



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:52 am BST

PDB ID : 3L7G
Title : Crystal structure of organophosphate anhydrolase/prolidase
Authors : Vyas, N.K.; Nickitenko, A.; Quioco, F.A.
Deposited on : 2009-12-28
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

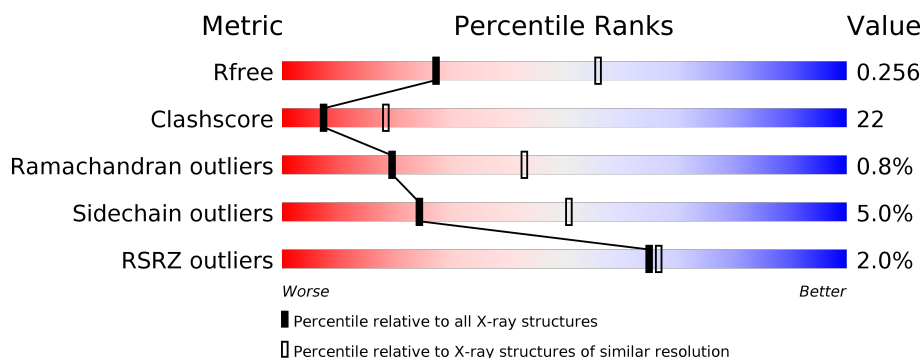
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	517	<div> <div>2%</div> <div>51% 28% • 18%</div> </div>
1	B	517	<div> <div>•</div> <div>50% 27% • 19%</div> </div>
1	C	517	<div> <div>2%</div> <div>45% 34% • 19%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10581 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

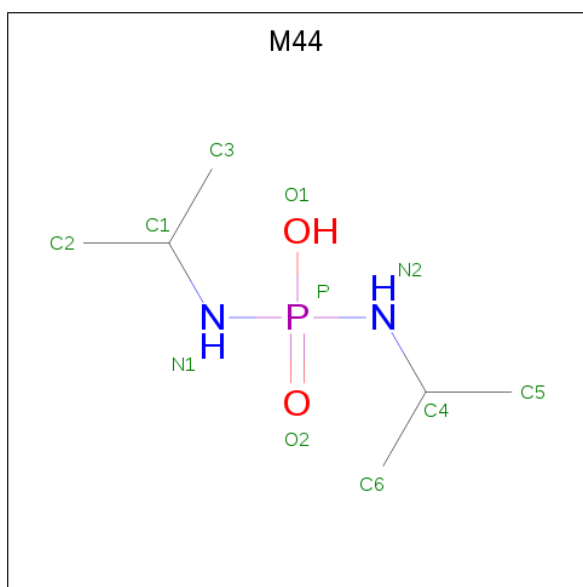
- Molecule 1 is a protein called Xaa-Pro dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3443	2208	589	632	14			
1	B	417	Total	C	N	O	S	0	0	0
			3392	2175	581	624	12			
1	C	417	Total	C	N	O	S	0	0	0
			3392	2175	581	624	12			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	PRO	ALA	SEE REMARK 999	UNP Q44238
A	283	MET	CYS	SEE REMARK 999	UNP Q44238
A	439	LEU	ALA	SEE REMARK 999	UNP Q44238
B	211	PRO	ALA	SEE REMARK 999	UNP Q44238
B	283	MET	CYS	SEE REMARK 999	UNP Q44238
B	439	LEU	ALA	SEE REMARK 999	UNP Q44238
C	211	PRO	ALA	SEE REMARK 999	UNP Q44238
C	283	MET	CYS	SEE REMARK 999	UNP Q44238
C	439	LEU	ALA	SEE REMARK 999	UNP Q44238

- Molecule 2 is N,N'-bis(1-methylethyl)phosphorodiamidic acid (three-letter code: M44) (formula: C₆H₁₇N₂O₂P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			11	6	2	2	1		
2	B	1	Total	C	N	O	P	0	0
			11	6	2	2	1		
2	C	1	Total	C	N	O	P	0	0
			11	6	2	2	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Mn	0	0
			4	4		
3	A	4	Total	Mn	0	0
			4	4		
3	C	3	Total	Mn	0	0
			3	3		

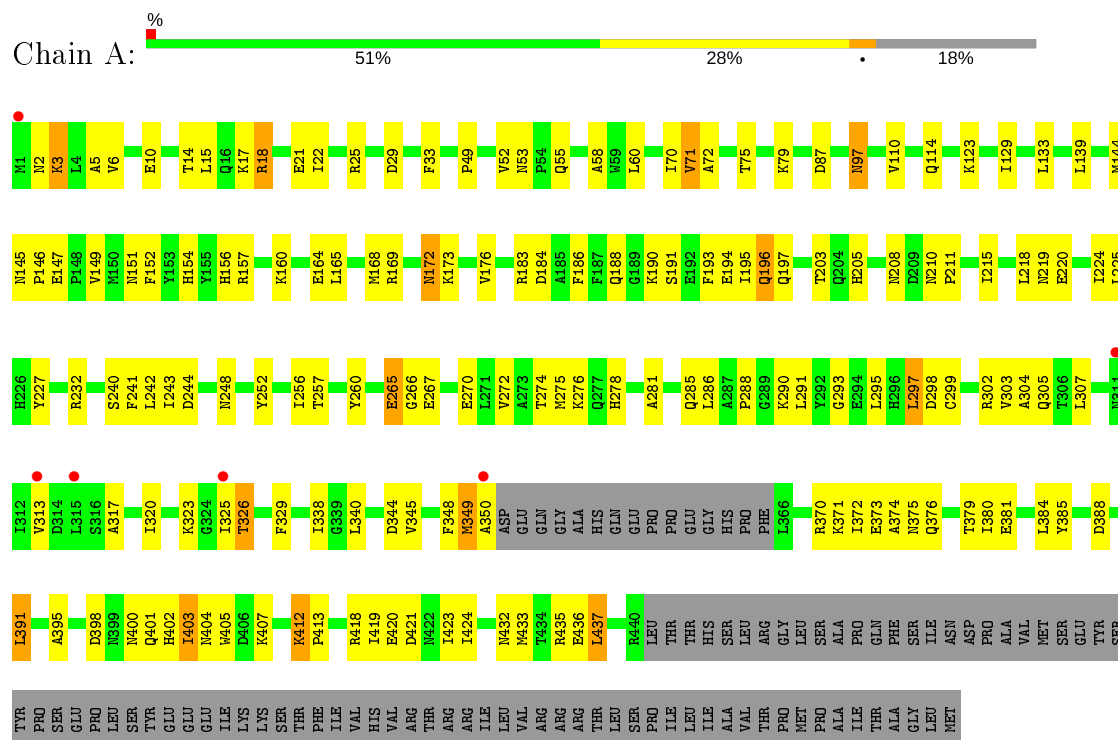
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		
4	B	103	Total	O	0	0
			103	103		
4	C	72	Total	O	0	0
			72	72		

3 Residue-property plots

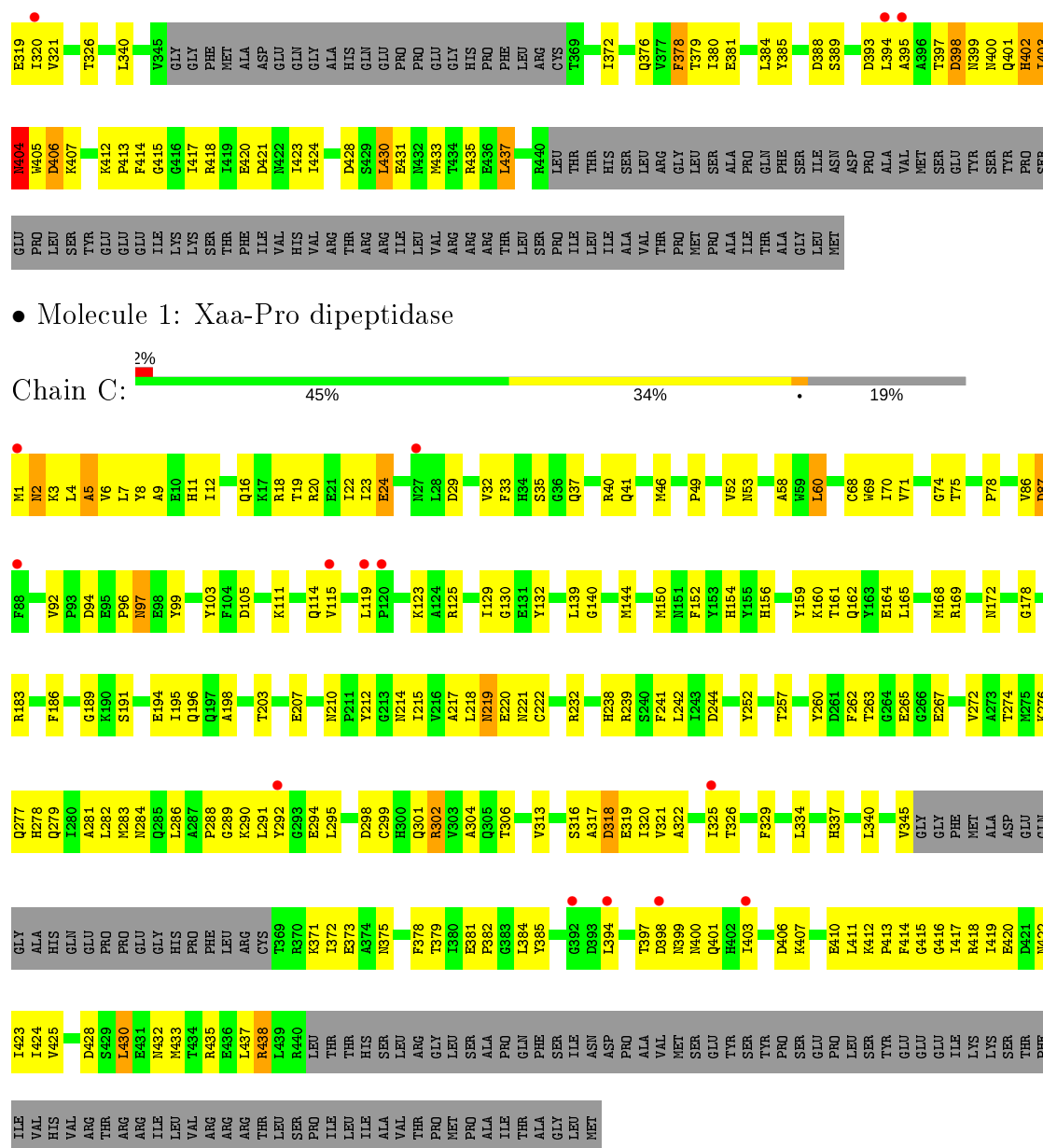
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Xaa-Pro dipeptidase



• Molecule 1: Xaa-Pro dipeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.35Å 143.93Å 219.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.73 – 2.70 60.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.4 (40.73-2.70) 91.2 (60.16-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.259 0.200 , 0.256	Depositor DCC
R_{free} test set	5495 reflections (8.27%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10581	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, M44

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	0.45	0/3534	0.69	0/4795
1	B	0.45	0/3482	0.67	0/4726
1	C	0.42	0/3482	0.63	1/4726 (0.0%)
All	All	0.44	0/10498	0.66	1/14247 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	105	ASP	N-CA-C	-5.11	97.20	111.00

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	3443	0	3318	150	0
1	B	3392	0	3271	141	0
1	C	3392	0	3271	168	0
2	A	11	0	16	0	0
2	B	11	0	16	0	0
2	C	11	0	16	0	0
3	A	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	3	0	0	0	0
4	A	135	0	0	6	0
4	B	103	0	0	4	0
4	C	72	0	0	5	0
All	All	10581	0	9908	452	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 22.

All (452) 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:B:55:GLN:HG2	1:B:129:ILE:HG21	1.32	1.06
1:A:164:GLU:HG2	1:A:252:TYR:OH	1.56	1.05
