Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:16 PM GMT

PDB ID	:	1ESN
Title	:	STRUCTURAL BASIS FOR THE FEEDBACK REGULATION OF ESCHERICHIA COLI PANTOTHENATE KINASE BY COENZYME A
Authors	:	Yun, M.; Park, C.G.; Kim, J.Y.; Rock, C.O.; Jackowski, S.; Park, H.W.
Deposited on	:	2000-04-10
Resolution	:	2.60 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 (i) symbol.

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

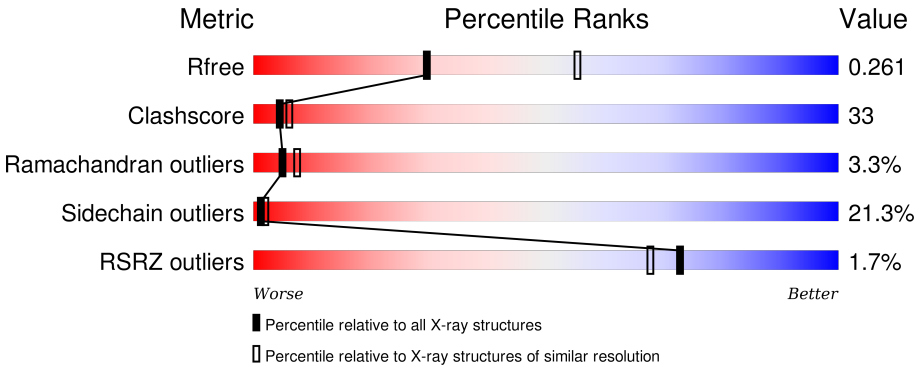
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	316	% 42% 41% 14%
1	B	316	% 48% 38% 11%
1	C	316	% 48% 35% 14%
1	D	316	3% 38% 44% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10498 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 PANTOTHENATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	Se	0	0	0
			2528	1623	434	465	6			
1	B	309	Total	C	N	O	Se	0	0	0
			2512	1614	431	461	6			
1	C	309	Total	C	N	O	Se	0	0	0
			2512	1614	431	461	6			
1	D	309	Total	C	N	O	Se	0	0	0
			2512	1614	431	461	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
A	29	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
A	142	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
A	153	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
A	208	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
A	275	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	9	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	29	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	142	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	153	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	208	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	275	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	9	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	29	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	142	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	153	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	208	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	275	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
D	9	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
D	29	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
D	142	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3

Continued on next page...

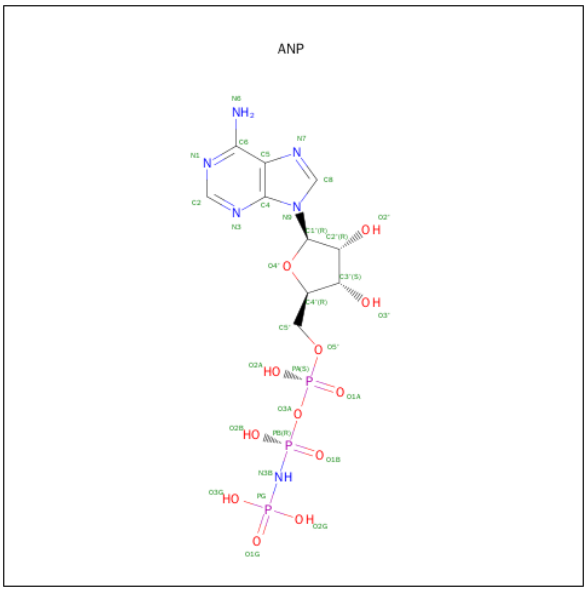
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	153	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
D	208	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
D	275	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3

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

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 10 6 12 3	0	0
3	B	1	Total C N O P 31 10 6 12 3	0	0
3	C	1	Total C N O P 31 10 6 12 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is water.

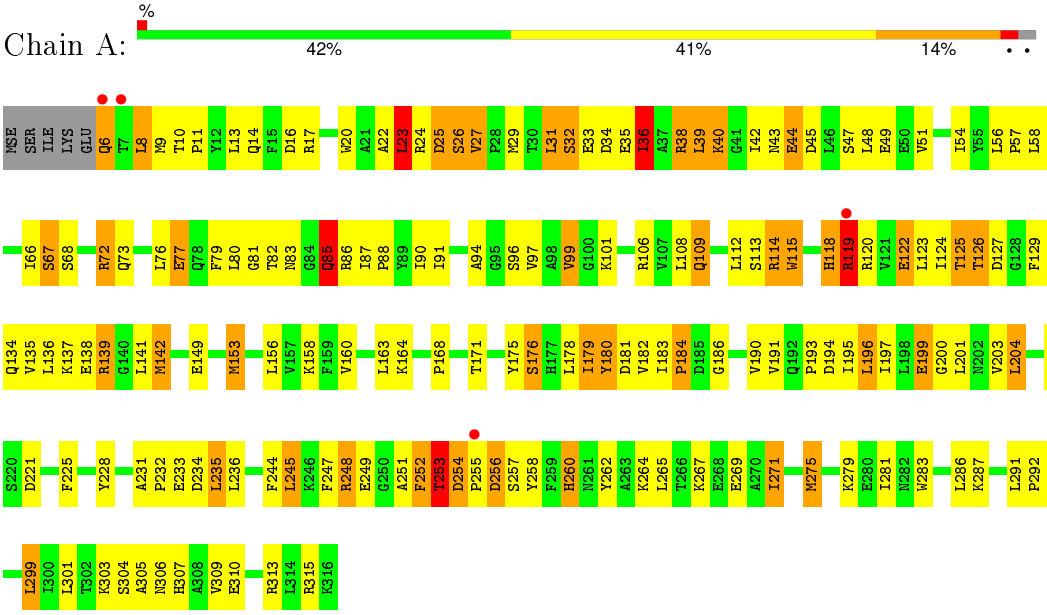
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	82	Total	O	0	0
			82	82		
4	C	81	Total	O	0	0
			81	81		
4	D	77	Total	O	0	0
			77	77		

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.

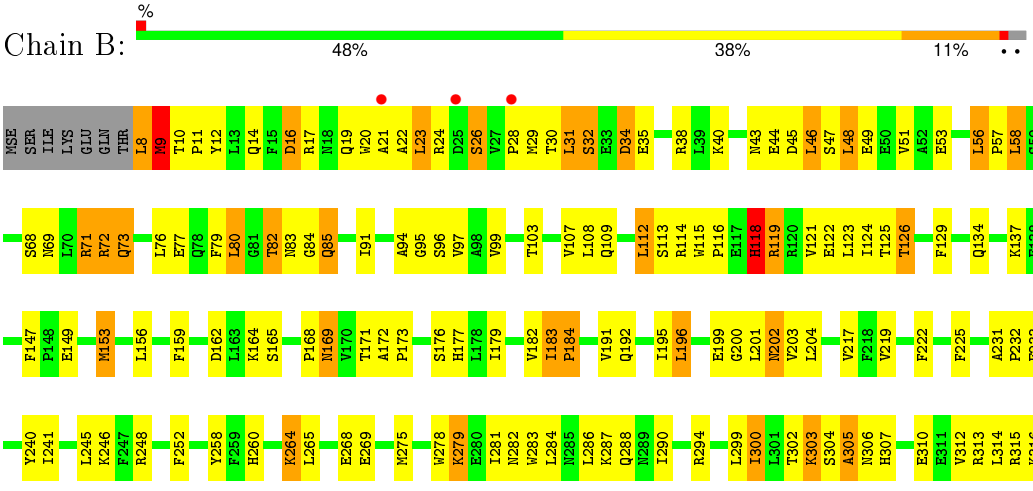
- Molecule 1: PANTOTHENATE KINASE

Chain A:



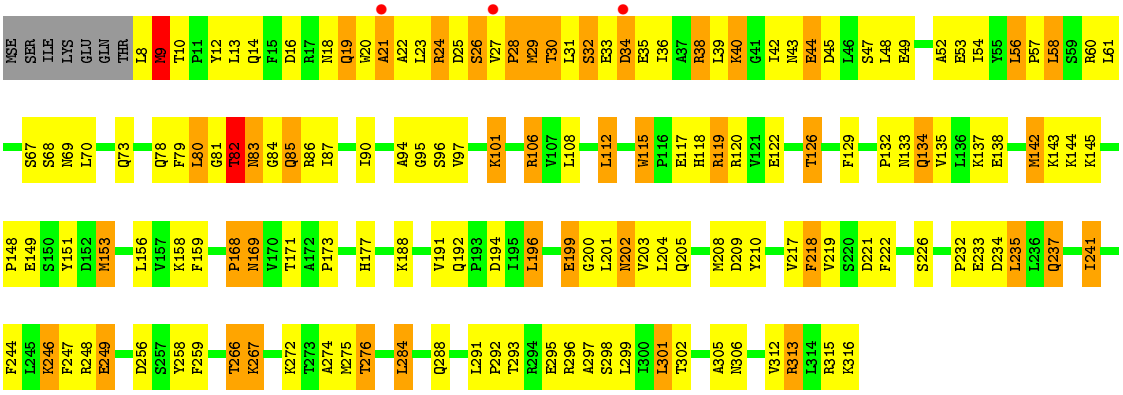
- Molecule 1: PANTOTHENATE KINASE

Chain B:



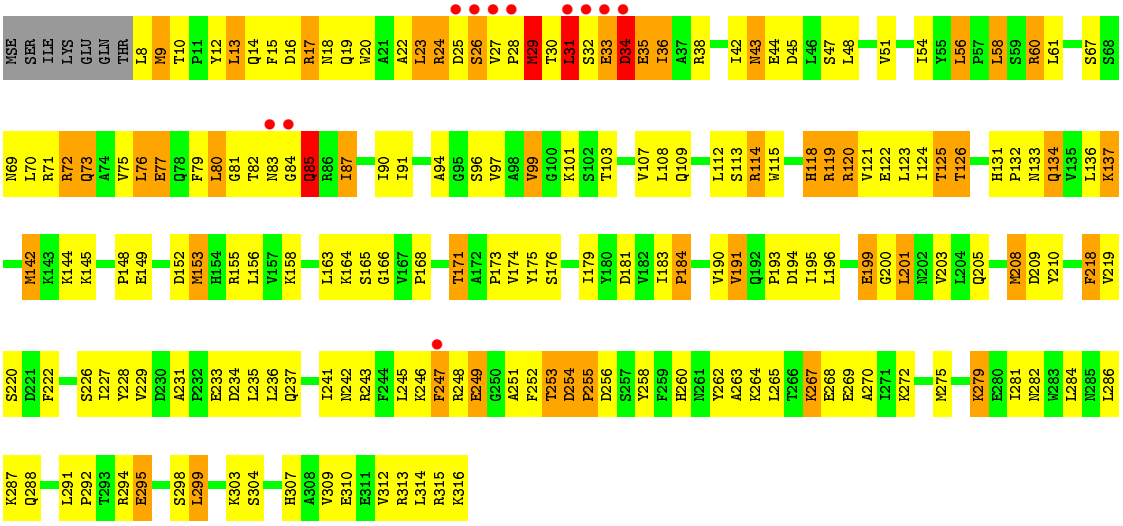
- Molecule 1: PANTOTHENATE KINASE

Chain C:



