LEU	2.1
1	D	548	ALA	2.1
1	D	498	GLN	2.1
1	D	496	ASP	2.1
1	D	521	GLU	2.1
1	C	547	GLU	2.1
1	C	496	ASP	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	MG	D	601	1/1	0.85	0.25	3.09	27,27,27,27	0
2	MG	C	601	1/1	0.80	0.21	1.87	29,29,29,29	0
2	MG	B	601	1/1	0.97	0.20	1.74	19,19,19,19	0
2	MG	A	601	1/1	0.95	0.18	0.60	23,23,23,23	0
3	TPP	C	600	26/26	0.97	0.17	-0.05	21,28,31,33	0
3	TPP	D	600	26/26	0.98	0.18	-0.06	22,28,31,32	0
3	TPP	B	600	26/26	0.98	0.17	-0.14	18,23,27,30	0
3	TPP	A	600	26/26	0.97	0.15	-0.66	19,24,26,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.