Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 01:57 PM EDT

PDB ID	:	3BN1
Title	:	Crystal structure of GDP-perosamine synthase
Authors	:	Cook, P.D.; Holden, H.M.
Deposited on	:	2007-12-13
Resolution	:	1.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35
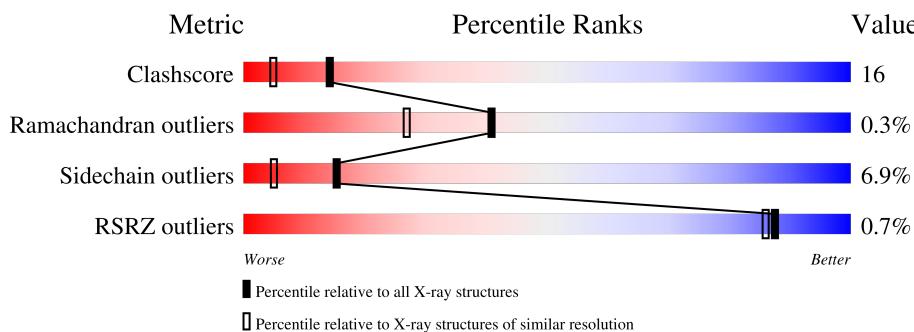
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
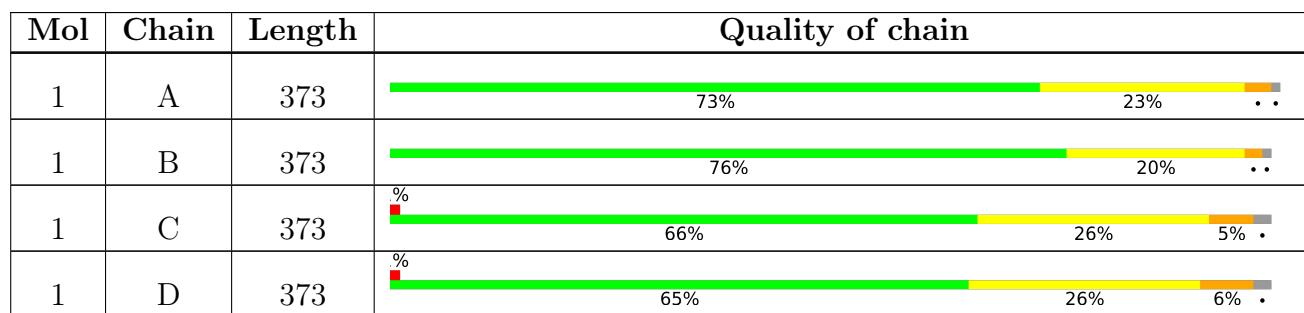
The reported resolution of this entry is 1.80 Å.

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	Percentile Ranks	Value
Clashscore		16
Ramachandran outliers		0.3%
Sidechain outliers		6.9%
RSRZ outliers		0.7%

Worse — *Better*

▉ Percentile relative to all X-ray structures
❑ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	373	73% / 23% / · ·
1	B	373	76% / 20% / · ·
1	C	373	.% / 66% / 26% / 5% ·
1	D	373	.% / 65% / 26% / 6% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	C	372	-	-	X	-
2	ACT	D	372	-	-	X	-

2　Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 12420 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.
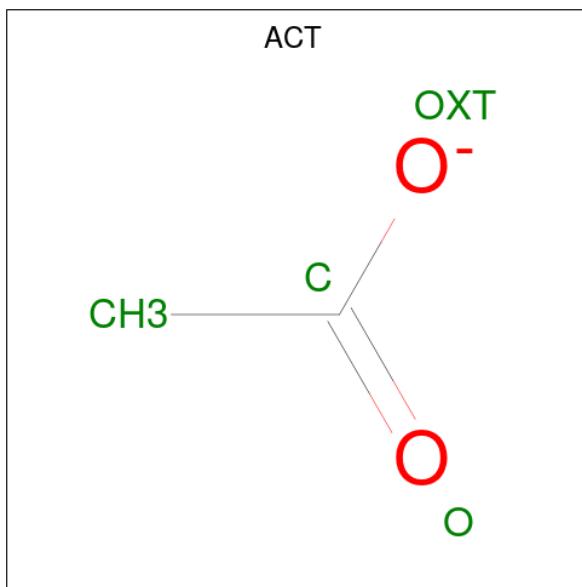
- Molecule 1 is a protein called Perosamine synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	368	Total 2852	C 1800	N 501	O 532	P 1	S 18	0	1	0
1	B	368	Total 2857	C 1806	N 501	O 531	P 1	S 18	0	2	0
1	C	365	Total 2830	C 1789	N 495	O 527	P 1	S 18	0	2	0
1	D	364	Total 2816	C 1777	N 493	O 526	P 1	S 19	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9A9H3
A	0	HIS	-	expression tag	UNP Q9A9H3
A	1	VAL	-	expression tag	UNP Q9A9H3
B	-1	GLY	-	expression tag	UNP Q9A9H3
B	0	HIS	-	expression tag	UNP Q9A9H3
B	1	VAL	-	expression tag	UNP Q9A9H3
C	-1	GLY	-	expression tag	UNP Q9A9H3
C	0	HIS	-	expression tag	UNP Q9A9H3
C	1	VAL	-	expression tag	UNP Q9A9H3
D	-1	GLY	-	expression tag	UNP Q9A9H3
D	0	HIS	-	expression tag	UNP Q9A9H3
D	1	VAL	-	expression tag	UNP Q9A9H3

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O^-

C

CH3

O

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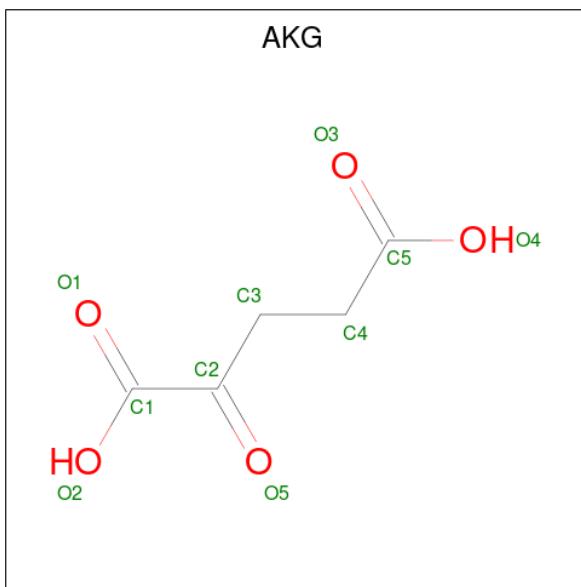
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).

