



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:10 PM UTC

PDB ID : 2W03 / pdb_00002w03
Title : Co-complex Structure of Achromobactin Synthetase Protein D (AcsD) with adenosine, sulfate and citrate from Pectobacterium Chrysanthemi
Authors : Schmelz, S.; McMahon, S.A.; Kadi, N.; Song, L.; Oves-Costales, D.; Oke, M.; Liu, H.; Johnson, K.A.; Carter, L.; White, M.F.; Challis, G.L.; Naismith, J.H.
Deposited on : 2008-08-08
Resolution : 2.95 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

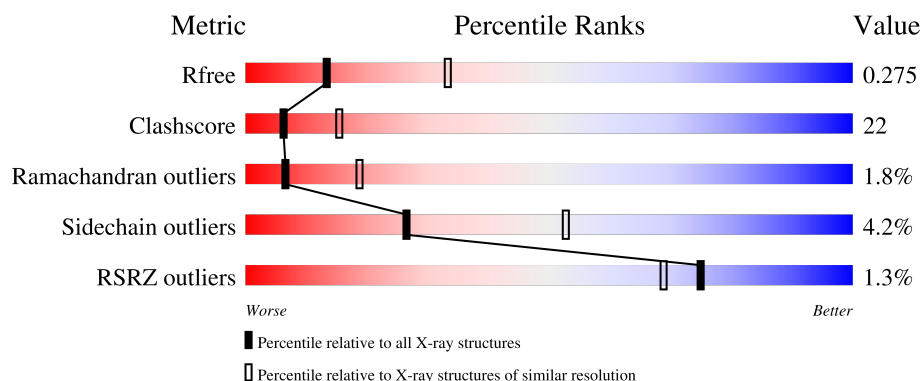
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	620	
1	B	620	

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
3	SO4	B	1589	-	-	X	-

2 Entry composition [i](#)

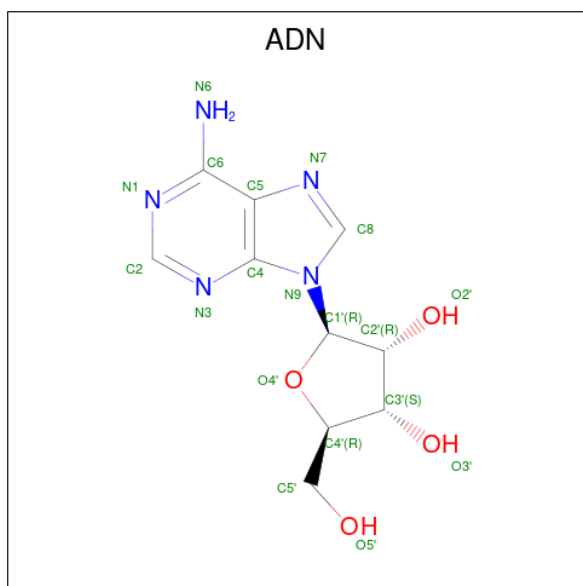
There are 5 unique types of molecules in this entry. The entry contains 9361 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACSD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	0	0	0
			4601	2926	834	821	20			
1	B	577	Total	C	N	O	S	0	0	0
			4626	2940	841	825	20			

- Molecule 2 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



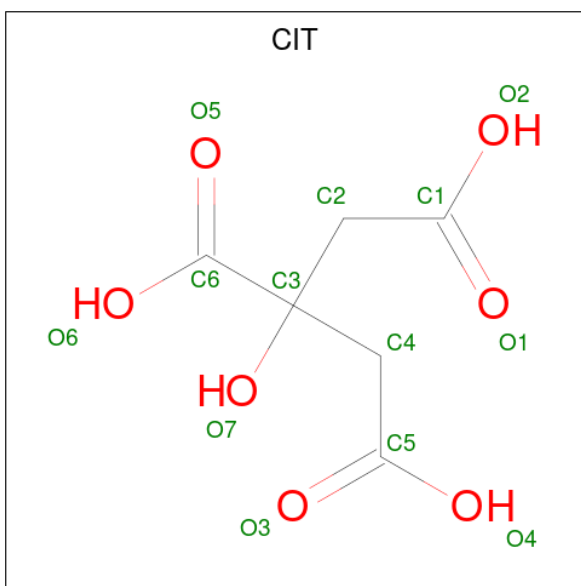
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total 33	O 33	0	0
5	B	40	Total 40	O 40	0	0

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.

