



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:32 am BST

PDB ID : 3ASJ
Title : Crystal structure of homoisocitrate dehydrogenase in complex with a designed inhibitor
Authors : Nango, E.; Kumasaka, T.; Eguchi, T.
Deposited on : 2010-12-13
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

<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

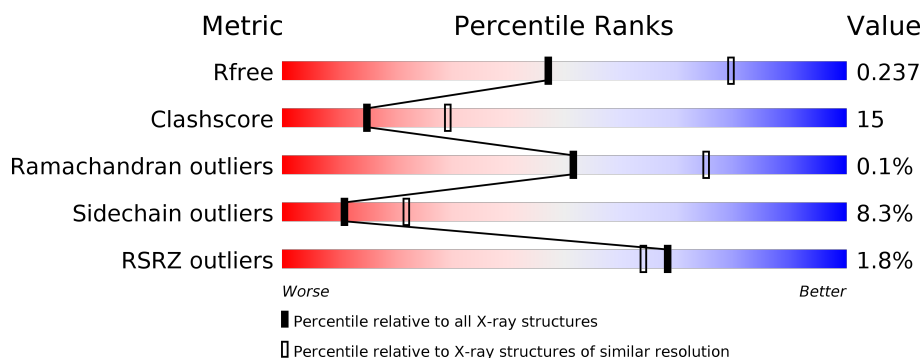
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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	334	<div> <div>0%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>•</div> </div> </div>
1	B	334	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>•</div> </div> </div>
1	C	334	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>•</div> </div> </div>
1	D	334	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>•</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MPD	A	1002	-	-	X	-
3	MPD	B	1001	-	-	X	-
3	MPD	C	1000	-	-	X	-
3	MPD	C	1001	-	-	X	-
3	MPD	C	1003	-	-	X	-
3	MPD	D	1001	-	-	X	-

2 Entry composition [i](#)

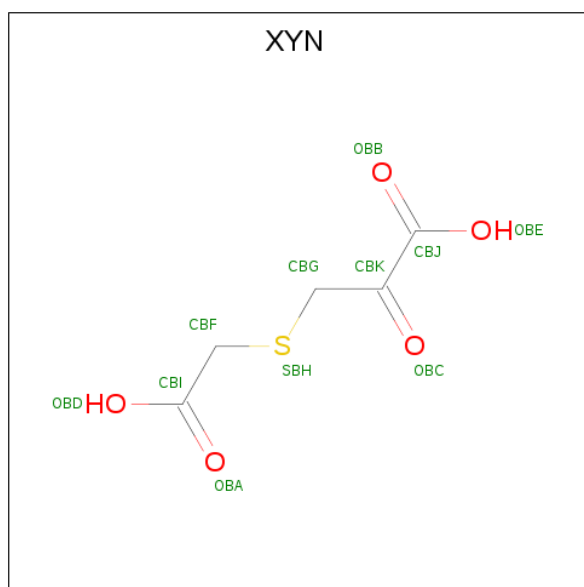
There are 5 unique types of molecules in this entry. The entry contains 10657 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Homoisocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2519	1590	448	474	7			
1	B	333	Total	C	N	O	S	0	0	0
			2519	1590	448	474	7			
1	C	333	Total	C	N	O	S	0	0	0
			2519	1590	448	474	7			
1	D	333	Total	C	N	O	S	0	1	0
			2527	1595	451	474	7			

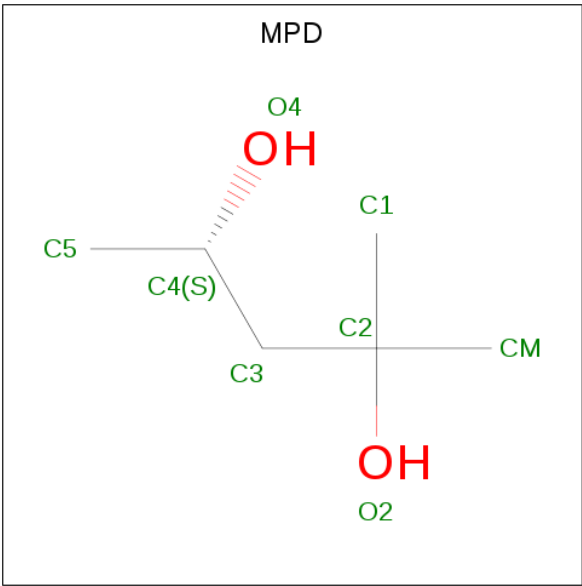
- Molecule 2 is 3-[(carboxymethyl)sulfanyl]-2-oxopropanoic acid (three-letter code: XYN) (formula: C₅H₆O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			11	5	5	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:

C₆H₁₄O₂).



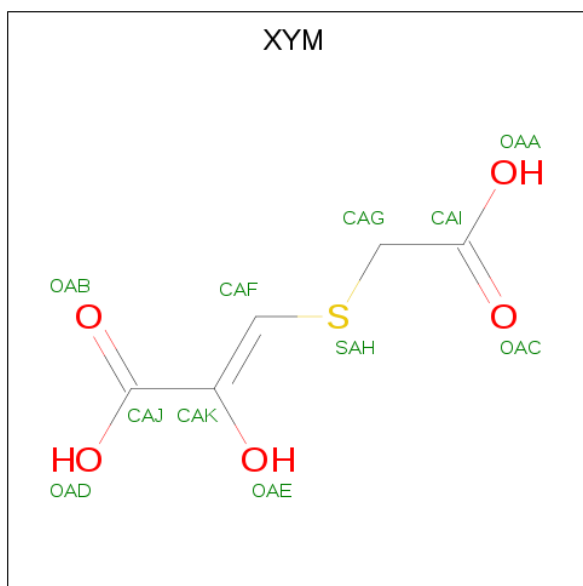
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0

- Molecule 4 is (2Z)-3-[(carboxymethyl)sulfanyl]-2-hydroxyprop-2-enoic acid (three-letter code: XYM) (formula: C₅H₆O₅S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O S 11 5 5 1	0	0
4	D	1	Total C O S 11 5 5 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	119	Total O 119 119	0	0

Continued on next page...