AKG

O3

O

OH O4

O1

O

C5

C3

C2

C4

C1

HO

O

O2

O5

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 10	C 5	O 5	0	0
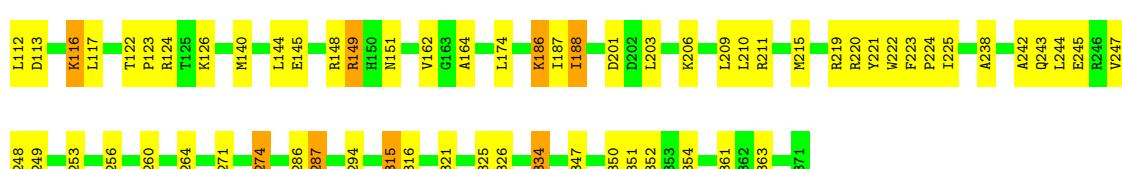
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	304	Total 304	O 304	0	0
5	B	284	Total 284	O 284	0	0
5	C	238	Total 238	O 238	0	0
5	D	216	Total 216	O 216	0	0
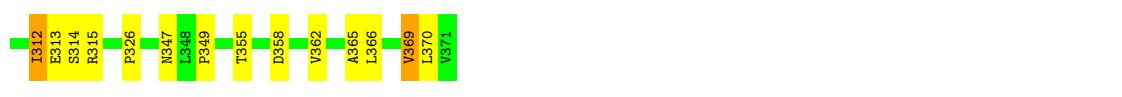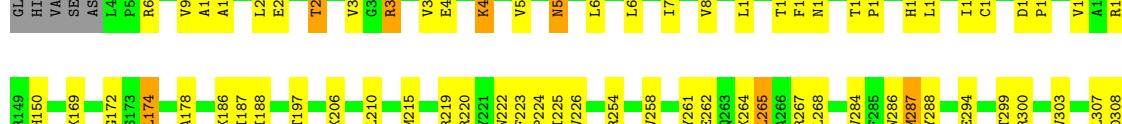
3 Residue-property plots ⓘ

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 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: Perosamine synthetase

Chain A:

• Molecule 1: Perosamine synthetase

Chain B:

• Molecule 1: Perosamine synthetase

Chain C:

Q263 K264 L265 A266 R267 G281 R282 H283 V284 F285 W286 M287 G295 L296 S297 T298 T299 R300 I304 K305 D306 L307 D308 A309 L310 G311 I312 E313 S314 R315 P316 V317 F318 H319 P320 M321 H322 I323 L335 K336 I337 A338 E339 N347 L348 P349 A352 T355 E356 A357 D358 I359 D360

R361 V362 I363 A364 A365 L366 D367 Q368 V369 L370 V371

• Molecule 1: Perosamine synthetase

Chain D:

65%   26%   6% ·

GLY HIS VAL SER ASP LEU PRO ARG ILE S8 V9 A10 A11 P12 R13 Y21 V22 L23 W30 K43 A46 D47 Y48 V51 A54 N58 P75 I80 V81 G97 V101 L102 R108 T109 F110 N111 L112 L117 E118 T122 P123 R124 T125 K126 M129

P130 L133 Q136 I137 C138 D139 M140 D141 P142 I143 L144 E145 R149 H150 N151 E160 G163 Y166 R167 G168 K169 K170 S171 G172 A178 N185 K186 I187 I188 I196 T197 M207 L210 R219 R220 Y221 W222 I225 A238 R246 V247 D248 E249 H250 L251

R254 E255 R256 V257 V258 G259 W260 Y261 E262 Q263 K264 L265 A266 R267 L268 R271 K274 L279 H283 V284 F285 W286 M287 L292 G293 E294 G295 L296 S297 L307 L310 G311 I312 E313 S314 R315 P316 M321 P325 D334 L335 K336 N347 L348 P349 T350 H351 A352

G353 L354 T355 E356 A357 D358 I359 D360 R361 V362 I363 L366 D367 Q368 V369 L370 V371

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.27Å 152.93Å 105.73Å 90.00° 102.09° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 35.48 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-1.80) 98.5 (35.48-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	0.80 (at 1.79Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.176 , 0.253 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	11.5	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 86.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12420	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NA, AKG, LLP, ACT

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	0.85	1/2884 (0.0%)	1.19	11/3920 (0.3%)
1	B	0.81	0/2892	1.18	5/3931 (0.1%)
1	C	0.80	3/2867 (0.1%)	1.14	2/3895 (0.1%)
1	D	0.74	0/2850	1.14	8/3872 (0.2%)
All	All	0.80	4/11493 (0.0%)	1.16	26/15618 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	371	VAL	C-OXT	8.03	1.38	1.23
1	C	371	VAL	CB-CG2	-6.85	1.38	1.52
1	C	295	GLY	C-O	-5.43	1.15	1.23
1	A	164	ALA	CA-CB	5.08	1.63	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	ARG	NE-CZ-NH2	9.19	124.90	120.30
1	B	148	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	D	11	ALA	C-N-CD	-8.68	101.50	120.60
1	C	300	ARG	NE-CZ-NH1	-8.55	116.02	120.30
1	B	148	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	108	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	211	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	287	MET	CG-SD-CE	-7.21	88.66	100.20
1	A	354	LEU	CB-CG-CD1	-7.12	98.89	111.00
1	D	149	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	334	ASP	CB-CG-OD2	5.83	123.54	118.30
1	D	133	LEU	CB-CG-CD1	-5.69	101.32	111.00
1	A	244	LEU	CA-CB-CG	5.63	128.26	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	271	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	D	149	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	B	300	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	D	292	LEU	CB-CG-CD1	5.42	120.22	111.00
1	D	334	ASP	CB-CG-OD1	-5.37	113.46	118.30
1	A	117	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	108	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	29	THR	N-CA-CB	5.31	120.38	110.30
1	A	201	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	211	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	124	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	D	188	ILE	CB-CA-C	5.00	121.61	111.60
1	A	315	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2852	0	2838	72	0
1	B	2857	0	2851	70	0
1	C	2830	0	2825	106	0
1	D	2816	0	2799	109	0
2	A	4	0	3	0	0
2	C	4	0	3	2	0
2	D	4	0	3	3	0
3	A	1	0	0	0	0
4	A	10	0	5	2	0
5	A	304	0	0	1	0
5	B	284	0	0	6	0
5	C	238	0	0	4	0
5	D	216	0	0	6	0
All	All	12420	0	11327	354	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 16.

