



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:47 PM UTC

PDB ID : 6ACX / pdb_00006acx
Title : Crystal structure of Mycobacterium smegmatis Mfd in complex with ADP + Pi at 3.5 Å resolution.
Authors : Putta, S.; Fox, G.C.; Walsh, M.A.; Rao, D.N.; Nagaraja, V.; Natesh, R.
Deposited on : 2018-07-27
Resolution : 3.50 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 ⓘ 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

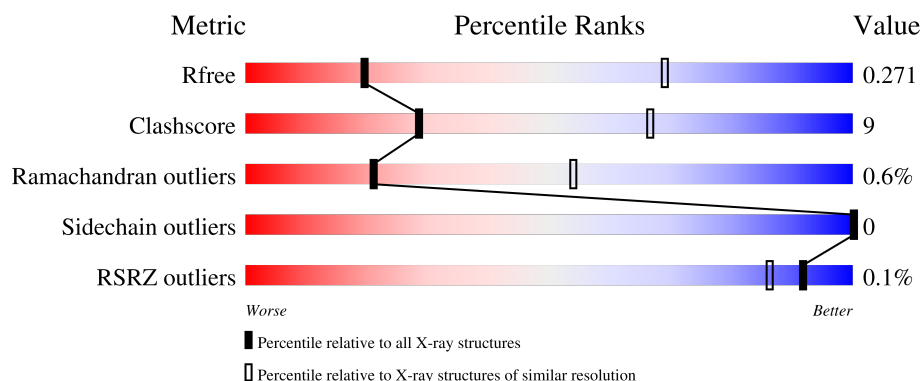
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	1235	
1	B	1235	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17349 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 Mycobacterium smegmatis Mfd.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1175	Total	C	N	O	S	0	0	0
			8626	5416	1539	1641	30			
1	B	1168	Total	C	N	O	S	0	0	0
			8539	5362	1515	1631	31			

There are 40 discrepancies between the modelled and reference sequences:

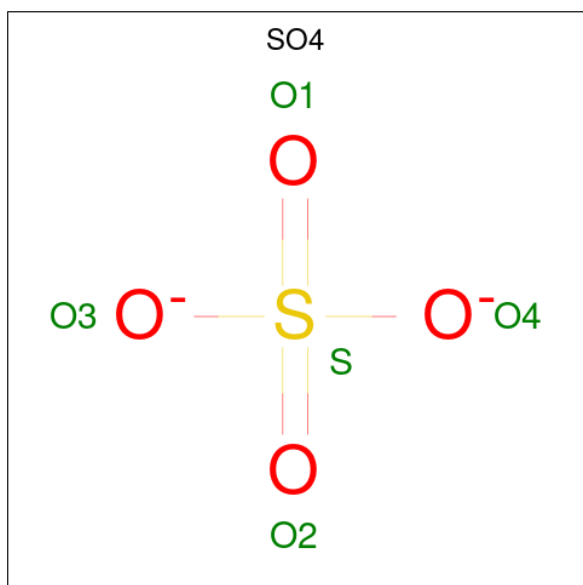
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP I7G7M2
A	-18	GLY	-	expression tag	UNP I7G7M2
A	-17	SER	-	expression tag	UNP I7G7M2
A	-16	SER	-	expression tag	UNP I7G7M2
A	-15	HIS	-	expression tag	UNP I7G7M2
A	-14	HIS	-	expression tag	UNP I7G7M2
A	-13	HIS	-	expression tag	UNP I7G7M2
A	-12	HIS	-	expression tag	UNP I7G7M2
A	-11	HIS	-	expression tag	UNP I7G7M2
A	-10	HIS	-	expression tag	UNP I7G7M2
A	-9	SER	-	expression tag	UNP I7G7M2
A	-8	SER	-	expression tag	UNP I7G7M2
A	-7	GLY	-	expression tag	UNP I7G7M2
A	-6	LEU	-	expression tag	UNP I7G7M2
A	-5	VAL	-	expression tag	UNP I7G7M2
A	-4	PRO	-	expression tag	UNP I7G7M2
A	-3	ARG	-	expression tag	UNP I7G7M2
A	-2	GLY	-	expression tag	UNP I7G7M2
A	-1	SER	-	expression tag	UNP I7G7M2
A	0	HIS	-	expression tag	UNP I7G7M2
B	-19	MET	-	initiating methionine	UNP I7G7M2
B	-18	GLY	-	expression tag	UNP I7G7M2
B	-17	SER	-	expression tag	UNP I7G7M2
B	-16	SER	-	expression tag	UNP I7G7M2
B	-15	HIS	-	expression tag	UNP I7G7M2

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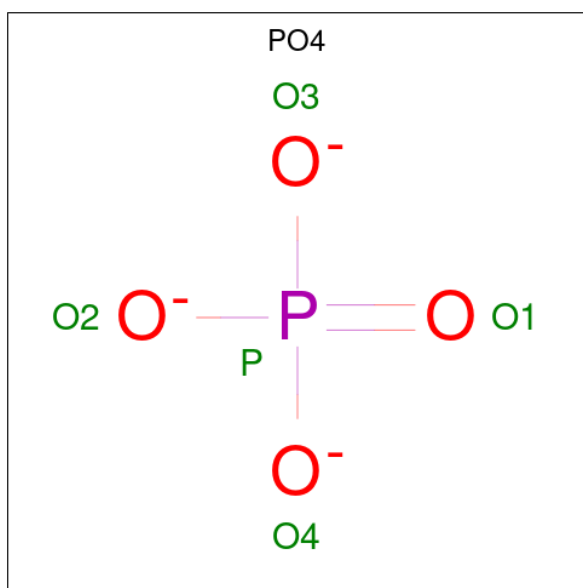
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP I7G7M2
B	-13	HIS	-	expression tag	UNP I7G7M2
B	-12	HIS	-	expression tag	UNP I7G7M2
B	-11	HIS	-	expression tag	UNP I7G7M2
B	-10	HIS	-	expression tag	UNP I7G7M2
B	-9	SER	-	expression tag	UNP I7G7M2
B	-8	SER	-	expression tag	UNP I7G7M2
B	-7	GLY	-	expression tag	UNP I7G7M2
B	-6	LEU	-	expression tag	UNP I7G7M2
B	-5	VAL	-	expression tag	UNP I7G7M2
B	-4	PRO	-	expression tag	UNP I7G7M2
B	-3	ARG	-	expression tag	UNP I7G7M2
B	-2	GLY	-	expression tag	UNP I7G7M2
B	-1	SER	-	expression tag	UNP I7G7M2
B	0	HIS	-	expression tag	UNP I7G7M2

