



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 10:02 AM EST

PDB ID : 1AHG
Title : ASPARTATE AMINOTRANSFERASE HEXAMUTANT
Authors : Malashkevich, V.N.; Jansonius, J.N.
Deposited on : 1995-02-22
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

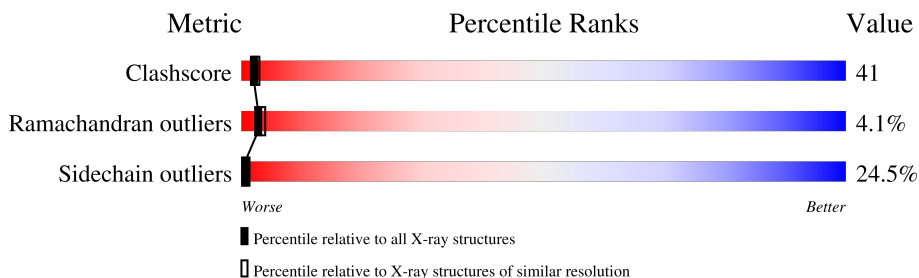
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	 34% 45% 20% .
1	B	396	 33% 47% 17% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6708 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.

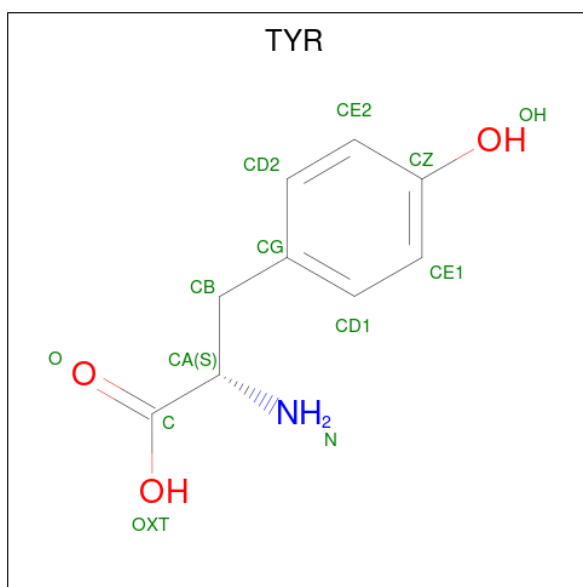
- Molecule 1 is a protein called Aspartate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3071	1942	533	583	13	0	0	0
1	B	396	3071	1942	533	583	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

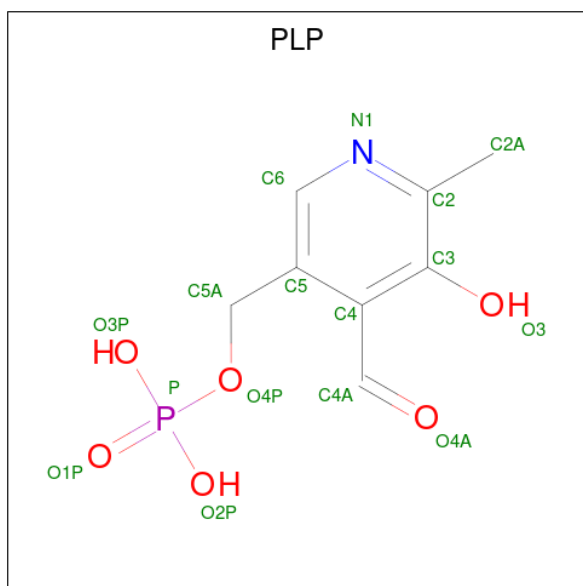
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LEU	VAL	engineered mutation	UNP P00509
A	41	TYR	LYS	engineered mutation	UNP P00509
A	47	ILE	THR	engineered mutation	UNP P00509
A	69	LEU	ASN	engineered mutation	UNP P00509
A	109	SER	THR	engineered mutation	UNP P00509
A	297	SER	ASN	engineered mutation	UNP P00509
B	39	LEU	VAL	engineered mutation	UNP P00509
B	41	TYR	LYS	engineered mutation	UNP P00509
B	47	ILE	THR	engineered mutation	UNP P00509
B	69	LEU	ASN	engineered mutation	UNP P00509
B	109	SER	THR	engineered mutation	UNP P00509
B	297	SER	ASN	engineered mutation	UNP P00509

- Molecule 2 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	13	9	1	3	0	0
2	B	1	13	9	1	3	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0
3	B	1	15	8	1	5	1	0	0

- Molecule 4 is water.

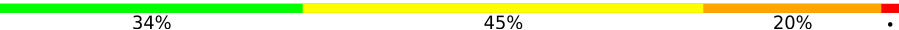
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total 249	O 249	0	0
4	B	261	Total 261	O 261	0	0

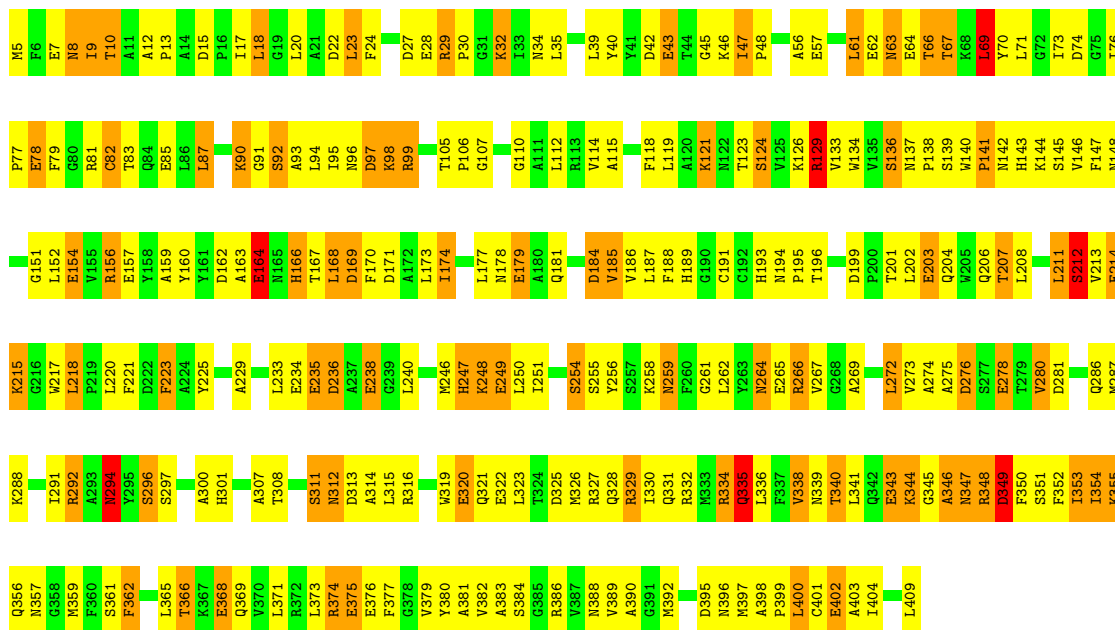
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

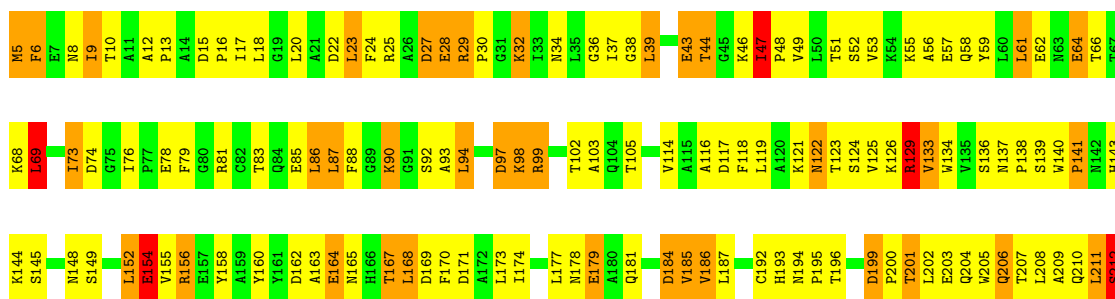
- Molecule 1: Aspartate aminotransferase