Chain A:

ARG	HIS	GLY	GLU	VAL	GLN	HIS	GLY	K545	Q546	E550	L551	D552	A553	L554	V560	A561	C562	K563	T564	N565	L566	V567	V568	R569	L570	A571	ALA	GLU	ALA	ASP	D480	ARG	D481	GLN	D482	A578	V581	R582	L583	V587	GLY	HIS	ALA	VAL	GLN	HIS	GLY	SER	GLU	VAL	GLN	HIS	ASP	VAL	ARG	HIS	GLU	GLU	ALA
W441	E442	L445	Q446	L450	V451	H452	Q453	Q454	Q459	D464	F465	E466	T471	G475	R477	Y478	L479	D480	D481	G482	L483	L492	L394	E496	R501	I502	M503	L506	F507	I508	L511	S512	D420	Q421	Y422	R428	P429	V430	L431	P527	L528	M529	V533	T540	T541	L545	S426	S432	L433	F434	F435	N436	H437	V440					
A351	E354	D356	S357	F360	R361	E362	Q363	T367	L368	R369	A378	E379	R380	S381	A384	G385	T386	L387	F388	V392	D393	L394	Q395	Q399	E408	A409	L410	A414	L415	L416	D420	Q421	Y422	R428	P429	V430	L431	P527	L528	M529	V533	T540	T541	L545	S426	S432	L433	F434	F435	N436	H437	V440							
W181	P182	A183	H184	L185	E193	A196	A199	H201	L200	H201	Q202	F203	E204	V205	T212	G213	A214	L217	T218	T219	V222	G225	F226	Q230	A231	A232	T238	H241	M242	P243	V244	F249	D252	A253	R254	V255	R260	L264	R265	D266	L267	E341	P342	G343	V344	R372													
W181	P182	A183	H184	L185	E193	A196	A199	H201	L200	H201	Q202	F203	E204	V205	T212	G213	A214	L217	T218	T219	V222	G225	F226	Q230	A231	A232	T238	H241	M242	P243	V244	F249	D252	A253	R254	V255	R260	L264	R265	D266	L267	E341	P342	G343	V344	R372													
W181	P182	A183	H184	L185	E193	A196	A199	H201	L200	H201	Q202	F203	E204	V205	T212	G213	A214	L217	T218	T219	V222	G225	F226	Q230	A231	A232	T238	H241	M242	P243	V244	F249	D252	A253	R254	V255	R260	L264	R265	D266	L267	E341	P342	G343	V344	R372													
W181	P182	A183	H184	L185	E193	A196	A199	H201	L200	H201	Q202	F203	E204	V205	T212	G213	A214	L217	T218	T219	V222	G225	F226	Q230	A231	A232	T238	H241	M242	P243	V244	F249	D252	A253	R254	V255	R260	L264	R265	D266	L267	E341	P342	G343	V344	R372													
W181	P182	A183	H184	L185	E193	A196	A199	H201	L200	H201	Q202	F203	E204	V205	T212	G213	A214	L217	T218	T219	V222	G225	F226	Q230	A231	A232	T238	H241	M242	P243	V244	F249	D252	A253	R254	V255	R260	L264	R265	D266	L267	E341	P342	G343	V344	R372													
W181	P182	A183	H184	L185	E193	A196	A199	H201	L200	H201	Q202	F203	E204	V205	T212	G213	A214	L217	T218	T219	V222	G225	F226	Q230	A231	A232	T238	H241	M242	P243	V244	F249	D252	A253	R254	V255	R260	L264	R265	D266	L267	E341	P342	G343	V344	R372													
W181	P182	A183	H184	L185	E193	A196	A199	H201	L200	H201	Q202	F203	E204	V205	T212	G213	A214	L217	T218	T219	V222	G225	F226	Q230	A231	A232	T238	H241	M242	P243	V244	F249	D252	A253	R254	V255	R260	L264	R265	D266	L267	E341	P342	G343	V344	R372													
W181	P182	A183	H184																																																								

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.65Å 69.14Å 94.19Å 95.43° 101.45° 95.06°	Depositor
Resolution (Å)	91.67 – 2.95 91.67 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (91.67-2.95) 98.2 (91.67-2.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.267 0.212 , 0.275	Depositor DCC
R_{free} test set	1474 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9361	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% 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: ADN, SO4, CIT

