Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 03:49 PM EDT

PDB ID	:	1OZ0
Title	:	CRYSTAL STRUCTURE OF THE HOMODIMERIC BIFUNCTIONAL TRANSFORMYLASE AND CYCLOHYDROLASE ENZYME AVIAN ATIC IN COMPLEX WITH A MULTISUBSTRATE ADDUCT INHIBITOR BETA-DADF.
Authors	:	Wolan, D.W.; Greasley, S.E.; Wall, M.J.; Benkovic, S.J.; Wilson, I.A.
Deposited on	:	2003-04-07
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

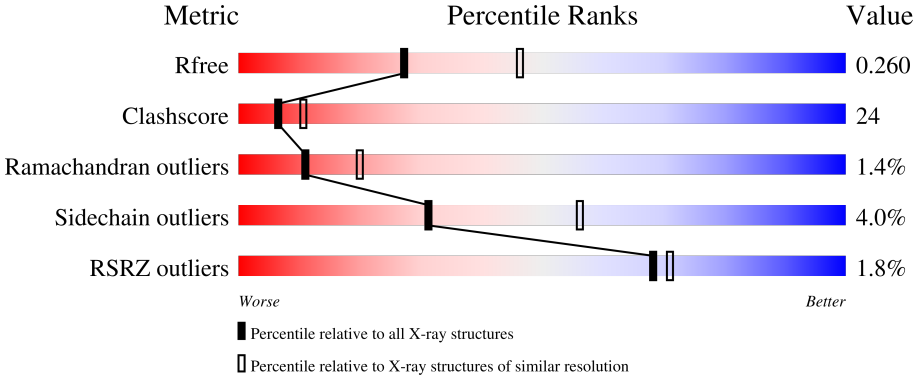
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	613	.% 54% 40% • •
1	B	613	2% 58% 35% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9526 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 Bifunctional purine biosynthesis protein PURH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	590	4511	2843	800	849	19	0	0	0
1	B	590	4511	2843	800	849	19	4	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P31335
A	-18	GLY	-	expression tag	UNP P31335
A	-17	SER	-	expression tag	UNP P31335
A	-16	SER	-	expression tag	UNP P31335
A	-15	HIS	-	expression tag	UNP P31335
A	-14	HIS	-	expression tag	UNP P31335
A	-13	HIS	-	expression tag	UNP P31335
A	-12	HIS	-	expression tag	UNP P31335
A	-11	HIS	-	expression tag	UNP P31335
A	-10	HIS	-	expression tag	UNP P31335
A	-9	SER	-	expression tag	UNP P31335
A	-8	SER	-	expression tag	UNP P31335
A	-7	GLY	-	expression tag	UNP P31335
A	-6	LEU	-	expression tag	UNP P31335
A	-5	VAL	-	expression tag	UNP P31335
A	-4	PRO	-	expression tag	UNP P31335
A	-3	ARG	-	expression tag	UNP P31335
A	-2	GLY	-	expression tag	UNP P31335
A	-1	SER	-	expression tag	UNP P31335
A	0	HIS	-	expression tag	UNP P31335
B	-19	MET	-	expression tag	UNP P31335
B	-18	GLY	-	expression tag	UNP P31335
B	-17	SER	-	expression tag	UNP P31335
B	-16	SER	-	expression tag	UNP P31335
B	-15	HIS	-	expression tag	UNP P31335

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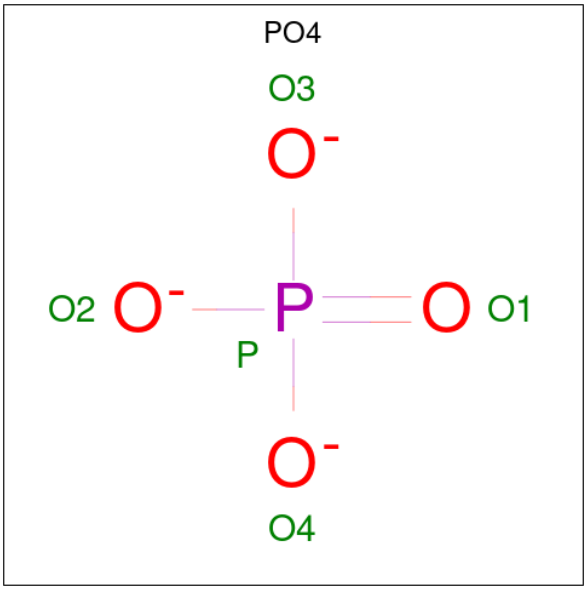
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P31335
B	-13	HIS	-	expression tag	UNP P31335
B	-12	HIS	-	expression tag	UNP P31335
B	-11	HIS	-	expression tag	UNP P31335
B	-10	HIS	-	expression tag	UNP P31335
B	-9	SER	-	expression tag	UNP P31335
B	-8	SER	-	expression tag	UNP P31335
B	-7	GLY	-	expression tag	UNP P31335
B	-6	LEU	-	expression tag	UNP P31335
B	-5	VAL	-	expression tag	UNP P31335
B	-4	PRO	-	expression tag	UNP P31335
B	-3	ARG	-	expression tag	UNP P31335
B	-2	GLY	-	expression tag	UNP P31335
B	-1	SER	-	expression tag	UNP P31335
B	0	HIS	-	expression tag	UNP P31335

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

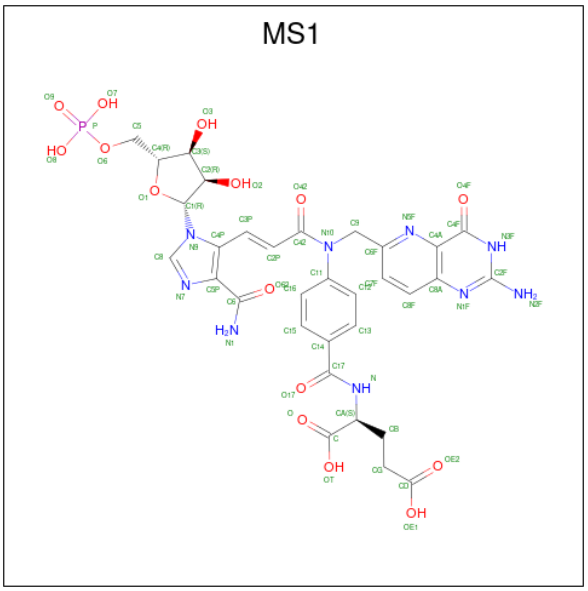
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P			
3	A	1	5	4	1		0	0
			Total	O	P			
3	B	1	5	4	1		0	0

- Molecule 4 is 2-[4-((2-AMINO-4-OXO-3,4-DIHYDRO-PYRIDO[3,2-D]PYRIMIDIN-6-YLMETHYL)-{3-[5-CARBAMOYL-3-(3,4- DIHYDROXY-5-PHOSPHONOOXYMETHYL-TETRAHYDRO-FURAN-2-YL)-3H-IMIDAZOL-4-YL]-ACRYLOYL}-AMINO)-BENZOYLAMINO]- PENTANEDIOIC ACID (three-letter code: MS1) (formula: $C_{32}H_{34}N_9O_{15}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	57	32	9	15	1	0	0
			Total	C	N	O	P		
4	B	1	57	32	9	15	1	0	0

- Molecule 5 is water.

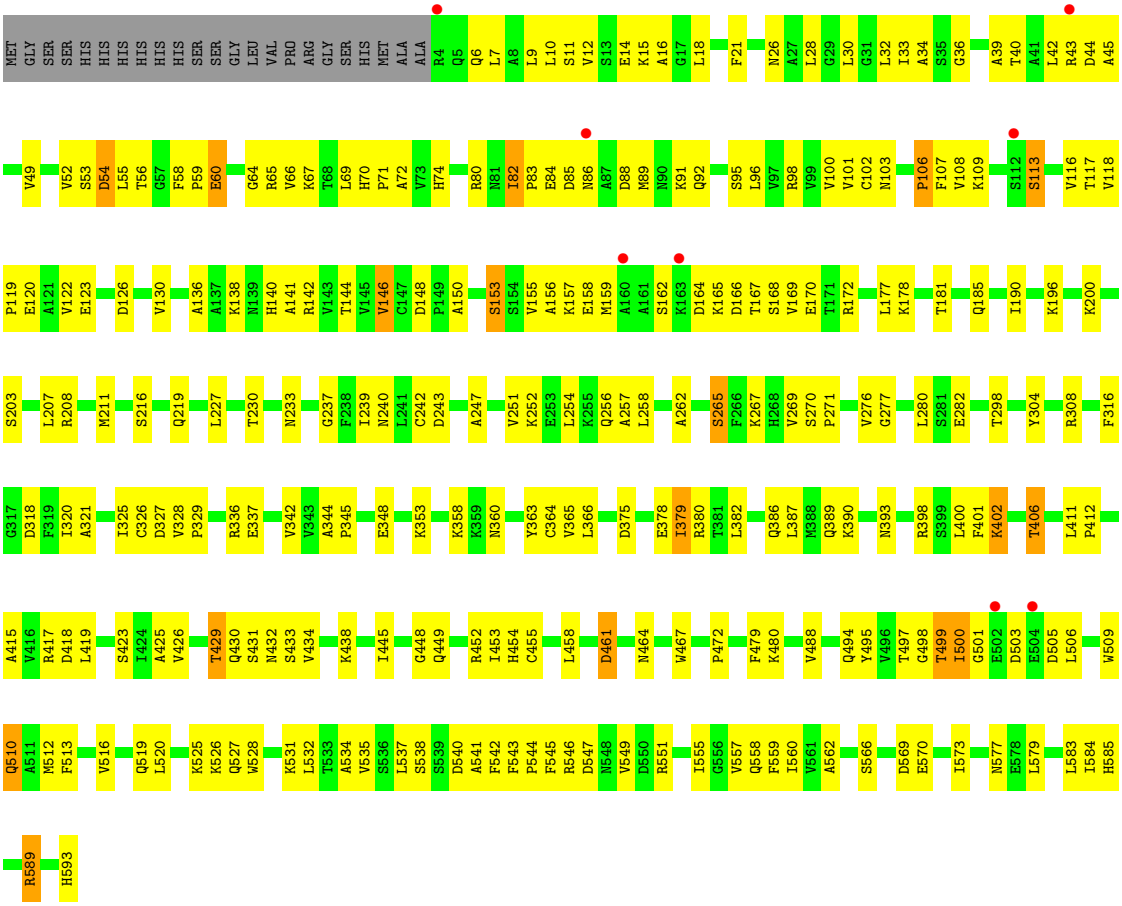
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	204	204	204	0	0
			Total	O		
5	B	174	174	174	0	0

3 Residue-property plots (i)

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.

