



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:33 PM GMT

PDB ID : 1G51
Title : ASPARTYL TRNA SYNTHETASE FROM THERMUS THERMOPHILUS
AT 2.4 Å RESOLUTION
Authors : Poterzsmann, A.; Delarue, M.; Thierry, J.C.; Moras, D.
Deposited on : 2000-10-30
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

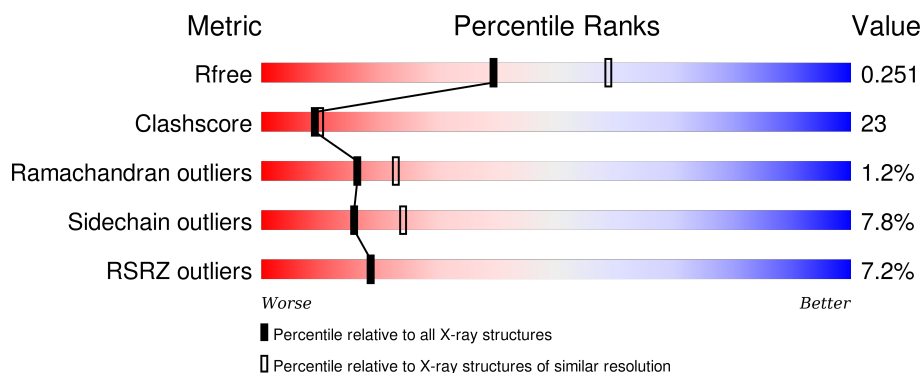
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	580	<div> <div>11%</div> <div>59%</div> <div>36%</div> <div>.</div> </div>
1	B	580	<div> <div>3%</div> <div>66%</div> <div>29%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10100 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 ASPARTYL-TRNA SYNTHETASE.

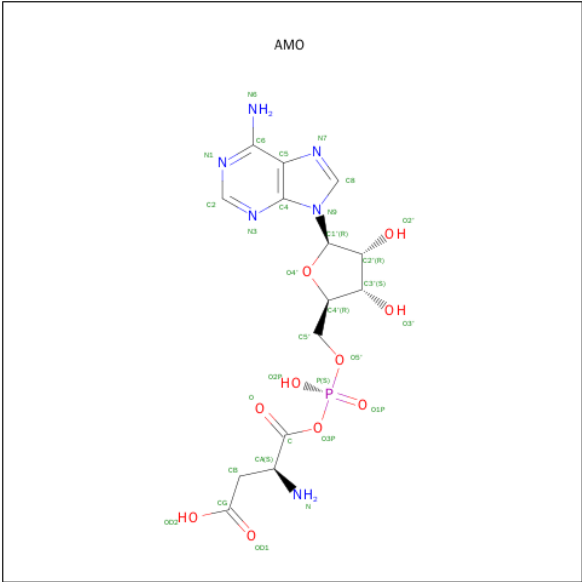
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	0	0
			4668	2980	840	837	11			
1	B	580	Total	C	N	O	S	0	0	0
			4668	2980	840	837	11			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



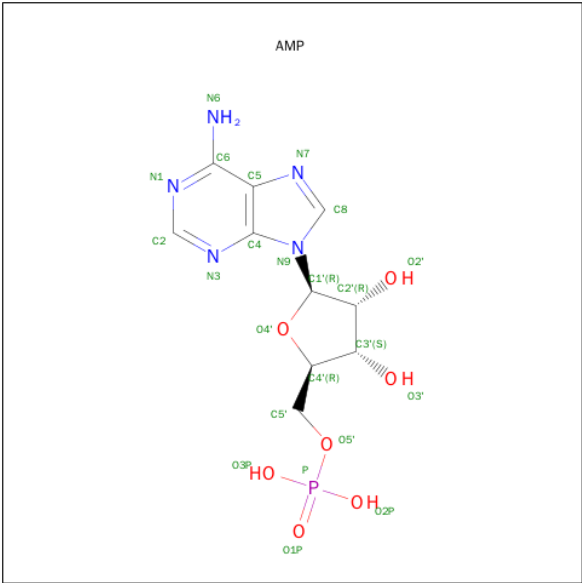
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ASPARTYL-ADENOSINE-5'-MONOPHOSPHATE (three-letter code: AMO) (formula: C₁₄H₁₉N₆O₁₀P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	14	6	10	1		
3	B	1	Total	C	N	O	P	0	0
			31	14	6	10	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

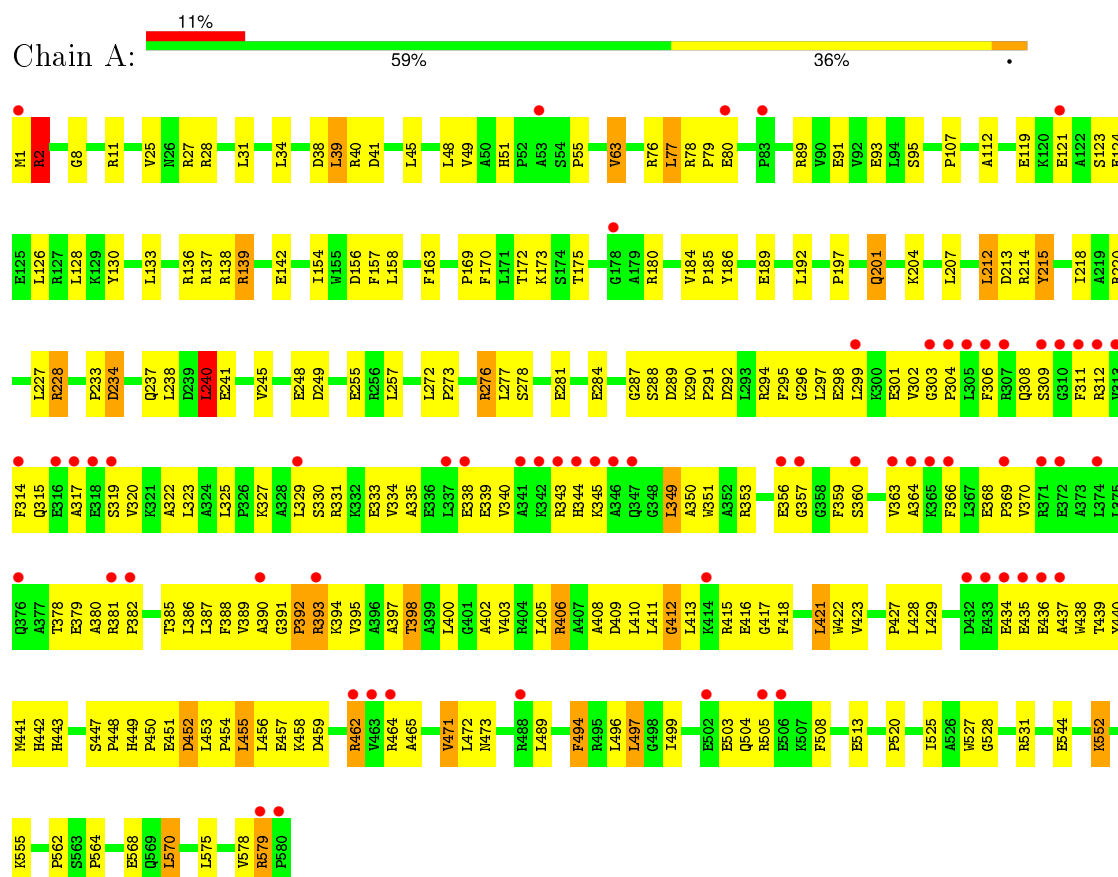
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	288	Total 288	O 288	0	0
5	B	381	Total 381	O 381	0	0