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



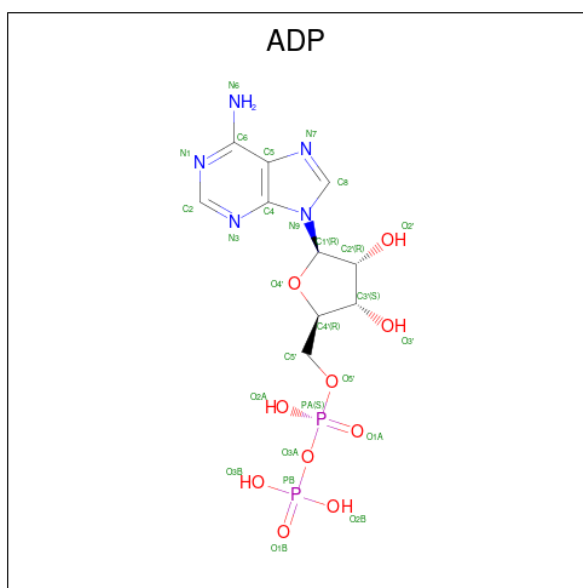
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

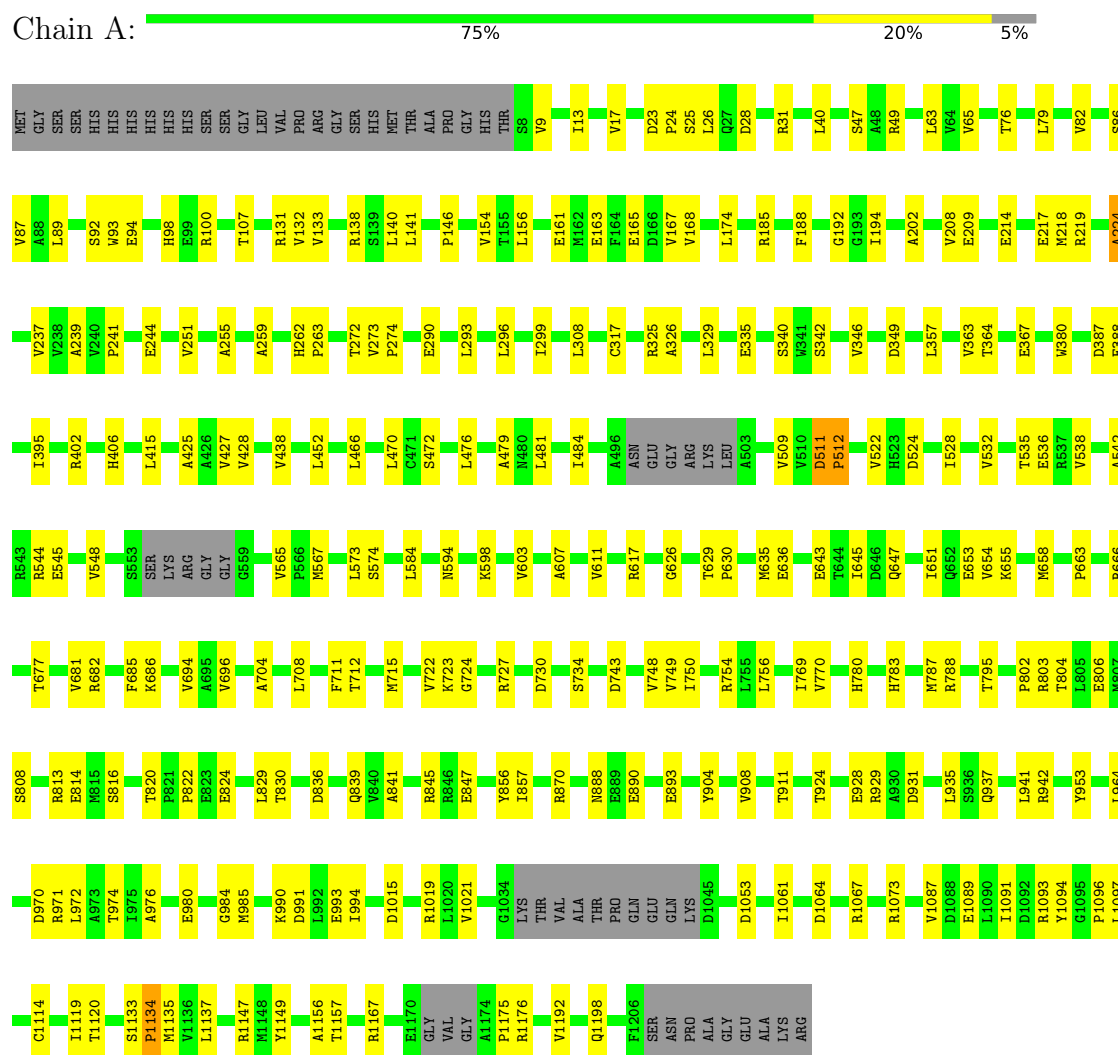
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total 54	O 54	0	0
5	B	51	Total 51	O 51	0	0

3 Residue-property plots

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: Mycobacterium smegmatis Mfd



• Molecule 1: Mycobacterium smegmatis Mfd



R1176	A988	I857	Y551	R396	I223	T76	MET
D1179	M989	H658	ALA	S397	A224	V82	GLY
L1180	K990	N859	SER	H406	I229	L89	SER
G1188	E993	R862	LYS	N407	V237	F90	HIS
L1191	I994	T863	ARG	I411	V238	P91	HIS
V1192	Y1028	E866	GLY	V419	A239	S92	HIS
L1193	R1029	R870	GLY	V439	T248	W93	HIS
D1200	K1035	E877	T560	E440	E94	E94	HIS
S1207	THR	V680	L563	E441	R100	R100	SER
ASN	VAL	V681	D571	L442	E106	E106	GLY
PRO	ALA	V881	Y576	G443	L126	L126	LEU
ALA	THR	V882	V577	E444	P285	P285	VAL
GLY	PRO	F728	GLY	A449	V133	V133	ARG
GLU	GLN	F899	GLY	T450	W134	W134	GLY
ALA	GLN	I906	GLU	I451	T135	T135	SER
LYS	LYS	L907	ALA	L452	D287	D287	HIS
D1045	D1045	V908	P582	E453	G288	G288	MET
V1052	V1052	T911	S583	T456	M289	M289	THR
D1053	D1053	R929	K596	V463	E290	E290	ALA
A1054	A1054	D931	E805	S472	S139	S139	PRO
Y1060	Y1060	T924	R608	V475	L140	L140	GLY
V1087	V1087	L925	V611	V495	L141	L141	HIS
I1091	I1091	R930	R617	ALA	E152	E152	THR
Y1094	Y1094	D931	R617	ASN	P153	P153	S8
G1095	G1095	L935	A624	GLU	V154	V154	I13
P1096	P1096	S936	L794	GLY	T155	T155	I13
L1097	L1097	Q937	T795	ARG	L156	L156	V17
L1104	L1104	L941	A798	LYS	M162	M162	L21
I1122	I1122	G946	G811	LEU	V167	V167	L26
T1129	T1129	R947	I812	ALA	R170	R170	I30
V1130	V1130	R951	R813	ALA	D180	D180	L42
R1131	R1131	R956	E814	F505	R191	R191	S47
L1132	L1132	P956	R815	V509	I194	I194	A48
S1133	S1133	P959	S816	VAL	L195	L195	R49
P1134	P1134	P959	P821	ASP	F198	F198	V52
L1137	L1137	A968	P822	P512	P205	P205	A55
A1141	A1141	Y969	V828	V522	V208	V208	L56
Y1149	Y1149	L972	V832	I528	E209	E209	L62
V1161	V1161	A973	R845	V532	V64	V64	L63
P1164	P1164	E980	R846	T535	W211	W211	V65
L1165	L1165	A983	E847	F536	S216	S216	T68
		G984	Q853	R537	E217	E217	E71
		N985	Y856	V548	M218	M218	A72

