



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:30 PM GMT

PDB ID : 1FWX
Title : CRYSTAL STRUCTURE OF NITROUS OXIDE REDUCTASE FROM P. DENITRIFICANS
Authors : Brown, K.; Djinovic-Carugo, K.; Haltia, T.; Cabrito, I.; Saraste, M.; Moura, J.J.; Moura, I.; Tegoni, M.; Cambillau, C.
Deposited on : 2000-09-25
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ 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) : 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

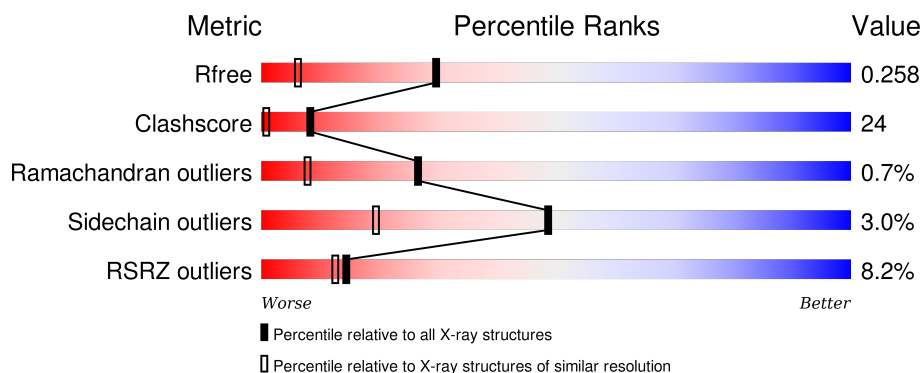
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	595	<div> <div>4%</div> <div>73% 25% ..</div> </div>
1	B	595	<div> <div>2%</div> <div>75% 21% ..</div> </div>
1	C	595	<div> <div>7%</div> <div>68% 28% ..</div> </div>
1	D	595	<div> <div>21%</div> <div>55% 41% ..</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	A	4904	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 21176 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 NITROUS OXIDE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4633	2913	796	892	32			
1	B	589	Total	C	N	O	S	0	0	0
			4619	2904	793	890	32			
1	C	590	Total	C	N	O	S	0	0	0
			4628	2910	795	891	32			
1	D	588	Total	C	N	O	S	0	0	0
			4611	2900	792	887	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	VAL	ALA	see remark 999	UNP Q51705
A	8	ALA	GLY	see remark 999	UNP Q51705
B	291	VAL	ALA	see remark 999	UNP Q51705
B	8	ALA	GLY	see remark 999	UNP Q51705
C	291	VAL	ALA	see remark 999	UNP Q51705
C	8	ALA	GLY	see remark 999	UNP Q51705
D	291	VAL	ALA	see remark 999	UNP Q51705
D	8	ALA	GLY	see remark 999	UNP Q51705

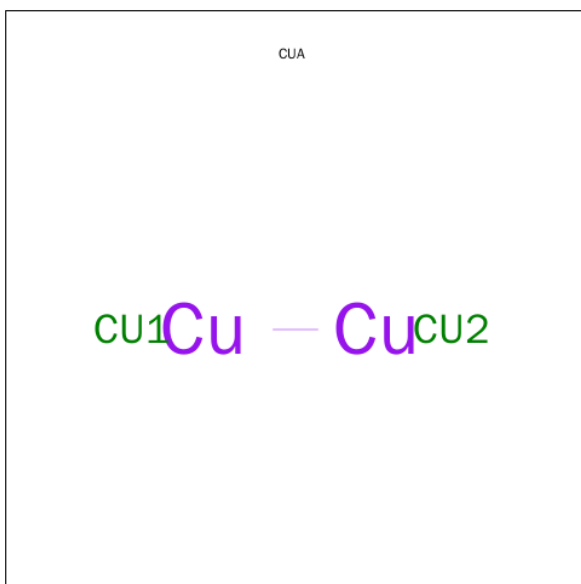
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

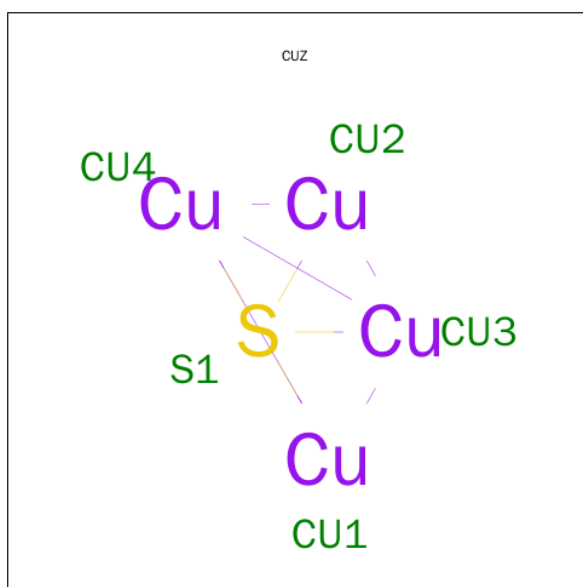
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Ca 3	0	0
3	A	3	Total 3	Ca 3	0	0
3	D	2	Total 2	Ca 2	0	0
3	C	3	Total 3	Ca 3	0	0

- Molecule 4 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 5 is (MU-4-SULFIDO)-TETRA-NUCLEAR COPPER ION (three-letter code: CUZ) (formula: Cu₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Cu	S	0	0
			5	4	1		
5	B	1	Total	Cu	S	0	0
			5	4	1		
5	C	1	Total	Cu	S	0	0
			5	4	1		
5	D	1	Total	Cu	S	0	0
			5	4	1		

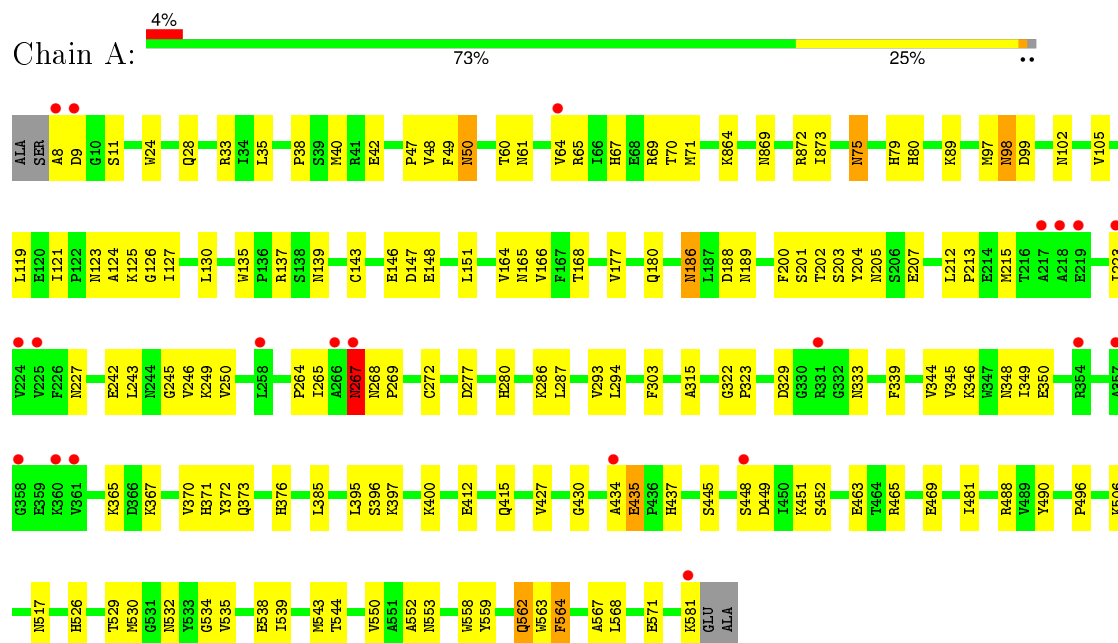
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	724	Total	O	0	0
			724	724		
6	B	750	Total	O	0	0
			750	750		
6	C	657	Total	O	0	0
			657	657		
6	D	511	Total	O	0	0
			511	511		

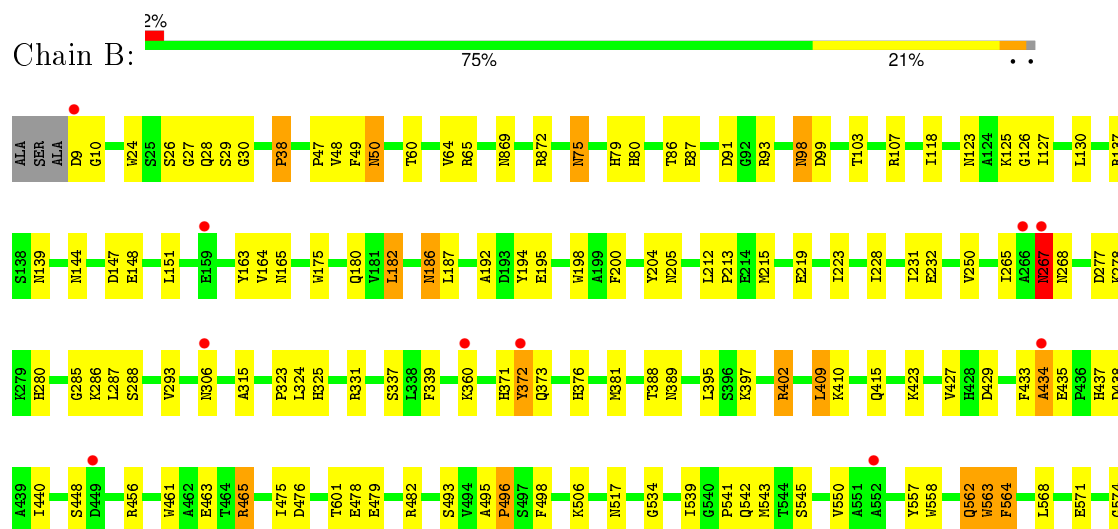
3 Residue-property plots

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.