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	0.89	1/4721 (0.0%)	1.17	16/6415 (0.2%)
1	B	0.91	0/4746	1.15	16/6448 (0.2%)
All	All	0.90	1/9467 (0.0%)	1.16	32/12863 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	3
1	B	0	3
All	All	2	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	THR	CA-CB	6.48	1.64	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ALA	N-CA-C	14.32	130.92	113.16
1	B	481	ASP	CB-CA-C	-9.90	105.15	116.54
1	A	302	ASN	N-CA-C	9.77	121.62	110.97
1	A	481	ASP	N-CA-C	8.71	122.90	111.75
1	A	477	ARG	N-CA-C	8.38	123.06	113.01
1	B	302	ASN	N-CA-C	7.49	119.08	111.07
1	B	288	HIS	N-CA-C	-6.93	98.55	109.50
1	A	482	ASP	N-CA-C	6.89	125.48	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	ASP	N-CA-C	6.52	118.21	108.31
1	A	8	VAL	N-CA-C	-6.50	104.69	111.58
1	B	363	GLN	N-CA-C	-6.34	105.68	113.41
1	B	184	HIS	N-CA-C	-5.93	105.91	113.02
1	A	104	CYS	CA-C-N	5.86	125.82	119.78
1	A	104	CYS	C-N-CA	5.86	125.82	119.78
1	B	263	VAL	N-CA-C	-5.83	103.62	111.44
1	B	62	ILE	CA-C-N	5.66	126.91	119.84
1	B	62	ILE	C-N-CA	5.66	126.91	119.84
1	A	512	SER	CA-C-N	5.63	127.82	120.28
1	A	512	SER	C-N-CA	5.63	127.82	120.28
1	B	568	VAL	CB-CA-C	-5.61	104.70	111.88
1	A	238	ILE	N-CA-C	5.51	115.52	107.37
1	A	354	GLU	N-CA-C	5.48	119.47	112.34
1	B	189	GLN	N-CA-C	-5.45	106.14	112.89
1	A	583	LEU	CA-C-N	5.38	125.38	119.90
1	A	583	LEU	C-N-CA	5.38	125.38	119.90
1	B	255	VAL	N-CA-C	5.33	116.11	110.72
1	B	301	THR	CB-CA-C	-5.30	110.02	117.23
1	B	351	ALA	N-CA-C	5.26	122.00	110.80
1	A	170	HIS	CA-C-N	5.23	125.28	119.32
1	A	170	HIS	C-N-CA	5.23	125.28	119.32
1	B	365	GLY	N-CA-C	5.20	117.44	111.36
1	B	354	GLU	N-CA-C	5.00	121.46	110.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	351	ALA	CA
1	A	482	ASP	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	GLY	Peptide
1	A	300	ILE	Peptide
1	A	480	ASP	Peptide
1	B	268	GLY	Peptide
1	B	327	ASP	Peptide
1	B	97	GLN	Peptide

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	4601	0	4519	183	0
1	B	4626	0	4545	227	0
2	A	19	0	13	0	0
2	B	19	0	13	4	0
3	A	5	0	0	0	0
3	B	5	0	0	2	0
4	B	13	0	5	1	0
5	A	33	0	0	0	0
5	B	40	0	0	5	0
All	All	9361	0	9095	410	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 22.