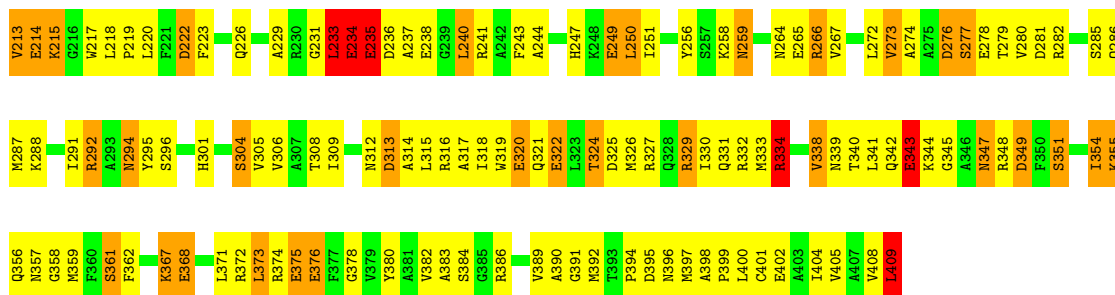
Chain A: 



- Molecule 1: Aspartate aminotransferase

Chain B: 





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.00Å 79.10Å 89.60Å 90.00° 118.67° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	90.5 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.250 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6708	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

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	0.98	25/3133 (0.8%)	1.33	34/4244 (0.8%)
1	B	0.96	21/3133 (0.7%)	1.33	34/4244 (0.8%)
All	All	0.97	46/6266 (0.7%)	1.33	68/8488 (0.8%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	GLU	CD-OE2	7.48	1.33	1.25
1	A	249	GLU	CD-OE2	6.69	1.33	1.25
1	A	203	GLU	CD-OE2	6.63	1.32	1.25
1	B	64	GLU	CD-OE2	6.52	1.32	1.25
1	A	234	GLU	CD-OE1	6.37	1.32	1.25
1	B	234	GLU	CD-OE2	6.24	1.32	1.25
1	B	320	GLU	CD-OE1	6.22	1.32	1.25
1	A	179	GLU	CD-OE2	6.21	1.32	1.25
1	B	43	GLU	CD-OE1	6.19	1.32	1.25
1	A	375	GLU	CD-OE1	6.13	1.32	1.25
1	A	235	GLU	CD-OE2	6.13	1.32	1.25
1	A	265	GLU	CD-OE1	6.09	1.32	1.25
1	A	154	GLU	CD-OE2	6.08	1.32	1.25
1	A	64	GLU	CD-OE2	6.07	1.32	1.25
1	A	43	GLU	CD-OE2	6.03	1.32	1.25
1	B	179	GLU	CD-OE2	5.97	1.32	1.25
1	A	376	GLU	CD-OE1	5.97	1.32	1.25
1	A	320	GLU	CD-OE1	5.95	1.32	1.25
1	B	249	GLU	CD-OE2	5.93	1.32	1.25
1	B	78	GLU	CD-OE1	5.90	1.32	1.25
1	B	203	GLU	CD-OE2	5.86	1.32	1.25
1	B	238	GLU	CD-OE2	5.86	1.32	1.25
1	A	78	GLU	CD-OE2	5.83	1.32	1.25
1	B	343	GLU	CD-OE2	5.75	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	GLU	CD-OE2	5.75	1.31	1.25
1	A	28	GLU	CD-OE1	5.73	1.31	1.25
1	B	28	GLU	CD-OE1	5.67	1.31	1.25
1	A	278	GLU	CD-OE1	5.65	1.31	1.25
1	B	375	GLU	CD-OE2	5.65	1.31	1.25
1	A	368	GLU	CD-OE1	5.62	1.31	1.25
1	A	164	GLU	CD-OE2	5.60	1.31	1.25
1	B	235	GLU	CD-OE2	5.60	1.31	1.25
1	B	214	GLU	CD-OE2	5.59	1.31	1.25
1	B	62	GLU	CD-OE2	5.54	1.31	1.25
1	A	343	GLU	CD-OE2	5.48	1.31	1.25
1	B	376	GLU	CD-OE2	5.47	1.31	1.25
1	A	85	GLU	CD-OE1	5.45	1.31	1.25
1	B	154	GLU	CD-OE1	5.39	1.31	1.25
1	B	85	GLU	CD-OE1	5.38	1.31	1.25
1	A	402	GLU	CD-OE2	5.36	1.31	1.25
1	A	57	GLU	CD-OE2	5.34	1.31	1.25
1	A	157	GLU	CD-OE2	5.08	1.31	1.25
1	A	214	GLU	CD-OE1	5.07	1.31	1.25
1	B	322	GLU	CD-OE2	5.07	1.31	1.25
1	A	238	GLU	CD-OE2	5.06	1.31	1.25
1	B	265	GLU	CD-OE1	5.03	1.31	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ASP	CB-CG-OD2	-7.88	111.20	118.30
1	B	329	ARG	NE-CZ-NH1	-7.67	116.47	120.30
1	B	276	ASP	CB-CG-OD2	-7.63	111.44	118.30
1	B	313	ASP	CB-CG-OD1	-7.62	111.44	118.30
1	B	395	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	B	329	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	B	27	ASP	CB-CG-OD1	-7.43	111.62	118.30
1	A	74	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	22	ASP	CB-CG-OD1	-7.19	111.83	118.30
1	B	222	ASP	CB-CG-OD1	6.97	124.58	118.30
1	A	74	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	99	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	B	97	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	B	266	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	B	27	ASP	N-CA-CB	6.56	122.42	110.60
1	B	169	ASP	CB-CG-OD1	6.56	124.20	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	B	169	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	169	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	B	368	GLU	N-CA-CB	6.36	122.05	110.60
1	B	167	THR	O-C-N	6.36	132.87	122.70
1	A	27	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	A	276	ASP	CB-CG-OD2	-6.32	112.62	118.30
1	B	276	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	184	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	A	281	ASP	CB-CG-OD1	-6.14	112.77	118.30
1	A	15	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	281	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	B	395	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	335	GLN	N-CA-CB	6.02	121.44	110.60
1	A	276	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	97	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	A	99	ARG	NE-CZ-NH1	-5.99	117.30	120.30
1	B	117	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	B	334	ARG	N-CA-CB	5.79	121.03	110.60
1	A	169	ASP	CB-CG-OD1	5.77	123.50	118.30
1	B	184	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	A	294	ASN	N-CA-CB	5.75	120.95	110.60
1	A	15	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	22	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	27	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	97	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	250	LEU	N-CA-CB	5.63	121.66	110.40
1	A	236	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	171	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	171	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	167	THR	CB-CA-C	-5.49	96.78	111.60
1	A	129	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	349	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	124	SER	N-CA-CB	5.43	118.65	110.50
1	A	171	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	22	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	A	27	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	117	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	97	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	313	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	162	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	B	409	LEU	N-CA-CB	5.21	120.82	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	266	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	129	ARG	N-CA-CB	5.19	119.94	110.60
1	B	281	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	222	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	334	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	316	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	B	349	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	162	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	184	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3071	0	3022	239	0
1	B	3071	0	3022	281	0
2	A	13	0	8	2	0
2	B	13	0	8	1	0
3	A	15	0	6	2	0
3	B	15	0	6	2	0
4	A	249	0	0	22	0
4	B	261	0	0	19	0
All	All	6708	0	6072	497	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 41.