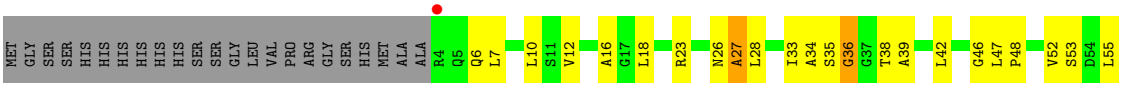
• Molecule 1: Bifunctional purine biosynthesis protein PURH

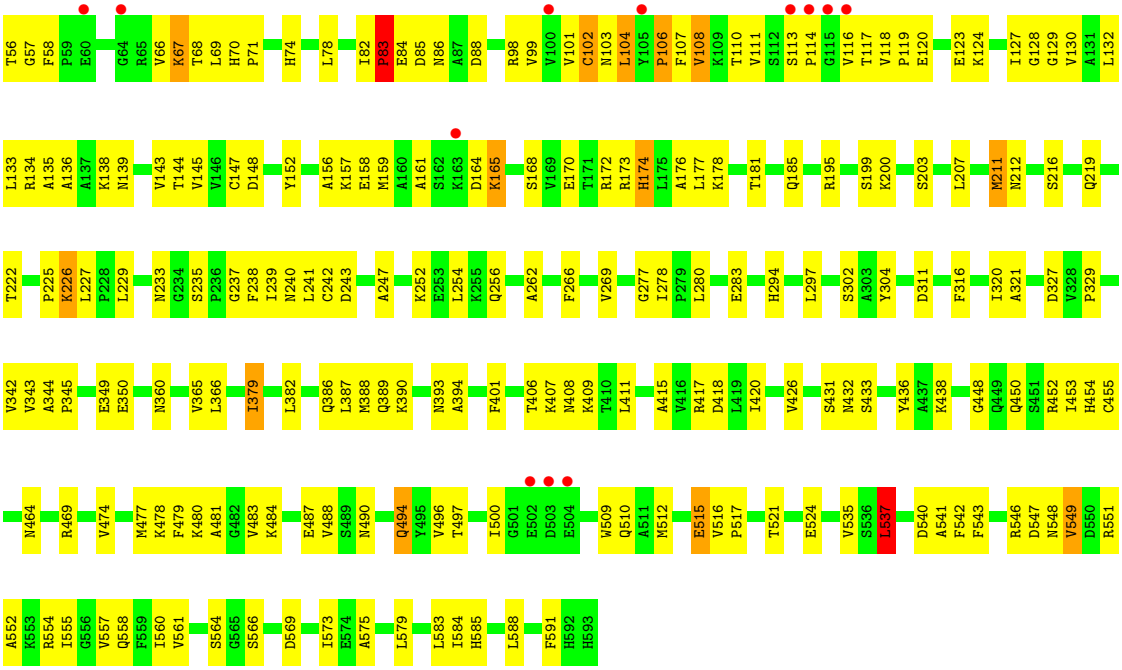
Chain A:



• Molecule 1: Bifunctional purine biosynthesis protein PURH

Chain B:




T56 G57 F58 P59 E60 G64 R65 V66 K67 T68 L69 H70 P71 H74 L78 I82 P83 E84 D85 N86 A87 D88 R98 V99 V100 V101 C102 N103 L104 Y105 P106 F107 V108 K109 T110 V111 S112 S113 P114 G115 V116 T117 V118 P119 E120 E123 K124 I127 G128 G129 V130 A131 L132
L133 R134 A135 A136 A137 K138 N139 V143 T144 V145 V146 C147 D148 Y152 A156 K157 E158 M159 A160 A161 S162 K163 D164 K165 S168 V169 E170 T171 R172 R173 H174 L175 A176 L177 K178 T181 Q185 R195 S199 K200 S203 L207 M211 N212 S216 Q219
T222 P225 K226 L227 P228 L229 N233 G234 S235 P236 G237 F238 I239 N240 L241 C242 D243 A247 K252 E253 L254 K255 Q256 A262 F266 V269 G277 I278 P279 L280 E283 H294 L297 S302 A303 Y304 D311 F316 I320 A321 D327 V328 P329
V342 V343 A344 P345 E349 E350 M360 V365 L366 I379 L382 Q386 L387 M388 Q389 K390 N393 A394 F401 T406 K407 N408 K409 T410 L411 A415 V416 R417 D418 L419 I420 V426 S431 N432 S433 Y436 A437 K438 G448 Q449 Q450 S451 R452 I453 H454 C455
N464 R469 V474 M477 K478 F479 K480 A481 G482 V483 K484 E487 V488 S489 N490 Q494 Y495 V496 T497 I500 G501 E502 D503 E504 W509 Q510 A511 M512 E515 V516 P517 T521 E524 V535 S536 L537 D540 A541 F542 F543 R546 D547 N548 V549 D550 R551
A552 K553 R554 I555 G556 V557 Q558 F559 I560 V561 S564 G565 S566 D569 I573 E574 A575 L579 L583 I584 H585 L588 F591 H592 H593

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.41Å 108.10Å 102.36Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 24.20 – 2.33	Depositor EDS
% Data completeness (in resolution range)	92.1 (50.00-2.50) 89.5 (24.20-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.269 0.207 , 0.260	Depositor DCC
R_{free} test set	3554 reflections (7.59%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.060 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9526	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, K, MS1

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	0.40	0/4595	0.64	0/6230
1	B	0.40	0/4595	0.64	1/6230 (0.0%)
All	All	0.40	0/9190	0.64	1/12460 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	537	LEU	CA-CB-CG	6.04	129.20	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4511	0	4561	242	0
1	B	4511	0	4561	208	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	57	0	31	6	0
4	B	57	0	31	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	204	0	0	29	0
5	B	174	0	0	22	0
All	All	9526	0	9184	435	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 24.