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.66Å 160.44Å 214.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.10 – 3.50 30.10 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.10-3.50) 96.5 (30.10-3.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.47Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: 000)	Depositor
R, R_{free}	0.226 , 0.273 0.227 , 0.271	Depositor DCC
R_{free} test set	1771 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	17349	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ADP, SO4

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	0.12	0/8781	0.32	1/11992 (0.0%)
1	B	0.11	0/8691	0.30	0/11874
All	All	0.11	0/17472	0.31	1/23866 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	VAL	N-CA-C	-5.19	107.41	112.29

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	8626	0	8374	156	0
1	B	8539	0	8256	145	0
2	A	15	0	0	4	0
2	B	5	0	0	0	0
3	A	5	0	0	0	0
4	A	27	0	12	3	0
4	B	27	0	12	2	0
5	A	54	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	51	0	0	1	0
All	All	17349	0	16654	299	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 9.

All (299) 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:511:ASP:H	1:A:512:PRO:HD3	1.36	0.89
1:A:617:ARG:HG3	1:A:663:PRO:HG2	1.67	0.76
1:B:968:ALA:O	1:B:972:LEU:HB2	1.87	0.75
1:B:832:VAL:HG12	1:B:956:PHE:HB2	1.72	0.72
1:A:251:VAL:HG23	1:A:296:LEU:HB3	1.71	0.71
1:B:674:TYR:HA	1:B:822:PRO:HG3	1.73	0.70
1:A:723:LYS:O	1:A:749:VAL:HA	1.93	0.69
1:B:929:ARG:HG2	1:B:959:PRO:HD3	1.73	0.69
1:A:273:VAL:HG23	1:A:274:PRO:HD3	1.75	0.69
1:A:804:THR:O	1:A:808:SER:HB3	1.93	0.68
1:A:857:ILE:HD12	1:A:941:LEU:HD13	1.76	0.68
1:B:704:ALA:O	1:B:708:LEU:HB2	1.94	0.67
1:A:788:ARG:HH21	1:A:813:ARG:HH12	1.43	0.67
1:B:734:SER:OG	1:B:754:ARG:NH2	2.27	0.66
1:B:535:THR:OG1	1:B:537:ARG:NH2	2.28	0.66
1:A:255:ALA:O	1:A:259:ALA:HB2	1.96	0.66
1:B:548:VAL:HA	1:B:563:LEU:O	1.96	0.66
1:B:211:TRP:HB2	1:B:216:SER:HB3	1.77	0.65
1:B:694:VAL:HG22	1:B:748:VAL:HG12	1.78	0.65
1:A:904:TYR:HE1	1:B:877:GLU:HB3	1.62	0.65
1:A:208:VAL:HG12	1:A:218:MET:HG2	1.79	0.64
1:A:98:HIS:NE2	1:A:357:LEU:O	2.30	0.64
1:B:522:VAL:HG23	1:B:576:TYR:HB2	1.80	0.64
1:A:822:PRO:HB2	4:A:1305:ADP:C6	2.33	0.64
1:B:222:ALA:HB2	1:B:229:ILE:HD11	1.80	0.64
1:A:511:ASP:H	1:A:512:PRO:CD	2.10	0.63
1:A:532:VAL:HB	1:A:548:VAL:HG23	1.80	0.63
1:B:532:VAL:HB	1:B:548:VAL:HG23	1.79	0.63
1:A:194:ILE:HG12	1:A:209:GLU:HG2	1.79	0.63
1:A:156:LEU:HB2	1:A:237:VAL:HG22	1.81	0.63
1:A:629:THR:HB	1:A:630:PRO:HD2	1.80	0.63
1:B:617:ARG:NH1	1:B:663:PRO:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:980:GLU:HA	1:B:985:MET:HG3	1.79	0.62
1:A:325:ARG:NH2	2:A:1301:SO4:O3	2.32	0.62
1:A:1167:ARG:CZ	1:A:1176:ARG:HH12	2.12	0.62
1:A:696:VAL:HG22	1:A:769:ILE:HB	1.81	0.62
1:B:154:VAL:HB	1:B:239:ALA:HB3	1.81	0.62
1:B:666:ARG:HA	1:B:814:GLU:O	2.00	0.62
1:A:1064:ASP:OD1	1:A:1067:ARG:NH2	2.31	0.62
1:A:724:GLY:HA2	1:A:750:ILE:O	1.99	0.61
1:A:870:ARG:NH2	1:A:928:GLU:OE2	2.33	0.61
1:A:734:SER:OG	1:A:754:ARG:NH2	2.33	0.61
1:B:985:MET:O	1:B:988:ALA:N	2.33	0.61
1:B:857:ILE:HD13	1:B:941:LEU:HD13	1.83	0.61
1:A:1091:ILE:HD13	1:A:1096:PRO:HA	1.83	0.60
1:B:969:TYR:O	1:B:973:ALA:HB2	2.01	0.60
1:A:185:ARG:NH2	1:A:202:ALA:O	2.35	0.60
1:A:1120:THR:HB	1:A:1134:PRO:HG3	1.83	0.60
1:A:1073:ARG:NH2	1:A:1089:GLU:OE2	2.35	0.59
1:A:364:THR:HG23	1:A:367:GLU:H	1.67	0.59
1:A:92:SER:HB2	1:A:138:ARG:HD2	1.85	0.58
1:B:72:ALA:O	1:B:76:THR:OG1	2.17	0.58
1:A:335:GLU:OE2	1:A:845:ARG:NH2	2.36	0.58
1:B:752:THR:OG1	1:B:753:HIS:N	2.34	0.58
1:A:836:ASP:HB3	1:A:839:GLN:HG3	1.87	0.57
1:A:427:VAL:HG11	1:A:438:VAL:HG11	1.86	0.57
