



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:06 PM UTC

PDB ID : 3UGJ / pdb_00003ugj
Title : Formyl Glycinamide ribonucleotide amidotransferase from *Salmonella Typhimurum*: Role of the ATP complexation and glutaminase domain in catalytic coupling
Authors : Morar, M.; Tanwar, A.S.; Panjikar, S.; Anand, R.
Deposited on : 2011-11-02
Resolution : 1.78 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

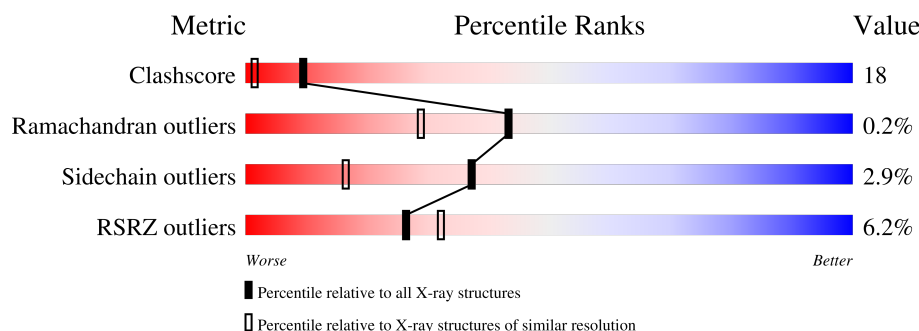
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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))
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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 $\leq 5\%$. 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	1303	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10759 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 Phosphoribosylformylglycinamide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1284	9884	6203	1766	1867	48	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

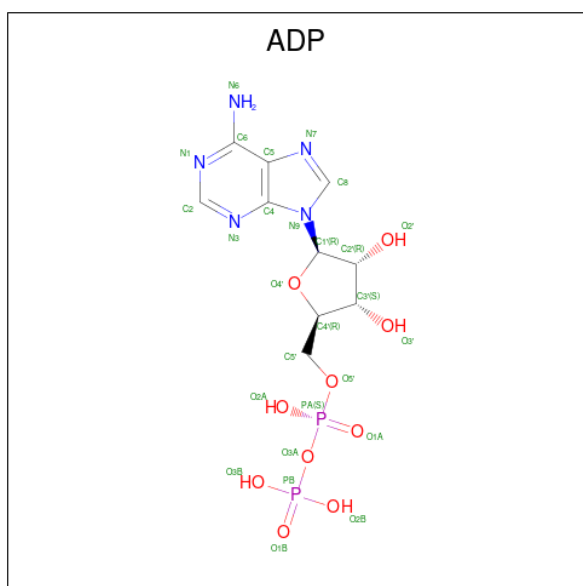
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P74881
A	-6	LEU	-	expression tag	UNP P74881
A	-5	VAL	-	expression tag	UNP P74881
A	-4	PRO	-	expression tag	UNP P74881
A	-3	ARG	-	expression tag	UNP P74881
A	-2	GLY	-	expression tag	UNP P74881
A	-1	SER	-	expression tag	UNP P74881
A	0	HIS	-	expression tag	UNP P74881

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0

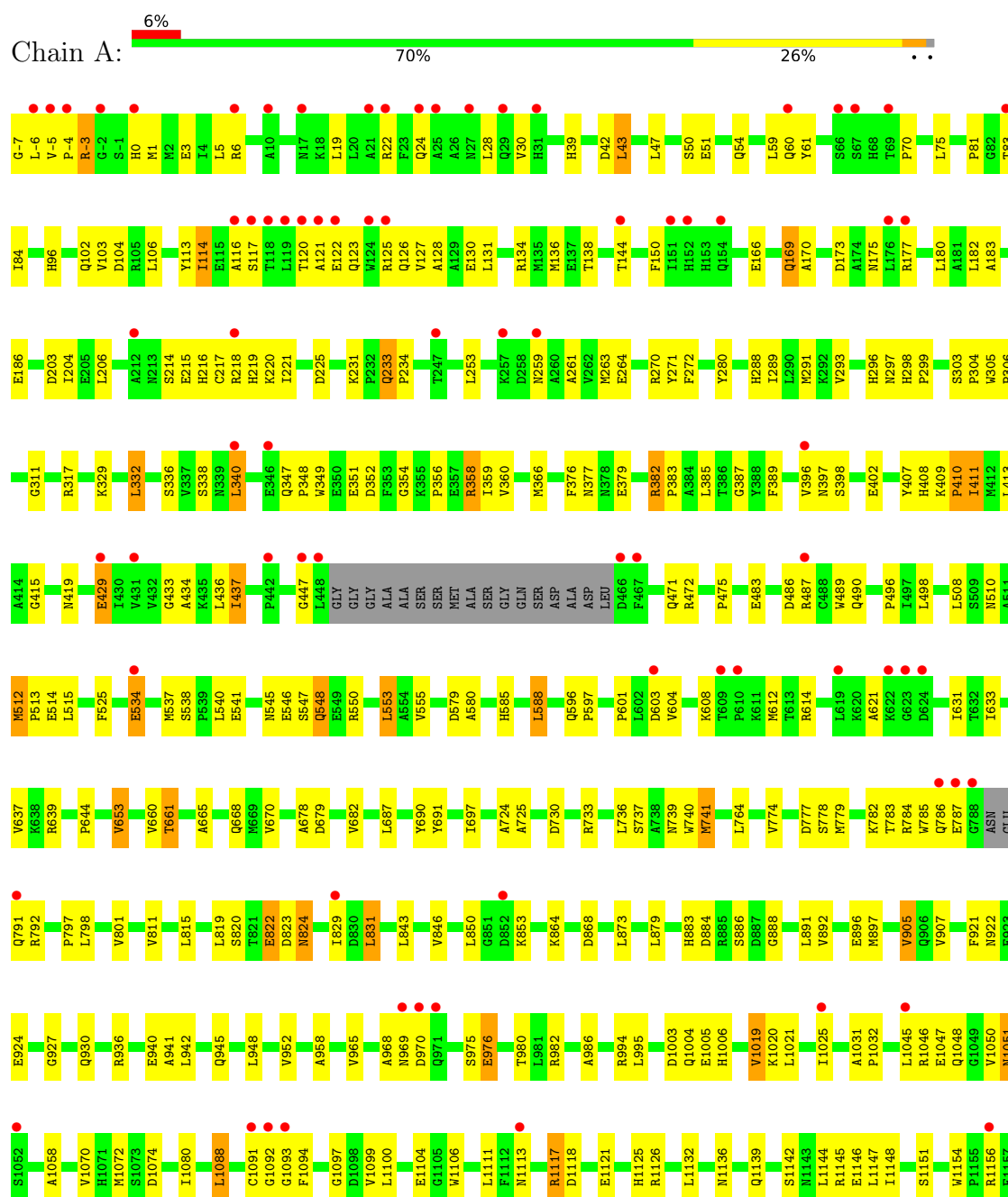
- Molecule 5 is water.