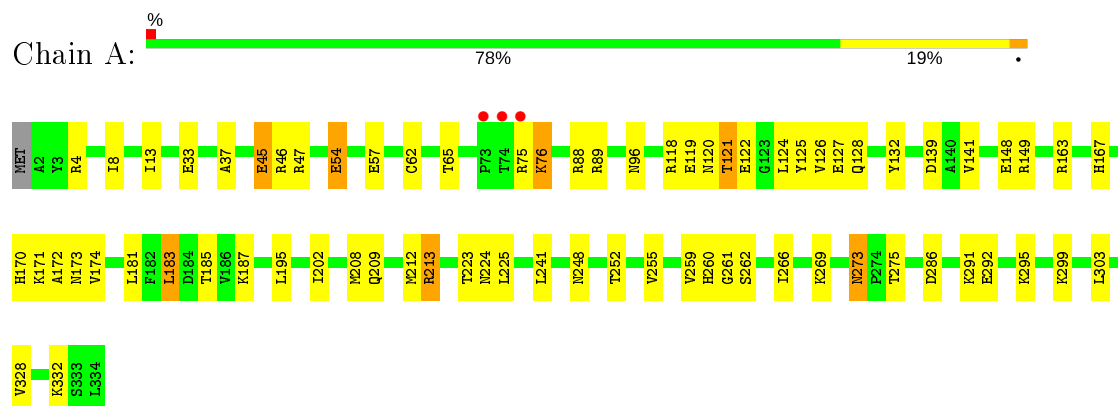
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	95	Total 95	O 95	0	0
5	C	79	Total 79	O 79	0	0
5	D	95	Total 95	O 95	0	0

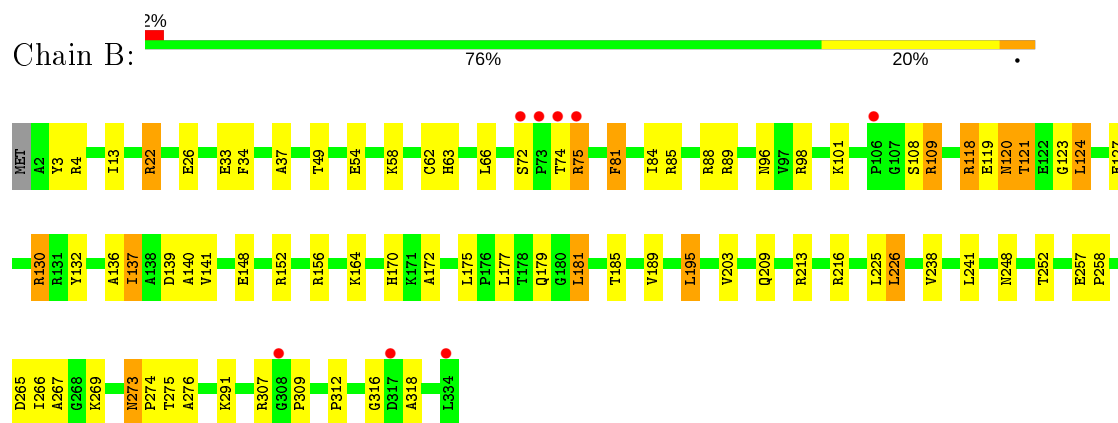
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

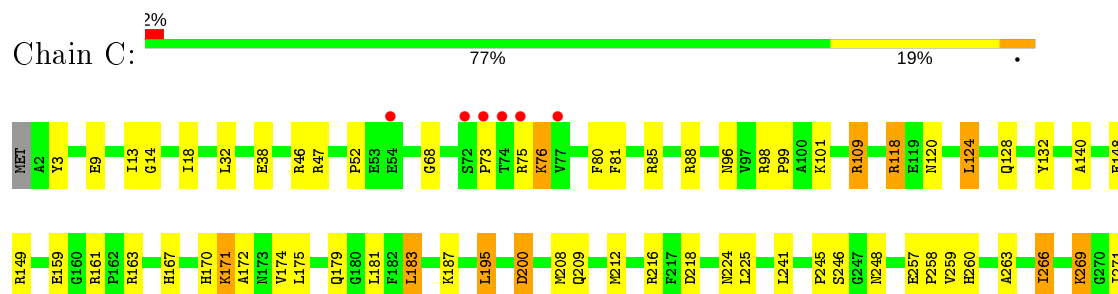
• Molecule 1: Homoisocitrate dehydrogenase

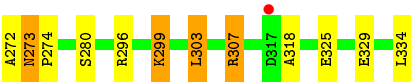


• Molecule 1: Homoisocitrate dehydrogenase

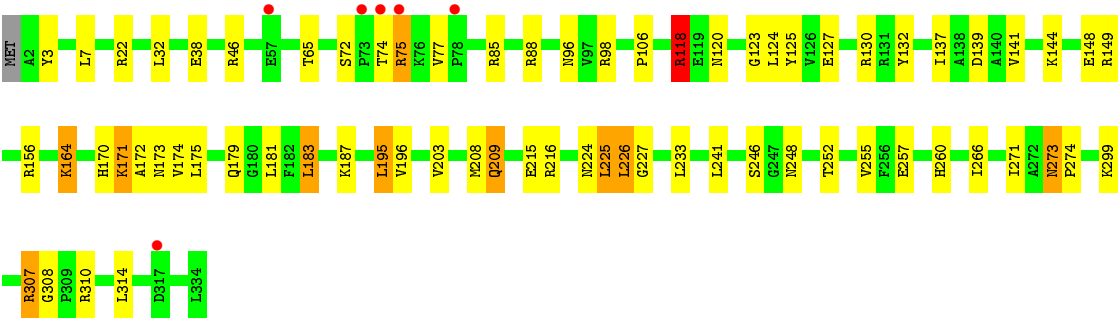
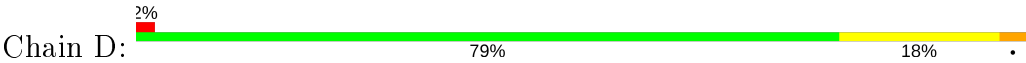


• Molecule 1: Homoisocitrate dehydrogenase





● Molecule 1: Homoisocitrate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	220.97Å 93.69Å 88.80Å 90.00° 97.68° 90.00°	Depositor
Resolution (Å)	44.02 – 2.60 44.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.02-2.60) 99.8 (44.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.169 , 0.231 0.174 , 0.237	Depositor DCC
R_{free} test set	2799 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10657	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, XYM, XYN

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	0.67	0/2560	0.75	0/3474
1	B	0.65	0/2560	0.75	1/3474 (0.0%)
1	C	0.65	0/2560	0.73	0/3474
1	D	0.66	0/2571	0.78	2/3488 (0.1%)
All	All	0.66	0/10251	0.75	3/13910 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	B	130	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	139	ASP	CB-CG-OD1	5.08	122.88	118.30

