



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:42 PM GMT

PDB ID : 1C3R  
Title : CRYSTAL STRUCTURE OF AN HDAC HOMOLOG COMPLEXED WITH TRICHOSTATIN A  
Authors : Finnin, M.S.; Donigian, J.R.; Pavletich, N.P.  
Deposited on : 1999-07-28  
Resolution : 2.00 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

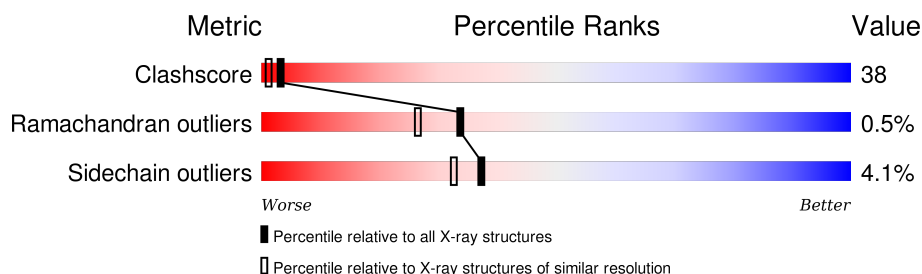
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	375	 57% 40% ..
1	B	375	 62% 35% ..

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6480 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 HDLP (HISTONE DEACETYLASE-LIKE PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2989	1930	494	557	8			
1	B	372	Total	C	N	O	S	0	0	0
			2989	1930	494	557	8			

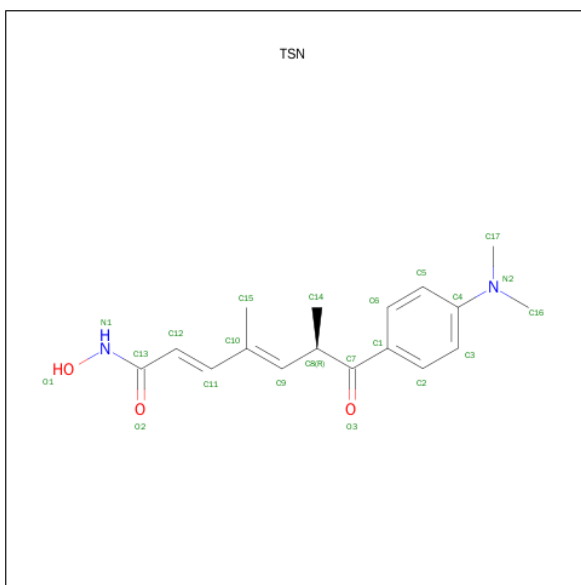
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	LYS	LEU	CONFLICT	UNP O67135
A	75	SER	CYS	ENGINEERED	UNP O67135
A	77	SER	CYS	ENGINEERED	UNP O67135
A	146	ASN	ASP	CONFLICT	UNP O67135
B	35	LYS	LEU	CONFLICT	UNP O67135
B	75	SER	CYS	ENGINEERED	UNP O67135
B	77	SER	CYS	ENGINEERED	UNP O67135
B	146	ASN	ASP	CONFLICT	UNP O67135

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is TRICHOSTATIN A (three-letter code: TSN) (formula: C<sub>17</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 22	C 17	N 2	O 3	0	0
3	B	1	Total 22	C 17	N 2	O 3	0	0

- Molecule 4 is water.

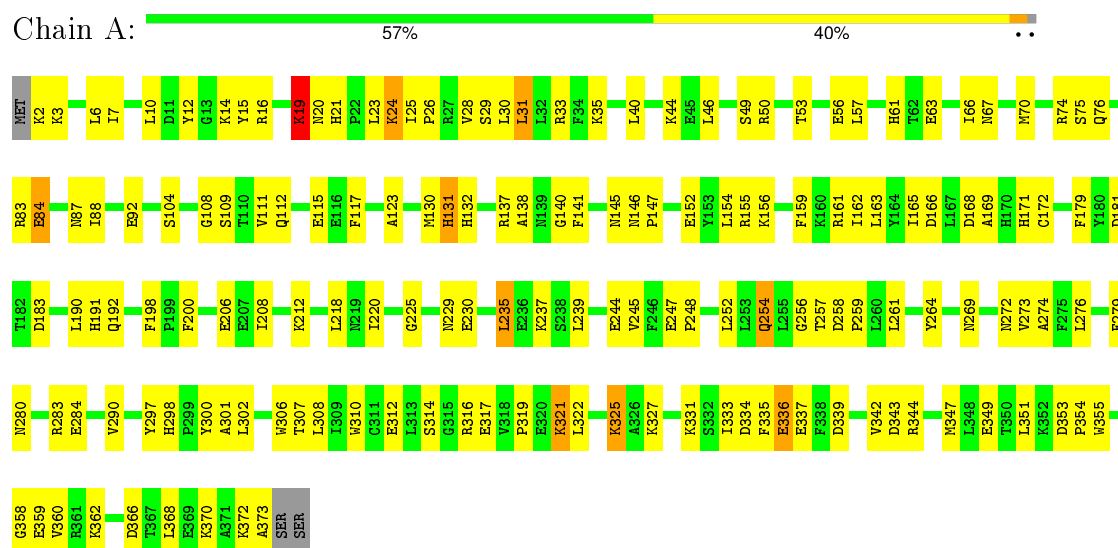
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	208	Total O 208 208	0	0
4	B	248	Total O 248 248	0	0