All (354) 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:206:LYS:HB2	1:C:206:LYS:NZ	1.77	0.99
1:C:359:ILE:HG22	1:C:363:ILE:HD11	1.51	0.92
1:D:219:ARG:HG2	1:D:222:TRP:CB	2.02	0.90
1:C:36:ARG:HH21	1:C:36:ARG:HG3	1.37	0.89
1:A:149:ARG:HG2	1:A:149:ARG:HH21	1.43	0.83
1:D:287[A]:MET:HG2	1:D:347:ASN:HB3	1.63	0.80
1:D:262:GLU:HG2	5:D:607:HOH:O	1.83	0.79
1:C:260:TRP:O	1:C:264:LYS:HG3	1.82	0.79
1:B:264:LYS:O	1:B:267:ARG:HG3	1.83	0.78
1:C:359:ILE:O	1:C:363:ILE:HD12	1.81	0.78
1:C:355:THR:HG23	1:C:358:ASP:OD2	1.84	0.77
1:C:264:LYS:HE2	1:C:360:ASP:OD1	1.85	0.77
1:D:219:ARG:HG2	1:D:222:TRP:HB3	1.65	0.77
1:C:186:LLP:H4'1	2:C:372:ACT:H1	1.67	0.76
1:A:287:MET:HE1	1:A:315:ARG:HD3	1.68	0.75
1:B:224:PRO:O	1:B:225[A]:ILE:HG13	1.88	0.74
1:D:219:ARG:HD2	5:D:637:HOH:O	1.88	0.73
1:D:268:LEU:HA	1:D:271:ARG:HH11	1.51	0.73
1:D:307:LEU:HD21	1:D:369:VAL:HG21	1.69	0.73
1:D:219:ARG:HG2	1:D:222:TRP:HB2	1.71	0.72
1:B:315:ARG:HG3	1:B:347:ASN:HD22	1.53	0.72
1:C:20:ASP:OD1	1:C:20:ASP:C	2.27	0.72
1:A:18:GLU:HG3	1:A:242:ALA:HB3	1.72	0.72
1:B:36:ARG:O	1:B:40:GLU:HG3	1.89	0.71
1:C:319:HIS:HB3	1:C:323:ILE:HD11	1.73	0.71
1:C:359:ILE:HG22	1:C:363:ILE:CD1	2.21	0.71
1:B:312:ILE:HD12	1:B:362:VAL:HA	1.73	0.71
1:D:279:LEU:N	1:D:279:LEU:HD23	2.06	0.70
1:B:219:ARG:HG2	1:B:222:TRP:CB	2.21	0.69
1:C:286:TRP:O	1:C:287:MET:HG2	1.90	0.69
1:D:58:ASN:H	1:D:58:ASN:HD22	1.39	0.69
1:C:264:LYS:HD3	1:C:363:ILE:HD13	1.74	0.69
1:D:13:ARG:HD2	1:D:352:ALA:HB3	1.76	0.68
1:D:13:ARG:HD2	1:D:352:ALA:CB	2.23	0.68
1:A:220:ARG:HG2	1:A:220:ARG:HH11	1.57	0.67
1:B:219:ARG:HG2	1:B:222:TRP:HB3	1.76	0.67
1:C:300:ARG:HD2	1:C:304:ILE:HD12	1.77	0.67
1:C:162:VAL:HG11	1:C:188[B]:ILE:HD12	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LYS:HD3	5:C:549:HOH:O	1.94	0.66
1:D:145:GLU:OE1	1:D:149:ARG:NH2	2.28	0.66
1:D:310:LEU:N	1:D:310:LEU:HD23	2.11	0.66
1:D:296:LEU:HD13	1:D:370:LEU:HD22	1.77	0.66
1:A:264:LYS:HB2	1:A:363:ILE:HD13	1.79	0.65
1:C:365:ALA:O	1:C:369:VAL:HG22	1.95	0.65
1:D:246:ARG:HH21	1:D:246:ARG:HB3	1.62	0.65
1:B:36:ARG:HD2	1:B:40:GLU:OE2	1.96	0.65
1:B:224:PRO:C	1:B:225[A]:ILE:HG13	2.17	0.64
1:A:28:THR:O	1:A:29[B]:THR:HG22	1.98	0.64
1:D:118:GLU:OE2	1:D:150:HIS:NE2	2.27	0.64
1:D:169:LYS:NZ	5:D:669:HOH:O	2.30	0.64
1:D:313:GLU:O	1:D:349:PRO:HG3	1.98	0.64
1:B:172:GLY:HA2	1:B:178:ALA:CB	2.28	0.63
1:D:81:VAL:O	1:D:102:LEU:HA	1.97	0.63
1:D:355:THR:O	1:D:358:ASP:HB2	1.97	0.63
1:C:206:LYS:HB2	1:C:206:LYS:HZ2	1.64	0.63
1:C:206:LYS:HB2	1:C:206:LYS:HZ1	1.64	0.63
1:B:73:ILE:HD13	1:B:73:ILE:N	2.14	0.63
1:D:220:ARG:HD3	1:D:221:TYR:CE2	2.33	0.63
1:D:58:ASN:HD22	1:D:58:ASN:N	1.95	0.62
1:D:141:ASP:HB2	1:D:142:PRO:HD3	1.82	0.62
1:C:312:ILE:HD11	1:C:361:ARG:HD2	1.80	0.62
1:A:274:LYS:NZ	1:A:274:LYS:HB3	2.15	0.62
1:C:36:ARG:HH21	1:C:36:ARG:CG	2.11	0.62
1:A:162:VAL:CG1	1:A:187:ILE:HB	2.30	0.61
1:D:187:ILE:HG22	1:D:188:ILE:HG23	1.82	0.61
1:A:249:GLU:OE1	1:A:249:GLU:N	2.26	0.61
1:D:220:ARG:HD3	1:D:221:TYR:CZ	2.36	0.60
1:A:220:ARG:HH11	1:A:220:ARG:CG	2.14	0.60
1:A:162:VAL:HG12	1:A:187:ILE:HB	1.82	0.60
1:D:46:ALA:HB2	1:D:54:ALA:HB2	1.82	0.60
1:D:321:MET:HA	1:D:321:MET:CE	2.32	0.60
1:A:116:LYS:HE2	1:A:334:ASP:OD2	2.02	0.60
1:C:254:ARG:HD3	1:C:285:PHE:O	2.02	0.60
1:C:13:ARG:HG3	1:C:13:ARG:HH11	1.66	0.60
1:A:219:ARG:HG2	1:A:222:TRP:HB2	1.84	0.59
1:C:30:TRP:HZ3	1:C:34:VAL:HG12	1.68	0.59
1:C:23:LEU:HD11	1:D:23:LEU:HD21	1.85	0.59
1:D:336:LYS:HD2	5:D:734:HOH:O	2.01	0.59
1:A:188:ILE:HD12	1:A:243:GLN:HB3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:TRP:CZ3	1:C:34:VAL:HG12	2.38	0.59
1:A:36:ARG:O	1:A:39:VAL:HG12	2.04	0.58
1:D:160:GLU:HG2	1:D:286:TRP:CE3	2.38	0.58
1:A:58:ASN:N	1:A:58:ASN:HD22	1.99	0.58
1:B:303:VAL:HG13	1:B:369:VAL:CG2	2.34	0.58
1:D:264:LYS:NZ	1:D:356:GLU:OE2	2.36	0.58
1:D:260:TRP:CD1	1:D:356:GLU:HG3	2.39	0.58
1:D:351:HIS:CD2	1:D:354:LEU:HG	2.38	0.58
1:D:258:VAL:O	1:D:262:GLU:HG3	2.04	0.57
1:A:58:ASN:HD22	1:A:58:ASN:H	1.52	0.57
1:A:245:GLU:OE2	5:A:626:HOH:O	2.17	0.57