- Molecule 1: PANTOTHENATE KINASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	130.08Å 130.08Å 281.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 43.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.5 (50.00-2.60) 84.5 (43.99-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.61Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.216 , 0.260 0.218 , 0.261	Depositor DCC
R_{free} test set	3633 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.1	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 77401 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10498	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: MG, ANP

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	0.50	0/2581	0.92	8/3494 (0.2%)
1	B	0.49	1/2565 (0.0%)	0.79	6/3472 (0.2%)
1	C	0.51	4/2565 (0.2%)	0.77	3/3472 (0.1%)
1	D	0.55	3/2565 (0.1%)	0.84	7/3472 (0.2%)
All	All	0.51	8/10276 (0.1%)	0.83	24/13910 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	142	MSE	CG-SE	-6.73	1.72	1.95
1	C	9	MSE	CG-SE	-5.55	1.76	1.95
1	C	275	MSE	CG-SE	-5.39	1.77	1.95
1	B	142	MSE	CG-SE	-5.38	1.77	1.95
1	C	142	MSE	CG-SE	-5.29	1.77	1.95
1	D	153	MSE	CG-SE	-5.19	1.77	1.95
1	C	153	MSE	CG-SE	-5.15	1.77	1.95
1	D	9	MSE	CG-SE	-5.11	1.78	1.95

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	ARG	NE-CZ-NH2	23.36	131.98	120.30
1	A	119	ARG	NE-CZ-NH1	-15.16	112.72	120.30
1	B	9	MSE	CA-CB-CG	8.59	127.91	113.30
1	D	142	MSE	CA-CB-CG	-7.98	99.73	113.30
1	B	142	MSE	CB-CG-SE	-7.37	90.59	112.70
1	D	153	MSE	CB-CG-SE	-7.37	90.60	112.70
1	A	119	ARG	NH1-CZ-NH2	-7.29	111.39	119.40
1	C	142	MSE	CB-CG-SE	-7.07	91.49	112.70
1	B	9	MSE	CB-CG-SE	-7.06	91.52	112.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	153	MSE	CB-CG-SE	-6.85	92.14	112.70
1	B	153	MSE	CB-CG-SE	-6.80	92.30	112.70
1	A	142	MSE	CB-CG-SE	-6.71	92.58	112.70
1	D	34	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	153	MSE	CB-CG-SE	-6.59	92.94	112.70
1	A	275	MSE	CB-CG-SE	-6.14	94.28	112.70
1	D	29	MSE	CA-CB-CG	6.13	123.72	113.30
1	C	142	MSE	CA-CB-CG	5.91	123.34	113.30
1	B	142	MSE	CA-CB-CG	5.80	123.17	113.30
1	A	142	MSE	CA-CB-CG	5.61	122.84	113.30
1	D	208	MSE	CB-CA-C	-5.35	99.70	110.40
1	D	153	MSE	CA-CB-CG	5.31	122.33	113.30
1	B	118	HIS	CA-C-N	-5.21	105.75	117.20
1	A	23	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	31	LEU	O-C-N	-5.12	114.51	122.70

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	2528	0	2540	152	0
1	B	2512	0	2524	148	0
1	C	2512	0	2524	173	0
1	D	2512	0	2525	228	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	0	0
3	C	31	0	13	1	0
3	D	31	0	13	0	0
4	A	66	0	0	1	0
4	B	82	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	81	0	0	3	0
4	D	77	0	0	2	0
All	All	10498	0	10165	662	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 33.

