Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:28 PM GMT

PDB ID	:	1TU5
Title	:	Crystal structure of bovine plasma copper-containing amine oxidase
Authors	:	Lunelli, M.; Di Paolo, M.L.; Biadene, M.; Calderone, V.; Scarpa, M.; Battistutta, R.; Rigo, A.; Zanotti, G.
Deposited on	:	2004-06-24
Resolution	:	2.37 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

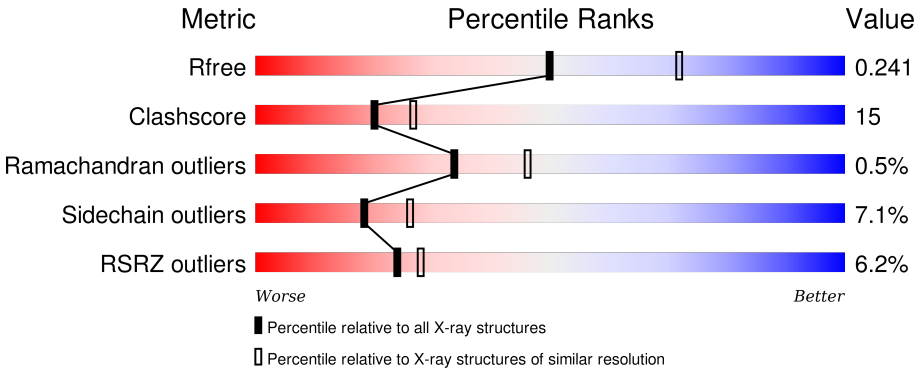
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	746	5% 59% 22% • 15%
1	B	746	5% 61% 21% • 15%

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	NAG	A	803	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10581 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 Copper amine oxidase, liver isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	0	0
			5018	3217	862	920	19			
1	B	633	Total	C	N	O	S	0	0	0
			5018	3217	862	920	19			

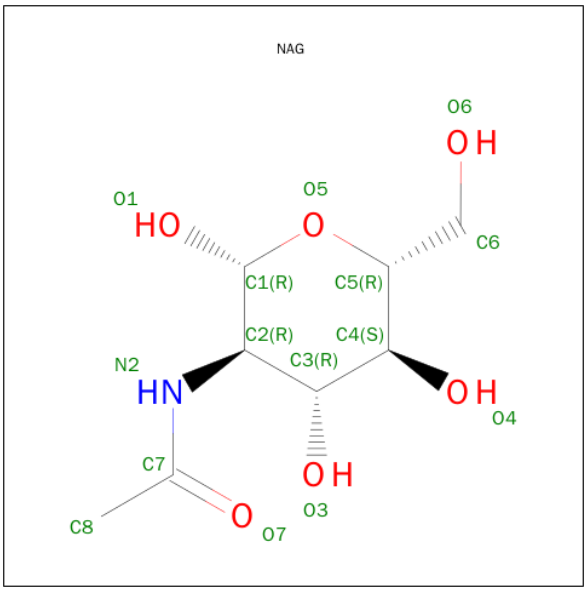
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	TPQ	TYR	MODIFIED RESIDUE	UNP Q29437
B	470	TPQ	TYR	MODIFIED RESIDUE	UNP Q29437

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

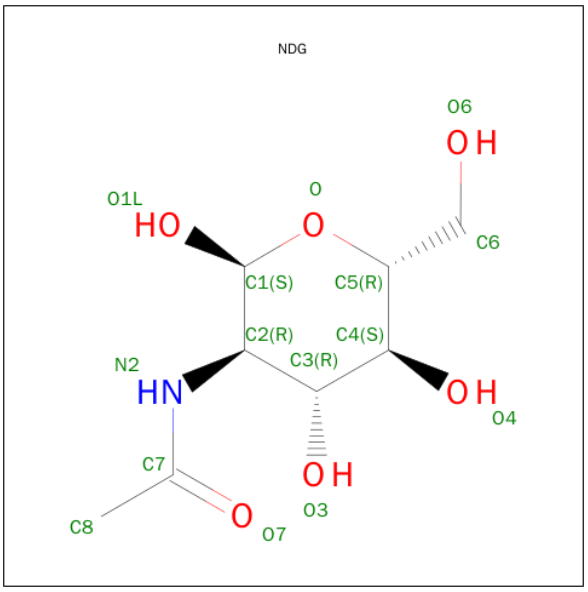
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cu	0	0
			1	1		
6	A	1	Total	Cu	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	2	Total	Ca	0	0
			2	2		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is water.

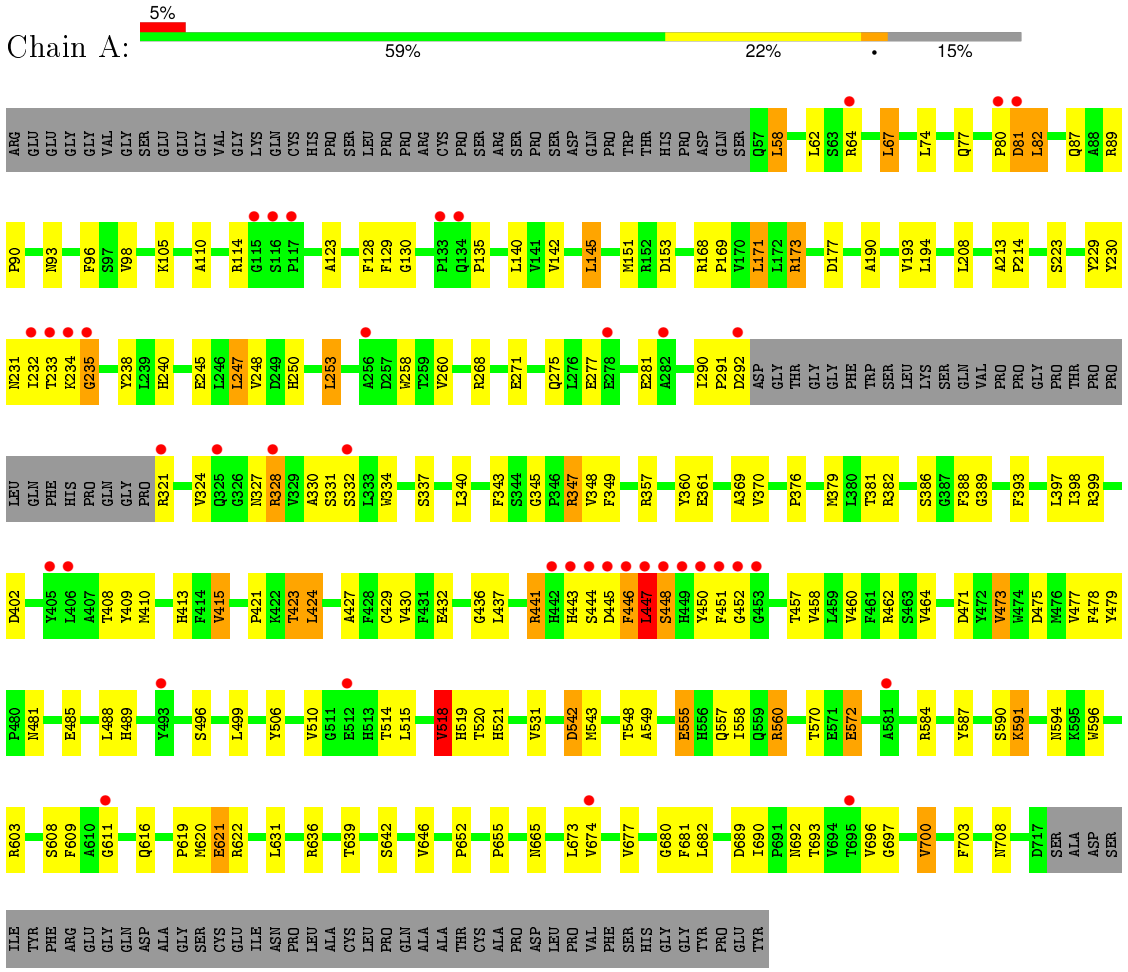
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	209	Total	O	0	0
			209	209		
9	B	201	Total	O	0	0
			201	201		