1:B:381:GLU:HB3	1:B:420:GLU:HB2	1.41	1.01
1:B:395:ALA:HA	1:B:400:ASN:HD22	1.30	0.97
1:A:71:VAL:HG13	1:A:79:LYS:HB3	1.47	0.97
1:A:55:GLN:HG2	1:A:129:ILE:HG21	1.48	0.94
1:A:3:LYS:H	1:A:3:LYS:HD3	1.34	0.93
1:A:169:ARG:HA	1:A:433:MET:HE2	1.57	0.86
1:B:71:VAL:HG13	1:B:79:LYS:HB3	1.58	0.85
1:C:32:VAL:HG22	1:C:71:VAL:HG22	1.61	0.80
1:C:169:ARG:HA	1:C:433:MET:CE	2.12	0.80
1:A:305:GLN:HE21	1:A:317:ALA:HB2	1.45	0.79
1:B:183:ARG:HD3	1:B:187:PHE:CE2	2.17	0.79
1:C:291:LEU:HD23	1:C:371:LYS:HG2	1.64	0.79
1:A:373:GLU:H	1:A:376:GLN:NE2	1.81	0.78
1:C:3:LYS:HG3	1:C:4:LEU:H	1.48	0.77
1:A:298:ASP:O	1:A:302:ARG:HG3	1.85	0.77
1:A:2:ASN:HB3	1:A:5:ALA:HB3	1.65	0.76
1:B:55:GLN:HG2	1:B:129:ILE:CG2	2.13	0.76
1:B:395:ALA:CA	1:B:400:ASN:HD22	1.98	0.76
1:A:381:GLU:HB3	1:A:420:GLU:HB2	1.69	0.75
1:C:169:ARG:HA	1:C:433:MET:HE1	1.68	0.75
1:A:370:ARG:HH11	1:A:370:ARG:HG2	1.52	0.74
1:C:238:HIS:HB3	1:C:262:PHE:CD2	2.22	0.74
1:A:169:ARG:HG2	1:A:433:MET:CE	2.18	0.73
1:C:437:LEU:O	1:C:438:ARG:HB2	1.89	0.73
1:A:210:ASN:HB2	1:A:211:PRO:HD2	1.71	0.73
1:C:290:LYS:HB3	1:C:372:ILE:HD12	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HB3	1:B:120:PRO:HD2	1.71	0.72
1:B:298:ASP:O	1:B:302:ARG:HG2	1.88	0.72
1:A:278:HIS:CE1	1:A:302:ARG:HB3	2.23	0.71
1:C:379:THR:HG22	1:C:422:ASN:ND2	2.04	0.71
1:A:191:SER:OG	1:A:194:GLU:HG3	1.90	0.71
1:A:320:ILE:HG22	1:A:326:THR:HG23	1.72	0.71
1:A:164:GLU:HG2	1:A:252:TYR:CZ	2.25	0.71
1:B:135:VAL:HG23	4:B:625:HOH:O	1.92	0.70
1:C:29:ASP:OD2	1:C:125:ARG:HB2	1.91	0.70
1:C:58:ALA:HA	1:C:340:LEU:HD11	1.72	0.70
1:A:14:THR:O	1:A:18:ARG:HG2	1.91	0.70
1:B:316:SER:OG	1:B:319:GLU:HG2	1.90	0.70
1:C:60:LEU:H	1:C:60:LEU:HD23	1.56	0.70
1:A:169:ARG:CA	1:A:433:MET:HE2	2.22	0.70
1:A:183:ARG:HG3	1:A:260:TYR:CE2	2.27	0.69
1:C:394:LEU:HG	1:C:403:ILE:HD11	1.74	0.69
1:B:18:ARG:NE	1:B:156:HIS:HB3	2.06	0.68
1:A:370:ARG:HD2	4:A:633:HOH:O	1.92	0.68
1:B:298:ASP:OD2	1:B:302:ARG:HD3	1.93	0.68
1:C:257:THR:HG22	1:C:418:ARG:O	1.94	0.68
1:A:299:CYS:O	1:A:303:VAL:HG23	1.92	0.68
1:A:432:ASN:ND2	1:A:435:ARG:HG3	2.09	0.67
1:B:111:LYS:HD3	1:B:114:GLN:NE2	2.09	0.67
1:C:186:PHE:CE1	1:C:241:PHE:HB2	2.30	0.67
1:C:6:VAL:HG23	1:C:7:LEU:N	2.10	0.67
1:A:348:PHE:HZ	1:B:430:LEU:HD13	1.58	0.66
1:C:298:ASP:O	1:C:302:ARG:HG2	1.95	0.66
1:A:3:LYS:H	1:A:3:LYS:CD	2.09	0.66
1:C:164:GLU:HG2	1:C:252:TYR:OH	1.94	0.66
1:C:286:LEU:HB2	1:C:430:LEU:HD21	1.77	0.66
1:B:169:ARG:CA	1:B:433:MET:HE1	2.26	0.66
1:B:33:PHE:HB2	1:B:70:ILE:HB	1.78	0.66
1:A:307:LEU:HD21	1:A:384:LEU:HD21	1.77	0.65
1:C:111:LYS:HB2	1:C:114:GLN:NE2	2.11	0.65
1:A:395:ALA:HB1	1:A:400:ASN:ND2	2.11	0.65
1:B:183:ARG:HD3	1:B:187:PHE:HE2	1.62	0.65
1:B:165:LEU:HD22	1:B:424:ILE:HD13	1.78	0.65
1:B:1:MET:HG3	1:B:2:ASN:N	2.11	0.65
1:C:222:CYS:HB2	1:C:415:GLY:HA3	1.77	0.65
1:B:385:TYR:OH	1:B:418:ARG:HD3	1.97	0.64
1:C:40:ARG:HG2	1:C:40:ARG:HH11	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ARG:HG3	1:C:260:TYR:CE2	2.33	0.64
1:A:388:ASP:HB3	1:A:412:LYS:NZ	2.12	0.64
1:A:424:ILE:HD11	1:A:433:MET:HE3	1.80	0.64
1:B:404:ASN:HD21	1:B:406:ASP:HB2	1.63	0.64
1:C:2:ASN:HB3	1:C:5:ALA:CB	2.28	0.64
1:A:184:ASP:O	1:A:188:GLN:HG3	1.98	0.63
1:C:412:LYS:N	1:C:413:PRO:HD2	2.14	0.63
1:A:3:LYS:HD3	1:A:3:LYS:N	2.11	0.63
1:C:37:GLN:HG3	1:C:132:TYR:CE2	2.34	0.63
1:A:349:MET:O	1:A:349:MET:HG3	1.99	0.63
1:B:169:ARG:HA	1:B:433:MET:HE1	1.80	0.63