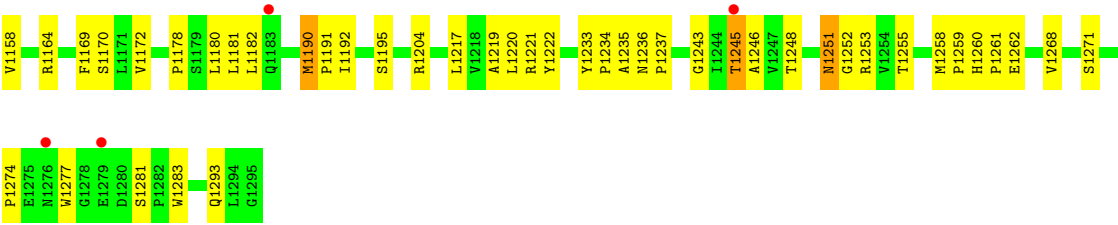
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	820	Total 820	O 820	0	0

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: Phosphoribosylformylglycinamide synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	145.98Å 145.98Å 141.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.78 30.00 – 1.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.78) 96.5 (30.00-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 1.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.240 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10759	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: SO4, ADP, MG

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	0.39	0/10096	0.93	43/13702 (0.3%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	GLU	CA-C-N	11.05	132.29	119.47
1	A	534	GLU	C-N-CA	11.05	132.29	119.47
1	A	779	MET	N-CA-C	9.19	123.20	112.72
1	A	303	SER	CA-C-N	7.66	127.20	119.24
1	A	303	SER	C-N-CA	7.66	127.20	119.24
1	A	409	LYS	N-CA-C	-7.55	94.96	108.47
1	A	1091	CYS	N-CA-C	7.46	120.15	110.53
1	A	311	GLY	N-CA-C	-6.90	104.14	112.49
1	A	724	ALA	N-CA-C	6.59	120.19	111.75
1	A	797	PRO	N-CA-C	-6.55	101.61	111.57
1	A	1019	VAL	N-CA-C	6.23	118.36	108.89
1	A	1051	ASN	N-CA-C	6.21	121.69	112.94
1	A	764	LEU	N-CA-C	6.11	117.63	110.97
1	A	347	GLN	CA-C-N	6.00	126.42	119.47
1	A	347	GLN	C-N-CA	6.00	126.42	119.47
1	A	385	LEU	N-CA-C	5.94	121.44	113.72
1	A	1236	ASN	N-CA-C	-5.93	96.72	109.01
1	A	653	VAL	N-CA-C	5.88	117.25	111.67
1	A	437	ILE	N-CA-C	5.85	117.86	108.85
1	A	691	TYR	N-CA-C	-5.82	102.84	110.53
1	A	407	TYR	N-CA-C	5.79	117.39	110.44
1	A	1148	ILE	N-CA-C	5.78	114.32	107.73
1	A	737	SER	N-CA-C	-5.77	99.78	109.07
1	A	548	GLN	N-CA-C	5.68	119.17	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1158	VAL	N-CA-C	5.59	115.64	108.82
1	A	289	ILE	N-CA-C	5.56	115.95	108.17
1	A	601	PRO	N-CA-C	-5.48	101.94	111.32
1	A	670	VAL	N-CA-C	5.38	116.22	108.48
1	A	798	LEU	N-CA-C	-5.30	102.21	110.10
1	A	824	ASN	N-CA-C	5.29	116.84	108.96
1	A	225	ASP	N-CA-C	-5.25	102.75	110.52
1	A	631	ILE	N-CA-C	5.23	116.82	108.87
1	A	965	VAL	N-CA-C	5.22	115.42	108.11
1	A	822	GLU	N-CA-C	-5.22	103.64	110.53
1	A	1126	ARG	CA-C-N	5.22	125.02	119.28
1	A	1126	ARG	C-N-CA	5.22	125.02	119.28
1	A	411	ILE	N-CA-C	-5.19	100.27	107.80
1	A	1237	PRO	N-CA-C	5.19	120.35	113.86
1	A	114	ILE	N-CA-C	5.17	115.30	107.80
1	A	233	GLN	CA-C-N	5.12	124.43	118.85
1	A	233	GLN	C-N-CA	5.12	124.43	118.85
1	A	270	ARG	N-CA-C	-5.10	102.31	109.96
1	A	736	LEU	N-CA-C	5.09	118.04	109.95

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	9884	0	9675	351	0
2	A	25	0	0	0	0
3	A	27	0	12	1	0
4	A	3	0	0	0	0
5	A	820	0	0	87	0
All	All	10759	0	9687	352	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 18.