1:B:611:VAL:HG21	1:B:1028:TYR:HB3	1.86	0.57
1:B:911:THR:HG22	1:B:941:LEU:HD21	1.87	0.57
1:B:862:ARG:HG3	1:B:863:THR:HG23	1.87	0.56
1:B:969:TYR:O	1:B:973:ALA:CB	2.53	0.56
1:A:65:VAL:HG21	1:A:140:LEU:HD22	1.87	0.56
1:A:935:LEU:HG	1:A:971:ARG:HG3	1.86	0.56
1:B:285:PRO:HB3	1:B:289:MET:HE1	1.86	0.56
1:A:522:VAL:HG22	1:A:528:ILE:HG12	1.87	0.56
1:B:442:LEU:HD12	1:B:449:ALA:HB2	1.88	0.56
1:A:654:VAL:HG12	1:A:658:MET:HE2	1.87	0.56
1:A:856:TYR:O	1:A:908:VAL:HA	2.06	0.56
1:B:1165:LEU:O	1:B:1176:ARG:NH1	2.39	0.56
1:A:168:VAL:HG23	1:A:188:PHE:CE2	2.41	0.55
1:A:685:PHE:HD2	1:A:715:MET:HG2	1.71	0.55
1:A:911:THR:HG22	1:A:941:LEU:HD21	1.89	0.55
1:A:174:LEU:HD22	1:A:241:PRO:HG3	1.88	0.55
1:A:255:ALA:O	1:A:259:ALA:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:SER:HB3	1:B:472:SER:HB2	1.88	0.55
1:B:681:VAL:HG21	1:B:714:ARG:HD3	1.87	0.55
1:A:13:ILE:HG13	1:A:82:VAL:HG12	1.87	0.55
1:A:168:VAL:HG23	1:A:188:PHE:HE2	1.70	0.55
1:A:727:ARG:NH2	1:A:893:GLU:OE1	2.40	0.55
1:B:856:TYR:O	1:B:908:VAL:HA	2.06	0.55
1:B:208:VAL:HG12	1:B:218:MET:HG2	1.88	0.54
1:B:335:GLU:OE2	1:B:845:ARG:NH2	2.40	0.54
1:B:726:SER:O	1:B:729:THR:OG1	2.24	0.54
1:A:524:ASP:OD2	1:A:1019:ARG:NH2	2.41	0.54
1:A:163:GLU:O	1:A:167:VAL:HG23	2.08	0.54
1:B:701:THR:HG21	1:B:727:ARG:H	1.71	0.54
1:A:26:LEU:HD21	1:A:395:ILE:HD11	1.90	0.53
1:B:94:GLU:HG2	1:B:951:ARG:HE	1.72	0.53
1:B:857:ILE:HD12	1:B:925:LEU:HD11	1.90	0.53
1:B:1052:VAL:HG13	1:B:1179:ASP:HA	1.91	0.53
1:B:811:GLY:HA3	1:B:1029:ARG:HE	1.74	0.53
1:B:624:ALA:HB2	1:B:661:PRO:HA	1.91	0.52
1:A:603:VAL:HG21	1:A:1021:VAL:HA	1.92	0.52
1:B:571:ASP:OD1	1:B:571:ASP:N	2.39	0.52
1:B:857:ILE:HD11	1:B:914:GLU:HG3	1.92	0.52
1:A:146:PRO:HD2	1:A:299:ILE:HD13	1.91	0.52
1:B:137:THR:HG22	1:B:322:VAL:HG13	1.92	0.52
1:B:1191:LEU:HD13	1:B:1200:ASP:HB2	1.92	0.52
1:B:712:THR:HG22	1:B:722:VAL:HG21	1.91	0.52
1:B:453:GLU:HG3	1:B:456:THR:HG21	1.90	0.52
1:A:49:ARG:HE	1:A:317:CYS:HB3	1.74	0.51
1:A:935:LEU:H	1:A:935:LEU:HD12	1.75	0.51
1:A:1087:VAL:HG13	1:A:1097:LEU:HD11	1.92	0.51
1:A:730:ASP:N	1:A:730:ASP:OD1	2.42	0.51
1:B:17:VAL:HG21	1:B:82:VAL:HG11	1.90	0.51
1:B:665:ASP:OD1	1:B:813:ARG:NE	2.44	0.51
1:A:262:HIS:NE2	1:A:349:ASP:O	2.43	0.51
1:B:990:LYS:HA	1:B:993:GLU:HG3	1.92	0.51
1:A:217:GLU:OE1	1:A:219:ARG:NH2	2.44	0.51
1:A:342:SER:O	1:A:346:VAL:HG23	2.10	0.51
1:B:63:LEU:HD22	1:B:308:LEU:HD11	1.93	0.51
1:B:65:VAL:HG21	1:B:140:LEU:HD22	1.91	0.51
1:B:180:ASP:O	1:B:191:ARG:NH1	2.22	0.51
1:A:651:ILE:HG22	1:A:655:LYS:HE3	1.92	0.50
1:B:880:VAL:HG22	1:B:906:ILE:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HB2	1:B:237:VAL:HG22	1.94	0.50
1:A:1147:ARG:NH1	2:A:1303:SO4:O1	2.38	0.50
1:A:100:ARG:NH2	1:A:340:SER:O	2.44	0.50
1:B:828:VAL:HG12	1:B:946:GLY:HA3	1.94	0.50
1:A:1133:SER:HB3	1:A:1134:PRO:HD3	1.93	0.50
1:B:194:ILE:HG12	1:B:209:GLU:HG3	1.92	0.50
1:A:803:ARG:HA	1:A:806:GLU:HB3	1.94	0.49
1:A:76:THR:HG21	1:A:89:LEU:HB2	1.94	0.49
1:A:1156:ALA:N	2:A:1302:SO4:O4	2.44	0.49
1:A:643:GLU:H	1:A:643:GLU:CD	2.20	0.49
1:A:783:HIS:CE1	1:A:787:MET:HE3	2.48	0.49
1:A:594:ASN:O	1:A:598:LYS:HG2	2.13	0.49
1:A:79:LEU:HD13	1:A:132:VAL:HG11	1.95	0.49
1:A:929:ARG:NH2	5:A:1403:HOH:O	2.46	0.48
1:B:21:LEU:HD23	1:B:26:LEU:HD13	1.95	0.48
1:B:52:VAL:O	1:B:55:ALA:HB3	2.12	0.48
1:A:565:VAL:HG21	1:A:573:LEU:HD11	1.95	0.48
1:A:1120:THR:H	1:A:1134:PRO:CG	2.26	0.48
1:A:991:ASP:HA	1:A:994:ILE:HG12	1.95	0.48
1:B:26:LEU:O	1:B:30:ILE:HG12	2.14	0.48
1:A:928:GLU:HG2	1:A:929:ARG:HG2	1.95	0.48
1:B:1054:ALA:HB1	1:B:1104:LEU:HA	1.95	0.48
1:B:330:ILE:HD11	1:B:364:THR:HA	1.96	0.48
1:A:415:LEU:HD22	1:A:425:ALA:HB1	1.96	0.47