• Molecule 1: NITROUS OXIDE REDUCTASE

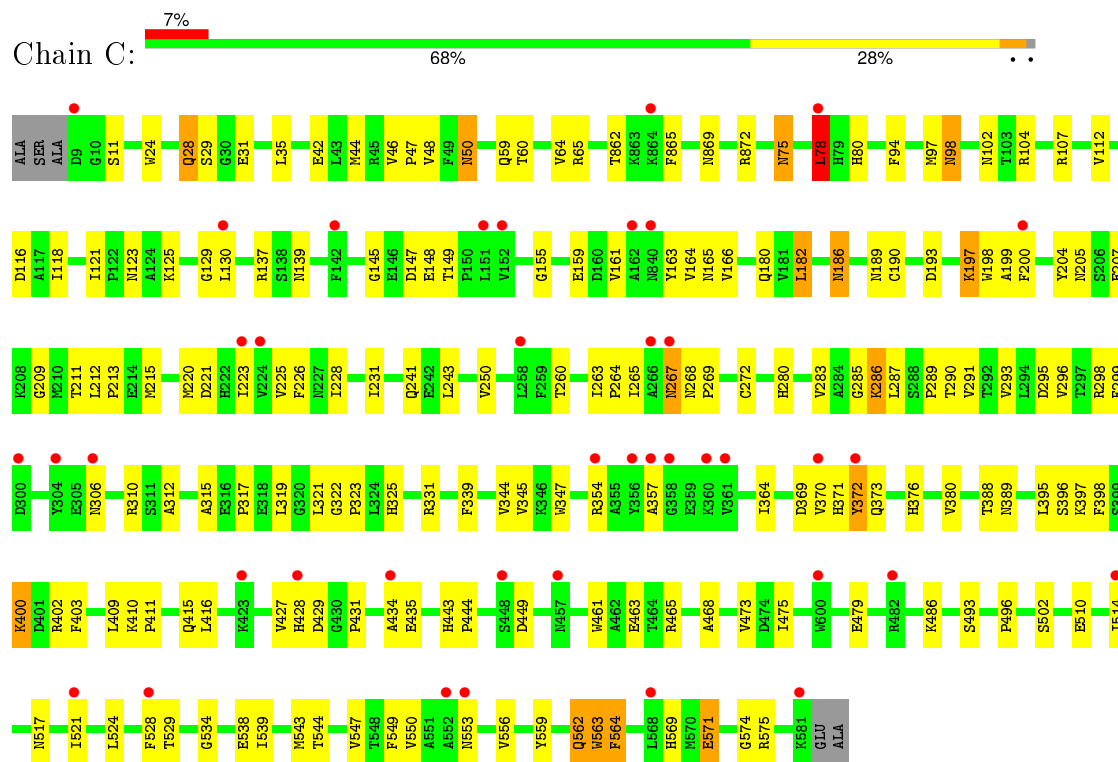


• Molecule 1: NITROUS OXIDE REDUCTASE

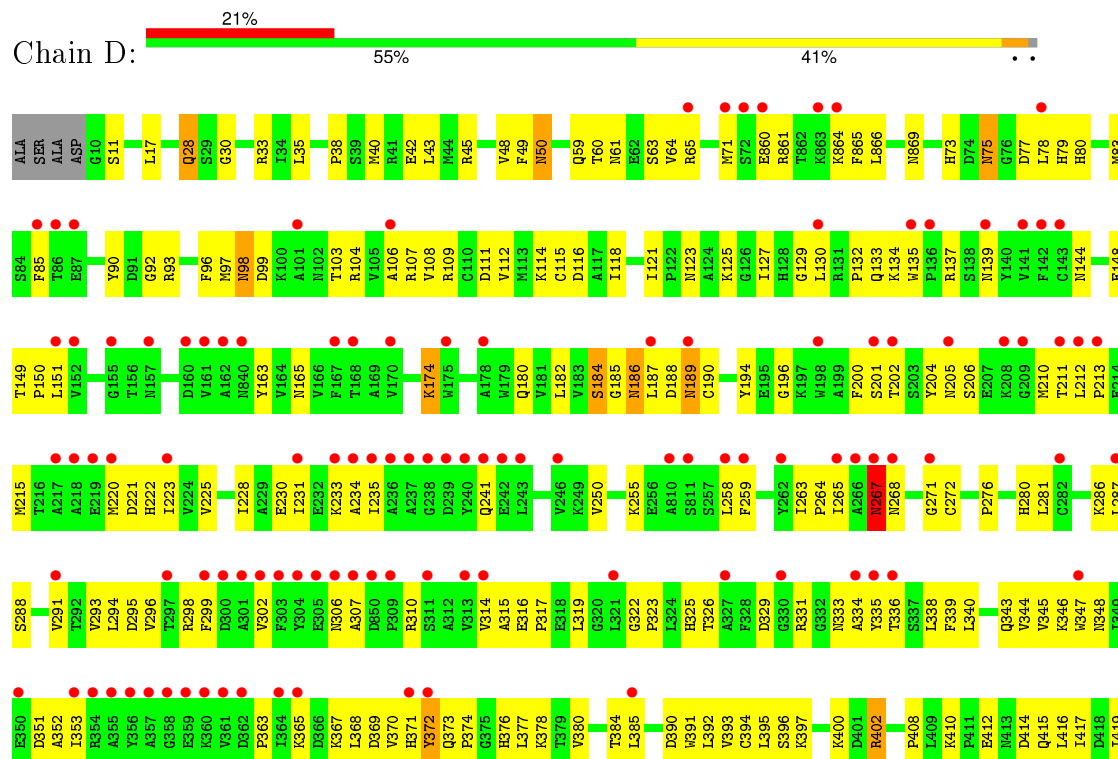


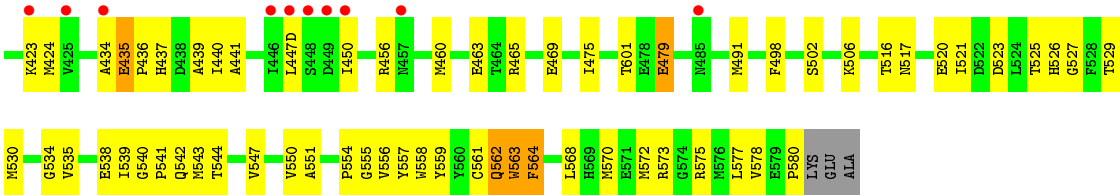


● Molecule 1: NITROUS OXIDE REDUCTASE



● Molecule 1: NITROUS OXIDE REDUCTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.59 Å 105.09 Å 116.70 Å 90.00° 110.69° 90.00°	Depositor
Resolution (Å)	29.83 – 1.60 29.82 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.4 (29.83-1.60) 89.5 (29.82-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.60 Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.241 , 0.264 0.239 , 0.258	Depositor DCC
R_{free} test set	1331 reflections (0.49%)	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 272420 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21176	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, CUZ, CUA, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/4744	0.71	2/6443 (0.0%)
1	B	0.35	0/4730	0.73	2/6425 (0.0%)
1	C	0.32	0/4739	0.70	5/6436 (0.1%)
1	D	0.30	0/4722	0.64	1/6414 (0.0%)
All	All	0.33	0/18935	0.69	10/25718 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	GLU	N-CA-C	10.92	140.48	111.00
1	C	435	GLU	N-CA-C	10.26	138.70	111.00
1	A	435	GLU	N-CA-C	9.79	137.44	111.00
1	B	267	ASN	N-CA-C	7.73	131.88	111.00
1	C	267	ASN	N-CA-C	7.54	131.37	111.00
1	D	435	GLU	N-CA-C	7.18	130.39	111.00
1	A	267	ASN	N-CA-C	6.84	129.46	111.00
1	C	449	ASP	CB-CA-C	-6.35	97.71	110.40
1	C	78	LEU	CA-CB-CG	5.09	127.02	115.30
1	C	145	GLY	N-CA-C	-5.01	100.58	113.10

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	4633	0	4443	180	0
1	B	4619	0	4425	156	0
1	C	4628	0	4438	234	0
1	D	4611	0	4421	347	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	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	724	0	0	83	0
6	B	750	0	0	67	0
6	C	657	0	0	127	0
6	D	511	0	0	203	0
All	All	21176	0	17727	879	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 24.