All (435) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:GLY:HA3	1:A:505:ASP:HB2	1.45	0.97
1:A:401:PHE:HB3	1:A:584:ILE:HD13	1.48	0.94
1:B:350:GLU:HB2	5:B:1125:HOH:O	1.70	0.90
1:B:283:GLU:HG3	5:B:1067:HOH:O	1.69	0.89
1:A:64:GLY:HA3	1:A:67:LYS:HE3	1.55	0.88
1:A:426:VAL:HA	1:A:429:THR:CG2	2.02	0.88
1:B:464:ASN:OD1	1:B:555:ILE:HD13	1.74	0.86
1:A:7:LEU:HD13	1:A:33:ILE:HD11	1.59	0.84
1:A:12:VAL:HB	1:A:103:ASN:ND2	1.91	0.83
1:A:411:LEU:HB3	5:A:1137:HOH:O	1.78	0.83
1:B:104:LEU:HD21	1:B:133:LEU:HD12	1.60	0.81
1:A:32:LEU:HD11	1:A:49:VAL:HG22	1.63	0.81
1:A:138:LYS:HD2	1:B:127:ILE:HD11	1.64	0.80
1:B:406:THR:HG23	1:B:583:LEU:HB3	1.64	0.80
1:A:200:LYS:HE2	5:A:1094:HOH:O	1.83	0.77
1:A:495:TYR:HA	1:A:500:ILE:HD11	1.67	0.76
1:A:510:GLN:OE1	1:A:516:VAL:HG11	1.85	0.76
1:A:98:ARG:HA	5:A:1199:HOH:O	1.86	0.76
1:A:88:ASP:HA	1:A:91:LYS:HE3	1.69	0.75
1:B:207:LEU:HD23	1:B:219:GLN:HA	1.69	0.75
1:B:452:ARG:NH2	1:B:541:ALA:HB3	2.03	0.74
1:A:118:VAL:HB	1:A:119:PRO:HD3	1.70	0.74
1:B:113:SER:HB2	1:B:114:PRO:HD2	1.68	0.73
1:A:379:ILE:HG22	5:B:1077:HOH:O	1.88	0.72
1:B:128:GLY:O	1:B:132:LEU:HG	1.89	0.72
1:B:200:LYS:NZ	5:B:1114:HOH:O	2.22	0.72
1:B:211:MET:HE2	1:B:239:ILE:HG12	1.71	0.72
1:A:537:LEU:HD23	1:A:538:SER:N	2.05	0.71
1:B:118:VAL:HB	1:B:119:PRO:HD3	1.73	0.70
1:A:208:ARG:NH2	4:B:1001:MS1:O8	2.24	0.69
1:B:48:PRO:HD2	5:B:1096:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:CD	1:B:127:ILE:HD11	2.23	0.69
1:B:130:VAL:O	1:B:134:ARG:HG3	1.92	0.68
1:A:32:LEU:HG	5:A:1012:HOH:O	1.94	0.68
1:B:110:THR:CG2	1:B:124:LYS:HD2	2.24	0.68
1:A:9:LEU:HD12	1:A:33:ILE:O	1.95	0.67
1:B:7:LEU:HB3	1:B:33:ILE:HD11	1.77	0.67
1:A:558:GLN:HB3	5:A:1158:HOH:O	1.94	0.67
1:B:207:LEU:HD11	1:B:241:LEU:HD11	1.76	0.67
1:A:452:ARG:NH2	1:A:541:ALA:HB3	2.09	0.67
1:B:113:SER:OG	1:B:116:VAL:HB	1.95	0.66
1:A:336:ARG:HG3	5:A:1173:HOH:O	1.95	0.66
1:B:46:GLY:O	1:B:47:LEU:HG	1.94	0.66
1:B:6:GLN:OE1	1:B:98:ARG:NH1	2.28	0.66
1:B:484:LYS:HB3	5:B:1178:HOH:O	1.96	0.66
1:A:12:VAL:HG23	1:A:15:LYS:HG3	1.79	0.65
1:A:181:THR:O	1:A:185:GLN:HG3	1.96	0.65
1:B:27:ALA:HB2	5:B:1123:HOH:O	1.95	0.65
1:B:479:PHE:CE2	1:B:488:VAL:HG13	2.31	0.64
1:A:7:LEU:HD13	1:A:33:ILE:CD1	2.28	0.64
1:A:82:ILE:HD13	1:A:82:ILE:H	1.61	0.64
1:A:83:PRO:HG2	1:A:84:GLU:OE1	1.97	0.64
1:A:401:PHE:HB3	1:A:584:ILE:CD1	2.26	0.64
1:B:110:THR:HG21	1:B:124:LYS:HD2	1.78	0.64
4:A:1002:MS1:C12	4:A:1002:MS1:C2P	2.74	0.64
1:B:7:LEU:HB3	1:B:33:ILE:CD1	2.27	0.63
1:A:526:LYS:NZ	1:A:526:LYS:HB3	2.14	0.63
1:B:389:GLN:HG3	1:B:390:LYS:O	1.99	0.63
1:B:33:ILE:N	1:B:33:ILE:HD12	2.13	0.63
1:B:104:LEU:HD21	1:B:133:LEU:CD1	2.29	0.63
1:A:402:LYS:NZ	1:A:402:LYS:HA	2.14	0.62
1:A:434:VAL:HG13	1:A:537:LEU:HD21	1.80	0.62
1:A:98:ARG:CB	5:A:1199:HOH:O	2.47	0.62
1:A:153:SER:O	1:A:157:LYS:HG3	2.00	0.62
1:B:226:LYS:HB2	1:B:226:LYS:NZ	2.14	0.62
1:A:10:LEU:HD22	1:A:42:LEU:HD21	1.80	0.61
1:B:252:LYS:O	1:B:256:GLN:HG3	1.99	0.61
1:A:65:ARG:NH2	1:A:123:GLU:OE1	2.27	0.61
1:B:521:THR:HG23	1:B:524:GLU:OE1	1.99	0.61
1:A:247:ALA:HB1	1:A:321:ALA:HB2	1.81	0.61
1:B:120:GLU:O	1:B:124:LYS:HG3	2.00	0.61
1:B:280:LEU:CD1	1:B:302:SER:HB3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HD12	1:A:325:ILE:H	1.66	0.61
1:B:34:ALA:HB3	1:B:39:ALA:HB2	1.81	0.61
1:A:400:LEU:HB2	5:A:1038:HOH:O	2.00	0.61
1:B:426:VAL:CG1	1:B:540:ASP:HB3	2.31	0.61
4:A:1002:MS1:C2P	4:A:1002:MS1:H12	2.31	0.60
1:B:18:LEU:HG	1:B:42:LEU:HD21	1.83	0.60
1:A:282:GLU:N	1:A:282:GLU:OE1	2.33	0.60
1:A:159:MET:O	1:A:162:SER:HB3	2.01	0.60
1:B:181:THR:HG22	1:B:185:GLN:HE21	1.66	0.60
1:B:252:LYS:HG2	1:B:256:GLN:HE21	1.65	0.60
4:A:1002:MS1:H52	1:B:239:ILE:HB	1.83	0.60
1:B:34:ALA:O	1:B:52:VAL:HG23	2.02	0.59
1:A:498:GLY:C	1:A:500:ILE:H	2.05	0.59
1:B:474:VAL:O	1:B:477:MET:HG3	2.01	0.59
1:A:117:THR:O	1:A:120:GLU:HB2	2.02	0.59
1:A:316:PHE:CG	4:B:1001:MS1:H7F	2.38	0.59
1:B:453:ILE:HD13	1:B:547:ASP:CG	2.23	0.59
1:A:458:LEU:HD12	5:A:1046:HOH:O	2.03	0.59
1:A:33:ILE:HD13	1:A:55:LEU:HD22	1.82	0.59
1:B:379:ILE:HD13	1:B:379:ILE:C	2.23	0.59
1:B:408:ASN:HB3	5:B:1156:HOH:O	2.03	0.59
1:A:80:ARG:HB2	1:A:82:ILE:HD12	1.85	0.59
1:A:393:ASN:ND2	5:A:1131:HOH:O	2.36	0.58
1:B:386:GLN:NE2	5:B:1030:HOH:O	2.36	0.58
1:A:159:MET:O	1:A:165:LYS:HA	2.03	0.58
1:A:454:HIS:ND1	5:A:1081:HOH:O	2.32	0.58
1:A:549:VAL:HG12	1:A:579:LEU:HD12	1.86	0.58
1:A:230:THR:HG23	5:A:1024:HOH:O	2.01	0.58
1:A:242:CYS:HA	1:B:382:LEU:HD21	1.84	0.58
1:A:82:ILE:HD13	1:A:85:ASP:HB2	1.86	0.58
1:A:426:VAL:HA	1:A:429:THR:HG21	1.85	0.57
1:A:32:LEU:CD1	1:A:49:VAL:HG22	2.33	0.57
1:A:82:ILE:CD1	1:A:85:ASP:HB2	2.35	0.57
1:A:169:VAL:HG23	1:A:170:GLU:H	1.67	0.57
1:A:380:ARG:HB2	5:B:1113:HOH:O	2.04	0.57
1:B:28:LEU:HB3	1:B:165:LYS:HD3	1.87	0.57
1:B:129:GLY:HA2	1:B:132:LEU:HD12	1.87	0.56
1:B:379:ILE:HD11	1:B:386:GLN:OE1	2.05	0.56
1:A:52:VAL:C	1:A:54:ASP:H	2.07	0.56
1:A:433:SER:HA	1:A:455:CYS:SG	2.45	0.56
1:B:453:ILE:HD13	1:B:547:ASP:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ALA:O	1:A:429:THR:HG22	2.05	0.56
1:B:252:LYS:HG2	1:B:256:GLN:NE2	2.20	0.56
1:A:64:GLY:HA3	1:A:67:LYS:CE	2.32	0.56
1:A:98:ARG:CA	5:A:1199:HOH:O	2.51	0.56
1:B:480:LYS:O	1:B:483:VAL:HG23	2.05	0.56
1:B:82:ILE:HG23	1:B:83:PRO:HD2	1.88	0.56
1:A:431:SER:O	1:A:448:GLY:HA2	2.05	0.56
1:A:589:ARG:HD3	5:A:1130:HOH:O	2.05	0.56
1:A:526:LYS:HB3	1:A:526:LYS:HZ3	1.70	0.56
1:B:542:PHE:CD1	1:B:566:SER:HB2	2.41	0.56
1:A:122:VAL:O	1:B:138:LYS:HE3	2.06	0.56
1:B:211:MET:HE2	1:B:239:ILE:CG1	2.35	0.56
1:A:169:VAL:HG23	1:A:170:GLU:N	2.21	0.55
1:A:402:LYS:HA	1:A:402:LYS:HZ3	1.72	0.55
1:A:382:LEU:HD21	1:B:242:CYS:HA	1.89	0.55
1:B:229:LEU:HD11	1:B:366:LEU:HB3	1.88	0.55
1:A:265:SER:OG	1:A:318:ASP:OD2	2.24	0.55
1:A:271:PRO:HG2	1:A:445:ILE:CD1	2.36	0.55
1:B:452:ARG:HH21	1:B:541:ALA:HB3	1.71	0.55
1:B:82:ILE:HG22	1:B:84:GLU:OE1	2.06	0.55
1:B:145:VAL:HG12	5:B:1022:HOH:O	2.06	0.55
1:A:12:VAL:O	1:A:15:LYS:HE3	2.06	0.55
1:B:509:TRP:HH2	1:B:517:PRO:HG2	1.70	0.55
1:A:32:LEU:HD12	1:A:49:VAL:HA	1.89	0.55
1:B:575:ALA:O	1:B:579:LEU:HG	2.07	0.55
1:B:12:VAL:HG12	1:B:102:CYS:HA	1.89	0.55
1:B:139:ASN:ND2	1:B:143:VAL:HG23	2.22	0.55
1:B:477:MET:HE2	1:B:517:PRO:HG3	1.89	0.55
1:A:43:ARG:HE	1:A:49:VAL:HB	1.72	0.55
1:B:136:ALA:HB1	1:B:145:VAL:HB	1.89	0.55
1:B:127:ILE:N	1:B:127:ILE:HD12	2.22	0.54
1:B:211:MET:CE	1:B:239:ILE:HG12	2.35	0.54
1:B:123:GLU:HG2	5:B:1079:HOH:O	2.07	0.54
1:B:552:ALA:O	1:B:555:ILE:HG22	2.07	0.54
1:A:390:LYS:HG3	1:B:216:SER:O	2.08	0.54
1:B:394:ALA:CB	1:B:588:LEU:HD11	2.37	0.54
1:A:64:GLY:HA2	5:A:1133:HOH:O	2.07	0.54
1:B:143:VAL:O	1:B:172:ARG:HD2	2.07	0.54
1:B:454:HIS:HB3	5:B:1102:HOH:O	2.08	0.54
1:A:501:GLY:HA3	1:A:505:ASP:CB	2.31	0.53
1:A:11:SER:O	1:A:102:CYS:HA	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:CYS:O	1:B:147:CYS:HA	2.09	0.53
1:A:252:LYS:O	1:A:256:GLN:HG3	2.08	0.53
1:A:398:ARG:NH1	1:A:398:ARG:HB2	2.23	0.53
1:A:461:ASP:HA	1:A:464:ASN:ND2	2.24	0.53
1:A:432:ASN:ND2	1:A:449:GLN:O	2.42	0.53
1:B:174:HIS:C	1:B:174:HIS:CD2	2.82	0.53
1:A:426:VAL:HA	1:A:429:THR:HG22	1.90	0.53
1:A:32:LEU:CD1	1:A:49:VAL:HA	2.39	0.53
1:A:555:ILE:HG13	1:A:555:ILE:O	2.08	0.53
1:B:551:ARG:HD3	1:B:554:ARG:HH21	1.74	0.53
1:A:438:LYS:NZ	1:A:534:ALA:HB3	2.24	0.52
1:B:203:SER:HA	1:B:227:LEU:HG	1.90	0.52
1:A:379:ILE:HD11	1:A:386:GLN:HG3	1.91	0.52
1:B:67:LYS:HE3	5:B:1088:HOH:O	2.09	0.52
1:B:207:LEU:HD11	1:B:241:LEU:CD1	2.39	0.52
1:A:498:GLY:O	1:A:500:ILE:N	2.43	0.52
1:B:111:VAL:HA	1:B:116:VAL:HG11	1.90	0.52
1:B:304:TYR:CE1	1:B:320:ILE:HG12	2.45	0.52
1:A:382:LEU:CD2	1:B:242:CYS:HA	2.40	0.52
1:A:544:PRO:HB2	1:A:545:PHE:CD2	2.45	0.52
1:A:28:LEU:HD22	1:A:165:LYS:HB3	1.91	0.52
1:A:542:PHE:CD1	1:A:566:SER:HB2	2.45	0.52
1:B:207:LEU:HD23	1:B:219:GLN:CA	2.39	0.52
1:A:106:PRO:C	1:A:108:VAL:N	2.64	0.52
1:B:394:ALA:HB1	1:B:588:LEU:HD11	1.92	0.51
1:A:242:CYS:HA	1:B:382:LEU:CD2	2.40	0.51
1:A:168:SER:HB3	5:A:1103:HOH:O	2.09	0.51
1:A:15:LYS:HA	5:A:1075:HOH:O	2.10	0.51
1:A:426:VAL:O	1:A:429:THR:HG23	2.10	0.51
1:B:280:LEU:N	1:B:280:LEU:HD12	2.24	0.51
1:A:98:ARG:HB2	5:A:1199:HOH:O	2.10	0.51
1:A:452:ARG:NH1	1:A:540:ASP:OD1	2.43	0.51
1:A:401:PHE:HA	1:A:584:ILE:HG21	1.93	0.51
1:B:10:LEU:O	1:B:38:THR:HG21	2.11	0.51
1:B:431:SER:O	1:B:448:GLY:HA2	2.10	0.51
1:B:117:THR:HG23	1:B:120:GLU:OE1	2.10	0.51
1:A:546:ARG:HG2	5:A:1090:HOH:O	2.11	0.51
1:A:569:ASP:O	1:A:573:ILE:HG13	2.11	0.51
1:B:23:ARG:HG2	1:B:47:LEU:HD21	1.93	0.51
1:B:546:ARG:O	1:B:549:VAL:HG13	2.10	0.51
1:A:178:LYS:HE2	1:B:225:PRO:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:VAL:HG22	1:B:579:LEU:HD12	1.92	0.51
1:B:211:MET:HE3	1:B:238:PHE:CD1	2.45	0.50
1:B:411:LEU:HD12	1:B:415:ALA:HB3	1.93	0.50
1:B:480:LYS:HD2	1:B:481:ALA:H	1.76	0.50
1:A:88:ASP:O	1:A:91:LYS:HB3	2.12	0.50
1:A:494:GLN:HB3	1:A:500:ILE:HA	1.93	0.50
1:B:487:GLU:HB3	1:B:512:MET:CE	2.41	0.50
1:B:541:ALA:HB2	1:B:591:PHE:CE1	2.47	0.50
1:A:431:SER:HB2	1:A:593:HIS:CE1	2.45	0.50
1:B:226:LYS:HB2	1:B:226:LYS:HZ2	1.75	0.50
1:A:527:GLN:NE2	5:A:1207:HOH:O	2.45	0.50
1:A:144:THR:HG21	1:A:167:THR:HG21	1.93	0.49
1:A:537:LEU:HD23	1:A:537:LEU:C	2.33	0.49
1:B:418:ASP:OD2	1:B:438:LYS:HA	2.12	0.49
1:A:308:ARG:CZ	1:A:337:GLU:HB3	2.41	0.49
1:A:21:PHE:CE1	1:A:156:ALA:HB2	2.46	0.49
1:A:237:GLY:H	1:A:240:ASN:HB2	1.78	0.49
1:B:394:ALA:HA	5:B:1074:HOH:O	2.13	0.49
1:A:500:ILE:HG13	1:A:519:GLN:OE1	2.12	0.49
1:A:558:GLN:NE2	5:A:1158:HOH:O	2.45	0.49
1:B:431:SER:CB	1:B:432:ASN:HA	2.41	0.49
1:A:56:THR:HG22	1:A:72:ALA:HB3	1.94	0.49
5:A:1203:HOH:O	1:B:239:ILE:HG13	2.12	0.49