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	2519	0	2582	60	0
1	B	2519	0	2582	81	0
1	C	2519	0	2582	95	0
1	D	2527	0	2595	66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	11	0	4	0	0
3	A	40	0	70	21	0
3	B	56	0	98	18	0
3	C	32	0	56	38	0
3	D	24	0	42	20	0
4	B	11	0	3	1	0
4	D	11	0	3	1	0
5	A	119	0	0	6	0
5	B	95	0	0	6	0
5	C	79	0	0	10	0
5	D	95	0	0	7	0
All	All	10657	0	10617	315	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (315) 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)
3:D:1001:MPD:C5	3:D:1001:MPD:HM1	1.55	1.24
3:D:1001:MPD:H52	3:D:1001:MPD:CM	1.73	1.18
3:C:1003:MPD:C5	3:C:1003:MPD:HM2	1.74	1.18
1:A:208:MET:HE1	1:B:241:LEU:CG	1.75	1.16
1:C:124:LEU:H	3:C:1001:MPD:H11	1.01	1.15
1:C:273:ASN:H	3:C:1003:MPD:HM3	1.05	1.09
1:A:208:MET:CE	1:B:241:LEU:HG	1.81	1.09
1:D:124:LEU:H	3:D:1001:MPD:H11	1.15	1.07
3:C:1001:MPD:HM1	3:C:1001:MPD:O4	1.50	1.06
1:C:124:LEU:HD23	3:C:1001:MPD:HM2	1.34	1.05
1:B:124:LEU:H	3:B:1001:MPD:H52	1.24	1.03
1:C:124:LEU:CD2	3:C:1001:MPD:HM2	1.90	1.01
3:A:1004:MPD:H12	3:A:1004:MPD:H52	1.42	1.01
3:C:1003:MPD:H52	3:C:1003:MPD:HM2	1.00	0.99
3:C:1003:MPD:H52	3:C:1003:MPD:CM	1.89	0.99
1:B:273:ASN:H	3:B:1003:MPD:HM3	1.25	0.99
3:D:1001:MPD:C5	3:D:1001:MPD:CM	2.38	0.97
3:C:1003:MPD:C5	3:C:1003:MPD:CM	2.44	0.95
1:A:170:HIS:HD2	1:A:172:ALA:H	1.15	0.95
1:B:81:PHE:H	1:B:81:PHE:HD1	1.16	0.94
1:C:18:ILE:HD11	1:C:68:GLY:HA2	1.51	0.93
1:A:208:MET:HE1	1:B:241:LEU:HG	0.93	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:HIS:HD2	1:C:172:ALA:H	1.11	0.92
1:B:124:LEU:HD22	3:B:1001:MPD:C1	2.00	0.92
3:C:1000:MPD:HM2	3:C:1000:MPD:H52	1.53	0.91
1:B:170:HIS:HD2	1:B:172:ALA:H	1.14	0.91
1:C:13:ILE:CD1	3:C:1003:MPD:H12	2.01	0.91
1:C:124:LEU:N	3:C:1001:MPD:H11	1.86	0.90
3:C:1000:MPD:HM2	3:C:1000:MPD:C5	2.00	0.90
1:A:122:GLU:HG2	3:A:1003:MPD:O2	1.70	0.90
1:C:307:ARG:HD3	5:C:1075:HOH:O	1.71	0.90
1:A:124:LEU:H	3:A:1002:MPD:HM2	1.35	0.89
1:D:170:HIS:HD2	1:D:172:ALA:H	1.14	0.88
1:D:85:ARG:NH1	1:D:127:GLU:HG3	1.87	0.88
1:D:124:LEU:HD12	3:D:1001:MPD:HM2	1.55	0.87
1:C:273:ASN:N	3:C:1003:MPD:HM3	1.89	0.87
1:B:140:ALA:HB1	3:B:1001:MPD:H13	1.57	0.84
1:C:18:ILE:CD1	1:C:68:GLY:HA2	2.09	0.83
1:C:179:GLN:HE21	3:C:1001:MPD:H4	1.43	0.82
1:B:124:LEU:HD22	3:B:1001:MPD:H12	1.63	0.81
1:D:75:ARG:HD2	1:D:77:VAL:HG22	1.63	0.81
1:A:88:ARG:HE	1:A:248:ASN:ND2	1.79	0.80
3:C:1001:MPD:O4	3:C:1001:MPD:CM	2.29	0.79
1:C:170:HIS:CD2	1:C:172:ALA:H	2.00	0.79
1:A:4:ARG:HD3	1:A:33:GLU:OE1	1.83	0.78
1:C:272:ALA:HB1	3:C:1003:MPD:H13	1.66	0.78
1:C:225:LEU:H	3:C:1001:MPD:H13	1.47	0.78
1:D:124:LEU:N	3:D:1001:MPD:H11	1.98	0.77
1:B:209:GLN:HE22	1:B:213:ARG:HE	1.33	0.77
3:D:1001:MPD:H52	3:D:1001:MPD:HM1	0.78	0.75
1:C:195:LEU:HD12	1:C:195:LEU:H	1.52	0.74
1:C:13:ILE:HD13	3:C:1003:MPD:H12	1.68	0.74
1:B:81:PHE:CD1	1:B:81:PHE:N	2.56	0.73
1:B:81:PHE:HD1	1:B:81:PHE:N	1.85	0.73
1:D:170:HIS:CD2	1:D:172:ALA:H	2.04	0.73
1:C:124:LEU:HD23	3:C:1001:MPD:CM	2.15	0.73
1:B:54:GLU:HG2	3:B:1006:MPD:HM2	1.71	0.72
1:C:118:ARG:HH12	3:C:1000:MPD:H31	1.53	0.72
3:C:1000:MPD:C5	3:C:1000:MPD:CM	2.67	0.72
1:C:225:LEU:HB3	3:C:1001:MPD:HM3	1.70	0.71
1:C:266:ILE:HG13	1:C:271:ILE:HD11	1.72	0.71
1:A:65:THR:HB	1:A:255:VAL:HG22	1.72	0.71
1:A:121:THR:HG22	1:A:122:GLU:HG3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1004:MPD:C1	3:A:1004:MPD:H52	2.20	0.71
1:C:109:ARG:CG	1:C:109:ARG:HH21	2.04	0.70
1:D:85:ARG:HH12	1:D:127:GLU:HG3	1.53	0.70
1:C:18:ILE:CD1	1:C:68:GLY:CA	2.69	0.70
1:A:119:GLU:OE2	1:A:121:THR:HB	1.91	0.69
1:B:203:VAL:HG21	1:B:226:LEU:HG	1.75	0.69
1:D:307:ARG:CD	5:D:1090:HOH:O	2.40	0.69
1:D:124:LEU:HD12	3:D:1001:MPD:CM	2.21	0.69
1:D:307:ARG:HD3	5:D:1090:HOH:O	1.91	0.69
1:C:18:ILE:HD11	1:C:68:GLY:CA	2.23	0.68
3:A:1002:MPD:O4	3:A:1002:MPD:H11	1.92	0.68
3:D:1003:MPD:H52	3:D:1003:MPD:H11	1.73	0.68
1:A:208:MET:SD	1:A:212:MET:HE1	2.34	0.68
1:B:124:LEU:N	3:B:1001:MPD:H52	2.06	0.67
1:D:174:VAL:HG23	1:D:175:LEU:HG	1.76	0.67
1:C:299:LYS:HB3	1:C:334:LEU:HD11	1.77	0.67
1:B:124:LEU:H	3:B:1001:MPD:C5	2.05	0.66
3:A:1002:MPD:O4	3:A:1002:MPD:C1	2.43	0.66
3:B:1001:MPD:H52	3:B:1001:MPD:H11	1.78	0.66
1:B:273:ASN:H	3:B:1003:MPD:CM	2.04	0.66
1:D:203:VAL:HG21	1:D:226:LEU:HG	1.78	0.66
3:A:1003:MPD:H52	3:A:1003:MPD:HM1	1.77	0.65
1:C:149:ARG:HD2	5:C:1073:HOH:O	1.97	0.65
1:C:109:ARG:HG2	1:C:109:ARG:HH21	1.63	0.64
1:C:208:MET:CE	1:D:241:LEU:HG	2.28	0.64
1:D:179:GLN:NE2	3:D:1001:MPD:H53	2.13	0.64
1:C:13:ILE:HD12	3:C:1003:MPD:H12	1.80	0.63
1:A:124:LEU:H	3:A:1002:MPD:CM	2.11	0.63
1:C:109:ARG:HB3	1:C:109:ARG:HH21	1.64	0.62
1:C:266:ILE:HG13	1:C:271:ILE:CD1	2.30	0.61
1:B:124:LEU:HD22	3:B:1001:MPD:H11	1.79	0.61
1:A:225:LEU:H	3:A:1002:MPD:HM3	1.63	0.61
1:C:171:LYS:NZ	4:D:1000:XYM:OAC	2.34	0.61
1:A:225:LEU:H	3:A:1002:MPD:CM	2.14	0.61
3:C:1001:MPD:HM1	3:C:1001:MPD:HO4	1.64	0.61
1:C:98:ARG:HD3	5:C:1042:HOH:O	2.01	0.61