1:B:13:ILE:HG13	1:B:82:VAL:HG12	1.96	0.47
1:B:832:VAL:HA	1:B:956:PHE:O	2.14	0.47
1:A:847:GLU:OE1	1:A:924:THR:OG1	2.24	0.47
1:A:325:ARG:O	1:A:329:LEU:HD22	2.13	0.47
1:A:681:VAL:HG12	1:A:711:PHE:CE1	2.50	0.47
1:B:287:ASP:OD1	1:B:288:GLY:N	2.47	0.47
1:B:847:GLU:OE1	1:B:924:THR:OG1	2.29	0.47
1:B:49:ARG:HE	1:B:317:CYS:HB3	1.77	0.47
1:A:802:PRO:HD3	1:A:993:GLU:HB3	1.96	0.47
1:A:1061:ILE:O	1:A:1067:ARG:NH1	2.48	0.47
1:B:396:ARG:HG3	1:B:475:VAL:HB	1.97	0.47
1:B:419:VAL:HG11	1:B:463:VAL:HG22	1.97	0.47
1:A:647:GLN:O	1:A:651:ILE:HG13	2.15	0.47
1:B:882:VAL:HA	1:B:908:VAL:O	2.15	0.47
1:B:1129:THR:HA	1:B:1164:PRO:HA	1.97	0.47
1:A:970:ASP:O	1:A:974:THR:HG23	2.14	0.47
1:A:161:GLU:HA	1:A:214:GLU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LEU:HD21	1:A:484:ILE:HD12	1.97	0.47
1:A:931:ASP:N	1:A:931:ASP:OD1	2.46	0.46
4:A:1305:ADP:H5'2	4:A:1305:ADP:C8	2.50	0.46
1:B:68:THR:OG1	1:B:71:GLU:OE1	2.22	0.46
1:B:198:PHE:CD2	1:B:205:PRO:HG3	2.51	0.46
1:A:635:MET:HE1	1:A:682:ARG:HG2	1.97	0.46
1:B:141:LEU:HD11	1:B:326:ALA:HB1	1.97	0.46
1:B:1137:LEU:HB3	1:B:1141:ALA:HB3	1.97	0.46
1:A:822:PRO:HB2	4:A:1305:ADP:N1	2.31	0.46
1:A:888:ASN:OD1	1:A:888:ASN:N	2.49	0.46
1:B:322:VAL:HG12	1:B:365:PHE:HE2	1.81	0.46
1:B:635:MET:HE1	1:B:682:ARG:HG2	1.97	0.46
1:A:406:HIS:CE1	1:B:396:ARG:HD2	2.51	0.46
1:B:407:ASN:O	1:B:411:ILE:HG12	2.15	0.46
1:B:696:VAL:HG22	1:B:769:ILE:HB	1.97	0.46
1:A:636:GLU:HG2	1:A:682:ARG:HD3	1.98	0.46
1:B:290:GLU:O	1:B:293:LEU:HB2	2.16	0.46
1:A:476:LEU:HD13	1:A:481:LEU:HD23	1.98	0.45
1:A:980:GLU:HA	1:A:985:MET:SD	2.56	0.45
1:B:439:VAL:HG22	1:B:449:ALA:HB1	1.98	0.45
1:A:28:ASP:OD1	1:A:31:ARG:NH2	2.49	0.45
1:A:584:LEU:HD23	1:A:584:LEU:HA	1.79	0.45
1:B:369:ARG:HG3	1:B:379:TRP:CG	2.51	0.45
1:B:788:ARG:HG2	1:B:793:VAL:HG11	1.97	0.45
1:B:1045:ASP:OD1	1:B:1045:ASP:N	2.48	0.45
1:B:1130:VAL:HB	1:B:1165:LEU:HD21	1.98	0.45
1:A:23:ASP:HB2	1:A:479:ALA:HB2	1.99	0.45
1:A:86:SER:HB3	1:A:131:ARG:HG3	1.97	0.45
1:A:387:ASP:OD1	1:A:388:GLU:N	2.48	0.45
1:A:666:ARG:HA	1:A:814:GLU:O	2.16	0.45
1:B:528:ILE:HD12	1:B:583:SER:HB2	1.97	0.45
1:B:937:GLN:O	1:B:941:LEU:HG	2.17	0.45
1:B:1133:SER:HB3	1:B:1134:PRO:HD3	1.98	0.45
1:A:402:ARG:NH2	1:B:397:SER:OG	2.30	0.45
1:A:1157:THR:OG1	2:A:1302:SO4:O1	2.29	0.45
1:B:305:THR:HG21	1:B:372:ALA:HB2	1.98	0.45
1:A:1114:CYS:HB3	1:A:1119:ILE:HB	1.97	0.45
1:B:440:GLU:O	1:B:444:GLU:HB2	2.17	0.45
1:B:704:ALA:O	1:B:708:LEU:CB	2.64	0.45
1:A:326:ALA:HA	1:A:329:LEU:HD23	1.99	0.44
1:B:342:SER:O	1:B:346:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:HD22	1:B:393:LEU:HD11	1.99	0.44
1:B:770:VAL:HB	1:B:795:THR:HG22	1.98	0.44
1:B:935:LEU:HD12	1:B:935:LEU:H	1.82	0.44
1:A:743:ASP:OD1	1:A:743:ASP:N	2.50	0.44
1:A:1149:TYR:HE1	1:A:1192:VAL:HG21	1.82	0.44
1:B:605:GLU:O	1:B:608:SER:OG	2.27	0.44
1:A:677:THR:O	1:A:681:VAL:HG13	2.17	0.44
1:A:904:TYR:CE1	1:B:877:GLU:HB3	2.48	0.44
1:A:40:LEU:HB3	1:A:380:TRP:CG	2.52	0.44
1:A:535:THR:OG1	1:A:536:GLU:N	2.50	0.44
1:B:1087:VAL:HG13	1:B:1097:LEU:HD11	1.99	0.44
1:A:937:GLN:O	1:A:941:LEU:HG	2.17	0.44
1:B:100:ARG:NH2	1:B:271:GLY:O	2.45	0.44
1:A:704:ALA:O	1:A:708:LEU:HB2	2.18	0.44
1:B:931:ASP:OD1	1:B:931:ASP:N	2.48	0.44
1:A:830:THR:OG1	1:A:942:ARG:NH1	2.50	0.43
1:B:364:THR:HG23	1:B:367:GLU:H	1.83	0.43
1:B:853:GLN:NE2	1:B:899:PHE:O	2.49	0.43
1:B:1060:TYR:CZ	1:B:1094:TYR:HB2	2.53	0.43
1:A:47:SER:HB3	1:A:472:SER:HB2	1.99	0.43
1:B:321:LYS:H	1:B:321:LYS:HD2	1.84	0.43
1:A:888:ASN:ND2	1:A:890:GLU:OE1	2.46	0.43
1:B:866:GLU:O	1:B:870:ARG:HG3	2.18	0.43
1:B:1161:VAL:HG11	1:B:1193:LEU:HD11	2.00	0.43
1:B:596:LYS:HB3	1:B:596:LYS:HE2	1.78	0.43