### 3 Residue-property plots

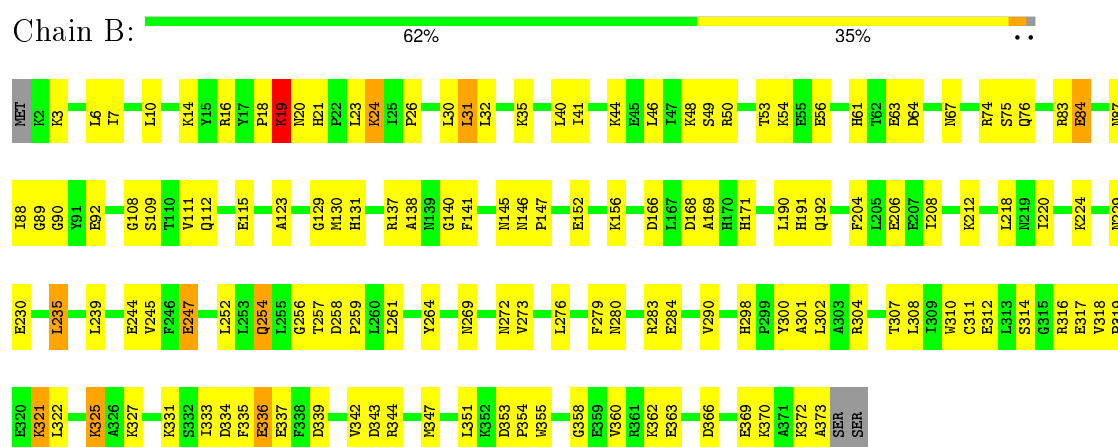
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: HDLP (HISTONE DEACETYLASE-LIKE PROTEIN)



#### • Molecule 1: HDLP (HISTONE DEACETYLASE-LIKE PROTEIN)



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.40Å 94.40Å 156.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.34	0/3060	0.62	0/4128
1	B	0.35	0/3060	0.63	0/4128
All	All	0.35	0/6120	0.63	0/8256

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2989	0	2960	234	0
1	B	2989	0	2960	216	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	21	1	0
3	B	22	0	21	0	0
4	A	208	0	0	101	1
4	B	248	0	0	87	0
All	All	6480	0	5962	450	1

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 38.

All (450) 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:325:LYS:H	1:B:325:LYS:HE3	0.99	1.15
1:A:325:LYS:H	1:A:325:LYS:HE3	0.98	1.11
1:B:325:LYS:N	1:B:325:LYS:HE3	1.68	1.09
1:A:254:GLN:NE2	1:A:256:GLY:H	1.51	1.06
1:A:321:LYS:HE3	1:A:321:LYS:H	0.93	1.06
1:B:321:LYS:HE3	1:B:321:LYS:H	0.92	1.06
1:A:75:SER:HB3	4:A:689:HOH:O	1.54	1.06
1:A:325:LYS:N	1:A:325:LYS:HE3	1.69	1.05
1:B:254:GLN:NE2	1:B:256:GLY:H	1.54	1.05
1:B:321:LYS:HB3	4:B:711:HOH:O	1.59	1.03
1:B:54:LYS:HE2	4:B:698:HOH:O	1.57	1.03
1:B:3:LYS:HD2	4:B:733:HOH:O	1.60	1.02
1:A:208:ILE:HB	4:A:557:HOH:O	1.58	1.01
1:B:208:ILE:HB	4:B:599:HOH:O	1.62	0.98
1:A:349:GLU:HG3	4:A:529:HOH:O	1.62	0.98
1:A:12:TYR:HB2	4:A:583:HOH:O	1.63	0.97
1:B:321:LYS:HE3	1:B:321:LYS:N	1.77	0.97
1:A:321:LYS:HE3	1:A:321:LYS:N	1.79	0.96
1:B:254:GLN:HE22	1:B:256:GLY:H	1.13	0.96
1:A:31:LEU:HD22	1:A:35:LYS:HE3	1.45	0.96
1:A:274:ALA:HB2	4:A:697:HOH:O	1.66	0.96
1:B:83:ARG:HG3	4:B:752:HOH:O	1.64	0.96
1:A:362:LYS:HB3	4:A:592:HOH:O	1.64	0.96
1:A:154:LEU:HB3	4:A:682:HOH:O	1.66	0.95
1:B:64:ASP:HB3	4:B:508:HOH:O	1.66	0.94
1:A:254:GLN:HE22	1:A:256:GLY:H	1.15	0.94
1:A:273:VAL:HB	4:A:604:HOH:O	1.68	0.94
1:A:283:ARG:HD3	4:A:527:HOH:O	1.66	0.93
1:B:321:LYS:CE	1:B:321:LYS:H	1.80	0.93
1:A:337:GLU:HG2	1:A:342:VAL:HG21	1.50	0.93
1:B:337:GLU:HG2	1:B:342:VAL:HG21	1.48	0.92
1:B:31:LEU:HD22	1:B:35:LYS:HE3	1.47	0.92
1:A:321:LYS:H	1:A:321:LYS:CE	1.82	0.92
1:B:276:LEU:HB2	4:B:737:HOH:O	1.69	0.91
1:B:353:ASP:HB3	4:B:666:HOH:O	1.70	0.91
1:A:200:PHE:N	4:A:511:HOH:O	2.05	0.89
1:A:49:SER:HA	4:A:710:HOH:O	1.72	0.89
1:B:14:LYS:HA	1:B:14:LYS:HE2	1.54	0.89
1:A:35:LYS:HG2	4:A:626:HOH:O	1.71	0.88
1:A:14:LYS:HE2	1:A:14:LYS:HA	1.54	0.88