1:A:97:ASN:HD22	1:A:97:ASN:H	1.45	0.62
1:B:183:ARG:HD3	1:B:187:PHE:CD2	2.34	0.62
1:A:49:PRO:HG3	1:A:208:ASN:ND2	2.14	0.62
1:A:265:GLU:OE1	1:A:266:GLY:N	2.32	0.62
1:B:113:ASP:OD1	1:B:114:GLN:HG3	1.99	0.62
1:B:301:GLN:NE2	1:B:321:VAL:HG21	2.15	0.62
1:C:398:ASP:O	1:C:401:GLN:HB3	1.99	0.62
1:A:186:PHE:CE1	1:A:241:PHE:HB2	2.34	0.62
1:A:403:ILE:HD11	1:A:405:TRP:CD2	2.34	0.62
1:A:320:ILE:HG23	1:A:325:ILE:CG1	2.29	0.62
1:C:178:GLY:HA3	1:C:203:THR:HG23	1.81	0.62
1:B:18:ARG:HD3	4:B:652:HOH:O	1.99	0.62
1:B:314:ASP:O	1:B:315:LEU:HD23	2.00	0.61
1:A:71:VAL:CG1	1:A:79:LYS:HB3	2.28	0.61
1:B:399:ASN:O	1:B:402:HIS:HB2	2.00	0.61
1:A:186:PHE:CD1	1:A:241:PHE:HB2	2.35	0.61
1:B:26:GLU:OE1	1:B:26:GLU:HA	2.00	0.61
1:A:401:GLN:HG3	1:A:402:HIS:CD2	2.35	0.61
1:A:151:ASN:ND2	1:A:350:ALA:HB2	2.17	0.60
1:A:2:ASN:HB3	1:A:5:ALA:CB	2.31	0.60
1:C:286:LEU:HD23	1:C:372:ILE:HD13	1.81	0.60
1:C:290:LYS:HE3	1:C:294:GLU:HB2	1.82	0.60
1:C:2:ASN:HB3	1:C:5:ALA:HB2	1.83	0.60
1:B:404:ASN:C	1:B:404:ASN:HD22	2.05	0.60
1:A:276:LYS:HE3	1:A:435:ARG:NH2	2.17	0.60
1:B:1:MET:HG3	1:B:2:ASN:H	1.65	0.60
1:B:65:ASN:HD22	1:B:66:PRO:HD2	1.66	0.60
1:A:348:PHE:CZ	1:B:430:LEU:HD13	2.35	0.60
1:C:207:GLU:O	1:C:210:ASN:OD1	2.20	0.60
1:A:286:LEU:HD23	1:A:372:ILE:HD13	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LYS:HG2	1:A:295:LEU:HD11	1.83	0.59
1:B:394:LEU:HD21	1:B:403:ILE:HG21	1.83	0.59
1:A:169:ARG:HG2	1:A:433:MET:HE3	1.83	0.59
1:A:22:ILE:HD13	1:A:152:PHE:CD1	2.37	0.59
1:B:172:ASN:O	1:B:176:VAL:HG23	2.03	0.59
1:B:18:ARG:CZ	1:B:156:HIS:HB3	2.33	0.59
1:A:404:ASN:ND2	1:A:407:LYS:HB2	2.17	0.59
1:C:381:GLU:HB3	1:C:420:GLU:HB2	1.85	0.59
1:C:144:MET:HA	1:C:144:MET:HE2	1.85	0.59
1:A:210:ASN:CB	1:A:211:PRO:HD2	2.31	0.59
1:A:380:ILE:O	1:A:420:GLU:HA	2.03	0.58
1:B:380:ILE:O	1:B:420:GLU:HA	2.03	0.58
1:A:97:ASN:N	1:A:97:ASN:HD22	2.01	0.58
1:C:278:HIS:ND1	1:C:302:ARG:HB3	2.18	0.58
1:C:283:MET:HG3	1:C:432:ASN:HD22	1.69	0.58
1:C:317:ALA:O	1:C:321:VAL:HG23	2.03	0.58
1:A:165:LEU:O	1:A:169:ARG:HG3	2.03	0.58
1:C:289:GLY:HA2	1:C:371:LYS:HD3	1.85	0.58
1:A:224:ILE:HB	1:A:227:TYR:HB2	1.86	0.58
1:A:278:HIS:ND1	1:A:302:ARG:HB3	2.19	0.58
1:A:412:LYS:HB3	1:A:413:PRO:HD3	1.84	0.58
1:C:97:ASN:H	1:C:97:ASN:HD22	1.52	0.57
1:A:349:MET:O	1:A:350:ALA:C	2.42	0.57
1:C:9:ALA:HA	1:C:103:TYR:CE2	2.40	0.57
1:B:423:ILE:N	1:B:423:ILE:HD12	2.19	0.57
1:A:288:PRO:HA	1:A:372:ILE:O	2.04	0.57
1:B:398:ASP:C	1:B:400:ASN:N	2.54	0.57
1:B:169:ARG:N	1:B:433:MET:HE1	2.20	0.57
1:A:172:ASN:O	1:A:176:VAL:HG13	2.05	0.57
1:C:407:LYS:O	1:C:411:LEU:HD23	2.05	0.56
1:C:41:GLN:NE2	1:C:46:MET:HB2	2.20	0.56
1:C:320:ILE:HG23	1:C:325:ILE:CG1	2.35	0.56
1:C:394:LEU:CG	1:C:403:ILE:HD11	2.35	0.56
1:C:12:ILE:HG13	1:C:103:TYR:CD2	2.41	0.56
1:C:319:GLU:O	1:C:322:ALA:HB3	2.06	0.56
1:B:79:LYS:HD2	1:B:107:GLU:HG3	1.86	0.56
1:B:132:TYR:N	1:B:132:TYR:CD1	2.73	0.56
1:B:69:TRP:HB2	1:B:81:ILE:HD12	1.88	0.56
1:A:291:LEU:HD22	1:A:371:LYS:HG2	1.89	0.55
1:B:120:PRO:HG2	1:B:123:LYS:HG2	1.88	0.55
1:A:193:PHE:O	1:A:197:GLN:HG2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:O	1:A:6:VAL:HG12	2.06	0.55
1:C:288:PRO:HA	1:C:372:ILE:O	2.07	0.55
1:B:65:ASN:HD21	1:B:83:TYR:HD2	1.55	0.54
1:C:278:HIS:O	1:C:282:LEU:HG	2.08	0.54
1:C:219:ASN:O	1:C:221:ASN:N	2.40	0.54
1:A:173:LYS:HA	1:A:437:LEU:HD21	1.90	0.54
1:B:403:ILE:HD11	1:B:405:TRP:CZ3	2.41	0.54
1:B:83:TYR:CZ	1:B:85:PRO:HG3	2.43	0.54