All (879) 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:326:THR:HG22	1:D:336:THR:HG22	1.19	1.14
1:B:456:ARG:HA	6:B:6235:HOH:O	1.54	1.04
1:D:547:VAL:HA	6:D:8122:HOH:O	1.58	1.04
1:D:71:MET:SD	6:D:8077:HOH:O	2.18	1.02
1:C:215:MET:HG2	6:C:7335:HOH:O	1.59	1.01
1:D:540:GLY:HA2	6:D:8240:HOH:O	1.59	1.01
1:D:860:GLU:HG3	1:D:864:LYS:HE2	1.44	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:SER:HB3	6:D:8189:HOH:O	1.63	0.99
1:A:550:VAL:H	1:B:869:ASN:HD21	1.10	0.98
1:D:392:LEU:HB3	6:D:8101:HOH:O	1.62	0.97
1:D:336:THR:HG23	1:D:347:TRP:HE1	1.29	0.97
1:B:371:HIS:H	1:B:415:GLN:HE22	1.07	0.96
1:C:553:ASN:ND2	1:D:865:PHE:HB2	1.80	0.96
1:D:540:GLY:HA3	6:D:8169:HOH:O	1.65	0.95
1:D:541:PRO:HD3	6:D:8240:HOH:O	1.64	0.95
1:C:104:ARG:HA	6:C:6962:HOH:O	1.66	0.94
1:D:371:HIS:H	1:D:415:GLN:HE22	1.02	0.94
1:C:28:GLN:HE21	1:C:28:GLN:H	1.04	0.94
1:D:134:LYS:HB2	6:D:8275:HOH:O	1.67	0.93
1:D:502:SER:HA	6:D:7910:HOH:O	1.67	0.93
1:A:105:VAL:HG22	6:A:5276:HOH:O	1.68	0.92
1:D:578:VAL:HB	6:D:7861:HOH:O	1.70	0.92
1:A:371:HIS:H	1:A:415:GLN:HE22	1.02	0.92
1:D:416:LEU:HA	6:D:8178:HOH:O	1.68	0.92
1:C:291:VAL:HG21	6:C:7096:HOH:O	1.69	0.91
1:B:148:GLU:HG3	1:B:165:ASN:HD21	1.36	0.91
1:D:210:MET:HB3	6:D:8300:HOH:O	1.70	0.91
1:D:194:TYR:HA	6:D:8275:HOH:O	1.70	0.91
1:D:28:GLN:H	1:D:28:GLN:HE21	1.15	0.91
1:C:129:GLY:HA3	6:C:7014:HOH:O	1.69	0.90
1:C:121:ILE:HG12	6:C:6962:HOH:O	1.71	0.90
1:B:65:ARG:HD2	1:B:463:GLU:OE2	1.71	0.90
1:C:371:HIS:H	1:C:415:GLN:HE22	1.10	0.90
1:D:371:HIS:H	1:D:415:GLN:NE2	1.70	0.90
1:A:452:SER:HA	6:B:6426:HOH:O	1.70	0.89
1:A:137:ARG:HH11	1:A:139:ASN:ND2	1.70	0.89
1:C:250:VAL:HB	6:C:7063:HOH:O	1.72	0.89
1:A:371:HIS:H	1:A:415:GLN:NE2	1.71	0.88
1:C:31:GLU:HB3	6:C:7454:HOH:O	1.73	0.88
1:A:69:ARG:HB3	6:A:5290:HOH:O	1.74	0.88
1:C:403:PHE:HA	6:C:7395:HOH:O	1.75	0.87
1:A:188:ASP:HB3	6:A:5348:HOH:O	1.73	0.87
1:A:869:ASN:HD21	1:B:550:VAL:H	1.17	0.87
1:C:869:ASN:HD21	1:D:550:VAL:H	1.22	0.87
1:C:241:GLN:HG3	6:C:7063:HOH:O	1.75	0.86
1:B:381:MET:HB2	6:B:6223:HOH:O	1.76	0.85
1:D:577:LEU:HD11	6:D:7871:HOH:O	1.76	0.85
1:A:49:PHE:HB3	6:A:5395:HOH:O	1.77	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASN:H	1:B:50:ASN:HD22	1.25	0.84
1:B:388:THR:HG23	6:B:6223:HOH:O	1.76	0.84
1:D:371:HIS:N	1:D:415:GLN:HE22	1.76	0.83
1:C:296:VAL:HB	6:C:7268:HOH:O	1.77	0.83
1:C:220:MET:HB3	6:C:6998:HOH:O	1.77	0.83
1:D:267:ASN:HB3	1:D:287:LEU:HB2	1.59	0.83
1:C:161:VAL:HG23	6:C:7192:HOH:O	1.77	0.83
1:D:48:VAL:HG11	6:D:8262:HOH:O	1.77	0.83
1:D:137:ARG:HH11	1:D:139:ASN:ND2	1.77	0.82
1:C:371:HIS:H	1:C:415:GLN:NE2	1.77	0.82
1:C:272:CYS:HB2	6:C:7324:HOH:O	1.80	0.82
1:A:50:ASN:HD22	1:A:50:ASN:H	1.28	0.81
1:C:486:LYS:HE2	6:C:7391:HOH:O	1.79	0.81
1:C:207:GLU:HB2	6:C:7143:HOH:O	1.79	0.81
1:B:9:ASP:OD1	1:B:10:GLY:N	2.13	0.81
1:C:289:PRO:HB3	6:C:7383:HOH:O	1.79	0.81
1:B:195:GLU:HA	6:B:6421:HOH:O	1.79	0.81
1:C:225:VAL:HG12	6:C:7399:HOH:O	1.81	0.81
1:C:155:GLY:HA3	6:D:7911:HOH:O	1.79	0.81
1:C:228:ILE:HG13	6:C:7373:HOH:O	1.79	0.80
1:A:371:HIS:N	1:A:415:GLN:HE22	1.79	0.80
1:A:448:SER:OG	6:A:5439:HOH:O	1.99	0.80
1:D:346:LYS:HD2	6:D:8187:HOH:O	1.81	0.80
1:B:123:ASN:HD22	1:B:180:GLN:HE22	1.29	0.80
1:C:123:ASN:HD22	1:C:180:GLN:HE22	1.27	0.80
1:A:148:GLU:HG3	1:A:165:ASN:HD21	1.45	0.80
1:A:168:THR:HB	6:A:5258:HOH:O	1.81	0.80
1:C:78:LEU:HD13	1:C:97:MET:HB2	1.62	0.80
1:D:535:VAL:HG22	6:D:8251:HOH:O	1.82	0.80
1:C:189:ASN:HB2	6:C:7324:HOH:O	1.82	0.79
1:C:286:LYS:HB3	6:C:7413:HOH:O	1.83	0.79
1:D:296:VAL:HG13	6:D:7891:HOH:O	1.82	0.79
1:D:302:VAL:HG22	6:D:8026:HOH:O	1.81	0.79
1:D:419:ILE:HG23	6:D:8101:HOH:O	1.81	0.78
1:C:321:LEU:HA	6:C:7383:HOH:O	1.82	0.78
1:B:148:GLU:HB2	6:B:6532:HOH:O	1.82	0.78
1:B:371:HIS:H	1:B:415:GLN:NE2	1.81	0.78
1:D:557:TYR:HE2	6:D:7861:HOH:O	1.67	0.78
1:A:143:CYS:SG	6:A:5258:HOH:O	2.41	0.78
1:D:353:ILE:HD11	6:D:8029:HOH:O	1.84	0.78
1:D:294:LEU:HD12	6:D:8132:HOH:O	1.82	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:GLU:HG2	6:D:8066:HOH:O	1.84	0.77
1:D:71:MET:CG	6:D:7990:HOH:O	2.32	0.77
1:A:177:VAL:HG11	1:A:246:VAL:HG21	1.67	0.77
1:A:564:PHE:HE1	6:A:5572:HOH:O	1.68	0.77
1:D:137:ARG:HH11	1:D:139:ASN:HD22	1.30	0.76
1:C:410:LYS:HD3	6:C:7235:HOH:O	1.84	0.76
1:A:180:GLN:HB2	6:A:5552:HOH:O	1.85	0.76
1:D:377:LEU:HD22	6:D:8047:HOH:O	1.86	0.76
1:C:107:ARG:HD2	1:C:116:ASP:OD2	1.83	0.76
1:A:67:HIS:HB3	6:A:5517:HOH:O	1.85	0.76
1:D:310:ARG:HG2	6:D:8052:HOH:O	1.85	0.76
1:B:198:TRP:HA	1:B:228:ILE:HD13	1.68	0.76
1:D:223:ILE:HG23	1:D:265:ILE:HG13	1.66	0.76
1:A:488:ARG:HB2	6:A:5225:HOH:O	1.85	0.76
1:C:198:TRP:HB3	6:C:7338:HOH:O	1.85	0.75
1:C:228:ILE:HD13	6:C:6839:HOH:O	1.87	0.75
1:D:125:LYS:HG3	1:D:149:THR:HG21	1.68	0.75
1:D:220:MET:HB3	6:D:8039:HOH:O	1.85	0.75
1:D:225:VAL:HG12	6:D:8065:HOH:O	1.85	0.75
1:D:35:LEU:HD13	1:D:42:GLU:HA	1.68	0.75
1:B:267:ASN:HB3	1:B:287:LEU:HB2	1.68	0.75
1:A:137:ARG:HH11	1:A:139:ASN:HD22	1.35	0.75
1:D:393:VAL:HA	6:D:8178:HOH:O	1.87	0.74
1:B:192:ALA:HA	6:B:6515:HOH:O	1.86	0.74
1:A:207:GLU:HB2	6:A:5455:HOH:O	1.87	0.74
1:C:550:VAL:H	1:D:869:ASN:HD21	1.35	0.74
1:C:243:LEU:HG	6:C:7063:HOH:O	1.87	0.74
1:C:50:ASN:H	1:C:50:ASN:HD22	1.32	0.74
1:D:115:CYS:SG	6:D:7943:HOH:O	2.46	0.74
1:D:271:GLY:HA2	6:D:7996:HOH:O	1.87	0.74
1:D:543:MET:HE3	6:D:8169:HOH:O	1.88	0.74
1:A:202:THR:HB	6:A:5348:HOH:O	1.85	0.74
1:A:245:GLY:HA2	6:A:5568:HOH:O	1.88	0.74
1:A:123:ASN:HD22	1:A:180:GLN:HE22	1.36	0.74
1:C:347:TRP:HB3	6:C:6950:HOH:O	1.87	0.74
1:B:137:ARG:HH11	1:B:139:ASN:ND2	1.86	0.74
1:D:417:ILE:HB	6:D:8101:HOH:O	1.86	0.73
1:C:369:ASP:HB3	6:C:7452:HOH:O	1.87	0.73
1:D:259:PHE:HA	6:D:8093:HOH:O	1.88	0.73
1:A:89:LYS:HE2	6:A:5385:HOH:O	1.89	0.73
1:C:148:GLU:HG3	6:C:7424:HOH:O	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:ILE:HB	6:B:6389:HOH:O	1.88	0.73
1:D:106:ALA:HB1	6:D:7943:HOH:O	1.89	0.73
1:B:26:SER:OG	6:B:6545:HOH:O	2.07	0.73
1:A:250:VAL:HG22	6:A:5552:HOH:O	1.89	0.72
1:D:93:ARG:HA	6:D:8164:HOH:O	1.89	0.72
1:D:516:THR:HB	6:D:8011:HOH:O	1.88	0.72
1:A:125:LYS:HE3	6:B:6544:HOH:O	1.88	0.72
1:C:223:ILE:HG23	1:C:265:ILE:HG13	1.71	0.72
1:B:498:PHE:HA	6:B:6478:HOH:O	1.89	0.72
1:D:526:HIS:HB3	6:D:7895:HOH:O	1.89	0.72
1:D:465:ARG:HG2	1:D:475:ILE:HD11	1.72	0.72
1:A:272:CYS:HB2	6:A:5209:HOH:O	1.90	0.71
1:B:215:MET:HB2	6:B:6186:HOH:O	1.90	0.71
1:D:326:THR:HG22	1:D:336:THR:CG2	2.10	0.71
1:C:517:ASN:HB2	1:C:539:ILE:HG22	1.71	0.71
1:D:114:LYS:N	6:D:8146:HOH:O	2.21	0.71
1:C:148:GLU:HG2	6:C:7031:HOH:O	1.90	0.71
1:C:263:ILE:HG22	6:C:7066:HOH:O	1.89	0.71
1:C:118:ILE:HD11	6:C:7072:HOH:O	1.89	0.71
1:B:30:GLY:N	6:B:6545:HOH:O	2.19	0.71
1:D:348:ASN:O	6:D:8250:HOH:O	2.09	0.71
1:B:461:TRP:HZ2	6:B:6235:HOH:O	1.74	0.70
1:C:575:ARG:HD2	6:D:8300:HOH:O	1.90	0.70
1:D:112:VAL:HG22	6:D:8304:HOH:O	1.91	0.70
1:D:475:ILE:HA	6:D:8068:HOH:O	1.91	0.70
1:C:149:THR:HA	6:C:7140:HOH:O	1.91	0.70
1:A:550:VAL:H	1:B:869:ASN:ND2	1.88	0.70
1:D:108:VAL:HG13	6:D:8146:HOH:O	1.91	0.70
1:A:212:LEU:HA	6:A:5452:HOH:O	1.91	0.70
1:A:265:ILE:HD11	6:A:5520:HOH:O	1.89	0.70
1:B:87:GLU:HG3	6:B:6455:HOH:O	1.91	0.70
1:B:465:ARG:NH2	1:B:476:ASP:OD2	2.23	0.70
1:C:371:HIS:N	1:C:415:GLN:HE22	1.87	0.70
1:C:286:LYS:HA	6:C:7309:HOH:O	1.92	0.70
1:B:285:GLY:O	6:B:6340:HOH:O	2.08	0.70
1:C:521:ILE:HG23	1:C:524:LEU:HB2	1.74	0.70
1:D:866:LEU:HD11	6:D:8087:HOH:O	1.92	0.69
1:D:575:ARG:N	6:D:7910:HOH:O	2.22	0.69
1:A:11:SER:HA	6:A:5461:HOH:O	1.91	0.69
1:B:575:ARG:HD3	6:B:5931:HOH:O	1.91	0.69
1:D:230:GLU:HB2	6:D:8093:HOH:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:MET:HB3	6:D:7982:HOH:O	1.93	0.69
1:A:869:ASN:ND2	1:B:550:VAL:H	1.89	0.69
1:C:285:GLY:HA2	6:C:7279:HOH:O	1.91	0.68
1:D:336:THR:CG2	1:D:347:TRP:HE1	2.04	0.68
1:C:28:GLN:NE2	1:C:28:GLN:H	1.85	0.68