4:A:1002:MS1:H7F	1:B:316:PHE:CG	2.47	0.49
1:A:528:TRP:O	1:A:531:LYS:HB2	2.13	0.49
1:A:12:VAL:HB	1:A:103:ASN:HD21	1.73	0.48
1:A:74:HIS:HB3	1:B:69:LEU:HD13	1.95	0.48
1:B:107:PHE:CE2	1:B:111:VAL:HG11	2.48	0.48
1:B:496:VAL:HG23	1:B:497:THR:HG23	1.95	0.48
1:A:84:GLU:OE1	1:A:84:GLU:N	2.36	0.48
1:A:430:GLN:HG3	5:B:1103:HOH:O	2.12	0.48
1:B:247:ALA:HB1	1:B:321:ALA:HB2	1.96	0.48
1:A:89:MET:HE2	1:A:96:LEU:HD23	1.96	0.48
1:A:267:LYS:HG2	1:B:450:GLN:HB3	1.94	0.48
1:A:418:ASP:OD2	1:A:438:LYS:HA	2.13	0.48
1:B:549:VAL:CG2	1:B:579:LEU:HD12	2.44	0.48
1:B:344:ALA:HB1	1:B:345:PRO:HD2	1.94	0.48
1:A:66:VAL:HA	1:A:69:LEU:HD12	1.95	0.48
1:A:141:ALA:HB2	5:A:1088:HOH:O	2.13	0.48
1:B:207:LEU:N	1:B:207:LEU:HD22	2.29	0.48
1:B:469:ARG:NH1	5:B:1041:HOH:O	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD11	1:A:85:ASP:CG	2.33	0.48
1:B:106:PRO:HB3	1:B:108:VAL:HG23	1.96	0.48
1:A:247:ALA:CB	1:A:321:ALA:HB2	2.42	0.48
1:A:406:THR:HG22	1:A:577:ASN:OD1	2.14	0.48
1:A:562:ALA:O	1:A:585:HIS:HA	2.14	0.48
1:B:233:ASN:HB3	1:B:365:VAL:HG23	1.95	0.48
1:B:500:ILE:HD11	1:B:509:TRP:CG	2.49	0.48
1:A:326:CYS:O	1:A:348:GLU:HG3	2.13	0.47
1:A:344:ALA:HB1	1:A:345:PRO:HD2	1.95	0.47
1:B:26:ASN:C	1:B:28:LEU:H	2.16	0.47
1:A:34:ALA:C	1:A:39:ALA:HB2	2.34	0.47
1:A:251:VAL:HG23	1:A:252:LYS:N	2.29	0.47
1:A:98:ARG:HG3	5:A:1190:HOH:O	2.14	0.47
1:A:358:LYS:HB2	1:A:363:TYR:HB2	1.97	0.47
1:B:327:ASP:OD1	1:B:329:PRO:HD2	2.14	0.47
1:A:196:LYS:HE2	1:A:219:GLN:NE2	2.30	0.47
1:A:258:LEU:HD13	1:A:417:ARG:HG3	1.96	0.47
1:B:56:THR:HB	1:B:70:HIS:CD2	2.49	0.47
1:B:254:LEU:HD23	1:B:262:ALA:HB1	1.96	0.47
1:B:342:VAL:HG22	1:B:343:VAL:N	2.30	0.47
1:B:583:LEU:HD12	1:B:584:ILE:N	2.30	0.47
1:A:80:ARG:HB2	1:A:82:ILE:CD1	2.44	0.47
1:B:535:VAL:HB	1:B:557:VAL:HA	1.97	0.47
1:A:500:ILE:HG22	1:A:501:GLY:N	2.30	0.47
1:A:177:LEU:HD21	1:B:195:ARG:HG2	1.97	0.47
1:A:520:LEU:HB2	1:A:525:LYS:HE3	1.97	0.47
1:A:70:HIS:ND1	1:A:71:PRO:HD2	2.30	0.47
1:A:375:ASP:HB3	5:A:1204:HOH:O	2.15	0.47
1:B:70:HIS:CG	1:B:71:PRO:HD2	2.50	0.47
1:A:583:LEU:HD12	1:A:584:ILE:H	1.80	0.46
1:A:106:PRO:C	1:A:108:VAL:H	2.18	0.46
1:A:589:ARG:HB3	1:B:212:ASN:OD1	2.15	0.46
1:B:393:ASN:HA	5:B:1019:HOH:O	2.15	0.46
1:B:401:PHE:HE2	1:B:420:ILE:HG13	1.80	0.46
1:B:547:ASP:OD1	1:B:548:ASN:N	2.47	0.46
1:A:254:LEU:HD23	1:A:262:ALA:HB1	1.97	0.46
1:A:316:PHE:CD1	4:B:1001:MS1:H7F	2.51	0.46
1:A:364:CYS:SG	1:A:366:LEU:HD21	2.55	0.46
1:A:243:ASP:OD1	1:A:269:VAL:N	2.46	0.46
1:A:257:ALA:HB2	5:A:1051:HOH:O	2.16	0.46
1:A:423:SER:O	1:A:426:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:HG22	1:B:144:THR:HB	1.96	0.46
1:A:480:LYS:HE3	1:A:513:PHE:O	2.15	0.46
1:A:80:ARG:CB	1:A:82:ILE:HD12	2.46	0.46
1:A:10:LEU:HD23	1:A:18:LEU:HD11	1.97	0.45
1:A:40:THR:HG22	1:A:44:ASP:OD2	2.16	0.45
1:B:148:ASP:CB	1:B:178:LYS:HE2	2.46	0.45
1:B:278:ILE:HD11	1:B:417:ARG:CZ	2.46	0.45
1:B:558:GLN:O	1:B:558:GLN:HG2	2.16	0.45
1:A:7:LEU:HD11	1:A:95:SER:HB2	1.97	0.45
1:A:320:ILE:O	1:A:342:VAL:HA	2.17	0.45
1:A:233:ASN:HB3	1:A:365:VAL:HG23	1.97	0.45
1:A:316:PHE:HB3	4:B:1001:MS1:H7F	1.97	0.45
4:A:1002:MS1:C12	4:A:1002:MS1:H2P	2.46	0.45
1:B:247:ALA:HA	1:B:266:PHE:CE1	2.52	0.45
1:B:478:LYS:HB2	1:B:515:GLU:HB3	1.98	0.45
1:A:52:VAL:C	1:A:54:ASP:N	2.69	0.45
1:B:74:HIS:O	1:B:78:LEU:N	2.42	0.45
1:B:490:ASN:O	1:B:494:GLN:HG2	2.17	0.45
1:A:570:GLU:HB2	5:A:1079:HOH:O	2.16	0.45
1:B:35:SER:O	1:B:36:GLY:C	2.55	0.45
1:B:108:VAL:HA	1:B:111:VAL:HG22	1.99	0.45
1:B:139:ASN:HD22	1:B:143:VAL:HG23	1.81	0.45
1:A:86:ASN:N	1:A:86:ASN:HD22	2.13	0.45
1:A:401:PHE:CB	1:A:584:ILE:HD13	2.34	0.45
1:B:172:ARG:HG3	1:B:172:ARG:HH11	1.82	0.45
1:A:126:ASP:OD1	1:A:130:VAL:HG23	2.17	0.45
1:A:148:ASP:OD2	1:A:150:ALA:HB3	2.16	0.45
1:B:7:LEU:HD13	1:B:33:ILE:HD11	1.97	0.45
1:A:159:MET:CE	1:A:166:ASP:HA	2.47	0.45
1:A:304:TYR:OH	1:A:308:ARG:NH1	2.49	0.45
1:B:406:THR:CG2	1:B:583:LEU:HB3	2.43	0.45
1:B:320:ILE:HG22	1:B:342:VAL:HG23	1.99	0.44
1:A:14:GLU:OE2	1:A:16:ALA:HB2	2.17	0.44
1:A:130:VAL:HG21	1:B:134:ARG:NH1	2.32	0.44
1:B:484:LYS:HB2	1:B:487:GLU:OE1	2.18	0.44
1:A:56:THR:HB	1:A:70:HIS:CD2	2.53	0.44
1:A:162:SER:C	1:A:164:ASP:H	2.20	0.44
1:A:328:VAL:N	1:A:329:PRO:HD2	2.32	0.44
1:B:543:PHE:HE2	1:B:560:ILE:HG21	1.83	0.44
1:A:82:ILE:HD13	1:A:82:ILE:N	2.29	0.44
1:A:258:LEU:HD12	1:A:276:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ASP:HB2	1:A:329:PRO:HD2	1.99	0.44
1:B:173:ARG:O	1:B:176:ALA:HB3	2.17	0.44
1:B:278:ILE:HD11	1:B:417:ARG:NH1	2.33	0.44
1:B:407:LYS:O	1:B:409:LYS:HG3	2.18	0.44
1:B:159:MET:C	1:B:161:ALA:H	2.20	0.44
1:B:401:PHE:HB3	1:B:584:ILE:HD13	1.99	0.44
1:A:43:ARG:C	1:A:45:ALA:N	2.71	0.44
1:A:452:ARG:HH21	1:A:541:ALA:HB3	1.79	0.44
1:B:53:SER:O	1:B:57:GLY:N	2.46	0.44
1:B:158:GLU:OE2	1:B:168:SER:N	2.50	0.44
1:A:140:HIS:C	1:A:142:ARG:N	2.72	0.44
1:A:271:PRO:HG2	1:A:445:ILE:HD13	2.00	0.44
1:A:389:GLN:HB3	1:B:238:PHE:CE2	2.53	0.44
1:B:537:LEU:HB3	1:B:560:ILE:HG12	1.99	0.43
1:B:555:ILE:O	1:B:555:ILE:HG13	2.18	0.43
1:A:64:GLY:CA	1:A:67:LYS:HG3	2.48	0.43
1:B:16:ALA:O	1:B:152:TYR:HE2	2.01	0.43
1:A:69:LEU:O	1:B:71:PRO:HD3	2.19	0.43
1:A:431:SER:HB3	1:A:432:ASN:HA	1.98	0.43
1:A:464:ASN:HD21	1:A:551:ARG:HH22	1.67	0.43
1:A:535:VAL:HB	1:A:557:VAL:HA	2.01	0.43
1:B:26:ASN:O	1:B:28:LEU:N	2.51	0.43
1:A:498:GLY:C	1:A:500:ILE:N	2.71	0.43
1:B:379:ILE:HA	1:B:387:LEU:O	2.19	0.43
1:A:9:LEU:HD12	1:A:10:LEU:N	2.34	0.43
1:B:67:LYS:HE2	5:B:1139:HOH:O	2.19	0.43
1:A:168:SER:O	1:A:172:ARG:HG3	2.19	0.43
4:A:1002:MS1:H7F	1:B:316:PHE:CD1	2.54	0.43
1:B:82:ILE:C	1:B:86:ASN:ND2	2.72	0.43
1:A:12:VAL:HB	1:A:103:ASN:HD22	1.79	0.43
1:A:58:PHE:CD1	1:A:59:PRO:HD2	2.54	0.43
1:A:426:VAL:CA	1:A:429:THR:CG2	2.87	0.43
1:A:320:ILE:HB	1:A:342:VAL:HB	2.00	0.43
1:A:378:GLU:OE2	1:A:389:GLN:NE2	2.49	0.43
1:B:104:LEU:CD2	1:B:133:LEU:HD12	2.42	0.43
1:B:311:ASP:HB3	5:B:1111:HOH:O	2.19	0.43
1:A:64:GLY:O	1:A:67:LYS:HG3	2.19	0.42
1:A:101:VAL:HG22	1:A:146:VAL:HG13	2.01	0.42
1:A:107:PHE:CE2	1:A:190:ILE:HA	2.54	0.42
1:A:230:THR:CG2	5:A:1024:HOH:O	2.63	0.42
1:B:222:THR:HG22	1:B:227:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:SER:HA	1:B:455:CYS:SG	2.59	0.42
1:A:207:LEU:HG	1:A:219:GLN:HA	2.01	0.42
1:B:431:SER:HB3	1:B:432:ASN:HA	2.01	0.42
1:A:91:LYS:NZ	1:A:92:GLN:HG2	2.35	0.42
1:A:177:LEU:O	1:A:177:LEU:HD12	2.20	0.42
1:B:10:LEU:HD23	1:B:18:LEU:HD11	2.01	0.42
1:B:564:SER:HB3	1:B:585:HIS:CG	2.54	0.42
1:A:52:VAL:O	1:A:54:ASP:N	2.52	0.42
1:A:60:GLU:OE2	1:A:67:LYS:HE2	2.19	0.42
1:A:113:SER:O	1:A:116:VAL:HG12	2.19	0.42
1:B:203:SER:HB3	1:B:226:LYS:HA	2.00	0.42
1:A:239:ILE:HB	4:B:1001:MS1:H51	2.01	0.42
1:B:99:VAL:HG12	1:B:101:VAL:HG23	2.02	0.42
1:A:431:SER:CB	1:A:432:ASN:HA	2.49	0.42
1:A:467:TRP:NE1	1:A:532:LEU:HB2	2.35	0.42
1:A:415:ALA:O	1:A:419:LEU:HG	2.19	0.42
1:A:510:GLN:HE21	1:A:510:GLN:HB2	1.50	0.42
1:B:164:ASP:O	1:B:165:LYS:C	2.58	0.42
1:B:170:GLU:O	1:B:173:ARG:N	2.52	0.42
1:B:500:ILE:HD12	1:B:500:ILE:HA	1.92	0.42
1:A:6:GLN:O	1:A:30:LEU:HD23	2.19	0.41
1:A:438:LYS:HZ3	1:A:534:ALA:HB3	1.83	0.41
1:A:461:ASP:HA	1:A:464:ASN:HD22	1.85	0.41
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.91	0.41
1:B:510:GLN:HG2	1:B:516:VAL:HG11	2.02	0.41
4:B:1001:MS1:H1	4:B:1001:MS1:H3P	1.75	0.41
1:A:74:HIS:CB	1:B:69:LEU:HD13	2.50	0.41
1:B:569:ASP:O	1:B:573:ILE:HG13	2.21	0.41
1:A:203:SER:HA	1:A:227:LEU:HG	2.03	0.41
1:A:479:PHE:CE2	1:A:488:VAL:HG13	2.55	0.41
1:B:247:ALA:CB	1:B:321:ALA:HB2	2.50	0.41
1:A:14:GLU:O	1:A:14:GLU:HG3	2.20	0.41
1:A:106:PRO:HB2	1:A:109:LYS:HG3	2.03	0.41
1:B:294:HIS:HA	1:B:297:LEU:HD12	2.01	0.41
1:A:7:LEU:CD1	1:A:33:ILE:HD11	2.40	0.41
1:A:506:LEU:O	1:A:510:GLN:HB2	2.20	0.41
1:B:103:ASN:HB3	1:B:147:CYS:O	2.20	0.41
1:B:247:ALA:HB2	1:B:266:PHE:CD1	2.54	0.41
1:B:436:TYR:CE2	1:B:555:ILE:HG21	2.55	0.41
1:A:211:MET:N	1:B:389:GLN:OE1	2.52	0.41
1:A:379:ILE:CG2	5:B:1077:HOH:O	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:TRP:CZ2	1:A:513:PHE:CZ	3.08	0.41
1:B:320:ILE:O	1:B:342:VAL:HA	2.21	0.41
1:A:497:THR:C	1:A:499:THR:H	2.23	0.41
1:B:66:VAL:O	1:B:68:THR:N	2.53	0.41
1:A:528:TRP:HH2	5:A:1196:HOH:O	2.03	0.41
1:B:78:LEU:HD21	1:B:135:ALA:HB1	2.03	0.41
1:B:278:ILE:CD1	1:B:417:ARG:CZ	2.99	0.41
1:A:100:VAL:HG21	1:A:136:ALA:HB2	2.01	0.41
1:A:542:PHE:CD1	1:A:542:PHE:C	2.94	0.41
1:A:555:ILE:O	1:A:555:ILE:CG1	2.69	0.41
1:B:68:THR:OG1	5:B:1086:HOH:O	2.22	0.41
1:B:83:PRO:O	1:B:84:GLU:C	2.57	0.41
1:B:156:ALA:C	1:B:158:GLU:H	2.24	0.41
1:B:349:GLU:OE1	1:B:349:GLU:N	2.54	0.41
1:A:219:GLN:HE21	1:B:388:MET:CE	2.34	0.41
1:A:353:LYS:HE3	1:A:353:LYS:HB2	1.95	0.41
1:A:543:PHE:HE2	1:A:560:ILE:HG21	1.86	0.41
1:A:583:LEU:HD12	1:A:584:ILE:N	2.36	0.41
1:B:26:ASN:C	1:B:28:LEU:N	2.75	0.41
1:B:28:LEU:CB	1:B:165:LYS:HD3	2.51	0.41
1:B:494:GLN:HG2	1:B:494:GLN:H	1.73	0.41
1:B:561:VAL:HG13	1:B:561:VAL:O	2.21	0.41
1:A:155:VAL:O	1:A:158:GLU:N	2.52	0.40
1:A:453:ILE:HD13	1:A:547:ASP:CG	2.42	0.40
1:B:47:LEU:HA	1:B:48:PRO:HD3	1.85	0.40
1:B:243:ASP:OD1	1:B:269:VAL:N	2.49	0.40
1:A:86:ASN:N	1:A:86:ASN:ND2	2.69	0.40
1:A:316:PHE:CB	4:B:1001:MS1:H7F	2.51	0.40
1:A:472:PRO:HD3	1:A:528:TRP:CZ3	2.56	0.40
1:B:34:ALA:C	1:B:52:VAL:HG23	2.42	0.40
1:B:113:SER:CB	1:B:114:PRO:HD2	2.45	0.40
1:B:237:GLY:H	1:B:240:ASN:HB2	1.85	0.40
1:A:298:THR:HG23	1:A:329:PRO:HG3	2.04	0.40
1:A:379:ILE:HA	1:A:387:LEU:O	2.21	0.40
1:A:412:PRO:HD2	1:A:559:PHE:CE2	2.56	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	588/613 (96%)	542 (92%)	39 (7%)	7 (1%)	13 24
1	B	588/613 (96%)	541 (92%)	38 (6%)	9 (2%)	10 18
All	All	1176/1226 (96%)	1083 (92%)	77 (6%)	16 (1%)	11 20