All (410) 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:124:ARG:CD	1:B:571:ALA:HA	1.67	1.23
1:B:124:ARG:HD3	1:B:571:ALA:CA	1.68	1.23
1:B:563:LYS:NZ	1:B:576:ARG:HH22	1.41	1.15
1:A:303:CYS:SG	1:A:305:ARG:NH2	2.29	1.05
1:B:476:ILE:HD13	1:B:492:LEU:HD13	1.32	1.04
1:B:423:GLN:HE22	1:B:536:GLN:HG3	0.92	1.03
1:B:423:GLN:NE2	1:B:536:GLN:HG3	1.75	1.01
1:B:503:MET:HE3	1:B:561:ALA:H	1.24	0.99
1:B:301:THR:HG21	2:B:1588:ADN:O2'	1.64	0.98
1:B:564:THR:O	1:B:568:VAL:HG23	1.65	0.97
1:B:563:LYS:HZ2	1:B:576:ARG:HH22	1.12	0.94
1:B:563:LYS:NZ	1:B:576:ARG:NH2	2.13	0.94
1:B:29:GLU:OE1	1:B:566:LEU:HB3	1.68	0.94
1:A:134:LEU:O	1:A:138:ARG:HG2	1.73	0.88
1:B:110:LEU:HD12	1:B:114:LEU:HD12	1.56	0.88
1:A:476:ILE:HD12	1:A:479:ILE:HD12	1.55	0.87
1:B:255:VAL:HA	1:B:258:LEU:HD12	1.58	0.86
1:B:425:ARG:HH21	1:B:425:ARG:HG3	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ILE:HG13	1:B:479:ILE:HD12	1.58	0.85
1:B:563:LYS:HZ2	1:B:576:ARG:NH2	1.73	0.85
1:B:136:SER:O	1:B:140:VAL:HG23	1.79	0.83
1:A:303:CYS:SG	1:A:305:ARG:CZ	2.67	0.83
1:B:287:ASP:HA	1:B:374:ARG:HD2	1.61	0.83
1:A:136:SER:O	1:A:140:VAL:HG23	1.80	0.82
1:B:563:LYS:HZ1	1:B:576:ARG:HH22	1.25	0.82
1:B:361:ARG:HD2	5:B:2023:HOH:O	1.81	0.80
1:A:98:ALA:HB3	1:A:100:GLY:HA2	1.63	0.79
1:A:181:TRP:HB2	1:A:182:PRO:HD2	1.64	0.79
1:B:182:PRO:HB2	1:B:184:HIS:CE1	2.18	0.79
1:B:245:GLN:OE1	1:B:296:LEU:HA	1.84	0.77
1:B:14:SER:OG	1:B:137:GLN:NE2	2.16	0.77
1:A:476:ILE:HD12	1:A:479:ILE:CD1	2.15	0.76
1:B:215:ASN:HD21	1:B:320:ARG:HB2	1.51	0.75
1:A:299:ARG:HA	1:A:303:CYS:O	1.86	0.75
1:A:428:ARG:HG2	1:A:540:ILE:HG12	1.68	0.74
1:B:299:ARG:HA	1:B:303:CYS:O	1.86	0.74
1:A:503:MET:HE3	1:A:561:ALA:CB	2.17	0.73
1:B:563:LYS:HZ1	1:B:576:ARG:NH2	1.81	0.73
1:B:444:HIS:HE1	1:B:446:GLN:HB3	1.53	0.72
1:B:164:GLN:OE1	1:B:195:GLN:HA	1.91	0.70
1:B:341:GLU:OE1	1:B:465:PHE:HB2	1.92	0.70
1:A:160:LEU:O	1:A:164:GLN:HG3	1.91	0.70
1:A:252:ASP:OD2	1:A:254:ARG:HB2	1.91	0.70
1:B:185:LEU:HD21	1:B:247:GLN:HG3	1.74	0.70
1:B:182:PRO:CB	1:B:184:HIS:CE1	2.74	0.70
1:B:503:MET:HE3	1:B:561:ALA:N	2.03	0.69
1:B:387:LEU:HD21	1:B:450:LEU:HD22	1.74	0.69
1:B:388:PHE:CE1	1:B:514:THR:HG23	2.26	0.69
1:A:503:MET:HE3	1:A:561:ALA:HB2	1.74	0.69
1:B:299:ARG:HE	1:B:569:ARG:HH22	1.38	0.69
1:B:314:SER:HB2	1:B:491:LEU:HD21	1.74	0.69
1:A:98:ALA:HB3	1:A:100:GLY:CA	2.23	0.69
1:B:167:TRP:O	1:B:177:LYS:HE3	1.93	0.69
1:A:309:TRP:HA	1:A:312:LEU:HD12	1.76	0.68
1:A:313:GLU:CD	1:A:361:ARG:HH22	2.02	0.68