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:THR:HB	4:B:742:HOH:O	1.73	0.88
1:A:280:ASN:HA	4:A:527:HOH:O	1.74	0.87
1:A:76:GLN:HB2	4:A:684:HOH:O	1.74	0.87
1:A:163:LEU:HD22	4:A:692:HOH:O	1.73	0.87
1:A:10:LEU:HG	4:A:554:HOH:O	1.75	0.86
1:A:347:MET:HB2	4:A:706:HOH:O	1.76	0.85
1:A:312:GLU:HB2	4:A:701:HOH:O	1.76	0.85
1:B:74:ARG:HD3	4:B:528:HOH:O	1.76	0.84
1:B:272:ASN:HA	4:B:570:HOH:O	1.77	0.83
1:B:88:ILE:HB	4:B:593:HOH:O	1.78	0.83
1:A:336:GLU:N	4:A:567:HOH:O	2.12	0.82
1:A:159:PHE:HB3	4:A:593:HOH:O	1.79	0.81
1:A:368:LEU:O	1:A:372:LYS:HG3	1.81	0.81
1:B:247:GLU:HG2	4:B:567:HOH:O	1.81	0.81
1:A:130:MET:H	1:A:146:ASN:HD21	1.29	0.81
1:A:212:LYS:HA	1:A:212:LYS:HE2	1.63	0.81
1:B:212:LYS:HA	1:B:212:LYS:HE2	1.63	0.80
1:A:334:ASP:HB2	4:A:589:HOH:O	1.80	0.80
1:A:347:MET:SD	4:A:559:HOH:O	2.40	0.79
1:A:248:PRO:HG3	4:A:692:HOH:O	1.83	0.78
1:A:16:ARG:HG2	4:A:521:HOH:O	1.83	0.78
1:B:308:LEU:HD13	4:B:737:HOH:O	1.82	0.78
1:B:130:MET:H	1:B:146:ASN:HD21	1.31	0.78
1:A:308:LEU:O	4:A:701:HOH:O	2.01	0.77
1:B:362:LYS:HD2	4:B:588:HOH:O	1.83	0.77
1:A:198:PHE:CE2	4:A:617:HOH:O	2.37	0.77
1:A:300:TYR:HD2	1:A:347:MET:HE3	1.50	0.76
1:A:111:VAL:O	1:A:115:GLU:HG3	1.87	0.75
1:A:344:ARG:HB3	1:A:347:MET:CE	2.18	0.74
1:B:19:LYS:HD2	4:B:615:HOH:O	1.86	0.74
1:A:104:SER:HB2	4:A:564:HOH:O	1.86	0.74
1:B:334:ASP:HB2	4:B:678:HOH:O	1.88	0.74
1:A:28:VAL:HA	4:A:651:HOH:O	1.88	0.74
1:B:344:ARG:HB3	1:B:347:MET:CE	2.16	0.74
1:B:254:GLN:HE22	1:B:256:GLY:N	1.86	0.73
1:B:347:MET:SD	4:B:654:HOH:O	2.45	0.73
1:A:254:GLN:HE22	1:A:256:GLY:N	1.86	0.73
1:A:276:LEU:HD13	4:A:701:HOH:O	1.88	0.73
1:B:21:HIS:HD2	1:B:23:LEU:H	1.36	0.73
1:A:25:ILE:HG22	4:A:566:HOH:O	1.89	0.72
1:A:15:TYR:HD1	4:A:702:HOH:O	1.72	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:CYS:HB3	4:B:560:HOH:O	1.89	0.71
1:B:18:PRO:HD3	4:B:690:HOH:O	1.89	0.71
1:A:21:HIS:HD2	1:A:23:LEU:H	1.36	0.71
1:A:321:LYS:HB3	4:A:543:HOH:O	1.90	0.71
1:A:3:LYS:N	4:A:510:HOH:O	2.23	0.71
1:B:300:TYR:HD2	1:B:347:MET:HE3	1.55	0.71
1:B:366:ASP:O	1:B:370:LYS:HD3	1.91	0.71
1:B:111:VAL:O	1:B:115:GLU:HG3	1.91	0.71
1:A:325:LYS:CE	1:A:325:LYS:H	1.91	0.70
1:A:300:TYR:CD2	1:A:347:MET:HE3	2.25	0.70
1:A:70:MET:SD	4:A:654:HOH:O	2.48	0.70
1:A:28:VAL:HG22	4:A:651:HOH:O	1.92	0.70
1:B:87:ASN:HB2	1:B:137:ARG:NE	2.06	0.70
1:A:256:GLY:O	4:A:624:HOH:O	2.10	0.70
1:A:87:ASN:HB2	1:A:137:ARG:NE	2.07	0.69
1:B:41:ILE:HG22	4:B:619:HOH:O	1.90	0.69
1:A:342:VAL:HG22	4:A:520:HOH:O	1.91	0.69
1:B:300:TYR:CD2	1:B:347:MET:HE3	2.27	0.69
1:B:32:LEU:HB3	4:B:677:HOH:O	1.91	0.69
1:B:53:THR:OG1	1:B:56:GLU:HG3	1.92	0.69
1:A:57:LEU:HD11	4:A:564:HOH:O	1.93	0.69
1:B:32:LEU:HD22	4:B:677:HOH:O	1.92	0.69
1:B:325:LYS:H	1:B:325:LYS:CE	1.92	0.68
1:B:273:VAL:HG23	4:B:608:HOH:O	1.92	0.68
1:B:208:ILE:HD13	4:B:510:HOH:O	1.92	0.68
1:A:14:LYS:HB3	4:A:674:HOH:O	1.92	0.68
1:A:366:ASP:O	1:A:370:LYS:HD3	1.93	0.68
1:A:74:ARG:CZ	4:A:689:HOH:O	2.42	0.67
1:B:373:ALA:N	4:B:696:HOH:O	2.26	0.67
1:B:362:LYS:HE2	1:B:362:LYS:H	1.60	0.67
1:B:24:LYS:HE3	4:B:627:HOH:O	1.94	0.67
1:B:41:ILE:N	4:B:619:HOH:O	2.29	0.66
1:A:53:THR:OG1	1:A:56:GLU:HG3	1.96	0.66
1:B:76:GLN:OE1	4:B:681:HOH:O	2.13	0.66
1:A:254:GLN:NE2	1:A:256:GLY:N	2.35	0.66
1:B:316:ARG:NH2	4:B:521:HOH:O	2.29	0.66
1:A:16:ARG:HH11	1:A:16:ARG:HG3	1.61	0.65
1:B:204:PHE:HZ	4:B:634:HOH:O	1.79	0.65
1:B:272:ASN:CB	4:B:608:HOH:O	2.43	0.65
1:A:359:GLU:HA	4:A:594:HOH:O	1.96	0.65