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	LYS
1	A	36	GLY
1	A	53	SER
1	A	499	THR
1	A	500	ILE
1	B	27	ALA
1	B	36	GLY
1	A	277	GLY
1	A	512	MET
1	B	157	LYS
1	B	515	GLU
1	B	83	PRO
1	B	106	PRO
1	B	165	LYS
1	A	106	PRO
1	B	277	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	484/502 (96%)	464 (96%)	20 (4%)	30	55
1	B	484/502 (96%)	465 (96%)	19 (4%)	32	57
All	All	968/1004 (96%)	929 (96%)	39 (4%)	31	56

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	54	ASP
1	A	60	GLU
1	A	82	ILE
1	A	113	SER
1	A	146	VAL
1	A	153	SER
1	A	216	SER
1	A	265	SER
1	A	270	SER
1	A	280	LEU
1	A	360	ASN
1	A	379	ILE
1	A	402	LYS
1	A	406	THR
1	A	429	THR
1	A	461	ASP
1	A	503	ASP
1	A	510	GLN
1	A	589	ARG
1	B	55	LEU
1	B	58	PHE
1	B	83	PRO
1	B	85	ASP
1	B	88	ASP
1	B	102	CYS
1	B	104	LEU
1	B	108	VAL
1	B	174	HIS
1	B	177	LEU
1	B	199	SER
1	B	211	MET
1	B	226	LYS
1	B	235	SER
1	B	360	ASN