1:B:666:ARG:NH2	1:B:816:SER:OG	2.51	0.43
1:B:1149:TYR:HE2	1:B:1192:VAL:HG21	1.83	0.43
1:A:17:VAL:HG21	1:A:82:VAL:HG11	2.00	0.43
1:B:1122:ILE:HG12	1:B:1132:LEU:HG	2.00	0.43
1:B:76:THR:HG21	1:B:89:LEU:HB2	2.00	0.43
1:A:272:THR:HG23	1:A:274:PRO:HD2	2.00	0.43
1:B:90:PHE:HB3	1:B:135:THR:HB	2.01	0.43
1:A:290:GLU:HA	1:A:293:LEU:HD13	2.00	0.43
1:A:655:LYS:HA	1:A:658:MET:HE3	2.01	0.43
1:B:643:GLU:OE1	1:B:643:GLU:N	2.40	0.43
1:A:722:VAL:HG12	1:A:748:VAL:CG1	2.49	0.43
1:B:276:MET:HG3	1:B:286:VAL:HG21	2.01	0.43
1:A:829:LEU:HD12	1:A:953:TYR:HE1	1.83	0.42
1:A:990:LYS:O	1:A:994:ILE:HG12	2.19	0.42
1:B:308:LEU:HB2	1:B:377:HIS:CE1	2.54	0.42
4:B:1302:ADP:H8	4:B:1302:ADP:H5'2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASP:OD2	1:A:25:SER:HB3	2.19	0.42
1:B:152:GLU:HB3	1:B:170:ARG:HH11	1.84	0.42
1:A:165:GLU:HA	1:A:168:VAL:HG12	2.00	0.42
1:B:92:SER:HB2	1:B:138:ARG:HD2	2.01	0.42
1:A:536:GLU:HA	1:A:544:ARG:O	2.19	0.42
1:A:574:SER:HB2	1:A:1015:ASP:HB3	2.02	0.42
1:A:972:LEU:O	1:A:976:ALA:HB2	2.18	0.42
1:B:990:LYS:O	1:B:994:ILE:HG12	2.20	0.42
1:A:87:VAL:HA	1:A:132:VAL:O	2.20	0.42
1:B:126:LEU:HD23	1:B:238:VAL:HG21	2.00	0.42
1:A:626:GLY:O	1:A:686:LYS:NZ	2.50	0.42
1:B:725:LEU:HD11	1:B:754:ARG:HE	1.85	0.42
1:A:154:VAL:HB	1:A:239:ALA:HB3	2.02	0.42
1:A:452:LEU:HB2	1:A:466:LEU:HD13	2.00	0.42
1:A:653:GLU:OE2	1:A:816:SER:OG	2.26	0.42
1:A:694:VAL:O	1:A:748:VAL:HA	2.20	0.42
1:A:1198:GLN:OE1	1:A:1198:GLN:N	2.51	0.42
1:B:106:GLU:H	1:B:106:GLU:HG2	1.69	0.42
1:A:538:VAL:HA	1:A:542:ALA:O	2.20	0.42
1:A:645:ILE:HG23	1:A:820:THR:HG21	2.02	0.42
1:B:788:ARG:HH21	1:B:795:THR:HG21	1.84	0.42
1:B:715:MET:HE1	1:B:748:VAL:HG11	2.01	0.42
1:A:63:LEU:HD22	1:A:308:LEU:HD11	2.01	0.41
1:A:63:LEU:HD12	1:A:133:VAL:O	2.20	0.41
1:B:63:LEU:HD12	1:B:133:VAL:O	2.18	0.41
1:B:674:TYR:CE1	1:B:821:PRO:HA	2.55	0.41
1:B:856:TYR:HB3	1:B:908:VAL:HG22	2.01	0.41
1:B:1180:LEU:HD23	1:B:1180:LEU:HA	1.75	0.41
1:A:708:LEU:O	1:A:712:THR:HG23	2.20	0.41
1:A:756:LEU:HD12	1:A:780:HIS:HB3	2.02	0.41
1:B:56:LEU:HB2	1:B:62:LEU:HD13	2.01	0.41
1:B:94:GLU:HG2	1:B:951:ARG:NE	2.34	0.41
1:A:94:GLU:OE2	1:A:107:THR:OG1	2.30	0.41
1:B:162:MET:HE2	1:B:167:VAL:HG22	2.03	0.41
1:A:23:ASP:HA	1:A:24:PRO:HD3	1.96	0.41
1:A:224:ALA:HA	1:A:509:VAL:H	1.85	0.41
1:B:671:ASP:CG	1:B:947:ARG:HH22	2.29	0.41
1:B:1091:ILE:HA	1:B:1095:GLY:O	2.20	0.41
1:A:428:VAL:HG21	1:A:470:LEU:HD12	2.03	0.41
1:A:93:TRP:NE1	1:A:244:GLU:OE2	2.52	0.41
1:B:135:THR:OG1	1:B:136:THR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:MET:HE3	1:B:635:MET:HB3	1.92	0.41
1:A:218:MET:HE2	1:A:218:MET:HB3	1.91	0.41
1:A:1135:MET:HE2	1:A:1137:LEU:HD21	2.02	0.41
1:B:248:THR:O	1:B:251:VAL:HG22	2.21	0.41
1:B:670:GLY:O	1:B:798:ALA:HA	2.21	0.41
1:B:721:THR:OG1	1:B:747:ASP:N	2.54	0.41
1:B:1188:GLY:O	1:B:1192:VAL:HG22	2.21	0.41
1:A:141:LEU:O	1:A:363:VAL:HG22	2.21	0.41
1:B:195:LEU:O	1:B:208:VAL:HG22	2.21	0.41
1:A:770:VAL:HB	1:A:795:THR:HG22	2.02	0.40
1:A:452:LEU:HD12	1:A:466:LEU:HB2	2.03	0.40
1:A:841:ALA:O	1:A:845:ARG:HG3	2.22	0.40
1:B:859:ASN:ND2	5:B:1401:HOH:O	2.36	0.40
1:A:273:VAL:HG21	1:A:346:VAL:CG1	2.52	0.40
1:A:1093:ARG:NH1	1:A:1094:TYR:OH	2.54	0.40
1:A:427:VAL:HA	1:A:484:ILE:O	2.21	0.40
1:A:607:ALA:O	1:A:611:VAL:HG22	2.21	0.40
1:B:708:LEU:O	1:B:712:THR:HG23	2.21	0.40
1:A:545:GLU:HG2	1:A:567:MET:HE3	2.02	0.40
1:A:964:LEU:HD23	1:A:964:LEU:H	1.87	0.40
1:B:822:PRO:HB2	4:B:1302:ADP:C2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1165/1235 (94%)	1101 (94%)	54 (5%)	10 (1%)	14 47
1	B	1156/1235 (94%)	1088 (94%)	64 (6%)	4 (0%)	36 67
All	All	2321/2470 (94%)	2189 (94%)	118 (5%)	14 (1%)	21 54