1:A:117:ALA:O	1:A:121:ILE:HD12	1.93	0.68
1:A:204:GLU:HB3	1:A:265:ARG:HB2	1.75	0.68
1:A:280:ILE:HG21	1:A:300:ILE:HD13	1.74	0.68
1:B:23:LEU:O	1:B:27:ILE:HD12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:PRO:CB	1:B:184:HIS:HE1	2.06	0.68
1:B:445:LEU:HD12	2:B:1588:ADN:HN62	1.58	0.68
1:B:476:ILE:CG1	1:B:479:ILE:HD12	2.24	0.67
1:A:297:ASN:ND2	1:A:306:LYS:HB3	2.08	0.67
1:A:508:ILE:HD12	1:A:562:CYS:HB2	1.77	0.67
1:A:134:LEU:HB3	1:A:138:ARG:NH1	2.10	0.67
1:B:301:THR:OG1	1:B:302:ASN:N	2.22	0.67
1:A:408:GLU:HG3	1:A:409:ALA:O	1.95	0.67
1:B:356:ASP:O	1:B:357:SER:C	2.39	0.66
1:B:175:ALA:HB1	1:B:178:ALA:HB2	1.77	0.66
1:B:299:ARG:NE	1:B:569:ARG:HH22	1.94	0.66
1:A:202:GLN:NE2	1:A:271:GLY:HA2	2.11	0.66
1:A:568:VAL:HG21	1:A:578:ALA:HB1	1.78	0.65
1:B:425:ARG:HG3	1:B:425:ARG:NH2	2.09	0.65
1:A:43:ASP:OD1	1:A:44:GLU:N	2.27	0.65
1:B:382:ILE:HD12	1:B:452:HIS:CD2	2.32	0.65
1:A:124:ARG:NH2	1:A:571:ALA:O	2.29	0.65
1:B:9:LEU:O	1:B:13:ILE:HG13	1.97	0.65
1:B:108:GLU:HB3	1:B:109:PRO:HD3	1.79	0.64
1:A:297:ASN:HD21	1:A:306:LYS:HB3	1.63	0.64
1:A:541:GLN:NE2	1:A:552:ASP:OD1	2.31	0.64
1:B:444:HIS:CE1	1:B:446:GLN:HB3	2.32	0.64
1:A:11:ARG:NH1	1:A:15:GLU:OE2	2.31	0.64
1:A:225:GLY:O	1:A:272:ARG:NH2	2.26	0.64
1:A:148:GLY:HA2	1:A:392:VAL:HG11	1.79	0.64
1:A:143:ILE:CD1	1:A:193:GLU:HG3	2.29	0.63
1:A:303:CYS:SG	1:A:305:ARG:NE	2.71	0.63
1:A:380:ARG:O	1:A:452:HIS:HD2	1.80	0.63
1:B:476:ILE:CD1	1:B:479:ILE:HD12	2.29	0.63
1:A:295:SER:HB3	1:A:306:LYS:HA	1.79	0.63
1:B:424:THR:HG22	1:B:428:ARG:HH21	1.63	0.62
1:B:215:ASN:ND2	1:B:320:ARG:HB2	2.13	0.62
1:A:170:HIS:HB3	1:A:173:HIS:HB2	1.81	0.62
1:B:30:PHE:C	1:B:33:PRO:HD2	2.25	0.61
1:B:110:LEU:CD1	1:B:114:LEU:HD12	2.29	0.61
1:B:86:SER:OG	1:B:512:SER:HB2	2.00	0.61
1:A:464:ASP:OD2	1:A:466:GLU:HB3	2.00	0.61
1:A:170:HIS:HB3	1:A:173:HIS:CB	2.31	0.61
1:B:281:ARG:HD3	1:B:294:GLY:O	2.01	0.61
1:A:280:ILE:HG21	1:A:300:ILE:CD1	2.30	0.60
1:B:303:CYS:H	1:B:305:ARG:HH11	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:GLN:HE22	1:B:536:GLN:CG	1.88	0.60
1:A:143:ILE:HD13	1:A:193:GLU:HG3	1.82	0.60
1:B:357:SER:O	1:B:361:ARG:HG3	2.02	0.60
1:A:380:ARG:HG2	1:A:452:HIS:O	2.00	0.60
1:B:129:LEU:O	1:B:133:ILE:HG13	2.01	0.60
1:B:541:GLN:HA	1:B:544:LEU:HD12	1.83	0.60
1:A:180:LEU:O	1:A:298:VAL:HG13	2.01	0.59
1:B:476:ILE:CD1	1:B:479:ILE:CD1	2.80	0.59
1:B:480:ASP:OD1	1:B:480:ASP:O	2.20	0.59
1:A:430:VAL:HG21	1:A:506:LEU:HD21	1.84	0.59