All (352) 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:358:ARG:H	1:A:358:ARG:HD3	1.06	1.12
1:A:340:LEU:HD11	1:A:644:PRO:HG2	1.38	1.05
1:A:261:ALA:HB2	1:A:774:VAL:HG13	1.39	1.02
1:A:639:ARG:HB3	1:A:846:VAL:HG21	1.38	1.00
1:A:1190:MET:HE2	1:A:1190:MET:H	1.26	0.98
1:A:1145:ARG:HD3	1:A:1154:TRP:HB2	1.48	0.94
1:A:358:ARG:H	1:A:358:ARG:CD	1.82	0.93
1:A:824:ASN:HD21	1:A:958:ALA:H	1.15	0.93
1:A:175:ASN:HD21	1:A:182:LEU:H	1.12	0.92
1:A:120:THR:HG23	1:A:123:GLN:HE21	1.35	0.91
1:A:653:VAL:HG22	5:A:2093:HOH:O	1.71	0.89
1:A:639:ARG:HB3	1:A:846:VAL:CG2	2.02	0.89
1:A:1178:PRO:HD2	5:A:2091:HOH:O	1.72	0.88
1:A:1190:MET:HE2	1:A:1190:MET:N	1.88	0.88
1:A:637:VAL:HG22	1:A:891:LEU:HD21	1.54	0.87
1:A:741:MET:HE2	1:A:778:SER:CB	2.04	0.87
1:A:741:MET:HE2	1:A:778:SER:HB3	1.56	0.86
1:A:253:LEU:HD21	1:A:264:GLU:HG3	1.55	0.86
1:A:633:ILE:HG22	5:A:2064:HOH:O	1.75	0.85
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.41	0.85
1:A:358:ARG:HD3	1:A:358:ARG:N	1.90	0.84
1:A:-3:ARG:HD2	1:A:150:PHE:HB2	1.58	0.84
1:A:340:LEU:H	1:A:340:LEU:HD12	1.42	0.82
1:A:429:GLU:CD	1:A:429:GLU:H	1.85	0.82
1:A:1111:LEU:HA	1:A:1117:ARG:HG3	1.62	0.81
1:A:534:GLU:HG3	1:A:537:MET:HG3	1.63	0.81
1:A:733:ARG:HG2	5:A:2103:HOH:O	1.80	0.80
1:A:1217:LEU:HA	5:A:2091:HOH:O	1.81	0.80
1:A:1178:PRO:HB2	5:A:2118:HOH:O	1.81	0.79
1:A:305:TRP:HB3	1:A:306:PRO:HD3	1.64	0.79
1:A:377:ASN:OD1	1:A:382:ARG:HD2	1.80	0.79
1:A:922:ASN:HD22	1:A:924:GLU:H	1.32	0.77
1:A:169:GLN:HE22	1:A:173:ASP:CG	1.93	0.77
1:A:396:VAL:HG11	1:A:850:LEU:HD22	1.66	0.77
1:A:820:SER:H	1:A:930:GLN:HE22	1.29	0.77
1:A:217:CYS:HB2	5:A:1970:HOH:O	1.87	0.75
1:A:498:LEU:HD13	1:A:555:VAL:HA	1.67	0.75
1:A:1219:ALA:C	1:A:1220:LEU:HD22	2.12	0.75
1:A:1245:THR:HG23	5:A:1299:HOH:O	1.87	0.75
1:A:336:SER:HB2	1:A:411:ILE:HB	1.69	0.74
1:A:740:TRP:O	1:A:741:MET:HE3	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1070:VAL:HG22	1:A:1080:ILE:HD13	1.70	0.74
1:A:351:GLU:HG2	5:A:2071:HOH:O	1.89	0.72
1:A:905:VAL:HG13	1:A:907:VAL:HG13	1.70	0.72
1:A:665:ALA:CB	1:A:811:VAL:HG11	2.20	0.72
1:A:1222:TYR:OH	1:A:1245:THR:HG21	1.89	0.72
1:A:545:ASN:HD22	1:A:547:SER:H	1.37	0.72
1:A:231:LYS:HG3	5:A:2072:HOH:O	1.88	0.71
1:A:941:ALA:O	1:A:945:GLN:HG3	1.91	0.71
1:A:1045:LEU:HG	1:A:1106:TRP:HZ2	1.56	0.71
1:A:1145:ARG:CD	1:A:1154:TRP:HB2	2.20	0.71
1:A:253:LEU:HD21	1:A:264:GLU:CG	2.21	0.71
1:A:261:ALA:HB2	1:A:774:VAL:CG1	2.18	0.70
1:A:843:LEU:O	1:A:846:VAL:HG12	1.91	0.70
1:A:1117:ARG:HD3	1:A:1147:LEU:HD11	1.72	0.70
1:A:348:PRO:HB2	5:A:1913:HOH:O	1.91	0.69
1:A:637:VAL:HG22	1:A:891:LEU:CD2	2.22	0.68
1:A:1252:GLY:HA2	5:A:2118:HOH:O	1.92	0.68
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.00	0.68
1:A:218:ARG:HD2	1:A:220:LYS:HG2	1.76	0.68
1:A:356:PRO:HG3	1:A:785:TRP:HB3	1.76	0.67
1:A:1004:GLN:NE2	1:A:1233:TYR:H	1.92	0.67
1:A:512:MET:HG3	1:A:525:PHE:CZ	2.30	0.67
1:A:639:ARG:HD3	5:A:1913:HOH:O	1.94	0.67
1:A:1251:ASN:ND2	1:A:1253:ARG:H	1.92	0.67
1:A:447:GLY:HA3	1:A:546:GLU:H	1.59	0.67
1:A:1156:ARG:HH21	1:A:1204:ARG:CZ	2.07	0.67
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.43	0.67
1:A:413:LEU:HD11	5:A:1941:HOH:O	1.95	0.66
1:A:740:TRP:C	1:A:741:MET:HE3	2.20	0.66
1:A:175:ASN:ND2	1:A:182:LEU:H	1.92	0.66
1:A:19:LEU:HA	5:A:1972:HOH:O	1.96	0.66
1:A:5:LEU:HD22	1:A:59:LEU:HD12	1.76	0.65
1:A:332:LEU:HD13	1:A:415:GLY:C	2.21	0.65
1:A:447:GLY:CA	1:A:546:GLU:H	2.10	0.65
1:A:317:ARG:HH22	1:A:548:GLN:NE2	1.95	0.65
1:A:221:ILE:HD13	1:A:612:MET:SD	2.37	0.64
1:A:1220:LEU:HD23	1:A:1246:ALA:CB	2.27	0.64
1:A:739:ASN:HB2	5:A:1941:HOH:O	1.95	0.64
1:A:96:HIS:HE1	1:A:103:VAL:O	1.80	0.64
1:A:261:ALA:CB	1:A:774:VAL:HG13	2.23	0.64
1:A:120:THR:HG23	1:A:123:GLN:NE2	2.09	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:PRO:HD3	1:A:660:VAL:HG13	1.79	0.63
1:A:183:ALA:HB3	1:A:186:GLU:HG3	1.80	0.63
1:A:483:GLU:OE1	1:A:487:ARG:NH2	2.31	0.63
1:A:349:TRP:HE3	5:A:1913:HOH:O	1.80	0.63
1:A:1:MET:HE3	5:A:2029:HOH:O	1.99	0.62
1:A:471:GLN:HE21	1:A:472:ARG:H	1.46	0.62
1:A:121:ALA:O	1:A:125:ARG:HD3	1.99	0.62
1:A:969:ASN:OD1	1:A:970:ASP:N	2.32	0.62
1:A:356:PRO:HG2	1:A:783:THR:CG2	2.30	0.62
1:A:976:GLU:HB3	5:A:1847:HOH:O	2.00	0.61
1:A:1245:THR:HG22	1:A:1259:PRO:HD3	1.82	0.61
1:A:127:VAL:HG12	5:A:2122:HOH:O	2.01	0.61
1:A:579:ASP:HB3	5:A:2104:HOH:O	2.00	0.61
1:A:733:ARG:N	5:A:2103:HOH:O	2.34	0.61
1:A:1088:LEU:HD23	1:A:1088:LEU:C	2.25	0.61
1:A:434:ALA:HB3	5:A:2120:HOH:O	2.00	0.60
1:A:682:VAL:HG11	1:A:811:VAL:HG13	1.83	0.60
1:A:1220:LEU:HB2	1:A:1246:ALA:HB3	1.83	0.60
1:A:791:GLN:HB3	5:A:2081:HOH:O	1.99	0.60
1:A:801:VAL:HB	5:A:1941:HOH:O	2.00	0.60
1:A:1190:MET:HE3	1:A:1283:TRP:CZ2	2.37	0.60
1:A:1156:ARG:HH21	1:A:1204:ARG:NH1	1.99	0.60
1:A:120:THR:OG1	1:A:123:GLN:HG3	2.01	0.60
1:A:1074:ASP:CB	1:A:1080:ILE:HD12	2.32	0.60
1:A:1:MET:HB3	5:A:2029:HOH:O	2.01	0.59
1:A:1219:ALA:O	1:A:1220:LEU:HD22	2.03	0.59
1:A:-3:ARG:HD3	1:A:42:ASP:OD1	2.03	0.59
1:A:218:ARG:HD2	1:A:220:LYS:CG	2.33	0.59
1:A:429:GLU:CD	1:A:429:GLU:N	2.60	0.59
1:A:215:GLU:HA	5:A:1865:HOH:O	2.02	0.58
1:A:1051:ASN:H	1:A:1093:GLY:HA3	1.67	0.58
1:A:396:VAL:HG12	1:A:397:ASN:N	2.18	0.58
1:A:379:GLU:HB3	1:A:475:PRO:HB2	1.86	0.58
1:A:1220:LEU:HD23	1:A:1246:ALA:HB3	1.86	0.58
1:A:51:GLU:CD	1:A:102:GLN:HE22	2.12	0.58
1:A:487:ARG:HH21	1:A:1046:ARG:NH2	2.02	0.57
1:A:1117:ARG:NH1	1:A:1117:ARG:HB3	2.19	0.57
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.86	0.57
1:A:1248:THR:HG23	5:A:2091:HOH:O	2.04	0.57
1:A:741:MET:HE2	1:A:778:SER:HB2	1.85	0.57
1:A:1113:ASN:HB3	5:A:1985:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLY:HA3	1:A:546:GLU:N	2.19	0.57
1:A:298:HIS:HB3	1:A:299:PRO:HD3	1.85	0.57
1:A:396:VAL:HB	5:A:2050:HOH:O	2.05	0.57
1:A:1146:GLU:HG3	1:A:1147:LEU:HD13	1.87	0.57
1:A:220:LYS:HE2	1:A:612:MET:HE3	1.86	0.56
1:A:792:ARG:HG3	5:A:2112:HOH:O	2.04	0.56
1:A:253:LEU:N	1:A:253:LEU:HD22	2.20	0.56
1:A:782:LYS:NZ	1:A:784:ARG:NH2	2.53	0.56
1:A:75:LEU:HD12	1:A:114:ILE:HD12	1.88	0.56
1:A:540:LEU:HD23	1:A:540:LEU:C	2.31	0.55
1:A:888:GLY:HA3	1:A:892:VAL:HG21	1.89	0.55
1:A:219:HIS:HD2	1:A:777:ASP:OD1	1.89	0.55
1:A:329:LYS:O	1:A:383:PRO:HD2	2.06	0.55
1:A:396:VAL:HG11	1:A:850:LEU:HB2	1.88	0.55
1:A:1169:PHE:CZ	1:A:1191:PRO:HB2	2.42	0.55
1:A:580:ALA:HB2	5:A:2120:HOH:O	2.06	0.55
1:A:515:LEU:HA	5:A:1989:HOH:O	2.05	0.54
1:A:968:ALA:O	1:A:969:ASN:CG	2.50	0.54
1:A:1145:ARG:HD3	1:A:1154:TRP:CB	2.31	0.54
1:A:1255:THR:HB	5:A:2018:HOH:O	2.07	0.54
1:A:131:LEU:HD12	5:A:2122:HOH:O	2.07	0.54
1:A:668:GLN:HG2	5:A:2093:HOH:O	2.07	0.54
1:A:1117:ARG:HB3	1:A:1117:ARG:HH11	1.73	0.54
1:A:354:GLY:O	1:A:408:HIS:HE1	1.90	0.54
1:A:433:GLY:HA2	5:A:2104:HOH:O	2.07	0.54
1:A:114:ILE:HD11	1:A:131:LEU:HD11	1.90	0.54
1:A:782:LYS:NZ	5:A:1428:HOH:O	2.40	0.54
1:A:1099:VAL:HG12	1:A:1100:LEU:HG	1.89	0.54
1:A:-5:VAL:CG1	1:A:-4:PRO:HD2	2.37	0.53
1:A:1144:LEU:HD22	1:A:1147:LEU:HD22	1.91	0.53
1:A:510:ASN:O	1:A:514:GLU:HG3	2.09	0.53
1:A:6:ARG:HG2	5:A:1580:HOH:O	2.07	0.53
1:A:1180:LEU:HD13	1:A:1252:GLY:C	2.33	0.53
1:A:1164:ARG:HD3	5:A:1350:HOH:O	2.08	0.53
1:A:-5:VAL:HB	5:A:2074:HOH:O	2.07	0.53
1:A:538:SER:OG	1:A:541:GLU:HG3	2.08	0.53
1:A:122:GLU:O	1:A:126:GLN:HG3	2.09	0.52
1:A:398:SER:HB2	5:A:2050:HOH:O	2.08	0.52
1:A:483:GLU:O	1:A:487:ARG:HG2	2.08	0.52
1:A:942:LEU:HD23	1:A:942:LEU:C	2.34	0.52
1:A:639:ARG:CB	1:A:846:VAL:HG21	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:HIS:HD2	5:A:1529:HOH:O	1.91	0.52
1:A:774:VAL:HG12	5:A:1550:HOH:O	2.08	0.52
1:A:349:TRP:CZ3	1:A:846:VAL:HG23	2.44	0.52
1:A:621:ALA:HA	5:A:2062:HOH:O	2.10	0.52
1:A:1271:SER:HA	5:A:2100:HOH:O	2.08	0.52
1:A:70:PRO:HB3	1:A:113:TYR:CE1	2.45	0.51
1:A:39:HIS:HD2	5:A:1458:HOH:O	1.92	0.51
1:A:-5:VAL:HG13	1:A:-4:PRO:HD2	1.92	0.51
1:A:639:ARG:NH1	5:A:1913:HOH:O	2.43	0.51
1:A:1190:MET:N	1:A:1190:MET:CE	2.68	0.51
1:A:128:ALA:HA	5:A:2122:HOH:O	2.10	0.51
1:A:177:ARG:HH11	1:A:177:ARG:HG2	1.74	0.51
1:A:682:VAL:CG1	1:A:811:VAL:HG13	2.40	0.51