1:C:183:LEU:HD22	1:C:187:LYS:HD2	1.83	0.61
1:A:328:VAL:O	1:A:332:LYS:HG3	2.00	0.61
3:A:1001:MPD:O2	3:A:1001:MPD:H52	2.01	0.60
1:C:179:GLN:NE2	3:C:1001:MPD:H4	2.15	0.60
1:C:109:ARG:NH2	1:C:109:ARG:HG2	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:GLN:HE21	3:D:1001:MPD:H53	1.68	0.59
3:D:1003:MPD:H53	3:D:1003:MPD:HM2	1.84	0.59
3:A:1001:MPD:O2	3:A:1001:MPD:C5	2.50	0.59
1:C:225:LEU:H	3:C:1001:MPD:C1	2.14	0.58
1:A:183:LEU:HD22	1:A:187:LYS:HD3	1.86	0.58
1:A:208:MET:SD	1:A:212:MET:CE	2.91	0.58
1:D:225:LEU:H	3:D:1001:MPD:H13	1.67	0.58
1:C:159:GLU:OE1	1:C:195:LEU:HD13	2.03	0.58
3:D:1002:MPD:CM	5:D:1091:HOH:O	2.52	0.58
1:C:46:ARG:HD2	5:C:1026:HOH:O	2.04	0.57
3:A:1003:MPD:H13	5:A:1052:HOH:O	2.04	0.57
1:B:137:ILE:HD12	1:D:137:ILE:HD12	1.86	0.57
1:C:75:ARG:O	1:C:76:LYS:HB3	2.04	0.57
1:C:96:ASN:HB3	1:C:118:ARG:HG2	1.87	0.57
1:C:109:ARG:CB	1:C:109:ARG:HH21	2.17	0.57
1:A:124:LEU:N	3:A:1002:MPD:HM2	2.14	0.56
1:B:225:LEU:H	3:B:1001:MPD:H51	1.70	0.56
1:D:225:LEU:HB2	3:D:1001:MPD:H13	1.87	0.56
1:A:170:HIS:CD2	1:A:172:ALA:H	2.07	0.56
1:A:120:ASN:HD21	1:A:248:ASN:HD22	1.52	0.56
3:C:1000:MPD:HM2	3:C:1000:MPD:H53	1.84	0.56
3:D:1002:MPD:HM3	5:D:1091:HOH:O	2.06	0.56
1:D:183:LEU:HD22	1:D:187:LYS:HD2	1.87	0.56
1:D:310:ARG:HG3	1:D:314:LEU:HB2	1.86	0.56
1:A:96:ASN:HD22	1:A:118:ARG:HG2	1.71	0.55
1:B:123:GLY:HA3	3:B:1001:MPD:H53	1.88	0.55
1:C:18:ILE:HD13	1:C:68:GLY:CA	2.35	0.55
1:A:225:LEU:CB	3:A:1002:MPD:HM1	2.37	0.55
1:B:22:ARG:NH2	1:B:34:PHE:CD1	2.75	0.55
1:B:4:ARG:HD3	1:B:33:GLU:OE1	2.06	0.55
1:B:49:THR:HG1	1:B:81:PHE:HZ	1.53	0.55
1:C:120:ASN:HD21	1:C:248:ASN:HD22	1.53	0.55
1:B:54:GLU:HG2	3:B:1006:MPD:CM	2.35	0.55
1:D:124:LEU:CD1	3:D:1001:MPD:HM2	2.31	0.55
3:C:1000:MPD:CM	3:C:1000:MPD:H53	2.37	0.55
1:C:167:HIS:HD2	5:C:1056:HOH:O	1.90	0.55
1:C:3:TYR:HB2	1:C:32:LEU:HD23	1.89	0.55
1:D:260:HIS:HE1	5:D:1004:HOH:O	1.90	0.54
1:A:124:LEU:HD11	1:B:124:LEU:HD21	1.89	0.54
1:B:170:HIS:CD2	1:B:172:ALA:H	2.07	0.54
1:D:183:LEU:HD22	1:D:187:LYS:CD	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:LEU:CD2	1:D:187:LYS:HD2	2.38	0.54
1:B:85:ARG:HH22	4:B:1000:XYM:HAG	1.72	0.54
1:B:119:GLU:OE1	1:B:121:THR:HB	2.08	0.53
1:A:225:LEU:HB3	3:A:1002:MPD:HM1	1.90	0.53
1:C:18:ILE:HD13	1:C:68:GLY:HA3	1.91	0.53
3:A:1004:MPD:C1	3:A:1004:MPD:C5	2.85	0.53
1:D:7:LEU:HD11	1:D:22[A]:ARG:HG3	1.91	0.53
1:D:88:ARG:HH21	1:D:248:ASN:HD21	1.57	0.53
3:B:1005:MPD:H11	3:B:1005:MPD:H53	1.90	0.53
1:B:37:ALA:HB2	1:B:58:LYS:HD3	1.90	0.53
1:A:292:GLU:OE2	1:A:295:LYS:HE3	2.09	0.52
1:A:46:ARG:O	1:A:47:ARG:HG3	2.09	0.52
1:B:124:LEU:CD2	3:B:1001:MPD:H12	2.36	0.52
1:C:163:ARG:HD3	5:C:1034:HOH:O	2.09	0.52
1:D:209:GLN:HE21	1:D:216:ARG:HH21	1.57	0.52
1:D:164:LYS:HG3	1:D:196:VAL:HA	1.91	0.52
1:A:223:THR:HB	3:A:1002:MPD:C1	2.40	0.52
1:C:124:LEU:HD22	3:C:1001:MPD:HM2	1.88	0.52
1:B:216:ARG:O	1:B:216:ARG:HG3	2.09	0.51
1:B:258:PRO:HB3	1:B:276:ALA:CB	2.40	0.51
1:D:164:LYS:HG2	1:D:195:LEU:O	2.11	0.51
1:B:273:ASN:ND2	1:B:275:THR:H	2.08	0.51
1:C:118:ARG:NH2	1:C:224:ASN:OD1	2.43	0.51
1:A:273:ASN:ND2	1:A:275:THR:H	2.08	0.51
1:A:125:TYR:HB2	1:A:224:ASN:ND2	2.26	0.51
1:C:118:ARG:NH1	3:C:1000:MPD:H31	2.24	0.51
1:B:258:PRO:HB3	1:B:276:ALA:HB1	1.92	0.50
1:B:4:ARG:CD	1:B:33:GLU:OE1	2.59	0.50
1:A:171:LYS:HE3	1:A:174:VAL:HG13	1.92	0.50
1:C:96:ASN:HB3	1:C:118:ARG:CG	2.42	0.50
1:D:144:LYS:O	1:D:148:GLU:HG3	2.11	0.50
1:D:88:ARG:HE	1:D:248:ASN:ND2	2.10	0.50
1:B:89:ARG:HG2	5:B:1096:HOH:O	2.10	0.50
1:B:273:ASN:HD22	1:B:274:PRO:N	2.09	0.50
1:B:309:PRO:HB2	1:B:318:ALA:HB2	1.93	0.50
1:C:299:LYS:HB3	1:C:334:LEU:CD1	2.41	0.50
1:A:45:GLU:HB2	5:A:1099:HOH:O	2.11	0.50
1:D:106:PRO:HD3	1:D:310:ARG:HH12	1.76	0.50
1:B:209:GLN:HE22	1:B:213:ARG:NE	2.08	0.49
1:C:13:ILE:HD11	1:C:260:HIS:CD2	2.47	0.49
1:C:124:LEU:HD21	1:D:124:LEU:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ARG:HD2	5:D:1090:HOH:O	2.06	0.49
1:A:208:MET:HE1	1:B:241:LEU:CD2	2.42	0.49
1:C:73:PRO:HD2	1:C:80:PHE:CE1	2.48	0.49
1:B:266:ILE:O	1:B:269:LYS:HB2	2.13	0.49
1:A:148:GLU:HG3	1:A:185:THR:CG2	2.43	0.49
1:B:22:ARG:NH2	1:B:26:GLU:OE2	2.46	0.49
3:A:1004:MPD:H12	3:A:1004:MPD:C5	2.25	0.48
1:A:208:MET:HG2	1:A:212:MET:HE2	1.95	0.48
1:D:96:ASN:HB3	1:D:118:ARG:HG2	1.95	0.48
1:C:174:VAL:HG23	1:C:175:LEU:HG	1.96	0.48
1:A:260:HIS:HD2	1:A:261:GLY:O	1.96	0.48
1:B:195:LEU:HB2	5:B:1092:HOH:O	2.12	0.48
1:C:13:ILE:CD1	3:C:1003:MPD:C1	2.85	0.48
1:C:209:GLN:OE1	1:C:216:ARG:NH2	2.39	0.48
1:C:76:LYS:O	1:C:76:LYS:CG	2.61	0.48
1:B:75:ARG:NH1	1:B:75:ARG:HB3	2.29	0.48
1:A:141:VAL:HG21	1:D:132:TYR:CZ	2.49	0.48
1:B:141:VAL:HG21	1:C:132:TYR:CZ	2.49	0.48
1:B:89:ARG:NE	5:B:1100:HOH:O	2.47	0.48
1:C:266:ILE:O	1:C:269:LYS:HB2	2.14	0.48
1:D:96:ASN:HD22	1:D:118:ARG:HG2	1.78	0.48
1:A:266:ILE:HA	1:A:269:LYS:HD2	1.95	0.47
1:B:273:ASN:HD22	1:B:274:PRO:CD	2.27	0.47
1:B:273:ASN:HD22	1:B:274:PRO:HD2	1.78	0.47
1:A:128:GLN:HE21	1:D:130:ARG:HG2	1.79	0.47