1:B:35:LYS:HB2	1:B:35:LYS:NZ	2.11	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:HH11	1:B:16:ARG:HG3	1.62	0.65
1:A:35:LYS:HB2	1:A:35:LYS:NZ	2.12	0.65
1:A:344:ARG:HB3	1:A:347:MET:HE2	1.78	0.64
1:B:254:GLN:NE2	1:B:256:GLY:N	2.38	0.64
1:A:261:LEU:HD13	1:A:269:ASN:HB3	1.78	0.64
1:B:257:THR:C	1:B:259:PRO:HD2	2.17	0.64
1:A:12:TYR:HA	4:A:702:HOH:O	1.97	0.64
1:A:316:ARG:NH2	4:A:535:HOH:O	2.30	0.64
1:A:362:LYS:H	1:A:362:LYS:HE2	1.62	0.64
1:A:257:THR:C	1:A:259:PRO:HD2	2.16	0.64
1:B:272:ASN:HB2	4:B:608:HOH:O	1.97	0.64
1:B:35:LYS:HB2	1:B:35:LYS:HZ2	1.63	0.63
1:B:40:LEU:HA	1:B:316:ARG:HH11	1.62	0.63
1:B:63:GLU:HG3	1:B:67:ASN:ND2	2.13	0.63
1:A:264:TYR:OH	1:A:337:GLU:HG3	1.99	0.63
1:A:152:GLU:OE2	4:A:531:HOH:O	2.14	0.63
1:B:88:ILE:HD11	1:B:138:ALA:HB2	1.81	0.63
1:A:168:ASP:HA	4:A:624:HOH:O	1.97	0.63
1:A:208:ILE:O	1:A:208:ILE:HG22	1.99	0.62
1:A:63:GLU:HG3	1:A:67:ASN:ND2	2.13	0.62
1:A:156:LYS:CD	4:A:531:HOH:O	2.46	0.62
1:A:88:ILE:HD11	1:A:138:ALA:HB2	1.81	0.62
1:B:208:ILE:O	1:B:208:ILE:HG22	1.99	0.62
1:A:7:ILE:HG23	4:A:710:HOH:O	1.98	0.62
1:A:145:ASN:OD1	1:A:147:PRO:HD2	1.99	0.62
1:B:317:GLU:C	4:B:560:HOH:O	2.36	0.62
1:B:322:LEU:HB3	4:B:561:HOH:O	1.98	0.62
1:B:90:GLY:N	4:B:752:HOH:O	2.33	0.62
1:B:49:SER:HA	1:B:112:GLN:HE22	1.65	0.62
1:B:264:TYR:OH	1:B:337:GLU:HG3	1.99	0.61
1:B:74:ARG:CZ	4:B:609:HOH:O	2.48	0.61
1:B:344:ARG:HB3	1:B:347:MET:HE2	1.81	0.61
1:A:40:LEU:HA	1:A:316:ARG:HH11	1.64	0.61
1:B:373:ALA:HB2	4:B:696:HOH:O	2.00	0.61
1:A:16:ARG:HG3	1:A:16:ARG:NH1	2.15	0.60
1:A:237:LYS:HD3	4:A:709:HOH:O	1.99	0.60
1:A:132:HIS:CD2	4:A:617:HOH:O	2.53	0.60
1:B:16:ARG:NH1	1:B:16:ARG:HG3	2.15	0.60
1:A:156:LYS:CG	4:A:664:HOH:O	2.48	0.60
1:B:261:LEU:HD13	1:B:269:ASN:HB3	1.82	0.60
1:B:276:LEU:CB	4:B:737:HOH:O	2.40	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LYS:HE2	4:A:531:HOH:O	2.00	0.60
1:B:372:LYS:HG3	4:B:628:HOH:O	2.01	0.60
1:A:307:THR:HG23	4:A:626:HOH:O	2.00	0.60
1:A:276:LEU:HD11	1:A:312:GLU:HG3	1.84	0.60
1:B:212:LYS:HE2	1:B:212:LYS:CA	2.31	0.60
1:B:92:GLU:HB2	4:B:647:HOH:O	2.02	0.60
1:B:327:LYS:N	4:B:561:HOH:O	2.33	0.60
1:B:276:LEU:HD11	1:B:312:GLU:HG3	1.84	0.59
1:A:212:LYS:CA	1:A:212:LYS:HE2	2.31	0.59
1:A:306:TRP:HB2	4:A:691:HOH:O	2.03	0.59
1:B:16:ARG:NH2	1:B:26:PRO:HG3	2.18	0.59
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.67	0.59
1:A:15:TYR:HB2	4:A:702:HOH:O	2.02	0.59
1:A:49:SER:HA	1:A:112:GLN:HE22	1.68	0.59
1:A:280:ASN:O	1:A:284:GLU:HG3	2.01	0.59
1:B:362:LYS:CE	1:B:362:LYS:H	2.16	0.59
1:B:40:LEU:N	4:B:619:HOH:O	2.35	0.59
1:B:18:PRO:HB3	4:B:690:HOH:O	2.03	0.58
1:B:369:GLU:HG3	4:B:639:HOH:O	2.02	0.58
1:B:273:VAL:HG13	4:B:557:HOH:O	2.03	0.58
1:B:19:LYS:HG2	4:B:714:HOH:O	2.01	0.58
1:B:21:HIS:CD2	1:B:23:LEU:H	2.21	0.58
1:B:316:ARG:CZ	4:B:521:HOH:O	2.51	0.58
1:B:276:LEU:HD11	1:B:312:GLU:CG	2.33	0.58
1:B:322:LEU:HD11	4:B:703:HOH:O	2.02	0.58
1:A:248:PRO:CG	4:A:692:HOH:O	2.47	0.57
1:A:50:ARG:H	1:A:112:GLN:NE2	2.02	0.57
1:A:16:ARG:NH2	1:A:26:PRO:HG3	2.19	0.57
1:B:130:MET:H	1:B:146:ASN:ND2	2.00	0.57
1:B:335:PHE:O	1:B:336:GLU:HB3	2.03	0.57
1:A:258:ASP:N	1:A:259:PRO:HD2	2.19	0.57
1:A:84:GLU:CD	1:A:84:GLU:H	2.06	0.57
1:A:335:PHE:O	1:A:336:GLU:HB3	2.04	0.57
1:B:145:ASN:OD1	1:B:147:PRO:HD2	2.03	0.57
1:B:61:HIS:CE1	1:B:145:ASN:H	2.22	0.57
1:B:280:ASN:O	1:B:284:GLU:HG3	2.04	0.57
1:A:35:LYS:HB2	1:A:35:LYS:HZ2	1.69	0.57
1:B:325:LYS:CE	1:B:325:LYS:N	2.58	0.57
1:B:84:GLU:CD	1:B:84:GLU:H	2.07	0.57
1:A:21:HIS:CD2	1:A:23:LEU:H	2.21	0.56