1:D:73:HIS:N	6:D:8087:HOH:O	2.26	0.68
1:D:97:MET:HG3	6:D:8262:HOH:O	1.93	0.68
1:B:231:ILE:HB	6:B:6166:HOH:O	1.94	0.68
1:B:187:LEU:HD22	6:B:6516:HOH:O	1.94	0.68
2:D:4908:CL:CL	6:D:7996:HOH:O	2.49	0.67
1:D:572:MET:HB3	6:D:7995:HOH:O	1.93	0.67
1:D:535:VAL:HG12	6:D:8198:HOH:O	1.94	0.67
1:C:148:GLU:CD	1:C:148:GLU:H	1.97	0.67
1:C:339:PHE:CE1	1:C:373:GLN:HB3	2.29	0.67
1:B:456:ARG:NH1	6:B:6235:HOH:O	2.28	0.67
1:C:212:LEU:HD11	1:D:568:LEU:HD13	1.76	0.67
1:A:202:THR:HG23	1:A:269:PRO:HG2	1.74	0.67
1:D:137:ARG:HB2	6:D:8246:HOH:O	1.95	0.67
1:B:557:TYR:HA	6:B:6544:HOH:O	1.93	0.67
1:A:70:THR:HG23	6:A:5290:HOH:O	1.94	0.67
1:A:348:ASN:HB2	1:A:365:LYS:HE3	1.76	0.67
1:C:293:VAL:HG13	6:C:7419:HOH:O	1.94	0.67
1:C:553:ASN:HD21	1:D:865:PHE:HB2	1.60	0.66
6:C:7165:HOH:O	1:D:149:THR:HB	1.94	0.66
1:D:78:LEU:HD13	1:D:97:MET:HB2	1.75	0.66
1:C:547:VAL:HG22	6:C:7415:HOH:O	1.95	0.66
1:D:402:ARG:HB3	6:D:8015:HOH:O	1.94	0.66
1:C:221:ASP:HB2	6:C:7427:HOH:O	1.96	0.66
1:D:109:ARG:HB3	6:D:8304:HOH:O	1.96	0.66
1:D:71:MET:HG2	6:D:7990:HOH:O	1.95	0.66
1:B:86:THR:HG23	6:B:6455:HOH:O	1.95	0.66
1:D:570:MET:HA	6:D:8201:HOH:O	1.96	0.66
1:D:61:ASN:N	6:D:8122:HOH:O	2.29	0.66
1:D:314:VAL:HG12	1:D:353:ILE:HG23	1.77	0.66
1:B:371:HIS:N	1:B:415:GLN:HE22	1.87	0.66
1:C:310:ARG:HG2	6:C:7066:HOH:O	1.94	0.66
1:D:351:ASP:HB2	6:D:8250:HOH:O	1.95	0.66
1:A:80:HIS:H	1:A:98:ASN:ND2	1.93	0.66
1:D:298:ARG:O	6:D:7928:HOH:O	2.13	0.65
1:B:456:ARG:NH2	6:B:6389:HOH:O	2.27	0.65
1:D:372:TYR:CD1	1:D:372:TYR:N	2.63	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:PHE:HB3	6:D:7946:HOH:O	1.94	0.65
1:C:199:ALA:N	6:C:7373:HOH:O	2.29	0.65
1:B:27:GLY:O	6:B:6545:HOH:O	2.14	0.65
1:C:865:PHE:HB2	6:C:7377:HOH:O	1.96	0.65
1:D:561:CYS:HB3	6:D:7995:HOH:O	1.95	0.65
1:D:415:GLN:HB2	6:D:8274:HOH:O	1.96	0.65
1:A:552:ALA:N	6:A:5417:HOH:O	2.29	0.65
1:A:127:ILE:HD12	6:A:5318:HOH:O	1.97	0.65
1:A:61:ASN:ND2	6:A:5221:HOH:O	2.29	0.65
1:D:365:LYS:HE3	6:D:7994:HOH:O	1.97	0.65
1:A:35:LEU:HD21	6:A:5511:HOH:O	1.97	0.65
1:D:416:LEU:HD12	6:D:8178:HOH:O	1.96	0.65
1:A:246:VAL:HG23	6:A:4947:HOH:O	1.96	0.65
1:A:567:ALA:HA	6:A:5572:HOH:O	1.97	0.65
1:C:312:ALA:HB2	6:C:7114:HOH:O	1.97	0.65
1:C:475:ILE:HD11	6:C:7081:HOH:O	1.97	0.64
1:D:121:ILE:HD12	1:D:127:ILE:HD13	1.79	0.64
1:C:534:GLY:HA2	1:D:75:ASN:HD21	1.63	0.64
1:D:228:ILE:HG13	6:D:8221:HOH:O	1.97	0.64
1:C:372:TYR:HB3	1:C:398:PHE:HB2	1.78	0.64
1:D:410:LYS:HD3	6:D:7898:HOH:O	1.96	0.64
1:C:121:ILE:N	6:C:6962:HOH:O	2.30	0.64
1:C:354:ARG:O	1:C:357:ALA:HB3	1.97	0.64
1:D:50:ASN:HD22	1:D:50:ASN:H	1.46	0.64
1:D:28:GLN:H	1:D:28:GLN:NE2	1.94	0.64
1:A:534:GLY:HA2	1:B:75:ASN:HD21	1.63	0.64
1:B:440:ILE:HG22	6:B:6224:HOH:O	1.98	0.64
1:C:268:ASN:N	1:C:269:PRO:HD3	2.12	0.64
1:D:121:ILE:HB	1:D:127:ILE:HD11	1.80	0.64
1:B:50:ASN:ND2	1:B:50:ASN:H	1.95	0.64
1:C:226:PHE:O	6:C:7373:HOH:O	2.15	0.64
1:C:46:VAL:HG22	6:C:7326:HOH:O	1.97	0.63
1:D:557:TYR:HB3	6:D:7992:HOH:O	1.99	0.63
1:C:265:ILE:N	6:C:6998:HOH:O	2.29	0.63
1:D:335:TYR:HE2	6:D:8187:HOH:O	1.81	0.63
6:A:5596:HOH:O	1:B:574:GLY:HA2	1.99	0.63
1:C:293:VAL:HB	1:C:315:ALA:HB3	1.81	0.63
1:D:265:ILE:N	6:D:8039:HOH:O	2.31	0.63
1:B:493:SER:HA	6:B:6478:HOH:O	1.98	0.63
1:C:280:HIS:HB3	6:C:7419:HOH:O	1.97	0.63
1:C:465:ARG:HB2	6:C:7081:HOH:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASN:ND2	1:A:50:ASN:H	1.96	0.63
1:D:447(D):LEU:O	1:D:450:ILE:HG13	1.98	0.63
1:D:397:LYS:HB3	6:D:7946:HOH:O	1.97	0.62
1:D:397:LYS:HD2	6:D:7946:HOH:O	1.99	0.62
1:A:137:ARG:NH1	1:A:139:ASN:HD22	1.98	0.62
1:D:542:GLN:HG2	6:D:7900:HOH:O	1.99	0.62
1:B:277:ASP:OD2	1:B:280:HIS:HD2	1.83	0.62
1:A:65:ARG:CZ	1:A:463:GLU:HG3	2.29	0.62
1:D:526:HIS:HB2	6:D:8220:HOH:O	2.00	0.62
1:D:45:ARG:HG3	6:D:8305:HOH:O	1.99	0.62
1:D:325:HIS:HB2	6:D:8047:HOH:O	1.99	0.62
1:D:395:LEU:HG	6:D:7989:HOH:O	1.99	0.62
1:A:581:LYS:HE3	6:A:5178:HOH:O	1.98	0.62
1:D:109:ARG:N	6:D:8146:HOH:O	2.33	0.62
1:A:535:VAL:HB	6:A:5306:HOH:O	1.99	0.62
1:B:339:PHE:CE1	1:B:373:GLN:HB3	2.35	0.62
1:C:65:ARG:HH11	1:C:463:GLU:HB2	1.65	0.62
1:A:75:ASN:HD21	1:B:534:GLY:HA2	1.64	0.61
1:A:143:CYS:O	6:A:5258:HOH:O	2.16	0.61
1:B:601:THR:HG22	1:B:479:GLU:H	1.64	0.61
1:A:269:PRO:O	6:A:5609:HOH:O	2.16	0.61
1:A:242:GLU:HG2	6:A:5568:HOH:O	2.01	0.61
1:A:212:LEU:HB3	1:A:213:PRO:HD3	1.83	0.61
1:A:215:MET:HB2	6:A:5452:HOH:O	1.99	0.61
1:D:554:PRO:HB2	6:D:7911:HOH:O	1.99	0.61
1:C:50:ASN:H	1:C:50:ASN:ND2	1.97	0.61
1:A:33:ARG:HB3	6:A:5511:HOH:O	2.00	0.61
1:C:44:MET:HG3	6:C:7326:HOH:O	2.01	0.61
1:D:575:ARG:HB2	6:D:7871:HOH:O	2.01	0.61
1:D:263:ILE:HG22	6:D:8052:HOH:O	2.01	0.61
1:C:211:THR:O	1:C:215:MET:HG3	2.01	0.61
1:C:112:VAL:HB	6:C:7106:HOH:O	2.00	0.61
1:A:530:MET:HB3	6:A:5306:HOH:O	2.01	0.61
1:C:28:GLN:N	1:C:28:GLN:HE21	1.88	0.61
1:D:302:VAL:HG23	6:D:7928:HOH:O	1.99	0.61
1:C:564:PHE:N	1:D:435:GLU:OE2	2.34	0.61
1:C:345:VAL:HG22	6:C:6950:HOH:O	2.00	0.61
1:B:437:HIS:HB3	6:B:6184:HOH:O	2.01	0.61
1:A:201:SER:HB3	6:A:5168:HOH:O	2.00	0.61
1:B:212:LEU:HD12	6:B:6186:HOH:O	2.00	0.60
1:D:65:ARG:HD2	1:D:463:GLU:OE2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HB3	6:A:5305:HOH:O	2.01	0.60
1:D:385:LEU:HD23	6:D:8292:HOH:O	2.01	0.60
1:C:50:ASN:CG	6:C:7454:HOH:O	2.38	0.60
1:A:168:THR:O	6:A:5258:HOH:O	2.17	0.60
1:D:866:LEU:CD1	6:D:8087:HOH:O	2.49	0.60
1:D:40:MET:HE2	6:D:8000:HOH:O	2.01	0.60
1:C:869:ASN:ND2	1:D:550:VAL:H	1.98	0.60
1:C:94:PHE:CE2	1:C:107:ARG:HD3	2.36	0.60
1:D:80:HIS:H	1:D:98:ASN:ND2	1.99	0.60
1:C:29:SER:O	6:C:7454:HOH:O	2.16	0.60
1:B:232:GLU:HG3	6:B:6381:HOH:O	2.01	0.60
1:D:465:ARG:HB3	6:D:8038:HOH:O	2.02	0.60
1:D:127:ILE:HG12	6:D:8234:HOH:O	2.01	0.60
1:B:80:HIS:H	1:B:98:ASN:ND2	2.00	0.60
1:B:123:ASN:HD22	1:B:180:GLN:NE2	1.99	0.60
1:B:107:ARG:NH1	6:B:6506:HOH:O	2.34	0.60
1:A:339:PHE:CE1	1:A:373:GLN:HB3	2.37	0.59
1:B:493:SER:OG	1:B:517:ASN:HA	2.03	0.59
1:D:393:VAL:HG22	6:D:8178:HOH:O	2.01	0.59
1:C:137:ARG:HH11	1:C:139:ASN:ND2	2.00	0.59
1:D:348:ASN:HB3	6:D:7994:HOH:O	2.01	0.59
1:D:502:SER:HB2	6:D:7871:HOH:O	2.01	0.59
1:C:575:ARG:CD	6:D:8300:HOH:O	2.47	0.59
1:A:8:ALA:O	1:A:9:ASP:HB2	2.02	0.59
1:B:402:ARG:HD3	1:B:429:ASP:OD2	2.03	0.59
1:A:873:ILE:HG22	6:A:5517:HOH:O	2.01	0.59
1:D:63:SER:HB2	6:D:8013:HOH:O	2.03	0.59
1:A:267:ASN:HB3	1:A:287:LEU:HB2	1.85	0.59
1:C:286:LYS:HE2	6:C:7413:HOH:O	2.01	0.58
1:D:520:GLU:HA	6:D:7900:HOH:O	2.02	0.58
1:D:148:GLU:H	1:D:148:GLU:CD	2.06	0.58
1:D:860:GLU:O	1:D:864:LYS:HG3	2.03	0.58
1:D:78:LEU:CD1	1:D:97:MET:HB2	2.33	0.58
1:D:233:LYS:HG3	1:D:234:ALA:N	2.19	0.58
1:A:562:GLN:HE21	1:A:562:GLN:H	1.52	0.58
1:D:440:ILE:HB	6:D:8141:HOH:O	2.03	0.58
1:B:517:ASN:HB2	1:B:539:ILE:HG22	1.86	0.58
6:C:7140:HOH:O	1:D:556:VAL:HG11	2.01	0.58
1:D:306:ASN:HB2	6:D:8116:HOH:O	2.03	0.58
1:B:60:THR:O	1:B:64:VAL:HG23	2.04	0.58
1:D:345:VAL:HG22	1:D:367:LYS:HG2	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ASN:HB3	1:C:287:LEU:HB2	1.85	0.58
1:C:75:ASN:HD21	1:D:534:GLY:HA2	1.69	0.58
1:D:861:ARG:HD2	6:D:8286:HOH:O	2.03	0.57
1:D:374:PRO:HA	1:D:396:SER:HA	1.85	0.57
1:C:265:ILE:HG22	6:C:7279:HOH:O	2.04	0.57
1:D:295:ASP:HB2	1:D:314:VAL:HG21	1.86	0.57
1:A:97:MET:HB2	6:A:5480:HOH:O	2.03	0.57
1:D:551:ALA:N	6:D:8167:HOH:O	2.37	0.57
1:D:562:GLN:HE21	1:D:562:GLN:H	1.52	0.57
1:B:212:LEU:HA	6:B:6186:HOH:O	2.04	0.57
1:D:109:ARG:CB	6:D:8304:HOH:O	2.52	0.57
1:C:125:LYS:HG3	1:C:149:THR:HG21	1.86	0.57
1:D:575:ARG:CZ	6:D:7871:HOH:O	2.52	0.57
1:B:423:LYS:HE3	6:B:6094:HOH:O	2.04	0.57
1:D:50:ASN:ND2	1:D:50:ASN:H	2.02	0.57
1:C:231:ILE:HB	6:C:7139:HOH:O	2.05	0.57
1:C:80:HIS:H	1:C:98:ASN:ND2	2.02	0.57
1:A:465:ARG:O	1:A:469:GLU:HG3	2.05	0.57
1:C:295:ASP:HB3	6:C:7097:HOH:O	2.04	0.57
1:D:400:LYS:N	6:D:7898:HOH:O	2.38	0.56
1:D:293:VAL:HG11	6:D:8029:HOH:O	2.04	0.56