All (497) 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:129:ARG:HB2	1:A:154:GLU:HB3	1.32	1.10
1:A:312:ASN:ND2	1:A:315:LEU:H	1.50	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:HD2	1:B:47:ILE:HG13	1.38	1.04
1:B:29:ARG:HH11	1:B:29:ARG:HG3	1.22	1.03
1:B:389:VAL:HG22	1:B:392:MET:HE1	1.54	0.90
1:A:46:LYS:HD2	1:A:47:ILE:H	1.38	0.88
1:B:200:PRO:HG2	1:B:205:TRP:CE2	2.09	0.87
1:A:366:THR:HG22	1:A:369:GLN:H	1.40	0.87
1:B:46:LYS:HD2	1:B:47:ILE:H	1.40	0.87
1:B:397:MET:HE3	1:B:400:LEU:HD13	1.56	0.85
1:B:212:SER:HB2	1:B:217:TRP:HE3	1.43	0.83
1:B:99:ARG:HH11	1:B:99:ARG:HG2	1.41	0.83
1:A:366:THR:HG22	1:A:369:GLN:N	1.92	0.83
1:A:258:LYS:HG2	1:A:359:MET:CE	2.09	0.83
1:B:389:VAL:HG22	1:B:392:MET:CE	2.08	0.82
1:A:292:ARG:HH12	1:B:15:ASP:HA	1.44	0.82
1:B:338:VAL:HG11	1:B:354:ILE:HD11	1.62	0.81
1:A:203:GLU:HG2	4:A:683:HOH:O	1.81	0.81
1:A:312:ASN:HD21	1:A:315:LEU:H	1.27	0.80
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.44	0.80
1:A:77:PRO:HB2	1:A:81:ARG:HH22	1.46	0.79
1:B:319:TRP:HA	1:B:322:GLU:HG3	1.63	0.79
1:B:170:PHE:CZ	1:B:208:LEU:HD21	2.19	0.78
1:A:173:LEU:HD13	1:A:177:LEU:HD12	1.65	0.78
1:B:83:THR:HG22	1:B:87:LEU:HD22	1.64	0.77
1:B:314:ALA:O	1:B:318:ILE:HG13	1.84	0.77
1:A:235:GLU:O	1:A:238:GLU:HG3	1.85	0.77
1:A:331:GLN:HB3	4:A:666:HOH:O	1.84	0.77
1:A:61:LEU:HD12	1:B:61:LEU:HD12	1.64	0.76
1:A:185:VAL:HG22	1:A:218:LEU:HB3	1.67	0.76
1:A:121:LYS:NZ	1:A:121:LYS:HB3	2.00	0.76
1:A:229:ALA:HB3	1:A:236:ASP:OD1	1.85	0.75
1:A:83:THR:HG22	1:A:87:LEU:HD22	1.69	0.75
1:B:98:LYS:HA	1:B:98:LYS:CE	2.16	0.74
1:A:142:ASN:O	1:A:146:VAL:HG22	1.86	0.74
1:A:258:LYS:HG2	1:A:359:MET:HE1	1.70	0.74
1:A:248:LYS:CG	1:A:275:ALA:HB2	2.15	0.74
1:A:46:LYS:O	1:A:48:PRO:HD3	1.88	0.74
1:B:220:LEU:HD12	1:B:251:ILE:HB	1.69	0.74
1:A:397:MET:HA	1:A:397:MET:CE	2.18	0.74
1:B:46:LYS:CD	1:B:47:ILE:HG13	2.14	0.73
1:B:46:LYS:O	1:B:48:PRO:HD3	1.88	0.73
1:B:170:PHE:CE2	1:B:174:ILE:HD11	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LYS:HA	1:B:98:LYS:HE2	1.70	0.73
1:B:88:PHE:O	1:B:241:ARG:HD3	1.89	0.72
1:A:129:ARG:HG3	1:A:156:ARG:HG2	1.71	0.72
1:B:164:GLU:HA	4:B:689:HOH:O	1.88	0.72
1:A:377:PHE:CD2	1:A:403:ALA:HB1	2.25	0.72
1:B:73:ILE:HG23	1:B:296:SER:O	1.89	0.72
1:B:332:ARG:HD2	4:B:611:HOH:O	1.89	0.72
1:B:397:MET:HA	1:B:397:MET:CE	2.19	0.71
1:B:204:GLN:O	1:B:208:LEU:HG	1.89	0.71
1:A:374:ARG:HG2	1:A:374:ARG:O	1.90	0.71
1:B:398:ALA:HB3	1:B:399:PRO:HD3	1.73	0.71
1:B:129:ARG:HG3	1:B:129:ARG:NH1	2.06	0.71
1:B:187:LEU:HD12	1:B:220:LEU:O	1.91	0.71
1:B:46:LYS:HD2	1:B:47:ILE:CG1	2.20	0.71
1:B:46:LYS:CD	1:B:47:ILE:H	2.03	0.71
1:B:99:ARG:HG2	1:B:99:ARG:NH1	2.05	0.70
1:B:212:SER:HB2	1:B:217:TRP:CE3	2.26	0.70
1:B:250:LEU:HD12	1:B:273:VAL:CG1	2.22	0.70
1:A:347:ASN:OD1	1:A:348:ARG:HG2	1.91	0.70
1:B:330:ILE:HG23	1:B:389:VAL:HG12	1.72	0.70
1:A:92:SER:HB3	1:A:95:ILE:HD12	1.74	0.70
1:B:18:LEU:HD12	1:B:37:ILE:HD12	1.73	0.69
1:A:63:ASN:HD22	1:A:63:ASN:N	1.90	0.69
1:A:312:ASN:HD22	1:A:315:LEU:H	1.34	0.69
1:A:276:ASP:O	1:A:280:VAL:HG22	1.92	0.69
1:A:69:LEU:HD21	1:B:47:ILE:CD1	2.22	0.69
1:B:200:PRO:HG2	1:B:205:TRP:NE1	2.08	0.69
1:A:194:ASN:HD22	3:A:500:PLP:H2A1	1.58	0.69
1:A:251:ILE:HD13	1:A:272:LEU:HD23	1.74	0.69
1:A:321:GLN:HG3	1:A:325:ASP:OD2	1.92	0.69
1:A:170:PHE:CE2	1:A:207:THR:HG21	2.28	0.69
1:A:206:GLN:HG3	4:A:751:HOH:O	1.93	0.68
1:B:129:ARG:HB3	1:B:154:GLU:HG2	1.74	0.68
1:A:170:PHE:HE2	1:A:207:THR:HG21	1.59	0.68
1:A:29:ARG:O	1:A:32:LYS:HG2	1.92	0.68
1:A:42:ASP:HB2	4:A:606:HOH:O	1.92	0.68
1:A:69:LEU:O	1:B:264:ASN:HB3	1.93	0.68
1:A:357:ASN:ND2	4:A:601:HOH:O	2.26	0.68
1:B:29:ARG:HG3	1:B:29:ARG:NH1	2.02	0.68
1:B:46:LYS:HD2	1:B:47:ILE:N	2.08	0.68
1:A:274:ALA:HB3	1:A:280:VAL:HG13	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ALA:HB3	1:A:399:PRO:HD3	1.75	0.67
1:A:389:VAL:O	1:A:392:MET:HB2	1.94	0.67
1:B:344:LYS:HD2	1:B:402:GLU:HG2	1.75	0.67
1:A:83:THR:HG22	1:A:87:LEU:CD2	2.25	0.67
1:B:207:THR:HG22	1:B:208:LEU:N	2.10	0.66
1:B:256:TYR:HA	1:B:259:ASN:HD21	1.61	0.66
1:A:170:PHE:CE2	1:A:174:ILE:HD11	2.30	0.66
1:B:123:THR:OG1	1:B:125:VAL:HG23	1.94	0.66
1:B:210:GLN:HB3	4:B:707:HOH:O	1.96	0.66
1:A:24:PHE:CE1	1:A:34:ASN:HB2	2.31	0.66
1:B:338:VAL:HG11	1:B:354:ILE:CD1	2.26	0.66
1:B:193:HIS:ND1	1:B:196:THR:OG1	2.29	0.65
1:B:87:LEU:O	1:B:241:ARG:NH1	2.29	0.65
1:B:29:ARG:NH2	1:B:374:ARG:O	2.30	0.65