1:A:117:PHE:HD1	4:A:565:HOH:O	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:PRO:HG2	1:A:351:LEU:HD12	1.87	0.56
1:B:156:LYS:N	1:B:156:LYS:HD2	2.20	0.56
1:A:272:ASN:HB2	1:A:353:ASP:OD2	2.05	0.56
1:B:61:HIS:HE1	1:B:145:ASN:H	1.52	0.56
1:B:258:ASP:N	1:B:259:PRO:HD2	2.21	0.56
1:B:156:LYS:CG	4:B:651:HOH:O	2.53	0.56
1:B:245:VAL:HG12	1:B:245:VAL:O	2.05	0.56
1:A:130:MET:H	1:A:146:ASN:ND2	2.00	0.56
1:B:19:LYS:HD2	1:B:20:ASN:H	1.71	0.56
1:A:208:ILE:HD13	4:A:514:HOH:O	2.04	0.56
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.70	0.56
1:A:362:LYS:H	1:A:362:LYS:CE	2.19	0.56
1:B:276:LEU:HD22	4:B:737:HOH:O	2.06	0.56
1:A:104:SER:CB	4:A:564:HOH:O	2.47	0.56
1:A:206:GLU:OE1	1:A:206:GLU:N	2.39	0.56
1:A:61:HIS:CE1	1:A:145:ASN:H	2.24	0.56
1:A:245:VAL:HG12	1:A:245:VAL:O	2.06	0.55
1:B:40:LEU:HA	1:B:316:ARG:NH1	2.21	0.55
1:A:181:ASP:CG	4:A:519:HOH:O	2.44	0.55
1:B:89:GLY:C	4:B:752:HOH:O	2.44	0.55
1:A:200:PHE:HB3	4:A:636:HOH:O	2.06	0.55
1:A:19:LYS:HD2	1:A:20:ASN:H	1.71	0.55
1:A:276:LEU:HD11	1:A:312:GLU:CG	2.37	0.55
1:B:272:ASN:HB3	4:B:608:HOH:O	2.07	0.55
1:A:322:LEU:HD13	4:A:599:HOH:O	2.07	0.55
1:B:319:PRO:HG2	1:B:351:LEU:HD12	1.88	0.55
1:A:156:LYS:N	1:A:156:LYS:HD2	2.22	0.55
1:B:362:LYS:HD3	1:B:362:LYS:N	2.21	0.55
1:B:363:GLU:OE1	4:B:635:HOH:O	2.18	0.55
1:B:342:VAL:HG23	1:B:343:ASP:N	2.22	0.54
1:A:112:GLN:NE2	4:A:710:HOH:O	2.39	0.54
1:A:342:VAL:HG23	1:A:343:ASP:N	2.22	0.54
1:B:272:ASN:HB2	1:B:353:ASP:OD2	2.07	0.54
1:B:317:GLU:CD	1:B:317:GLU:H	2.11	0.54
1:A:319:PRO:HG2	1:A:351:LEU:CD1	2.37	0.54
1:B:50:ARG:H	1:B:112:GLN:NE2	2.05	0.54
1:A:61:HIS:HE1	1:A:145:ASN:H	1.56	0.54
1:B:14:LYS:CE	1:B:14:LYS:HA	2.33	0.54
1:A:347:MET:HE2	4:A:706:HOH:O	2.08	0.54
1:A:327:LYS:N	4:A:599:HOH:O	2.41	0.54
1:A:229:ASN:HD22	1:A:358:GLY:H	1.56	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:HD22	4:B:742:HOH:O	2.08	0.53
1:B:19:LYS:HG3	4:B:613:HOH:O	2.07	0.53
1:A:317:GLU:H	1:A:317:GLU:CD	2.11	0.53
1:A:162:ILE:HG13	4:A:593:HOH:O	2.08	0.53
1:B:353:ASP:HB2	1:B:354:PRO:HD2	1.90	0.53
1:A:161:ARG:N	4:A:593:HOH:O	2.42	0.53
1:A:179:PHE:HE2	4:A:705:HOH:O	1.92	0.53
1:B:166:ASP:OD2	1:B:254:GLN:HG2	2.08	0.53
1:B:272:ASN:CA	4:B:570:HOH:O	2.47	0.53
1:B:156:LYS:HG2	4:B:651:HOH:O	2.07	0.53
1:A:40:LEU:HA	1:A:316:ARG:NH1	2.23	0.53
1:B:353:ASP:CB	4:B:666:HOH:O	2.42	0.52
1:A:140:GLY:O	1:A:141:PHE:HB2	2.09	0.52
1:A:14:LYS:CE	1:A:14:LYS:HA	2.33	0.52
1:B:206:GLU:OE1	1:B:206:GLU:N	2.41	0.52
1:B:319:PRO:HG2	1:B:351:LEU:CD1	2.40	0.52
1:A:3:LYS:CA	4:A:510:HOH:O	2.57	0.52
1:A:302:LEU:HD23	1:A:302:LEU:C	2.30	0.52
1:B:308:LEU:HB3	4:B:737:HOH:O	2.08	0.52
1:A:24:LYS:HE3	4:A:625:HOH:O	2.09	0.52
1:B:140:GLY:O	1:B:141:PHE:HB2	2.09	0.52
1:B:108:GLY:O	1:B:112:GLN:HG3	2.10	0.52
1:B:109:SER:HA	1:B:112:GLN:HE21	1.75	0.51
1:B:224:LYS:HE3	4:B:598:HOH:O	2.09	0.51
1:B:10:LEU:HD13	4:B:633:HOH:O	2.11	0.51
1:A:276:LEU:CD1	4:A:701:HOH:O	2.52	0.51
1:A:166:ASP:CG	1:A:254:GLN:HG2	2.31	0.51
1:B:166:ASP:CG	1:B:254:GLN:HG2	2.31	0.51
1:B:74:ARG:HG3	1:B:75:SER:N	2.25	0.51
1:B:16:ARG:CZ	1:B:26:PRO:HG3	2.41	0.51
1:B:302:LEU:C	1:B:302:LEU:HD23	2.31	0.51
1:A:31:LEU:CD2	4:A:691:HOH:O	2.59	0.50
1:A:74:ARG:HG3	1:A:75:SER:N	2.26	0.50
1:A:300:TYR:HD2	1:A:347:MET:CE	2.22	0.50
1:A:353:ASP:HB2	1:A:354:PRO:HD2	1.92	0.50
1:B:7:ILE:HD13	1:B:123:ALA:HB1	1.93	0.50
1:B:337:GLU:HG2	1:B:342:VAL:CG2	2.31	0.50
1:B:362:LYS:H	1:B:362:LYS:CD	2.25	0.50
1:B:40:LEU:C	1:B:316:ARG:NH1	2.65	0.50
1:A:50:ARG:H	1:A:112:GLN:HE22	1.58	0.50