1:C:136:GLN:HB2	1:C:283:HIS:CD2	2.40	0.57
1:D:21:TYR:HB3	1:D:238:ALA:HB1	1.87	0.57
1:D:307:LEU:HB3	1:D:312:ILE:HB	1.87	0.57
1:B:9:VAL:HA	1:B:349:PRO:HA	1.87	0.56
1:B:313:GLU:O	1:B:349:PRO:HG3	2.05	0.56
1:D:172:GLY:HA2	1:D:178:ALA:CB	2.35	0.56
1:D:321:MET:HA	1:D:321:MET:HE2	1.87	0.56
1:A:4:LEU:O	1:A:4:LEU:HG	2.04	0.56
1:C:105:ASN:HD21	1:C:338:ALA:HA	1.69	0.56
1:B:122:THR:HB	1:B:123:PRO:CD	2.35	0.56
1:C:313:GLU:O	1:C:349:PRO:HG3	2.06	0.56
1:A:149:ARG:HG2	1:A:149:ARG:NH2	2.16	0.56
1:D:296:LEU:CD1	1:D:370:LEU:HD22	2.36	0.56
1:A:4:LEU:N	1:A:4:LEU:HD23	2.20	0.56
1:B:9:VAL:HG23	1:B:313:GLU:O	2.05	0.56
1:C:310:LEU:N	1:C:310:LEU:HD12	2.21	0.56
1:C:361:ARG:O	1:C:364:ALA:HB3	2.06	0.56
1:C:30:TRP:HZ3	1:C:34:VAL:CG1	2.19	0.56
1:C:359:ILE:C	1:C:363:ILE:HD12	2.26	0.55
1:A:58:ASN:H	1:A:58:ASN:ND2	2.04	0.55
1:C:306:ASP:O	1:C:309:ALA:N	2.39	0.55
1:A:253:ALA:HA	1:A:256:ARG:NH2	2.21	0.55
1:A:67:ALA:O	1:A:71:MET:HG3	2.07	0.55
1:C:9:VAL:N	1:C:313:GLU:HG2	2.21	0.55
1:D:315:ARG:HB2	1:D:316:PRO:HD2	1.88	0.55
1:B:254:ARG:O	1:B:258:VAL:HG23	2.07	0.54
1:C:315:ARG:HB2	1:C:316:PRO:HD2	1.88	0.54
1:C:337:ILE:N	1:C:337:ILE:HD13	2.21	0.54
1:C:121:ILE:HD13	1:C:152:LEU:HD11	1.88	0.54
1:C:81:VAL:O	1:C:102:LEU:HA	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LYS:NZ	5:C:584:HOH:O	2.29	0.54
1:A:219:ARG:HG2	1:A:222:TRP:CB	2.38	0.54
1:D:366:LEU:HA	1:D:369:VAL:HG22	1.88	0.54
1:D:9:VAL:HB	1:D:313:GLU:HG2	1.89	0.53
1:C:18:GLU:HG3	1:C:242:ALA:HB3	1.89	0.53
1:C:309:ALA:HB3	1:C:310:LEU:HD12	1.91	0.53
1:D:310:LEU:O	1:D:361:ARG:NH2	2.37	0.53
1:A:315:ARG:HB2	1:A:316:PRO:HD2	1.90	0.53
1:C:75:PRO:HA	1:C:97:GLY:O	2.09	0.53
1:D:58:ASN:H	1:D:58:ASN:ND2	2.06	0.53
1:D:371:VAL:OXT	1:D:371:VAL:HG12	2.08	0.53
1:A:29[B]:THR:HG23	1:A:29[B]:THR:O	2.08	0.53
1:D:220:ARG:HH11	1:D:220:ARG:CG	2.21	0.53
1:C:254:ARG:NH2	1:C:286:TRP:O	2.41	0.52
1:C:9:VAL:H	1:C:313:GLU:HG2	1.73	0.52
1:C:283:HIS:CE1	1:C:285:PHE:H	2.28	0.52
1:A:66:LEU:HD11	1:A:210:LEU:HB2	1.92	0.52
1:D:51:VAL:HG21	1:D:197:THR:HB	1.91	0.52
1:D:355:THR:O	1:D:359:ILE:HG12	2.10	0.52
1:C:43[B]:LYS:HD2	1:C:47:ASP:OD1	2.10	0.52
1:A:21:TYR:HB3	1:A:238:ALA:HB1	1.90	0.52
1:D:186:LLP:H4'1	2:D:372:ACT:H3	1.92	0.52
1:D:210:LEU:CD2	1:D:225:ILE:HD12	2.40	0.52
1:D:117:LEU:O	1:D:118:GLU:C	2.46	0.52
1:B:39:VAL:HG22	1:B:40:GLU:N	2.26	0.52
1:B:225[A]:ILE:HG23	5:B:722:HOH:O	2.09	0.51
1:A:220:ARG:NH1	1:A:221:TYR:CE1	2.78	0.51
1:B:81:VAL:O	1:B:102:LEU:HA	2.09	0.51
1:C:206:LYS:NZ	1:C:206:LYS:CB	2.63	0.51
1:C:306:ASP:O	1:C:307:LEU:C	2.48	0.51
1:A:315:ARG:NH2	4:A:374:AKG:O2	2.43	0.51
1:C:109:THR:O	1:C:110:PHE:HB2	2.11	0.51
1:C:295:GLY:O	1:C:296:LEU:C	2.49	0.51
1:A:144:LEU:O	1:A:148:ARG:HG3	2.10	0.51
1:B:6:ARG:HH22	1:B:308:ASP:HA	1.76	0.51
1:D:9:VAL:HA	1:D:349:PRO:HB3	1.93	0.51
1:A:220:ARG:CG	1:A:220:ARG:NH1	2.73	0.50
1:C:253:ALA:CB	1:C:352:ALA:HB1	2.41	0.50
1:D:163:GLY:HA3	1:D:251:LEU:HD11	1.94	0.50
1:B:366:LEU:HD22	1:B:370:LEU:HD11	1.93	0.50
1:C:295:GLY:O	1:C:296:LEU:O	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LEU:HB3	1:B:312:ILE:HB	1.93	0.50
1:C:219:ARG:HG2	1:C:222:TRP:CB	2.41	0.50
1:D:9:VAL:H	1:D:313:GLU:HG2	1.76	0.50
1:D:220:ARG:CG	1:D:220:ARG:NH1	2.73	0.50
1:C:220:ARG:HD3	1:C:221:TYR:CZ	2.47	0.49
1:C:306:ASP:O	1:C:310:LEU:HD13	2.12	0.49
1:D:139:ASP:O	1:D:142:PRO:HD2	2.11	0.49
1:D:315:ARG:HB2	1:D:316:PRO:CD	2.42	0.49
1:B:169:LYS:HD2	1:B:174:LEU:CD2	2.42	0.49
1:C:355:THR:OG1	1:C:357:ALA:HB3	2.12	0.49
1:C:186:LLP:OP3	2:C:372:ACT:OXT	2.29	0.49
1:D:187:ILE:HD11	1:D:286:TRP:HA	1.94	0.49
1:B:51:VAL:HG21	1:B:197:THR:HB	1.93	0.49
1:D:124:ARG:HG3	1:D:124:ARG:NH2	2.27	0.49
1:A:58:ASN:N	1:A:58:ASN:ND2	2.61	0.48
1:A:112:LEU:C	1:A:112:LEU:HD23	2.34	0.48
1:D:260:TRP:CG	1:D:356:GLU:HG3	2.48	0.48
1:B:312:ILE:CD1	1:B:362:VAL:HA	2.41	0.48
1:D:122:THR:HB	1:D:123:PRO:HD2	1.95	0.48
1:D:250:HIS:O	1:D:254:ARG:HG3	2.12	0.48
1:B:109:THR:O	1:B:110:PHE:HB2	2.14	0.48
1:B:299:THR:O	1:B:303:VAL:HG23	2.14	0.48