1:C:263:ALA:HB1	1:C:266:ILE:CG2	2.45	0.47
1:D:156:ARG:NE	5:D:1048:HOH:O	2.47	0.47
1:C:13:ILE:HD13	3:C:1003:MPD:C1	2.42	0.47
1:C:260:HIS:HE1	5:C:1069:HOH:O	1.98	0.47
1:B:13:ILE:HG22	1:B:267:ALA:HA	1.96	0.47
3:C:1003:MPD:H53	3:C:1003:MPD:CM	2.41	0.47
3:D:1002:MPD:O2	3:D:1002:MPD:H52	2.14	0.47
1:A:167:HIS:HD2	5:A:1009:HOH:O	1.97	0.47
1:A:76:LYS:HE3	1:A:76:LYS:O	2.15	0.47
1:B:123:GLY:HA3	3:B:1001:MPD:C5	2.45	0.46
1:B:98:ARG:HD3	5:B:1088:HOH:O	2.14	0.46
1:C:303:LEU:O	1:C:307:ARG:HD2	2.14	0.46
1:C:98:ARG:HD2	1:C:246:SER:HB3	1.98	0.46
1:A:139:ASP:OD2	1:D:130:ARG:HD2	2.16	0.46
1:D:118:ARG:HB2	1:D:227:GLY:HA3	1.97	0.46
1:C:273:ASN:HD22	1:C:274:PRO:HD2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:TYR:HB2	1:D:224:ASN:ND2	2.31	0.46
1:A:13:ILE:HG12	1:A:262:SER:O	2.16	0.45
1:B:152:ARG:O	1:B:156:ARG:HG3	2.17	0.45
1:C:208:MET:HG2	1:C:212:MET:HE2	1.97	0.45
1:D:215:GLU:CD	1:D:215:GLU:H	2.20	0.45
1:B:273:ASN:HD22	1:B:273:ASN:C	2.19	0.45
1:B:312:PRO:HA	1:B:316:GLY:O	2.16	0.45
1:C:183:LEU:HD22	1:C:187:LYS:CD	2.46	0.45
1:A:4:ARG:HG2	1:A:62:CYS:SG	2.56	0.45
1:A:260:HIS:HE1	5:A:1007:HOH:O	2.00	0.45
1:B:96:ASN:HB3	1:B:118:ARG:HG2	1.98	0.45
1:C:88:ARG:HE	1:C:248:ASN:ND2	2.15	0.45
1:C:257:GLU:HG2	1:C:258:PRO:O	2.17	0.45
1:D:106:PRO:HD3	1:D:310:ARG:NH1	2.30	0.45
1:D:170:HIS:HD2	1:D:172:ALA:N	1.97	0.45
1:B:156:ARG:HD2	5:B:1077:HOH:O	2.16	0.44
1:A:208:MET:CE	1:B:241:LEU:CG	2.65	0.44
1:D:98:ARG:HD2	1:D:246:SER:HB3	1.98	0.44
1:A:223:THR:HB	3:A:1002:MPD:H13	2.00	0.44
1:D:65:THR:HB	1:D:255:VAL:HG22	2.00	0.44
1:A:209:GLN:HE22	1:A:213:ARG:HH21	1.66	0.44
1:B:120:ASN:ND2	5:B:1056:HOH:O	2.50	0.44
1:B:130:ARG:HG2	1:C:128:GLN:NE2	2.33	0.44
3:B:1005:MPD:C1	3:B:1005:MPD:H53	2.47	0.44
1:C:318:ALA:HA	5:C:1080:HOH:O	2.17	0.44
1:A:132:TYR:CZ	1:D:141:VAL:HG21	2.52	0.43
1:D:225:LEU:HB3	3:D:1001:MPD:HM3	2.00	0.43
1:C:241:LEU:HG	1:D:208:MET:SD	2.58	0.43
1:C:9:GLU:O	1:C:14:GLY:HA3	2.18	0.43
1:A:173:ASN:ND2	1:A:202:ILE:HD13	2.34	0.43
1:C:109:ARG:NH2	1:C:109:ARG:CG	2.70	0.43
1:C:47:ARG:HH11	1:C:52:PRO:HB3	1.84	0.43
1:B:132:TYR:OH	1:C:128:GLN:HG3	2.19	0.43
1:D:85:ARG:NH1	1:D:127:GLU:CG	2.69	0.43
1:A:88:ARG:HE	1:A:248:ASN:HD21	1.59	0.43
1:C:76:LYS:O	1:C:76:LYS:HG2	2.19	0.43
1:A:171:LYS:HE3	1:A:174:VAL:CG1	2.48	0.43
1:B:137:ILE:HD12	1:D:137:ILE:CD1	2.48	0.43
1:C:140:ALA:HB1	3:C:1001:MPD:H53	2.01	0.43
1:C:208:MET:HE1	1:D:241:LEU:HG	1.98	0.43
1:B:88:ARG:HH21	1:B:248:ASN:HD21	1.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:LYS:HD2	1:D:203:VAL:HG12	2.01	0.42
1:C:85:ARG:HG2	5:C:1083:HOH:O	2.19	0.42
1:B:175:LEU:O	1:B:179:GLN:HB2	2.19	0.42
1:C:118:ARG:HH12	3:C:1000:MPD:C3	2.25	0.42
1:C:208:MET:SD	1:C:212:MET:HE1	2.58	0.42
1:C:161:ARG:NH2	1:C:218:ASP:OD1	2.52	0.42
1:A:259:VAL:O	1:A:259:VAL:HG12	2.20	0.42
1:A:8:ILE:HG12	1:A:37:ALA:HB3	2.02	0.42
1:B:130:ARG:HG2	1:C:128:GLN:HE21	1.84	0.42
1:A:208:MET:CE	1:B:241:LEU:CD2	2.98	0.42
1:D:96:ASN:HB3	1:D:118:ARG:CG	2.50	0.42
1:C:149:ARG:CD	5:C:1073:HOH:O	2.62	0.42
1:D:171:LYS:HE2	1:D:173:ASN:OD1	2.20	0.42
1:D:273:ASN:HD22	1:D:274:PRO:HD2	1.85	0.42
1:A:88:ARG:HH21	1:A:248:ASN:HD21	1.68	0.42
1:B:85:ARG:HD3	1:B:127:GLU:OE1	2.19	0.42
1:C:299:LYS:HA	1:C:299:LYS:HD3	1.87	0.42
1:B:118:ARG:HG3	1:B:118:ARG:O	2.19	0.42
1:B:3:TYR:HA	1:B:63:HIS:CE1	2.55	0.41
1:C:98:ARG:CZ	1:C:259:VAL:HG21	2.50	0.41
1:A:273:ASN:HD22	1:A:273:ASN:C	2.23	0.41
1:B:238:VAL:O	1:B:238:VAL:HG23	2.19	0.41
3:C:1000:MPD:O4	1:D:171:LYS:NZ	2.52	0.41
1:B:109:ARG:HB3	1:B:109:ARG:HE	1.37	0.41
1:B:148:GLU:HG3	1:B:185:THR:HG21	2.02	0.41
1:B:4:ARG:O	1:B:62:CYS:HB3	2.20	0.41
1:B:88:ARG:HE	1:B:248:ASN:ND2	2.18	0.41
1:C:170:HIS:HE1	1:C:200:ASP:OD1	2.03	0.41
1:D:3:TYR:HB2	1:D:32:LEU:HD23	2.02	0.41
1:C:208:MET:HE3	1:D:241:LEU:HG	2.03	0.41
1:B:120:ASN:HD22	1:B:120:ASN:HA	1.74	0.41
1:A:286:ASP:HB2	3:A:1001:MPD:H11	2.03	0.41
1:B:273:ASN:ND2	1:B:273:ASN:C	2.74	0.41
1:C:81:PHE:CD1	1:C:81:PHE:N	2.89	0.41
1:B:136:ALA:C	1:B:137:ILE:HG12	2.41	0.41
1:B:49:THR:OG1	1:B:81:PHE:HZ	2.03	0.41
1:C:99:PRO:HG2	1:C:245:PRO:HG2	2.03	0.41
1:D:266:ILE:HD12	1:D:271:ILE:HD11	2.03	0.41
1:C:88:ARG:HH12	3:C:1000:MPD:H32	1.86	0.40
1:A:149:ARG:HD2	5:A:1015:HOH:O	2.20	0.40
1:A:54:GLU:HB3	5:A:1074:HOH:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:O	1:B:181:LEU:HB2	2.22	0.40
1:D:233:LEU:C	1:D:233:LEU:HD23	2.42	0.40
1:B:130:ARG:NH2	1:B:139:ASP:OD1	2.54	0.40
1:D:123:GLY:HA3	3:D:1001:MPD:C1	2.51	0.40
1:D:85:ARG:HH11	1:D:127:GLU:HG3	1.79	0.40
1:D:38:GLU:OE2	1:D:46:ARG:NH2	2.54	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	331/334 (99%)	312 (94%)	19 (6%)	0	100	100
1	B	331/334 (99%)	313 (95%)	18 (5%)	0	100	100
1	C	331/334 (99%)	311 (94%)	20 (6%)	0	100	100
1	D	332/334 (99%)	317 (96%)	14 (4%)	1 (0%)	41	64
All	All	1325/1336 (99%)	1253 (95%)	71 (5%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	308	GLY