1:A:267:GLU:O	1:A:270:GLU:HB2	2.07	0.54
1:B:278:HIS:ND1	1:B:302:ARG:HB3	2.23	0.54
1:B:58:ALA:HA	1:B:340:LEU:HD11	1.89	0.54
1:A:385:TYR:OH	1:A:418:ARG:HD3	2.07	0.54
1:C:32:VAL:HA	1:C:70:ILE:O	2.08	0.53
1:C:119:LEU:HD12	1:C:139:LEU:HD22	1.90	0.53
1:C:6:VAL:CG2	1:C:7:LEU:N	2.72	0.53
1:C:16:GLN:HA	1:C:16:GLN:OE1	2.07	0.53
1:C:33:PHE:HB2	1:C:70:ILE:HB	1.90	0.53
1:B:424:ILE:HB	1:B:431:GLU:HB3	1.90	0.53
1:B:71:VAL:CG1	1:B:79:LYS:HB3	2.33	0.53
1:C:165:LEU:HD22	1:C:424:ILE:HD13	1.91	0.53
1:C:183:ARG:HG3	1:C:260:TYR:CZ	2.44	0.53
1:A:169:ARG:HG2	1:A:433:MET:HE2	1.87	0.53
1:B:398:ASP:O	1:B:401:GLN:HG3	2.09	0.52
1:A:388:ASP:HB3	1:A:412:LYS:HZ2	1.72	0.52
1:C:210:ASN:HD22	1:C:214:ASN:ND2	2.07	0.52
1:C:320:ILE:HG22	1:C:326:THR:HG23	1.92	0.52
1:B:424:ILE:HD11	1:B:433:MET:HE2	1.89	0.52
1:C:49:PRO:HA	4:C:631:HOH:O	2.08	0.52
1:A:17:LYS:O	1:A:21:GLU:HG3	2.10	0.52
1:A:160:LYS:HE2	1:A:168:MET:HE1	1.91	0.52
1:C:115:VAL:HG13	1:C:139:LEU:HD21	1.90	0.52
1:A:370:ARG:HH11	1:A:370:ARG:CG	2.23	0.52
1:C:23:ILE:HG13	1:C:24:GLU:N	2.26	0.51
1:C:40:ARG:HG2	1:C:40:ARG:NH1	2.25	0.51
1:A:219:ASN:HA	1:A:240:SER:OG	2.11	0.51
1:C:60:LEU:N	1:C:60:LEU:HD23	2.25	0.51
1:C:20:ARG:HD3	1:C:75:THR:HG22	1.91	0.51
1:C:320:ILE:HG23	1:C:325:ILE:HG12	1.91	0.51
1:B:19:THR:O	1:B:22:ILE:HG22	2.11	0.51
1:A:381:GLU:HB3	1:A:420:GLU:CB	2.40	0.50
1:A:329:PHE:HB3	1:A:384:LEU:HD22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ILE:HB	1:C:244:ASP:HB3	1.93	0.50
1:C:397:THR:HG22	1:C:398:ASP:N	2.26	0.50
1:A:257:THR:HB	1:A:420:GLU:HB3	1.94	0.50
1:C:313:VAL:HG11	1:C:325:ILE:CD1	2.42	0.50
1:C:274:THR:O	1:C:277:GLN:HB2	2.11	0.50
1:A:374:ALA:O	1:A:375:ASN:HB2	2.12	0.50
1:B:279:GLN:OE1	1:B:435:ARG:NH1	2.44	0.50
1:B:60:LEU:HD22	1:B:70:ILE:HD11	1.93	0.50
1:C:295:LEU:HD11	1:C:372:ILE:HD11	1.92	0.50
1:B:211:PRO:HG2	1:B:212:TYR:CD1	2.47	0.50
1:B:315:LEU:HD11	1:B:402:HIS:ND1	2.27	0.50
1:C:298:ASP:O	1:C:301:GLN:HB3	2.12	0.50
1:C:394:LEU:HG	1:C:403:ILE:CD1	2.40	0.50
1:C:86:VAL:O	1:C:87:ASP:HB3	2.12	0.50
1:B:111:LYS:HD3	1:B:114:GLN:HE22	1.74	0.50
1:C:257:THR:HB	1:C:420:GLU:HB3	1.94	0.50
1:C:437:LEU:O	1:C:438:ARG:CB	2.59	0.50
1:C:92:VAL:HG13	1:C:92:VAL:O	2.12	0.50
1:A:379:THR:HA	1:A:421:ASP:O	2.12	0.49
1:A:370:ARG:HG2	1:A:370:ARG:NH1	2.26	0.49
1:A:381:GLU:HA	1:A:419:ILE:O	2.12	0.49
1:B:378:PHE:CD1	1:B:378:PHE:N	2.81	0.49
1:C:299:CYS:SG	1:C:334:LEU:HD13	2.52	0.49
1:C:313:VAL:HB	1:C:320:ILE:HD11	1.94	0.49
1:B:274:THR:HG21	1:B:306:THR:HG23	1.94	0.49
1:A:381:GLU:CB	1:A:420:GLU:HB2	2.40	0.49
1:B:395:ALA:CB	1:B:400:ASN:HD22	2.25	0.49
1:C:257:THR:HG21	1:C:418:ARG:HB3	1.94	0.49
1:A:295:LEU:HD12	1:A:295:LEU:H	1.78	0.49
1:B:393:ASP:O	1:B:397:THR:HG23	2.12	0.49
1:A:18:ARG:CZ	1:A:156:HIS:HB3	2.43	0.49
1:B:403:ILE:HD11	1:B:405:TRP:CE3	2.48	0.49
1:B:97:ASN:HD22	1:B:97:ASN:H	1.60	0.49
1:C:189:GLY:HA2	1:C:238:HIS:NE2	2.28	0.49
1:A:25:ARG:NH2	1:B:428:ASP:OD2	2.46	0.49
1:A:215:ILE:HB	1:A:244:ASP:HB3	1.94	0.49
1:B:372:ILE:HG23	1:B:378:PHE:CZ	2.48	0.49
1:B:83:TYR:CZ	1:B:85:PRO:CG	2.96	0.49
1:C:210:ASN:ND2	1:C:212:TYR:O	2.46	0.49
1:A:293:GLY:O	1:A:297:LEU:HD22	2.12	0.49
1:B:320:ILE:HG22	1:B:326:THR:HG23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ASP:C	1:B:400:ASN:H	2.15	0.48
1:C:60:LEU:N	1:C:60:LEU:CD2	2.76	0.48
1:C:60:LEU:H	1:C:60:LEU:CD2	2.25	0.48
1:B:404:ASN:ND2	1:B:407:LYS:H	2.12	0.48