3 Residue-property plots (i)

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

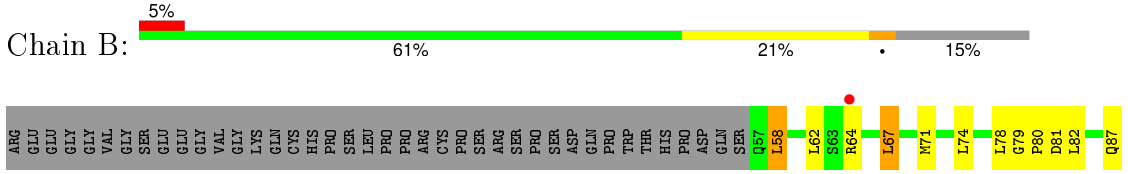
- Molecule 1: Copper amine oxidase, liver isozyme

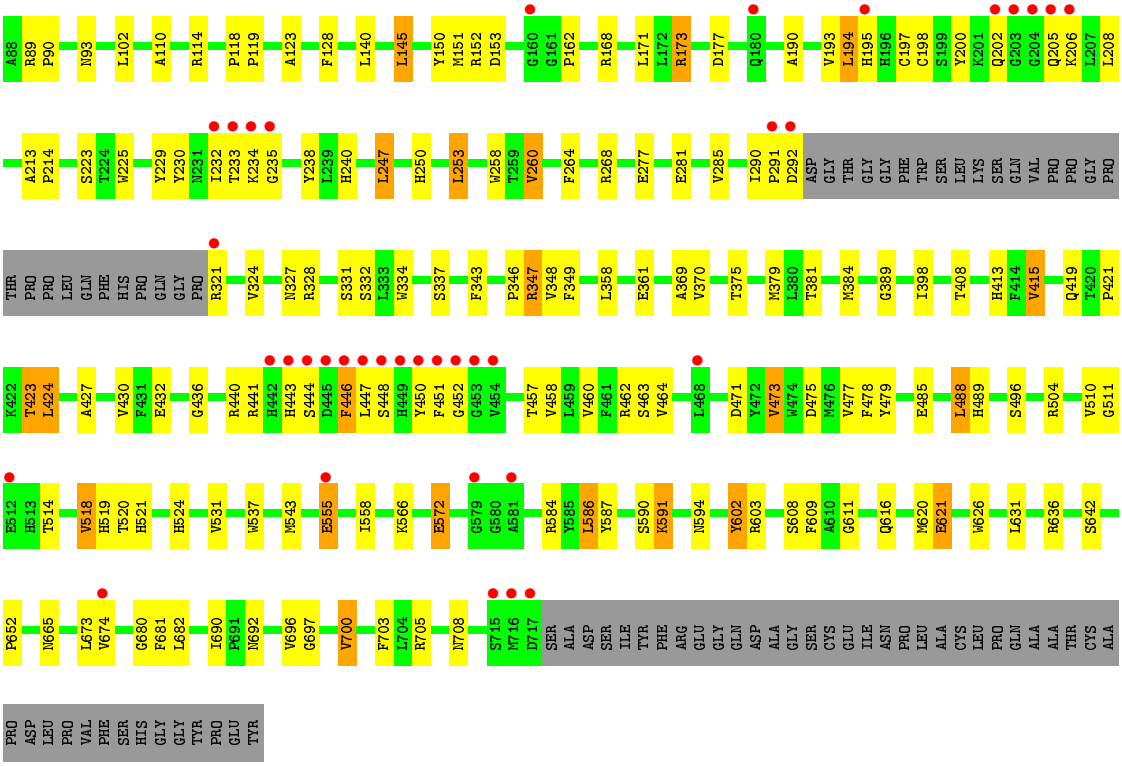
Chain A:



- Molecule 1: Copper amine oxidase, liver isozyme

Chain B:




A88 R89 P90 N93 L102 A110 R114 P118 P119 A123 F128 L140 L145 Y150 M151 R152 D153 G160 G161 P162 R168 L171 I172 R173 D177 Q180 A190 V193 L194 H195 H196 C197 C198 S199 Y200 K201 Q202 G203 G204 Q205 K206 L207 L208
A213 P214 S223 T224 W225 Y229 Y230 N231 I232 T233 K234 G235 Y238 L239 H240 L247 H250 L253 W258 T259 V260 F264 R268 E277 E281 V285 I290 P291 D292 ASP GLY THR GLY GLY PHE TRP SER LEU LYS SER GLN VAL PRO PRO GLY PRO
THR PRO PRO LEU GLN PHE HIS PRO GLN GLY PRO R321 V324 N327 R328 S331 S332 L333 W334 S337 F343 P346 R347 V348 F349 L358 E361 A369 V370 T375 M379 L380 T381 M384 G389 I398 T408 H413 F414 V415 Q419 T420 P421
K422 T423 L424 A427 V430 F431 E432 G436 R440 R441 H442 H443 S444 D445 F446 L447 S448 H449 Y450 F451 G452 G453 Y454 T457 V458 L459 V460 F461 R462 S463 V464 L468 D471 Y472 V473 W474 D475 M476 V477 F478 Y479 E485 L488 H489 S496 R504 V510 G511
E512 H513 T514 V518 H519 T520 H521 H524 V531 W537 M543 E555 I558 K566 E572 G579 G580 A581 R584 Y585 L586 Y587 S590 K591 N594 Y602 R603 S608 F609 A610 G611 Q616 M620 E621 W626 L631 R636 S642
P652 N665 L673 V674 G680 F681 L682 I690 P691 N692 V696 G697 V700 F703 L704 R705 N708 S715 M716 D717 SER ALA ASP SER ILE TYR PHE ARG GLU GLY GLN ASP ALA GLY SER CYS GLU ILE ASN PRO LEU ALA CYS LEU PRO GLN ALA ALA THR CYS ALA
PRO ASP LEU PRO VAL PHE SER HIS GLY GLY TYR PRO GLU TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.68Å 131.19Å 134.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.37 27.85 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.7 (25.00-2.37) 93.8 (27.85-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.237 0.215 , 0.241	Depositor DCC
R_{free} test set	3719 reflections (7.08%)	DCC
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.7	EDS
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 52570 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10581	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, CA, NDG, TPQ, CU

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	0.57	2/5156 (0.0%)	0.83	7/7025 (0.1%)
1	B	0.55	0/5156	0.79	6/7025 (0.1%)
All	All	0.56	2/10312 (0.0%)	0.81	13/14050 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	VAL	CB-CG1	-6.81	1.38	1.52
1	A	142	VAL	CB-CG2	5.38	1.64	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	448	SER	N-CA-C	-9.93	84.20	111.00
1	A	446	PHE	N-CA-C	8.70	134.49	111.00
1	A	447	LEU	CA-CB-CG	-8.53	95.69	115.30
1	B	448	SER	N-CA-C	-8.41	88.30	111.00
1	B	446	PHE	N-CA-C	6.98	129.84	111.00
1	A	145	LEU	CA-CB-CG	-6.36	100.68	115.30
1	A	142	VAL	CG1-CB-CG2	6.10	120.66	110.90
1	A	145	LEU	CB-CG-CD2	-5.96	100.87	111.00
1	A	518	VAL	CB-CA-C	-5.78	100.41	111.40
1	B	145	LEU	CA-CB-CG	-5.57	102.50	115.30
1	B	518	VAL	CB-CA-C	-5.55	100.86	111.40
1	B	384	MET	N-CA-C	-5.35	96.56	111.00
1	B	145	LEU	C-N-CD	-5.12	109.34	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5018	0	4801	165	0
1	B	5018	0	4802	139	0
2	A	42	0	37	2	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
4	A	14	0	13	4	0
5	B	42	0	37	6	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
9	A	209	0	0	5	0
9	B	201	0	0	3	0
All	All	10581	0	9716	292	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 15.