All (662) 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:C:29:MSE:HE3	1:C:56:LEU:CD2	1.63	1.25
1:C:313:ARG:HH11	1:C:313:ARG:HB2	1.10	1.15
1:C:29:MSE:HE3	1:C:56:LEU:HD23	1.17	1.12
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.20	1.03
1:A:118:HIS:O	1:A:119:ARG:CZ	2.07	1.02
1:D:24:ARG:HH11	1:D:24:ARG:HB2	1.17	1.02
1:B:202:ASN:H	1:B:202:ASN:HD22	0.99	0.98
1:D:32:SER:O	1:D:35:GLU:HG2	1.65	0.95
1:D:120:ARG:NH1	1:D:193:PRO:HA	1.81	0.95
1:D:251:ALA:C	1:D:253:THR:H	1.66	0.94
1:D:29:MSE:HG3	1:D:56:LEU:HD22	1.53	0.91
1:D:137:LYS:HG2	1:D:142:MSE:HE3	1.52	0.90
1:B:29:MSE:HG3	1:B:56:LEU:HD22	1.52	0.90
1:A:248:ARG:HB3	1:A:251:ALA:HB3	1.52	0.89
1:D:16:ASP:H	1:D:19:GLN:HE21	1.19	0.89
1:C:29:MSE:HE3	1:C:56:LEU:HD22	1.52	0.89
1:C:29:MSE:CE	1:C:56:LEU:HD23	2.00	0.89
1:D:26:SER:HB2	1:D:60:ARG:NH2	1.87	0.88
1:D:24:ARG:HH11	1:D:24:ARG:CB	1.86	0.88
1:B:237:GLN:HG3	1:B:278:TRP:CD1	2.08	0.87
1:C:39:LEU:HA	1:C:42:ILE:HD12	1.56	0.86
1:D:153:MSE:HE1	1:D:219:VAL:HG21	1.57	0.86
1:B:48:LEU:H	1:B:48:LEU:HD12	1.41	0.86
1:B:23:LEU:HD13	1:B:23:LEU:H	1.41	0.85
1:D:33:GLU:HG2	1:D:34:ASP:N	1.92	0.85
1:C:218:PHE:CE2	1:D:208:MSE:HE2	2.11	0.84
1:D:120:ARG:HB2	1:D:194:ASP:OD1	1.77	0.84
1:D:29:MSE:HE2	1:D:56:LEU:HD23	1.59	0.84
1:C:202:ASN:H	1:C:202:ASN:HD22	1.26	0.83
1:B:202:ASN:ND2	1:B:202:ASN:H	1.75	0.83
1:C:133:ASN:HD21	1:C:145:LYS:NZ	1.76	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ASP:OD2	1:D:256:ASP:HB2	1.78	0.83
1:C:29:MSE:SE	1:C:60:ARG:HE	2.12	0.82
1:B:43:ASN:OD1	1:B:45:ASP:HB2	1.79	0.82
1:D:32:SER:C	1:D:36:ILE:HG13	2.00	0.81
1:B:29:MSE:HG3	1:B:56:LEU:CD2	2.10	0.81
1:C:126:THR:HG21	1:C:202:ASN:HD21	1.44	0.81
1:A:114:ARG:HG3	1:A:114:ARG:NH1	1.89	0.80
1:C:21:ALA:HB1	1:C:53:GLU:HG2	1.60	0.80
1:C:43:ASN:O	1:C:44:GLU:HG3	1.81	0.80
1:B:202:ASN:N	1:B:202:ASN:HD22	1.73	0.79
1:C:80:LEU:HA	1:D:23:LEU:HD22	1.62	0.79
1:D:33:GLU:O	1:D:36:ILE:HB	1.83	0.79
1:B:153:MSE:CE	1:B:219:VAL:HG23	2.13	0.78
1:A:6:GLN:NE2	1:A:8:LEU:HD11	1.99	0.78
1:B:26:SER:HB2	1:B:60:ARG:HH21	1.47	0.78
1:A:153:MSE:CE	1:A:219:VAL:HG23	2.14	0.78
1:A:160:VAL:HA	1:A:163:LEU:HD12	1.65	0.78
1:B:96:SER:HB2	1:B:286:LEU:HD13	1.66	0.77
1:C:31:LEU:HD21	1:C:56:LEU:HD21	1.65	0.77
1:A:142:MSE:HE2	1:A:258:TYR:CG	2.19	0.77
1:C:126:THR:HG21	1:C:202:ASN:ND2	2.00	0.77
1:D:251:ALA:HB3	1:D:253:THR:HG23	1.66	0.76
1:B:21:ALA:HB1	1:B:53:GLU:HG2	1.66	0.76
1:D:251:ALA:C	1:D:253:THR:N	2.39	0.76
1:A:248:ARG:HB3	1:A:251:ALA:CB	2.15	0.76
1:D:43:ASN:HD22	1:D:45:ASP:H	1.30	0.76
1:B:116:PRO:HA	1:B:119:ARG:HH21	1.51	0.76
1:C:208:MSE:HE2	1:D:218:PHE:CZ	2.21	0.76
1:D:33:GLU:N	1:D:36:ILE:HG13	2.01	0.75
1:B:21:ALA:CB	1:B:53:GLU:HG2	2.16	0.75
1:B:10:THR:HG23	1:B:12:TYR:H	1.51	0.75
1:C:27:VAL:O	1:C:29:MSE:HG2	1.86	0.75
1:D:153:MSE:HE1	1:D:219:VAL:CG2	2.17	0.74
1:D:133:ASN:HA	1:D:142:MSE:HE2	1.69	0.74
1:A:96:SER:HB2	1:A:286:LEU:HD13	1.70	0.74
1:D:29:MSE:HE2	1:D:56:LEU:CD2	2.17	0.74
1:B:119:ARG:HG3	1:B:119:ARG:O	1.88	0.74
1:D:73:GLN:HE21	1:D:87:ILE:HD11	1.51	0.74
1:A:6:GLN:HE21	1:A:8:LEU:HD11	1.51	0.74
1:D:120:ARG:HH12	1:D:193:PRO:HA	1.51	0.73
1:D:265:LEU:HD22	1:D:269:GLU:HB3	1.67	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:GLU:O	1:D:38:ARG:N	2.21	0.73
1:C:313:ARG:CB	1:C:313:ARG:HH11	1.95	0.73
1:A:40:LYS:HE3	1:A:48:LEU:HD11	1.69	0.73
1:A:31:LEU:H	1:A:31:LEU:HD12	1.52	0.73
1:D:15:PHE:HA	1:D:19:GLN:NE2	2.04	0.72
1:B:153:MSE:HE1	1:B:219:VAL:HG23	1.71	0.72
1:D:43:ASN:ND2	1:D:45:ASP:HB2	2.05	0.72
1:C:29:MSE:CG	1:C:60:ARG:HH21	2.02	0.72
1:A:118:HIS:O	1:A:119:ARG:NE	2.22	0.71
1:D:84:GLY:O	1:D:85:GLN:HB3	1.90	0.71
1:B:85:GLN:H	1:C:191:VAL:HG21	1.54	0.71
1:D:73:GLN:NE2	1:D:87:ILE:HD11	2.03	0.71
1:C:120:ARG:HB2	1:C:194:ASP:OD1	1.90	0.71
1:A:269:GLU:HG3	4:A:5114:HOH:O	1.89	0.71
1:D:26:SER:HB2	1:D:60:ARG:HH21	1.54	0.71
1:C:52:ALA:HA	1:C:56:LEU:HD12	1.70	0.71
1:A:178:LEU:HD22	1:A:178:LEU:N	2.05	0.71
1:A:134:GLN:O	1:A:138:GLU:HG3	1.91	0.71
1:A:66:ILE:HD13	1:A:195:ILE:HD11	1.72	0.71
1:C:208:MSE:HE2	1:D:218:PHE:CE2	2.26	0.70
1:B:126:THR:HB	1:B:200:GLY:HA3	1.73	0.70
1:A:114:ARG:CG	1:A:114:ARG:HH11	2.00	0.70
1:B:153:MSE:HE1	1:B:219:VAL:CG2	2.22	0.70
1:D:33:GLU:HG2	1:D:34:ASP:H	1.52	0.70
1:B:29:MSE:HE2	1:B:56:LEU:CD2	2.22	0.69
1:B:109:GLN:HG3	1:B:121:VAL:HG23	1.74	0.69
1:C:313:ARG:HB2	1:C:313:ARG:NH1	1.96	0.69
1:B:121:VAL:HG23	1:B:121:VAL:O	1.92	0.69
1:A:43:ASN:OD1	1:A:45:ASP:HB2	1.92	0.69
1:D:33:GLU:O	1:D:34:ASP:C	2.29	0.69
1:D:247:PHE:CE2	1:D:248:ARG:HB2	2.28	0.69
1:A:153:MSE:HE1	1:A:219:VAL:CG2	2.23	0.69
1:D:251:ALA:O	1:D:253:THR:N	2.26	0.69
1:C:202:ASN:ND2	1:C:202:ASN:H	1.91	0.69
1:B:31:LEU:HB2	1:B:35:GLU:OE1	1.92	0.69
1:C:126:THR:HB	1:C:200:GLY:HA3	1.73	0.69
1:D:125:THR:HG23	4:D:5180:HOH:O	1.90	0.69
1:C:153:MSE:CE	1:C:219:VAL:HG23	2.22	0.69
1:C:106:ARG:HG2	1:C:106:ARG:NH1	2.07	0.69
1:C:202:ASN:N	1:C:202:ASN:HD22	1.88	0.69
1:A:253:THR:O	1:A:254:ASP:HB2	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:LYS:HG2	1:D:142:MSE:CE	2.23	0.69
1:D:153:MSE:CE	1:D:219:VAL:CG2	2.70	0.69
1:D:24:ARG:HB2	1:D:24:ARG:NH1	2.00	0.69
1:C:106:ARG:HG2	1:C:106:ARG:HH11	1.57	0.69
1:D:101:LYS:HE2	1:D:201:LEU:HD23	1.75	0.68
1:A:153:MSE:CE	1:A:219:VAL:CG2	2.72	0.68
1:C:218:PHE:HE2	1:D:208:MSE:HE2	1.57	0.68
1:A:26:SER:O	1:A:27:VAL:HB	1.92	0.68
1:C:153:MSE:CE	1:C:219:VAL:CG2	2.72	0.68
1:B:303:LYS:NZ	1:B:307:HIS:ND1	2.42	0.68
1:D:47:SER:O	1:D:51:VAL:HG23	1.95	0.67
1:B:283:TRP:HE3	1:B:284:LEU:HD23	1.60	0.67
1:C:244:PHE:O	1:C:248:ARG:HG2	1.93	0.67
1:C:12:TYR:HB3	1:C:313:ARG:HG2	1.75	0.67
1:D:43:ASN:HD21	1:D:45:ASP:HB2	1.60	0.67
1:B:20:TRP:HA	1:B:23:LEU:HD11	1.75	0.66
1:C:218:PHE:CZ	1:D:208:MSE:HE2	2.31	0.66
1:C:26:SER:HB2	1:C:60:ARG:HH12	1.59	0.66
1:A:85:GLN:O	1:A:85:GLN:HG2	1.95	0.66
1:D:281:ILE:HG22	1:D:282:ASN:N	2.10	0.66
1:A:56:LEU:HB3	1:A:57:PRO:HD3	1.78	0.66
1:D:267:LYS:CD	1:D:267:LYS:H	2.09	0.66
1:C:276:THR:HG23	4:C:5151:HOH:O	1.96	0.65
1:C:153:MSE:HE1	1:C:219:VAL:CG2	2.26	0.65
1:D:126:THR:HB	1:D:200:GLY:HA3	1.77	0.65
1:C:80:LEU:HD12	1:C:82:THR:CG2	2.26	0.65
1:C:218:PHE:CZ	1:D:208:MSE:CE	2.79	0.65
1:A:204:LEU:HB3	1:A:293:THR:HB	1.79	0.65
1:C:169:ASN:HD22	1:C:169:ASN:H	1.44	0.65
1:C:153:MSE:HE1	1:C:219:VAL:HG21	1.77	0.65
1:B:235:LEU:HD21	1:B:305:ALA:HA	1.79	0.65
1:D:16:ASP:H	1:D:19:GLN:NE2	1.94	0.64
1:C:33:GLU:O	1:C:34:ASP:HB2	1.95	0.64
1:B:8:LEU:O	1:B:8:LEU:HD12	1.97	0.64
1:C:54:ILE:O	1:C:57:PRO:HD2	1.98	0.64
1:C:241:ILE:HG23	1:C:274:ALA:HB3	1.79	0.64
1:D:27:VAL:HG12	1:D:60:ARG:NH2	2.12	0.64
1:C:299:LEU:HD21	1:C:301:LEU:CD1	2.28	0.64
1:B:16:ASP:OD2	1:B:19:GLN:HG3	1.98	0.64
1:D:67:SER:HA	1:D:70:LEU:HD12	1.80	0.63
1:A:72:ARG:HD2	1:A:76:LEU:HD11	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:CG2	1:C:60:ARG:HD2	2.29	0.63
1:B:76:LEU:O	1:B:80:LEU:HD12	1.98	0.63
1:C:133:ASN:O	1:C:137:LYS:HG3	1.99	0.62
1:C:299:LEU:HD21	1:C:301:LEU:HD13	1.81	0.62
1:C:133:ASN:HD21	1:C:145:LYS:HZ3	1.46	0.62
1:A:135:VAL:O	1:A:139:ARG:HD2	1.98	0.62
1:B:29:MSE:HE2	1:B:56:LEU:HD21	1.82	0.62
1:D:16:ASP:N	1:D:19:GLN:HE21	1.95	0.62
1:D:94:ALA:HB2	1:D:203:VAL:CG2	2.30	0.62
1:B:31:LEU:HD12	1:B:31:LEU:N	2.15	0.62
1:C:20:TRP:C	1:C:22:ALA:H	2.03	0.62
1:A:20:TRP:HA	1:A:23:LEU:HD22	1.82	0.62
1:D:48:LEU:HD12	1:D:48:LEU:H	1.64	0.62
1:D:80:LEU:N	1:D:80:LEU:HD23	2.15	0.62
1:D:267:LYS:H	1:D:267:LYS:HD2	1.63	0.62
1:D:282:ASN:H	1:D:282:ASN:ND2	1.98	0.61
1:C:246:LYS:HD3	1:C:247:PHE:CE1	2.35	0.61
1:D:133:ASN:HB3	1:D:142:MSE:HE1	1.82	0.61
1:D:67:SER:HB2	1:D:71:ARG:NH1	2.16	0.61
1:B:159:PHE:CE1	1:B:172:ALA:HB2	2.36	0.61
1:B:82:THR:O	1:B:83:ASN:HB2	1.99	0.61
1:A:126:THR:HB	1:A:200:GLY:HA3	1.81	0.61
1:C:40:LYS:HE3	1:C:44:GLU:HA	1.81	0.61
1:C:218:PHE:CE2	1:D:208:MSE:CE	2.84	0.61
1:A:66:ILE:HD13	1:A:195:ILE:CD1	2.30	0.61
1:B:275:MSE:O	1:B:279:LYS:HG3	2.00	0.61
1:D:145:LYS:HE2	1:D:175:TYR:OH	2.00	0.60
1:C:133:ASN:HD21	1:C:145:LYS:HZ1	1.47	0.60
1:C:237:GLN:O	1:C:241:ILE:HG12	2.01	0.60
1:C:80:LEU:HD12	1:C:82:THR:HG21	1.84	0.60
1:D:31:LEU:HA	1:D:114:ARG:HH21	1.67	0.60
1:D:136:LEU:HB2	1:D:142:MSE:HE2	1.84	0.60
1:A:90:ILE:HD12	1:A:164:LYS:HE2	1.83	0.60
1:B:142:MSE:HE2	1:B:258:TYR:CG	2.36	0.60
1:A:153:MSE:HE1	1:A:219:VAL:HG23	1.84	0.60
1:B:85:GLN:H	1:C:191:VAL:CG2	2.15	0.60
1:C:232:PRO:HG2	1:C:235:LEU:HD22	1.84	0.60
1:C:26:SER:HB2	1:C:60:ARG:NH1	2.17	0.59
1:C:34:ASP:O	1:C:38:ARG:NH1	2.35	0.59
1:D:267:LYS:HG2	1:D:268:GLU:H	1.67	0.59
1:D:227:ILE:HG12	1:D:299:LEU:HD22	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TRP:O	1:B:23:LEU:HD13	2.01	0.59
1:C:284:LEU:O	1:C:288:GLN:HG2	2.03	0.59
1:A:120:ARG:HB2	1:A:194:ASP:OD1	2.03	0.59
1:C:126:THR:CG2	1:C:202:ASN:HD21	2.15	0.59
1:C:30:THR:C	1:C:31:LEU:HD23	2.24	0.58
1:D:253:THR:OG1	1:D:263:ALA:HB2	2.02	0.58
1:D:134:GLN:H	1:D:134:GLN:CD	1.97	0.58
1:D:120:ARG:HH11	1:D:193:PRO:HA	1.63	0.58
1:D:73:GLN:HA	1:D:73:GLN:OE1	2.02	0.58
1:A:153:MSE:HE1	1:A:219:VAL:HG21	1.86	0.58
1:A:245:LEU:HD11	1:A:271:ILE:HG22	1.85	0.58
1:C:43:ASN:O	1:C:44:GLU:CG	2.50	0.58
1:A:20:TRP:O	1:A:23:LEU:HD22	2.03	0.58
1:C:134:GLN:HG3	1:C:135:VAL:N	2.17	0.58
1:D:79:PHE:HB3	1:D:80:LEU:HD23	1.86	0.58
1:C:27:VAL:HG21	1:C:60:ARG:HD2	1.85	0.57
1:D:20:TRP:C	1:D:22:ALA:H	2.06	0.57
1:B:248:ARG:HG3	1:B:252:PHE:CE1	2.39	0.57
1:C:36:ILE:N	1:C:36:ILE:HD13	2.19	0.57
1:C:60:ARG:NH1	1:D:79:PHE:HE2	2.01	0.57
1:B:10:THR:OG1	1:B:11:PRO:CD	2.52	0.57
1:D:27:VAL:HG12	1:D:60:ARG:CZ	2.34	0.57
1:A:123:LEU:C	1:A:123:LEU:HD23	2.25	0.57
1:B:313:ARG:HG3	1:B:313:ARG:HH11	1.70	0.57
1:C:9:MSE:CE	1:D:166:GLY:HA3	2.35	0.57
1:A:101:LYS:HE3	1:A:201:LEU:HD12	1.87	0.57