1:B:424:THR:HG22	1:B:428:ARG:NH2	2.18	0.59
1:A:337:VAL:HG21	1:A:459:GLN:OE1	2.03	0.59
1:A:356:ASP:O	1:A:357:SER:C	2.44	0.59
1:B:182:PRO:HB3	1:B:184:HIS:HE1	1.67	0.58
1:A:388:PHE:CZ	1:A:514:THR:HG23	2.38	0.58
1:B:252:ASP:HB3	1:B:255:VAL:HG23	1.85	0.58
1:A:68:LEU:HD12	1:A:72:LEU:CD2	2.33	0.58
1:A:380:ARG:O	1:A:452:HIS:CD2	2.56	0.58
1:A:428:ARG:O	1:A:432:SER:OG	2.20	0.58
1:B:233:SER:O	1:B:236:HIS:HB2	2.03	0.58
1:B:424:THR:CG2	1:B:428:ARG:HH21	2.17	0.58
1:A:222:VAL:HG12	1:A:226:PHE:HE2	1.68	0.58
1:B:308:ALA:HA	1:B:362:GLU:OE2	2.04	0.58
1:B:406:TYR:HB2	1:B:410:LEU:HD11	1.86	0.58
1:A:173:HIS:O	1:A:176:PRO:HD3	2.03	0.57
1:A:26:LEU:HD22	1:A:114:LEU:HD22	1.87	0.57
1:B:388:PHE:CZ	1:B:514:THR:HG23	2.39	0.57
1:B:19:LEU:HD13	1:B:19:LEU:C	2.30	0.57
1:B:94:TYR:CE1	1:B:104:CYS:HB2	2.40	0.57
1:B:98:ALA:HA	1:B:100:GLY:N	2.19	0.57
1:A:249:PHE:O	1:A:255:VAL:HG21	2.04	0.56
1:A:332:THR:HB	1:A:436:ASN:HD22	1.70	0.56
1:B:29:GLU:HG2	1:B:564:THR:HB	1.87	0.56
1:A:481:ASP:O	1:A:483:ILE:N	2.36	0.56
1:A:181:TRP:HB2	1:A:182:PRO:CD	2.36	0.56
1:B:151:ARG:HG2	1:B:153:ASP:OD1	2.05	0.56
1:A:241:MET:HE1	1:A:249:PHE:CD1	2.40	0.56
1:A:503:MET:HG2	1:A:560:VAL:HG13	1.88	0.56
1:B:55:ASP:OD1	1:B:55:ASP:C	2.48	0.56
1:B:110:LEU:HD12	1:B:114:LEU:CD1	2.33	0.56
1:B:157:GLN:HA	1:B:157:GLN:OE1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HD11	1:B:58:ASP:HA	1.87	0.55
1:B:293:LYS:HE3	3:B:1589:SO4:O2	2.07	0.55
1:A:503:MET:CG	1:A:560:VAL:HG13	2.36	0.55
1:A:200:LEU:HD21	1:A:283:TRP:CD2	2.41	0.55
1:B:60:LYS:O	1:B:90:LEU:HD12	2.07	0.55
1:B:140:VAL:HG22	1:B:177:LYS:HG3	1.88	0.55
1:A:381:SER:HA	1:A:450:LEU:O	2.07	0.55
1:B:433:LEU:HD22	1:B:439:VAL:HB	1.89	0.55
1:B:324:GLN:O	1:B:328:GLN:HB3	2.07	0.54
1:B:481:ASP:O	1:B:483:ILE:N	2.38	0.54
1:A:354:GLU:HA	1:A:357:SER:HB3	1.89	0.54
1:B:179:ARG:C	1:B:180:LEU:HG	2.31	0.54
1:B:182:PRO:HB3	1:B:184:HIS:CE1	2.43	0.54
1:B:278:ALA:HB3	1:B:383:MET:HE1	1.89	0.54
1:A:169:GLY:O	1:A:171:PRO:HD3	2.08	0.54
1:A:314:SER:O	1:A:318:ILE:HG12	2.08	0.54
1:B:301:THR:CG2	2:B:1588:ADN:O2'	2.47	0.54
1:A:79:ASP:HB3	1:A:90:LEU:HD11	1.89	0.54
1:B:201:HIS:HA	1:B:269:GLN:HA	1.90	0.54
1:B:266:ASP:OD1	1:B:267:LEU:O	2.25	0.54
1:B:385:GLY:HA2	1:B:445:LEU:HB3	1.89	0.54
1:B:7:ASP:HA	1:B:10:SER:OG	2.07	0.54
1:B:143:ILE:HG23	1:B:193:GLU:HB3	1.90	0.53
1:B:75:PHE:HB2	1:B:102:TRP:CH2	2.43	0.53
1:A:568:VAL:HG21	1:A:578:ALA:CB	2.38	0.53
1:B:98:ALA:HA	1:B:100:GLY:CA	2.37	0.53