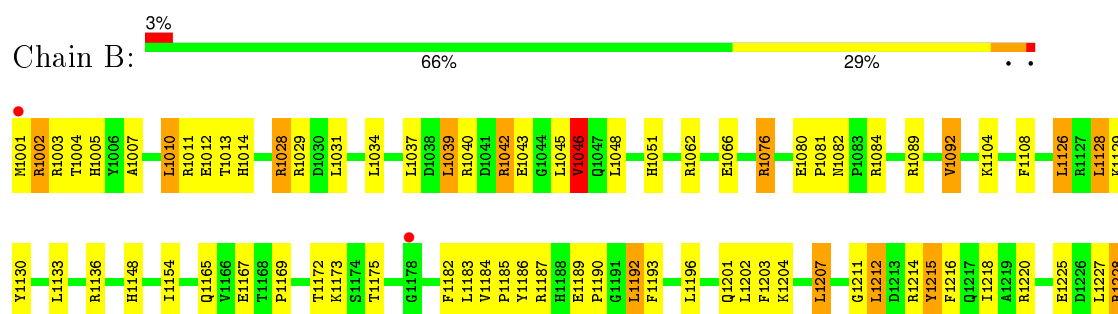
3 Residue-property plots

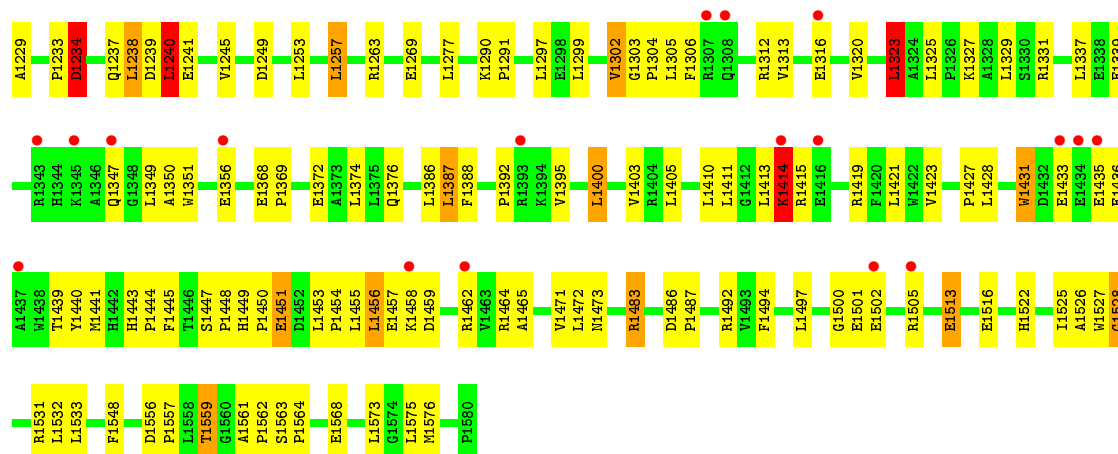
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ASPARTYL-TRNA SYNTHETASE



• Molecule 1: ASPARTYL-TRNA SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.13Å 155.50Å 171.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.00 – 2.40 14.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.3 (14.00-2.40) 91.4 (14.00-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.251 0.194 , 0.251	Depositor DCC
R_{free} test set	4443 reflections (7.67%)	DCC
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 60454 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, SO4, AMO

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	0.62	0/4780	0.84	7/6467 (0.1%)
1	B	0.65	0/4780	0.91	14/6467 (0.2%)
All	All	0.63	0/9560	0.88	21/12934 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	LEU	CA-CB-CG	8.87	135.71	115.30
1	B	1240	LEU	CA-CB-CG	8.74	135.40	115.30
1	A	2	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	B	1212	LEU	C-N-CA	-6.83	104.62	121.70
1	A	212	LEU	N-CA-C	-6.36	93.82	111.00
1	B	1046	VAL	CB-CA-C	-6.29	99.45	111.40
1	B	1212	LEU	N-CA-C	-5.96	94.91	111.00
1	B	1234	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	218	ILE	N-CA-C	-5.75	95.46	111.00
1	B	1323	LEU	CA-CB-CG	5.70	128.40	115.30
1	B	1238	LEU	N-CA-C	-5.67	95.69	111.00
1	B	1218	ILE	N-CA-C	-5.66	95.72	111.00
1	A	156	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	528	GLY	N-CA-C	-5.49	99.39	113.10
1	B	1356	GLU	N-CA-C	-5.41	96.40	111.00
1	B	1003	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	41	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	B	1207	LEU	CA-CB-CG	5.16	127.16	115.30
1	B	1182	PHE	N-CA-C	-5.15	97.09	111.00
1	B	1528	GLY	N-CA-C	-5.12	100.31	113.10
1	B	1028	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4668	0	4679	276	0
1	B	4668	0	4676	181	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	31	0	17	5	0
3	B	31	0	17	3	0
4	B	23	0	12	0	0
5	A	288	0	0	21	0
5	B	381	0	0	25	0
All	All	10100	0	9401	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 23.