1:A:113:SER:O	1:A:119:ARG:HA	2.04	0.57
1:C:108:LEU:O	1:C:112:LEU:HB2	2.04	0.57
1:B:126:THR:HG21	1:B:202:ASN:HD21	1.70	0.57
1:A:248:ARG:HG3	1:A:262:TYR:HB3	1.87	0.57
1:C:177:HIS:HB2	4:C:5275:HOH:O	2.04	0.56
1:D:191:VAL:O	1:D:191:VAL:HG22	2.03	0.56
1:D:253:THR:O	1:D:260:HIS:HD2	1.88	0.56
1:D:123:LEU:O	1:D:124:ILE:HD13	2.05	0.56
1:C:95:GLY:O	1:C:201:LEU:HD23	2.05	0.56
1:C:29:MSE:HG2	1:C:60:ARG:HH21	1.70	0.56
1:A:96:SER:OG	1:A:97:VAL:N	2.39	0.56
1:D:275:MSE:O	1:D:279:LYS:HG3	2.05	0.56
1:B:268:GLU:H	1:B:268:GLU:CD	2.09	0.56
1:B:31:LEU:CD1	1:B:31:LEU:N	2.68	0.56
1:D:20:TRP:HA	1:D:23:LEU:CD1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLN:NE2	1:A:8:LEU:CD1	2.68	0.56
1:D:262:TYR:O	1:D:265:LEU:HB2	2.06	0.56
1:C:168:PRO:HD3	1:D:9:MSE:HE1	1.86	0.56
1:D:38:ARG:O	1:D:42:ILE:HG13	2.06	0.56
1:B:26:SER:HB2	1:B:60:ARG:NH2	2.19	0.56
1:B:20:TRP:C	1:B:22:ALA:H	2.09	0.56
1:D:134:GLN:OE1	1:D:134:GLN:N	2.26	0.56
1:D:77:GLU:HG3	1:D:82:THR:HB	1.87	0.56
1:C:90:ILE:HG23	1:C:196:LEU:HD23	1.87	0.56
1:D:282:ASN:HD22	1:D:282:ASN:H	1.53	0.56
1:D:103:THR:O	1:D:107:VAL:HG23	2.06	0.56
1:C:81:GLY:O	1:C:83:ASN:N	2.39	0.56
1:A:101:LYS:HB3	1:A:199:GLU:HG3	1.88	0.56
1:D:61:LEU:HD21	1:D:314:LEU:CD1	2.36	0.55
1:C:101:LYS:HE3	1:C:201:LEU:HD23	1.87	0.55
1:D:79:PHE:HD1	1:D:80:LEU:CD2	2.18	0.55
1:D:153:MSE:CE	1:D:219:VAL:HG22	2.37	0.55
1:C:218:PHE:HZ	1:D:208:MSE:CE	2.19	0.55
1:B:49:GLU:OE2	1:B:49:GLU:N	2.40	0.55
1:D:123:LEU:C	1:D:124:ILE:HD13	2.26	0.55
1:D:163:LEU:CD1	1:D:196:LEU:HD13	2.36	0.55
1:A:176:SER:HB2	1:A:183:ILE:HD11	1.88	0.55
1:C:83:ASN:OD1	1:C:84:GLY:N	2.35	0.55
1:C:9:MSE:HE3	1:D:165:SER:O	2.07	0.55
1:D:163:LEU:HD11	1:D:196:LEU:HD13	1.89	0.55
1:C:133:ASN:ND2	1:C:145:LYS:NZ	2.52	0.55
1:A:275:MSE:HE2	1:A:279:LYS:HE2	1.89	0.55
1:B:299:LEU:HD12	1:B:314:LEU:HD13	1.89	0.55
1:C:36:ILE:HG23	1:C:48:LEU:HD21	1.88	0.54
1:C:60:ARG:HH11	1:D:79:PHE:HE2	1.55	0.54
1:D:247:PHE:C	1:D:251:ALA:HB2	2.27	0.54
1:C:40:LYS:CE	1:C:44:GLU:HA	2.37	0.54
1:A:252:PHE:O	1:A:253:THR:C	2.44	0.54
1:D:72:ARG:HD2	1:D:76:LEU:HD11	1.89	0.54
1:B:76:LEU:O	1:B:80:LEU:CD1	2.55	0.54
1:B:153:MSE:CE	1:B:219:VAL:CG2	2.83	0.54
1:C:169:ASN:ND2	1:C:169:ASN:H	2.05	0.54
1:D:67:SER:HB2	1:D:71:ARG:HH12	1.71	0.54
1:C:80:LEU:CA	1:D:23:LEU:HD22	2.35	0.54
1:D:247:PHE:C	1:D:247:PHE:CD2	2.80	0.54
1:B:29:MSE:HE2	1:B:56:LEU:HD23	1.87	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ARG:HH11	1:C:106:ARG:CG	2.18	0.54
1:D:281:ILE:O	1:D:284:LEU:HB2	2.06	0.54
1:B:94:ALA:HB2	1:B:203:VAL:HG23	1.89	0.54
1:D:255:PRO:HA	1:D:260:HIS:CG	2.43	0.54
1:D:133:ASN:O	1:D:137:LYS:HG3	2.07	0.54
1:A:132:PRO:HG3	1:A:182:VAL:HG21	1.90	0.54
1:C:27:VAL:H	1:C:60:ARG:NH1	2.06	0.53
1:A:31:LEU:HD12	1:A:31:LEU:N	2.22	0.53
1:A:32:SER:HB3	1:A:35:GLU:OE2	2.08	0.53
1:A:123:LEU:O	1:A:124:ILE:HD13	2.08	0.53
1:C:9:MSE:HE3	1:D:166:GLY:HA3	1.91	0.53
1:C:16:ASP:OD2	1:C:18:ASN:HB2	2.08	0.53
1:B:121:VAL:HG12	1:B:195:ILE:HB	1.90	0.53
1:A:133:ASN:O	1:A:137:LYS:HG3	2.08	0.53
1:D:13:LEU:O	1:D:313:ARG:HA	2.09	0.53
1:D:97:VAL:HG11	1:D:243:ARG:CZ	2.39	0.53
1:B:46:LEU:HD22	1:B:51:VAL:HG23	1.91	0.53
1:A:118:HIS:C	1:A:119:ARG:HG3	2.28	0.53
1:D:254:ASP:O	1:D:256:ASP:N	2.41	0.53
1:D:255:PRO:HA	1:D:260:HIS:CD2	2.44	0.53
1:B:283:TRP:CH2	1:B:287:LYS:HD2	2.43	0.53
1:C:32:SER:O	1:C:36:ILE:HG12	2.09	0.53
1:D:249:GLU:HG3	1:D:270:ALA:HB2	1.89	0.53
1:C:144:LYS:HE2	4:C:5053:HOH:O	2.08	0.53
1:B:237:GLN:HG3	1:B:278:TRP:NE1	2.22	0.53
1:C:208:MSE:HE2	1:D:218:PHE:HZ	1.71	0.53
1:B:162:ASP:O	1:B:165:SER:HB2	2.09	0.53
1:B:126:THR:HG21	1:B:202:ASN:ND2	2.24	0.53
1:C:142:MSE:HE2	1:C:258:TYR:CG	2.44	0.53
1:D:133:ASN:N	1:D:133:ASN:HD22	2.06	0.52
1:C:301:LEU:HD12	1:C:312:VAL:HG22	1.91	0.52
1:C:29:MSE:HG3	1:C:60:ARG:HH21	1.71	0.52
1:C:13:LEU:O	1:C:313:ARG:HA	2.09	0.52
1:A:129:PHE:CE2	1:A:156:LEU:HA	2.44	0.52
1:C:87:ILE:HG13	1:D:316:LYS:HB3	1.90	0.52
1:A:183:ILE:CG2	1:A:186:GLY:HA3	2.38	0.52
1:D:16:ASP:OD2	1:D:18:ASN:HB2	2.09	0.52
1:A:221:ASP:O	1:B:315:ARG:NH2	2.42	0.52
1:C:21:ALA:O	1:C:24:ARG:HG2	2.09	0.52
1:B:94:ALA:HB2	1:B:203:VAL:CG2	2.40	0.52
1:A:183:ILE:HG21	1:A:186:GLY:HA3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:PRO:O	1:C:210:TYR:HE2	1.92	0.52
1:D:131:HIS:HB2	1:D:136:LEU:HD21	1.91	0.51
1:D:24:ARG:HH11	1:D:24:ARG:CG	2.23	0.51
1:B:96:SER:HB2	1:B:286:LEU:CD1	2.39	0.51
1:D:265:LEU:HD13	1:D:270:ALA:HA	1.93	0.51
1:A:82:THR:HG21	1:A:85:GLN:HE22	1.74	0.51
1:B:9:MSE:HE2	1:B:316:LYS:NZ	2.25	0.51
1:B:20:TRP:HA	1:B:23:LEU:CD1	2.40	0.51
1:B:232:PRO:HD2	1:B:235:LEU:HD12	1.92	0.51
1:C:169:ASN:HD22	1:C:169:ASN:N	2.05	0.51
1:A:183:ILE:HG22	1:A:186:GLY:N	2.25	0.51
1:D:90:ILE:HD12	1:D:164:LYS:HD3	1.92	0.51
1:B:31:LEU:O	1:B:31:LEU:HD13	2.11	0.51
1:D:247:PHE:CD2	1:D:248:ARG:HB2	2.46	0.51
1:A:94:ALA:HB2	1:A:203:VAL:CG2	2.41	0.51
1:C:21:ALA:CB	1:C:53:GLU:HG2	2.35	0.51
1:D:19:GLN:O	1:D:22:ALA:HB3	2.11	0.51
1:C:148:PRO:O	1:C:210:TYR:CE2	2.64	0.51
1:B:121:VAL:CG2	1:B:121:VAL:O	2.59	0.50
1:B:61:LEU:HD11	1:B:65:TYR:HE1	1.76	0.50
1:A:253:THR:O	1:A:254:ASP:CB	2.59	0.50
1:C:86:ARG:HD2	1:C:192:GLN:HB3	1.94	0.50
1:D:133:ASN:OD1	1:D:181:ASP:HB2	2.11	0.50
1:D:26:SER:HB2	1:D:60:ARG:HH22	1.70	0.50
1:D:120:ARG:HH12	1:D:193:PRO:CA	2.24	0.50
1:D:248:ARG:HD3	1:D:253:THR:CG2	2.41	0.50
1:C:35:GLU:HA	1:C:38:ARG:HD2	1.92	0.50
1:A:275:MSE:HE3	1:A:279:LYS:HG3	1.94	0.50
1:D:122:GLU:HG2	1:D:190:VAL:HG22	1.93	0.50
1:C:31:LEU:O	1:C:32:SER:HB3	2.11	0.50
1:D:253:THR:O	1:D:254:ASP:C	2.50	0.50
1:C:43:ASN:HD21	3:C:403:ANP:H2'	1.75	0.50
1:D:131:HIS:CE1	1:D:152:ASP:HB2	2.47	0.50
1:B:283:TRP:CE3	1:B:284:LEU:HD23	2.44	0.50
1:D:284:LEU:O	1:D:288:GLN:HG2	2.12	0.50
1:C:315:ARG:HH22	1:D:164:LYS:HG2	1.75	0.50
1:C:80:LEU:HA	1:D:23:LEU:CD2	2.37	0.50
1:A:125:THR:HB	1:A:199:GLU:OE1	2.12	0.50
1:A:179:ILE:O	1:A:180:TYR:HD2	1.93	0.50
1:C:299:LEU:CD2	1:C:301:LEU:HD13	2.41	0.50
1:C:90:ILE:HD12	1:C:222:PHE:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLU:HG2	1:C:200:GLY:N	2.28	0.49
1:A:85:GLN:HG3	1:A:87:ILE:HD11	1.94	0.49
1:D:126:THR:CB	1:D:200:GLY:HA3	2.42	0.49
1:C:35:GLU:O	1:C:38:ARG:HB2	2.12	0.49
1:B:122:GLU:HB3	1:B:196:LEU:HD12	1.94	0.49
1:B:103:THR:O	1:B:107:VAL:HG23	2.11	0.49
1:D:43:ASN:C	1:D:43:ASN:HD22	2.15	0.49
1:D:71:ARG:O	1:D:75:VAL:HG23	2.12	0.49
1:C:156:LEU:O	1:C:156:LEU:HD12	2.12	0.49
1:C:80:LEU:HD12	1:C:82:THR:HG22	1.95	0.49
1:A:178:LEU:N	1:A:178:LEU:CD2	2.74	0.49
1:C:293:THR:O	1:C:296:ARG:HB2	2.12	0.49
1:B:202:ASN:ND2	1:B:202:ASN:N	2.45	0.49
1:B:10:THR:OG1	1:B:11:PRO:HD2	2.13	0.49
1:B:121:VAL:HA	1:B:195:ILE:O	2.12	0.49
1:B:77:GLU:HA	1:B:82:THR:CG2	2.42	0.49
1:C:54:ILE:C	1:C:57:PRO:HD2	2.33	0.49
1:D:35:GLU:O	1:D:36:ILE:C	2.50	0.49
1:B:116:PRO:CA	1:B:119:ARG:HH21	2.24	0.49
1:D:133:ASN:N	1:D:133:ASN:ND2	2.58	0.49
1:A:8:LEU:N	1:A:8:LEU:HD12	2.28	0.49
1:B:294:ARG:HG2	1:B:300:ILE:CD1	2.43	0.49
1:C:29:MSE:HE2	1:C:56:LEU:C	2.33	0.49
1:B:235:LEU:CD2	1:B:305:ALA:HA	2.42	0.49
1:C:94:ALA:HB2	1:C:203:VAL:CG2	2.42	0.49
1:A:136:LEU:HD22	1:A:141:LEU:HB2	1.95	0.49
1:D:96:SER:O	1:D:101:LYS:HE3	2.13	0.49
1:A:304:SER:HB3	1:A:310:GLU:CG	2.43	0.49
1:D:133:ASN:HD21	1:D:145:LYS:NZ	2.11	0.48
1:A:77:GLU:HG3	1:A:82:THR:HB	1.94	0.48
1:B:142:MSE:HE2	1:B:258:TYR:CD2	2.48	0.48
1:D:19:GLN:O	1:D:23:LEU:HG	2.13	0.48
1:D:79:PHE:HD1	1:D:80:LEU:HD22	1.77	0.48
1:B:21:ALA:HB2	1:B:53:GLU:HG2	1.92	0.48
1:A:43:ASN:C	1:A:45:ASP:H	2.17	0.48
1:D:27:VAL:CG1	1:D:60:ARG:CZ	2.91	0.48
1:C:58:LEU:O	1:C:61:LEU:HB3	2.12	0.48
1:D:72:ARG:O	1:D:76:LEU:HD12	2.14	0.48
1:D:247:PHE:O	1:D:251:ALA:HB2	2.14	0.48
1:D:133:ASN:O	1:D:142:MSE:CE	2.62	0.48
1:D:27:VAL:HG23	1:D:28:PRO:HD2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:VAL:HG11	1:D:229:VAL:HB	1.96	0.48
1:C:29:MSE:HE2	1:C:56:LEU:O	2.13	0.48
1:B:286:LEU:HA	1:B:290:ILE:HB	1.96	0.48
1:D:174:VAL:HG12	1:D:183:ILE:HD12	1.95	0.48
1:A:88:PRO:HB3	1:A:193:PRO:O	2.14	0.48
1:D:20:TRP:HA	1:D:23:LEU:HD11	1.95	0.48
1:A:72:ARG:HG3	1:B:68:SER:CB	2.44	0.48
1:D:31:LEU:O	1:D:31:LEU:HD12	2.14	0.48
1:D:99:VAL:CG1	1:D:229:VAL:HB	2.43	0.48
1:D:12:TYR:HB3	1:D:313:ARG:HB3	1.96	0.47
1:B:268:GLU:N	1:B:268:GLU:CD	2.67	0.47
1:A:34:ASP:CG	1:A:38:ARG:HH12	2.18	0.47
1:B:124:ILE:HD13	1:B:196:LEU:HD11	1.96	0.47
1:C:218:PHE:O	1:C:221:ASP:HB2	2.13	0.47
1:A:256:ASP:CA	1:A:260:HIS:HB2	2.44	0.47
1:B:264:LYS:HG2	1:B:264:LYS:H	1.33	0.47
1:A:56:LEU:CB	1:A:57:PRO:HD3	2.44	0.47
1:B:32:SER:HB3	1:B:35:GLU:OE2	2.15	0.47
1:D:32:SER:O	1:D:33:GLU:O	2.33	0.47
1:D:248:ARG:HH11	1:D:253:THR:HG22	1.79	0.47
1:D:13:LEU:HD13	1:D:316:LYS:HG3	1.97	0.47
1:C:169:ASN:ND2	1:C:169:ASN:O	2.47	0.47
1:C:134:GLN:O	1:C:138:GLU:HG3	2.13	0.47
1:A:176:SER:O	1:A:180:TYR:HA	2.15	0.47
1:D:12:TYR:CE2	1:D:315:ARG:HG2	2.49	0.47
1:D:267:LYS:CD	1:D:267:LYS:N	2.78	0.47
1:B:275:MSE:O	1:B:279:LYS:CG	2.61	0.47
1:A:248:ARG:O	1:A:251:ALA:HB2	2.15	0.47
1:A:275:MSE:CE	1:A:279:LYS:HE2	2.45	0.47
1:B:9:MSE:CE	1:B:316:LYS:HZ1	2.28	0.47
1:C:94:ALA:HB2	1:C:203:VAL:HG23	1.96	0.47
1:A:25:ASP:HB2	1:B:79:PHE:HD1	1.80	0.47
1:C:29:MSE:HG2	1:C:60:ARG:NH2	2.31	0.46
1:C:68:SER:OG	1:D:72:ARG:HG3	2.14	0.46
1:A:11:PRO:HA	1:B:165:SER:HA	1.95	0.46
1:A:293:THR:HG22	4:B:5184:HOH:O	2.15	0.46
1:D:48:LEU:N	1:D:48:LEU:HD12	2.30	0.46
1:D:132:PRO:HB2	1:D:134:GLN:HG2	1.96	0.46
1:D:231:ALA:HB3	1:D:236:LEU:HD21	1.97	0.46
1:D:291:LEU:HB3	1:D:292:PRO:HD3	1.95	0.46
1:C:39:LEU:O	1:C:42:ILE:HB	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:LYS:HB3	1:D:137:LYS:NZ	2.29	0.46
1:B:96:SER:OG	1:B:97:VAL:N	2.48	0.46
1:B:109:GLN:CG	1:B:121:VAL:HG23	2.43	0.46