1:C:564:PHE:CD2	1:D:397:LYS:HE3	2.40	0.56
1:D:196:GLY:N	6:D:8194:HOH:O	2.38	0.56
1:D:344:VAL:HG23	1:D:370:VAL:CG1	2.35	0.56
1:C:400:LYS:N	6:C:7235:HOH:O	2.37	0.56
1:A:365:LYS:HB3	6:A:5288:HOH:O	2.05	0.56
1:C:11:SER:HA	6:C:7301:HOH:O	2.06	0.56
1:B:228:ILE:N	1:B:228:ILE:HD12	2.21	0.56
1:A:189:ASN:HB2	6:A:5209:HOH:O	2.04	0.56
1:B:48:VAL:HG12	6:B:6156:HOH:O	2.05	0.56
1:D:109:ARG:N	6:D:7833:HOH:O	2.37	0.56
1:C:468:ALA:HB1	1:C:473:VAL:HG23	1.86	0.56
1:D:144:ASN:HD21	1:D:190:CYS:HB3	1.69	0.56
1:C:60:THR:O	1:C:64:VAL:HG23	2.06	0.56
1:D:96:PHE:HE2	6:D:8236:HOH:O	1.88	0.56
1:C:521:ILE:HG23	1:C:524:LEU:CB	2.36	0.56
1:D:322:GLY:HA3	1:D:340:LEU:HD13	1.88	0.56
1:C:493:SER:OG	1:C:517:ASN:HA	2.06	0.56
1:B:164:VAL:HG12	6:B:6011:HOH:O	2.04	0.56
1:D:555:GLY:N	6:D:7861:HOH:O	2.39	0.55
1:B:465:ARG:HH22	1:B:476:ASP:CG	2.08	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:VAL:H	1:D:869:ASN:ND2	2.03	0.55
1:C:197:LYS:HG3	1:C:198:TRP:NE1	2.21	0.55
1:C:402:ARG:HA	6:C:7221:HOH:O	2.06	0.55
1:A:349:ILE:HD13	6:A:5450:HOH:O	2.05	0.55
1:A:864:LYS:HG2	6:B:6327:HOH:O	2.06	0.55
1:C:215:MET:HE2	6:C:7054:HOH:O	2.05	0.55
1:C:290:THR:CG2	6:C:7417:HOH:O	2.54	0.55
1:A:517:ASN:HB2	1:A:539:ILE:HG22	1.87	0.55
1:A:445:SER:O	1:A:448:SER:OG	2.24	0.55
1:D:376:HIS:HB2	1:D:437:HIS:O	2.06	0.55
1:A:246:VAL:HG22	6:A:5552:HOH:O	2.07	0.55
1:C:137:ARG:HH11	1:C:139:ASN:HD22	1.55	0.55
1:D:393:VAL:HG13	6:D:8000:HOH:O	2.05	0.55
1:D:447(D):LEU:HD22	1:D:450:ILE:HD11	1.88	0.55
1:C:402:ARG:HD2	1:C:429:ASP:OD2	2.07	0.55
1:C:529:THR:O	1:C:559:TYR:HA	2.06	0.55
1:C:268:ASN:HB2	6:C:7413:HOH:O	2.07	0.55
1:B:80:HIS:CD2	6:B:6184:HOH:O	2.60	0.55
1:D:28:GLN:HE21	1:D:28:GLN:N	1.96	0.55
1:C:862:THR:HG23	6:C:7356:HOH:O	2.07	0.55
1:A:146:GLU:HG3	6:A:5325:HOH:O	2.07	0.55
1:B:288:SER:CB	6:B:6340:HOH:O	2.54	0.54
1:C:148:GLU:HB3	1:C:165:ASN:HD21	1.70	0.54
1:A:80:HIS:HB2	6:A:5305:HOH:O	2.07	0.54
1:A:80:HIS:H	1:A:98:ASN:HD21	1.55	0.54
1:D:187:LEU:HG	6:D:8112:HOH:O	2.07	0.54
1:D:414:ASP:HB3	6:D:7989:HOH:O	2.06	0.54
1:C:344:VAL:HG23	1:C:370:VAL:HG11	1.90	0.54
1:A:202:THR:HG21	1:A:269:PRO:C	2.28	0.54
6:C:7031:HOH:O	1:D:558:TRP:HZ2	1.90	0.54
1:A:35:LEU:HD22	1:A:42:GLU:HA	1.88	0.54
1:A:430:GLY:HA3	6:A:5223:HOH:O	2.08	0.54
1:D:517:ASN:HB2	1:D:539:ILE:HG22	1.90	0.54
1:A:33:ARG:HD3	6:A:5511:HOH:O	2.06	0.54
1:A:42:GLU:HG3	6:A:5511:HOH:O	2.06	0.54
1:D:144:ASN:HB3	1:D:187:LEU:CB	2.38	0.54
1:B:438:ASP:HB2	6:B:6184:HOH:O	2.08	0.54
1:B:47:PRO:HA	1:B:50:ASN:HD21	1.72	0.54
1:A:280:HIS:HB2	6:A:5450:HOH:O	2.07	0.54
1:D:547:VAL:HG21	6:D:8251:HOH:O	2.08	0.53
1:C:465:ARG:NE	6:C:7081:HOH:O	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ARG:NH1	1:D:139:ASN:HD22	2.02	0.53
1:B:9:ASP:OD1	1:B:427:VAL:CG1	2.56	0.53
1:C:287:LEU:HD21	6:D:8008:HOH:O	2.07	0.53
1:C:364:ILE:HA	6:C:6950:HOH:O	2.08	0.53
1:A:558:TRP:HZ2	6:B:6532:HOH:O	1.91	0.53
1:D:79:HIS:H	1:D:98:ASN:HD21	1.56	0.53
1:D:133:GLN:OE1	1:D:139:ASN:HB2	2.08	0.53
1:A:127:ILE:HG23	6:A:5318:HOH:O	2.09	0.53
1:D:65:ARG:HH11	1:D:463:GLU:HG3	1.73	0.53
1:D:539:ILE:HB	6:D:8220:HOH:O	2.08	0.53
1:D:344:VAL:HG23	1:D:370:VAL:HG13	1.90	0.53
1:B:410:LYS:NZ	6:B:6426:HOH:O	2.41	0.53
1:C:125:LYS:HD2	6:D:8206:HOH:O	2.07	0.53
1:D:369:ASP:HB3	6:D:8244:HOH:O	2.08	0.53
1:B:137:ARG:HH11	1:B:139:ASN:HD22	1.55	0.53
1:D:121:ILE:HD12	1:D:127:ILE:CD1	2.37	0.53
1:C:371:HIS:CE1	6:C:7452:HOH:O	2.62	0.53
1:C:521:ILE:CG2	1:C:524:LEU:HB2	2.38	0.53
1:C:473:VAL:HG12	1:C:479:GLU:OE1	2.09	0.53
1:C:331:ARG:HG3	1:C:389:ASN:OD1	2.09	0.53
1:D:329:ASP:OD2	1:D:333:ASN:HB2	2.08	0.53
1:D:202:THR:HG22	1:D:223:ILE:HG22	1.91	0.53
1:D:109:ARG:O	6:D:8146:HOH:O	2.18	0.53
1:C:75:ASN:HD21	1:C:102:ASN:HD21	1.56	0.53
1:C:260:THR:C	6:C:7250:HOH:O	2.46	0.53
1:A:481:ILE:HB	6:A:5225:HOH:O	2.08	0.53
1:D:291:VAL:CG2	1:D:319:LEU:HD12	2.39	0.53
1:D:521:ILE:N	1:D:521:ILE:HD12	2.24	0.53
1:D:456:ARG:HG2	6:D:8261:HOH:O	2.08	0.52
1:C:562:GLN:H	1:C:562:GLN:HE21	1.54	0.52
1:C:215:MET:HA	6:C:7143:HOH:O	2.10	0.52
1:D:397:LYS:HE2	6:D:8306:HOH:O	2.08	0.52
1:D:272:CYS:HB3	6:D:7947:HOH:O	2.09	0.52
1:B:288:SER:HB3	6:B:6340:HOH:O	2.08	0.52
1:D:165:ASN:CG	1:D:186:ASN:HA	2.30	0.52
1:D:71:MET:HG3	6:D:8272:HOH:O	2.10	0.52
1:C:372:TYR:HB2	1:C:398:PHE:O	2.09	0.52
1:C:290:THR:HG22	6:C:7417:HOH:O	2.09	0.52
1:D:288:SER:HB2	6:D:7951:HOH:O	2.09	0.52
1:C:373:GLN:HE21	1:C:398:PHE:HD2	1.58	0.52
1:D:395:LEU:N	1:D:395:LEU:HD12	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:GLN:HE21	1:B:562:GLN:H	1.55	0.52
1:C:190:CYS:N	6:C:7014:HOH:O	2.43	0.52
1:D:288:SER:CB	6:D:7951:HOH:O	2.57	0.52
1:D:316:GLU:N	1:D:317:PRO:HD3	2.24	0.52
6:C:7106:HOH:O	1:D:408:PRO:HD2	2.09	0.52
1:A:202:THR:HG21	1:A:269:PRO:O	2.10	0.52
1:D:412:GLU:HG3	1:D:435:GLU:HA	1.92	0.52
1:D:189:ASN:CB	6:D:7996:HOH:O	2.57	0.52
1:B:26:SER:C	6:B:6545:HOH:O	2.47	0.52
1:C:75:ASN:ND2	1:C:102:ASN:HD21	2.08	0.51
1:C:269:PRO:HD3	6:C:7427:HOH:O	2.10	0.51
1:C:286:LYS:HB2	6:C:7430:HOH:O	2.10	0.51
1:C:468:ALA:O	1:C:473:VAL:HG22	2.10	0.51
1:D:212:LEU:HB3	1:D:213:PRO:HD3	1.92	0.51
1:D:368:LEU:HD23	1:D:417:ILE:HD13	1.93	0.51
1:B:267:ASN:CB	6:B:6340:HOH:O	2.57	0.51
1:D:573:ARG:NH2	6:D:8057:HOH:O	2.43	0.51
1:D:326:THR:HB	6:D:8182:HOH:O	2.10	0.51
1:C:321:LEU:HD23	6:C:7383:HOH:O	2.10	0.51
1:C:550:VAL:HG23	1:C:550:VAL:O	2.09	0.51
1:D:116:ASP:N	6:D:7833:HOH:O	2.42	0.51
1:D:506:LYS:HE2	6:D:8100:HOH:O	2.10	0.51
1:B:331:ARG:HD3	1:B:389:ASN:OD1	2.11	0.51
1:D:103:THR:HA	6:D:8217:HOH:O	2.10	0.51
1:D:241:GLN:HB2	6:D:8033:HOH:O	2.10	0.51
6:C:7112:HOH:O	1:D:30:GLY:HA3	2.10	0.51
1:C:182:LEU:HD13	1:C:250:VAL:HG11	1.93	0.51
1:C:159:GLU:HA	6:C:7192:HOH:O	2.11	0.51
1:D:334:ALA:HB1	6:D:8182:HOH:O	2.09	0.51
1:D:204:TYR:HA	1:D:268:ASN:HA	1.93	0.51
1:A:186:ASN:ND2	1:A:205:ASN:H	2.09	0.51
1:B:79:HIS:H	1:B:98:ASN:HD21	1.56	0.51
1:B:175:TRP:N	6:B:6506:HOH:O	2.44	0.51
1:C:562:GLN:HB3	6:C:7425:HOH:O	2.10	0.51
1:C:319:LEU:HB2	6:C:7134:HOH:O	2.11	0.51
1:D:127:ILE:HA	1:D:144:ASN:O	2.10	0.51
1:D:439:ALA:HB1	6:D:8173:HOH:O	2.10	0.51
1:D:557:TYR:CE2	6:D:7861:HOH:O	2.52	0.51
1:C:287:LEU:HG	6:C:7413:HOH:O	2.11	0.51
1:A:385:LEU:HB2	6:A:5385:HOH:O	2.11	0.51
1:D:363:PRO:CB	6:D:8250:HOH:O	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:HIS:HE1	6:B:5864:HOH:O	1.92	0.51
1:D:340:LEU:N	1:D:340:LEU:HD12	2.26	0.51
1:D:380:VAL:HA	1:D:441:ALA:HB3	1.93	0.51
1:C:372:TYR:CB	1:C:398:PHE:HB2	2.41	0.50
1:B:198:TRP:CA	1:B:228:ILE:HD13	2.40	0.50
1:C:267:ASN:HA	6:C:7427:HOH:O	2.11	0.50
1:C:538:GLU:HG3	6:C:7330:HOH:O	2.10	0.50
1:C:198:TRP:NE1	6:C:7268:HOH:O	2.43	0.50
6:A:5452:HOH:O	1:B:571:GLU:HB3	2.12	0.50
1:A:223:ILE:HG23	1:A:265:ILE:HG13	1.93	0.50
1:D:85:PHE:HE2	6:D:8042:HOH:O	1.94	0.50
1:B:163:TYR:HD1	6:B:6532:HOH:O	1.94	0.50
1:C:264:PRO:O	6:C:7066:HOH:O	2.18	0.50
1:A:79:HIS:H	1:A:98:ASN:HD21	1.60	0.50
1:B:80:HIS:H	1:B:98:ASN:HD21	1.59	0.50
1:A:124:ALA:HB2	1:A:166:VAL:HB	1.94	0.50
1:D:144:ASN:HB3	1:D:187:LEU:HB3	1.94	0.50
1:C:468:ALA:HB1	1:C:473:VAL:CG2	2.42	0.50
1:D:130:LEU:HB3	6:D:8134:HOH:O	2.12	0.50
1:D:601:THR:OG1	1:D:479:GLU:HG2	2.12	0.50
1:D:132:PRO:HA	6:D:7998:HOH:O	2.12	0.50
1:C:571:GLU:OE1	1:C:571:GLU:N	2.44	0.50
1:A:558:TRP:CD1	1:B:147:ASP:HB3	2.47	0.49
1:C:47:PRO:HA	1:C:50:ASN:HD21	1.77	0.49
1:D:83:MET:HB3	1:D:90:TYR:CD1	2.47	0.49
1:A:126:GLY:HA2	6:A:5264:HOH:O	2.12	0.49
1:D:469:GLU:N	6:D:8191:HOH:O	2.45	0.49
1:C:204:TYR:HA	1:C:268:ASN:HA	1.94	0.49
1:C:317:PRO:C	6:C:7417:HOH:O	2.51	0.49
1:D:258:LEU:HG	6:D:8311:HOH:O	2.11	0.49
1:D:78:LEU:C	1:D:78:LEU:HD12	2.33	0.49
1:A:412:GLU:HG3	1:A:435:GLU:HA	1.93	0.49
1:D:130:LEU:C	1:D:130:LEU:HD23	2.31	0.49
1:C:130:LEU:HD23	1:C:130:LEU:C	2.33	0.49
1:D:109:ARG:C	6:D:8304:HOH:O	2.51	0.49