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Mol	Chain	Res	Type
1	B	379	ILE
1	B	494	GLN
1	B	537	LEU
1	B	549	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	26	ASN
1	A	81	ASN
1	A	86	ASN
1	A	139	ASN
1	A	219	GLN
1	A	510	GLN
1	A	527	GLN
1	B	5	GLN
1	B	81	ASN
1	B	86	ASN
1	B	139	ASN
1	B	174	HIS
1	B	185	GLN
1	B	256	GLN
1	B	408	ASN
1	B	494	GLN
1	B	510	GLN
1	B	558	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	B	1006	-	4,4,4	1.63	0	6,6,6	0.42	0
4	MS1	B	1001	-	57,61,61	2.63	24 (42%)	73,89,89	3.69	35 (47%)
3	PO4	A	1005	-	4,4,4	1.63	0	6,6,6	0.43	0
4	MS1	A	1002	-	57,61,61	3.66	22 (38%)	73,89,89	3.56	29 (39%)

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	MS1	B	1001	-	-	10/38/64/64	0/5/5/5
4	MS1	A	1002	-	-	8/38/64/64	0/5/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	MS1	C42-N10	-19.23	1.11	1.36
4	B	1001	MS1	C4A-C4F	8.47	1.55	1.41
4	A	1002	MS1	C11-N10	8.21	1.60	1.43
4	A	1002	MS1	C4A-C4F	7.47	1.54	1.41
4	B	1001	MS1	C11-N10	6.96	1.57	1.43
4	B	1001	MS1	C2F-N3F	6.33	1.46	1.35
4	A	1002	MS1	C2F-N3F	6.33	1.46	1.35
4	B	1001	MS1	C8A-N1F	5.37	1.46	1.37
4	A	1002	MS1	C2P-C42	5.16	1.56	1.48
4	A	1002	MS1	OE2-CD	4.52	1.37	1.22
4	B	1001	MS1	OE2-CD	4.51	1.37	1.22
4	A	1002	MS1	C13-C14	4.40	1.46	1.39
4	A	1002	MS1	C12-C11	4.27	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	MS1	C9-N10	3.88	1.53	1.46
4	A	1002	MS1	C16-C11	3.86	1.46	1.39
4	B	1001	MS1	C16-C11	3.64	1.46	1.39
4	A	1002	MS1	C8A-N1F	3.59	1.43	1.37
4	B	1001	MS1	C2-C1	-3.55	1.48	1.53
4	B	1001	MS1	C15-C14	3.42	1.45	1.39
4	A	1002	MS1	P-O9	3.38	1.61	1.50
4	B	1001	MS1	P-O9	3.25	1.61	1.50
4	A	1002	MS1	C12-C13	3.21	1.44	1.38
4	B	1001	MS1	C8F-C7F	3.09	1.43	1.36
4	B	1001	MS1	C9-N10	3.09	1.52	1.46
4	B	1001	MS1	C2P-C42	3.07	1.53	1.48
4	B	1001	MS1	C4F-N3F	2.92	1.38	1.33
4	A	1002	MS1	C15-C16	2.83	1.43	1.38
4	B	1001	MS1	C12-C11	2.73	1.44	1.39
4	B	1001	MS1	C2P-C3P	2.64	1.39	1.33
4	A	1002	MS1	C15-C14	2.64	1.43	1.39
4	B	1001	MS1	C7F-C6F	2.60	1.44	1.38
4	A	1002	MS1	C2P-C3P	2.57	1.39	1.33
4	B	1001	MS1	C12-C13	2.42	1.43	1.38
4	B	1001	MS1	OT-C	2.36	1.38	1.30
4	A	1002	MS1	O1-C1	2.34	1.44	1.41
4	B	1001	MS1	C4A-C8A	2.31	1.47	1.43
4	B	1001	MS1	C15-C16	2.26	1.42	1.38
4	B	1001	MS1	CB-CA	2.21	1.58	1.53
4	A	1002	MS1	C17-N	-2.20	1.29	1.34
4	A	1002	MS1	OT-C	2.15	1.37	1.30
4	B	1001	MS1	C42-N10	-2.10	1.33	1.36
4	A	1002	MS1	C2F-N2F	2.08	1.38	1.33
4	A	1002	MS1	C8-N7	2.08	1.38	1.35
4	B	1001	MS1	C2F-N2F	2.07	1.38	1.33
4	B	1001	MS1	CA-N	2.06	1.50	1.45
4	A	1002	MS1	C4P-N9	2.00	1.40	1.36