1:C:252:ALA:O	1:C:255:GLU:HB2	2.14	0.48
1:A:10:ALA:O	1:A:11:ALA:HB2	2.14	0.48
1:B:219:ARG:HG2	1:B:222:TRP:HB2	1.94	0.48
1:C:310:LEU:N	1:C:310:LEU:CD1	2.76	0.48
1:A:149:ARG:NH2	1:A:149:ARG:CG	2.76	0.48
1:C:36:ARG:CG	1:C:36:ARG:NH2	2.75	0.48
1:B:365:ALA:O	1:B:369:VAL:HG13	2.13	0.48
1:D:166:TYR:CD1	1:D:167:ARG:HG3	2.49	0.48
1:D:185:ASN:OD1	1:D:185:ASN:C	2.51	0.48
1:A:81:VAL:O	1:A:102:LEU:HA	2.13	0.47
1:B:315:ARG:HG3	1:B:347:ASN:HB2	1.95	0.47
1:D:137:ILE:HD11	1:D:171:SER:HB3	1.95	0.47
1:C:18:GLU:O	1:C:22:VAL:HG23	2.14	0.47
1:C:138:CYS:O	1:C:140:MET:HG2	2.14	0.47
1:D:287[B]:MET:HE2	1:D:287[B]:MET:HB2	1.79	0.47
1:B:122:THR:HB	1:B:123:PRO:HD2	1.97	0.47
1:C:317:VAL:O	1:C:318:PHE:C	2.52	0.47
1:B:24:GLU:OE1	1:B:36:ARG:NH1	2.44	0.47
1:C:267:ARG:HH22	1:C:364:ALA:HA	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ARG:HD2	1:D:352:ALA:HB1	1.94	0.47
1:C:315:ARG:HG3	1:C:347:ASN:HB2	1.97	0.46
1:D:80:ILE:HA	1:D:101:VAL:O	2.15	0.46
1:D:260:TRP:O	1:D:264:LYS:HG3	2.15	0.46
1:A:264:LYS:HB2	1:A:363:ILE:CD1	2.44	0.46
1:B:24:GLU:CD	1:B:36:ARG:HH11	2.19	0.46
1:B:169:LYS:HD2	1:B:174:LEU:HD23	1.98	0.46
1:C:186:LLP:O	1:C:187:ILE:C	2.53	0.46
1:A:13:ARG:HD3	1:A:352:ALA:HB3	1.97	0.46
1:D:122:THR:HB	1:D:123:PRO:CD	2.46	0.46
1:C:67:ALA:O	1:C:71:MET:HG3	2.16	0.46
1:C:210:LEU:HD23	1:C:225:ILE:CD1	2.45	0.46
1:A:315:ARG:HB2	1:A:316:PRO:CD	2.46	0.46
1:B:141:ASP:HB2	1:B:142:PRO:CD	2.46	0.46
1:D:210:LEU:HD21	1:D:225:ILE:HD12	1.97	0.46
1:D:321:MET:CE	1:D:321:MET:CA	2.93	0.46
1:A:30:TRP:CZ3	1:A:34:VAL:HG23	2.51	0.46
1:A:223:PHE:O	1:B:326:PRO:HD3	2.15	0.46
1:B:169:LYS:HD3	5:B:914:HOH:O	2.15	0.46
1:C:83:SER:O	1:C:321:MET:HG2	2.15	0.46
1:D:186:LLP:OP3	2:D:372:ACT:O	2.34	0.46
1:D:268:LEU:HA	1:D:271:ARG:NH1	2.26	0.46
1:B:137:ILE:HG22	1:B:138:CYS:O	2.16	0.46
1:D:9:VAL:CB	1:D:313:GLU:HG2	2.45	0.45
1:D:351:HIS:NE2	1:D:354:LEU:CD2	2.79	0.45
1:B:111:ASN:OD1	1:B:133:LEU:HB2	2.16	0.45
1:B:141:ASP:N	1:B:142:PRO:HD2	2.31	0.45
1:A:30:TRP:HZ3	1:A:34:VAL:CG2	2.30	0.45
1:B:262:GLU:OE2	1:B:288:TYR:OH	2.18	0.45
1:A:21:TYR:OH	1:A:245:GLU:OE2	2.27	0.45
1:B:303:VAL:HG13	1:B:369:VAL:HG23	1.98	0.45
1:C:306:ASP:O	1:C:309:ALA:HB3	2.17	0.45
1:D:307:LEU:CD2	1:D:369:VAL:HG21	2.45	0.45
1:A:4:LEU:N	1:A:4:LEU:CD2	2.79	0.45
1:B:210:LEU:HD21	1:B:225[B]:ILE:HD12	1.99	0.45
1:D:112:LEU:C	1:D:112:LEU:HD23	2.37	0.45
1:D:166:TYR:CE1	1:D:167:ARG:HG3	2.52	0.45
1:A:99:THR:HA	1:A:100:PRO:HD3	1.78	0.45
1:B:141:ASP:HB2	1:B:142:PRO:HD3	1.99	0.45
1:D:294:GLU:O	1:D:294:GLU:HG3	2.17	0.45
1:A:37:PHE:CD2	1:A:238:ALA:HB2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASP:CB	1:B:142:PRO:CD	2.95	0.45
1:B:223:PHE:CD1	1:B:223:PHE:N	2.84	0.45
1:B:225[A]:ILE:HG22	1:B:226:VAL:N	2.32	0.45
1:D:261:TYR:O	1:D:265:LEU:HB2	2.16	0.45
1:D:136:GLN:HB2	1:D:283:HIS:CD2	2.52	0.45
1:B:172:GLY:HA2	1:B:178:ALA:HB3	1.98	0.44
1:B:215:MET:HE3	5:B:765:HOH:O	2.17	0.44
1:D:297:SER:H	1:D:371:VAL:C	2.19	0.44
1:C:335:LEU:O	1:C:339:GLU:HG3	2.17	0.44
1:A:10:ALA:HA	1:A:351:HIS:HB3	1.99	0.44
1:A:325:PRO:HB2	1:A:326:PRO:HD3	1.99	0.44
1:B:64:LEU:O	1:B:68:LEU:HG	2.18	0.44
1:C:23:LEU:HD23	1:C:23:LEU:HA	1.67	0.44
1:C:300:ARG:HD2	1:C:304:ILE:CD1	2.43	0.44
1:B:261:TYR:O	1:B:265:LEU:HD23	2.17	0.44
1:B:315:ARG:NH2	5:B:798:HOH:O	2.50	0.44
1:D:265:LEU:HD12	1:D:363:ILE:HD11	1.98	0.44
1:A:36:ARG:CG	1:A:37:PHE:N	2.80	0.44
1:C:9:VAL:HA	1:C:349:PRO:HA	1.99	0.44
1:C:36:ARG:HG2	5:C:517:HOH:O	2.18	0.44
1:B:146:VAL:O	1:B:150:HIS:HD2	2.01	0.44
1:D:109:THR:O	1:D:110:PHE:HB2	2.17	0.44
1:D:370:LEU:HA	1:D:370:LEU:HD23	1.47	0.44
1:A:112:LEU:HD23	1:A:113:ASP:N	2.33	0.43
1:C:141:ASP:N	1:C:142:PRO:HD2	2.33	0.43
1:C:298:THR:HG22	1:C:371:VAL:OXT	2.18	0.43
1:C:307:LEU:HD23	1:C:307:LEU:HA	1.78	0.43
1:D:75:PRO:HA	1:D:97:GLY:O	2.18	0.43
1:A:4:LEU:HD12	1:A:361:ARG:NH2	2.34	0.43
1:A:80:ILE:HA	1:A:101:VAL:O	2.18	0.43
1:B:39:VAL:CG2	1:B:40:GLU:N	2.79	0.43
1:C:21:TYR:HB3	1:C:238:ALA:HB1	1.99	0.43
1:C:222:TRP:CZ2	1:D:325:PRO:HD3	2.54	0.43