1:B:40:ARG:HD2	1:B:44:ASP:O	2.13	0.48
1:C:191:SER:OG	1:C:194:GLU:HG3	2.13	0.48
1:A:265:GLU:CD	1:A:266:GLY:N	2.67	0.48
1:B:155:TYR:CD2	1:C:428:ASP:HB3	2.48	0.48
1:A:320:ILE:HG23	1:A:325:ILE:HG12	1.95	0.48
1:C:8:TYR:CZ	1:C:12:ILE:HD11	2.48	0.48
1:B:22:ILE:HD13	1:B:152:PHE:CG	2.49	0.48
1:C:274:THR:HG21	1:C:306:THR:HG23	1.96	0.48
1:C:411:LEU:N	1:C:411:LEU:HD22	2.29	0.48
1:B:404:ASN:C	1:B:404:ASN:ND2	2.64	0.48
1:B:239:ARG:HB3	1:B:414:PHE:CE1	2.49	0.48
1:A:401:GLN:HG3	1:A:402:HIS:H	1.78	0.48
1:C:281:ALA:CB	1:C:302:ARG:NH2	2.77	0.48
1:A:114:GLN:NE2	4:A:617:HOH:O	2.43	0.48
1:B:55:GLN:HE22	1:B:153:TYR:HB3	1.79	0.48
1:C:410:GLU:C	1:C:411:LEU:HD22	2.34	0.48
1:A:146:PRO:HB2	1:A:149:VAL:HG23	1.96	0.48
1:B:35:SER:HB3	1:B:68:CYS:HB2	1.96	0.48
1:B:433:MET:O	1:B:437:LEU:HD22	2.14	0.48
1:C:319:GLU:HA	1:C:322:ALA:CB	2.44	0.48
1:C:35:SER:HB3	1:C:68:CYS:HB2	1.96	0.48
1:C:381:GLU:HB3	1:C:420:GLU:CB	2.44	0.48
1:A:304:ALA:HB2	1:A:326:THR:CG2	2.44	0.47
1:C:178:GLY:HA3	1:C:203:THR:CG2	2.44	0.47
1:A:191:SER:O	1:A:195:ILE:HG13	2.13	0.47
1:C:37:GLN:HG3	1:C:132:TYR:CD2	2.49	0.47
1:A:403:ILE:HD12	1:A:403:ILE:C	2.34	0.47
1:B:19:THR:O	1:B:23:ILE:HG23	2.15	0.47
1:B:69:TRP:HB2	1:B:81:ILE:HB	1.97	0.47
1:A:196:GLN:HE21	1:A:196:GLN:HA	1.80	0.47
1:A:168:MET:HG2	1:A:252:TYR:HB3	1.96	0.47
1:B:196:GLN:HA	1:B:196:GLN:HE21	1.78	0.47
1:A:403:ILE:HD12	1:A:404:ASN:N	2.29	0.47
1:B:395:ALA:HA	1:B:400:ASN:ND2	2.13	0.47
1:B:52:VAL:HG22	1:B:53:ASN:N	2.30	0.47
1:C:111:LYS:HD2	1:C:114:GLN:NE2	2.29	0.47
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:THR:HG22	1:A:278:HIS:CD2	2.49	0.47
1:B:165:LEU:O	1:B:169:ARG:HG3	2.14	0.47
1:C:263:THR:HG23	4:C:620:HOH:O	2.13	0.47
1:C:411:LEU:C	1:C:413:PRO:HD2	2.35	0.47
1:A:291:LEU:CD2	1:A:371:LYS:HG2	2.44	0.47
1:C:18:ARG:CZ	1:C:156:HIS:HB3	2.45	0.47
1:B:165:LEU:HD22	1:B:424:ILE:CD1	2.44	0.47
1:B:394:LEU:HD23	1:B:403:ILE:HD13	1.97	0.47
1:B:424:ILE:HD11	1:B:433:MET:CE	2.45	0.47
1:A:183:ARG:HG3	1:A:260:TYR:CZ	2.48	0.47
1:B:216:VAL:HG23	1:B:230:PHE:HE1	1.79	0.47
1:C:218:LEU:O	1:C:221:ASN:HB2	2.14	0.47
1:A:220:GLU:HG3	1:A:413:PRO:HA	1.96	0.47
1:A:55:GLN:HG2	1:A:129:ILE:CG2	2.33	0.47
1:B:412:LYS:HB3	1:B:413:PRO:HD3	1.96	0.46
1:C:400:ASN:HA	1:C:403:ILE:HD12	1.96	0.46
1:A:164:GLU:CG	1:A:252:TYR:OH	2.45	0.46
1:A:348:PHE:HZ	1:B:430:LEU:CD1	2.28	0.46
1:B:29:ASP:OD2	1:B:125:ARG:HB2	2.15	0.46
1:C:375:ASN:N	1:C:425:VAL:O	2.44	0.46
1:A:424:ILE:HD11	1:A:433:MET:CE	2.45	0.46
1:C:159:TYR:OH	1:C:373:GLU:HG3	2.14	0.46
1:C:302:ARG:HG2	1:C:302:ARG:H	1.47	0.46
1:C:52:VAL:HG22	1:C:53:ASN:N	2.31	0.46
1:A:272:VAL:O	1:A:275:MET:HB2	2.15	0.46
1:B:246:GLY:HA3	1:B:254:ALA:O	2.15	0.46
1:C:168:MET:HG2	1:C:252:TYR:HB3	1.98	0.46
1:C:320:ILE:HG12	1:C:325:ILE:HD11	1.97	0.46
1:A:123:LYS:HD2	1:A:139:LEU:O	2.15	0.46
1:B:164:GLU:HG2	1:B:252:TYR:OH	2.16	0.46
1:C:189:GLY:HA2	1:C:238:HIS:CD2	2.51	0.46
1:C:169:ARG:CA	1:C:433:MET:CE	2.89	0.46
1:A:432:ASN:O	1:A:436:GLU:HG3	2.16	0.46
1:B:178:GLY:HA2	1:B:202:ALA:HB3	1.97	0.46
1:B:25:ARG:HG3	1:C:169:ARG:NH2	2.31	0.46
1:C:319:GLU:HA	1:C:322:ALA:HB3	1.98	0.46
1:A:313:VAL:HG11	1:A:320:ILE:HG12	1.98	0.46
1:C:379:THR:O	1:C:381:GLU:HG2	2.16	0.46
1:A:256:ILE:HG22	1:A:257:THR:N	2.31	0.45
1:C:283:MET:HG2	1:C:423:ILE:HG12	1.97	0.45
1:A:388:ASP:HB3	1:A:412:LYS:HZ1	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ILE:HG12	1:A:423:ILE:HD13	1.98	0.45