1:A:248:ARG:NH1	1:A:265:LEU:HB2	2.31	0.46
1:B:20:TRP:CZ3	1:B:312:VAL:HG11	2.50	0.46
1:C:33:GLU:O	1:C:34:ASP:CB	2.61	0.46
1:C:96:SER:OG	1:C:97:VAL:N	2.49	0.46
1:D:20:TRP:HA	1:D:23:LEU:HD12	1.98	0.46
1:A:118:HIS:HB3	1:A:194:ASP:HB3	1.98	0.46
1:A:79:PHE:CZ	1:B:23:LEU:HD23	2.50	0.46
1:A:293:THR:O	1:A:296:ARG:HB2	2.16	0.46
1:A:22:ALA:O	1:A:24:ARG:HG2	2.16	0.46
1:B:48:LEU:CD1	1:B:48:LEU:H	2.17	0.46
1:D:10:THR:C	1:D:12:TYR:H	2.19	0.46
1:A:254:ASP:O	1:A:255:PRO:C	2.54	0.46
1:B:29:MSE:CG	1:B:56:LEU:HD22	2.35	0.46
1:A:47:SER:O	1:A:51:VAL:HG23	2.16	0.46
1:D:242:ASN:O	1:D:246:LYS:HG3	2.16	0.46
1:D:126:THR:CG2	1:D:200:GLY:HA3	2.46	0.46
1:B:58:LEU:O	1:B:61:LEU:HB3	2.16	0.46
1:D:171:THR:HG22	4:D:5132:HOH:O	2.15	0.46
1:D:133:ASN:HA	1:D:142:MSE:CE	2.42	0.45
1:C:85:GLN:HE21	1:D:9:MSE:SE	2.50	0.45
1:C:47:SER:HB2	1:C:49:GLU:OE1	2.16	0.45
1:A:247:PHE:N	1:A:247:PHE:CD1	2.84	0.45
1:D:133:ASN:CA	1:D:142:MSE:CE	2.94	0.45
1:D:303:LYS:HE2	1:D:307:HIS:O	2.16	0.45
1:C:27:VAL:HG23	1:C:60:ARG:NH1	2.31	0.45
1:D:101:LYS:HB3	1:D:199:GLU:HG3	1.98	0.45
1:D:121:VAL:HA	1:D:195:ILE:O	2.17	0.45
1:A:313:ARG:HG3	1:A:313:ARG:HH11	1.81	0.45
1:C:31:LEU:HD23	1:C:31:LEU:N	2.32	0.45
1:D:97:VAL:CG1	1:D:243:ARG:CZ	2.94	0.45
1:C:241:ILE:HG23	1:C:274:ALA:CB	2.45	0.45
1:D:176:SER:HB3	1:D:179:ILE:HG12	1.98	0.45
1:D:137:LYS:CG	1:D:142:MSE:CE	2.93	0.45
1:B:10:THR:HG22	4:B:5186:HOH:O	2.16	0.45
1:D:96:SER:OG	1:D:97:VAL:N	2.50	0.45
1:C:316:LYS:NZ	1:D:165:SER:O	2.48	0.45
1:A:190:VAL:HG12	1:A:193:PRO:HD3	1.99	0.45
1:D:248:ARG:HD3	1:D:248:ARG:HA	1.68	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ASN:HD21	1:D:145:LYS:HZ1	1.63	0.45
1:B:24:ARG:HB3	1:B:57:PRO:HB3	1.99	0.45
1:B:153:MSE:HE1	1:B:219:VAL:HG21	1.98	0.45
1:A:8:LEU:HB2	1:A:9:MSE:H	1.22	0.45
1:A:27:VAL:O	1:A:27:VAL:HG12	2.16	0.45
1:A:183:ILE:HA	1:A:184:PRO:HD2	1.69	0.45
1:C:226:SER:OG	1:C:297:ALA:HA	2.17	0.45
1:D:20:TRP:C	1:D:22:ALA:N	2.69	0.45
1:A:256:ASP:HA	1:A:260:HIS:HB2	1.98	0.45
1:D:281:ILE:CG2	1:D:282:ASN:N	2.80	0.45
1:C:101:LYS:HE3	1:C:201:LEU:CD2	2.47	0.45
1:A:34:ASP:OD1	1:A:35:GLU:N	2.47	0.45
1:D:90:ILE:HD12	1:D:222:PHE:O	2.17	0.45
1:A:122:GLU:HB3	1:A:196:LEU:HD22	1.99	0.45
1:C:249:GLU:HG2	1:C:259:PHE:CD1	2.52	0.45
1:D:133:ASN:CA	1:D:142:MSE:HE2	2.44	0.44
1:A:127:ASP:O	1:A:130:LEU:HD12	2.17	0.44
1:C:115:TRP:HD1	1:C:117:GLU:OE1	2.00	0.44
1:C:20:TRP:C	1:C:22:ALA:N	2.68	0.44
1:B:313:ARG:CG	1:B:313:ARG:HH11	2.30	0.44
1:A:299:LEU:HD21	1:A:301:LEU:HD21	2.00	0.44
1:C:119:ARG:NH1	1:C:119:ARG:HG2	2.32	0.44
1:C:19:GLN:HB2	1:C:19:GLN:HE21	1.61	0.44
1:B:108:LEU:O	1:B:112:LEU:HB2	2.17	0.44
1:B:147:PHE:HE1	1:B:281:ILE:HG22	1.82	0.44
1:D:153:MSE:HE2	1:D:219:VAL:CG2	2.47	0.44
1:A:43:ASN:O	1:A:45:ASP:N	2.51	0.44
1:C:27:VAL:HA	1:C:28:PRO:HD2	1.79	0.44
1:C:156:LEU:O	1:C:159:PHE:HB3	2.17	0.44
1:B:156:LEU:O	1:B:156:LEU:HD12	2.17	0.44
1:A:40:LYS:H	1:A:40:LYS:HG2	1.63	0.44
1:C:129:PHE:CZ	1:C:173:PRO:HD2	2.52	0.44
1:C:24:ARG:HB3	1:C:57:PRO:HG3	1.99	0.44
1:D:131:HIS:HB2	1:D:136:LEU:CD2	2.48	0.44
1:B:123:LEU:O	1:B:124:ILE:HD12	2.17	0.44
1:A:191:VAL:O	1:A:191:VAL:HG13	2.18	0.44
1:C:67:SER:HA	1:C:70:LEU:HD12	1.99	0.44
1:A:101:LYS:HE2	1:A:101:LYS:HB2	1.63	0.44
1:A:133:ASN:HB2	1:A:181:ASP:OD2	2.18	0.44
1:C:129:PHE:CE2	1:C:156:LEU:HA	2.52	0.44
1:A:91:ILE:HA	1:A:225:PHE:O	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD22	1:A:269:GLU:HB3	1.99	0.44
1:C:299:LEU:HD21	1:C:301:LEU:HD11	1.99	0.44
1:B:73:GLN:O	1:B:77:GLU:HB2	2.18	0.44
1:B:191:VAL:HG22	1:B:191:VAL:O	2.18	0.44
1:D:226:SER:O	1:D:298:SER:HB2	2.17	0.44
1:A:85:GLN:HB3	1:A:85:GLN:HE21	1.62	0.43
1:D:133:ASN:ND2	1:D:133:ASN:H	2.16	0.43
1:A:34:ASP:HB2	1:A:38:ARG:NH1	2.33	0.43
1:D:29:MSE:CE	1:D:56:LEU:CD2	2.92	0.43
1:B:113:SER:O	1:B:119:ARG:HA	2.17	0.43
1:A:106:ARG:O	1:A:109:GLN:HG2	2.18	0.43
1:A:231:ALA:HB3	1:A:236:LEU:HD21	2.00	0.43
1:D:252:PHE:O	1:D:253:THR:C	2.57	0.43
1:B:20:TRP:C	1:B:22:ALA:N	2.71	0.43
1:B:283:TRP:CZ3	1:B:287:LYS:HD2	2.53	0.43
1:B:299:LEU:HD23	1:B:300:ILE:N	2.34	0.43
1:D:183:ILE:HA	1:D:184:PRO:HD2	1.77	0.43
1:B:231:ALA:HB3	1:B:236:LEU:HD13	2.00	0.43
1:B:29:MSE:SE	1:B:60:ARG:HD2	2.69	0.43
1:B:137:LYS:HD3	1:B:258:TYR:CE1	2.53	0.43
1:A:175:TYR:OH	1:A:180:TYR:HB2	2.19	0.43
1:A:25:ASP:HB2	1:B:79:PHE:CD1	2.53	0.43
1:B:304:SER:HB3	1:B:310:GLU:HG2	2.00	0.43
1:A:118:HIS:C	1:A:119:ARG:CG	2.86	0.43
1:D:35:GLU:CG	1:D:36:ILE:H	2.31	0.43
1:D:248:ARG:HD3	1:D:253:THR:HG22	2.00	0.43
1:C:126:THR:HG23	1:C:151:TYR:HE2	1.83	0.43
1:A:72:ARG:HB3	1:A:72:ARG:HE	1.78	0.43
1:D:123:LEU:HD12	1:D:124:ILE:N	2.34	0.43
1:D:228:TYR:CD1	1:D:294:ARG:HA	2.53	0.43
1:A:60:ARG:HD3	1:A:60:ARG:HA	1.90	0.43
1:D:24:ARG:NH1	1:D:24:ARG:CG	2.82	0.43
1:C:221:ASP:O	1:D:315:ARG:NH2	2.52	0.43
1:A:10:THR:HB	1:A:11:PRO:CD	2.49	0.43
1:D:304:SER:HB3	1:D:310:GLU:CG	2.49	0.43
1:A:232:PRO:HD2	1:A:235:LEU:CD2	2.48	0.43
1:B:303:LYS:HE2	1:B:307:HIS:O	2.18	0.42
1:A:72:ARG:NH1	1:B:65:TYR:CD2	2.87	0.42
1:C:266:THR:O	1:C:267:LYS:C	2.57	0.42
1:D:118:HIS:O	1:D:194:ASP:CG	2.57	0.42
1:B:29:MSE:CG	1:B:56:LEU:CD2	2.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:N	1:B:57:PRO:HD2	2.34	0.42
1:B:118:HIS:HB2	1:B:119:ARG:H	1.20	0.42
1:C:217:VAL:HG21	1:D:295:GLU:HB2	2.01	0.42
1:D:113:SER:O	1:D:119:ARG:HD2	2.20	0.42
1:B:240:TYR:OH	1:B:282:ASN:ND2	2.52	0.42
1:A:244:PHE:O	1:A:248:ARG:N	2.36	0.42
1:D:282:ASN:N	1:D:282:ASN:ND2	2.66	0.42
1:C:234:ASP:OD1	1:C:235:LEU:N	2.52	0.42
1:B:94:ALA:CB	1:B:204:LEU:HD12	2.49	0.42
1:B:9:MSE:HE2	1:B:316:LYS:HZ3	1.83	0.42
1:C:204:LEU:HB3	1:C:293:THR:HB	2.01	0.42
1:C:79:PHE:CE1	1:D:23:LEU:O	2.72	0.42
1:B:169:ASN:ND2	1:B:191:VAL:HA	2.34	0.42
1:D:155:ARG:CZ	1:D:173:PRO:HD3	2.49	0.42
1:D:17:ARG:HH11	1:D:17:ARG:HG2	1.84	0.42
1:B:123:LEU:C	1:B:124:ILE:HD12	2.39	0.42
1:A:13:LEU:O	1:A:313:ARG:HA	2.20	0.42
1:A:315:ARG:NH2	1:B:222:PHE:CD2	2.88	0.42
1:C:21:ALA:C	1:C:24:ARG:HG2	2.40	0.42
1:D:29:MSE:CE	1:D:56:LEU:HD23	2.41	0.42
1:A:248:ARG:HH12	1:A:265:LEU:HB2	1.84	0.42
1:C:235:LEU:HA	1:C:235:LEU:HD12	1.85	0.42
1:A:99:VAL:HG12	1:A:101:LYS:HG3	2.01	0.42
1:D:237:GLN:O	1:D:241:ILE:HG13	2.19	0.42
1:A:29:MSE:HB3	1:A:56:LEU:HD22	2.00	0.42
1:C:9:MSE:CE	1:D:166:GLY:C	2.88	0.42
1:B:164:LYS:HG3	1:B:222:PHE:HB3	2.02	0.42
1:A:283:TRP:CZ2	1:A:287:LYS:HE2	2.55	0.42
1:D:148:PRO:O	1:D:210:TYR:CE2	2.73	0.42
1:A:228:TYR:CD2	1:A:294:ARG:HG3	2.55	0.42
1:A:267:LYS:O	1:A:271:ILE:HG23	2.19	0.42
1:D:91:ILE:HD12	1:D:195:ILE:CG2	2.50	0.42
1:A:39:LEU:O	1:A:42:ILE:HB	2.20	0.42
1:C:27:VAL:HG23	1:C:60:ARG:HH11	1.84	0.41
1:C:133:ASN:ND2	1:C:145:LYS:HZ1	2.16	0.41
1:B:80:LEU:CD1	1:B:82:THR:HG22	2.49	0.41
1:D:291:LEU:N	1:D:292:PRO:CD	2.83	0.41
1:B:34:ASP:OD2	1:B:34:ASP:N	2.52	0.41
1:D:20:TRP:CZ3	1:D:312:VAL:HG11	2.55	0.41
1:C:153:MSE:CE	1:C:219:VAL:HG21	2.41	0.41
1:B:77:GLU:HA	1:B:82:THR:HG23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:LEU:O	1:D:61:LEU:HB3	2.20	0.41
1:B:94:ALA:HB3	1:B:204:LEU:HD12	2.02	0.41
1:B:129:PHE:CZ	1:B:173:PRO:HD2	2.55	0.41
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.93	0.41
1:B:91:ILE:HA	1:B:225:PHE:O	2.21	0.41
1:B:43:ASN:C	1:B:45:ASP:H	2.23	0.41
1:A:32:SER:OG	1:A:33:GLU:N	2.53	0.41
1:D:109:GLN:HA	1:D:121:VAL:HG11	2.02	0.41
1:B:71:ARG:HB2	1:B:71:ARG:HE	1.62	0.41
1:D:205:GLN:HB3	1:D:209:ASP:OD2	2.21	0.41
1:C:43:ASN:C	1:C:45:ASP:H	2.24	0.41
1:B:265:LEU:HA	1:B:269:GLU:OE1	2.20	0.41
1:B:23:LEU:H	1:B:23:LEU:CD1	2.21	0.41
1:D:85:GLN:HG2	1:D:85:GLN:O	2.21	0.41
1:A:204:LEU:HB3	1:A:293:THR:CB	2.49	0.41
1:D:94:ALA:HB2	1:D:203:VAL:HG22	2.01	0.41
1:B:9:MSE:HE3	1:B:316:LYS:HZ1	1.86	0.41
1:A:68:SER:OG	1:B:72:ARG:HG3	2.20	0.41
1:D:153:MSE:HB2	1:D:156:LEU:HB3	2.03	0.41
1:D:253:THR:O	1:D:254:ASP:O	2.39	0.41
1:A:153:MSE:HB2	1:A:156:LEU:HB3	2.01	0.41
1:A:115:TRP:O	1:A:119:ARG:HG3	2.21	0.41
1:A:303:LYS:HD3	1:A:307:HIS:O	2.21	0.41
1:B:183:ILE:HA	1:B:184:PRO:HD2	1.67	0.41
1:B:19:GLN:O	1:B:23:LEU:CD1	2.68	0.41
1:A:40:LYS:CE	1:A:48:LEU:HD11	2.46	0.41
1:A:54:ILE:O	1:A:57:PRO:HD2	2.21	0.41
1:A:33:GLU:O	1:A:36:ILE:HB	2.20	0.41
1:A:291:LEU:HB3	1:A:292:PRO:HD3	2.02	0.41
1:D:34:ASP:O	1:D:35:GLU:C	2.57	0.41
1:C:20:TRP:O	1:C:22:ALA:N	2.54	0.41
1:A:42:ILE:HA	1:A:106:ARG:NH2	2.36	0.41
1:B:49:GLU:O	1:B:53:GLU:HB2	2.21	0.40
1:D:96:SER:O	1:D:101:LYS:CE	2.70	0.40
1:B:306:ASN:O	1:B:307:HIS:HB2	2.22	0.40
1:A:306:ASN:O	1:A:307:HIS:HB2	2.19	0.40
1:D:54:ILE:HG21	1:D:309:VAL:HG21	2.03	0.40
1:C:132:PRO:HG2	1:C:135:VAL:HG23	2.02	0.40
1:A:299:LEU:HD21	1:A:301:LEU:CD2	2.52	0.40
1:A:91:ILE:O	1:A:197:ILE:HA	2.21	0.40
1:C:291:LEU:HB3	1:C:292:PRO:HD3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:MSE:CE	1:C:56:LEU:O	2.69	0.40
1:D:133:ASN:ND2	1:D:145:LYS:NZ	2.70	0.40
1:C:122:GLU:HB3	1:C:196:LEU:HD12	2.03	0.40
1:A:179:ILE:O	1:A:180:TYR:CD2	2.73	0.40
1:C:246:LYS:HD3	1:C:247:PHE:HE1	1.83	0.40
1:A:315:ARG:NH2	1:B:222:PHE:HD2	2.20	0.40
1:A:63:ASN:O	1:A:67:SER:HB3	2.21	0.40
1:B:237:GLN:O	1:B:241:ILE:HD12	2.21	0.40
1:D:43:ASN:C	1:D:45:ASP:H	2.25	0.40
1:A:96:SER:HB2	1:A:286:LEU:CD1	2.43	0.40
1:D:94:ALA:HB2	1:D:203:VAL:HG23	2.02	0.40
1:A:183:ILE:HG22	1:A:183:ILE:O	2.21	0.40
1:A:149:GLU:HG3	1:A:212:HIS:NE2	2.36	0.40
1:C:205:GLN:HB3	1:C:209:ASP:OD2	2.22	0.40
1:B:95:GLY:O	1:B:201:LEU:HD23	2.22	0.40
1:A:17:ARG:HG3	1:A:309:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	309/316 (98%)	266 (86%)	29 (9%)	14 (4%)	3 4
1	B	307/316 (97%)	275 (90%)	26 (8%)	6 (2%)	9 18
1	C	307/316 (97%)	268 (87%)	29 (9%)	10 (3%)	5 7
1	D	307/316 (97%)	266 (87%)	30 (10%)	11 (4%)	4 6
All	All	1230/1264 (97%)	1075 (87%)	114 (9%)	41 (3%)	5 7