1:B:249:PHE:CE1	1:B:255:VAL:HG11	2.44	0.53
1:B:226:PHE:CZ	1:B:345:VAL:HG12	2.44	0.53
1:B:15:GLU:HG2	1:B:107:PHE:CG	2.44	0.53
1:B:224:ASP:OD1	1:B:229:GLN:HB2	2.08	0.53
1:A:226:PHE:CZ	1:A:368:LEU:HG	2.44	0.53
1:B:387:LEU:CD2	1:B:450:LEU:HD22	2.38	0.53
1:A:321:LEU:CD1	1:A:478:TYR:HB3	2.39	0.53
1:A:336:LEU:HD22	1:A:433:LEU:HD11	1.90	0.53
1:B:341:GLU:HB2	1:B:465:PHE:CD2	2.44	0.53
1:A:309:TRP:O	1:A:312:LEU:HB2	2.09	0.53
1:B:503:MET:CE	1:B:561:ALA:H	2.11	0.53
1:B:299:ARG:NE	1:B:569:ARG:NH2	2.57	0.53
1:B:340:ALA:O	1:B:369:ARG:HG3	2.09	0.53
1:A:279:SER:HB3	1:A:446:GLN:NE2	2.24	0.52
1:B:111:VAL:O	1:B:112:ALA:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:LEU:O	1:B:511:LEU:HD12	2.08	0.52
1:A:385:GLY:HA2	1:A:445:LEU:HB3	1.91	0.52
1:B:173:HIS:ND1	1:B:174:PRO:HD2	2.24	0.52
1:B:376:THR:O	1:B:380:ARG:NH1	2.43	0.52
1:A:25:CYS:SG	1:A:174:PRO:HD3	2.50	0.52
1:A:324:GLN:O	1:A:328:GLN:HB2	2.08	0.52
1:A:511:LEU:O	1:A:512:SER:C	2.51	0.52
1:B:124:ARG:NH1	1:B:571:ALA:O	2.43	0.52
1:B:55:ASP:OD1	1:B:57:ALA:N	2.37	0.52
1:A:74:LEU:C	1:A:74:LEU:HD23	2.35	0.51
1:A:212:ILE:HG21	1:A:219:PRO:HA	1.92	0.51
1:B:526:ALA:HB3	1:B:527:PRO:CD	2.40	0.51
1:A:266:ASP:OD1	1:A:267:LEU:O	2.29	0.51
1:B:503:MET:HE2	1:B:561:ALA:CB	2.40	0.51
1:B:110:LEU:CD1	1:B:114:LEU:CD1	2.89	0.51
1:A:119:GLU:HG2	1:A:125:LYS:HA	1.91	0.51
1:A:290:TYR:HB2	1:A:368:LEU:HD22	1.92	0.51
1:B:446:GLN:HG3	2:B:1588:ADN:O4'	2.11	0.51
1:B:551:LEU:O	1:B:555:ILE:HG13	2.10	0.51
1:B:19:LEU:HD13	1:B:19:LEU:O	2.11	0.51
1:B:30:PHE:O	1:B:33:PRO:HD2	2.11	0.51
1:B:245:GLN:OE1	1:B:297:ASN:N	2.41	0.50
1:A:434:PHE:CD2	1:A:440:VAL:HG22	2.47	0.50
1:B:508:ILE:HG21	1:B:562:CYS:SG	2.51	0.50
1:A:11:ARG:HG2	1:A:15:GLU:OE2	2.12	0.50
1:A:230:GLN:O	1:A:232:ALA:N	2.44	0.50
1:A:437:HIS:O	1:A:475:GLY:HA2	2.12	0.50
1:B:474:LEU:O	1:B:477:ARG:HG2	2.12	0.50
1:B:124:ARG:HD3	1:B:571:ALA:HA	0.74	0.49
1:B:249:PHE:O	1:B:255:VAL:HG21	2.13	0.49
1:A:184:HIS:CE1	1:A:185:LEU:CD2	2.95	0.49
1:A:242:HIS:ND1	1:A:244:VAL:HB	2.27	0.49
1:A:170:HIS:H	1:A:176:PRO:HB3	1.78	0.49
1:A:554:LEU:HD11	1:A:560:VAL:HG22	1.93	0.49
1:A:199:ALA:HA	1:A:273:VAL:HA	1.94	0.49
1:A:205:VAL:HG12	1:A:264:ILE:CG2	2.42	0.49
1:A:49:PRO:O	1:A:50:PRO:C	2.56	0.49
1:A:387:LEU:HD21	1:A:450:LEU:HD22	1.94	0.49
1:A:242:HIS:CE1	1:A:244:VAL:HB	2.47	0.49
1:B:576:ARG:HD2	1:B:577:GLN:H	1.76	0.49
1:A:284:PHE:CE1	1:A:286:ASP:OD1	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:GLU:HG3	1:B:501:ARG:HD3	1.95	0.49