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	511	ASP
1	A	1134	PRO
1	B	1134	PRO
1	A	512	PRO
1	A	1053	ASP
1	A	1175	PRO
1	B	224	ALA
1	A	824	GLU
1	A	224	ALA
1	A	263	PRO
1	A	984	GLY
1	A	192	GLY
1	B	346	VAL
1	B	451	ILE

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	851/988 (86%)	851 (100%)	0	100	100
1	B	842/988 (85%)	842 (100%)	0	100	100
All	All	1693/1976 (86%)	1693 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	526	HIS
1	A	1142	GLN
1	A	1194	ASN
1	B	384	GLN
1	B	418	HIS
1	B	790	HIS

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Mol	Chain	Res	Type
1	B	937	GLN
1	B	1005	GLN
1	B	1008	HIS
1	B	1194	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	1304	-	4,4,4	0.96	0	6,6,6	0.49	0
2	SO4	A	1302	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	1303	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	1301	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	A	1301	-	4,4,4	0.23	0	6,6,6	0.08	0
4	ADP	A	1305	-	28,29,29	1.41	5 (17%)	43,45,45	1.76	7 (16%)
4	ADP	B	1302	-	28,29,29	1.43	5 (17%)	43,45,45	1.84	8 (18%)

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	ADP	A	1305	-	-	6/16/32/32	0/3/3/3
4	ADP	B	1302	-	-	5/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1302	ADP	C5-C4	4.81	1.47	1.39
4	A	1305	ADP	C5-C4	4.65	1.47	1.39
4	B	1302	ADP	C5-C6	2.62	1.48	1.41
4	A	1305	ADP	C5-C6	2.55	1.48	1.41
4	B	1302	ADP	C5-N7	-2.39	1.34	1.39
4	A	1305	ADP	C5-N7	-2.39	1.34	1.39
4	A	1305	ADP	C8-N7	2.21	1.35	1.31
4	B	1302	ADP	C8-N7	2.17	1.35	1.31
4	A	1305	ADP	C4-N9	-2.04	1.33	1.37
4	B	1302	ADP	PA-O3A	2.02	1.61	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1302	ADP	C5-C4-N3	-5.89	118.60	126.72
4	A	1305	ADP	C5-C4-N3	-5.50	119.15	126.72
4	B	1302	ADP	N3-C4-N9	4.82	135.37	127.17
4	A	1305	ADP	N3-C4-N9	4.37	134.60	127.17
4	B	1302	ADP	C2-N3-C4	3.62	120.68	111.83
4	A	1305	ADP	C2-N3-C4	3.51	120.40	111.83
4	B	1302	ADP	C4-C5-N7	-3.25	106.86	110.58
4	A	1305	ADP	N3-C2-N1	-3.20	123.74	128.58
4	B	1302	ADP	N3-C2-N1	-3.13	123.84	128.58
4	A	1305	ADP	C4-C5-N7	-3.11	107.02	110.58
4	B	1302	ADP	C4-N9-C8	2.55	108.41	105.74
4	B	1302	ADP	C3'-C2'-C1'	2.52	106.23	101.46
4	B	1302	ADP	C5-N7-C8	2.43	107.27	103.45
4	A	1305	ADP	C4-N9-C8	2.40	108.26	105.74
4	A	1305	ADP	C5-N7-C8	2.23	106.95	103.45

There are no chirality outliers.

All (11) torsion outliers are listed below:

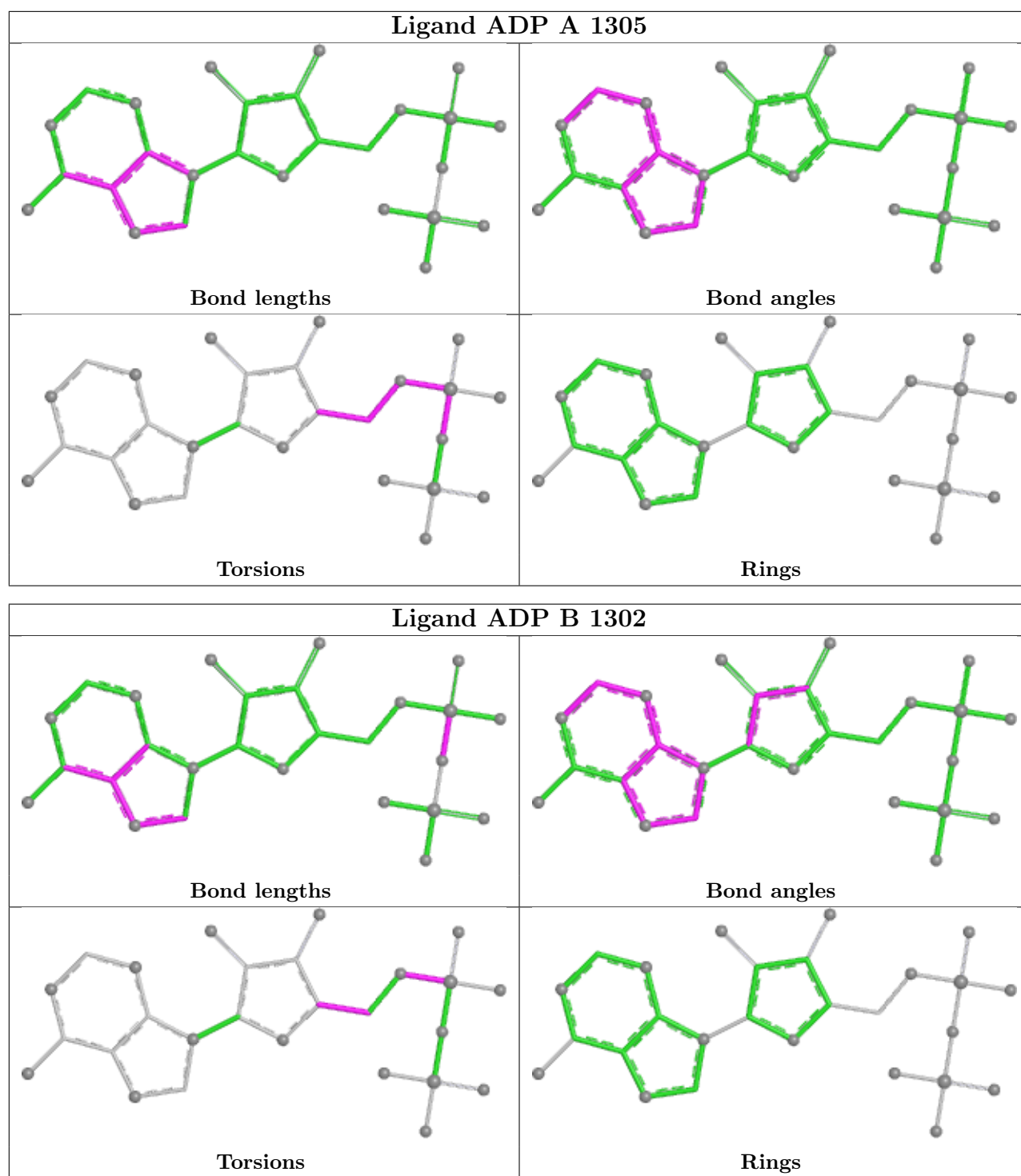
Mol	Chain	Res	Type	Atoms
4	A	1305	ADP	PB-O3A-PA-O5'
4	A	1305	ADP	C5'-O5'-PA-O3A
4	B	1302	ADP	C5'-O5'-PA-O1A
4	B	1302	ADP	C5'-O5'-PA-O2A
4	B	1302	ADP	C5'-O5'-PA-O3A
4	A	1305	ADP	C3'-C4'-C5'-O5'
4	A	1305	ADP	O4'-C4'-C5'-O5'
4	B	1302	ADP	C3'-C4'-C5'-O5'
4	B	1302	ADP	O4'-C4'-C5'-O5'
4	A	1305	ADP	C4'-C5'-O5'-PA
4	A	1305	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1302	SO4	2	0
2	A	1303	SO4	1	0
2	A	1301	SO4	1	0
4	A	1305	ADP	3	0
4	B	1302	ADP	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1175/1235 (95%)	-0.18	0 100 100	31, 64, 104, 132	0
1	B	1168/1235 (94%)	-0.13	2 (0%) 91 82	32, 71, 111, 135	0
All	All	2343/2470 (94%)	-0.16	2 (0%) 92 86	31, 67, 108, 135	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	983	ALA	2.3
1	B	406	HIS	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(Å ²)	Q<0.9
3	PO4	A	1304	5/5	0.76	0.16	87,94,97,105	0
2	SO4	A	1303	5/5	0.77	0.10	86,89,102,111	0
4	ADP	B	1302	27/27	0.77	0.11	81,103,115,136	0