1:A:58:ALA:HA	1:A:340:LEU:HD11	1.98	0.45
1:B:169:ARG:HG2	1:B:433:MET:CE	2.47	0.45
1:B:224:ILE:HB	1:B:227:TYR:HB2	1.98	0.45
1:B:83:TYR:CE1	1:B:85:PRO:HG3	2.52	0.45
1:A:3:LYS:HA	1:A:6:VAL:HG12	1.97	0.45
1:B:158:ALA:O	1:B:376:GLN:HG2	2.17	0.45
1:A:432:ASN:CG	1:A:435:ARG:HG3	2.37	0.45
1:B:242:LEU:C	1:B:242:LEU:HD23	2.37	0.45
1:C:304:ALA:HB2	1:C:326:THR:HG21	1.98	0.45
1:B:404:ASN:OD1	1:B:407:LYS:HB2	2.17	0.45
1:C:276:LYS:HE3	1:C:435:ARG:HH12	1.79	0.45
1:C:318:ASP:O	1:C:322:ALA:N	2.48	0.45
1:A:110:VAL:CG2	1:A:114:GLN:HE22	2.29	0.45
1:C:7:LEU:HD22	1:C:162:GLN:HB3	1.97	0.45
1:B:403:ILE:HD11	1:B:405:TRP:CH2	2.52	0.44
1:B:50:PHE:O	1:B:51:LYS:HD3	2.17	0.44
1:C:115:VAL:CG1	1:C:139:LEU:HD21	2.48	0.44
1:B:55:GLN:HE22	1:B:153:TYR:CB	2.31	0.44
1:B:4:LEU:HG	1:B:163:TYR:HE1	1.83	0.44
1:A:203:THR:OG1	1:A:205:HIS:HB2	2.17	0.44
1:B:412:LYS:N	1:B:413:PRO:CD	2.80	0.44
1:A:401:GLN:HG3	1:A:402:HIS:N	2.33	0.44
1:B:97:ASN:H	1:B:97:ASN:ND2	2.15	0.44
1:C:272:VAL:HA	1:C:417:ILE:HD13	1.99	0.44
1:A:304:ALA:HB1	1:A:320:ILE:HB	1.98	0.44
1:B:388:ASP:O	1:B:389:SER:C	2.56	0.44
1:B:404:ASN:HD22	1:B:406:ASP:H	1.66	0.44
1:C:69:TRP:NE1	1:C:115:VAL:HG21	2.33	0.44
1:C:19:THR:O	1:C:23:ILE:HG23	2.17	0.44
1:A:15:LEU:HA	1:A:18:ARG:HG3	1.99	0.44
1:C:3:LYS:CG	1:C:4:LEU:H	2.19	0.44
1:B:191:SER:O	1:B:195:ILE:HG13	2.19	0.43
1:C:291:LEU:HB2	1:C:294:GLU:HG3	1.98	0.43
1:C:169:ARG:HG2	1:C:433:MET:HE2	2.00	0.43
1:A:173:LYS:HA	1:A:437:LEU:CD2	2.48	0.43
1:B:115:VAL:HG13	1:B:116:GLU:N	2.33	0.43
1:B:271:LEU:O	1:B:275:MET:HG2	2.18	0.43
1:C:242:LEU:C	1:C:242:LEU:HD23	2.38	0.43
1:C:278:HIS:CE1	1:C:302:ARG:HB3	2.53	0.43
1:C:6:VAL:CG2	1:C:7:LEU:H	2.30	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASP:O	4:A:648:HOH:O	2.21	0.43
1:B:205:HIS:NE2	1:B:247:ALA:HB1	2.33	0.43
1:B:169:ARG:HG2	1:B:433:MET:HE2	2.00	0.43
1:C:22:ILE:HB	1:C:152:PHE:CE2	2.53	0.43
1:C:291:LEU:O	1:C:292:TYR:C	2.56	0.43
1:A:323:LYS:HE3	1:A:402:HIS:CE1	2.53	0.43
1:C:1:MET:HG2	1:C:2:ASN:N	2.33	0.43
1:C:320:ILE:HG23	1:C:325:ILE:HD11	1.99	0.43
1:C:2:ASN:HB3	1:C:5:ALA:HB3	1.99	0.43
1:C:385:TYR:OH	1:C:418:ARG:HD3	2.18	0.43
1:B:41:GLN:NE2	1:B:46:MET:HB2	2.33	0.43
1:A:25:ARG:HH22	1:B:428:ASP:CG	2.22	0.43
1:C:217:ALA:O	1:C:241:PHE:HD1	2.01	0.43
1:C:6:VAL:HG23	1:C:7:LEU:H	1.80	0.43
1:B:169:ARG:NH1	4:B:671:HOH:O	2.52	0.42
1:B:192:GLU:HG2	1:B:218:LEU:HD22	2.01	0.42
1:C:195:ILE:O	1:C:198:ALA:HB3	2.19	0.42
1:C:97:ASN:N	1:C:97:ASN:HD22	2.17	0.42
1:A:190:LYS:HB3	1:A:194:GLU:HB2	2.01	0.42
1:B:41:GLN:NE2	1:B:46:MET:CB	2.83	0.42
1:C:123:LYS:HD2	1:C:140:GLY:HA3	2.01	0.42
1:C:19:THR:HA	1:C:22:ILE:HG22	2.01	0.42
1:A:281:ALA:O	1:A:285:GLN:HG3	2.20	0.42
1:A:52:VAL:HG22	1:A:53:ASN:N	2.34	0.42
1:C:284:ASN:HD22	1:C:284:ASN:HA	1.61	0.42
1:A:154:HIS:CD2	1:A:345:VAL:HG21	2.55	0.42
1:B:215:ILE:O	1:B:243:ILE:HA	2.19	0.42
1:C:16:GLN:NE2	1:C:78:PRO:HD3	2.34	0.42
1:C:18:ARG:O	1:C:22:ILE:HG22	2.18	0.42
1:C:337:HIS:ND1	4:C:600:HOH:O	2.37	0.42
1:A:72:ALA:HB1	4:A:637:HOH:O	2.19	0.42
1:A:320:ILE:HG23	1:A:325:ILE:HG13	1.99	0.42
1:A:403:ILE:HD12	1:A:405:TRP:N	2.35	0.42
1:C:329:PHE:CD1	1:C:329:PHE:N	2.86	0.42
1:B:4:LEU:HA	1:B:4:LEU:HD12	1.87	0.42
1:B:65:ASN:HD22	1:B:66:PRO:CD	2.30	0.42
1:C:283:MET:HG3	1:C:432:ASN:ND2	2.34	0.42
1:A:242:LEU:C	1:A:242:LEU:HD23	2.40	0.42
1:B:403:ILE:HG13	1:B:403:ILE:O	2.16	0.42