1:A:1178:PRO:O	1:A:1180:LEU:HD12	2.11	0.51
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.94	0.50
1:A:1005:GLU:HB2	1:A:1234:PRO:HD3	1.93	0.50
1:A:1251:ASN:HD22	1:A:1252:GLY:N	2.09	0.50
1:A:486:ASP:HA	1:A:489:TRP:NE1	2.27	0.50
1:A:508:LEU:CD1	1:A:550:ARG:NH1	2.74	0.50
1:A:220:LYS:HE3	5:A:1931:HOH:O	2.11	0.50
1:A:125:ARG:HD2	5:A:2046:HOH:O	2.11	0.50
1:A:995:LEU:C	1:A:995:LEU:HD12	2.37	0.50
1:A:358:ARG:CD	1:A:358:ARG:N	2.59	0.50
1:A:815:LEU:HD13	1:A:879:LEU:HB2	1.93	0.50
1:A:994:ARG:HD2	1:A:1003:ASP:OD1	2.12	0.50
1:A:1146:GLU:HG2	5:A:1620:HOH:O	2.12	0.50
1:A:1222:TYR:CZ	1:A:1245:THR:HG21	2.46	0.50
1:A:1074:ASP:HB3	1:A:1080:ILE:HD12	1.93	0.49
1:A:815:LEU:CD1	1:A:879:LEU:HD12	2.42	0.49
1:A:349:TRP:CE3	1:A:846:VAL:HG23	2.47	0.49
1:A:1006:HIS:HE1	5:A:1417:HOH:O	1.95	0.49
1:A:1180:LEU:HD13	1:A:1252:GLY:O	2.12	0.49
1:A:1251:ASN:C	1:A:1251:ASN:ND2	2.69	0.49
1:A:114:ILE:HD13	1:A:127:VAL:HG11	1.94	0.49
1:A:486:ASP:HA	1:A:489:TRP:CD1	2.47	0.49
1:A:1132:LEU:HA	5:A:2018:HOH:O	2.11	0.49
1:A:1251:ASN:HD22	1:A:1253:ARG:H	1.60	0.49
1:A:515:LEU:HD23	1:A:515:LEU:C	2.37	0.49
1:A:665:ALA:CB	1:A:811:VAL:CG1	2.89	0.49
1:A:219:HIS:N	5:A:1854:HOH:O	2.46	0.49
1:A:1025:ILE:HD11	1:A:1281:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLY:N	1:A:546:GLU:H	2.10	0.49
1:A:136:MET:HB3	5:A:1701:HOH:O	2.13	0.49
1:A:815:LEU:CD1	1:A:879:LEU:HB2	2.43	0.48
1:A:259:ASN:HB2	5:A:1404:HOH:O	2.14	0.48
1:A:948:LEU:O	1:A:952:VAL:HG23	2.13	0.48
1:A:1181:LEU:HD12	5:A:2018:HOH:O	2.14	0.48
1:A:0:HIS:HB3	1:A:43:LEU:O	2.13	0.48
1:A:402:GLU:HB2	5:A:1944:HOH:O	2.13	0.48
1:A:28:LEU:HD13	1:A:127:VAL:HG22	1.95	0.48
1:A:1192:ILE:HD13	1:A:1259:PRO:HB2	1.95	0.48
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.96	0.48
1:A:329:LYS:NZ	1:A:419:ASN:HD21	2.13	0.47
1:A:1121:GLU:O	1:A:1125:HIS:HD2	1.96	0.47
1:A:220:LYS:HG3	5:A:1865:HOH:O	2.12	0.47
1:A:1136:ASN:HA	1:A:1139:GLN:OE1	2.13	0.47
1:A:24:GLN:HB3	5:A:2057:HOH:O	2.14	0.47
1:A:633:ILE:C	5:A:2064:HOH:O	2.57	0.47
1:A:1104:GLU:HG3	5:A:1831:HOH:O	2.15	0.47
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.98	0.47
1:A:545:ASN:ND2	1:A:547:SER:H	2.10	0.47
1:A:50:SER:O	1:A:54:GLN:HG3	2.15	0.47
1:A:396:VAL:CG1	1:A:850:LEU:HB2	2.44	0.47
1:A:668:GLN:NE2	5:A:2093:HOH:O	2.46	0.47
1:A:782:LYS:HE3	1:A:784:ARG:NH2	2.29	0.47
1:A:782:LYS:HZ1	1:A:784:ARG:NH2	2.13	0.47
1:A:508:LEU:HD13	1:A:550:ARG:NH1	2.30	0.47
1:A:1145:ARG:HH11	1:A:1145:ARG:HB3	1.79	0.47
1:A:352:ASP:C	5:A:2071:HOH:O	2.58	0.47
1:A:864:LYS:HE2	1:A:868:ASP:OD2	2.15	0.47
1:A:1145:ARG:HD2	1:A:1151:SER:O	2.15	0.47
1:A:1259:PRO:O	1:A:1261:PRO:HD3	2.14	0.46
1:A:253:LEU:HD23	1:A:263:MET:C	2.40	0.46
1:A:608:LYS:HA	5:A:1953:HOH:O	2.14	0.46
1:A:725:ALA:HB1	1:A:815:LEU:HB2	1.96	0.46
1:A:1245:THR:HG22	1:A:1258:MET:HB2	1.97	0.46
1:A:1047:GLU:HG3	1:A:1048:GLN:N	2.29	0.46
1:A:980:THR:HB	5:A:1847:HOH:O	2.14	0.46
1:A:668:GLN:HA	1:A:678:ALA:HB3	1.96	0.46
1:A:356:PRO:HD2	1:A:359:ILE:HD11	1.98	0.46
1:A:437:ILE:HB	1:A:553:LEU:HD23	1.98	0.46
1:A:1234:PRO:O	1:A:1235:ALA:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-5:VAL:CG1	1:A:-4:PRO:CD	2.94	0.45
1:A:175:ASN:ND2	1:A:180:LEU:HB2	2.20	0.45
1:A:75:LEU:HD12	1:A:114:ILE:CD1	2.46	0.45
1:A:81:PRO:HD3	1:A:138:THR:HG21	1.99	0.45
1:A:297:ASN:HB3	1:A:410:PRO:O	2.16	0.45
1:A:376:PHE:CD1	1:A:475:PRO:HG3	2.52	0.45
1:A:436:LEU:HD21	5:A:2120:HOH:O	2.17	0.45
1:A:5:LEU:HD12	1:A:5:LEU:N	2.31	0.45
1:A:332:LEU:C	1:A:332:LEU:HD22	2.41	0.45
1:A:1248:THR:CG2	5:A:2118:HOH:O	2.64	0.45
1:A:396:VAL:CG1	1:A:397:ASN:N	2.79	0.45
1:A:496:PRO:O	1:A:498:LEU:HD12	2.17	0.45
1:A:741:MET:CE	1:A:778:SER:HB3	2.38	0.45
1:A:975:SER:O	1:A:976:GLU:HG2	2.17	0.45
1:A:288:HIS:O	1:A:419:ASN:HA	2.17	0.45
1:A:169:GLN:NE2	1:A:173:ASP:CG	2.69	0.44
1:A:216:HIS:C	5:A:1854:HOH:O	2.59	0.44
1:A:130:GLU:HG3	5:A:1921:HOH:O	2.17	0.44
1:A:387:GLY:HA2	1:A:697:ILE:HD12	1.99	0.44
1:A:922:ASN:ND2	1:A:924:GLU:H	2.08	0.44
1:A:123:GLN:O	1:A:127:VAL:HG23	2.18	0.44
1:A:1156:ARG:NH2	1:A:1204:ARG:NH1	2.63	0.44
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.53	0.44
1:A:891:LEU:HD23	1:A:921:PHE:CE1	2.52	0.44
1:A:293:VAL:HB	1:A:739:ASN:HD21	1.82	0.44
1:A:396:VAL:CG1	1:A:850:LEU:HD22	2.41	0.44
1:A:1217:LEU:CD2	5:A:2091:HOH:O	2.66	0.44
1:A:873:LEU:CD2	1:A:942:LEU:HD13	2.48	0.44
1:A:1019:VAL:HG12	1:A:1020:LYS:N	2.33	0.44
1:A:166:GLU:HB2	1:A:170:ALA:HB2	1.99	0.43
1:A:356:PRO:HD2	1:A:359:ILE:CD1	2.48	0.43
1:A:585:HIS:HB3	5:A:2041:HOH:O	2.17	0.43
1:A:976:GLU:HG3	5:A:1879:HOH:O	2.17	0.43
1:A:1025:ILE:HD11	1:A:1281:SER:CA	2.48	0.43
1:A:1050:VAL:HG13	1:A:1092:GLY:O	2.17	0.43
1:A:665:ALA:HB3	1:A:811:VAL:HG11	1.98	0.43
1:A:1031:ALA:HB3	1:A:1032:PRO:HD3	2.00	0.43
1:A:-7:GLY:O	1:A:3:GLU:HG3	2.19	0.43
1:A:30:VAL:HA	1:A:116:ALA:HB2	2.00	0.43
1:A:730:ASP:CG	5:A:2103:HOH:O	2.61	0.43
1:A:1019:VAL:CG1	1:A:1020:LYS:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1170:SER:O	1:A:1191:PRO:HA	2.19	0.43
1:A:338:SER:OG	1:A:408:HIS:HD2	2.02	0.42
1:A:690:TYR:CE1	1:A:1268:VAL:HG11	2.54	0.42
1:A:1099:VAL:O	1:A:1100:LEU:HB2	2.18	0.42
1:A:603:ASP:OD2	1:A:604:VAL:HG23	2.19	0.42
1:A:660:VAL:O	1:A:661:THR:HG23	2.19	0.42
1:A:787:GLU:HG2	1:A:792:ARG:CZ	2.48	0.42
1:A:1245:THR:CG2	1:A:1259:PRO:HD3	2.48	0.42
1:A:304:PRO:HG3	1:A:360:VAL:HG21	2.00	0.42
1:A:214:SER:N	5:A:1970:HOH:O	2.52	0.42
1:A:633:ILE:O	1:A:637:VAL:HG23	2.20	0.42
1:A:687:LEU:HD13	1:A:1058:ALA:HB2	2.02	0.42
1:A:1004:GLN:HE21	1:A:1233:TYR:H	1.66	0.42
1:A:-6:LEU:HG	5:A:2029:HOH:O	2.20	0.42
1:A:263:MET:HG2	1:A:291:MET:HE1	2.01	0.42
1:A:329:LYS:HZ2	1:A:419:ASN:HD21	1.67	0.42
1:A:936:ARG:O	1:A:940:GLU:HG3	2.19	0.42
1:A:-5:VAL:HG12	1:A:-4:PRO:N	2.34	0.42
1:A:588:LEU:O	1:A:597:PRO:HD2	2.19	0.42
1:A:1025:ILE:HD11	1:A:1281:SER:C	2.44	0.42
1:A:1217:LEU:HD23	5:A:2091:HOH:O	2.19	0.42
1:A:687:LEU:HD13	1:A:1058:ALA:CB	2.50	0.42
1:A:982:ARG:HH12	1:A:986:ALA:HB2	1.85	0.42
1:A:340:LEU:HD11	1:A:644:PRO:CG	2.28	0.42
1:A:853:LYS:HE2	5:A:2105:HOH:O	2.20	0.42
1:A:1094:PHE:HB3	1:A:1097:GLY:HA2	2.02	0.42
1:A:332:LEU:HD22	1:A:332:LEU:O	2.19	0.41
1:A:1142:SER:O	1:A:1145:ARG:HG3	2.20	0.41
1:A:786:GLN:HA	5:A:2112:HOH:O	2.20	0.41
1:A:829:ILE:HG22	1:A:831:LEU:HD13	2.02	0.41
1:A:1172:VAL:HG23	1:A:1190:MET:HE1	2.02	0.41
1:A:103:VAL:HG11	1:A:106:LEU:HG	2.02	0.41
1:A:437:ILE:HB	1:A:553:LEU:CD2	2.49	0.41
1:A:819:LEU:HG	1:A:897:MET:HB3	2.02	0.41
1:A:1180:LEU:HD23	1:A:1293:GLN:CD	2.45	0.41
1:A:83:THR:HG22	1:A:84:ILE:N	2.35	0.41
1:A:366:MET:HE2	1:A:389:PHE:CE1	2.55	0.41
1:A:436:LEU:CD2	5:A:2120:HOH:O	2.68	0.41
1:A:822:GLU:O	1:A:823:ASP:C	2.61	0.41
1:A:332:LEU:CD1	1:A:415:GLY:C	2.92	0.41
1:A:396:VAL:HG11	1:A:850:LEU:CD2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:ASP:HB3	5:A:2103:HOH:O	2.20	0.41
1:A:1190:MET:HE3	1:A:1283:TRP:HZ2	1.82	0.41
1:A:498:LEU:HD12	1:A:498:LEU:N	2.35	0.41
1:A:884:ASP:HA	1:A:927:GLY:HA3	2.02	0.41
1:A:1117:ARG:NH1	1:A:1118:ASP:OD1	2.54	0.41
3:A:2005:ADP:HI'	5:A:2093:HOH:O	2.20	0.41
1:A:233:GLN:HA	1:A:234:PRO:HD3	1.86	0.41
1:A:272:PHE:CG	1:A:490:GLN:HG2	2.56	0.41
1:A:512:MET:HB3	1:A:513:PRO:HD3	2.02	0.41
1:A:1072:MET:HE3	1:A:1072:MET:HB3	1.83	0.41
1:A:1221:ARG:HA	1:A:1243:GLY:O	2.21	0.41
1:A:203:ASP:OD1	1:A:204:ILE:N	2.54	0.41
1:A:387:GLY:HA2	1:A:697:ILE:CD1	2.51	0.41
1:A:1019:VAL:HG12	1:A:1021:LEU:HG	2.02	0.41
1:A:22:ARG:CZ	5:A:1972:HOH:O	2.69	0.40
1:A:782:LYS:CE	1:A:784:ARG:NH2	2.84	0.40
1:A:218:ARG:HB3	5:A:1865:HOH:O	2.20	0.40
1:A:1121:GLU:O	1:A:1125:HIS:CD2	2.75	0.40
1:A:1274:PRO:HD2	1:A:1277:TRP:CE2	2.56	0.40
1:A:668:GLN:CG	5:A:2093:HOH:O	2.68	0.40
1:A:134:ARG:HG2	5:A:1968:HOH:O	2.21	0.40
1:A:221:ILE:CD1	1:A:614:ARG:NH1	2.84	0.40
1:A:1190:MET:HE2	1:A:1190:MET:CA	2.50	0.40
1:A:883:HIS:CE1	1:A:896:GLU:HB2	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	1278/1303 (98%)	1224 (96%)	51 (4%)	3 (0%)	43 29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	SER
1	A	661	THR
1	A	886	SER