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1002	MS1	C3P-C2P-C42	15.99	151.85	120.51
4	B	1001	MS1	C3P-C2P-C42	15.84	151.57	120.51
4	B	1001	MS1	C4P-C3P-C2P	12.38	147.42	126.21
4	A	1002	MS1	C4P-C3P-C2P	11.95	146.69	126.21
4	B	1001	MS1	C5P-C4P-N9	9.96	113.32	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1001	MS1	O1-C1-C2	9.51	120.82	106.93
4	A	1002	MS1	C5P-C4P-N9	8.78	112.70	108.14
4	A	1002	MS1	O1-C1-C2	7.16	117.39	106.93
4	A	1002	MS1	C11-N10-C42	-6.72	115.72	123.52
4	A	1002	MS1	O42-C42-N10	-6.02	113.61	120.87
4	B	1001	MS1	CG-CB-CA	5.39	123.23	113.16
4	A	1002	MS1	C4A-C4F-N3F	-5.21	116.30	123.43
4	B	1001	MS1	O42-C42-N10	4.95	126.85	120.87
4	A	1002	MS1	C8-N9-C4P	-4.94	96.51	105.88
4	B	1001	MS1	CA-N-C17	-4.93	109.53	121.60
4	B	1001	MS1	O42-C42-C2P	-4.73	112.22	122.06
4	A	1002	MS1	O42-C42-C2P	-4.67	112.34	122.06
4	A	1002	MS1	C2F-N3F-C4F	4.51	123.09	115.93
4	B	1001	MS1	C4A-C4F-N3F	-4.41	117.40	123.43
4	B	1001	MS1	C2F-N3F-C4F	4.40	122.93	115.93
4	A	1002	MS1	C6F-C9-N10	4.32	119.76	112.76
4	A	1002	MS1	O62-C6-N1	-4.24	116.55	122.58
4	B	1001	MS1	O62-C6-N1	-4.20	116.61	122.58
4	B	1001	MS1	N1F-C2F-N3F	-4.19	121.63	127.22
4	A	1002	MS1	N1F-C2F-N3F	-4.16	121.68	127.22
4	B	1001	MS1	C3-C2-C1	-3.86	95.17	100.98
4	A	1002	MS1	C16-C11-N10	3.75	125.66	120.18
4	B	1001	MS1	C16-C11-N10	3.67	125.55	120.18
4	B	1001	MS1	C5P-C6-N1	3.62	121.46	115.75
4	B	1001	MS1	CB-CA-N	3.49	117.93	110.88
4	B	1001	MS1	C4F-C4A-N5F	3.49	122.58	118.60
4	B	1001	MS1	C6F-C9-N10	3.44	118.33	112.76
4	A	1002	MS1	C5P-C6-N1	3.41	121.14	115.75
4	A	1002	MS1	OE2-CD-CG	-3.35	112.32	123.08
4	A	1002	MS1	C4F-C4A-N5F	3.32	122.39	118.60
4	B	1001	MS1	OE2-CD-CG	-3.29	112.50	123.08
4	B	1001	MS1	C5-C4-C3	-3.10	103.58	115.18
4	A	1002	MS1	OE1-CD-CG	3.07	123.89	114.03
4	B	1001	MS1	C6F-N5F-C4A	3.02	122.01	118.45
4	A	1002	MS1	C4A-C8A-N1F	-2.99	119.32	121.68
4	B	1001	MS1	C8-N9-C4P	-2.96	100.28	105.88
4	A	1002	MS1	CA-N-C17	-2.92	114.46	121.60
4	B	1001	MS1	OE1-CD-CG	2.88	123.27	114.03
4	B	1001	MS1	C16-C11-C12	-2.83	113.39	119.16
4	B	1001	MS1	O2-C2-C3	2.70	120.57	111.82
4	A	1002	MS1	O2-C2-C3	2.66	120.43	111.82
4	B	1001	MS1	C15-C16-C11	2.63	123.79	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1001	MS1	C11-N10-C42	2.60	126.54	123.52
4	A	1002	MS1	CB-CA-N	-2.60	105.61	110.88
4	B	1001	MS1	O1-C4-C3	2.49	110.05	105.11
4	B	1001	MS1	C13-C12-C11	2.43	123.52	120.32
4	A	1002	MS1	O1-C4-C3	2.34	109.74	105.11
4	B	1001	MS1	C2-C3-C4	2.32	107.16	102.64
4	B	1001	MS1	C14-C17-N	2.23	121.35	117.06
4	A	1002	MS1	C12-C13-C14	2.23	123.38	120.78
4	A	1002	MS1	C15-C16-C11	2.22	123.25	120.32
4	B	1001	MS1	O17-C17-N	-2.20	118.40	122.45
4	B	1001	MS1	C2F-N1F-C8A	2.15	121.65	116.33
4	B	1001	MS1	C8F-C8A-N1F	2.11	121.91	118.69
4	A	1002	MS1	C2F-N1F-C8A	2.11	121.55	116.33
4	A	1002	MS1	C6F-N5F-C4A	2.10	120.92	118.45
4	A	1002	MS1	C15-C14-C13	-2.05	115.67	118.59
4	A	1002	MS1	C8F-C8A-N1F	2.05	121.82	118.69
4	B	1001	MS1	C8F-C8A-C4A	-2.01	117.82	119.83

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	MS1	C5-O6-P-O8
4	B	1001	MS1	C5-O6-P-O8
4	B	1001	MS1	C5-O6-P-O7
4	B	1001	MS1	N-CA-CB-CG
4	B	1001	MS1	C-CA-CB-CG
4	B	1001	MS1	O1-C4-C5-O6
4	B	1001	MS1	C3-C4-C5-O6
4	B	1001	MS1	C3P-C2P-C42-O42
4	A	1002	MS1	C12-C11-N10-C42
4	A	1002	MS1	C3P-C2P-C42-O42
4	A	1002	MS1	O42-C42-N10-C9
4	B	1001	MS1	C3P-C2P-C42-N10
4	A	1002	MS1	C6F-C9-N10-C42
4	A	1002	MS1	C16-C11-N10-C42
4	A	1002	MS1	OE1-CD-CG-CB
4	B	1001	MS1	C5-O6-P-O9
4	A	1002	MS1	OE2-CD-CG-CB
4	B	1001	MS1	C6F-C9-N10-C42

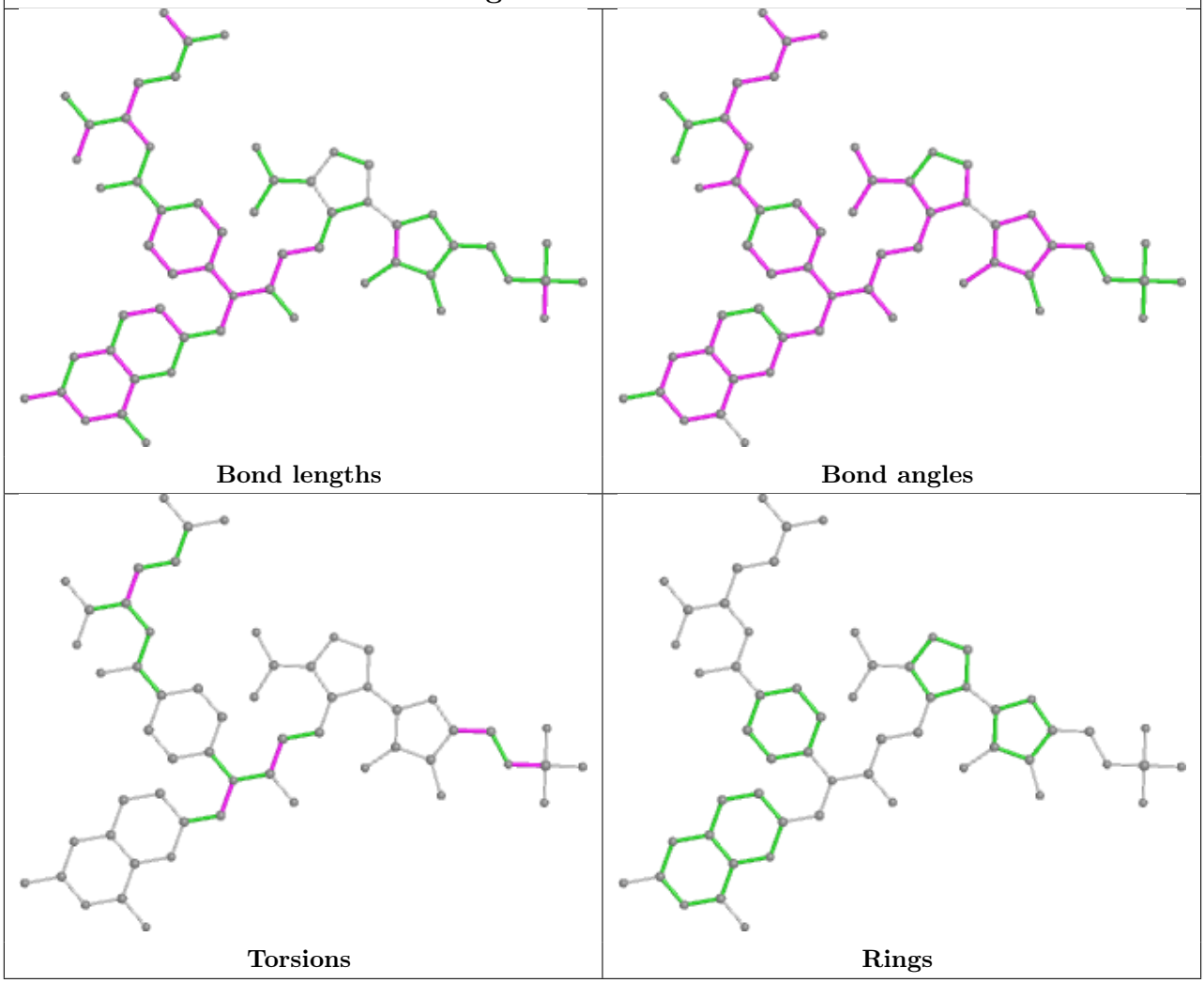
There are no ring outliers.

2 monomers are involved in 13 short contacts:

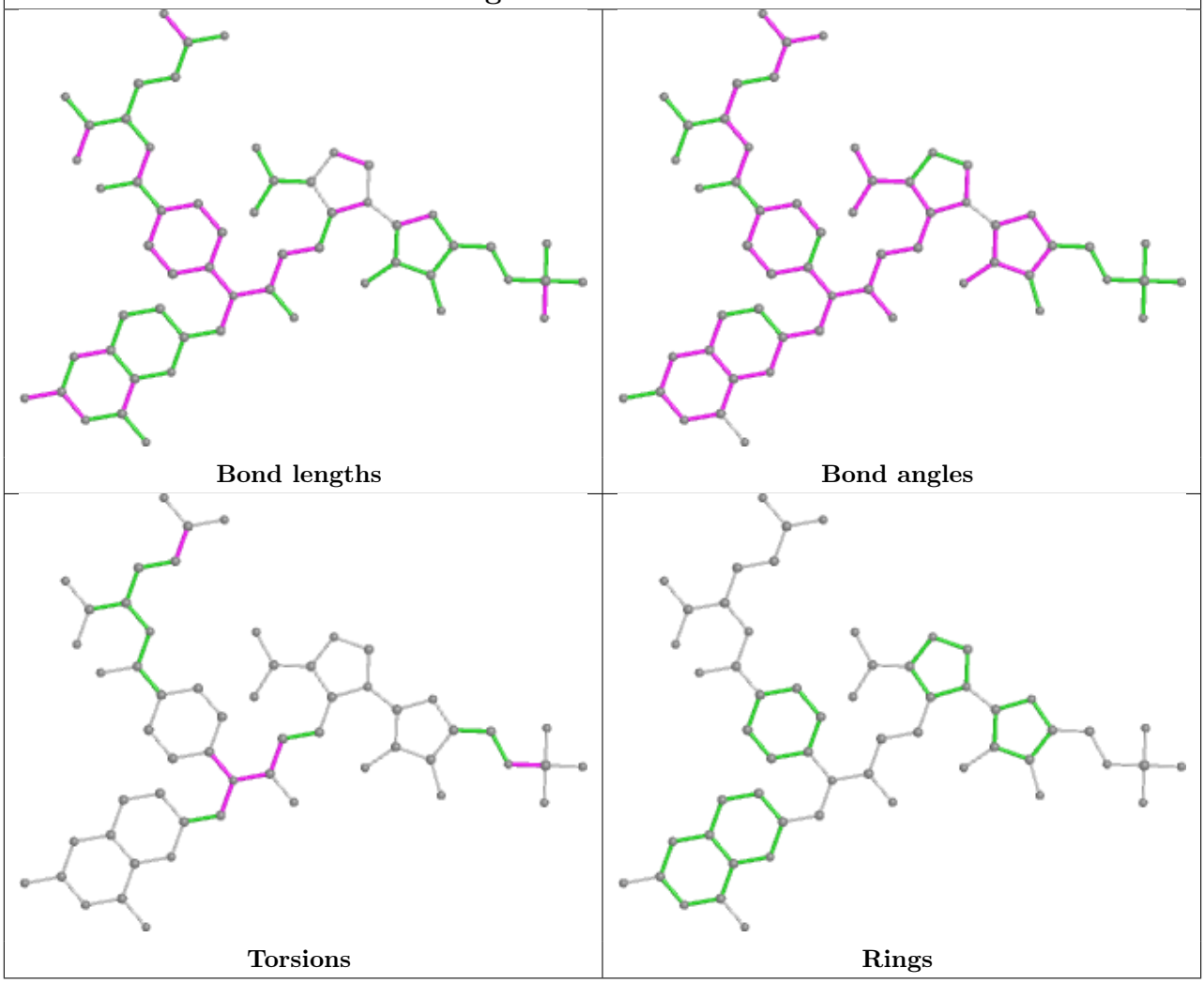
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	MS1	7	0
4	A	1002	MS1	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MS1 B 1001