All (292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LYS:N	1:A:591:LYS:HD3	1.63	1.09
1:B:232:ILE:HG12	1:B:240:HIS:CD2	1.87	1.08
1:B:591:LYS:H	1:B:591:LYS:CD	1.62	1.07
1:B:591:LYS:HD2	1:B:591:LYS:N	1.65	1.07
1:A:591:LYS:CD	1:A:591:LYS:H	1.63	1.02
1:B:477:VAL:HG22	1:B:485:GLU:HB3	1.40	1.01
1:B:110:ALA:HB2	1:B:114:ARG:HH11	1.25	1.00
1:B:591:LYS:HD2	1:B:591:LYS:H	0.84	0.98
1:A:591:LYS:HD3	1:A:591:LYS:H	0.80	0.95
1:A:477:VAL:HG22	1:A:485:GLU:HB3	1.49	0.94
5:B:801:NAG:H61	5:B:802:NAG:H83	1.53	0.90
1:B:324:VAL:HG11	1:B:408:THR:HG21	1.54	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ALA:HA	1:A:114:ARG:NH1	1.86	0.88
1:A:462:ARG:HG3	1:A:475:ASP:OD1	1.75	0.87
1:A:324:VAL:HG11	1:A:408:THR:HG21	1.55	0.87
1:B:87:GLN:HA	1:B:173:ARG:HD2	1.56	0.86
1:B:110:ALA:HA	1:B:114:ARG:HE	1.41	0.85
1:B:324:VAL:CG1	1:B:408:THR:HG21	2.09	0.83
1:B:67:LEU:HG	1:B:415:VAL:HG12	1.61	0.83
1:B:74:LEU:HD23	1:B:151:MET:HE2	1.59	0.82
1:B:110:ALA:CB	1:B:114:ARG:HH11	1.93	0.81
1:B:477:VAL:CG2	1:B:485:GLU:HB3	2.11	0.81
1:A:477:VAL:CG2	1:A:485:GLU:HB3	2.11	0.80
1:B:110:ALA:HB2	1:B:114:ARG:NH1	1.96	0.80
1:A:324:VAL:CG1	1:A:408:THR:HG21	2.11	0.79
1:B:462:ARG:HG3	1:B:475:ASP:OD1	1.82	0.79
1:A:87:GLN:HA	1:A:173:ARG:HD2	1.66	0.78
1:A:665:ASN:OD1	4:A:804:NDG:H8C1	1.84	0.77
1:A:89:ARG:NH1	1:A:173:ARG:HD3	2.00	0.75
5:B:801:NAG:C6	5:B:802:NAG:H83	2.17	0.75
1:A:110:ALA:HA	1:A:114:ARG:HH11	1.51	0.74
1:A:347:ARG:HG3	1:A:349:PHE:CE1	2.25	0.72
1:A:424:LEU:HD13	1:A:427:ALA:HB2	1.72	0.72
1:A:347:ARG:HD3	9:A:1064:HOH:O	1.89	0.71
1:A:616:GLN:HA	1:A:621:GLU:HG2	1.73	0.70
1:A:58:LEU:HD23	1:A:58:LEU:H	1.59	0.67
1:A:413:HIS:CD2	1:A:423:THR:HB	2.29	0.67
1:B:213:ALA:HA	1:B:214:PRO:O	1.95	0.67
5:B:801:NAG:H61	5:B:802:NAG:C8	2.25	0.66
1:A:277:GLU:O	1:A:281:GLU:HG2	1.96	0.66
1:B:321:ARG:NH1	1:B:457:THR:HG21	2.12	0.65
1:A:74:LEU:HD23	1:A:151:MET:HE2	1.78	0.65
1:A:611:GLY:O	1:B:543:MET:SD	2.55	0.65
1:A:321:ARG:NH2	1:A:432:GLU:OE2	2.29	0.65
1:A:67:LEU:HG	1:A:415:VAL:HG12	1.79	0.64
1:A:347:ARG:HG3	1:A:349:PHE:HE1	1.61	0.64
1:B:232:ILE:CG1	1:B:240:HIS:CD2	2.76	0.63
1:B:347:ARG:HG3	1:B:349:PHE:CE1	2.33	0.63
1:A:557:GLN:HB2	9:A:1077:HOH:O	1.97	0.63
1:A:213:ALA:HA	1:A:214:PRO:O	1.98	0.63
1:A:74:LEU:HD23	1:A:151:MET:CE	2.29	0.63
1:B:89:ARG:NH1	1:B:173:ARG:HD3	2.13	0.63
1:B:555:GLU:CD	1:B:555:GLU:H	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:802:NAG:O3	2:A:802:NAG:H83	1.99	0.62
1:A:81:ASP:O	1:A:93:ASN:HB2	1.98	0.62
1:A:510:VAL:CG2	1:A:690:ILE:HD11	2.30	0.62
1:B:277:GLU:O	1:B:281:GLU:HG2	1.99	0.62
1:B:230:TYR:HE1	1:B:290:ILE:HG22	1.65	0.61
1:A:402:ASP:OD1	1:B:441:ARG:HD2	2.01	0.61
1:A:58:LEU:H	1:A:58:LEU:CD2	2.14	0.60
1:A:584:ARG:NE	1:B:611:GLY:HA2	2.16	0.60
1:A:558:ILE:HD11	1:B:379:MET:O	2.02	0.60
1:B:74:LEU:CD2	1:B:151:MET:HE2	2.32	0.60
1:A:596:TRP:CZ2	1:B:511:GLY:HA2	2.37	0.60
1:B:58:LEU:H	1:B:58:LEU:HD23	1.65	0.59
1:A:506:TYR:O	1:A:518:VAL:HG22	2.02	0.59
1:B:537:TRP:HZ3	1:B:591:LYS:HG3	1.65	0.59
1:A:74:LEU:CD2	1:A:151:MET:HE2	2.31	0.59
1:A:268:ARG:HH21	1:A:268:ARG:HG3	1.66	0.59
1:A:473:VAL:HG13	1:A:489:HIS:HB2	1.84	0.59
1:B:102:LEU:HD21	1:B:347:ARG:NH2	2.18	0.58
1:A:555:GLU:CD	1:A:555:GLU:H	2.06	0.58
1:A:572:GLU:HG2	4:A:804:NDG:O6	2.03	0.58
1:A:543:MET:SD	1:B:611:GLY:O	2.62	0.58
1:B:424:LEU:HD13	1:B:427:ALA:HB2	1.85	0.58
1:A:462:ARG:NH2	1:B:436:GLY:O	2.37	0.58
1:A:413:HIS:HD2	1:A:423:THR:HB	1.67	0.57
1:B:232:ILE:C	1:B:234:LYS:H	2.06	0.57
1:B:473:VAL:HG13	1:B:489:HIS:HB2	1.87	0.57
1:B:636:ARG:HH11	1:B:636:ARG:HG3	1.68	0.57
1:B:636:ARG:HB2	1:B:674:VAL:CG2	2.34	0.57
1:A:232:ILE:HG22	1:A:234:LYS:H	1.69	0.57
1:B:531:VAL:O	1:B:590:SER:HB3	2.03	0.56
1:B:587:TYR:HB3	1:B:603:ARG:HB3	1.86	0.56
1:B:324:VAL:HG11	1:B:408:THR:CG2	2.31	0.56
1:B:74:LEU:HD23	1:B:151:MET:CE	2.33	0.56
1:A:636:ARG:HB2	1:A:674:VAL:HG23	1.87	0.56
1:A:424:LEU:HD13	1:A:427:ALA:CB	2.35	0.56
1:B:620:MET:HB2	1:B:652:PRO:HB2	1.88	0.56
1:B:268:ARG:NH2	1:B:285:VAL:HG22	2.21	0.56
1:A:130:GLY:HA2	1:A:135:PRO:HB3	1.87	0.56
1:A:370:VAL:O	1:A:519:HIS:HA	2.06	0.56
1:A:587:TYR:HB3	1:A:603:ARG:HB3	1.88	0.56
1:A:531:VAL:O	1:A:590:SER:HB3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:VAL:CG2	1:B:690:ILE:HD11	2.36	0.55
3:A:803:NAG:H3	3:A:803:NAG:O7	2.06	0.55
1:B:616:GLN:HA	1:B:621:GLU:HG2	1.89	0.55
1:A:105:LYS:HE3	1:A:360:TYR:CG	2.41	0.55
1:A:229:TYR:CD2	1:A:238:TYR:HA	2.42	0.54
1:A:570:THR:HG21	4:A:804:NDG:H8C2	1.90	0.54
1:B:58:LEU:H	1:B:58:LEU:CD2	2.20	0.54
1:B:64:ARG:NH1	1:B:423:THR:HG22	2.22	0.54
1:B:443:HIS:ND1	1:B:444:SER:N	2.55	0.53
1:A:398:ILE:HD13	1:B:452:GLY:HA2	1.90	0.53
1:B:510:VAL:HB	1:B:690:ILE:HD12	1.91	0.53
1:B:370:VAL:O	1:B:519:HIS:HA	2.09	0.53
1:A:570:THR:HG21	4:A:804:NDG:C8	2.39	0.52
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.74	0.52
1:B:128:PHE:CZ	1:B:168:ARG:HB2	2.44	0.52
1:A:321:ARG:NH2	1:A:457:THR:CG2	2.73	0.52
1:A:67:LEU:HB3	1:A:421:PRO:HG3	1.91	0.52
1:A:620:MET:HB2	1:A:652:PRO:HB2	1.91	0.52
1:B:225:TRP:CE2	1:B:247:LEU:HG	2.45	0.52
1:A:436:GLY:O	1:B:462:ARG:NH2	2.43	0.52
1:B:78:LEU:HD12	1:B:82:LEU:HD11	1.92	0.52
1:A:443:HIS:ND1	1:A:444:SER:N	2.57	0.52
1:A:114:ARG:HG3	1:A:114:ARG:NH1	2.25	0.51
1:A:636:ARG:HB2	1:A:674:VAL:CG2	2.40	0.51
1:B:229:TYR:CD2	1:B:238:TYR:HA	2.45	0.51
1:A:223:SER:HB3	1:A:247:LEU:HD22	1.92	0.51
1:A:347:ARG:HG2	1:A:347:ARG:O	2.09	0.51
1:B:81:ASP:O	1:B:93:ASN:HB2	2.11	0.51
1:B:67:LEU:HB3	1:B:421:PRO:HG3	1.94	0.50
1:B:446:PHE:HB3	1:B:447:LEU:HD22	1.92	0.50
1:B:510:VAL:HB	1:B:690:ILE:CD1	2.41	0.50
1:A:689:ASP:CB	1:A:693:THR:HG22	2.42	0.50
1:A:324:VAL:HG11	1:A:408:THR:CG2	2.36	0.50
1:B:213:ALA:HA	1:B:214:PRO:C	2.32	0.50
1:B:424:LEU:HD13	1:B:427:ALA:CB	2.41	0.50
1:A:328:ARG:NH1	1:A:330:ALA:HB2	2.27	0.50
1:B:572:GLU:OE2	1:B:665:ASN:N	2.44	0.50
1:A:90:PRO:HB2	1:A:253:LEU:HA	1.94	0.50
1:A:446:PHE:HB3	1:A:447:LEU:HD22	1.94	0.50
1:A:499:LEU:HD12	1:A:515:LEU:HB2	1.94	0.49
1:B:347:ARG:HG3	1:B:349:PHE:HE1	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PHE:CZ	1:A:168:ARG:HB2	2.47	0.49
1:A:611:GLY:HA2	1:B:584:ARG:NE	2.26	0.49
1:B:608:SER:HA	1:B:700:VAL:HG22	1.95	0.49
1:B:343:PHE:HA	1:B:389:GLY:HA2	1.95	0.49
1:A:291:PRO:O	1:A:292:ASP:HB2	2.12	0.49
1:B:346:PRO:HG3	1:B:463:SER:OG	2.12	0.49
1:B:90:PRO:HB2	1:B:253:LEU:HA	1.93	0.49
1:B:140:LEU:HD23	1:B:153:ASP:HA	1.95	0.49
1:A:616:GLN:HA	1:A:621:GLU:CG	2.41	0.49
1:B:413:HIS:CD2	1:B:423:THR:HB	2.47	0.49
1:A:67:LEU:HD12	1:A:98:VAL:HG22	1.94	0.49
1:A:464:VAL:HG22	1:A:473:VAL:HB	1.95	0.48
1:B:208:LEU:C	1:B:208:LEU:HD12	2.33	0.48