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	1028/1041 (99%)	998 (97%)	30 (3%)	37 16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ARG
1	A	43	LEU
1	A	47	LEU
1	A	60	GLN
1	A	104	ASP
1	A	144	THR
1	A	169	GLN
1	A	206	LEU
1	A	296	HIS
1	A	332	LEU
1	A	340	LEU
1	A	358	ARG
1	A	382	ARG
1	A	410	PRO
1	A	429	GLU
1	A	512	MET
1	A	553	LEU
1	A	588	LEU
1	A	596	GLN
1	A	741	MET
1	A	831	LEU
1	A	905	VAL

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Mol	Chain	Res	Type
1	A	976	GLU
1	A	1088	LEU
1	A	1117	ARG
1	A	1182	LEU
1	A	1190	MET
1	A	1195	SER
1	A	1245	THR
1	A	1251	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	54	GLN
1	A	60	GLN
1	A	68	HIS
1	A	96	HIS
1	A	123	GLN
1	A	169	GLN
1	A	175	ASN
1	A	202	ASN
1	A	216	HIS
1	A	219	HIS
1	A	259	ASN
1	A	276	ASN
1	A	283	HIS
1	A	298	HIS
1	A	339	ASN
1	A	347	GLN
1	A	408	HIS
1	A	419	ASN
1	A	445	ASN
1	A	471	GLN
1	A	490	GLN
1	A	545	ASN
1	A	548	GLN
1	A	585	HIS
1	A	739	ASN
1	A	746	HIS
1	A	824	ASN
1	A	862	GLN
1	A	883	HIS