Ligand MS1 A 1002



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	590/613 (96%)	-0.17	8 (1%)	75	77	21, 40, 70, 87	0
1	B	590/613 (96%)	-0.20	13 (2%)	62	65	21, 40, 68, 82	1 (0%)
All	All	1180/1226 (96%)	-0.18	21 (1%)	68	71	21, 40, 69, 87	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	PRO	3.6
1	A	4	ARG	3.4
1	B	115	GLY	3.4
1	B	503	ASP	3.1
1	A	160	ALA	3.0
1	A	502	GLU	3.0
1	B	502	GLU	2.9
1	B	116	VAL	2.9
1	A	112	SER	2.7
1	B	113	SER	2.7
1	A	504	GLU	2.6
1	B	4	ARG	2.6
1	B	64	GLY	2.4
1	A	86	ASN	2.3
1	B	60	GLU	2.2
1	B	163	LYS	2.2
1	B	105	TYR	2.2
1	A	43	ARG	2.2
1	B	100	VAL	2.1
1	B	504	GLU	2.1
1	A	163	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

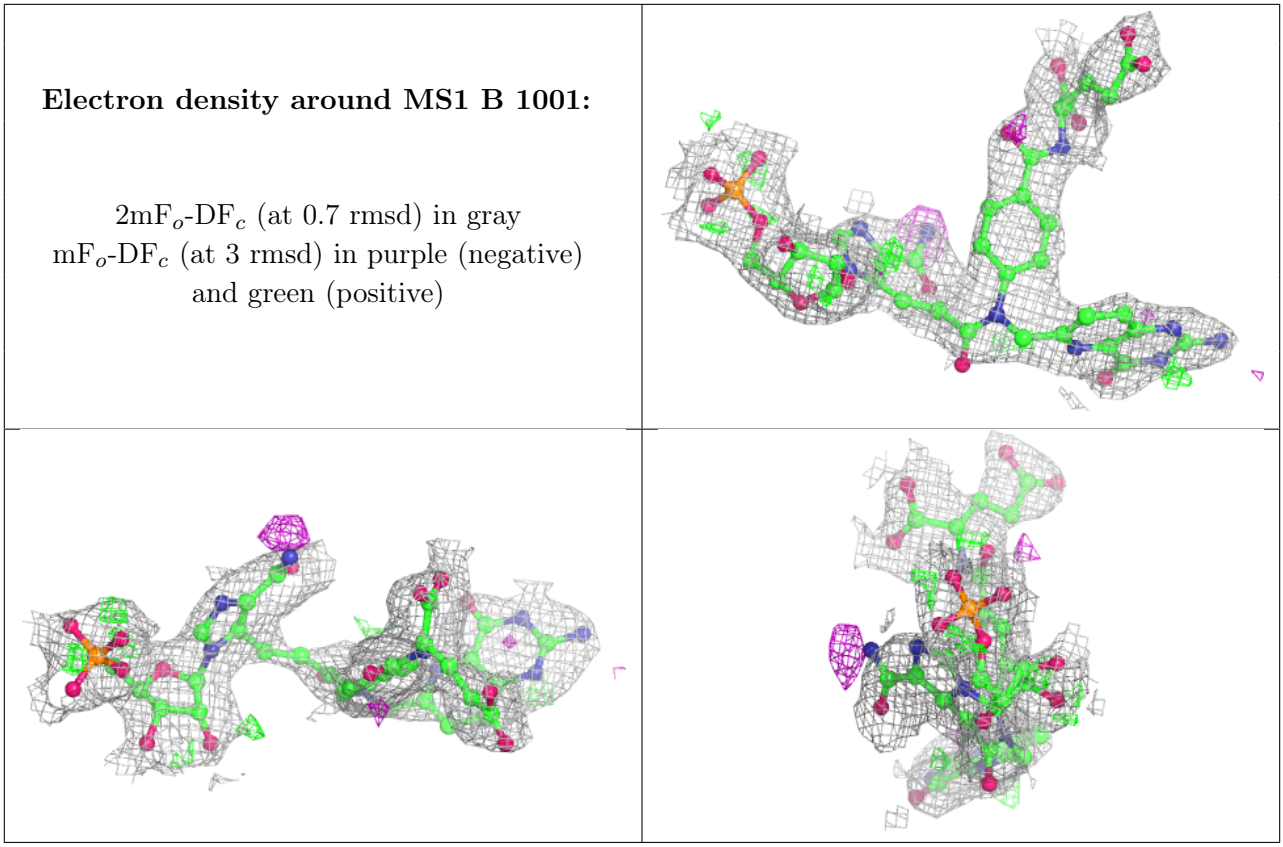
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MS1	B	1001	57/57	0.87	0.19	47,57,65,66	0
3	PO4	B	1006	5/5	0.90	0.15	81,81,81,82	0
4	MS1	A	1002	57/57	0.91	0.15	38,50,58,58	0
2	K	A	1004	1/1	0.92	0.14	42,42,42,42	0
3	PO4	A	1005	5/5	0.94	0.12	97,97,97,98	0
2	K	B	1003	1/1	0.98	0.09	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

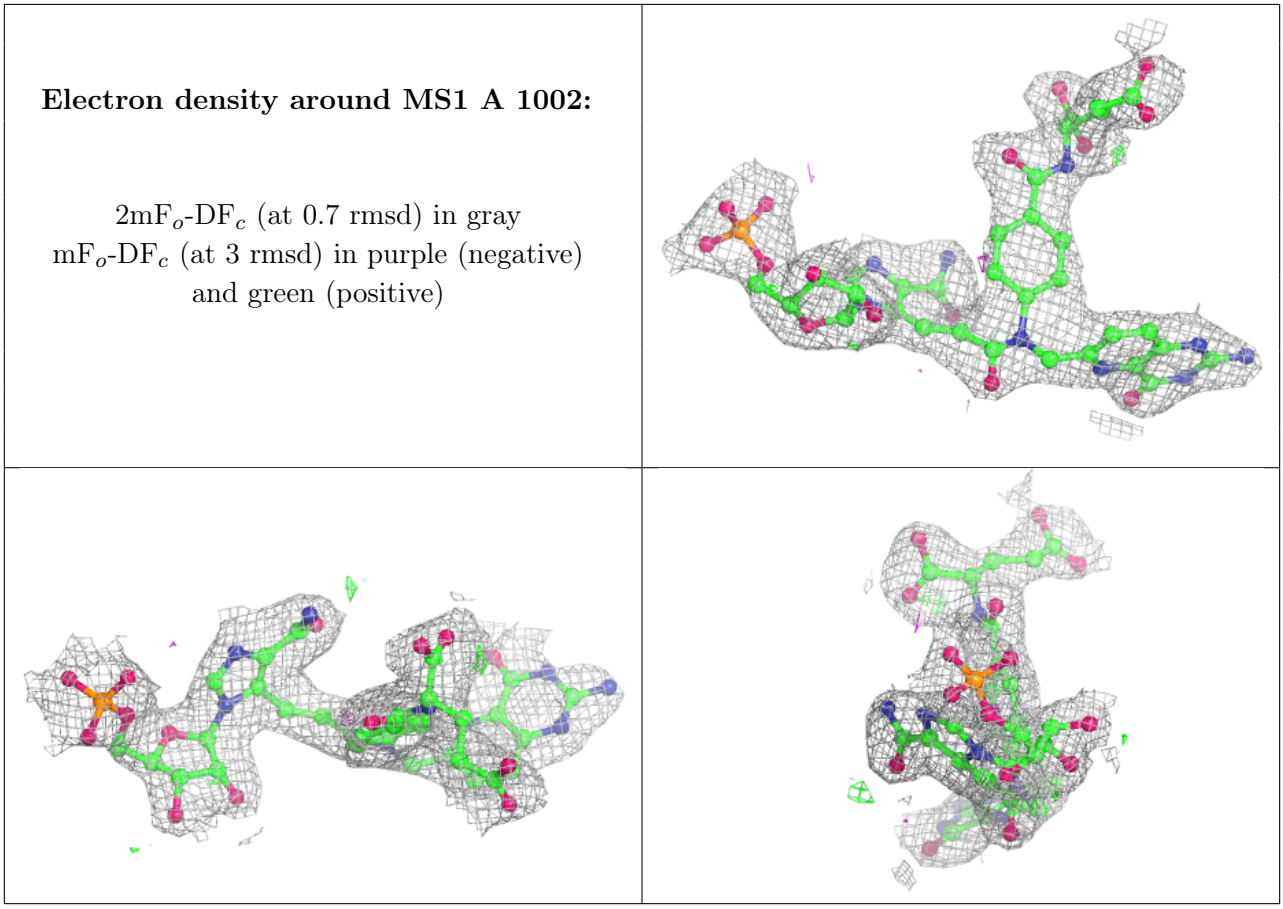
Electron density around MS1 B 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MS1 A 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.