5:B:801:NAG:H61	5:B:802:NAG:C7	2.44	0.48
1:A:321:ARG:NH2	1:A:457:THR:HG23	2.27	0.48
1:B:488:LEU:HD12	1:B:489:HIS:N	2.28	0.48
1:A:64:ARG:HD2	1:A:421:PRO:HB2	1.95	0.48
1:A:410:MET:HE1	1:A:430:VAL:HG23	1.94	0.48
1:B:477:VAL:HG23	1:B:479:TYR:CE1	2.48	0.48
1:B:110:ALA:CA	1:B:114:ARG:HH11	2.26	0.48
1:A:609:PHE:O	1:A:681:PHE:HA	2.13	0.48
1:A:596:TRP:O	1:B:504:ARG:NH2	2.47	0.48
1:A:447:LEU:HD13	1:A:447:LEU:N	2.25	0.48
1:B:62:LEU:HD11	1:B:123:ALA:HB2	1.94	0.48
1:A:703:PHE:CZ	1:B:697:GLY:HA2	2.48	0.48
1:B:162:PRO:HG3	5:B:800:NDG:H8C3	1.96	0.48
1:B:591:LYS:N	1:B:591:LYS:CD	2.42	0.47
1:A:230:TYR:HE1	1:A:290:ILE:HG22	1.78	0.47
1:B:232:ILE:O	1:B:234:LYS:N	2.46	0.47
1:B:321:ARG:HD3	1:B:432:GLU:OE1	2.14	0.47
1:A:697:GLY:HA2	1:B:703:PHE:CZ	2.49	0.47
1:B:334:TRP:CE2	1:B:478:PHE:HB3	2.49	0.47
1:B:173:ARG:NH1	1:B:177:ASP:OD1	2.48	0.47
1:A:87:GLN:CA	1:A:173:ARG:HD2	2.41	0.47
1:A:334:TRP:CE2	1:A:478:PHE:HB3	2.49	0.47
1:B:190:ALA:HB1	1:B:193:VAL:CG1	2.45	0.47
1:B:195:HIS:ND1	1:B:200:TYR:O	2.47	0.47
1:A:213:ALA:HA	1:A:214:PRO:C	2.35	0.47
1:A:96:PHE:CZ	1:A:169:PRO:HG2	2.50	0.47
1:B:190:ALA:O	1:B:194:LEU:HB2	2.13	0.47
1:A:430:VAL:HA	1:A:460:VAL:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LEU:N	1:B:447:LEU:HD22	2.29	0.47
1:A:560:ARG:HG3	9:A:929:HOH:O	2.15	0.46
1:B:358:LEU:HD22	1:B:602:TYR:CE1	2.50	0.46
1:B:524:HIS:HB2	1:B:626:TRP:CE3	2.51	0.46
1:B:223:SER:HB3	1:B:247:LEU:HD22	1.95	0.46
1:A:452:GLY:HA2	1:B:398:ILE:HD13	1.98	0.46
1:A:596:TRP:CH2	1:B:511:GLY:HA2	2.51	0.46
1:B:608:SER:HA	1:B:700:VAL:CG2	2.45	0.46
1:A:496:SER:HB3	1:A:514:THR:HG23	1.98	0.46
1:A:696:VAL:O	1:B:705:ARG:NH2	2.44	0.46
1:B:250:HIS:HA	1:B:258:TRP:CD1	2.51	0.46
1:B:369:ALA:HA	1:B:520:THR:O	2.15	0.46
1:B:636:ARG:HB2	1:B:674:VAL:HG23	1.98	0.46
3:A:803:NAG:O7	3:A:803:NAG:C3	2.64	0.46
1:A:548:THR:HG22	1:A:549:ALA:O	2.16	0.46
1:A:58:LEU:HD23	1:A:58:LEU:N	2.25	0.46
1:B:441:ARG:HA	1:B:452:GLY:O	2.16	0.46
1:A:140:LEU:HD23	1:A:153:ASP:HA	1.98	0.46
1:B:586:LEU:HD22	1:B:631:LEU:HD21	1.98	0.45
1:A:190:ALA:HB1	1:A:193:VAL:CG1	2.46	0.45
1:B:79:GLY:N	1:B:80:PRO:HD2	2.31	0.45
1:B:464:VAL:HG22	1:B:473:VAL:HB	1.98	0.45
1:A:379:MET:O	1:B:558:ILE:HD11	2.17	0.45
1:A:327:ASN:O	1:A:337:SER:HA	2.17	0.45
1:A:129:PHE:CG	2:A:800:NAG:H62	2.51	0.45
1:A:321:ARG:CZ	1:A:432:GLU:OE1	2.65	0.45
1:B:71:MET:HE2	1:B:419:GLN:HA	1.99	0.45
1:A:321:ARG:HH22	1:A:457:THR:HG23	1.81	0.44
1:A:81:ASP:HB2	1:A:93:ASN:HD22	1.82	0.44
1:A:128:PHE:HE1	1:A:171:LEU:HD13	1.81	0.44
1:A:268:ARG:NH2	9:A:1100:HOH:O	2.50	0.44
1:A:343:PHE:HA	1:A:389:GLY:HA2	1.98	0.44
1:A:349:PHE:CD2	1:A:361:GLU:HB2	2.53	0.44
1:A:689:ASP:OD1	1:A:693:THR:HG22	2.17	0.44
1:A:447:LEU:HD12	1:A:447:LEU:HA	1.60	0.44
1:B:521:HIS:O	1:B:680:GLY:HA3	2.17	0.44
1:B:587:TYR:HB3	1:B:603:ARG:CB	2.47	0.44
1:A:90:PRO:HB2	1:A:253:LEU:O	2.17	0.44
1:A:448:SER:HB3	1:A:450:TYR:CE1	2.52	0.44
1:A:631:LEU:HD13	1:A:677:VAL:HG22	2.00	0.44
1:A:510:VAL:O	1:A:690:ILE:HD12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:LEU:HD13	1:A:447:LEU:H	1.81	0.44
1:B:110:ALA:HA	1:B:114:ARG:NE	2.21	0.43
1:A:245:GLU:OE2	1:A:376:PRO:HB2	2.18	0.43
1:B:264:PHE:CZ	1:B:375:THR:HG22	2.53	0.43
1:A:622:ARG:HH12	1:A:655:PRO:HD2	1.83	0.43
1:B:537:TRP:CZ3	1:B:591:LYS:HG3	2.49	0.43
1:A:208:LEU:HD23	1:A:231:ASN:ND2	2.33	0.43
1:A:619:PRO:HD2	9:B:2011:HOH:O	2.17	0.43
1:B:291:PRO:O	1:B:292:ASP:HB2	2.17	0.43
1:B:430:VAL:HA	1:B:460:VAL:O	2.17	0.43
1:B:67:LEU:HA	1:B:67:LEU:HD12	1.92	0.43
1:B:213:ALA:O	1:B:381:THR:HA	2.18	0.43
1:A:471:ASP:OD2	1:B:441:ARG:NE	2.50	0.43
1:B:205:GLN:NE2	1:B:206:LYS:H	2.17	0.43
1:B:232:ILE:C	1:B:234:LYS:N	2.72	0.43
1:A:477:VAL:HG23	1:A:479:TYR:CE1	2.53	0.43
1:A:397:LEU:HD13	1:A:429:CYS:HB3	1.99	0.43
1:B:150:TYR:CD1	1:B:152:ARG:HD2	2.54	0.43
1:B:496:SER:HB3	1:B:514:THR:HG23	2.00	0.43
1:A:80:PRO:O	1:A:82:LEU:N	2.47	0.43
1:A:340:LEU:HD12	1:A:345:GLY:C	2.39	0.43
1:A:481:ASN:ND2	1:B:696:VAL:HG21	2.34	0.43
1:A:689:ASP:CG	1:A:693:THR:HG22	2.40	0.42
1:A:357:ARG:HD2	9:A:947:HOH:O	2.19	0.42
1:A:462:ARG:NH1	1:A:475:ASP:OD2	2.52	0.42
1:A:173:ARG:NH1	1:A:177:ASP:OD1	2.51	0.42
1:A:98:VAL:O	1:A:415:VAL:HG13	2.20	0.42
1:A:441:ARG:HA	1:A:452:GLY:O	2.19	0.42
1:A:399:ARG:HG2	1:A:409:TYR:CZ	2.55	0.42
1:A:521:HIS:O	1:A:680:GLY:HA3	2.19	0.42
1:B:616:GLN:HA	1:B:621:GLU:CG	2.48	0.42
1:A:230:TYR:CE1	1:A:290:ILE:HG22	2.53	0.42
1:B:586:LEU:HD22	1:B:631:LEU:CD2	2.49	0.42
5:B:802:NAG:C1	5:B:802:NAG:O7	2.67	0.42
1:A:462:ARG:CG	1:A:475:ASP:OD1	2.58	0.42
1:B:58:LEU:N	1:B:58:LEU:HD23	2.33	0.42
1:B:268:ARG:HH21	1:B:285:VAL:HG22	1.83	0.42
1:A:608:SER:HA	1:A:700:VAL:HG22	2.02	0.42
1:B:609:PHE:O	1:B:681:PHE:HA	2.18	0.42
1:B:347:ARG:HD3	9:B:2079:HOH:O	2.20	0.42
1:A:478:PHE:N	1:A:478:PHE:CD1	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:PHE:CD2	1:B:361:GLU:HB2	2.55	0.42
1:A:250:HIS:HA	1:A:258:TRP:CD1	2.55	0.42
1:A:594:ASN:HB3	1:A:708:ASN:O	2.20	0.42
1:A:281:GLU:HA	1:A:281:GLU:OE1	2.20	0.41
1:B:327:ASN:O	1:B:337:SER:HA	2.20	0.41
1:A:437:LEU:HD11	1:B:489:HIS:CD2	2.55	0.41
1:B:590:SER:HB2	1:B:591:LYS:HD2	2.01	0.41
1:A:462:ARG:HG3	1:A:462:ARG:HH11	1.85	0.41
1:A:213:ALA:O	1:A:381:THR:HA	2.21	0.41
1:A:145:LEU:HA	1:A:145:LEU:HD23	1.65	0.41
1:A:77:GLN:HB2	1:A:151:MET:HE1	2.01	0.41
1:A:386:SER:O	1:A:646:VAL:HG13	2.21	0.41
1:B:197:CYS:C	1:B:198:CYS:SG	2.99	0.41
1:A:232:ILE:HD12	1:A:240:HIS:CD2	2.56	0.41
1:A:268:ARG:NH2	1:A:268:ARG:HG3	2.32	0.41
1:A:128:PHE:CD1	1:A:168:ARG:HD2	2.55	0.41
1:A:321:ARG:HH22	1:A:457:THR:CG2	2.34	0.41
1:A:98:VAL:HG22	1:A:415:VAL:CG1	2.51	0.41
1:A:62:LEU:HD11	1:A:123:ALA:HB2	2.02	0.41
1:A:587:TYR:HB3	1:A:603:ARG:CB	2.51	0.41
1:A:234:LYS:HB3	1:A:235:GLY:H	1.52	0.40
1:A:689:ASP:HB3	1:A:693:THR:HG22	2.02	0.40
1:B:118:PRO:HA	1:B:119:PRO:HD3	1.95	0.40
1:A:81:ASP:O	1:A:81:ASP:OD2	2.38	0.40
1:A:608:SER:HA	1:A:700:VAL:CG2	2.51	0.40
1:A:271:GLU:HB2	1:A:275:GLN:OE1	2.22	0.40
1:A:114:ARG:CG	1:A:114:ARG:HH11	2.34	0.40
1:A:542:ASP:OD1	1:A:584:ARG:NH1	2.47	0.40
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.84	0.40
1:B:496:SER:HB3	1:B:514:THR:CG2	2.52	0.40
1:A:369:ALA:HA	1:A:520:THR:O	2.22	0.40
1:B:260:VAL:HG13	9:B:1960:HOH:O	2.21	0.40
1:A:388:PHE:HB3	1:A:393:PHE:CE2	2.56	0.40
1:B:594:ASN:HB3	1:B:708:ASN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	628/746 (84%)	592 (94%)	33 (5%)	3 (0%)	34	46
1	B	628/746 (84%)	594 (95%)	31 (5%)	3 (0%)	34	46
All	All	1256/1492 (84%)	1186 (94%)	64 (5%)	6 (0%)	34	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	THR
1	A	81	ASP
1	A	235	GLY
1	A	233	THR
1	B	235	GLY
1	B	450	TYR