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:B:1431:TRP:CH2	1:B:1436:GLU:HA	1.92	1.04
1:A:301:GLU:OE2	1:A:319:SER:HB2	1.59	1.00
1:A:214:ARG:HG2	5:B:2657:HOH:O	1.61	1.00
1:A:394:LYS:HE2	1:A:398:THR:HG21	1.42	1.00
1:A:499:ILE:HG13	1:A:503:GLU:HB3	1.48	0.95
1:A:459:ASP:HB3	1:A:462:ARG:HG2	1.47	0.94
1:A:393:ARG:HD2	1:A:394:LYS:H	1.31	0.93
1:A:303:GLY:HA2	1:A:320:VAL:HG22	1.50	0.92
1:B:1559:THR:HG22	1:B:1561:ALA:H	1.31	0.92
1:A:393:ARG:CD	1:A:394:LYS:H	1.83	0.91
1:A:137:ARG:HH22	1:A:139:ARG:HH12	1.13	0.90
1:B:1011:ARG:H	1:B:1014:HIS:HD2	1.20	0.89
1:A:393:ARG:HD2	1:A:394:LYS:N	1.88	0.88
1:A:389:VAL:CG1	1:A:400:LEU:HB2	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:HD23	1:A:462:ARG:HD3	1.55	0.87
1:A:394:LYS:O	1:A:398:THR:HG22	1.75	0.86
1:B:1204:LYS:HE2	1:B:1241:GLU:OE1	1.76	0.85
1:A:79:PRO:HG2	1:A:80:GLU:OE1	1.76	0.85
1:A:213:ASP:N	5:A:2638:HOH:O	2.11	0.84
1:B:1439:THR:HG22	1:B:1440:TYR:H	1.41	0.83
1:A:297:LEU:HB3	1:A:323:LEU:HD12	1.60	0.83
1:A:276:ARG:O	1:A:277:LEU:HD23	1.79	0.83
1:B:1042:ARG:HD3	1:B:1043:GLU:OE1	1.79	0.83
1:B:1327:LYS:HB2	1:B:1411:LEU:HD12	1.60	0.83
1:A:339:GLU:O	1:A:343:ARG:HG2	1.79	0.83
1:B:1241:GLU:OE2	1:B:1483:ARG:HD2	1.78	0.82
1:A:455:LEU:H	1:A:455:LEU:HD12	1.43	0.82
1:A:389:VAL:HG11	1:A:400:LEU:HB2	1.59	0.81
1:A:455:LEU:CD1	1:A:455:LEU:H	1.94	0.81
1:B:1040:ARG:HB2	1:B:1045:LEU:HD23	1.62	0.81
1:A:80:GLU:HG2	1:A:80:GLU:O	1.81	0.80
1:B:1323:LEU:HD22	1:B:1387:LEU:HB2	1.64	0.79
1:B:1012:GLU:OE1	1:B:1089:ARG:HD3	1.82	0.79
1:A:137:ARG:HH22	1:A:139:ARG:NH1	1.80	0.78
1:A:329:LEU:HD23	1:A:411:LEU:HD21	1.65	0.77
1:A:323:LEU:HD22	1:A:400:LEU:HD11	1.65	0.77
1:A:578:VAL:HG21	5:B:2481:HOH:O	1.85	0.77
1:B:1439:THR:HG22	1:B:1440:TYR:N	1.99	0.77
1:B:1316:GLU:HG3	5:B:2488:HOH:O	1.85	0.76
1:A:455:LEU:HD12	1:A:455:LEU:N	2.01	0.76
1:A:2:ARG:NH2	1:B:1245:VAL:HG12	1.99	0.76
1:A:408:ALA:HA	1:A:413:LEU:HD12	1.68	0.76
1:A:570:LEU:HD22	1:A:575:LEU:HB2	1.66	0.76
1:B:1327:LYS:HB2	1:B:1411:LEU:CD1	2.15	0.76
1:A:392:PRO:HD2	1:A:395:VAL:HG21	1.67	0.75
1:A:394:LYS:HD3	1:A:395:VAL:N	2.02	0.75
1:A:394:LYS:NZ	1:A:395:VAL:HG12	2.02	0.75
1:A:499:ILE:CG1	1:A:503:GLU:HB3	2.16	0.75
1:B:1431:TRP:CZ3	1:B:1433:GLU:HA	2.21	0.75
1:A:392:PRO:HB2	1:A:395:VAL:HG22	1.68	0.75
1:A:204:LYS:HE3	1:A:241:GLU:OE1	1.87	0.75
1:A:303:GLY:CA	1:A:320:VAL:HG22	2.17	0.74
1:A:330:SER:O	1:A:334:VAL:HG23	1.88	0.74
1:A:409:ASP:OD2	1:A:415:ARG:NH1	2.21	0.74
1:B:1220:ARG:HD2	1:B:1234:ASP:OD2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:SER:OG	1:A:281:GLU:HG2	1.88	0.73
1:A:311:PHE:HB2	1:A:366:PHE:CE1	2.24	0.73
1:B:1421:LEU:CD2	1:B:1471:VAL:HG22	2.19	0.72
1:A:394:LYS:HZ3	1:A:395:VAL:HG12	1.55	0.72
1:A:139:ARG:NH2	1:A:544:GLU:OE1	2.22	0.72
1:A:393:ARG:HH12	1:A:395:VAL:HG13	1.55	0.71
1:A:227:LEU:O	1:A:552:LYS:HD2	1.91	0.71
1:A:173:LYS:HB2	1:B:1559:THR:CG2	2.21	0.71
1:B:1431:TRP:CZ2	1:B:1436:GLU:HA	2.26	0.70
1:A:273:PRO:HB2	5:A:2356:HOH:O	1.92	0.69
1:B:1458:LYS:HE2	1:B:1459:ASP:HB2	1.74	0.69
1:A:295:PHE:CE2	1:A:408:ALA:HB2	2.28	0.68
1:A:353:ARG:HH11	1:A:353:ARG:HG3	1.59	0.68
1:B:1201:GLN:O	1:B:1204:LYS:HG2	1.94	0.68
1:B:1439:THR:CG2	1:B:1440:TYR:H	2.06	0.67
1:A:449:HIS:ND1	1:A:450:PRO:HD2	2.09	0.67
1:A:418:PHE:HB3	1:A:472:LEU:HD11	1.77	0.67
1:B:1011:ARG:H	1:B:1014:HIS:CD2	2.10	0.67
1:B:1128:LEU:HB3	1:B:1557:PRO:HG2	1.75	0.67
1:A:320:VAL:HG12	1:A:390:ALA:CB	2.24	0.67
1:A:303:GLY:N	1:A:304:PRO:HD2	2.10	0.67
1:A:389:VAL:HG12	1:A:400:LEU:HB2	1.75	0.67
1:A:349:LEU:HD23	1:A:388:PHE:O	1.95	0.67
1:B:1007:ALA:HB1	1:B:1046:VAL:HG22	1.77	0.67
1:A:381:ARG:HB3	1:A:382:PRO:CD	2.26	0.66
1:A:391:GLY:O	1:A:392:PRO:O	2.13	0.66
1:A:325:LEU:HD11	1:A:329:LEU:HD11	1.77	0.65
1:A:173:LYS:HB2	1:B:1559:THR:HG23	1.78	0.65
1:A:413:LEU:O	1:A:415:ARG:HG3	1.97	0.65
1:A:40:ARG:HB3	1:A:45:LEU:HD23	1.79	0.65
1:A:451:GLU:C	1:A:453:LEU:H	1.99	0.64
1:A:439:THR:HG22	1:A:440:TYR:H	1.62	0.64