1:A:13:PRO:HD2	4:A:742:HOH:O	1.97	0.65
1:B:143:HIS:NE2	1:B:222:ASP:OD2	2.30	0.65
1:B:250:LEU:HD12	1:B:273:VAL:HG13	1.79	0.65
1:A:63:ASN:N	1:A:63:ASN:ND2	2.45	0.65
4:A:608:HOH:O	1:B:68:LYS:HB2	1.96	0.64
1:B:99:ARG:NH1	1:B:274:ALA:O	2.29	0.64
1:B:99:ARG:NH2	4:B:606:HOH:O	2.29	0.64
1:B:202:LEU:HD12	1:B:202:LEU:O	1.97	0.64
1:B:356:GLN:OE1	1:B:361:SER:HA	1.96	0.64
1:A:110:GLY:O	1:A:114:VAL:HG23	1.97	0.64
1:A:348:ARG:NH2	4:A:603:HOH:O	2.28	0.64
1:A:229:ALA:HB3	1:A:236:ASP:CG	2.17	0.64
1:A:10:THR:HG23	4:A:716:HOH:O	1.97	0.64
1:B:27:ASP:OD2	1:B:29:ARG:NH1	2.29	0.64
1:A:99:ARG:O	1:A:280:VAL:HG11	1.98	0.64
1:A:212:SER:HB2	1:A:217:TRP:CE3	2.33	0.64
1:B:348:ARG:NH2	4:B:608:HOH:O	2.30	0.64
1:B:347:ASN:HB2	1:B:409:LEU:HD12	1.80	0.63
1:A:374:ARG:NH2	4:A:602:HOH:O	2.26	0.63
1:A:225:TYR:CE1	1:A:258:LYS:HD3	2.33	0.63
1:A:258:LYS:HG2	1:A:359:MET:HE3	1.79	0.63
1:B:94:LEU:HD11	1:B:244:ALA:HB1	1.80	0.63
1:B:134:TRP:HA	1:B:156:ARG:O	1.98	0.63
1:B:277:SER:HA	1:B:280:VAL:HG12	1.81	0.63
1:A:400:LEU:HD12	1:A:401:CYS:N	2.13	0.62
1:A:12:ALA:HB2	1:B:286:GLN:NE2	2.14	0.62
1:A:215:LYS:NZ	4:A:615:HOH:O	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLU:HA	1:B:273:VAL:O	2.00	0.62
1:A:352:PHE:O	1:A:355:LYS:HG3	2.00	0.62
1:B:372:ARG:HG3	1:B:372:ARG:O	1.98	0.61
1:A:321:GLN:HE21	1:A:325:ASP:CG	2.02	0.61
1:B:83:THR:CG2	1:B:87:LEU:HD22	2.30	0.61
1:B:372:ARG:O	1:B:376:GLU:HB3	2.01	0.61
1:A:129:ARG:HD3	1:A:156:ARG:HG3	1.82	0.61
1:A:71:LEU:HB2	4:A:628:HOH:O	2.00	0.61
1:B:259:ASN:H	1:B:259:ASN:HD22	1.48	0.61
1:B:372:ARG:HG2	1:B:408:VAL:HG11	1.82	0.61
2:B:501:TYR:N	3:B:500:PLP:O3	2.33	0.61
1:A:93:ALA:O	1:A:97:ASP:N	2.29	0.61
1:A:105:THR:O	1:A:107:GLY:N	2.32	0.61
1:A:193:HIS:ND1	1:A:196:THR:OG1	2.30	0.61
1:B:133:VAL:HB	1:B:185:VAL:HG12	1.81	0.61
1:B:332:ARG:NH1	4:B:611:HOH:O	2.30	0.61
1:A:373:LEU:HA	1:A:377:PHE:HD2	1.66	0.60
1:A:381:ALA:N	4:A:605:HOH:O	2.28	0.60
1:A:262:LEU:HD23	1:B:68:LYS:HD3	1.82	0.60
1:A:312:ASN:ND2	1:A:315:LEU:N	2.35	0.60
1:B:29:ARG:NH2	1:B:378:GLY:HA2	2.17	0.60
1:A:8:ASN:OD1	1:A:8:ASN:N	2.30	0.60
1:A:211:LEU:O	1:A:214:GLU:N	2.34	0.60
1:B:305:VAL:O	1:B:308:THR:HB	2.02	0.60
1:B:229:ALA:HB3	1:B:236:ASP:OD2	2.02	0.59
1:A:212:SER:HB2	1:A:217:TRP:HE3	1.65	0.59
1:B:344:LYS:CD	1:B:402:GLU:HG2	2.32	0.59
1:A:78:GLU:CD	1:A:81:ARG:HH21	2.06	0.59
1:A:321:GLN:NE2	1:A:325:ASP:OD1	2.34	0.59
1:A:40:TYR:OH	1:A:329:ARG:HD3	2.02	0.59
1:A:264:ASN:HB3	1:B:69:LEU:O	2.02	0.59
1:A:259:ASN:N	1:A:259:ASN:HD22	1.99	0.59
1:B:29:ARG:O	1:B:32:LYS:HD3	2.02	0.59
1:A:12:ALA:HB1	4:A:742:HOH:O	2.02	0.59
1:A:344:LYS:HD3	1:A:402:GLU:HG2	1.84	0.59
1:A:201:THR:OG1	1:A:204:GLN:HG3	2.02	0.59
1:A:373:LEU:HD21	1:A:404:ILE:HA	1.84	0.59
1:A:397:MET:HA	1:A:397:MET:HE2	1.84	0.59
1:A:17:ILE:O	1:A:20:LEU:HB2	2.02	0.59
1:A:251:ILE:CD1	1:A:272:LEU:HD23	2.33	0.59
1:B:114:VAL:HG12	1:B:287:MET:HE2	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLU:HG2	4:A:614:HOH:O	2.03	0.58
1:B:170:PHE:CE2	1:B:207:THR:HG21	2.37	0.58
1:A:156:ARG:HE	1:A:156:ARG:HA	1.67	0.58
1:A:34:ASN:HA	1:A:380:TYR:HB2	1.83	0.58
1:B:46:LYS:CG	1:B:47:ILE:H	2.16	0.58
1:A:10:THR:O	1:B:286:GLN:NE2	2.33	0.58
1:B:46:LYS:NZ	1:B:47:ILE:HG13	2.19	0.58
1:B:53:VAL:O	1:B:57:GLU:HG3	2.04	0.58
1:A:69:LEU:HD21	1:B:47:ILE:HD13	1.86	0.58
1:A:292:ARG:NH1	1:B:15:ASP:HA	2.15	0.58
1:A:78:GLU:HA	1:A:78:GLU:OE1	2.03	0.57
1:A:366:THR:HB	1:A:369:GLN:OE1	2.03	0.57
1:A:327:ARG:HG2	1:A:331:GLN:HE21	1.68	0.57
1:A:166:HIS:ND1	1:A:166:HIS:N	2.52	0.57
1:A:259:ASN:ND2	1:A:259:ASN:H	2.02	0.57
1:A:322:GLU:O	1:A:326:MET:HG3	2.03	0.57
1:A:46:LYS:NZ	1:B:66:THR:HB	2.20	0.57
1:A:191:CYS:HA	1:A:199:ASP:OD2	2.03	0.57
1:A:256:TYR:HA	1:A:259:ASN:HD21	1.70	0.56
1:B:140:TRP:CD1	1:B:141:PRO:HD2	2.39	0.56
1:B:321:GLN:NE2	1:B:325:ASP:OD1	2.34	0.56
1:B:28:GLU:OE1	1:B:28:GLU:HA	2.05	0.56
1:B:357:ASN:HB3	4:B:729:HOH:O	2.05	0.56
1:B:64:GLU:OE1	1:B:68:LYS:NZ	2.38	0.56
1:B:326:MET:O	1:B:330:ILE:HG13	2.06	0.56
1:A:66:THR:O	1:B:49:VAL:HG23	2.05	0.56
1:B:83:THR:HG22	1:B:87:LEU:CD2	2.35	0.56
1:A:69:LEU:HD21	1:B:47:ILE:HD12	1.87	0.56
1:A:99:ARG:NH1	1:A:274:ALA:O	2.36	0.56
1:A:400:LEU:HD12	1:A:400:LEU:C	2.26	0.56
1:B:237:ALA:O	1:B:241:ARG:HG3	2.05	0.56
1:B:160:TYR:CE1	1:B:168:LEU:HD21	2.41	0.55
1:A:141:PRO:HG3	4:A:793:HOH:O	2.05	0.55
1:A:73:ILE:HG23	1:A:296:SER:O	2.06	0.55