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	530/623 (85%)	491 (93%)	39 (7%)	17	24
1	B	530/623 (85%)	494 (93%)	36 (7%)	20	28
All	All	1060/1246 (85%)	985 (93%)	75 (7%)	18	26

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	67	LEU
1	A	82	LEU
1	A	171	LEU
1	A	173	ARG
1	A	194	LEU
1	A	247	LEU
1	A	248	VAL
1	A	253	LEU
1	A	260	VAL
1	A	328	ARG
1	A	331	SER
1	A	332	SER
1	A	347	ARG
1	A	348	VAL
1	A	382	ARG
1	A	415	VAL
1	A	423	THR
1	A	424	LEU
1	A	441	ARG
1	A	445	ASP
1	A	447	LEU
1	A	451	PHE
1	A	458	VAL
1	A	473	VAL
1	A	488	LEU
1	A	518	VAL
1	A	542	ASP
1	A	555	GLU
1	A	560	ARG
1	A	572	GLU
1	A	591	LYS
1	A	621	GLU
1	A	639	THR
1	A	642	SER
1	A	673	LEU
1	A	682	LEU
1	A	692	ASN
1	A	700	VAL
1	B	58	LEU
1	B	67	LEU
1	B	171	LEU
1	B	173	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	194	LEU
1	B	202	GLN
1	B	247	LEU
1	B	253	LEU
1	B	260	VAL
1	B	328	ARG
1	B	331	SER
1	B	332	SER
1	B	347	ARG
1	B	348	VAL
1	B	415	VAL
1	B	423	THR
1	B	424	LEU
1	B	440	ARG
1	B	451	PHE
1	B	458	VAL
1	B	471	ASP
1	B	473	VAL
1	B	488	LEU
1	B	518	VAL
1	B	555	GLU
1	B	566	LYS
1	B	572	GLU
1	B	586	LEU
1	B	591	LYS
1	B	602	TYR
1	B	621	GLU
1	B	642	SER
1	B	673	LEU
1	B	682	LEU
1	B	692	ASN
1	B	700	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	205	GLN
1	A	279	GLN
1	A	413	HIS
1	A	456	GLN
1	A	559	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	616	GLN
1	A	712	GLN
1	B	184	ASN
1	B	205	GLN
1	B	231	ASN
1	B	279	GLN
1	B	413	HIS
1	B	442	HIS
1	B	456	GLN
1	B	489	HIS
1	B	559	GLN
1	B	692	ASN
1	B	712	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPQ	A	470	1	13,14,15	2.92	6 (46%)	15,19,21	1.61	2 (13%)
1	TPQ	B	470	1	13,14,15	2.90	5 (38%)	15,19,21	1.94	3 (20%)