1:A:376:HIS:HB2	1:A:437:HIS:O	2.13	0.49
1:A:202:THR:HG22	1:A:203:SER:N	2.28	0.49
1:A:75:ASN:O	6:A:5395:HOH:O	2.20	0.49
1:D:424:MET:HG2	6:D:8187:HOH:O	2.11	0.49
1:A:535:VAL:N	6:A:5306:HOH:O	2.46	0.49
1:A:212:LEU:HD11	1:B:568:LEU:HD13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:HB3	1:B:213:PRO:HD3	1.94	0.49
1:D:123:ASN:HD22	1:D:180:GLN:HE22	1.60	0.49
1:B:65:ARG:NH1	1:B:463:GLU:HG3	2.27	0.49
1:D:322:GLY:N	1:D:323:PRO:HD3	2.28	0.49
1:D:538:GLU:HB2	1:D:563:TRP:CH2	2.48	0.48
1:C:48:VAL:H	1:C:50:ASN:ND2	2.11	0.48
1:A:8:ALA:HB2	6:A:5611:HOH:O	2.13	0.48
1:A:372:TYR:N	1:A:372:TYR:CD1	2.80	0.48
1:B:29:SER:N	6:B:6545:HOH:O	2.45	0.48
1:C:322:GLY:N	1:C:323:PRO:HD3	2.28	0.48
1:C:164:VAL:HG12	6:C:7050:HOH:O	2.13	0.48
1:C:197:LYS:HG3	1:C:198:TRP:CD1	2.48	0.48
1:D:267:ASN:CB	6:D:7951:HOH:O	2.62	0.48
1:D:299:PHE:C	6:D:7928:HOH:O	2.51	0.48
1:D:307:ALA:CB	6:D:8026:HOH:O	2.62	0.48
1:D:352:ALA:N	6:D:8250:HOH:O	2.46	0.48
1:C:461:TRP:HD1	6:C:7081:HOH:O	1.97	0.48
1:A:562:GLN:HG3	1:B:28:GLN:HB3	1.94	0.48
1:C:298:ARG:NH1	6:C:7444:HOH:O	2.47	0.48
1:C:64:VAL:HG11	1:C:872:ARG:NH2	2.28	0.48
1:D:180:GLN:HB2	1:D:250:VAL:HG22	1.94	0.48
1:D:111:ASP:OD1	6:D:8304:HOH:O	2.19	0.48
1:A:38:PRO:HD3	6:A:5296:HOH:O	2.14	0.48
1:D:370:VAL:HG11	1:D:394:CYS:SG	2.54	0.48
1:A:8:ALA:N	1:A:427:VAL:HG11	2.29	0.48
1:D:562:GLN:N	1:D:562:GLN:HE21	2.12	0.48
1:D:61:ASN:ND2	6:D:8096:HOH:O	2.43	0.48
1:D:572:MET:HE2	6:D:7895:HOH:O	2.12	0.48
1:C:166:VAL:HG22	1:C:182:LEU:HD12	1.95	0.48
1:C:556:VAL:HB	6:C:7165:HOH:O	2.13	0.48
1:A:562:GLN:HE21	1:A:562:GLN:N	2.11	0.48
1:C:298:ARG:HB2	6:C:7097:HOH:O	2.12	0.48
1:D:60:THR:O	1:D:64:VAL:HG23	2.14	0.48
1:A:202:THR:HB	6:A:5209:HOH:O	2.13	0.48
1:D:137:ARG:HD3	1:D:139:ASN:HD21	1.78	0.48
1:C:310:ARG:CG	6:C:7066:HOH:O	2.57	0.48
1:D:33:ARG:HG2	6:D:8205:HOH:O	2.13	0.48
6:C:7122:HOH:O	1:D:523:ASP:HA	2.14	0.48
1:D:184:SER:OG	1:D:255:LYS:HG3	2.13	0.48
1:C:550:VAL:HG22	1:D:869:ASN:ND2	2.29	0.48
1:C:299:PHE:HA	6:C:7114:HOH:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LYS:HE3	1:D:174:LYS:HA	1.95	0.48
1:A:60:THR:O	1:A:64:VAL:HG23	2.14	0.48
1:C:223:ILE:O	1:C:223:ILE:HG13	2.14	0.47
1:D:189:ASN:HB3	6:D:7996:HOH:O	2.14	0.47
1:D:182:LEU:HD13	1:D:250:VAL:CG1	2.44	0.47
1:D:529:THR:O	1:D:559:TYR:HA	2.13	0.47
1:C:80:HIS:H	1:C:98:ASN:HD21	1.61	0.47
1:B:542:GLN:O	6:B:6235:HOH:O	2.20	0.47
1:A:121:ILE:CD1	6:A:5276:HOH:O	2.62	0.47
1:D:264:PRO:O	1:D:265:ILE:HD13	2.14	0.47
1:D:259:PHE:HD1	6:D:8093:HOH:O	1.97	0.47
1:A:280:HIS:HE1	6:A:5045:HOH:O	1.97	0.47
1:D:80:HIS:H	1:D:98:ASN:HD21	1.62	0.47
1:C:268:ASN:O	1:C:286:LYS:HE2	2.15	0.47
1:A:147:ASP:HB3	1:B:558:TRP:CD1	2.49	0.47
1:D:106:ALA:CB	6:D:7943:HOH:O	2.56	0.47
1:D:103:THR:CA	6:D:8217:HOH:O	2.63	0.47
6:A:5448:HOH:O	1:B:324:LEU:HD11	2.15	0.47
1:A:322:GLY:N	1:A:323:PRO:HD3	2.30	0.47
1:D:104:ARG:HD3	6:D:7977:HOH:O	2.14	0.47
1:C:298:ARG:HD2	6:C:7097:HOH:O	2.13	0.47
1:A:47:PRO:HA	1:A:50:ASN:HD21	1.79	0.47
1:A:64:VAL:HG11	1:A:872:ARG:NH2	2.29	0.47
1:D:106:ALA:HB3	6:D:8157:HOH:O	2.15	0.47
1:C:299:PHE:HD2	6:C:7114:HOH:O	1.98	0.47
1:D:322:GLY:CA	1:D:340:LEU:HD13	2.45	0.47
1:D:204:TYR:HB2	1:D:268:ASN:HB3	1.97	0.47
1:B:325:HIS:CE1	1:B:376:HIS:CE1	3.03	0.47
1:B:186:ASN:ND2	1:B:205:ASN:H	2.13	0.47
1:D:384:THR:HA	6:D:8042:HOH:O	2.14	0.46
1:C:198:TRP:HA	6:C:7373:HOH:O	2.13	0.46
1:D:73:HIS:CG	6:D:8087:HOH:O	2.67	0.46
1:A:538:GLU:OE2	1:B:409:LEU:HG	2.15	0.46
1:B:482:ARG:HB3	6:B:6274:HOH:O	2.15	0.46
1:D:11:SER:HA	6:D:8245:HOH:O	2.15	0.46
1:D:397:LYS:HG2	6:D:8306:HOH:O	2.15	0.46
1:B:461:TRP:CZ2	6:B:6235:HOH:O	2.55	0.46
1:B:601:THR:HG23	1:B:479:GLU:HG2	1.97	0.46
1:C:562:GLN:N	1:C:562:GLN:HE21	2.12	0.46
1:A:135:TRP:HB2	6:A:5261:HOH:O	2.16	0.46
1:D:378:LYS:HD3	6:D:8252:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:VAL:HG21	1:D:374:PRO:HG3	1.97	0.46
1:A:571:GLU:HG2	6:B:6186:HOH:O	2.15	0.46
1:D:291:VAL:HG23	1:D:319:LEU:HD12	1.98	0.46
1:C:344:VAL:HG23	1:C:370:VAL:CG1	2.46	0.46
1:A:532:ASN:ND2	1:B:125:LYS:HD2	2.31	0.46
1:A:449:ASP:O	1:A:449:ASP:OD1	2.34	0.46
1:D:542:GLN:HB3	6:D:8261:HOH:O	2.15	0.46
1:A:202:THR:CG2	1:A:203:SER:N	2.79	0.46
1:C:94:PHE:CD2	1:C:107:ARG:HD3	2.50	0.46
1:C:550:VAL:HG22	1:D:869:ASN:CG	2.35	0.46
1:D:165:ASN:ND2	1:D:186:ASN:HA	2.30	0.46
1:C:35:LEU:HD22	1:C:42:GLU:HA	1.97	0.46
1:C:502:SER:HA	1:C:575:ARG:O	2.15	0.46
1:B:219:GLU:HG3	6:B:6441:HOH:O	2.15	0.46
1:B:461:TRP:CZ3	1:B:543:MET:HG3	2.50	0.46
1:C:209:GLY:CA	6:C:7335:HOH:O	2.64	0.46
1:D:554:PRO:C	6:D:7861:HOH:O	2.53	0.46
1:B:381:MET:HE3	6:B:6223:HOH:O	2.16	0.46
1:D:317:PRO:CG	1:D:352:ALA:HB1	2.46	0.46
1:B:223:ILE:HG23	1:B:265:ILE:HG13	1.98	0.46
1:D:326:THR:CG2	1:D:336:THR:HG22	2.14	0.46
1:A:165:ASN:CG	1:A:186:ASN:HA	2.36	0.46
1:C:163:TYR:HD1	6:C:7031:HOH:O	1.98	0.46
1:D:385:LEU:HA	6:D:8292:HOH:O	2.15	0.46
1:D:331:ARG:HD2	6:D:8238:HOH:O	2.16	0.46
1:B:541:PRO:O	1:B:542:GLN:HB2	2.16	0.45
1:D:231:ILE:HG13	6:D:8093:HOH:O	2.16	0.45
1:D:103:THR:HG23	1:D:127:ILE:HG13	1.98	0.45
1:D:250:VAL:HB	6:D:8033:HOH:O	2.16	0.45
1:B:495:ALA:HA	1:B:496:PRO:HA	1.79	0.45
1:A:164:VAL:HG12	6:A:5077:HOH:O	2.15	0.45
1:C:416:LEU:O	1:C:427:VAL:HG22	2.16	0.45
1:D:527:GLY:HA2	1:D:539:ILE:HD12	1.98	0.45
1:A:246:VAL:HG22	1:A:249:LYS:N	2.30	0.45
1:A:490:TYR:HE1	6:A:5225:HOH:O	1.98	0.45
6:C:7395:HOH:O	1:D:17:LEU:CD2	2.65	0.45
1:D:35:LEU:HD13	1:D:42:GLU:CA	2.44	0.45
1:B:64:VAL:HG11	1:B:872:ARG:CZ	2.46	0.45
1:D:186:ASN:ND2	1:D:205:ASN:H	2.13	0.45
1:B:562:GLN:HE21	1:B:562:GLN:N	2.14	0.45
1:D:394:CYS:HB3	6:D:8274:HOH:O	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:GLU:CD	6:C:7391:HOH:O	2.55	0.45
1:D:293:VAL:HB	1:D:315:ALA:HB3	1.98	0.45
1:D:272:CYS:N	6:D:7996:HOH:O	2.49	0.45
1:C:473:VAL:HB	6:C:7303:HOH:O	2.15	0.45
1:D:49:PHE:CE2	1:D:99:ASP:HB2	2.51	0.45
1:B:288:SER:N	6:B:6340:HOH:O	2.49	0.45
1:D:135:TRP:HB2	6:D:8211:HOH:O	2.16	0.45
1:C:186:ASN:ND2	1:C:205:ASN:H	2.15	0.45
1:B:437:HIS:CB	6:B:6184:HOH:O	2.63	0.45
1:A:372:TYR:O	1:A:396:SER:HB3	2.15	0.45
1:D:287:LEU:HD23	6:D:8168:HOH:O	2.16	0.45
1:D:338:LEU:HD11	1:D:345:VAL:HG21	1.99	0.45
1:C:306:ASN:HB2	6:C:7431:HOH:O	2.16	0.45
1:B:127:ILE:HA	1:B:144:ASN:O	2.17	0.45
1:D:223:ILE:O	1:D:223:ILE:HG13	2.16	0.45
1:C:65:ARG:NH1	1:C:463:GLU:HB2	2.31	0.45
1:A:435:GLU:OE2	1:B:564:PHE:HB2	2.16	0.44
1:A:869:ASN:HD21	1:B:550:VAL:N	1.98	0.44
1:D:231:ILE:O	1:D:235:ILE:HG12	2.17	0.44
1:C:431:PRO:HA	6:C:7400:HOH:O	2.16	0.44
1:B:182:LEU:HD13	1:B:250:VAL:CG1	2.48	0.44
1:D:351:ASP:HB2	6:D:7994:HOH:O	2.17	0.44
1:D:276:PRO:HA	6:D:8292:HOH:O	2.17	0.44
1:A:543:MET:HG2	1:A:544:THR:N	2.32	0.44
1:B:49:PHE:CE2	1:B:99:ASP:HB2	2.53	0.44
1:A:400:LYS:HG2	6:B:6378:HOH:O	2.16	0.44
1:B:126:GLY:HA2	6:B:6442:HOH:O	2.16	0.44
1:A:568:LEU:HD13	1:B:212:LEU:HD11	2.00	0.44
1:A:350:GLU:HG2	6:A:5155:HOH:O	2.17	0.44
1:B:278:LYS:HE2	6:B:6472:HOH:O	2.17	0.44
1:C:574:GLY:HA2	6:D:8248:HOH:O	2.18	0.44
1:D:371:HIS:C	1:D:372:TYR:CG	2.90	0.44
1:A:345:VAL:HG22	1:A:367:LYS:HG2	2.00	0.44
1:C:380:VAL:HB	1:C:388:THR:OG1	2.17	0.44
1:D:525:THR:HA	6:D:8240:HOH:O	2.17	0.44
1:D:129:GLY:HA3	1:D:189:ASN:HA	2.00	0.44
1:D:363:PRO:HA	6:D:7994:HOH:O	2.18	0.44
1:B:130:LEU:HD23	1:B:130:LEU:C	2.38	0.44
1:D:417:ILE:HD11	6:D:8274:HOH:O	2.17	0.44
1:C:534:GLY:HA2	1:D:75:ASN:ND2	2.32	0.44
1:B:98:ASN:H	1:B:98:ASN:HD22	1.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:TYR:HA	1:B:268:ASN:HA	2.00	0.44
1:C:268:ASN:N	1:C:269:PRO:CD	2.80	0.44
1:A:532:ASN:ND2	1:B:125:LYS:CD	2.80	0.44
1:A:451:LYS:HE2	6:A:5629:HOH:O	2.18	0.44
1:B:198:TRP:HA	1:B:228:ILE:CD1	2.45	0.44
1:D:116:ASP:HA	1:D:460:MET:HE3	2.00	0.44
1:D:529:THR:HA	6:D:8198:HOH:O	2.16	0.43
1:A:395:LEU:N	1:A:395:LEU:HD12	2.32	0.43
1:D:118:ILE:HD12	6:D:8150:HOH:O	2.17	0.43