1:B:1455:LEU:HD23	1:B:1462:ARG:HD3	1.80	0.64
1:A:494:PHE:O	1:A:499:ILE:HG22	1.96	0.64
1:A:353:ARG:HG3	1:A:353:ARG:NH1	2.12	0.64
1:B:1257:LEU:HD13	1:B:1527:TRP:CH2	2.33	0.64
1:B:1431:TRP:HZ3	1:B:1433:GLU:HA	1.63	0.63
1:A:299:LEU:HD22	1:A:400:LEU:CD1	2.29	0.63
1:A:330:SER:OG	1:A:333:GLU:HG3	1.98	0.63
1:B:1455:LEU:H	1:B:1455:LEU:HD12	1.63	0.63
1:B:1453:LEU:O	1:B:1456:LEU:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:PRO:HD2	1:A:441:MET:HE3	1.79	0.63
1:A:400:LEU:HA	1:A:403:VAL:HG22	1.80	0.63
1:A:331:ARG:HD2	1:A:334:VAL:HB	1.81	0.63
1:A:51:HIS:HE1	1:A:76:ARG:HH12	1.47	0.63
1:A:393:ARG:H	1:A:393:ARG:CD	2.08	0.62
1:A:340:VAL:HG21	1:A:406:ARG:HG3	1.81	0.62
1:B:1372:GLU:HB2	5:B:2333:HOH:O	1.98	0.62
1:A:451:GLU:O	1:A:453:LEU:N	2.32	0.62
1:A:406:ARG:HH11	1:A:406:ARG:HG3	1.65	0.62
1:A:325:LEU:HG	1:A:387:LEU:HD13	1.81	0.62
1:B:1350:ALA:HB3	1:B:1388:PHE:HB2	1.81	0.62
1:B:1323:LEU:HD23	1:B:1323:LEU:C	2.21	0.61
1:B:1028:ARG:HG3	1:B:1037:LEU:CD2	2.29	0.61
1:A:339:GLU:HA	5:A:2652:HOH:O	1.98	0.61
1:A:442:HIS:HE1	3:A:831:AMO:OD2	1.83	0.61
1:B:1436:GLU:HG2	5:B:2664:HOH:O	2.00	0.61
1:B:1421:LEU:HD21	1:B:1471:VAL:HG22	1.81	0.61
1:B:1154:ILE:HD13	1:B:1238:LEU:HD22	1.83	0.61
1:A:323:LEU:HD22	1:A:400:LEU:CD1	2.30	0.61
1:B:1331:ARG:HD2	5:B:2414:HOH:O	2.01	0.61
1:A:298:GLU:HG3	5:A:2074:HOH:O	2.00	0.60
1:B:1313:VAL:HG13	5:B:2443:HOH:O	2.01	0.60
1:A:302:VAL:HG23	1:A:320:VAL:HG23	1.83	0.60
1:A:77:LEU:HD13	1:A:78:ARG:N	2.17	0.60
1:B:1556:ASP:OD1	1:B:1559:THR:HB	2.01	0.60
1:A:368:GLU:HB2	1:A:369:PRO:HD3	1.84	0.60
1:A:392:PRO:CB	1:A:393:ARG:CZ	2.79	0.60
1:A:245:VAL:HG12	1:B:1002:ARG:HH12	1.66	0.60
1:B:1303:GLY:N	1:B:1304:PRO:HD2	2.16	0.60
1:B:1225:GLU:HG2	5:B:2413:HOH:O	2.01	0.60
1:A:79:PRO:CG	1:A:80:GLU:OE1	2.50	0.60
1:B:1299:LEU:HD22	1:B:1400:LEU:HD13	1.84	0.60
1:B:1108:PHE:HD2	1:B:1126:LEU:HD13	1.67	0.60
1:A:325:LEU:HB2	1:A:385:THR:HG22	1.84	0.60
1:B:1048:LEU:HD23	1:B:1092:VAL:HG13	1.84	0.60
1:A:27:ARG:HD3	5:A:2517:HOH:O	2.02	0.60
1:B:1451:GLU:OE2	1:B:1464:ARG:NH2	2.34	0.59
1:A:40:ARG:CB	1:A:45:LEU:HD23	2.32	0.59
1:A:212:LEU:C	5:A:2638:HOH:O	2.38	0.59
1:A:451:GLU:O	1:A:454:PRO:HD2	2.02	0.59
1:B:1329:LEU:HD23	1:B:1411:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LYS:HE2	5:A:2398:HOH:O	2.02	0.59
1:A:453:LEU:HB2	1:A:454:PRO:HD3	1.83	0.58
1:A:287:GLY:HA3	1:A:397:ALA:O	2.03	0.58
1:A:234:ASP:OD2	5:A:2313:HOH:O	2.17	0.58
1:B:1029:ARG:HH11	1:B:1031:LEU:HD11	1.68	0.58
1:A:499:ILE:HD11	1:A:504:GLN:N	2.19	0.58
1:A:406:ARG:HH11	1:A:406:ARG:CG	2.16	0.58
1:B:1455:LEU:H	1:B:1455:LEU:CD1	2.16	0.58
1:A:51:HIS:CE1	1:A:76:ARG:HH12	2.20	0.58
1:B:1419:ARG:NE	5:B:2057:HOH:O	2.36	0.58
1:A:292:ASP:OD1	1:A:294:ARG:HD3	2.04	0.57
1:A:8:GLY:O	1:A:11:ARG:NH2	2.37	0.57
1:B:1129:LYS:HD3	1:B:1130:TYR:CE1	2.39	0.57
1:B:1455:LEU:HD12	1:B:1455:LEU:N	2.19	0.57
1:A:334:VAL:O	1:A:338:GLU:HG3	2.04	0.57
1:B:1483:ARG:HG3	1:B:1522:HIS:CD2	2.40	0.57
1:A:180:ARG:HE	1:B:1187:ARG:NH2	2.03	0.57
1:A:40:ARG:HB3	1:A:45:LEU:CD2	2.35	0.57
1:A:439:THR:HG22	1:A:440:TYR:N	2.18	0.57
1:A:185:PRO:HD2	1:B:1183:LEU:O	2.05	0.57
1:A:320:VAL:HG12	1:A:390:ALA:HB2	1.86	0.56
1:B:1257:LEU:HD13	1:B:1527:TRP:CZ2	2.39	0.56
1:A:154:ILE:HD13	1:A:238:LEU:HD22	1.87	0.56
1:B:1451:GLU:O	1:B:1454:PRO:HD2	2.06	0.56
1:A:27:ARG:HD2	1:A:38:ASP:OD2	2.04	0.56
1:A:325:LEU:HD11	1:A:387:LEU:HD21	1.86	0.56
1:A:55:PRO:HG2	1:A:95:SER:O	2.05	0.56
1:A:220:ARG:HD2	1:A:234:ASP:OD1	2.06	0.56
1:B:1337:LEU:HD22	1:B:1403:VAL:HG13	1.88	0.56
1:B:1253:LEU:C	1:B:1253:LEU:HD13	2.26	0.55
1:B:1189:GLU:CG	1:B:1192:LEU:HD22	2.36	0.55
1:B:1234:ASP:OD1	5:B:2642:HOH:O	2.18	0.55
1:A:452:ASP:HA	1:A:455:LEU:HD13	1.88	0.55
1:A:248:GLU:OE2	1:A:276:ARG:NH2	2.39	0.55
1:A:1:MET:O	1:A:2:ARG:C	2.45	0.55
1:A:443:HIS:HE1	3:A:831:AMO:OD2	1.90	0.55
1:A:309:SER:H	1:A:315:GLN:NE2	2.05	0.55
1:B:1040:ARG:NH2	1:B:1066:GLU:OE2	2.40	0.55
1:A:555:LYS:HG2	1:A:562:PRO:HD2	1.88	0.55