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	254	ASP
1	B	85	GLN
1	C	28	PRO
1	C	82	THR
1	C	85	GLN
1	D	33	GLU
1	D	34	ASP
1	D	36	ILE
1	A	85	GLN
1	A	252	PHE
1	A	253	THR
1	B	84	GLY
1	B	305	ALA
1	C	305	ALA
1	D	255	PRO
1	A	257	SER
1	B	168	PRO
1	C	21	ALA
1	C	26	SER
1	C	83	ASN
1	C	168	PRO
1	D	29	MSE
1	D	81	GLY
1	D	253	THR
1	A	27	VAL
1	A	44	GLU
1	A	81	GLY
1	A	305	ALA
1	D	85	GLN
1	A	38	ARG
1	A	168	PRO
1	B	28	PRO
1	B	184	PRO
1	C	38	ARG
1	A	184	PRO
1	C	32	SER
1	D	254	ASP
1	A	36	ILE
1	D	168	PRO
1	D	184	PRO

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	280/278 (101%)	223 (80%)	57 (20%)	1 2
1	B	278/278 (100%)	216 (78%)	62 (22%)	1 2
1	C	278/278 (100%)	222 (80%)	56 (20%)	1 2
1	D	278/278 (100%)	216 (78%)	62 (22%)	1 2
All	All	1114/1112 (100%)	877 (79%)	237 (21%)	1 2