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	263/264 (100%)	243 (92%)	20 (8%)	13	26
1	B	263/264 (100%)	237 (90%)	26 (10%)	8	15
1	C	263/264 (100%)	241 (92%)	22 (8%)	11	21
1	D	264/264 (100%)	245 (93%)	19 (7%)	14	29
All	All	1053/1056 (100%)	966 (92%)	87 (8%)	11	22

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	54	GLU
1	A	57	GLU
1	A	75	ARG
1	A	76	LYS
1	A	89	ARG
1	A	121	THR
1	A	126	VAL
1	A	127	GLU
1	A	163	ARG
1	A	181	LEU
1	A	183	LEU
1	A	195	LEU
1	A	213	ARG
1	A	241	LEU
1	A	252	THR
1	A	273	ASN
1	A	291	LYS
1	A	299	LYS
1	A	303	LEU
1	B	22	ARG
1	B	66	LEU
1	B	72	SER
1	B	74	THR
1	B	75	ARG
1	B	81	PHE
1	B	84	ILE
1	B	101	LYS
1	B	108	SER
1	B	109	ARG
1	B	118	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	120	ASN
1	B	121	THR
1	B	124	LEU
1	B	137	ILE
1	B	164	LYS
1	B	181	LEU
1	B	189	VAL
1	B	195	LEU
1	B	226	LEU
1	B	252	THR
1	B	257	GLU
1	B	265	ASP
1	B	273	ASN
1	B	291	LYS
1	B	307	ARG
1	C	38	GLU
1	C	76	LYS
1	C	101	LYS
1	C	109	ARG
1	C	118	ARG
1	C	124	LEU
1	C	148	GLU
1	C	171	LYS
1	C	181	LEU
1	C	183	LEU
1	C	195	LEU
1	C	200	ASP
1	C	266	ILE
1	C	269	LYS
1	C	273	ASN
1	C	280	SER
1	C	296	ARG
1	C	299	LYS
1	C	303	LEU
1	C	307	ARG
1	C	325	GLU
1	C	329	GLU
1	D	72	SER
1	D	74	THR
1	D	75	ARG
1	D	118	ARG
1	D	120	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	149	ARG
1	D	164	LYS
1	D	171	LYS
1	D	181	LEU
1	D	183	LEU
1	D	195	LEU
1	D	209	GLN
1	D	225	LEU
1	D	226	LEU
1	D	252	THR
1	D	257	GLU
1	D	273	ASN
1	D	299	LYS
1	D	307	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	128	GLN
1	A	167	HIS
1	A	170	HIS
1	A	205	ASN
1	A	248	ASN
1	A	260	HIS
1	A	273	ASN
1	B	96	ASN
1	B	120	ASN
1	B	167	HIS
1	B	170	HIS
1	B	209	GLN
1	B	248	ASN
1	B	273	ASN
1	C	96	ASN
1	C	128	GLN
1	C	167	HIS
1	C	170	HIS
1	C	205	ASN
1	C	248	ASN
1	C	260	HIS
1	C	273	ASN
1	D	96	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	120	ASN
1	D	170	HIS
1	D	197	ASN
1	D	199	GLN
1	D	209	GLN
1	D	248	ASN
1	D	260	HIS
1	D	273	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](#)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MPD	B	1006	-	7,7,7	0.35	0	9,10,10	0.77	0
3	MPD	A	1005	-	7,7,7	0.27	0	9,10,10	0.55	0
3	MPD	B	1007	-	7,7,7	0.44	0	9,10,10	0.92	0
3	MPD	B	1003	-	7,7,7	0.36	0	9,10,10	0.65	0
3	MPD	A	1003	-	7,7,7	0.40	0	9,10,10	0.99	0
3	MPD	D	1003	-	7,7,7	0.43	0	9,10,10	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MPD	B	1002	-	7,7,7	0.30	0	9,10,10	0.51	0
3	MPD	C	1000	-	7,7,7	0.43	0	9,10,10	0.83	0
3	MPD	B	1005	-	7,7,7	0.39	0	9,10,10	0.55	0
2	XYN	A	1000	-	4,10,10	1.05	0	4,12,12	2.67	3 (75%)
3	MPD	A	1002	-	7,7,7	0.37	0	9,10,10	1.52	1 (11%)
3	MPD	C	1003	-	7,7,7	0.30	0	9,10,10	0.56	0
4	XYM	D	1000	-	3,10,10	1.45	1 (33%)	2,12,12	2.07	1 (50%)
3	MPD	D	1001	-	7,7,7	0.42	0	9,10,10	1.93	3 (33%)
3	MPD	C	1001	-	7,7,7	0.51	0	9,10,10	1.34	2 (22%)
3	MPD	A	1001	-	7,7,7	0.27	0	9,10,10	0.54	0
3	MPD	B	1004	-	7,7,7	0.31	0	9,10,10	0.99	0
3	MPD	C	1002	-	7,7,7	0.28	0	9,10,10	0.89	0
4	XYM	B	1000	-	3,10,10	1.91	1 (33%)	2,12,12	2.40	1 (50%)
3	MPD	B	1001	-	7,7,7	0.52	0	9,10,10	1.18	2 (22%)
3	MPD	A	1004	-	7,7,7	0.25	0	9,10,10	0.66	0
3	MPD	D	1002	-	7,7,7	0.34	0	9,10,10	0.71	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
3	MPD	B	1006	-	-	1/5/5/5	-
3	MPD	A	1005	-	-	5/5/5/5	-
3	MPD	B	1007	-	-	1/5/5/5	-
3	MPD	B	1003	-	-	1/5/5/5	-
3	MPD	A	1003	-	-	4/5/5/5	-
3	MPD	D	1003	-	-	2/5/5/5	-
3	MPD	B	1002	-	-	3/5/5/5	-
3	MPD	C	1000	-	-	2/5/5/5	-
3	MPD	B	1005	-	-	1/5/5/5	-
2	XYN	A	1000	-	-	3/4/10/10	-
3	MPD	A	1002	-	-	3/5/5/5	-
3	MPD	C	1003	-	-	2/5/5/5	-
4	XYM	D	1000	-	-	2/2/10/10	-
3	MPD	D	1001	-	-	4/5/5/5	-
3	MPD	C	1001	-	-	2/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	A	1001	-	-	2/5/5/5	-
3	MPD	B	1004	-	-	0/5/5/5	-
3	MPD	C	1002	-	-	2/5/5/5	-
4	XYM	B	1000	-	-	1/2/10/10	-
3	MPD	B	1001	-	-	4/5/5/5	-
3	MPD	A	1004	-	-	1/5/5/5	-
3	MPD	D	1002	-	-	4/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1000	XYM	CAF-SAH	-2.70	1.69	1.73
4	D	1000	XYM	OAE-CAK	2.18	1.36	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	MPD	CM-C2-C1	-3.59	103.09	110.57
2	A	1000	XYN	CBF-SBH-CBG	-3.58	96.39	101.15
4	B	1000	XYM	CAG-SAH-CAF	-3.16	95.03	100.20
2	A	1000	XYN	CBK-CBG-SBH	-3.04	101.84	111.49
3	D	1001	MPD	O2-C2-C3	3.01	121.09	109.80
3	D	1001	MPD	O2-C2-C1	-2.70	99.40	108.08
3	C	1001	MPD	O2-C2-CM	-2.69	99.44	108.08
3	D	1001	MPD	CM-C2-C1	2.56	115.91	110.57
3	B	1001	MPD	C5-C4-C3	2.46	123.26	111.69
4	D	1000	XYM	OAE-CAK-CAF	-2.41	118.42	122.77
3	C	1001	MPD	O2-C2-C3	2.25	118.26	109.80
3	B	1001	MPD	O4-C4-C3	-2.12	102.81	111.36
2	A	1000	XYN	OBC-CBK-CBG	-2.09	117.71	120.55