1:A:380:ALA:CB	1:A:386:LEU:HD21	2.37	0.55
1:A:392:PRO:HB3	1:A:393:ARG:CZ	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:HG3	1:A:89:ARG:HH11	1.72	0.54
1:A:276:ARG:HG3	1:A:422:TRP:HB2	1.87	0.54
1:B:1297:LEU:HD13	1:B:1325:LEU:HD23	1.89	0.54
1:A:281:GLU:HA	1:A:284:GLU:HB2	1.90	0.54
1:A:435:GLU:O	1:A:437:ALA:N	2.37	0.54
1:A:76:ARG:NH1	1:A:93:GLU:HG3	2.23	0.54
1:A:80:GLU:N	1:A:80:GLU:OE1	2.41	0.54
1:B:1451:GLU:C	1:B:1453:LEU:H	2.10	0.54
1:B:1458:LYS:HG2	1:B:1459:ASP:N	2.23	0.53
1:A:578:VAL:HG23	5:A:2662:HOH:O	2.07	0.53
1:A:180:ARG:HD2	1:B:1187:ARG:HE	1.73	0.53
1:B:1421:LEU:HD23	1:B:1471:VAL:HG22	1.89	0.53
1:A:393:ARG:NH1	1:A:395:VAL:HG13	2.24	0.53
1:B:1453:LEU:HB2	1:B:1454:PRO:HD3	1.89	0.53
1:A:255:GLU:HB3	1:A:272:LEU:HD22	1.91	0.53
1:A:350:ALA:HB3	1:A:388:PHE:HB2	1.90	0.53
1:A:568:GLU:HG3	5:A:2585:HOH:O	2.08	0.52
1:B:1040:ARG:HB2	1:B:1045:LEU:CD2	2.37	0.52
1:A:138:ARG:O	1:A:142:GLU:HG3	2.09	0.52
1:A:325:LEU:HD12	1:A:385:THR:CG2	2.39	0.52
5:A:2070:HOH:O	1:B:1513:GLU:HG2	2.08	0.52
1:B:1487:PRO:HG3	1:B:1516:GLU:HG2	1.92	0.52
1:A:499:ILE:HD11	1:A:503:GLU:C	2.30	0.52
1:A:505:ARG:HH11	1:A:505:ARG:HG2	1.75	0.52
1:B:1263:ARG:NH1	5:B:2098:HOH:O	2.41	0.52
1:B:1062:ARG:NH2	5:B:2376:HOH:O	2.42	0.52
1:A:455:LEU:HA	1:A:458:LYS:HD3	1.92	0.52
1:A:325:LEU:CD1	1:A:329:LEU:HD11	2.39	0.52
1:B:1211:GLY:C	1:B:1212:LEU:O	2.45	0.52
1:A:322:ALA:HB2	1:A:388:PHE:CD2	2.45	0.52
1:A:578:VAL:HG23	1:A:578:VAL:O	2.09	0.51
1:A:180:ARG:HE	1:B:1187:ARG:HH21	1.57	0.51
1:A:353:ARG:HB2	1:A:360:SER:HB2	1.93	0.51
1:B:1563:SER:HB2	1:B:1564:PRO:HD2	1.92	0.51
1:B:1215:TYR:C	1:B:1215:TYR:CD2	2.84	0.51
1:B:1001:MET:O	1:B:1002:ARG:C	2.48	0.51
1:A:421:LEU:CD2	1:A:471:VAL:HG22	2.40	0.51
1:A:392:PRO:HB3	1:A:393:ARG:NE	2.25	0.51
1:A:121:GLU:HA	5:A:2485:HOH:O	2.11	0.51
1:B:1459:ASP:OD1	1:B:1462:ARG:HD2	2.10	0.50
1:A:308:GLN:HA	1:A:315:GLN:HE22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PHE:HB3	1:A:364:ALA:HB1	1.93	0.50
1:A:299:LEU:HD23	1:A:299:LEU:N	2.25	0.50
1:A:340:VAL:CG1	1:A:403:VAL:HG12	2.41	0.50
1:A:308:GLN:CA	1:A:315:GLN:HE22	2.24	0.50
1:B:1290:LYS:N	1:B:1291:PRO:HD3	2.25	0.50
1:B:1568:GLU:HG3	5:B:2197:HOH:O	2.11	0.50
1:A:451:GLU:N	1:A:451:GLU:OE1	2.44	0.50
1:A:451:GLU:O	1:A:454:PRO:CD	2.59	0.50
1:B:1028:ARG:HG3	1:B:1037:LEU:HD23	1.93	0.50
1:B:1457:GLU:HB2	5:B:2185:HOH:O	2.11	0.50
1:A:288:SER:HA	5:A:2475:HOH:O	2.11	0.50
1:B:1421:LEU:HD21	1:B:1471:VAL:CG2	2.42	0.50
1:A:459:ASP:HB3	1:A:462:ARG:CG	2.31	0.50
1:A:2:ARG:HA	5:A:2116:HOH:O	2.11	0.50
1:B:1302:VAL:HG13	1:B:1306:PHE:HE1	1.77	0.50
1:B:1505:ARG:HG2	1:B:1505:ARG:HH11	1.77	0.49
1:A:400:LEU:HD22	1:A:403:VAL:CG2	2.42	0.49
1:B:1443:HIS:HB2	1:B:1444:PRO:HD2	1.92	0.49
1:A:409:ASP:CG	1:A:415:ARG:HH12	2.14	0.49
1:A:303:GLY:HA2	1:A:320:VAL:CG2	2.32	0.49
1:A:411:LEU:O	1:A:412:GLY:C	2.49	0.49
1:A:394:LYS:HD3	1:A:395:VAL:HG13	1.95	0.49
1:A:49:VAL:HG21	1:A:91:GLU:OE2	2.13	0.49
1:A:429:LEU:HD13	1:A:438:TRP:HB3	1.93	0.49
1:A:578:VAL:CG1	1:B:1576:MET:HB3	2.42	0.49
1:A:505:ARG:HH11	1:A:505:ARG:CG	2.25	0.49
1:A:392:PRO:HB2	1:A:393:ARG:CZ	2.43	0.49
1:A:320:VAL:HG12	1:A:390:ALA:HB1	1.94	0.49
1:A:2:ARG:HH22	1:B:1245:VAL:HG12	1.76	0.49
1:A:421:LEU:HD21	1:A:471:VAL:HG22	1.93	0.49
1:A:237:GLN:HB2	1:A:527:TRP:O	2.13	0.49
1:A:451:GLU:C	1:A:453:LEU:N	2.66	0.49
1:B:1457:GLU:OE2	1:B:1492:ARG:HD3	2.13	0.49
1:B:1076:ARG:HH11	1:B:1076:ARG:HB3	1.78	0.49
1:A:392:PRO:HB2	1:A:395:VAL:CG2	2.41	0.48
1:A:173:LYS:HB2	1:B:1559:THR:HG21	1.91	0.48
1:A:290:LYS:N	1:A:291:PRO:HD3	2.27	0.48
1:B:1428:LEU:HA	1:B:1465:ALA:HB2	1.95	0.48
1:B:1303:GLY:HA2	1:B:1320:VAL:HG23	1.94	0.48
1:A:464:ARG:NH1	5:A:2073:HOH:O	2.46	0.48
1:A:410:LEU:C	1:A:412:GLY:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:CD1	1:A:233:PRO:HD3	2.43	0.48
1:B:1253:LEU:HD13	1:B:1253:LEU:O	2.13	0.48
1:A:317:ALA:HB1	1:A:391:GLY:H	1.79	0.48
1:A:406:ARG:CG	1:A:406:ARG:NH1	2.76	0.48