1:C:411:PRO:HB2	6:C:7400:HOH:O	2.17	0.43
1:D:221:ASP:O	1:D:222:HIS:HB3	2.17	0.43
1:D:59:GLN:CD	6:D:8251:HOH:O	2.56	0.43
1:C:369:ASP:CB	6:C:7452:HOH:O	2.55	0.43
1:D:281:LEU:N	6:D:7891:HOH:O	2.51	0.43
1:C:372:TYR:N	1:C:372:TYR:CD1	2.82	0.43
1:B:93:ARG:HD2	6:B:6316:HOH:O	2.18	0.43
1:B:293:VAL:HB	1:B:315:ALA:HB3	2.00	0.43
1:A:227:ASN:HB2	1:A:303:PHE:CE2	2.53	0.43
1:A:215:MET:HA	6:A:5455:HOH:O	2.17	0.43
1:C:372:TYR:O	1:C:396:SER:HB3	2.18	0.43
1:D:144:ASN:HB3	1:D:187:LEU:HB2	1.99	0.43
1:D:525:THR:CB	6:D:8240:HOH:O	2.67	0.43
1:A:553:ASN:N	6:A:5417:HOH:O	2.51	0.43
1:A:397:LYS:HE3	1:B:564:PHE:CD2	2.54	0.43
1:A:69:ARG:NE	6:A:5290:HOH:O	2.52	0.43
1:C:267:ASN:N	6:C:7427:HOH:O	2.51	0.43
1:A:177:VAL:CG1	1:A:246:VAL:HG21	2.42	0.43
1:D:49:PHE:CZ	1:D:99:ASP:HB2	2.54	0.43
1:D:436:PRO:HB3	6:D:8060:HOH:O	2.18	0.43
1:A:293:VAL:HB	1:A:315:ALA:HB3	2.01	0.43
1:C:212:LEU:N	1:C:213:PRO:HD2	2.33	0.43
1:C:317:PRO:HD2	6:C:7086:HOH:O	2.17	0.43
1:A:28:GLN:HB3	1:B:562:GLN:HG3	2.00	0.43
1:B:506:LYS:HD2	6:B:6085:HOH:O	2.17	0.43
1:C:397:LYS:HD3	6:C:7350:HOH:O	2.18	0.43
1:C:209:GLY:C	6:C:7335:HOH:O	2.57	0.43
1:B:118:ILE:HD11	6:B:6156:HOH:O	2.18	0.43
1:D:498:PHE:HD2	6:D:7982:HOH:O	2.02	0.43
1:D:530:MET:HG3	6:D:8310:HOH:O	2.19	0.43
1:B:579:GLU:HA	1:B:580:PRO:HD3	1.93	0.43
1:C:123:ASN:HD22	1:C:180:GLN:NE2	2.04	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:C	6:A:5609:HOH:O	2.56	0.43
1:D:424:MET:CG	6:D:8187:HOH:O	2.67	0.43
1:A:123:ASN:HD22	1:A:180:GLN:NE2	2.09	0.43
1:D:390:ASP:OD1	1:D:391:TRP:N	2.49	0.43
1:B:10:GLY:HA3	1:B:38:PRO:HB2	2.01	0.42
1:C:549:PHE:HB3	6:C:7415:HOH:O	2.19	0.42
1:C:395:LEU:N	1:C:395:LEU:HD12	2.34	0.42
1:D:38:PRO:HB2	1:D:416:LEU:HD21	2.01	0.42
1:D:258:LEU:HD12	1:D:258:LEU:N	2.33	0.42
1:C:416:LEU:HB3	1:C:428:HIS:HB2	2.01	0.42
1:C:397:LYS:HE3	1:D:564:PHE:CD2	2.53	0.42
1:A:121:ILE:HD11	6:A:5276:HOH:O	2.18	0.42
1:A:75:ASN:ND2	1:A:102:ASN:HD21	2.17	0.42
1:C:225:VAL:HG13	6:C:7338:HOH:O	2.18	0.42
1:D:73:HIS:CD2	6:D:8087:HOH:O	2.72	0.42
1:A:277:ASP:OD2	1:A:280:HIS:HD2	2.03	0.42
1:B:91:ASP:CG	1:B:93:ARG:HD3	2.39	0.42
1:D:267:ASN:HB2	6:D:7951:HOH:O	2.18	0.42
1:B:601:THR:HG22	1:B:478:GLU:N	2.35	0.42
1:D:543:MET:HG2	1:D:544:THR:N	2.33	0.42
1:C:182:LEU:HD13	1:C:250:VAL:CG1	2.49	0.42
1:A:71:MET:HE3	6:A:5517:HOH:O	2.19	0.42
1:A:529:THR:O	1:A:559:TYR:HA	2.19	0.42
1:C:325:HIS:CE1	1:C:376:HIS:CE1	3.07	0.42
1:D:280:HIS:HE1	6:D:8021:HOH:O	2.02	0.42
1:C:193:ASP:OD2	1:C:197:LYS:HG2	2.20	0.42
1:A:243:LEU:O	1:A:246:VAL:HG12	2.19	0.42
1:B:64:VAL:HG11	1:B:872:ARG:NH2	2.35	0.42
1:A:344:VAL:HG23	1:A:370:VAL:HG11	2.00	0.42
1:D:541:PRO:O	1:D:542:GLN:HB2	2.19	0.42
1:A:119:LEU:O	6:A:5276:HOH:O	2.22	0.42
1:A:75:ASN:HD21	1:A:102:ASN:HD21	1.68	0.42
1:D:288:SER:N	6:D:7951:HOH:O	2.52	0.42
1:A:448:SER:CB	6:A:5439:HOH:O	2.63	0.42
1:A:148:GLU:H	1:A:148:GLU:CD	2.23	0.42
1:C:563:TRP:O	1:C:564:PHE:C	2.56	0.42
1:D:118:ILE:HG12	6:D:7943:HOH:O	2.18	0.42
1:A:223:ILE:O	1:A:223:ILE:HG13	2.20	0.42
1:C:98:ASN:HD22	1:C:98:ASN:H	1.67	0.42
1:C:528:PHE:N	1:C:562:GLN:HE22	2.17	0.42
1:D:479:GLU:HG2	1:D:479:GLU:H	1.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ASP:N	6:D:8189:HOH:O	2.51	0.42
1:D:469:GLU:CA	6:D:8191:HOH:O	2.67	0.42
1:B:395:LEU:N	1:B:395:LEU:HD12	2.35	0.42
1:D:538:GLU:HG2	1:D:539:ILE:N	2.34	0.42
1:B:539:ILE:HG13	1:B:545:SER:OG	2.20	0.42
1:D:108:VAL:HA	6:D:7833:HOH:O	2.20	0.42
1:C:263:ILE:CG2	6:C:7066:HOH:O	2.58	0.42
1:A:526:HIS:CD2	6:A:5239:HOH:O	2.71	0.42
1:C:147:ASP:HB3	1:D:558:TRP:CD1	2.55	0.42
1:D:45:ARG:HG2	6:D:8205:HOH:O	2.20	0.42
1:C:543:MET:HG2	1:C:544:THR:N	2.33	0.42
1:B:372:TYR:CD1	1:B:372:TYR:N	2.84	0.42
1:B:456:ARG:HD2	6:B:6235:HOH:O	2.20	0.41
1:B:448:SER:CB	6:B:6256:HOH:O	2.68	0.41
1:B:50:ASN:N	1:B:50:ASN:HD22	2.05	0.41
6:C:7157:HOH:O	1:D:573:ARG:HD3	2.19	0.41
1:D:423:LYS:HE3	6:D:8216:HOH:O	2.19	0.41
1:C:223:ILE:HG21	1:C:283:VAL:HG21	2.01	0.41
1:D:339:PHE:CE1	1:D:373:GLN:HB3	2.55	0.41
1:A:75:ASN:ND2	1:B:534:GLY:HA2	2.33	0.41
1:A:143:CYS:N	6:A:5258:HOH:O	2.52	0.41
1:A:564:PHE:CD2	1:B:397:LYS:HE3	2.55	0.41
1:A:65:ARG:NH1	1:A:463:GLU:HG3	2.34	0.41
1:D:517:ASN:HB3	1:D:540:GLY:O	2.21	0.41
1:B:65:ARG:HH12	1:B:463:GLU:H	1.67	0.41
1:C:180:GLN:HB2	1:C:250:VAL:HG22	2.01	0.41
1:A:204:TYR:HA	1:A:268:ASN:HA	2.03	0.41
1:B:228:ILE:CD1	1:B:228:ILE:H	2.33	0.41
1:C:569:HIS:HB3	6:C:7456:HOH:O	2.20	0.41
1:C:226:PHE:C	6:C:7399:HOH:O	2.59	0.41
1:D:77:ASP:CG	1:D:79:HIS:HE2	2.24	0.41
1:A:532:ASN:HD21	1:B:125:LYS:CD	2.32	0.41
1:A:346:LYS:NZ	6:A:5507:HOH:O	2.54	0.41
1:C:205:ASN:CG	6:C:7335:HOH:O	2.58	0.41
1:D:860:GLU:CG	1:D:864:LYS:HE2	2.33	0.41
1:B:48:VAL:H	1:B:50:ASN:ND2	2.18	0.41
1:D:475:ILE:HG12	6:D:7920:HOH:O	2.21	0.41
1:C:264:PRO:HB3	6:C:7152:HOH:O	2.20	0.41
6:C:7371:HOH:O	1:D:103:THR:HB	2.20	0.41
1:B:601:THR:CG2	1:B:479:GLU:H	2.33	0.41
1:D:78:LEU:HD12	1:D:79:HIS:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PRO:O	1:A:265:ILE:HD13	2.21	0.41
1:D:562:GLN:NE2	1:D:562:GLN:H	2.15	0.41
1:D:211:THR:O	1:D:215:MET:HG3	2.21	0.41
1:D:134:LYS:HD3	6:D:8042:HOH:O	2.21	0.41
1:C:155:GLY:O	1:D:580:PRO:HD3	2.21	0.41
6:C:7395:HOH:O	1:D:17:LEU:HD22	2.20	0.41
1:A:202:THR:CG2	1:A:269:PRO:HG2	2.47	0.41
1:A:48:VAL:H	1:A:50:ASN:ND2	2.19	0.41
1:B:228:ILE:H	1:B:228:ILE:HD12	1.84	0.41
1:B:228:ILE:N	1:B:228:ILE:CD1	2.83	0.41
1:C:521:ILE:CG2	1:C:524:LEU:CB	2.98	0.41
1:D:414:ASP:N	6:D:7979:HOH:O	2.53	0.41
1:B:438:ASP:N	6:B:6184:HOH:O	2.53	0.41
1:A:562:GLN:NE2	1:A:562:GLN:H	2.19	0.41
1:C:411:PRO:HB3	1:D:43:LEU:O	2.21	0.41
1:B:49:PHE:CZ	1:B:99:ASP:HB2	2.56	0.41
1:C:443:HIS:HA	1:C:444:PRO:HD3	1.94	0.41
1:A:130:LEU:C	1:A:130:LEU:HD23	2.41	0.41
1:D:83:MET:SD	1:D:92:GLY:HA2	2.60	0.41
1:B:103:THR:HA	6:B:6442:HOH:O	2.20	0.41
1:C:514:ILE:N	1:C:514:ILE:HD12	2.36	0.41
1:A:506:LYS:HD2	6:A:5527:HOH:O	2.20	0.41
1:D:371:HIS:CE1	6:D:8244:HOH:O	2.74	0.40
1:A:49:PHE:CE2	1:A:99:ASP:HB2	2.56	0.40
1:B:194:TYR:O	6:B:6421:HOH:O	2.22	0.40
1:C:221:ASP:HB3	6:C:7337:HOH:O	2.21	0.40
1:D:230:GLU:HA	1:D:233:LYS:HG2	2.03	0.40
1:C:264:PRO:N	6:C:7066:HOH:O	2.53	0.40
1:C:59:GLN:NE2	1:C:534:GLY:O	2.52	0.40
1:A:329:ASP:OD2	1:A:333:ASN:HB2	2.21	0.40
1:C:50:ASN:HD22	1:C:50:ASN:N	2.10	0.40
1:B:228:ILE:HG23	6:B:6381:HOH:O	2.21	0.40
1:C:364:ILE:HG23	6:C:6950:HOH:O	2.20	0.40
1:A:98:ASN:ND2	6:A:5480:HOH:O	2.53	0.40
1:D:440:ILE:N	6:D:8173:HOH:O	2.52	0.40
1:D:107:ARG:HD2	6:D:8236:HOH:O	2.21	0.40
1:D:343:GLN:HA	1:D:370:VAL:HG22	2.03	0.40
1:A:371:HIS:HD2	1:A:415:GLN:OE1	2.03	0.40
1:B:65:ARG:HH11	1:B:463:GLU:HG3	1.87	0.40
1:A:186:ASN:HD21	1:A:204:TYR:H	1.68	0.40
1:B:563:TRP:O	1:B:564:PHE:C	2.60	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:PRO:HA	1:B:337:SER:O	2.22	0.40
1:B:433:PHE:CG	1:B:434:ALA:N	2.89	0.40
1:D:377:LEU:HA	1:D:393:VAL:O	2.21	0.40
1:D:410:LYS:HB3	6:D:7898:HOH:O	2.21	0.40
1:C:538:GLU:HA	6:C:7330:HOH:O	2.21	0.40
1:D:185:GLY:HA3	1:D:206:SER:HA	2.04	0.40
1:D:103:THR:N	6:D:8217:HOH:O	2.50	0.40
1:C:529:THR:HB	6:C:7425:HOH:O	2.22	0.40
1:A:40:MET:HB3	6:A:5223:HOH:O	2.22	0.40
1:A:64:VAL:HG11	1:A:872:ARG:CZ	2.51	0.40
1:D:150:PRO:HD3	1:D:163:TYR:CE2	2.57	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	589/595 (99%)	557 (95%)	29 (5%)	3 (0%)	34	12
1	B	587/595 (99%)	561 (96%)	23 (4%)	3 (0%)	34	12
1	C	588/595 (99%)	553 (94%)	31 (5%)	4 (1%)	26	8
1	D	586/595 (98%)	545 (93%)	35 (6%)	6 (1%)	19	4
All	All	2350/2380 (99%)	2216 (94%)	118 (5%)	16 (1%)	26	8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	B	434	ALA
1	D	267	ASN
1	A	434	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	267	ASN
1	B	286	LYS
1	C	286	LYS
1	C	434	ALA
1	D	286	LYS
1	A	286	LYS
1	C	372	TYR
1	D	189	ASN
1	D	372	TYR
1	D	434	ALA
1	C	400	LYS
1	D	184	SER