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
1	TPQ	A	470	1	-	0/4/22/24	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	B	470	1	-	0/4/22/24	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	470	TPQ	C1-C2	-8.16	1.38	1.49
1	A	470	TPQ	C1-C2	-8.02	1.38	1.49
1	A	470	TPQ	C4-C5	-2.68	1.38	1.47
1	B	470	TPQ	C4-C5	-2.28	1.40	1.47
1	A	470	TPQ	C6-C5	-2.14	1.38	1.44
1	B	470	TPQ	C3-C4	2.26	1.39	1.35
1	A	470	TPQ	C3-C4	2.27	1.39	1.35
1	B	470	TPQ	O2-C2	2.92	1.32	1.24
1	A	470	TPQ	O2-C2	3.08	1.33	1.24
1	B	470	TPQ	O5-C5	3.10	1.33	1.24
1	A	470	TPQ	O5-C5	3.20	1.33	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	470	TPQ	C1-C6-C5	-5.06	119.89	122.97
1	A	470	TPQ	C1-C6-C5	-4.26	120.37	122.97
1	A	470	TPQ	C6-C1-C2	2.28	120.05	118.44
1	B	470	TPQ	C3-C2-C1	2.52	120.19	118.30
1	B	470	TPQ	C6-C1-C2	2.63	120.30	118.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