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	LEU
1	A	14	GLN
1	A	16	ASP
1	A	23	LEU
1	A	25	ASP
1	A	26	SER
1	A	31	LEU
1	A	32	SER
1	A	36	ILE
1	A	39	LEU
1	A	40	LYS
1	A	44	GLU
1	A	49	GLU
1	A	58	LEU
1	A	59	SER
1	A	60	ARG
1	A	67	SER
1	A	72	ARG
1	A	73	GLN
1	A	77	GLU
1	A	80	LEU
1	A	85	GLN
1	A	86	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	99	VAL
1	A	108	LEU
1	A	109	GLN
1	A	114	ARG
1	A	115	TRP
1	A	118	HIS
1	A	119	ARG
1	A	122	GLU
1	A	125	THR
1	A	126	THR
1	A	139	ARG
1	A	158	LYS
1	A	171	THR
1	A	176	SER
1	A	179	ILE
1	A	180	TYR
1	A	196	LEU
1	A	199	GLU
1	A	204	LEU
1	A	218	PHE
1	A	233	GLU
1	A	234	ASP
1	A	235	LEU
1	A	245	LEU
1	A	248	ARG
1	A	249	GLU
1	A	253	THR
1	A	256	ASP
1	A	260	HIS
1	A	264	LYS
1	A	271	ILE
1	A	281	ILE
1	A	299	LEU
1	B	8	LEU
1	B	9	MSE
1	B	14	GLN
1	B	16	ASP
1	B	17	ARG
1	B	23	LEU
1	B	26	SER
1	B	30	THR
1	B	31	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	32	SER
1	B	34	ASP
1	B	38	ARG
1	B	40	LYS
1	B	44	GLU
1	B	46	LEU
1	B	47	SER
1	B	48	LEU
1	B	56	LEU
1	B	58	LEU
1	B	60	ARG
1	B	69	ASN
1	B	71	ARG
1	B	72	ARG
1	B	73	GLN
1	B	80	LEU
1	B	82	THR
1	B	99	VAL
1	B	112	LEU
1	B	114	ARG
1	B	115	TRP
1	B	118	HIS
1	B	119	ARG
1	B	125	THR
1	B	126	THR
1	B	134	GLN
1	B	139	ARG
1	B	143	LYS
1	B	149	GLU
1	B	169	ASN
1	B	171	THR
1	B	176	SER
1	B	177	HIS
1	B	179	ILE
1	B	182	VAL
1	B	183	ILE
1	B	192	GLN
1	B	196	LEU
1	B	199	GLU
1	B	202	ASN
1	B	217	VAL
1	B	233	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	236	LEU
1	B	237	GLN
1	B	245	LEU
1	B	246	LYS
1	B	260	HIS
1	B	264	LYS
1	B	279	LYS
1	B	288	GLN
1	B	300	ILE
1	B	302	THR
1	B	303	LYS
1	C	8	LEU
1	C	9	MSE
1	C	10	THR
1	C	14	GLN
1	C	19	GLN
1	C	23	LEU
1	C	24	ARG
1	C	25	ASP
1	C	29	MSE
1	C	30	THR
1	C	34	ASP
1	C	40	LYS
1	C	44	GLU
1	C	56	LEU
1	C	58	LEU
1	C	69	ASN
1	C	73	GLN
1	C	78	GLN
1	C	80	LEU
1	C	82	THR
1	C	101	LYS
1	C	106	ARG
1	C	112	LEU
1	C	115	TRP
1	C	118	HIS
1	C	119	ARG
1	C	126	THR
1	C	134	GLN
1	C	143	LYS
1	C	149	GLU
1	C	158	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	169	ASN
1	C	171	THR
1	C	188	LYS
1	C	196	LEU
1	C	199	GLU
1	C	202	ASN
1	C	218	PHE
1	C	233	GLU
1	C	235	LEU
1	C	237	GLN
1	C	241	ILE
1	C	246	LYS
1	C	249	GLU
1	C	256	ASP
1	C	266	THR
1	C	267	LYS
1	C	272	LYS
1	C	276	THR
1	C	284	LEU
1	C	295	GLU
1	C	298	SER
1	C	301	LEU
1	C	302	THR
1	C	306	ASN
1	C	313	ARG
1	D	8	LEU
1	D	13	LEU
1	D	14	GLN
1	D	17	ARG
1	D	23	LEU
1	D	24	ARG
1	D	25	ASP
1	D	26	SER
1	D	29	MSE
1	D	30	THR
1	D	31	LEU
1	D	35	GLU
1	D	43	ASN
1	D	44	GLU
1	D	56	LEU
1	D	58	LEU
1	D	60	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	69	ASN
1	D	72	ARG
1	D	73	GLN
1	D	76	LEU
1	D	77	GLU
1	D	80	LEU
1	D	83	ASN
1	D	85	GLN
1	D	87	ILE
1	D	99	VAL
1	D	108	LEU
1	D	112	LEU
1	D	114	ARG
1	D	115	TRP
1	D	118	HIS
1	D	119	ARG
1	D	120	ARG
1	D	125	THR
1	D	126	THR
1	D	134	GLN
1	D	137	LYS
1	D	144	LYS
1	D	149	GLU
1	D	158	LYS
1	D	171	THR
1	D	191	VAL
1	D	199	GLU
1	D	201	LEU
1	D	218	PHE
1	D	220	SER
1	D	233	GLU
1	D	234	ASP
1	D	235	LEU
1	D	245	LEU
1	D	247	PHE
1	D	249	GLU
1	D	258	TYR
1	D	264	LYS
1	D	267	LYS
1	D	272	LYS
1	D	279	LYS
1	D	286	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	287	LYS
1	D	295	GLU
1	D	299	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	69	ASN
1	A	73	GLN
1	A	85	GLN
1	A	109	GLN
1	A	154	HIS
1	A	192	GLN
1	A	242	ASN
1	A	261	ASN
1	B	14	GLN
1	B	19	GLN
1	B	169	ASN
1	B	202	ASN
1	B	237	GLN
1	B	260	HIS
1	B	282	ASN
1	C	14	GLN
1	C	18	ASN
1	C	19	GLN
1	C	69	ASN
1	C	85	GLN
1	C	133	ASN
1	C	169	ASN
1	C	202	ASN
1	C	306	ASN
1	D	19	GLN
1	D	43	ASN
1	D	69	ASN
1	D	133	ASN
1	D	154	HIS
1	D	260	HIS
1	D	282	ASN
1	D	306	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ANP	A	401	2	27,33,33	1.67	4 (14%)	30,52,52	2.02	5 (16%)
3	ANP	B	402	2	27,33,33	1.63	6 (22%)	30,52,52	1.98	5 (16%)
3	ANP	C	403	2	27,33,33	1.57	5 (18%)	30,52,52	1.94	4 (13%)
3	ANP	D	404	2	27,33,33	1.57	4 (14%)	30,52,52	1.95	4 (13%)