5.3.2 Protein sidechains ⓘ

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	501/503 (100%)	489 (98%)	12 (2%)	57	27
1	B	500/503 (99%)	481 (96%)	19 (4%)	40	13
1	C	501/503 (100%)	485 (97%)	16 (3%)	46	18
1	D	499/503 (99%)	485 (97%)	14 (3%)	51	22
All	All	2001/2012 (100%)	1940 (97%)	61 (3%)	48	19

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	50	ASN
1	A	75	ASN
1	A	98	ASN
1	A	151	LEU
1	A	186	ASN
1	A	200	PHE
1	A	294	LEU
1	A	496	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	562	GLN
1	A	563	TRP
1	A	564	PHE
1	B	24	TRP
1	B	38	PRO
1	B	50	ASN
1	B	75	ASN
1	B	98	ASN
1	B	151	LEU
1	B	182	LEU
1	B	186	ASN
1	B	200	PHE
1	B	306	ASN
1	B	360	LYS
1	B	372	TYR
1	B	402	ARG
1	B	409	LEU
1	B	465	ARG
1	B	496	PRO
1	B	562	GLN
1	B	563	TRP
1	B	564	PHE
1	C	24	TRP
1	C	28	GLN
1	C	50	ASN
1	C	75	ASN
1	C	78	LEU
1	C	98	ASN
1	C	182	LEU
1	C	186	ASN
1	C	197	LYS
1	C	200	PHE
1	C	409	LEU
1	C	496	PRO
1	C	562	GLN
1	C	563	TRP
1	C	564	PHE
1	C	571	GLU
1	D	28	GLN
1	D	50	ASN
1	D	75	ASN
1	D	98	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	151	LEU
1	D	174	LYS
1	D	186	ASN
1	D	200	PHE
1	D	267	ASN
1	D	402	ARG
1	D	479	GLU
1	D	562	GLN
1	D	563	TRP
1	D	564	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	61	ASN
1	A	869	ASN
1	A	75	ASN
1	A	98	ASN
1	A	139	ASN
1	A	144	ASN
1	A	165	ASN
1	A	180	GLN
1	A	186	ASN
1	A	189	ASN
1	A	280	HIS
1	A	371	HIS
1	A	373	GLN
1	A	415	GLN
1	A	485	ASN
1	A	562	GLN
1	B	50	ASN
1	B	61	ASN
1	B	869	ASN
1	B	75	ASN
1	B	98	ASN
1	B	139	ASN
1	B	144	ASN
1	B	165	ASN
1	B	180	GLN
1	B	186	ASN
1	B	189	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	241	GLN
1	B	280	HIS
1	B	306	ASN
1	B	371	HIS
1	B	373	GLN
1	B	415	GLN
1	B	428	HIS
1	B	562	GLN
1	C	28	GLN
1	C	50	ASN
1	C	61	ASN
1	C	869	ASN
1	C	75	ASN
1	C	98	ASN
1	C	139	ASN
1	C	165	ASN
1	C	180	GLN
1	C	186	ASN
1	C	189	ASN
1	C	280	HIS
1	C	371	HIS
1	C	373	GLN
1	C	415	GLN
1	C	562	GLN
1	D	28	GLN
1	D	50	ASN
1	D	61	ASN
1	D	869	ASN
1	D	75	ASN
1	D	98	ASN
1	D	139	ASN
1	D	144	ASN
1	D	840	ASN
1	D	165	ASN
1	D	180	GLN
1	D	186	ASN
1	D	189	ASN
1	D	267	ASN
1	D	280	HIS
1	D	371	HIS
1	D	373	GLN
1	D	415	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	428	HIS
1	D	562	GLN

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 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 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	$\# Z > 2$
4	CUA	A	4701	1	0,1,1	0.00	-	0,0,0	0.00	-
5	CUZ	A	4801	1	0,9,9	0.00	-	0,24,24	0.00	-
4	CUA	B	4701	1	0,1,1	0.00	-	0,0,0	0.00	-
5	CUZ	B	5801	1	0,9,9	0.00	-	0,24,24	0.00	-
4	CUA	C	4701	1	0,1,1	0.00	-	0,0,0	0.00	-
5	CUZ	C	6801	1	0,9,9	0.00	-	0,24,24	0.00	-
4	CUA	D	4701	1	0,1,1	0.00	-	0,0,0	0.00	-
5	CUZ	D	7801	1	0,9,9	0.00	-	0,24,24	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
4	CUA	A	4701	1	-	0/0/0/0	0/0/0/0
5	CUZ	A	4801	1	-	0/0/42/42	0/0/5/5
4	CUA	B	4701	1	-	0/0/0/0	0/0/0/0
5	CUZ	B	5801	1	-	0/0/42/42	0/0/5/5
4	CUA	C	4701	1	-	0/0/0/0	0/0/0/0
5	CUZ	C	6801	1	-	0/0/42/42	0/0/5/5
4	CUA	D	4701	1	-	0/0/0/0	0/0/0/0
5	CUZ	D	7801	1	-	0/0/42/42	0/0/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	591/595 (99%)	0.38	21 (3%) 46 43	10, 18, 28, 39	0
1	B	589/595 (98%)	0.13	10 (1%) 73 71	10, 16, 25, 32	0
1	C	590/595 (99%)	0.59	40 (6%) 20 19	15, 23, 31, 42	0
1	D	588/595 (98%)	1.22	122 (20%) 1 1	17, 31, 40, 46	158 (26%)
All	All	2358/2380 (99%)	0.58	193 (8%) 14 12	10, 21, 37, 46	158 (6%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	302	VAL	8.5
1	D	361	VAL	6.7
1	C	360	LYS	5.6
1	D	449	ASP	5.6
1	D	306	ASN	5.5
1	D	218	ALA	5.1
1	D	267	ASN	5.1
1	C	358	GLY	5.1
1	D	307	ALA	5.0
1	D	135	TRP	4.9
1	D	238	GLY	4.8
1	D	356	TYR	4.7
1	C	357	ALA	4.6
1	D	372	TYR	4.6
1	A	9	ASP	4.6
1	D	212	LEU	4.5
1	C	361	VAL	4.5
1	A	360	LYS	4.5
1	D	189	ASN	4.5
1	D	236	ALA	4.5
1	D	235	ILE	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	219	GLU	4.5
1	A	434	ALA	4.4
1	D	355	ALA	4.4
1	D	360	LYS	4.4
1	D	167	PHE	4.3
1	D	259	PHE	4.3
1	C	581	LYS	4.3
1	A	8	ALA	4.3
1	D	354	ARG	4.2
1	C	9	ASP	4.2
1	D	152	VAL	4.2
1	A	266	ALA	4.2
1	D	161	VAL	4.2
1	D	223	ILE	4.1
1	D	301	ALA	4.0
1	A	581	LYS	4.0
1	D	303	PHE	4.0
1	D	151	LEU	3.9
1	D	217	ALA	3.8
1	D	357	ALA	3.8
1	D	864	LYS	3.8
1	C	151	LEU	3.8
1	D	299	PHE	3.8
1	C	356	TYR	3.7
1	D	213	PRO	3.7
1	D	840	ASN	3.7
1	A	361	VAL	3.7
1	B	360	LYS	3.6
1	D	446	ILE	3.6
1	D	187	LEU	3.6
1	D	258	LEU	3.6
1	B	434	ALA	3.5
1	D	327	ALA	3.5
1	D	358	GLY	3.5
1	D	198	TRP	3.5
1	D	850	ASP	3.5
1	D	304	TYR	3.5
1	D	297	THR	3.4
1	D	309	PRO	3.4
1	C	306	ASN	3.4
1	C	568	LEU	3.3
1	D	246	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	314	VAL	3.3
1	A	448	SER	3.3
1	D	201	SER	3.3
1	C	521	ILE	3.2
1	D	359	GLU	3.2
1	D	86	THR	3.2
1	D	810	ALA	3.2
1	D	240	TYR	3.2
1	C	434	ALA	3.1
1	A	267	ASN	3.1
1	D	364	ILE	3.1
1	D	450	ILE	3.1
1	D	136	PRO	3.1
1	D	448	SER	3.1
1	D	266	ALA	3.0
1	D	65	ARG	3.0
1	B	266	ALA	3.0
1	A	357	ALA	2.9
1	A	219	GLU	2.9
1	C	553	ASN	2.9
1	D	860	GLU	2.9
1	D	141	VAL	2.9
1	D	268	ASN	2.8
1	D	291	VAL	2.8
1	D	162	ALA	2.8
1	C	304	TYR	2.8
1	D	287	LEU	2.8
1	D	282	CYS	2.8
1	D	334	ALA	2.7
1	B	9	ASP	2.7
1	C	162	ALA	2.7
1	D	265	ILE	2.7
1	D	305	GLU	2.7
1	D	239	ASP	2.7
1	D	350	GLU	2.7
1	D	485	ASN	2.7
1	C	840	ASN	2.7
1	C	266	ALA	2.7
1	B	372	TYR	2.6
1	B	306	ASN	2.6
1	D	139	ASN	2.6
1	D	157	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	168	THR	2.6
1	C	258	LEU	2.6
1	D	142	PHE	2.6
1	A	354	ARG	2.6
1	D	175	TRP	2.6
1	D	262	TYR	2.6
1	D	202	THR	2.5
1	D	231	ILE	2.5
1	A	218	ALA	2.5
1	D	209	GLY	2.5
1	A	217	ALA	2.5
1	D	362	ASP	2.5
1	D	85	PHE	2.5
1	D	78	LEU	2.5
1	D	434	ALA	2.5
1	C	300	ASP	2.4
1	D	811	SER	2.4
1	C	354	ARG	2.4
1	A	331	ARG	2.4
1	D	71	MET	2.4
1	C	267	ASN	2.4
1	D	205	ASN	2.4
1	C	552	ALA	2.4
1	D	311	SER	2.4
1	D	313	VAL	2.4
1	D	233	LYS	2.4
1	D	385	LEU	2.3
1	B	267	ASN	2.3
1	D	447(D)	LEU	2.3
1	C	514	ILE	2.3
1	D	271	GLY	2.3
1	D	208	LYS	2.3
1	A	223	ILE	2.3
1	B	552	ALA	2.3
1	D	87	GLU	2.3
1	D	300	ASP	2.3
1	C	528	PHE	2.3
1	C	864	LYS	2.3
1	D	242	GLU	2.3
1	D	365	LYS	2.3
1	C	428	HIS	2.2
1	C	448	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	101	ALA	2.2
1	D	211	THR	2.2
1	D	863	LYS	2.2
1	D	220	MET	2.2
1	D	155	GLY	2.2
1	D	241	GLN	2.2
1	D	321	LEU	2.2
1	C	600	TRP	2.2
1	D	347	TRP	2.2
1	D	335	TYR	2.2
1	C	152	VAL	2.2
1	D	336	THR	2.2
1	D	143	CYS	2.2
1	C	130	LEU	2.2
1	D	353	ILE	2.2
1	B	449	ASP	2.2
1	C	423	LYS	2.2
1	A	258	LEU	2.1
1	D	130	LEU	2.1
1	D	457	ASN	2.1
1	D	234	ALA	2.1
1	D	237	ALA	2.1
1	D	371	HIS	2.1
1	C	223	ILE	2.1
1	A	224	VAL	2.1
1	C	372	TYR	2.1
1	D	423	LYS	2.1
1	A	358	GLY	2.1
1	D	160	ASP	2.1
1	A	225	VAL	2.1
1	C	224	VAL	2.1
1	C	370	VAL	2.1
1	D	170	VAL	2.1
1	D	72	SER	2.1
1	D	178	ALA	2.1
1	D	425	VAL	2.0
1	C	457	ASN	2.0
1	B	159	GLU	2.0
1	D	330	GLY	2.0
1	C	142	PHE	2.0
1	C	78	LEU	2.0
1	D	243	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	64	VAL	2.0
1	D	106	ALA	2.0
1	C	482	ARG	2.0
1	C	200	PHE	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, 95th 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(\AA^2)	Q<0.9
3	CA	A	4904	1/1	0.59	0.21	2.86	74,74,74,74	0
3	CA	C	4910	1/1	0.76	0.12	-0.20	66,66,66,66	0
5	CUZ	D	7801	5/5	0.93	0.10	-1.20	31,31,32,32	0
3	CA	D	4903	1/1	0.89	0.11	-1.29	36,36,36,36	0
2	CL	D	4908	1/1	0.95	0.08	-1.52	32,32,32,32	0
3	CA	A	4903	1/1	0.98	0.05	-1.57	21,21,21,21	0
3	CA	B	4903	1/1	1.00	0.03	-1.74	13,13,13,13	0
3	CA	C	4903	1/1	0.99	0.06	-1.76	17,17,17,17	0
3	CA	D	4904	1/1	0.98	0.05	-1.77	25,25,25,25	0
3	CA	C	4905	1/1	1.00	0.07	-2.18	22,22,22,22	0
5	CUZ	C	6801	5/5	0.98	0.07	-2.44	21,21,21,22	0
3	CA	A	4905	1/1	0.99	0.03	-2.82	17,17,17,17	0
4	CUA	A	4701	2/2	1.00	0.02	-2.99	10,10,10,10	0
3	CA	B	4905	1/1	0.99	0.03	-3.07	14,14,14,14	0
4	CUA	C	4701	2/2	0.98	0.06	-3.35	24,24,24,25	0
2	CL	C	4907	1/1	0.99	0.04	-4.42	18,18,18,18	0
2	CL	A	4901	1/1	0.99	0.05	-4.81	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CUA	D	4701	2/2	0.99	0.06	-4.98	17,17,17,18	0
4	CUA	B	4701	2/2	0.99	0.03	-5.18	17,17,17,17	0
2	CL	B	4906	1/1	1.00	0.04	-5.32	12,12,12,12	0
5	CUZ	B	5801	5/5	0.99	0.04	-5.45	14,15,15,15	0
5	CUZ	A	4801	5/5	0.98	0.05	-6.51	18,19,19,20	0
3	CA	B	4909	1/1	0.88	0.11	-	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.