1:A:46:LYS:HD2	1:A:47:ILE:N	2.15	0.55
1:B:213:VAL:HG12	1:B:214:GLU:N	2.22	0.55
1:B:152:LEU:HD13	1:B:152:LEU:N	2.22	0.55
1:A:73:ILE:HG22	1:A:291:ILE:HG21	1.89	0.55
1:A:312:ASN:HD21	1:A:314:ALA:HB3	1.72	0.55
1:A:129:ARG:CD	1:A:156:ARG:HG3	2.37	0.55
1:B:170:PHE:CE1	1:B:208:LEU:HD21	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ALA:HB3	1:B:236:ASP:CG	2.27	0.55
1:A:112:LEU:O	1:A:115:ALA:HB3	2.07	0.54
1:A:248:LYS:HG2	1:A:275:ALA:HB2	1.86	0.54
1:B:170:PHE:HE2	1:B:207:THR:HG21	1.72	0.54
1:B:355:LYS:HG2	1:B:355:LYS:O	2.07	0.54
1:B:389:VAL:HA	1:B:392:MET:HE2	1.90	0.54
1:A:96:ASN:ND2	4:A:622:HOH:O	2.41	0.54
1:B:404:ILE:O	1:B:409:LEU:HD23	2.07	0.54
1:B:73:ILE:HG13	4:B:672:HOH:O	2.06	0.54
1:A:83:THR:CG2	1:A:87:LEU:HD22	2.37	0.54
1:A:259:ASN:N	1:A:259:ASN:ND2	2.53	0.54
1:A:287:MET:O	1:A:291:ILE:HG13	2.08	0.54
1:A:5:MET:CE	1:B:125:VAL:HG22	2.38	0.53
1:A:338:VAL:HG22	1:A:339:ASN:N	2.23	0.53
1:A:90:LYS:NZ	1:A:90:LYS:HB3	2.20	0.53
1:B:372:ARG:HG2	1:B:408:VAL:CG1	2.39	0.53
1:A:233:LEU:HD21	1:A:323:LEU:CD2	2.39	0.53
1:B:93:ALA:O	1:B:97:ASP:N	2.39	0.53
1:A:76:ILE:O	1:A:79:PHE:HB3	2.08	0.53
1:A:264:ASN:C	1:A:264:ASN:HD22	2.12	0.53
1:A:292:ARG:HG2	1:A:292:ARG:O	2.08	0.53
2:A:501:TYR:N	3:A:500:PLP:O3	2.41	0.53
1:A:247:HIS:ND1	1:A:247:HIS:N	2.56	0.53
1:A:121:LYS:NZ	1:A:121:LYS:O	2.41	0.53
1:A:148:ASN:O	1:A:151:GLY:N	2.30	0.53
1:A:213:VAL:HG23	1:A:247:HIS:CE1	2.44	0.53
1:A:328:GLN:O	1:A:332:ARG:HG3	2.09	0.53
1:B:149:SER:HB2	4:B:634:HOH:O	2.07	0.53
1:B:348:ARG:NH1	1:B:409:LEU:HB2	2.23	0.53
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.38	0.53
1:A:133:VAL:HG13	1:A:185:VAL:HG12	1.90	0.52
1:B:345:GLY:O	1:B:405:VAL:HG13	2.09	0.52
1:B:129:ARG:HD3	1:B:154:GLU:OE2	2.10	0.52
1:B:17:ILE:O	1:B:20:LEU:HB2	2.09	0.52
1:B:43:GLU:CD	1:B:43:GLU:H	2.12	0.52
1:B:122:ASN:N	1:B:122:ASN:ND2	2.57	0.52
1:B:304:SER:HA	4:B:702:HOH:O	2.09	0.52
1:A:204:GLN:O	1:A:208:LEU:HG	2.10	0.52
1:B:241:ARG:HD2	4:B:685:HOH:O	2.10	0.52
1:A:356:GLN:OE1	1:A:361:SER:HA	2.09	0.51
1:A:73:ILE:HG22	1:A:291:ILE:CG2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ASP:O	1:B:98:LYS:HB2	2.09	0.51
1:B:233:LEU:O	1:B:235:GLU:N	2.43	0.51
1:A:56:ALA:HB1	1:A:308:THR:HG21	1.91	0.51
1:B:373:LEU:HD13	1:B:408:VAL:HG21	1.91	0.51
1:B:334:ARG:NH2	1:B:358:GLY:O	2.43	0.51
1:A:365:LEU:HG	1:A:369:GLN:HB3	1.92	0.51
1:A:46:LYS:CD	1:A:47:ILE:H	2.17	0.51
1:A:382:VAL:HG12	1:A:383:ALA:N	2.24	0.51
1:B:46:LYS:CE	1:B:47:ILE:HG13	2.40	0.51
1:B:34:ASN:HA	1:B:380:TYR:HB2	1.93	0.51
1:A:134:TRP:NE1	1:A:184:ASP:OD2	2.37	0.51
1:A:160:TYR:O	1:A:168:LEU:HD23	2.10	0.51
1:A:350:PHE:HA	1:A:352:PHE:CE1	2.46	0.51
1:B:398:ALA:N	1:B:399:PRO:HD2	2.25	0.51
1:B:400:LEU:C	1:B:400:LEU:HD23	2.31	0.51
1:A:288:LYS:O	1:A:291:ILE:HB	2.11	0.51
1:B:29:ARG:HH22	1:B:378:GLY:HA2	1.76	0.51
1:B:247:HIS:H	1:B:247:HIS:CD2	2.29	0.51
1:A:366:THR:HG23	1:A:368:GLU:H	1.76	0.51
1:B:179:GLU:O	1:B:179:GLU:HG3	2.10	0.51
1:B:74:ASP:OD1	1:B:74:ASP:N	2.41	0.50
1:B:129:ARG:NH1	1:B:184:ASP:OD2	2.44	0.50
1:B:396:ASN:O	1:B:399:PRO:HD2	2.11	0.50
1:A:42:ASP:O	1:A:45:GLY:N	2.38	0.50
1:B:320:GLU:O	1:B:324:THR:HG22	2.12	0.50
1:A:396:ASN:O	1:A:399:PRO:HD2	2.11	0.50
1:B:240:LEU:HD23	1:B:240:LEU:O	2.12	0.50
1:B:308:THR:HG22	1:B:309:ILE:N	2.26	0.50
1:A:207:THR:HG22	1:A:208:LEU:N	2.27	0.50
1:A:374:ARG:HA	1:A:379:VAL:O	2.12	0.50
1:B:6:PHE:HA	1:B:9:ILE:HG13	1.92	0.50
1:B:86:LEU:O	1:B:226:GLN:OE1	2.30	0.50
1:B:349:ASP:OD1	1:B:351:SER:OG	2.30	0.50
1:A:307:ALA:O	1:A:311:SER:OG	2.29	0.50
1:A:316:ARG:O	1:A:319:TRP:N	2.44	0.50
1:A:345:GLY:O	1:A:346:ALA:O	2.30	0.50
1:B:99:ARG:HG2	1:B:274:ALA:O	2.11	0.50
1:A:67:THR:OG1	1:B:47:ILE:HB	2.12	0.50
1:A:229:ALA:HB3	1:A:236:ASP:OD2	2.11	0.50
1:B:102:THR:HG22	1:B:103:ALA:N	2.26	0.50
1:B:234:GLU:HG3	1:B:241:ARG:NH2	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LEU:HG	4:B:678:HOH:O	2.12	0.49
1:A:99:ARG:HD2	1:A:274:ALA:O	2.12	0.49
1:A:187:LEU:C	1:A:187:LEU:HD23	2.33	0.49
1:B:371:LEU:O	1:B:371:LEU:HD23	2.12	0.49
1:A:91:GLY:O	1:A:96:ASN:ND2	2.43	0.49
1:A:156:ARG:HA	1:A:156:ARG:NE	2.26	0.49
1:A:164:GLU:HB3	4:A:655:HOH:O	2.12	0.49
1:B:170:PHE:CZ	1:B:174:ILE:HD11	2.47	0.49
1:B:389:VAL:HG22	1:B:392:MET:HE2	1.90	0.49
1:B:398:ALA:HB3	1:B:399:PRO:CD	2.42	0.49
1:A:187:LEU:HD23	1:A:187:LEU:O	2.12	0.49
1:A:359:MET:N	4:A:627:HOH:O	2.45	0.49