1:A:33:ARG:HG3	4:A:554:HOH:O	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:CYS:CB	4:B:560:HOH:O	2.53	0.50
1:A:7:ILE:HD13	1:A:123:ALA:HB1	1.94	0.50
1:B:300:TYR:HD2	1:B:347:MET:CE	2.23	0.49
1:B:7:ILE:HD12	1:B:7:ILE:N	2.26	0.49
1:A:272:ASN:H	1:A:353:ASP:CG	2.15	0.49
1:A:16:ARG:CZ	1:A:26:PRO:HG3	2.41	0.49
1:B:318:VAL:N	4:B:560:HOH:O	2.45	0.49
1:A:362:LYS:N	1:A:362:LYS:HD3	2.27	0.49
1:A:2:LYS:C	4:A:510:HOH:O	2.49	0.49
1:A:229:ASN:ND2	1:A:358:GLY:H	2.11	0.49
1:B:272:ASN:H	1:B:353:ASP:CG	2.16	0.49
1:A:108:GLY:O	1:A:112:GLN:HG3	2.12	0.49
1:A:31:LEU:HG	4:A:691:HOH:O	2.12	0.49
1:A:109:SER:HA	1:A:112:GLN:HE21	1.78	0.49
1:A:155:ARG:NH2	4:A:580:HOH:O	2.45	0.49
1:A:7:ILE:HD12	1:A:7:ILE:N	2.27	0.49
1:B:88:ILE:CB	4:B:593:HOH:O	2.49	0.48
1:A:334:ASP:OD1	4:A:566:HOH:O	2.20	0.48
1:A:310:TRP:CE2	1:A:314:SER:OG	2.66	0.48
1:B:334:ASP:OD2	4:B:655:HOH:O	2.19	0.48
1:A:3:LYS:HA	4:A:510:HOH:O	2.13	0.48
1:A:322:LEU:HB3	4:A:599:HOH:O	2.13	0.48
1:A:166:ASP:OD2	1:A:254:GLN:HG2	2.13	0.48
1:A:373:ALA:HB2	4:A:591:HOH:O	2.12	0.48
1:B:362:LYS:N	1:B:362:LYS:CD	2.76	0.48
1:B:363:GLU:HB2	4:B:635:HOH:O	2.14	0.48
1:B:298:HIS:HD2	1:B:301:ALA:H	1.61	0.48
1:B:169:ALA:O	1:B:192:GLN:HG3	2.14	0.48
1:A:322:LEU:CD1	4:A:599:HOH:O	2.62	0.48
1:B:204:PHE:CZ	4:B:634:HOH:O	2.55	0.47
1:A:63:GLU:HG3	1:A:67:ASN:HD21	1.78	0.47
1:B:44:LYS:HD3	1:B:44:LYS:C	2.34	0.47
1:B:339:ASP:HB3	1:B:342:VAL:CG1	2.45	0.47
1:A:15:TYR:CD1	4:A:702:HOH:O	2.55	0.47
1:B:63:GLU:HG3	1:B:67:ASN:HD21	1.79	0.47
1:A:339:ASP:HB3	1:A:342:VAL:CG1	2.45	0.47
1:B:344:ARG:HB3	1:B:347:MET:HE1	1.95	0.47
1:A:156:LYS:CE	4:A:531:HOH:O	2.59	0.47
1:A:337:GLU:HG2	1:A:342:VAL:CG2	2.32	0.47
1:B:310:TRP:CE2	1:B:314:SER:OG	2.68	0.47
1:A:155:ARG:CZ	4:A:580:HOH:O	2.63	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLN:HE21	1:A:256:GLY:H	1.52	0.46
1:B:3:LYS:HE2	4:B:731:HOH:O	2.15	0.46
1:A:171:HIS:HB2	1:A:191:HIS:CD2	2.50	0.46
1:A:342:VAL:O	1:A:343:ASP:HB3	2.15	0.46
1:B:229:ASN:HD22	1:B:358:GLY:H	1.62	0.46
1:A:248:PRO:HD3	4:A:692:HOH:O	2.16	0.46
1:A:152:GLU:CD	4:A:705:HOH:O	2.53	0.46
1:A:248:PRO:CD	4:A:692:HOH:O	2.64	0.46
1:B:48:LYS:NZ	4:B:682:HOH:O	2.39	0.46
1:B:50:ARG:H	1:B:112:GLN:HE22	1.64	0.46
1:A:7:ILE:CD1	1:A:123:ALA:HB1	2.45	0.46
1:B:369:GLU:CD	4:B:726:HOH:O	2.54	0.46
1:A:325:LYS:CE	1:A:325:LYS:N	2.58	0.46
1:A:40:LEU:C	1:A:316:ARG:NH1	2.69	0.46
1:B:171:HIS:HB2	1:B:191:HIS:CD2	2.50	0.46
1:A:140:GLY:HA3	4:A:617:HOH:O	2.16	0.46
1:B:335:PHE:O	1:B:336:GLU:CB	2.63	0.46
1:B:230:GLU:HG2	1:B:360:VAL:HA	1.97	0.46
1:B:190:LEU:HD22	1:B:220:ILE:HB	1.98	0.45
1:A:331:LYS:HB3	1:A:331:LYS:NZ	2.32	0.45
1:B:311:CYS:SG	4:B:560:HOH:O	2.61	0.45
1:B:342:VAL:O	1:B:343:ASP:HB3	2.16	0.45
1:A:190:LEU:HD22	1:A:220:ILE:HB	1.99	0.45
1:A:258:ASP:N	1:A:259:PRO:CD	2.80	0.45
1:A:21:HIS:O	1:A:24:LYS:HD2	2.17	0.45
1:B:84:GLU:CD	1:B:84:GLU:N	2.69	0.45
1:B:7:ILE:CD1	1:B:123:ALA:HB1	2.46	0.45
1:A:44:LYS:C	1:A:44:LYS:HD3	2.36	0.45
1:A:169:ALA:O	1:A:192:GLN:HG3	2.17	0.45
1:B:369:GLU:CG	4:B:639:HOH:O	2.63	0.45
1:A:298:HIS:HD2	1:A:301:ALA:H	1.64	0.45
1:A:335:PHE:O	1:A:336:GLU:CB	2.64	0.45
1:A:156:LYS:HG3	4:A:664:HOH:O	2.15	0.45
1:A:84:GLU:CD	1:A:84:GLU:N	2.70	0.45
1:A:244:GLU:O	1:A:244:GLU:HG2	2.17	0.45
1:A:297:TYR:N	1:A:297:TYR:CD1	2.84	0.45
1:A:362:LYS:CD	1:A:362:LYS:H	2.30	0.44
1:B:322:LEU:HD13	4:B:561:HOH:O	2.17	0.44
1:A:168:ASP:HB2	1:A:254:GLN:NE2	2.32	0.44
1:A:321:LYS:CB	4:A:543:HOH:O	2.59	0.44