1:C:69:TRP:CE2	1:C:115:VAL:HG21	2.54	0.42
1:A:133:LEU:HD22	1:A:144:MET:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ALA:CB	1:A:400:ASN:ND2	2.80	0.42
1:B:99:TYR:CD1	1:B:100:TRP:N	2.88	0.42
1:B:4:LEU:HD21	1:B:249:PHE:HE2	1.83	0.42
1:A:160:LYS:HG2	1:A:168:MET:CE	2.50	0.42
1:A:157:ARG:NE	1:A:340:LEU:HD12	2.35	0.42
1:C:129:ILE:HD12	1:C:150:MET:SD	2.60	0.42
1:B:222:CYS:HB2	1:B:415:GLY:HA3	2.01	0.41
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.87	0.41
1:C:282:LEU:C	1:C:284:ASN:N	2.73	0.41
1:C:417:ILE:HG22	1:C:418:ARG:N	2.35	0.41
1:C:279:GLN:HG3	1:C:419:ILE:O	2.19	0.41
1:A:33:PHE:HB2	1:A:70:ILE:HB	2.03	0.41
1:B:97:ASN:N	1:B:97:ASN:ND2	2.68	0.41
1:B:98:GLU:O	1:B:99:TYR:C	2.59	0.41
1:B:404:ASN:ND2	1:B:406:ASP:H	2.17	0.41
1:C:267:GLU:HG3	1:C:410:GLU:OE2	2.20	0.41
1:C:329:PHE:O	1:C:384:LEU:HA	2.21	0.41
1:A:3:LYS:O	1:A:6:VAL:CG1	2.67	0.41
1:A:87:ASP:HA	4:A:702:HOH:O	2.19	0.41
1:B:127:ALA:HA	1:B:143:LEU:HB2	2.03	0.41
1:C:53:ASN:ND2	1:C:130:GLY:HA2	2.35	0.41
1:C:372:ILE:HG23	1:C:378:PHE:CE1	2.55	0.41
1:C:20:ARG:NH1	1:C:74:GLY:O	2.49	0.41
1:A:290:LYS:CG	1:A:295:LEU:HD11	2.49	0.41
1:A:350:ALA:HB2	4:A:722:HOH:O	2.21	0.41
1:A:403:ILE:HD12	1:A:404:ASN:C	2.41	0.41
1:B:67:HIS:CD2	1:B:112:PRO:HG3	2.56	0.41
1:A:432:ASN:HD21	1:A:435:ARG:HG3	1.85	0.41
1:B:97:ASN:HD22	1:B:97:ASN:N	2.17	0.41
1:C:5:ALA:HA	1:C:99:TYR:CD2	2.56	0.41
1:A:183:ARG:O	1:A:184:ASP:C	2.59	0.41
1:A:338:ILE:HA	1:A:344:ASP:HB2	2.03	0.41
1:B:119:LEU:HB3	1:B:120:PRO:CD	2.48	0.41
1:B:22:ILE:HB	1:B:152:PHE:CE2	2.56	0.41
1:B:86:VAL:HG23	1:B:86:VAL:O	2.21	0.41
1:C:397:THR:C	1:C:399:ASN:H	2.24	0.41
1:C:97:ASN:ND2	4:C:639:HOH:O	2.54	0.41
1:A:370:ARG:CG	1:A:370:ARG:NH1	2.80	0.41
1:B:299:CYS:O	1:B:303:VAL:HG23	2.21	0.41
1:C:154:HIS:HB3	1:C:345:VAL:HB	2.03	0.41
1:A:225:LEU:HD21	1:A:385:TYR:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LYS:HD2	1:C:160:LYS:N	2.36	0.41
1:C:169:ARG:CG	1:C:433:MET:HE2	2.51	0.40
1:C:214:ASN:ND2	4:C:602:HOH:O	2.54	0.40
1:C:416:GLY:C	1:C:417:ILE:HG13	2.41	0.40
1:A:22:ILE:HD13	1:A:152:PHE:CG	2.55	0.40
1:B:210:ASN:ND2	4:B:666:HOH:O	2.54	0.40
1:C:316:SER:O	1:C:317:ALA:C	2.58	0.40
1:A:144:MET:O	1:A:145:ASN:C	2.59	0.40
1:A:157:ARG:CD	1:A:340:LEU:HD12	2.52	0.40
1:B:379:THR:HA	1:B:421:ASP:O	2.21	0.40
1:C:382:PRO:HD2	1:C:419:ILE:O	2.21	0.40
1:B:417:ILE:HG22	1:B:418:ARG:N	2.36	0.40
1:C:239:ARG:HB3	1:C:414:PHE:CE2	2.57	0.40
1:C:8:TYR:O	1:C:11:HIS:HB3	2.22	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	421/517 (81%)	386 (92%)	33 (8%)	2 (0%)	29	54
1	B	413/517 (80%)	384 (93%)	28 (7%)	1 (0%)	47	73
1	C	413/517 (80%)	372 (90%)	34 (8%)	7 (2%)	9	23
All	All	1247/1551 (80%)	1142 (92%)	95 (8%)	10 (1%)	19	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	220	GLU
1	A	349	MET
1	C	5	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	87	ASP
1	C	438	ARG
1	C	219	ASN
1	C	265	GLU
1	B	404	ASN
1	C	96	PRO
1	A	412	LYS

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	360/443 (81%)	339 (94%)	21 (6%)	20	43
1	B	356/443 (80%)	335 (94%)	21 (6%)	19	43
1	C	356/443 (80%)	344 (97%)	12 (3%)	37	66
All	All	1072/1329 (81%)	1018 (95%)	54 (5%)	24	51

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	10	GLU
1	A	18	ARG
1	A	60	LEU
1	A	71	VAL
1	A	75	THR
1	A	97	ASN
1	A	147	GLU
1	A	172	ASN
1	A	196	GLN
1	A	218	LEU
1	A	232	ARG
1	A	243	ILE
1	A	248	ASN