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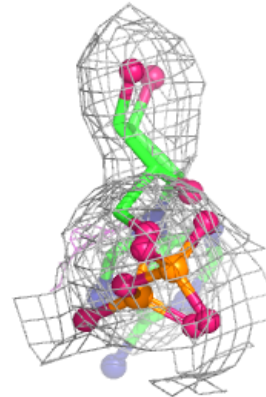
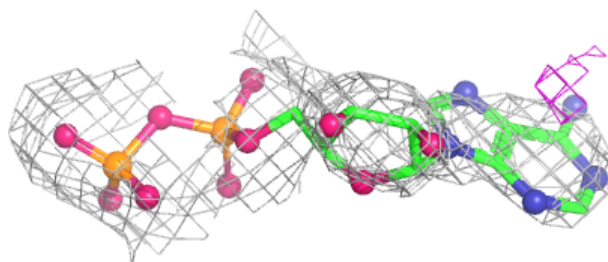
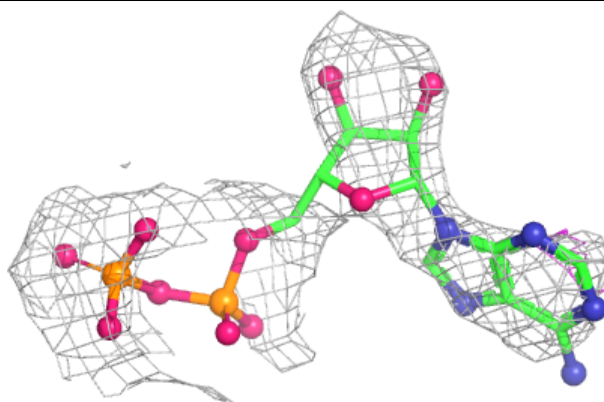
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ADP	A	1305	27/27	0.87	0.10	71,95,107,111	0
2	SO4	B	1301	5/5	0.89	0.09	48,56,63,66	0
2	SO4	A	1301	5/5	0.95	0.07	46,48,54,56	0
2	SO4	A	1302	5/5	0.97	0.05	52,64,65,68	0

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.

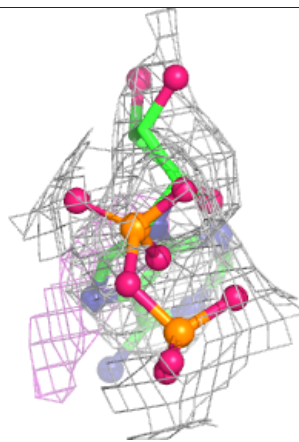
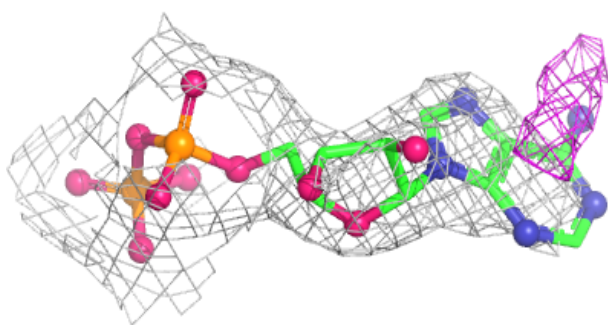
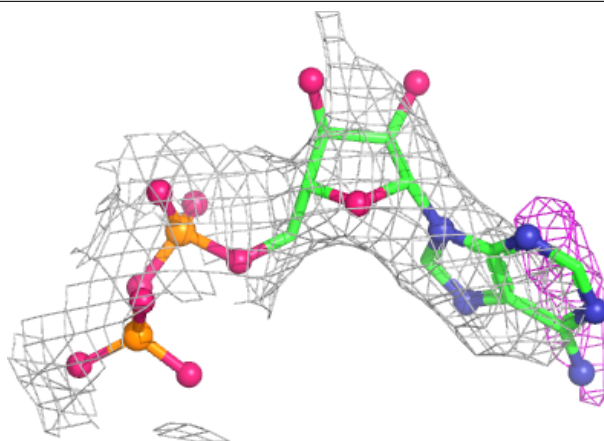
Electron density around ADP B 1302:

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 ADP A 1305:

$2mF_o - DF_c$ (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.