1:B:258:ASP:N	1:B:259:PRO:CD	2.81	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASN:HB2	4:A:656:HOH:O	2.16	0.44
1:A:74:ARG:HD3	4:A:666:HOH:O	2.17	0.44
1:A:362:LYS:CD	1:A:362:LYS:N	2.80	0.44
1:B:235:LEU:HD22	1:B:239:LEU:HG	2.00	0.44
1:B:261:LEU:HA	1:B:269:ASN:HA	1.99	0.44
1:B:229:ASN:ND2	1:B:358:GLY:H	2.16	0.44
1:B:304:ARG:O	4:B:742:HOH:O	2.21	0.44
1:B:244:GLU:HG2	1:B:244:GLU:O	2.17	0.44
1:B:168:ASP:HB2	1:B:254:GLN:NE2	2.32	0.44
1:A:12:TYR:CG	4:A:614:HOH:O	2.56	0.44
1:A:333:ILE:HG22	1:A:334:ASP:N	2.32	0.44
1:B:89:GLY:CA	4:B:752:HOH:O	2.65	0.43
1:A:261:LEU:HA	1:A:269:ASN:HA	2.00	0.43
1:B:6:LEU:HB2	1:B:310:TRP:CZ3	2.53	0.43
1:A:168:ASP:HB2	1:A:254:GLN:CD	2.39	0.43
1:B:35:LYS:CB	1:B:35:LYS:NZ	2.80	0.43
1:B:129:GLY:N	1:B:146:ASN:HD21	2.16	0.43
1:B:333:ILE:HG22	1:B:334:ASP:N	2.33	0.43
1:B:21:HIS:O	1:B:24:LYS:HD2	2.18	0.43
1:A:252:LEU:HG	1:A:290:VAL:HB	2.01	0.43
1:A:28:VAL:HB	4:A:614:HOH:O	2.18	0.43
1:B:252:LEU:HG	1:B:290:VAL:HB	2.00	0.43
1:B:276:LEU:CD2	4:B:737:HOH:O	2.66	0.43
1:A:230:GLU:HG2	1:A:360:VAL:HA	2.01	0.43
1:B:272:ASN:HB3	1:B:308:LEU:CD1	2.48	0.42
1:A:163:LEU:HD21	1:A:165:ILE:HD11	2.00	0.42
1:B:14:LYS:NZ	4:B:707:HOH:O	2.51	0.42
1:A:6:LEU:C	1:A:6:LEU:HD13	2.39	0.42
1:B:74:ARG:NH1	1:B:74:ARG:HG3	2.34	0.42
1:A:155:ARG:HB2	4:A:531:HOH:O	2.20	0.42
1:A:31:LEU:HD22	1:A:35:LYS:CE	2.34	0.42
1:B:334:ASP:OD1	1:B:334:ASP:O	2.38	0.42
1:B:318:VAL:HA	4:B:560:HOH:O	2.19	0.42
1:B:146:ASN:N	1:B:147:PRO:CD	2.83	0.42
1:B:298:HIS:CD2	1:B:301:ALA:H	2.37	0.42
1:B:373:ALA:O	4:B:553:HOH:O	2.21	0.42
1:A:235:LEU:HD22	1:A:239:LEU:HG	2.01	0.42
1:B:6:LEU:C	1:B:6:LEU:HD13	2.40	0.42
1:B:331:LYS:NZ	1:B:331:LYS:HB3	2.35	0.42
1:A:344:ARG:HB3	1:A:347:MET:HE1	1.99	0.42
1:A:29:SER:HB3	4:A:583:HOH:O	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD21	4:A:691:HOH:O	2.19	0.42
1:B:264:TYR:HH	1:B:337:GLU:HG3	1.85	0.42
1:B:318:VAL:CA	4:B:560:HOH:O	2.68	0.42
1:B:168:ASP:HB2	1:B:254:GLN:CD	2.40	0.41
1:B:276:LEU:O	1:B:279:PHE:HB3	2.20	0.41
1:B:370:LYS:NZ	4:B:574:HOH:O	2.51	0.41
1:A:6:LEU:HB2	1:A:310:TRP:CZ3	2.55	0.41
1:A:74:ARG:HG3	1:A:74:ARG:NH1	2.35	0.41
1:A:335:PHE:CG	1:A:336:GLU:N	2.88	0.41
1:A:225:GLY:HA2	1:A:269:ASN:ND2	2.35	0.41
1:B:146:ASN:ND2	1:B:147:PRO:HD3	2.35	0.41
1:B:140:GLY:O	1:B:141:PHE:CB	2.68	0.41
1:A:6:LEU:O	1:A:46:LEU:HD12	2.19	0.41
1:A:339:ASP:O	1:A:342:VAL:HG13	2.21	0.41
1:B:279:PHE:CZ	1:B:283:ARG:HD2	2.56	0.41
1:A:67:ASN:HA	4:A:654:HOH:O	2.19	0.41
1:A:19:LYS:CD	1:A:20:ASN:H	2.34	0.41
1:A:297:TYR:OH	3:A:502:TSN:O2	2.32	0.41
1:B:322:LEU:CD1	4:B:561:HOH:O	2.68	0.41
1:A:183:ASP:HB3	1:A:212:LYS:O	2.21	0.41
1:A:140:GLY:O	1:A:141:PHE:CB	2.69	0.41
1:A:316:ARG:CZ	4:A:535:HOH:O	2.67	0.41
1:B:322:LEU:CD1	4:B:703:HOH:O	2.66	0.41
1:A:131:HIS:HD1	1:A:172:CYS:HB3	1.85	0.41
1:A:306:TRP:CB	4:A:691:HOH:O	2.66	0.41
1:B:339:ASP:O	1:B:342:VAL:HG13	2.21	0.41
1:B:308:LEU:CD1	4:B:737:HOH:O	2.57	0.41
1:B:272:ASN:ND2	4:B:570:HOH:O	2.53	0.41
1:B:276:LEU:HD11	1:B:312:GLU:HG2	2.02	0.41
1:A:229:ASN:HD22	1:A:358:GLY:N	2.17	0.41
1:B:224:LYS:CE	4:B:598:HOH:O	2.68	0.41
1:B:171:HIS:CD2	1:B:191:HIS:CE1	3.09	0.41
1:A:12:TYR:HD2	4:A:702:HOH:O	2.04	0.40
1:A:276:LEU:O	1:A:279:PHE:HB3	2.21	0.40
1:A:146:ASN:N	1:A:147:PRO:CD	2.84	0.40
1:B:6:LEU:O	1:B:46:LEU:HD12	2.20	0.40
1:A:21:HIS:HE1	1:A:92:GLU:O	2.04	0.40
1:A:28:VAL:CG2	4:A:614:HOH:O	2.70	0.40
1:B:152:GLU:OE2	1:B:152:GLU:HA	2.22	0.40
1:A:272:ASN:HB3	1:A:308:LEU:CD1	2.52	0.40
1:A:61:HIS:HB2	1:A:66:ILE:HD11	2.04	0.40