1	A	265	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	297	LEU
1	A	326	THR
1	A	391	LEU
1	A	398	ASP
1	A	403	ILE
1	A	437	LEU
1	B	60	LEU
1	B	65	ASN
1	B	94	ASP
1	B	97	ASN
1	B	116	GLU
1	B	172	ASN
1	B	183	ARG
1	B	196	GLN
1	B	218	LEU
1	B	232	ARG
1	B	248	ASN
1	B	267	GLU
1	B	378	PHE
1	B	384	LEU
1	B	398	ASP
1	B	402	HIS
1	B	403	ILE
1	B	404	ASN
1	B	406	ASP
1	B	430	LEU
1	B	437	LEU
1	C	2	ASN
1	C	24	GLU
1	C	60	LEU
1	C	94	ASP
1	C	97	ASN
1	C	172	ASN
1	C	196	GLN
1	C	232	ARG
1	C	302	ARG
1	C	318	ASP
1	C	406	ASP
1	C	430	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	97	ASN
1	A	114	GLN
1	A	137	GLN
1	A	151	ASN
1	A	177	GLN
1	A	188	GLN
1	A	196	GLN
1	A	197	GLN
1	A	208	ASN
1	A	214	ASN
1	A	250	ASN
1	A	284	ASN
1	A	305	GLN
1	A	337	HIS
1	A	375	ASN
1	A	376	GLN
1	A	402	HIS
1	B	41	GLN
1	B	55	GLN
1	B	65	ASN
1	B	90	HIS
1	B	97	ASN
1	B	151	ASN
1	B	156	HIS
1	B	177	GLN
1	B	188	GLN
1	B	196	GLN
1	B	204	GLN
1	B	208	ASN
1	B	210	ASN
1	B	214	ASN
1	B	250	ASN
1	B	301	GLN
1	B	311	ASN
1	B	400	ASN
1	B	404	ASN
1	C	2	ASN
1	C	27	ASN
1	C	41	GLN
1	C	55	GLN
1	C	97	ASN
1	C	114	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	151	ASN
1	C	188	GLN
1	C	196	GLN
1	C	208	ASN
1	C	214	ASN
1	C	284	ASN
1	C	296	HIS
1	C	375	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	M44	B	518	3	7,10,10	1.25	1 (14%)	6,14,14	0.85	0
2	M44	A	518	3	7,10,10	1.08	1 (14%)	6,14,14	1.05	1 (16%)
2	M44	C	518	3	7,10,10	0.81	0	6,14,14	0.88	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
2	M44	B	518	3	-	2/8/10/10	-
2	M44	A	518	3	-	2/8/10/10	-
2	M44	C	518	3	-	2/8/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	518	M44	P-O2	2.83	1.51	1.46
2	A	518	M44	P-O2	2.48	1.50	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	518	M44	C2-C1-N1	-2.01	106.96	110.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	518	M44	C1-N1-P-O2
2	A	518	M44	C1-N1-P-N2
2	C	518	M44	C1-N1-P-N2
2	B	518	M44	C1-N1-P-N2
2	A	518	M44	C1-N1-P-O2
2	B	518	M44	C1-N1-P-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	425/517 (82%)	-0.12	6 (1%) 75 77	8, 33, 69, 86	0
1	B	417/517 (80%)	0.05	7 (1%) 70 72	12, 40, 73, 85	0
1	C	417/517 (80%)	0.20	12 (2%) 51 52	21, 47, 83, 98	0
All	All	1259/1551 (81%)	0.04	25 (1%) 65 67	8, 39, 75, 98	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	4.3
1	C	394	LEU	3.8
1	B	313	VAL	3.5
1	A	1	MET	3.4
1	C	120	PRO	3.3
1	B	320	ILE	3.2
1	B	312	ILE	3.2
1	A	313	VAL	3.0
1	C	325	ILE	3.0
1	C	115	VAL	2.9
1	B	394	LEU	2.7
1	A	311	ASN	2.6
1	C	119	LEU	2.6
1	B	315	LEU	2.5
1	A	325	ILE	2.4
1	C	27	ASN	2.4
1	A	350	ALA	2.3
1	C	398	ASP	2.3
1	B	395	ALA	2.2
1	C	403	ILE	2.1
1	A	315	LEU	2.1
1	C	292	TYR	2.1
1	C	392	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	88	PHE	2.0
1	B	116	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	MN	B	522	1/1	0.94	0.14	56,56,56,56	0
3	MN	C	521	1/1	0.96	0.07	66,66,66,66	0
3	MN	B	521	1/1	0.97	0.16	47,47,47,47	0
3	MN	A	521	1/1	0.97	0.12	50,50,50,50	0
3	MN	A	522	1/1	0.97	0.15	39,39,39,39	0
2	M44	C	518	11/11	0.98	0.18	44,47,49,50	0
2	M44	B	518	11/11	0.98	0.15	36,38,41,41	0
3	MN	C	520	1/1	0.99	0.10	33,33,33,33	0
3	MN	C	519	1/1	0.99	0.12	34,34,34,34	0
3	MN	B	520	1/1	0.99	0.15	24,24,24,24	0
2	M44	A	518	11/11	0.99	0.17	33,37,37,38	0
3	MN	A	520	1/1	0.99	0.12	20,20,20,20	0
3	MN	A	519	1/1	1.00	0.12	26,26,26,26	0
3	MN	B	519	1/1	1.00	0.12	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.