1:D:141:ASP:N	1:D:142:PRO:CD	2.81	0.43
1:D:350:THR:O	1:D:351:HIS:HB3	2.18	0.43
1:D:139:ASP:O	1:D:143:ILE:HG13	2.18	0.43
1:D:187:ILE:HD12	5:D:689:HOH:O	2.18	0.43
1:D:219:ARG:CG	1:D:222:TRP:HB2	2.44	0.43
1:D:256:ARG:HD2	1:D:260:TRP:CZ2	2.54	0.43
1:C:247:VAL:HG13	1:C:248:ASP:N	2.33	0.43
1:C:13:ARG:HH11	1:C:13:ARG:CG	2.29	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ALA:O	1:C:360:ASP:HB2	2.19	0.43
1:C:253:ALA:HB3	1:C:352:ALA:CB	2.49	0.42
1:D:283:HIS:CE1	1:D:285:PHE:H	2.37	0.42
1:C:206:LYS:HZ2	1:C:206:LYS:CB	2.29	0.42
1:D:210:LEU:CD2	1:D:225:ILE:CD1	2.97	0.42
1:C:9:VAL:HG23	1:C:313:GLU:O	2.18	0.42
1:A:215:MET:HB2	1:A:223:PHE:CE1	2.53	0.42
1:B:264:LYS:HG2	1:B:267:ARG:NH2	2.34	0.42
1:C:219:ARG:HG2	1:C:222:TRP:HB3	2.02	0.42
1:D:30:TRP:N	1:D:30:TRP:CD1	2.87	0.42
1:D:336:LYS:HE3	5:D:682:HOH:O	2.18	0.42
1:A:286:TRP:C	1:A:287:MET:HG2	2.38	0.42
1:C:48:TYR:CZ	1:C:170:LYS:HE2	2.54	0.42
1:C:210:LEU:HD23	1:C:225:ILE:HD12	2.00	0.42
1:D:263:GLN:HG2	1:D:264:LYS:HG2	2.00	0.42
1:A:71:MET:HG2	1:A:203:LEU:HD11	2.02	0.42
1:A:223:PHE:HA	1:A:224:PRO:HD2	1.82	0.42
1:B:223:PHE:HA	1:B:224:PRO:HD2	1.88	0.42
1:D:186:LLP:H4'1	2:D:372:ACT:CH3	2.49	0.42
1:B:34:VAL:HG23	1:B:34:VAL:O	2.19	0.42
1:B:132:HIS:CE1	1:B:137:ILE:HG23	2.55	0.42
1:D:129:MET:HA	1:D:130:PRO:HD2	1.88	0.42
1:B:219:ARG:HD2	5:B:916:HOH:O	2.19	0.41
1:B:355:THR:O	1:B:358:ASP:HB2	2.20	0.41
1:C:172:GLY:HA2	1:C:178:ALA:CB	2.50	0.41
1:C:219:ARG:HG2	1:C:222:TRP:HB2	2.01	0.41
1:C:355:THR:O	1:C:358:ASP:HB2	2.20	0.41
1:C:247:VAL:CG1	1:C:248:ASP:N	2.83	0.41
1:C:355:THR:OG1	1:C:358:ASP:N	2.50	0.41
1:A:75:PRO:HA	1:A:97:GLY:O	2.20	0.41
1:C:306:ASP:HB3	1:C:369:VAL:HG11	2.02	0.41
1:A:209:LEU:HG	1:A:225:ILE:HD11	2.03	0.41
1:C:165:THR:O	1:C:281:GLY:HA3	2.20	0.41
1:D:122:THR:CB	1:D:123:PRO:CD	2.98	0.41
1:A:25:CYS:HB3	1:A:30:TRP:O	2.20	0.41
1:D:247:VAL:HG13	1:D:248:ASP:N	2.36	0.41
1:A:30:TRP:CZ3	1:A:34:VAL:CG2	3.04	0.41
1:A:140:MET:HG3	1:A:174:LEU:HD13	2.02	0.41
1:B:268:LEU:HD23	1:B:268:LEU:HA	1.75	0.41
1:B:286:TRP:C	1:B:287:MET:HG2	2.39	0.41
1:A:106:ASP:OD2	1:A:108:ARG:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:THR:HB	1:A:123:PRO:HD2	2.03	0.41
1:A:321:MET:CE	1:A:321:MET:HA	2.51	0.41
1:B:10:ALA:O	1:B:11:ALA:HB2	2.20	0.41
1:B:188:ILE:HD13	1:B:188:ILE:HG21	1.83	0.41
1:C:359:ILE:O	1:C:360:ASP:C	2.59	0.41
1:B:23:LEU:HA	1:B:23:LEU:HD23	1.74	0.41
1:B:58:ASN:H	1:B:58:ASN:HD22	1.68	0.41
1:B:9:VAL:CG2	1:B:314:SER:HA	2.51	0.41
1:C:284:VAL:O	1:C:285:PHE:C	2.59	0.41
1:A:145:GLU:OE2	1:A:149:ARG:NE	2.36	0.40
1:A:247:VAL:HG13	1:A:248:ASP:N	2.35	0.40
1:C:265:LEU:HA	1:C:265:LEU:HD23	1.70	0.40
1:A:286:TRP:O	1:A:287:MET:HG2	2.21	0.40
1:A:315:ARG:HG2	1:A:347:ASN:HB2	2.03	0.40
1:C:9:VAL:CG2	1:C:314:SER:HA	2.51	0.40
1:C:223:PHE:HA	1:C:224:PRO:HD2	1.83	0.40
1:C:253:ALA:CB	1:C:352:ALA:CB	3.00	0.40
1:D:9:VAL:HG23	1:D:313:GLU:HG2	2.02	0.40
1:C:118:GLU:HG3	5:C:499:HOH:O	2.21	0.40
1:D:23:LEU:HA	1:D:23:LEU:HD23	1.77	0.40
1:D:48:TYR:CZ	1:D:170:LYS:HE2	2.56	0.40
1:D:178:ALA:HB3	1:D:197:THR:OG1	2.21	0.40
1:A:186:LLP:OP3	4:A:374:AKG:O3	2.39	0.40
1:B:43:LYS:HG2	5:B:873:HOH:O	2.20	0.40
1:D:196:ILE:HG21	1:D:207:MET:HE2	2.03	0.40
1:A:260:TRP:O	1:A:264:LYS:HG3	2.21	0.40
1:B:187:ILE:CD1	1:B:284:VAL:HG23	2.51	0.40
1:C:48:TYR:CE1	1:C:247:VAL:HG11	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/373 (98%)	357 (98%)	8 (2%)	1 (0%)	41	27
1	B	367/373 (98%)	352 (96%)	15 (4%)	0	100	100
1	C	364/373 (98%)	343 (94%)	18 (5%)	3 (1%)	19	7
1	D	362/373 (97%)	342 (94%)	19 (5%)	1 (0%)	41	27
All	All	1459/1492 (98%)	1394 (96%)	60 (4%)	5 (0%)	41	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	296	LEU
1	C	352	ALA
1	A	11	ALA
1	C	318	PHE
1	D	12	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/301 (99%)	282 (95%)	16 (5%)	22	9
1	B	299/301 (99%)	288 (96%)	11 (4%)	34	19
1	C	296/301 (98%)	270 (91%)	26 (9%)	10	3
1	D	294/301 (98%)	265 (90%)	29 (10%)	8	2
All	All	1187/1204 (99%)	1105 (93%)	82 (7%)	15	5