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	ANP	A	401	2	-	0/12/38/38	0/3/3/3
3	ANP	B	402	2	-	0/12/38/38	0/3/3/3
3	ANP	C	403	2	-	0/12/38/38	0/3/3/3
3	ANP	D	404	2	-	0/12/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ANP	O4'-C1'	-4.60	1.35	1.41
3	B	402	ANP	O4'-C1'	-4.14	1.36	1.41
3	C	403	ANP	O4'-C1'	-3.59	1.36	1.41
3	D	404	ANP	O4'-C1'	-3.52	1.36	1.41
3	C	403	ANP	C6-N6	-2.35	1.27	1.34
3	A	401	ANP	C6-N6	-2.30	1.27	1.34
3	B	402	ANP	C6-N6	-2.27	1.27	1.34
3	B	402	ANP	C2'-C3'	-2.18	1.47	1.53
3	D	404	ANP	C6-N6	-2.08	1.28	1.34
3	B	402	ANP	PG-O2G	-2.04	1.51	1.56
3	D	404	ANP	PG-O2G	-2.01	1.51	1.56
3	C	403	ANP	C2-N1	2.12	1.37	1.33
3	A	401	ANP	C2-N1	2.22	1.38	1.33
3	B	402	ANP	C2-N1	2.29	1.38	1.33
3	C	403	ANP	PB-O3A	2.73	1.62	1.59
3	C	403	ANP	PG-O1G	3.91	1.50	1.46
3	B	402	ANP	PG-O1G	4.42	1.51	1.46
3	A	401	ANP	PG-O1G	4.45	1.51	1.46
3	D	404	ANP	PG-O1G	4.64	1.51	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	ANP	N3-C2-N1	-7.86	122.88	128.89
3	D	404	ANP	N3-C2-N1	-7.81	122.91	128.89
3	A	401	ANP	N3-C2-N1	-7.76	122.95	128.89
3	C	403	ANP	N3-C2-N1	-7.55	123.11	128.89
3	A	401	ANP	O1G-PG-N3B	-4.68	104.72	111.90
3	C	403	ANP	O1G-PG-N3B	-3.98	105.79	111.90
3	D	404	ANP	O1G-PG-N3B	-3.87	105.96	111.90
3	B	402	ANP	O1G-PG-N3B	-3.85	105.99	111.90
3	A	401	ANP	C1'-N9-C4	-2.75	122.79	126.94
3	D	404	ANP	C1'-N9-C4	-2.43	123.28	126.94
3	B	402	ANP	C1'-N9-C4	-2.20	123.63	126.94
3	C	403	ANP	C1'-N9-C4	-2.19	123.64	126.94
3	B	402	ANP	C4'-O4'-C1'	2.11	112.03	109.72
3	A	401	ANP	C4'-O4'-C1'	2.14	112.07	109.72
3	A	401	ANP	C2-N1-C6	3.76	125.49	118.77
3	C	403	ANP	C2-N1-C6	3.82	125.59	118.77
3	D	404	ANP	C2-N1-C6	3.84	125.62	118.77
3	B	402	ANP	C2-N1-C6	3.90	125.74	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	ANP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	305/316 (96%)	-0.25	4 (1%)	79 75	24, 41, 67, 96	0
1	B	303/316 (95%)	-0.38	3 (0%)	84 81	24, 38, 66, 92	0
1	C	303/316 (95%)	-0.35	3 (0%)	84 81	24, 40, 71, 91	0
1	D	303/316 (95%)	-0.23	11 (3%)	46 38	23, 40, 74, 90	0
All	All	1214/1264 (96%)	-0.30	21 (1%)	73 68	23, 40, 71, 96	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	33	GLU	3.7
1	D	28	PRO	3.7
1	C	27	VAL	3.6
1	A	6	GLN	3.3
1	A	7	THR	3.3
1	D	84	GLY	3.1
1	B	25	ASP	3.0
1	D	31	LEU	2.9
1	B	21	ALA	2.8
1	C	34	ASP	2.6
1	D	83	ASN	2.6
1	D	247	PHE	2.5
1	A	119	ARG	2.5
1	B	28	PRO	2.5
1	D	27	VAL	2.4
1	D	26	SER	2.4
1	D	34	ASP	2.4
1	D	32	SER	2.2
1	D	25	ASP	2.1
1	C	21	ALA	2.1
1	A	255	PRO	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	ANP	A	401	31/31	0.97	0.15	0.58	31,40,43,45	0
3	ANP	B	402	31/31	0.98	0.14	0.38	30,39,46,50	0
3	ANP	D	404	31/31	0.97	0.14	0.34	32,42,48,52	0
3	ANP	C	403	31/31	0.97	0.14	0.09	29,39,45,53	0
2	MG	C	503	1/1	0.91	0.22	-	33,33,33,33	0
2	MG	D	504	1/1	0.96	0.23	-	30,30,30,30	0
2	MG	B	502	1/1	0.92	0.20	-	27,27,27,27	0
2	MG	A	501	1/1	0.93	0.31	-	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.