1:B:343:GLU:HG3	1:B:343:GLU:O	2.12	0.49
1:B:259:ASN:H	1:B:259:ASN:ND2	2.10	0.49
1:A:329:ARG:HH11	1:A:329:ARG:CG	2.25	0.49
1:B:226:GLN:NE2	4:B:618:HOH:O	2.37	0.49
1:B:295:TYR:O	1:B:296:SER:HB3	2.12	0.49
1:B:29:ARG:HH11	1:B:29:ARG:CG	2.10	0.49
1:B:116:ALA:HB3	4:B:624:HOH:O	2.13	0.49
1:B:220:LEU:CD1	1:B:251:ILE:HB	2.40	0.49
1:B:274:ALA:HB3	1:B:280:VAL:HB	1.94	0.48
1:B:389:VAL:O	1:B:391:GLY:N	2.46	0.48
1:A:254:SER:O	1:A:269:ALA:N	2.39	0.48
1:A:286:GLN:NE2	1:B:12:ALA:HB2	2.29	0.48
1:B:333:MET:CE	1:B:394:PRO:HD3	2.43	0.48
1:B:160:TYR:CD1	1:B:168:LEU:HD21	2.48	0.48
1:A:248:LYS:HG3	1:A:275:ALA:HB2	1.93	0.48
1:A:274:ALA:CB	1:A:280:VAL:HG13	2.43	0.48
1:A:335:GLN:OE1	1:A:354:ILE:HG23	2.14	0.48
1:B:136:SER:N	1:B:158:TYR:CE1	2.82	0.48
1:B:192:CYS:N	1:B:199:ASP:OD2	2.41	0.48
1:B:313:ASP:N	1:B:313:ASP:OD1	2.45	0.48
1:A:46:LYS:HZ3	1:B:66:THR:HB	1.78	0.48
1:B:129:ARG:CB	1:B:154:GLU:HG2	2.41	0.48
1:B:181:GLN:O	1:B:184:ASP:HB2	2.14	0.48
1:B:234:GLU:HG3	1:B:241:ARG:HH21	1.78	0.48
1:B:256:TYR:HD2	1:B:267:VAL:HG12	1.79	0.48
1:B:231:GLY:O	1:B:233:LEU:O	2.32	0.48
1:A:67:THR:OG1	1:B:47:ILE:O	2.30	0.47
1:B:18:LEU:HD12	1:B:37:ILE:CD1	2.42	0.47
1:A:366:THR:O	1:A:369:GLN:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LEU:HD12	1:B:273:VAL:HG11	1.96	0.47
1:A:201:THR:HG23	1:A:204:GLN:HG3	1.96	0.47
1:B:327:ARG:O	1:B:331:GLN:HG3	2.15	0.47
1:A:69:LEU:CD2	1:B:47:ILE:HD12	2.44	0.47
1:A:185:VAL:CG2	1:A:218:LEU:HB3	2.41	0.47
1:B:162:ASP:OD2	1:B:165:ASN:HB2	2.15	0.47
1:A:134:TRP:HA	1:A:156:ARG:O	2.14	0.47
1:A:336:LEU:O	1:A:340:THR:OG1	2.30	0.47
1:B:98:LYS:HA	1:B:98:LYS:NZ	2.29	0.47
1:B:247:HIS:CD2	1:B:247:HIS:N	2.82	0.47
1:B:329:ARG:CG	1:B:329:ARG:HH11	2.27	0.47
1:B:185:VAL:CG2	1:B:218:LEU:HB3	2.45	0.47
1:A:344:LYS:NZ	1:A:402:GLU:OE2	2.32	0.46
1:B:404:ILE:HG22	1:B:409:LEU:CD2	2.45	0.46
1:A:123:THR:O	1:A:124:SER:OG	2.30	0.46
1:B:24:PHE:CZ	1:B:34:ASN:HB2	2.50	0.46
1:B:202:LEU:O	1:B:206:GLN:NE2	2.48	0.46
1:B:233:LEU:HD21	1:B:319:TRP:CH2	2.50	0.46
1:A:373:LEU:HB3	1:A:379:VAL:HB	1.96	0.46
1:A:213:VAL:HG12	1:A:214:GLU:N	2.30	0.46
1:B:338:VAL:HG22	1:B:339:ASN:N	2.30	0.46
1:A:220:LEU:C	1:A:220:LEU:HD23	2.36	0.46
1:A:137:ASN:HA	1:A:138:PRO:HA	1.59	0.46
1:B:27:ASP:OD2	1:B:380:TYR:OH	2.29	0.46
1:B:186:VAL:HG12	1:B:217:TRP:HB3	1.97	0.46
1:B:195:PRO:HB3	1:B:386:ARG:HD3	1.98	0.45
1:B:294:ASN:C	1:B:294:ASN:HD22	2.20	0.45
1:B:397:MET:HE2	1:B:401:CYS:SG	2.56	0.45
1:A:78:GLU:O	1:A:82:CYS:HB2	2.16	0.45
1:A:98:LYS:HA	1:A:98:LYS:HD2	1.56	0.45
1:B:24:PHE:CE1	1:B:34:ASN:HB2	2.51	0.45
1:B:46:LYS:NZ	1:B:47:ILE:CD1	2.80	0.45
1:A:9:ILE:HD13	1:B:122:ASN:HB3	1.99	0.45
1:A:194:ASN:HA	1:A:195:PRO:HA	1.59	0.45
1:A:366:THR:CG2	1:A:368:GLU:H	2.29	0.45
1:B:133:VAL:O	1:B:155:VAL:HA	2.17	0.45
1:B:251:ILE:HG13	1:B:272:LEU:HD12	1.98	0.45
1:B:324:THR:HB	1:B:327:ARG:NH2	2.32	0.45
1:B:348:ARG:NH1	1:B:409:LEU:CD1	2.80	0.45
1:A:186:VAL:HG21	1:A:217:TRP:CE3	2.51	0.45
1:B:329:ARG:CG	1:B:329:ARG:NH1	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:MET:HA	1:B:397:MET:HE2	1.98	0.45
1:B:37:ILE:HG23	1:B:39:LEU:HD22	1.99	0.45
1:B:163:ALA:O	1:B:165:ASN:N	2.50	0.45
1:B:207:THR:HG22	1:B:208:LEU:HD23	1.99	0.45
1:A:136:SER:OG	1:A:138:PRO:O	2.29	0.45
1:B:129:ARG:HD3	1:B:154:GLU:HG2	1.99	0.45
1:B:314:ALA:O	1:B:317:ALA:HB3	2.17	0.45
1:B:305:VAL:HG12	1:B:306:VAL:N	2.29	0.44
1:B:355:LYS:HB2	4:B:772:HOH:O	2.17	0.44
1:A:170:PHE:CD2	1:A:174:ILE:CD1	3.00	0.44
1:A:312:ASN:HD22	1:A:315:LEU:N	2.05	0.44
1:B:102:THR:CG2	1:B:103:ALA:N	2.80	0.44
1:B:291:ILE:HG23	1:B:295:TYR:CE1	2.52	0.44
1:B:266:ARG:N	1:B:266:ARG:HD2	2.31	0.44
1:B:389:VAL:HG13	1:B:392:MET:HE2	1.99	0.44
1:A:292:ARG:HH22	1:B:16:PRO:CD	2.30	0.44
1:A:349:ASP:OD1	1:A:351:SER:OG	2.33	0.44
1:A:388:ASN:O	1:A:392:MET:HE3	2.17	0.44
1:A:140:TRP:CZ2	1:A:142:ASN:HB2	2.53	0.44
1:A:18:LEU:HD12	2:A:501:TYR:CZ	2.53	0.44
1:B:148:ASN:HB3	4:B:652:HOH:O	2.17	0.44
1:A:40:TYR:CE2	1:A:326:MET:HB3	2.52	0.44
1:A:83:THR:O	1:A:87:LEU:HD22	2.18	0.44
1:A:181:GLN:O	1:A:184:ASP:HB2	2.18	0.44
1:B:251:ILE:CG1	1:B:272:LEU:HD12	2.48	0.44
1:B:312:ASN:OD1	1:B:315:LEU:HB2	2.18	0.44
1:B:52:SER:HB2	1:B:309:ILE:HD13	2.00	0.44
1:B:129:ARG:HD3	1:B:154:GLU:CD	2.38	0.44
1:B:205:TRP:O	1:B:209:ALA:HB2	2.17	0.44
1:B:288:LYS:O	1:B:291:ILE:N	2.48	0.44
1:B:220:LEU:HD11	1:B:251:ILE:CG2	2.48	0.43