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	8	SER
1	A	36	ARG
1	A	43	LYS
1	A	52	LYS
1	A	58	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	116	LYS
1	A	126	LYS
1	A	149	ARG
1	A	151	ASN
1	A	188	ILE
1	A	206	LYS
1	A	274	LYS
1	A	287	MET
1	A	294	GLU
1	A	350	THR
1	B	29	THR
1	B	36	ARG
1	B	43	LYS
1	B	58	ASN
1	B	174	LEU
1	B	206	LYS
1	B	220	ARG
1	B	265	LEU
1	B	294	GLU
1	B	312	ILE
1	B	369	VAL
1	C	9	VAL
1	C	20	ASP
1	C	29	THR
1	C	36	ARG
1	C	52	LYS
1	C	126	LYS
1	C	145	GLU
1	C	148	ARG
1	C	170	LYS
1	C	174	LEU
1	C	206	LYS
1	C	246	ARG
1	C	254	ARG
1	C	256	ARG
1	C	262	GLU
1	C	264	LYS
1	C	265	LEU
1	C	283	HIS
1	C	296	LEU
1	C	297	SER
1	C	299	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	310	LEU
1	C	313	GLU
1	C	320	PRO
1	C	361	ARG
1	C	367	ASP
1	D	9	VAL
1	D	43	LYS
1	D	58	ASN
1	D	126	LYS
1	D	145	GLU
1	D	151	ASN
1	D	167	ARG
1	D	187	ILE
1	D	188	ILE
1	D	220	ARG
1	D	246	ARG
1	D	254	ARG
1	D	255	GLU
1	D	256	ARG
1	D	263	GLN
1	D	265	LEU
1	D	267	ARG
1	D	274	LYS
1	D	279	LEU
1	D	283	HIS
1	D	287[A]	MET
1	D	287[B]	MET
1	D	292	LEU
1	D	294	GLU
1	D	297	SER
1	D	310	LEU
1	D	312	ILE
1	D	361	ARG
1	D	368	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	B	58	ASN
1	B	150	HIS
1	B	218	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	347	ASN
1	C	91	ASN
1	C	105	ASN
1	C	263	GLN
1	D	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	LLP	B	186	1	23,24,25	1.31	4 (17%)	25,32,34	1.56	6 (24%)
1	LLP	D	186	1	23,24,25	1.09	2 (8%)	25,32,34	1.57	6 (24%)
1	LLP	C	186	1	23,24,25	1.33	3 (13%)	25,32,34	2.15	8 (32%)
1	LLP	A	186	1	23,24,25	1.13	1 (4%)	25,32,34	1.69	8 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	B	186	1	-	5/16/17/19	0/1/1/1
1	LLP	D	186	1	-	5/16/17/19	0/1/1/1
1	LLP	C	186	1	-	5/16/17/19	0/1/1/1
1	LLP	A	186	1	-	5/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	LLP	C4-C5	2.93	1.45	1.42
1	A	186	LLP	P-OP1	2.84	1.59	1.50
1	D	186	LLP	P-OP1	2.71	1.59	1.50
1	C	186	LLP	P-OP1	2.60	1.58	1.50
1	C	186	LLP	C3-C2	-2.47	1.38	1.40
1	C	186	LLP	C4-C4'	2.33	1.51	1.46
1	B	186	LLP	P-OP1	2.28	1.57	1.50
1	B	186	LLP	C3-C2	-2.16	1.38	1.40
1	B	186	LLP	C4-C4'	2.05	1.50	1.46
1	D	186	LLP	C4-C4'	2.01	1.50	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	LLP	C4-C3-C2	5.60	123.65	120.19
1	C	186	LLP	C3-C4-C5	-4.91	114.49	118.26
1	C	186	LLP	CE-NZ-C4'	3.58	129.89	118.90
1	B	186	LLP	CE-NZ-C4'	3.41	129.37	118.90
1	A	186	LLP	CE-NZ-C4'	3.37	129.25	118.90
1	A	186	LLP	OP4-C5'-C5	3.33	115.70	109.35
1	D	186	LLP	C3-C4-C5	-3.32	115.71	118.26
1	A	186	LLP	CD-CG-CB	3.11	124.64	113.62
1	D	186	LLP	CE-NZ-C4'	3.06	128.29	118.90
1	C	186	LLP	CD-CG-CB	3.01	124.29	113.62
1	D	186	LLP	C2'-C2-C3	-2.99	117.19	120.89
1	B	186	LLP	C3-C4-C5	-2.77	116.14	118.26
1	C	186	LLP	C5-C4-C4'	2.69	125.98	121.56
1	C	186	LLP	C2'-C2-C3	-2.60	117.68	120.89
1	B	186	LLP	CD-CG-CB	2.55	122.66	113.62
1	A	186	LLP	O3-C3-C2	2.52	122.99	117.49
1	B	186	LLP	C5-C4-C4'	2.45	125.59	121.56
1	B	186	LLP	OP4-P-OP1	2.43	113.30	106.47
1	D	186	LLP	C4-C4'-NZ	-2.43	113.17	124.31
1	C	186	LLP	C2'-C2-N1	2.29	122.13	117.67
1	B	186	LLP	C4-C4'-NZ	-2.25	114.00	124.31
1	A	186	LLP	OP2-P-OP4	2.24	112.71	106.73
1	A	186	LLP	C4-C4'-NZ	-2.16	114.39	124.31
1	C	186	LLP	C4-C4'-NZ	-2.13	114.52	124.31
1	D	186	LLP	C5-C4-C4'	2.07	124.96	121.56
1	A	186	LLP	OP4-P-OP1	-2.04	100.76	106.47
1	D	186	LLP	CG-CD-CE	-2.03	106.49	113.57
1	A	186	LLP	C5-C4-C4'	2.01	124.87	121.56