1:A:89:ARG:HG3	1:A:89:ARG:NH1	2.29	0.48
1:B:1240:LEU:HD22	1:B:1525:ILE:HG22	1.96	0.48
1:A:393:ARG:CD	1:A:393:ARG:N	2.77	0.47
1:A:299:LEU:HD22	1:A:400:LEU:HD12	1.96	0.47
1:A:378:THR:O	1:A:379:GLU:HB2	2.14	0.47
1:A:434:GLU:CD	1:A:434:GLU:H	2.17	0.47
1:A:80:GLU:O	1:A:80:GLU:CG	2.55	0.47
1:A:570:LEU:HD11	1:B:1193:PHE:HZ	1.79	0.47
1:A:353:ARG:HH11	1:A:353:ARG:CG	2.22	0.47
1:B:1133:LEU:O	1:B:1136:ARG:HB2	2.15	0.47
1:B:1029:ARG:NH1	1:B:1031:LEU:HD11	2.29	0.47
1:B:1173:LYS:HA	5:B:2182:HOH:O	2.15	0.47
1:B:1249:ASP:HA	5:B:2467:HOH:O	2.14	0.47
1:A:394:LYS:HE2	1:A:398:THR:CG2	2.30	0.47
1:A:172:THR:OG1	1:A:173:LYS:N	2.43	0.47
1:A:335:ALA:HA	1:A:338:GLU:OE1	2.15	0.47
1:A:180:ARG:CD	1:B:1187:ARG:HE	2.26	0.47
1:A:564:PRO:HD3	1:B:1192:LEU:CD1	2.45	0.47
1:A:359:PHE:CB	1:A:364:ALA:HB1	2.45	0.47
1:A:289:ASP:O	1:A:423:VAL:HG21	2.15	0.47
1:B:1372:GLU:O	1:B:1376:GLN:HB2	2.15	0.47
1:B:1228:ARG:NE	5:B:2474:HOH:O	2.47	0.47
1:A:289:ASP:C	1:A:291:PRO:HD3	2.35	0.47
1:A:393:ARG:HD2	1:A:393:ARG:N	2.29	0.47
1:A:395:VAL:HA	1:A:398:THR:HG23	1.97	0.46
1:A:394:LYS:O	1:A:398:THR:CG2	2.56	0.46
1:B:1531:ARG:NH1	3:B:1831:AMO:H2'2	2.30	0.46
1:A:429:LEU:HD13	1:A:438:TRP:CB	2.46	0.46
1:B:1080:GLU:HA	1:B:1081:PRO:HD2	1.75	0.46
1:A:312:ARG:HA	1:A:315:GLN:HB3	1.97	0.46
1:B:1415:ARG:HG3	5:B:2650:HOH:O	2.15	0.46
1:B:1454:PRO:C	1:B:1456:LEU:H	2.20	0.46
1:B:1108:PHE:CD2	1:B:1126:LEU:HD13	2.50	0.46
1:A:169:PRO:HG3	1:B:1548:PHE:HB2	1.97	0.46
1:A:363:VAL:O	1:A:363:VAL:HG22	2.16	0.46
1:B:1202:LEU:HD21	1:B:1445:PHE:CZ	2.51	0.46
1:A:240:LEU:HD22	1:A:525:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1202:LEU:HB2	5:B:2453:HOH:O	2.16	0.45
1:B:1327:LYS:HD2	1:B:1411:LEU:HD12	1.98	0.45
1:A:201:GLN:OE1	3:A:831:AMO:N	2.49	0.45
1:B:1189:GLU:CD	1:B:1192:LEU:HD22	2.37	0.45
1:B:1076:ARG:NH1	1:B:1076:ARG:HB3	2.31	0.45
1:B:1447:SER:HA	1:B:1448:PRO:HD3	1.84	0.45
1:B:1062:ARG:NH1	5:B:2192:HOH:O	2.46	0.45
1:B:1169:PRO:HG2	1:B:1203:PHE:CZ	2.52	0.45
1:A:303:GLY:N	1:A:304:PRO:CD	2.79	0.45
1:B:1329:LEU:CD2	1:B:1411:LEU:HD21	2.47	0.45
1:A:215:TYR:C	1:A:215:TYR:CD2	2.88	0.45
1:A:428:LEU:HA	1:A:465:ALA:HB2	1.99	0.45
1:B:1392:PRO:HG2	1:B:1395:VAL:CG2	2.47	0.45
1:B:1439:THR:CG2	1:B:1440:TYR:N	2.65	0.45
1:A:1:MET:O	1:A:2:ARG:O	2.34	0.45
1:B:1451:GLU:OE1	1:B:1451:GLU:C	2.55	0.45
1:A:392:PRO:HD2	1:A:395:VAL:CG2	2.40	0.45
1:B:1526:ALA:CB	3:B:1831:AMO:HB2	2.47	0.45
1:A:299:LEU:HD13	1:A:400:LEU:HD12	1.99	0.45
1:A:380:ALA:HB2	1:A:386:LEU:HD21	1.99	0.45
1:B:1500:GLY:O	1:B:1502:GLU:N	2.49	0.45
1:A:325:LEU:CD1	1:A:387:LEU:HD11	2.47	0.45
1:B:1237:GLN:HA	1:B:1527:TRP:O	2.17	0.45
1:B:1029:ARG:NH2	5:B:2146:HOH:O	2.50	0.45
1:A:340:VAL:HG12	1:A:403:VAL:HG12	1.98	0.44
1:B:1351:TRP:HA	1:B:1386:LEU:O	2.18	0.44
1:A:184:VAL:HG22	1:B:1184:VAL:HG22	1.99	0.44
1:A:344:HIS:NE2	1:A:402:ALA:CB	2.80	0.44
1:A:189:GLU:HB3	1:A:192:LEU:HD12	1.99	0.44
1:A:25:VAL:HG21	1:A:63:VAL:HG13	1.99	0.44
1:B:1302:VAL:HG22	1:B:1305:LEU:HD12	1.98	0.44
1:A:213:ASP:HB3	5:B:2657:HOH:O	2.18	0.44
1:A:325:LEU:HD21	1:A:387:LEU:HD22	2.00	0.44
1:B:1528:GLY:HA3	3:B:1831:AMO:H1'	1.99	0.44
1:A:137:ARG:NH2	1:A:139:ARG:NH1	2.59	0.44
1:A:249:ASP:OD1	1:B:1002:ARG:HD3	2.17	0.44
1:B:1368:GLU:HB2	1:B:1369:PRO:HD3	2.00	0.44
1:B:1290:LYS:O	1:B:1290:LYS:HG3	2.18	0.44
1:A:429:LEU:CD2	1:A:497:LEU:HD11	2.47	0.44
1:B:1172:THR:OG1	1:B:1173:LYS:N	2.49	0.44
1:B:1082:ASN:ND2	1:B:1084:ARG:HH21	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LYS:HZ2	1:A:395:VAL:HG12	1.82	0.43
1:A:452:ASP:OD1	1:A:464:ARG:HG2	2.18	0.43
1:A:427:PRO:HG2	1:A:441:MET:HE2	2.01	0.43
1:B:1302:VAL:HG13	1:B:1306:PHE:CE1	2.52	0.43
1:A:447:SER:HA	1:A:448:PRO:HD3	1.89	0.43
1:A:393:ARG:H	1:A:393:ARG:HD2	1.79	0.43
1:A:297:LEU:O	1:A:323:LEU:HD12	2.18	0.43
1:A:531:ARG:NH1	3:A:831:AMO:H2'2	2.34	0.43
1:A:427:PRO:CG	1:A:441:MET:HE2	2.48	0.43
1:B:1413:LEU:HA	1:B:1413:LEU:HD23	1.90	0.43