1:A:70:TYR:OH	3:B:500:PLP:O2P	2.29	0.43
1:B:118:PHE:O	1:B:122:ASN:ND2	2.46	0.43
1:B:156:ARG:HD3	1:B:156:ARG:HA	1.76	0.43
1:A:398:ALA:N	1:A:399:PRO:HD2	2.33	0.43
1:B:256:TYR:HA	1:B:259:ASN:ND2	2.31	0.43
1:A:23:LEU:HD13	1:A:23:LEU:HA	1.63	0.43
1:A:233:LEU:HD21	1:A:323:LEU:HD21	2.00	0.43
1:A:5:MET:N	1:A:7:GLU:OE1	2.51	0.43
1:A:29:ARG:HA	1:A:30:PRO:HD3	1.73	0.43
1:A:359:MET:O	1:A:389:VAL:N	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ILE:O	1:A:409:LEU:HG	2.18	0.43
1:B:56:ALA:O	1:B:59:TYR:HB3	2.18	0.43
1:B:133:VAL:HB	1:B:185:VAL:CG1	2.47	0.43
1:B:194:ASN:HA	1:B:195:PRO:HA	1.70	0.43
1:B:219:PRO:HG3	1:B:247:HIS:CE1	2.53	0.43
1:A:61:LEU:HD11	1:B:58:GLN:HG3	2.01	0.43
1:B:212:SER:CB	1:B:217:TRP:CE3	2.99	0.43
1:B:250:LEU:O	1:B:273:VAL:HG13	2.18	0.43
1:A:195:PRO:HB3	1:A:386:ARG:HD3	2.00	0.43
1:A:323:LEU:O	1:A:326:MET:N	2.52	0.43
1:B:46:LYS:CG	1:B:47:ILE:N	2.80	0.43
1:B:158:TYR:CD2	1:B:173:LEU:HD13	2.54	0.43
1:B:38:GLY:C	1:B:359:MET:HE1	2.39	0.43
1:B:233:LEU:N	1:B:233:LEU:CD1	2.80	0.43
1:A:98:LYS:HA	1:A:98:LYS:CE	2.42	0.42
1:B:215:LYS:HA	1:B:215:LYS:HD2	1.79	0.42
1:B:340:THR:O	1:B:344:LYS:HB2	2.19	0.42
1:A:140:TRP:O	1:A:142:ASN:N	2.52	0.42
1:B:114:VAL:CG1	1:B:287:MET:HE2	2.47	0.42
1:B:38:GLY:CA	1:B:359:MET:HE1	2.50	0.42
1:B:279:THR:O	1:B:282:ARG:N	2.52	0.42
1:B:292:ARG:O	1:B:292:ARG:HG2	2.20	0.42
1:B:382:VAL:HG11	4:B:682:HOH:O	2.19	0.42
1:A:29:ARG:H	1:A:29:ARG:HG2	1.73	0.42
1:A:249:GLU:HB3	1:B:6:PHE:CE2	2.54	0.42
1:B:44:THR:H	1:B:44:THR:HG23	1.51	0.42
1:B:137:ASN:HA	1:B:138:PRO:HA	1.58	0.42
1:B:199:ASP:HB3	1:B:200:PRO:HD2	2.02	0.42
1:B:211:LEU:O	1:B:214:GLU:N	2.52	0.42
1:B:338:VAL:O	1:B:341:LEU:N	2.52	0.42
1:A:98:LYS:CA	1:A:98:LYS:HE3	2.49	0.42
1:A:159:ALA:O	1:A:173:LEU:HD22	2.19	0.42
1:A:362:PHE:HD1	1:A:362:PHE:HA	1.65	0.42
1:B:129:ARG:HH22	1:B:181:GLN:HG3	1.83	0.42
1:A:343:GLU:HG2	4:A:720:HOH:O	2.18	0.42
1:B:206:GLN:HE21	1:B:206:GLN:HB2	1.58	0.42
1:B:76:ILE:O	1:B:79:PHE:HB3	2.20	0.42
1:B:122:ASN:N	1:B:122:ASN:HD22	2.18	0.42
1:B:205:TRP:HE3	1:B:243:PHE:HE1	1.68	0.42
1:B:397:MET:O	1:B:400:LEU:HB3	2.20	0.42
1:B:259:ASN:HD22	1:B:259:ASN:N	2.10	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:HD2	4:B:660:HOH:O	2.20	0.42
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.47	0.42
1:A:71:LEU:HD11	1:A:300:ALA:HB2	2.02	0.42
1:A:129:ARG:HG3	1:A:156:ARG:CG	2.46	0.42
1:A:329:ARG:CG	1:A:329:ARG:NH1	2.80	0.42
1:B:220:LEU:HD11	1:B:251:ILE:HG21	2.01	0.42
1:B:348:ARG:HH12	1:B:409:LEU:HB2	1.85	0.42
1:A:167:THR:OG1	1:A:168:LEU:N	2.53	0.41
1:A:185:VAL:HG12	1:A:185:VAL:O	2.20	0.41
1:A:218:LEU:HG	1:B:5:MET:HE3	2.02	0.41
1:A:223:PHE:HD1	1:A:223:PHE:HA	1.67	0.41
1:A:377:PHE:CG	1:A:403:ALA:HB1	2.54	0.41
1:B:8:ASN:ND2	4:B:632:HOH:O	2.53	0.41
1:B:15:ASP:OD1	1:B:16:PRO:HD2	2.19	0.41
1:B:160:TYR:O	1:B:168:LEU:HD23	2.20	0.41
1:B:201:THR:H	1:B:201:THR:HG23	1.41	0.41
1:B:354:ILE:H	1:B:354:ILE:HG12	1.43	0.41
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.61	0.41
1:A:170:PHE:CE2	1:A:174:ILE:CD1	3.02	0.41
1:A:353:ILE:HD13	1:A:361:SER:HB2	2.03	0.41
1:B:185:VAL:CG2	1:B:218:LEU:HD23	2.50	0.41
1:B:324:THR:HB	1:B:327:ARG:HH22	1.85	0.41
1:A:69:LEU:HG	1:B:47:ILE:HD12	2.03	0.41
1:B:170:PHE:CZ	1:B:208:LEU:CD2	3.00	0.41
1:B:373:LEU:HD12	1:B:373:LEU:HA	1.74	0.41
1:A:141:PRO:HD3	4:A:604:HOH:O	2.20	0.41
1:A:349:ASP:CG	1:A:351:SER:HG	2.23	0.41
1:B:167:THR:HB	1:B:168:LEU:H	1.38	0.41
1:B:200:PRO:HA	1:B:204:GLN:OE1	2.21	0.41
1:B:367:LYS:HE3	1:B:383:ALA:O	2.21	0.41
1:A:24:PHE:CD1	1:A:34:ASN:HB2	2.56	0.41
1:B:94:LEU:CD1	1:B:244:ALA:HB1	2.48	0.41
1:A:188:PHE:O	1:A:221:PHE:HA	2.21	0.40
1:B:177:LEU:O	1:B:217:TRP:HZ2	2.04	0.40
1:A:249:GLU:HA	1:A:273:VAL:O	2.22	0.40
1:A:294:ASN:C	1:A:294:ASN:HD22	2.23	0.40
1:B:322:GLU:O	1:B:325:ASP:HB2	2.20	0.40
1:A:143:HIS:O	1:A:147:PHE:HD2	2.03	0.40
1:A:261:GLY:HA2	4:A:671:HOH:O	2.22	0.40
1:B:99:ARG:HH11	1:B:99:ARG:CG	2.20	0.40
1:B:139:SER:OG	1:B:140:TRP:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HG23	1:A:389:VAL:CG1	2.51	0.40
1:A:77:PRO:HB2	1:A:81:ARG:NH2	2.26	0.40
1:B:152:LEU:HA	1:B:152:LEU:HD12	1.61	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	394/396 (100%)	331 (84%)	48 (12%)	15 (4%)	3	4
1	B	394/396 (100%)	328 (83%)	49 (12%)	17 (4%)	2	3
All	All	788/792 (100%)	659 (84%)	97 (12%)	32 (4%)	3	3