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	MPD	O2-C2-C3-C4
3	A	1003	MPD	CM-C2-C3-C4
3	D	1003	MPD	C2-C3-C4-C5
3	C	1000	MPD	C2-C3-C4-O4
3	C	1000	MPD	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1000	XYN	SBH-CBG-CBK-OBC
2	A	1000	XYN	SBH-CBG-CBK-CBJ
3	C	1003	MPD	C2-C3-C4-O4
4	D	1000	XYM	CAK-CAF-SAH-CAG
3	D	1001	MPD	O2-C2-C3-C4
3	D	1001	MPD	CM-C2-C3-C4
3	A	1001	MPD	C2-C3-C4-O4
3	A	1001	MPD	C2-C3-C4-C5
4	B	1000	XYM	CAK-CAF-SAH-CAG
3	B	1001	MPD	C1-C2-C3-C4
4	D	1000	XYM	CAI-CAG-SAH-CAF
3	A	1005	MPD	O2-C2-C3-C4
3	B	1007	MPD	O2-C2-C3-C4
3	B	1001	MPD	O2-C2-C3-C4
3	D	1002	MPD	O2-C2-C3-C4
2	A	1000	XYN	CBI-CBF-SBH-CBG
3	C	1003	MPD	C2-C3-C4-C5
3	A	1004	MPD	C2-C3-C4-C5
3	C	1001	MPD	C2-C3-C4-O4
3	C	1002	MPD	C2-C3-C4-O4
3	B	1001	MPD	C2-C3-C4-O4
3	A	1005	MPD	C1-C2-C3-C4
3	A	1005	MPD	CM-C2-C3-C4
3	A	1003	MPD	C1-C2-C3-C4
3	A	1002	MPD	C1-C2-C3-C4
3	D	1001	MPD	C1-C2-C3-C4
3	D	1002	MPD	C1-C2-C3-C4
3	D	1002	MPD	CM-C2-C3-C4
3	B	1002	MPD	O2-C2-C3-C4
3	A	1002	MPD	O2-C2-C3-C4
3	B	1006	MPD	C2-C3-C4-C5
3	A	1005	MPD	C2-C3-C4-C5
3	B	1003	MPD	C2-C3-C4-C5
3	A	1003	MPD	C2-C3-C4-C5
3	B	1002	MPD	C2-C3-C4-C5
3	B	1005	MPD	C2-C3-C4-C5
3	D	1001	MPD	C2-C3-C4-C5
3	C	1001	MPD	C2-C3-C4-C5
3	C	1002	MPD	C2-C3-C4-C5
3	B	1001	MPD	C2-C3-C4-C5
3	D	1002	MPD	C2-C3-C4-C5
3	A	1005	MPD	C2-C3-C4-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	1003	MPD	C2-C3-C4-O4
3	B	1002	MPD	C2-C3-C4-O4
3	A	1002	MPD	C2-C3-C4-O4