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	186	LLP	CG-CD-CE-NZ
1	B	186	LLP	CG-CD-CE-NZ
1	C	186	LLP	CG-CD-CE-NZ
1	D	186	LLP	C5-C4-C4'-NZ
1	D	186	LLP	CG-CD-CE-NZ
1	D	186	LLP	CA-CB-CG-CD
1	D	186	LLP	C3-C4-C4'-NZ
1	A	186	LLP	CA-CB-CG-CD
1	C	186	LLP	CA-CB-CG-CD
1	B	186	LLP	CA-CB-CG-CD
1	A	186	LLP	C3-C4-C4'-NZ
1	C	186	LLP	C3-C4-C4'-NZ
1	B	186	LLP	C3-C4-C4'-NZ
1	A	186	LLP	CD-CE-NZ-C4'
1	D	186	LLP	CD-CE-NZ-C4'
1	C	186	LLP	CD-CE-NZ-C4'
1	B	186	LLP	CD-CE-NZ-C4'
1	C	186	LLP	C5-C4-C4'-NZ
1	A	186	LLP	C5-C4-C4'-NZ
1	B	186	LLP	C5-C4-C4'-NZ

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	186	LLP	3	0
1	C	186	LLP	3	0
1	A	186	LLP	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is 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	$\#|Z| > 2$
2	ACT	A	372	-	3,3,3	0.90	0	3,3,3	0.64	0
4	AKG	A	374	-	9,9,9	1.79	2 (22%)	11,11,11	1.39	1 (9%)
2	ACT	C	372	-	3,3,3	1.95	1 (33%)	3,3,3	0.89	0
2	ACT	D	372	-	3,3,3	0.82	0	3,3,3	1.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AKG	A	374	-	-	2/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	374	AKG	C2-C1	-4.07	1.48	1.53
2	C	372	ACT	O-C	3.20	1.37	1.22
4	A	374	AKG	O4-C5	2.26	1.38	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	374	AKG	C3-C4-C5	-2.33	108.59	113.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	374	AKG	C3-C4-C5-O4
4	A	374	AKG	C3-C4-C5-O3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	374	AKG	2	0
2	C	372	ACT	2	0
2	D	372	ACT	3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	367/373 (98%)	-0.72	1 (0%)	94	92	6, 14, 38, 75	0
1	B	367/373 (98%)	-0.61	1 (0%)	94	92	5, 15, 45, 86	0
1	C	364/373 (97%)	-0.43	3 (0%)	86	84	7, 18, 56, 83	0
1	D	363/373 (97%)	-0.39	5 (1%)	75	72	7, 20, 58, 82	0
All	All	1461/1492 (97%)	-0.54	10 (0%)	87	86	5, 16, 50, 86	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	LEU	4.2
1	C	371	VAL	3.3
1	D	355	THR	2.6
1	D	259	GLY	2.4
1	C	310	LEU	2.4
1	D	359	ILE	2.3
1	D	260	TRP	2.3
1	D	256	ARG	2.2
1	A	4	LEU	2.2
1	C	260	TRP	2.1

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

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	A	186	24/25	0.97	0.11	7,12,19,33	0
1	LLP	C	186	24/25	0.97	0.13	8,15,27,99	0

Continued on next page...

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
1	LLP	B	186	24/25	0.98	0.13	4,10,22,30	0
1	LLP	D	186	24/25	0.98	0.13	7,15,28,34	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	NA	A	373	1/1	0.82	0.10	42,42,42,42	0
2	ACT	C	372	4/4	0.94	0.14	14,22,22,25	0
4	AKG	A	374	10/10	0.94	0.15	16,29,99,99	0
2	ACT	D	372	4/4	0.95	0.15	13,16,22,38	0
2	ACT	A	372	4/4	0.96	0.10	11,14,15,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.