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Mol	Chain	Res	Type
1	A	916	HIS
1	A	922	ASN
1	A	930	GLN
1	A	993	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1053	HIS
1	A	1061	HIS
1	A	1084	ASN
1	A	1125	HIS
1	A	1176	GLN
1	A	1251	ASN
1	A	1260	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	ADP	A	2005	4	28,29,29	1.12	2 (7%)	43,45,45	1.75	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	2003	-	4,4,4	0.39	0	6,6,6	0.07	0
2	SO4	A	2002	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	A	2009	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	A	2001	-	4,4,4	0.39	0	6,6,6	0.08	0
2	SO4	A	2004	-	4,4,4	0.32	0	6,6,6	0.08	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	ADP	A	2005	4	-	2/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2005	ADP	C5-N7	-3.21	1.33	1.39
3	A	2005	ADP	C4-N9	-2.02	1.33	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2005	ADP	N3-C2-N1	-5.59	120.12	128.58
3	A	2005	ADP	C5-C4-N3	-5.07	119.74	126.72
3	A	2005	ADP	C2-N3-C4	3.99	121.58	111.83
3	A	2005	ADP	N3-C4-N9	3.68	133.43	127.17
3	A	2005	ADP	N9-C8-N7	-2.62	110.22	113.94
3	A	2005	ADP	C5-N7-C8	2.62	107.56	103.45
3	A	2005	ADP	C4-C5-N7	-2.53	107.69	110.58
3	A	2005	ADP	O2B-PB-O3A	2.13	111.79	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