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	SER
1	A	301	HIS
1	A	346	ALA
1	B	233	LEU
1	B	234	GLU
1	A	92	SER
1	A	164	GLU
1	A	212	SER
1	B	69	LEU
1	B	90	LYS
1	B	164	GLU
1	B	201	THR
1	B	211	LEU
1	B	212	SER
1	B	301	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	141	PRO
1	A	163	ALA
1	A	211	LEU
1	A	266	ARG
1	B	36	GLY
1	B	390	ALA
1	A	169	ASP
1	A	320	GLU
1	A	390	ALA
1	B	92	SER
1	B	347	ASN
1	A	69	LEU
1	B	30	PRO
1	B	141	PRO
1	A	106	PRO
1	B	13	PRO
1	B	47	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	320/320 (100%)	238 (74%)	82 (26%)	0 1
1	B	320/320 (100%)	246 (77%)	74 (23%)	1 1
All	All	640/640 (100%)	484 (76%)	156 (24%)	0 1

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	9	ILE
1	A	10	THR
1	A	18	LEU
1	A	23	LEU
1	A	29	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	32	LYS
1	A	35	LEU
1	A	39	LEU
1	A	43	GLU
1	A	47	ILE
1	A	61	LEU
1	A	63	ASN
1	A	66	THR
1	A	67	THR
1	A	69	LEU
1	A	82	CYS
1	A	87	LEU
1	A	90	LYS
1	A	94	LEU
1	A	98	LYS
1	A	118	PHE
1	A	119	LEU
1	A	121	LYS
1	A	126	LYS
1	A	129	ARG
1	A	139	SER
1	A	144	LYS
1	A	145	SER
1	A	152	LEU
1	A	156	ARG
1	A	166	HIS
1	A	168	LEU
1	A	174	ILE
1	A	178	ASN
1	A	179	GLU
1	A	185	VAL
1	A	189	HIS
1	A	202	LEU
1	A	207	THR
1	A	212	SER
1	A	215	LYS
1	A	218	LEU
1	A	223	PHE
1	A	240	LEU
1	A	246	MET
1	A	247	HIS
1	A	248	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	250	LEU
1	A	254	SER
1	A	255	SER
1	A	259	ASN
1	A	264	ASN
1	A	267	VAL
1	A	272	LEU
1	A	278	GLU
1	A	280	VAL
1	A	292	ARG
1	A	294	ASN
1	A	296	SER
1	A	297	SER
1	A	311	SER
1	A	312	ASN
1	A	329	ARG
1	A	334	ARG
1	A	335	GLN
1	A	338	VAL
1	A	340	THR
1	A	341	LEU
1	A	344	LYS
1	A	347	ASN
1	A	348	ARG
1	A	349	ASP
1	A	353	ILE
1	A	354	ILE
1	A	355	LYS
1	A	362	PHE
1	A	366	THR
1	A	371	LEU
1	A	375	GLU
1	A	384	SER
1	A	400	LEU
1	B	5	MET
1	B	6	PHE
1	B	9	ILE
1	B	10	THR
1	B	23	LEU
1	B	25	ARG
1	B	29	ARG
1	B	32	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	39	LEU
1	B	44	THR
1	B	47	ILE
1	B	51	THR
1	B	55	LYS
1	B	61	LEU
1	B	69	LEU
1	B	73	ILE
1	B	81	ARG
1	B	86	LEU
1	B	87	LEU
1	B	90	LYS
1	B	94	LEU
1	B	98	LYS
1	B	99	ARG
1	B	105	THR
1	B	119	LEU
1	B	121	LYS
1	B	122	ASN
1	B	124	SER
1	B	126	LYS
1	B	129	ARG
1	B	133	VAL
1	B	144	LYS
1	B	145	SER
1	B	152	LEU
1	B	154	GLU
1	B	156	ARG
1	B	168	LEU
1	B	178	ASN
1	B	185	VAL
1	B	186	VAL
1	B	199	ASP
1	B	206	GLN
1	B	212	SER
1	B	213	VAL
1	B	215	LYS
1	B	223	PHE
1	B	233	LEU
1	B	235	GLU
1	B	240	LEU
1	B	258	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	259	ASN
1	B	273	VAL
1	B	276	ASP
1	B	277	SER
1	B	285	SER
1	B	292	ARG
1	B	294	ASN
1	B	304	SER
1	B	324	THR
1	B	334	ARG
1	B	338	VAL
1	B	342	GLN
1	B	343	GLU
1	B	351	SER
1	B	354	ILE
1	B	355	LYS
1	B	361	SER
1	B	362	PHE
1	B	367	LYS
1	B	368	GLU
1	B	373	LEU
1	B	375	GLU
1	B	384	SER
1	B	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	84	GLN
1	A	142	ASN
1	A	165	ASN
1	A	189	HIS
1	A	210	GLN
1	A	226	GLN
1	A	259	ASN
1	A	264	ASN
1	A	312	ASN
1	A	328	GLN
1	A	331	GLN
1	A	357	ASN
1	A	388	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	63	ASN
1	B	96	ASN
1	B	148	ASN
1	B	165	ASN
1	B	206	GLN
1	B	226	GLN
1	B	247	HIS
1	B	259	ASN
1	B	328	GLN
1	B	339	ASN
1	B	342	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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
3	PLP	A	500	2	15,15,16	1.66	3 (20%)	20,22,23	2.04	6 (30%)
2	TYR	B	501	3	12,13,13	0.76	0	16,17,17	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	B	500	2	15,15,16	1.65	2 (13%)	20,22,23	2.15	6 (30%)
2	TYR	A	501	3	12,13,13	0.74	0	16,17,17	0.72	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	PLP	A	500	2	-	2/6/6/8	0/1/1/1
2	TYR	B	501	3	-	4/8/8/8	0/1/1/1
3	PLP	B	500	2	-	3/6/6/8	0/1/1/1
2	TYR	A	501	3	-	0/8/8/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	PLP	C4A-C4	-4.55	1.42	1.51
3	A	500	PLP	C4A-C4	-3.82	1.43	1.51
3	A	500	PLP	C5-C4	2.68	1.43	1.40
3	A	500	PLP	P-O3P	-2.51	1.45	1.54
3	B	500	PLP	P-O3P	-2.28	1.46	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	PLP	C6-C5-C4	5.47	122.46	118.16
3	A	500	PLP	C6-C5-C4	3.94	121.26	118.16
3	A	500	PLP	C4A-C4-C5	3.88	124.93	120.94
3	B	500	PLP	C5-C6-N1	-3.41	118.14	123.82
3	A	500	PLP	O4P-C5A-C5	3.37	115.77	109.35
3	B	500	PLP	C2A-C2-C3	3.11	124.73	120.89
3	A	500	PLP	C3-C4-C5	-2.96	115.54	118.74
3	A	500	PLP	C5A-C5-C6	-2.89	114.63	119.37
3	B	500	PLP	O4P-C5A-C5	-2.84	103.94	109.35
3	B	500	PLP	C3-C2-N1	-2.81	117.13	120.77
3	B	500	PLP	C6-N1-C2	2.59	123.97	119.17
3	A	500	PLP	C5-C6-N1	-2.43	119.78	123.82
2	A	501	TYR	OXT-C-CA	2.07	120.42	113.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	PLP	C4-C5-C5A-O4P
3	A	500	PLP	C6-C5-C5A-O4P
3	B	500	PLP	C4-C5-C5A-O4P
2	B	501	TYR	OXT-C-CA-CB
3	B	500	PLP	C6-C5-C5A-O4P
2	B	501	TYR	O-C-CA-CB
2	B	501	TYR	CA-CB-CG-CD2
3	B	500	PLP	C5A-O4P-P-O3P
2	B	501	TYR	CA-CB-CG-CD1

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	PLP	2	0
2	B	501	TYR	1	0
3	B	500	PLP	2	0
2	A	501	TYR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.