All (1) 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)
4:A:543:HOH:O	4:A:553:HOH:O[1_655]	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	370/375 (99%)	348 (94%)	20 (5%)	2 (0%)	34	26
1	B	370/375 (99%)	350 (95%)	18 (5%)	2 (0%)	34	26
All	All	740/750 (99%)	698 (94%)	38 (5%)	4 (0%)	34	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	B	19	LYS
1	A	336	GLU
1	B	336	GLU

### 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	317/321 (99%)	304 (96%)	13 (4%)	37	32
1	B	317/321 (99%)	304 (96%)	13 (4%)	37	32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	634/642 (99%)	608 (96%)	26 (4%)	37	32

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	24	LYS
1	A	30	LEU
1	A	31	LEU
1	A	84	GLU
1	A	131	HIS
1	A	218	LEU
1	A	235	LEU
1	A	247	GLU
1	A	254	GLN
1	A	321	LYS
1	A	325	LYS
1	A	355	TRP
1	B	19	LYS
1	B	24	LYS
1	B	30	LEU
1	B	31	LEU
1	B	84	GLU
1	B	131	HIS
1	B	218	LEU
1	B	235	LEU
1	B	247	GLU
1	B	254	GLN
1	B	321	LYS
1	B	325	LYS
1	B	355	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	61	HIS
1	A	112	GLN
1	A	146	ASN
1	A	217	ASN
1	A	229	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	254	GLN
1	A	272	ASN
1	B	21	HIS
1	B	61	HIS
1	B	112	GLN
1	B	146	ASN
1	B	217	ASN
1	B	229	ASN
1	B	254	GLN
1	B	272	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	TSN	A	502	2	21,22,22	1.33	4 (19%)	23,29,29	1.00	0
3	TSN	B	504	2	21,22,22	1.42	3 (14%)	23,29,29	1.02	1 (4%)

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	TSN	A	502	2	-	0/23/23/23	0/1/1/1
3	TSN	B	504	2	-	0/23/23/23	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	TSN	C5-C4	2.08	1.43	1.39
3	A	502	TSN	C6-C1	2.26	1.43	1.39
3	A	502	TSN	C13-N1	2.27	1.37	1.33
3	B	504	TSN	C5-C4	2.55	1.44	1.39
3	B	504	TSN	C6-C1	2.70	1.43	1.39
3	A	502	TSN	C3-C4	3.21	1.45	1.39
3	B	504	TSN	C3-C4	3.66	1.46	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504	TSN	C3-C2-C1	2.13	123.23	120.76

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
3	A	502	TSN	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 ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.