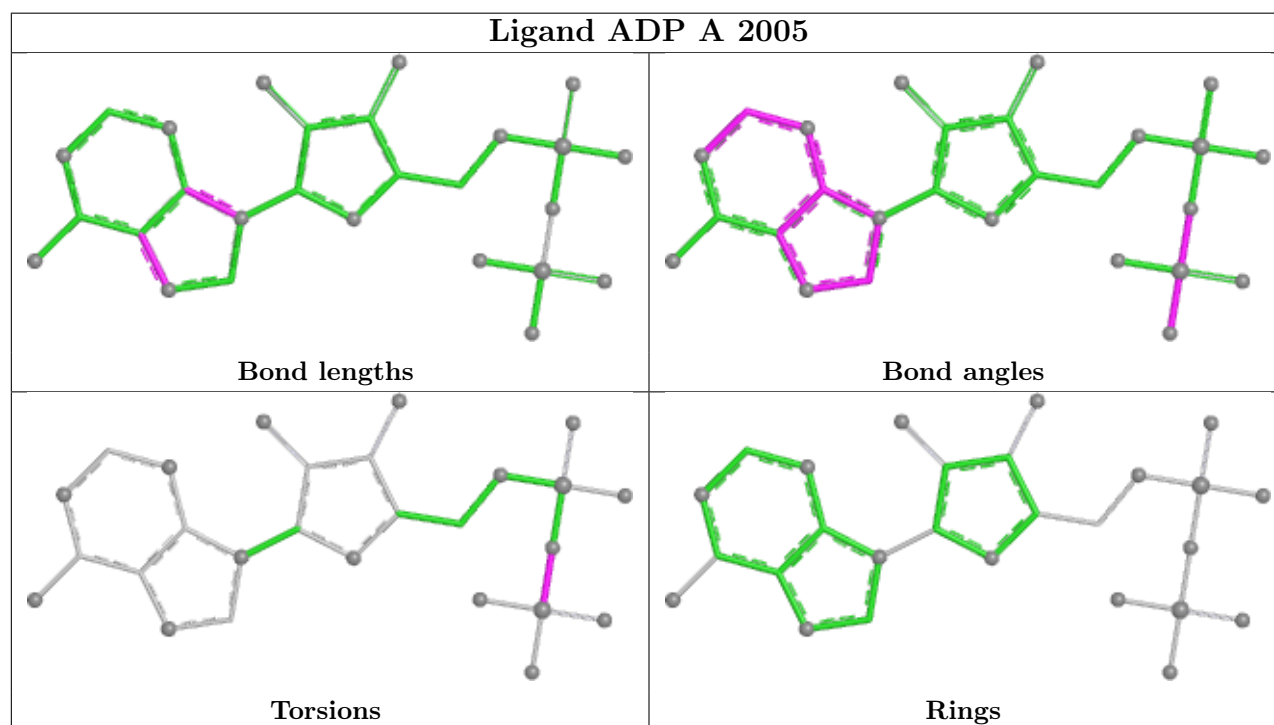
Mol	Chain	Res	Type	Atoms
3	A	2005	ADP	PA-O3A-PB-O2B
3	A	2005	ADP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2005	ADP	1	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 than 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.