1:A:175:THR:HG22	5:A:2247:HOH:O	2.18	0.43
1:A:564:PRO:HD3	1:B:1192:LEU:HD12	2.01	0.43
1:A:570:LEU:HD11	1:B:1193:PHE:CZ	2.53	0.43
1:B:1187:ARG:HG3	1:B:1187:ARG:HH11	1.82	0.43
1:A:107:PRO:HG3	1:A:130:TYR:CD1	2.54	0.43
1:B:1039:LEU:HG	1:B:1048:LEU:HD11	2.01	0.43
1:A:220:ARG:NH2	1:B:1167:GLU:HB3	2.34	0.43
1:A:351:TRP:HA	1:A:386:LEU:O	2.18	0.43
1:B:1187:ARG:HB3	1:B:1573:LEU:HD23	2.00	0.43
1:A:578:VAL:CG2	5:A:2662:HOH:O	2.65	0.43
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.84	0.43
1:A:157:PHE:CD2	1:A:257:LEU:HD13	2.54	0.43
1:B:1010:LEU:HD23	1:B:1046:VAL:HG11	2.01	0.42
1:B:1227:LEU:CD1	1:B:1233:PRO:HD3	2.49	0.42
1:A:213:ASP:HA	5:A:2087:HOH:O	2.18	0.42
1:A:320:VAL:HG23	1:A:320:VAL:O	2.20	0.42
1:A:325:LEU:HD11	1:A:387:LEU:CD2	2.48	0.42
1:A:570:LEU:HD22	1:A:575:LEU:CB	2.43	0.42
1:B:1129:LYS:HE2	5:B:2344:HOH:O	2.19	0.42
1:B:1449:HIS:CG	1:B:1450:PRO:HD2	2.54	0.42
1:B:1238:LEU:HD21	1:B:1257:LEU:HD11	2.01	0.42
1:A:112:ALA:HB3	1:A:119:GLU:HG2	2.02	0.42
1:B:1042:ARG:CD	1:B:1043:GLU:OE1	2.60	0.42
1:A:27:ARG:HG2	1:A:28:ARG:N	2.35	0.42
1:B:1405:LEU:HD23	1:B:1405:LEU:HA	1.81	0.42
1:A:294:ARG:HD2	1:A:473:ASN:CG	2.40	0.42
1:A:454:PRO:HB2	1:A:455:LEU:HD12	2.00	0.42
1:B:1216:PHE:HA	1:B:1239:ASP:O	2.20	0.42
1:B:1034:LEU:HA	1:B:1034:LEU:HD12	1.90	0.42
1:A:158:LEU:HB3	1:A:163:PHE:HB2	2.02	0.42
1:A:295:PHE:CZ	1:A:408:ALA:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1349:LEU:HD12	1:B:1388:PHE:O	2.20	0.42
1:B:1175:THR:HG22	5:B:2345:HOH:O	2.19	0.42
1:A:505:ARG:NH1	1:A:505:ARG:CG	2.83	0.42
1:B:1427:PRO:HD2	1:B:1441:MET:CE	2.50	0.42
1:A:434:GLU:OE2	1:A:434:GLU:N	2.52	0.42
1:B:1327:LYS:HB2	1:B:1411:LEU:HD11	2.01	0.42
1:A:578:VAL:CG2	1:A:578:VAL:O	2.68	0.42
1:A:443:HIS:CE1	3:A:831:AMO:OD2	2.72	0.42
1:A:416:GLU:HG3	1:A:417:GLY:N	2.34	0.42
1:B:1312:ARG:O	1:B:1316:GLU:HG2	2.19	0.41
1:A:363:VAL:HG22	1:A:366:PHE:HB2	2.02	0.41
1:A:494:PHE:O	1:A:499:ILE:CG2	2.66	0.41
1:A:137:ARG:HH12	1:A:139:ARG:HH11	1.67	0.41
1:B:1214:ARG:HA	1:B:1241:GLU:O	2.20	0.41
1:A:133:LEU:O	1:A:136:ARG:HB2	2.20	0.41
1:B:1451:GLU:C	1:B:1453:LEU:N	2.73	0.41
1:A:345:LYS:HD2	1:A:394:LYS:NZ	2.36	0.41
1:B:1028:ARG:HG3	1:B:1037:LEU:HD21	2.02	0.41
1:A:39:LEU:HG	1:A:48:LEU:HD11	2.01	0.41
1:A:170:PHE:O	1:A:197:PRO:HD3	2.21	0.41
1:A:227:LEU:HD13	1:A:233:PRO:HD3	2.01	0.41
1:B:1486:ASP:OD2	1:B:1486:ASP:C	2.57	0.41
1:A:343:ARG:HD3	5:A:2292:HOH:O	2.20	0.41
1:A:456:LEU:HD11	1:A:496:LEU:HD22	2.02	0.41
1:A:212:LEU:CA	5:A:2638:HOH:O	2.68	0.41
1:B:1440:TYR:CD1	1:B:1444:PRO:HD3	2.56	0.41
1:A:333:GLU:OE2	1:A:410:LEU:HB3	2.20	0.41
1:B:1185:PRO:HB2	1:B:1573:LEU:HD22	2.03	0.41
1:B:1034:LEU:HD11	1:B:1051:HIS:ND1	2.36	0.41
1:A:186:TYR:CG	1:B:1562:PRO:HG3	2.56	0.41
1:A:450:PRO:HG2	1:A:451:GLU:OE1	2.20	0.41
1:A:331:ARG:CZ	1:A:351:TRP:HZ2	2.33	0.41
1:B:1400:LEU:HD23	1:B:1400:LEU:HA	1.92	0.41
1:A:562:PRO:HG3	1:B:1186:TYR:CG	2.56	0.41
1:A:306:PHE:CE2	1:A:314:PHE:HD2	2.39	0.41
1:B:1414:LYS:CD	1:B:1414:LYS:H	2.33	0.41
1:B:1277:LEU:O	1:B:1423:VAL:HA	2.21	0.41
1:A:494:PHE:CZ	1:A:508:PHE:CD2	3.08	0.41
1:B:1323:LEU:CD2	1:B:1323:LEU:C	2.89	0.41
1:B:1455:LEU:HB3	1:B:1459:ASP:HB3	2.02	0.41
1:B:1148:HIS:C	1:B:1148:HIS:CD2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLU:HG3	5:A:2292:HOH:O	2.21	0.40
1:A:25:VAL:HG21	1:A:63:VAL:CG1	2.51	0.40
1:A:214:ARG:CD	5:B:2657:HOH:O	2.69	0.40
1:A:349:LEU:HD23	1:A:350:ALA:H	1.86	0.40
1:B:1004:THR:C	1:B:1005:HIS:ND1	2.75	0.40
1:B:1472:LEU:O	1:B:1473:ASN:C	2.59	0.40
1:B:1048:LEU:CD2	1:B:1092:VAL:HG13	2.50	0.40
1:B:1212:LEU:HD23	1:B:1212:LEU:HA	1.87	0.40
1:B:1263:ARG:HD3	1:B:1269:GLU:OE1	2.22	0.40
1:A:228:ARG:HG2	1:A:228:ARG:NH1	2.35	0.40
1:A:579:ARG:HG2	1:A:579:ARG:NH1	2.35	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	578/580 (100%)	536 (93%)	33 (6%)	9 (2%)	12	16
1	B	578/580 (100%)	543 (94%)	30 (5%)	5 (1%)	21	30
All	All	1156/1160 (100%)	1079 (93%)	63 (5%)	14 (1%)	16	23