6 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	800	1,2	14,14,15	0.56	0	15,19,21	0.89	1 (6%)
2	NAG	A	801	2	14,14,15	0.68	0	15,19,21	0.62	0
2	NAG	A	802	2	14,14,15	1.09	1 (7%)	15,19,21	1.04	1 (6%)
5	NDG	B	800	1,5	14,14,15	0.78	0	15,19,21	1.28	2 (13%)
5	NAG	B	801	5	14,14,15	0.54	0	15,19,21	0.96	1 (6%)
5	NAG	B	802	5	14,14,15	0.73	0	15,19,21	0.88	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	800	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	801	2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	1/6/23/26	0/1/1/1
5	NDG	B	800	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	801	5	-	0/6/23/26	0/1/1/1
5	NAG	B	802	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	NAG	C1-C2	3.53	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	801	NAG	C2-N2-C7	-2.72	119.55	123.04
2	A	802	NAG	C3-C4-C5	-2.55	105.75	110.20
5	B	800	NDG	C2-N2-C7	-2.49	119.84	123.04
5	B	802	NAG	C2-N2-C7	-2.12	120.32	123.04
2	A	800	NAG	C2-N2-C7	-2.11	120.32	123.04
5	B	800	NDG	C1-O-C5	3.16	116.26	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	802	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	NAG	1	0
2	A	802	NAG	1	0
5	B	800	NDG	1	0
5	B	801	NAG	4	0
5	B	802	NAG	5	0

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	NAG	A	803	1	14,14,15	0.70	0	15,19,21	0.97	0
4	NDG	A	804	1	14,14,15	0.57	0	15,19,21	0.77	1 (6%)
3	NAG	B	804	1	14,14,15	0.74	0	15,19,21	0.91	1 (6%)

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	NAG	A	803	1	-	0/6/23/26	0/1/1/1
4	NDG	A	804	1	-	1/6/23/26	0/1/1/1
3	NAG	B	804	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	804	NAG	C2-N2-C7	-2.37	119.99	123.04
4	A	804	NDG	C2-N2-C7	-2.28	120.11	123.04

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	NDG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	NAG	2	0
4	A	804	NDG	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	632/746 (84%)	0.36	40 (6%)	23	27	11, 25, 50, 114	0
1	B	632/746 (84%)	0.43	38 (6%)	25	29	9, 25, 48, 115	0
All	All	1264/1492 (84%)	0.40	78 (6%)	24	28	9, 25, 49, 115	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	PHE	17.2
1	A	447	LEU	15.6
1	B	451	PHE	15.1
1	A	444	SER	15.0
1	A	450	TYR	14.9
1	B	444	SER	14.6
1	A	448	SER	14.4
1	B	450	TYR	14.0
1	A	449	HIS	12.9
1	B	447	LEU	12.6
1	B	445	ASP	11.8
1	A	446	PHE	11.2
1	B	448	SER	11.2
1	A	451	PHE	10.6
1	B	233	THR	10.2
1	A	443	HIS	9.8
1	B	449	HIS	9.5
1	B	716	MET	8.0
1	B	203	GLY	7.6
1	B	443	HIS	7.3
1	A	235	GLY	7.2
1	A	445	ASP	7.1
1	A	442	HIS	7.0
1	B	717	ASP	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	233	THR	5.8
1	B	715	SER	5.8
1	A	452	GLY	4.9
1	B	204	GLY	4.6
1	B	234	LYS	4.6
1	B	292	ASP	4.4
1	B	235	GLY	4.4
1	B	453	GLY	4.3
1	B	232	ILE	3.8
1	A	232	ILE	3.8
1	A	453	GLY	3.7
1	A	81	ASP	3.7
1	A	234	LYS	3.7
1	B	442	HIS	3.7
1	A	512	GLU	3.4
1	B	160	GLY	3.4
1	B	202	GLN	3.4
1	B	555	GLU	3.4
1	A	321	ARG	3.4
1	A	282	ALA	3.3
1	A	80	PRO	3.3
1	A	117	PRO	3.2
1	B	291	PRO	3.1
1	B	454	VAL	3.1
1	B	579	GLY	3.0
1	B	180	GLN	3.0
1	A	611	GLY	2.9
1	B	321	ARG	2.9
1	B	452	GLY	2.9
1	B	205	GLN	2.8
1	B	206	LYS	2.8
1	A	493	TYR	2.7
1	A	115	GLY	2.7
1	A	581	ALA	2.6
1	B	581	ALA	2.6
1	A	133	PRO	2.5
1	A	674	VAL	2.4
1	A	116	SER	2.4
1	B	468	LEU	2.4
1	A	328	ARG	2.4
1	A	292	ASP	2.3
1	B	512	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	325	GLN	2.2
1	A	405	TYR	2.2
1	B	195	HIS	2.2
1	A	278	GLU	2.2
1	A	332	SER	2.2
1	A	256	ALA	2.1
1	A	134	GLN	2.1
1	A	695	THR	2.1
1	B	64	ARG	2.1
1	A	406	LEU	2.0
1	A	64	ARG	2.0
1	B	674	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	TPQ	B	470	14/15	0.82	0.21	-	40,53,55,56	0
1	TPQ	A	470	14/15	0.85	0.18	-	40,50,52,52	0

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	800	14/15	0.93	0.13	0.47	29,30,32,36	0
5	NDG	B	800	14/15	0.94	0.12	-0.77	29,31,35,35	0
2	NAG	A	801	14/15	0.89	0.15	-	28,44,49,55	0
5	NAG	B	802	14/15	0.69	0.41	-	61,64,66,67	0
5	NAG	B	801	14/15	0.91	0.22	-	35,42,49,55	0
2	NAG	A	802	14/15	0.68	0.47	-	63,70,73,74	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	803	14/15	0.77	0.42	-0.27	48,49,51,52	0
8	CL	B	1905	1/1	0.98	0.10	-0.84	25,25,25,25	0
7	CA	A	902	1/1	0.99	0.10	-0.96	18,18,18,18	0
7	CA	B	1902	1/1	0.99	0.06	-1.80	23,23,23,23	0
7	CA	B	1903	1/1	0.99	0.05	-2.10	23,23,23,23	0
7	CA	A	903	1/1	0.98	0.03	-2.99	19,19,19,19	0
3	NAG	B	804	14/15	0.70	0.50	-	57,60,62,63	0
6	CU	A	901	1/1	1.00	0.08	-	21,21,21,21	0
8	CL	A	904	1/1	0.94	0.08	-	32,32,32,32	0
8	CL	B	1904	1/1	0.98	0.09	-	32,32,32,32	0
6	CU	B	901	1/1	0.99	0.07	-	23,23,23,23	0
4	NDG	A	804	14/15	0.80	0.53	-	64,67,67,68	0

6.5 Other polymers (i)

There are no such residues in this entry.