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	1284/1303 (98%)	0.37	80 (6%)	26 32	8, 15, 21, 48	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	448	LEU	8.1
1	A	788	GLY	7.0
1	A	466	ASP	6.2
1	A	118	THR	5.3
1	A	447	GLY	4.8
1	A	-5	VAL	4.5
1	A	25	ALA	4.4
1	A	1091	CYS	4.2
1	A	121	ALA	4.2
1	A	119	LEU	3.9
1	A	152	HIS	3.9
1	A	120	THR	3.8
1	A	117	SER	3.8
1	A	969	ASN	3.8
1	A	66	SER	3.7
1	A	1092	GLY	3.6
1	A	27	ASN	3.6
1	A	1045	LEU	3.5
1	A	24	GLN	3.5
1	A	624	ASP	3.4
1	A	429	GLU	3.4
1	A	6	ARG	3.4
1	A	1093	GLY	3.3
1	A	609	THR	3.2
1	A	29	GLN	3.1
1	A	467	PHE	3.1
1	A	122	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	116	ALA	3.0
1	A	154	GLN	2.9
1	A	442	PRO	2.9
1	A	603	ASP	2.9
1	A	259	ASN	2.9
1	A	247	THR	2.8
1	A	67	SER	2.8
1	A	1245	THR	2.7
1	A	1025	ILE	2.7
1	A	177	ARG	2.7
1	A	396	VAL	2.7
1	A	1113	ASN	2.7
1	A	970	ASP	2.7
1	A	791	GLN	2.6
1	A	60	GLN	2.6
1	A	83	THR	2.6
1	A	623	GLY	2.6
1	A	1279	GLU	2.6
1	A	786	GLN	2.6
1	A	1156	ARG	2.6
1	A	487	ARG	2.5
1	A	534	GLU	2.5
1	A	1052	SER	2.5
1	A	257	LYS	2.4
1	A	144	THR	2.4
1	A	622	LYS	2.4
1	A	31	HIS	2.4
1	A	787	GLU	2.4
1	A	125	ARG	2.4
1	A	-4	PRO	2.3
1	A	1183	GLN	2.3
1	A	-2	GLY	2.3
1	A	22	ARG	2.3
1	A	610	PRO	2.3
1	A	431	VAL	2.3
1	A	346	GLU	2.2
1	A	69	THR	2.2
1	A	1276	ASN	2.2
1	A	10	ALA	2.2
1	A	340	LEU	2.2
1	A	619	LEU	2.2
1	A	151	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	-6	LEU	2.2
1	A	176	LEU	2.2
1	A	852	ASP	2.1
1	A	21	ALA	2.1
1	A	212	ALA	2.1
1	A	17	ASN	2.1
1	A	124	TRP	2.1
1	A	971	GLN	2.1
1	A	218	ARG	2.1
1	A	0	HIS	2.1
1	A	829	ILE	2.1

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 oligosaccharides in this entry.

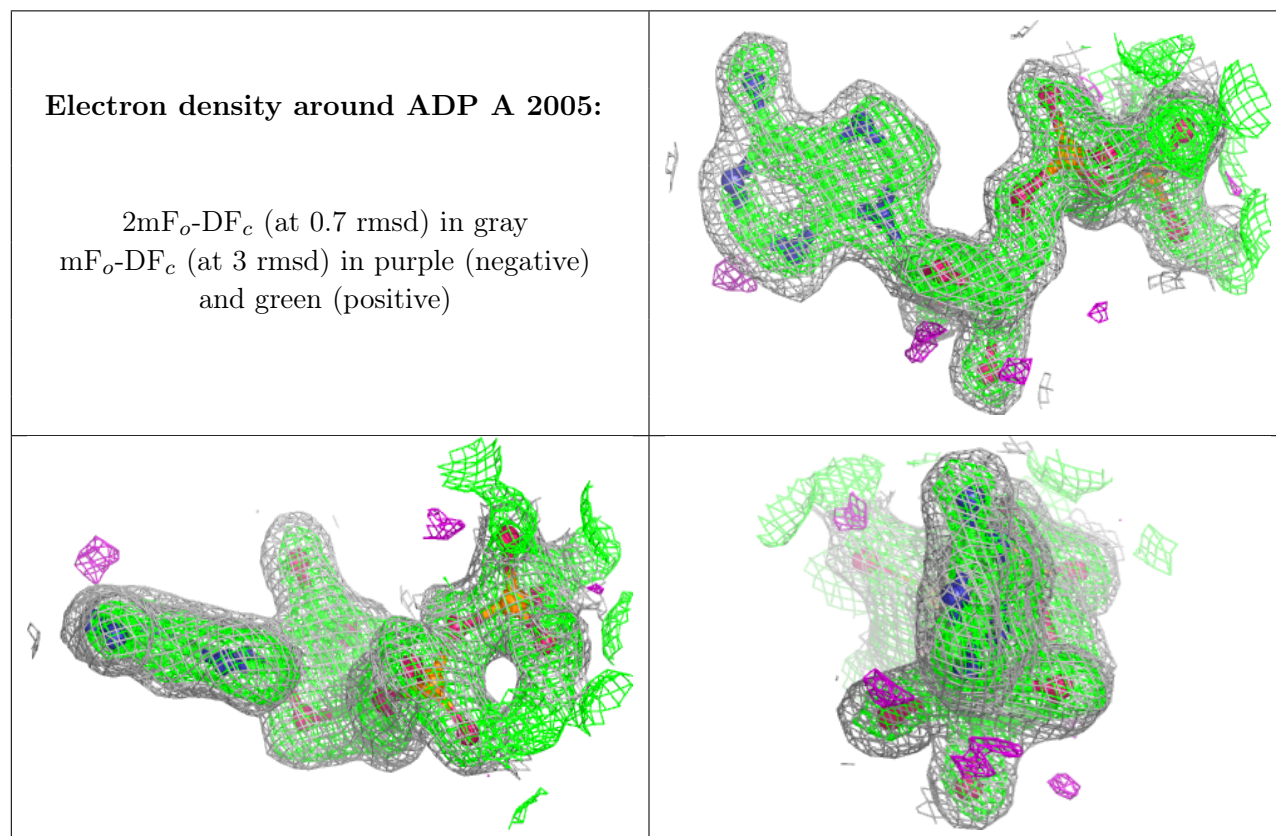
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
4	MG	A	2008	1/1	0.70	0.15	21,21,21,21	0
2	SO4	A	2003	5/5	0.85	0.17	38,40,41,42	0
4	MG	A	2006	1/1	0.86	0.13	20,20,20,20	0
4	MG	A	2007	1/1	0.87	0.12	21,21,21,21	0
2	SO4	A	2001	5/5	0.88	0.21	40,41,42,42	0
3	ADP	A	2005	27/27	0.93	0.23	6,14,15,16	27
2	SO4	A	2009	5/5	0.94	0.14	39,40,40,42	0
2	SO4	A	2002	5/5	0.95	0.14	31,33,36,36	0
2	SO4	A	2004	5/5	0.97	0.11	33,34,35,36	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.