There are no ring outliers.

16 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1006	MPD	2	0
3	B	1003	MPD	2	0
3	A	1003	MPD	3	0
3	D	1003	MPD	2	0
3	C	1000	MPD	10	0
3	B	1005	MPD	2	0
3	A	1002	MPD	11	0
3	C	1003	MPD	13	0
4	D	1000	XYM	1	0
3	D	1001	MPD	15	0
3	C	1001	MPD	15	0
3	A	1001	MPD	3	0
4	B	1000	XYM	1	0
3	B	1001	MPD	12	0
3	A	1004	MPD	4	0
3	D	1002	MPD	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	333/334 (99%)	-0.58	3 (0%) 84 82	20, 29, 49, 78	0
1	B	333/334 (99%)	-0.46	8 (2%) 59 53	20, 31, 52, 76	0
1	C	333/334 (99%)	-0.36	7 (2%) 63 58	21, 32, 55, 80	0
1	D	333/334 (99%)	-0.47	6 (1%) 68 64	21, 30, 48, 74	0
All	All	1332/1336 (99%)	-0.47	24 (1%) 68 64	20, 30, 53, 80	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	THR	5.7
1	D	74	THR	5.5
1	B	74	THR	5.5
1	A	75	ARG	5.1
1	B	75	ARG	5.1
1	C	74	THR	4.6
1	C	73	PRO	3.4
1	B	73	PRO	3.3
1	B	308	GLY	3.2
1	C	317	ASP	3.0
1	C	75	ARG	3.0
1	D	73	PRO	2.9
1	D	75	ARG	2.9
1	A	73	PRO	2.6
1	D	78	PRO	2.6
1	D	317	ASP	2.6
1	B	334	LEU	2.5
1	D	57	GLU	2.4
1	C	77	VAL	2.4
1	C	54	GLU	2.3
1	B	72	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	72	SER	2.1
1	B	106	PRO	2.1
1	B	317	ASP	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
4	XYM	D	1000	11/11	0.71	0.36	48,54,58,58	11
3	MPD	A	1003	8/8	0.85	0.25	34,37,37,37	8
2	XYN	A	1000	11/11	0.85	0.32	29,40,45,46	11
3	MPD	B	1003	8/8	0.85	0.22	37,39,40,41	8
3	MPD	C	1003	8/8	0.87	0.27	36,36,38,40	8
3	MPD	B	1005	8/8	0.87	0.33	46,47,48,49	8
4	XYM	B	1000	11/11	0.87	0.27	41,45,50,52	11
3	MPD	A	1004	8/8	0.87	0.26	25,30,36,39	8
3	MPD	B	1001	8/8	0.88	0.27	21,26,30,36	0
3	MPD	A	1005	8/8	0.90	0.26	31,32,35,36	8
3	MPD	B	1006	8/8	0.90	0.21	38,39,40,41	8
3	MPD	D	1002	8/8	0.90	0.28	28,29,29,32	8
3	MPD	C	1001	8/8	0.91	0.24	23,25,27,27	0
3	MPD	C	1002	8/8	0.91	0.26	34,36,37,38	8
3	MPD	B	1007	8/8	0.92	0.17	36,39,42,42	0
3	MPD	B	1004	8/8	0.93	0.17	31,33,36,37	8
3	MPD	C	1000	8/8	0.93	0.36	30,31,32,32	8
3	MPD	D	1003	8/8	0.94	0.17	34,35,37,38	0
3	MPD	D	1001	8/8	0.94	0.23	17,20,22,22	0
3	MPD	A	1002	8/8	0.94	0.24	21,27,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MPD	A	1001	8/8	0.94	0.19	33,35,36,37	8
3	MPD	B	1002	8/8	0.94	0.15	38,39,40,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.