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	392	PRO
1	A	436	GLU
1	A	452	ASP
1	B	1414	LYS
1	A	296	GLY
1	B	1501	GLU

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Mol	Chain	Res	Type
1	A	357	GLY
1	B	1456	LEU
1	B	1002	ARG
1	A	201	GLN
1	B	1229	ALA
1	A	370	VAL
1	A	412	GLY

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	483/483 (100%)	448 (93%)	35 (7%)	18	28
1	B	483/483 (100%)	443 (92%)	40 (8%)	14	21
All	All	966/966 (100%)	891 (92%)	75 (8%)	16	24

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	34	LEU
1	A	39	LEU
1	A	63	VAL
1	A	77	LEU
1	A	123	SER
1	A	124	GLU
1	A	126	LEU
1	A	128	LEU
1	A	139	ARG
1	A	207	LEU
1	A	215	TYR
1	A	228	ARG
1	A	234	ASP
1	A	240	LEU
1	A	276	ARG

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Mol	Chain	Res	Type
1	A	349	LEU
1	A	356	GLU
1	A	393	ARG
1	A	398	THR
1	A	405	LEU
1	A	406	ARG
1	A	421	LEU
1	A	455	LEU
1	A	457	GLU
1	A	462	ARG
1	A	471	VAL
1	A	489	LEU
1	A	494	PHE
1	A	497	LEU
1	A	513	GLU
1	A	520	PRO
1	A	552	LYS
1	A	570	LEU
1	A	579	ARG
1	B	1010	LEU
1	B	1013	THR
1	B	1039	LEU
1	B	1042	ARG
1	B	1046	VAL
1	B	1076	ARG
1	B	1092	VAL
1	B	1104	LYS
1	B	1126	LEU
1	B	1128	LEU
1	B	1165	GLN
1	B	1190	PRO
1	B	1192	LEU
1	B	1196	LEU
1	B	1207	LEU
1	B	1215	TYR
1	B	1228	ARG
1	B	1234	ASP
1	B	1240	LEU
1	B	1257	LEU
1	B	1302	VAL
1	B	1323	LEU
1	B	1339	GLU

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Mol	Chain	Res	Type
1	B	1347	GLN
1	B	1374	LEU
1	B	1387	LEU
1	B	1400	LEU
1	B	1410	LEU
1	B	1414	LYS
1	B	1431	TRP
1	B	1435	GLU
1	B	1451	GLU
1	B	1483	ARG
1	B	1494	PHE
1	B	1497	LEU
1	B	1513	GLU
1	B	1532	LEU
1	B	1533	LEU
1	B	1559	THR
1	B	1575	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	315	GLN
1	A	442	HIS
1	A	443	HIS
1	B	1014	HIS
1	B	1047	GLN
1	B	1260	HIS
1	B	1344	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

5 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$
2	SO4	A	1901	-	4,4,4	0.39	0	6,6,6	0.18	0
3	AMO	A	831	-	23,33,33	0.91	1 (4%)	24,49,49	0.73	1 (4%)
3	AMO	B	1831	-	23,33,33	0.87	1 (4%)	24,49,49	0.96	2 (8%)
4	AMP	B	800	-	20,25,25	0.74	0	22,38,38	1.07	2 (9%)
2	SO4	B	901	-	4,4,4	0.35	0	6,6,6	0.15	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	SO4	A	1901	-	-	0/0/0/0	0/0/0/0
3	AMO	A	831	-	-	0/15/39/39	0/3/3/3
3	AMO	B	1831	-	-	0/15/39/39	0/3/3/3
4	AMP	B	800	-	-	0/6/26/26	0/3/3/3
2	SO4	B	901	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1831	AMO	P-O3P	2.60	1.66	1.60
3	A	831	AMO	P-O3P	3.20	1.67	1.60

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	800	AMP	O3'-C3'-C2'	-2.58	103.45	111.83
3	B	1831	AMO	O3P-P-O1P	-2.19	101.15	108.38
3	A	831	AMO	O2P-P-O3P	2.11	110.69	104.16
4	B	800	AMP	O3P-P-O1P	2.75	119.43	110.58
3	B	1831	AMO	O3P-P-O5'	2.88	110.36	102.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	831	AMO	5	0
3	B	1831	AMO	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	580/580 (100%)	0.13	64 (11%) 7 7	14, 39, 86, 102	0
1	B	580/580 (100%)	-0.37	20 (3%) 49 49	13, 31, 64, 93	0
All	All	1160/1160 (100%)	-0.12	84 (7%) 18 18	13, 34, 81, 102	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	PRO	6.2
1	B	1434	GLU	5.5
1	A	434	GLU	5.2
1	A	307	ARG	5.2
1	A	365	LYS	5.1
1	A	311	PHE	5.1
1	A	313	VAL	4.7
1	B	1433	GLU	4.7
1	A	369	PRO	4.6
1	A	305	LEU	4.6
1	A	317	ALA	4.5
1	A	580	PRO	4.3
1	B	1502	GLU	4.2
1	A	374	LEU	4.2
1	A	393	ARG	4.0
1	A	309	SER	4.0
1	A	316	GLU	3.9
1	A	338	GLU	3.9
1	A	376	GLN	3.9
1	A	579	ARG	3.7
1	A	437	ALA	3.6
1	A	345	LYS	3.6
1	A	436	GLU	3.6
1	A	343	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	414	LYS	3.5
1	A	337	LEU	3.5
1	A	381	ARG	3.4
1	A	435	GLU	3.3
1	B	1001	MET	3.3
1	A	502	GLU	3.2
1	B	1307	ARG	3.2
1	A	347	GLN	3.1
1	A	319	SER	3.1
1	A	364	ALA	3.1
1	A	506	GLU	3.1
1	A	462	ARG	3.0
1	A	433	GLU	3.0
1	B	1393	ARG	3.0
1	A	346	ALA	3.0
1	A	371	ARG	2.9
1	B	1505	ARG	2.9
1	A	318	GLU	2.9
1	A	366	PHE	2.8
1	A	312	ARG	2.8
1	B	1462	ARG	2.8
1	A	314	PHE	2.8
1	A	372	GLU	2.8
1	A	178	GLY	2.8
1	A	357	GLY	2.7
1	A	363	VAL	2.7
1	A	80	GLU	2.7
1	B	1435	GLU	2.6
1	A	53	ALA	2.6
1	A	464	ARG	2.6
1	A	382	PRO	2.6
1	A	121	GLU	2.5
1	B	1458	LYS	2.5
1	A	390	ALA	2.5
1	A	463	VAL	2.5
1	A	310	GLY	2.5
1	A	341	ALA	2.5
1	B	1416	GLU	2.4
1	A	306	PHE	2.4
1	B	1343	ARG	2.4
1	A	1	MET	2.4
1	A	505	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	356	GLU	2.3
1	B	1308	GLN	2.3
1	B	1356	GLU	2.3
1	A	329	LEU	2.3
1	B	1414	LYS	2.3
1	A	303	GLY	2.2
1	A	342	LYS	2.2
1	B	1437	ALA	2.2
1	A	299	LEU	2.2
1	A	488	ARG	2.2
1	B	1178	GLY	2.1
1	B	1347	GLN	2.1
1	A	432	ASP	2.1
1	A	83	PRO	2.1
1	B	1345	LYS	2.0
1	A	360	SER	2.0
1	B	1316	GLU	2.0
1	A	344	HIS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	AMP	B	800	23/23	0.77	0.25	1.65	73,82,96,98	0
2	SO4	B	901	5/5	0.98	0.15	0.32	68,69,70,70	0
3	AMO	B	1831	31/31	0.98	0.10	-0.19	17,26,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	AMO	A	831	31/31	0.97	0.09	-0.68	25,28,30,32	0
2	SO4	A	1901	5/5	0.96	0.10	-	69,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.