1:A:526:ALA:HB3	1:A:527:PRO:HD3	1.95	0.49
1:B:401:PHE:CD2	1:B:402:LEU:HD23	2.48	0.49
1:A:50:PRO:HA	1:A:53:TYR:CE1	2.48	0.48
1:B:472:ASP:OD2	1:B:494:SER:HA	2.13	0.48
1:B:568:VAL:O	1:B:571:ALA:HB3	2.13	0.48
1:A:11:ARG:O	1:A:15:GLU:HG3	2.14	0.48
1:A:202:GLN:NE2	1:A:271:GLY:CA	2.76	0.48
1:B:541:GLN:NE2	1:B:552:ASP:OD1	2.46	0.48
1:B:272:ARG:HD3	1:B:285:ILE:HD13	1.96	0.48
1:B:511:LEU:O	1:B:512:SER:C	2.56	0.48
1:A:24:ASN:O	1:A:28:LYS:HD2	2.13	0.48
1:A:318:ILE:O	1:A:322:PHE:HD2	1.96	0.48
1:B:360:PHE:C	1:B:362:GLU:N	2.71	0.48
1:A:126:ASN:OD1	1:A:128:GLU:HB2	2.13	0.48
1:B:129:LEU:O	1:B:129:LEU:HD12	2.12	0.48
1:A:428:ARG:HG3	1:A:540:ILE:HD11	1.96	0.48
1:B:476:ILE:HD11	1:B:479:ILE:CD1	2.43	0.48
1:B:74:LEU:C	1:B:74:LEU:HD23	2.39	0.48
1:B:337:VAL:HG21	1:B:459:GLN:HG2	1.95	0.48
1:A:260:ARG:O	1:A:260:ARG:HG2	2.13	0.48
1:A:79:ASP:CB	1:A:90:LEU:HD11	2.43	0.47
1:A:564:THR:HG21	1:A:581:VAL:HG13	1.95	0.47
1:B:547:PRO:O	5:B:2037:HOH:O	2.20	0.47
1:A:111:VAL:O	1:A:112:ALA:C	2.57	0.47
1:B:489:GLN:O	1:B:489:GLN:HG3	2.13	0.47
1:A:503:MET:HE3	1:A:561:ALA:HB3	1.94	0.47
1:A:503:MET:HG2	1:A:560:VAL:CG1	2.45	0.47
1:B:170:HIS:ND1	1:B:171:PRO:HD2	2.29	0.47
1:B:228:ASP:O	1:B:231:PRO:HD2	2.14	0.47
1:A:515:ILE:HG22	1:A:516:LEU:N	2.30	0.47
1:B:226:PHE:CE2	1:B:368:LEU:HG	2.49	0.47
1:B:577:GLN:NE2	5:B:2039:HOH:O	2.46	0.47
1:A:134:LEU:HB3	1:A:138:ARG:HH12	1.79	0.47
1:A:393:ASP:OD1	1:A:395:GLN:HB2	2.15	0.47
1:A:526:ALA:HB3	1:A:527:PRO:CD	2.44	0.47
1:B:299:ARG:C	1:B:300:ILE:HG12	2.39	0.47
1:A:218:THR:O	1:A:219:PRO:C	2.56	0.47
1:B:170:HIS:HB3	1:B:173:HIS:HB3	1.97	0.47
1:B:303:CYS:H	1:B:305:ARG:NH1	2.12	0.47
1:B:321:LEU:HD13	1:B:478:TYR:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:THR:HG22	1:A:495:ARG:HA	1.96	0.46
1:B:246:ALA:O	1:B:250:MET:HE2	2.14	0.46
1:A:196:ALA:O	1:A:276:PRO:HD2	2.15	0.46
1:B:68:LEU:O	1:B:70:ASP:N	2.49	0.46
1:B:97:GLN:O	1:B:98:ALA:HB3	2.16	0.46
1:B:576:ARG:CD	1:B:577:GLN:H	2.29	0.46
1:A:281:ARG:NH1	1:A:293:LYS:HE2	2.31	0.45
1:A:122:ALA:HB3	1:A:570:LEU:HD23	1.98	0.45
1:A:154:ALA:N	1:A:155:PRO:HD2	2.32	0.45
1:A:422:TYR:HE2	1:A:450:LEU:HD13	1.81	0.45
1:B:258:LEU:HB3	1:B:264:ILE:HG12	1.98	0.45
1:B:503:MET:HE2	1:B:561:ALA:HB3	1.98	0.45
1:B:122:ALA:C	1:B:124:ARG:H	2.24	0.45
1:B:208:ASP:HB3	1:B:350:ALA:HB2	1.98	0.45
1:B:256:GLN:HB3	1:B:260:ARG:HH22	1.82	0.45
1:A:214:ALA:HB2	1:A:222:VAL:HG21	1.99	0.45
1:B:116:ALA:HA	1:B:119:GLU:OE1	2.15	0.45
1:A:184:HIS:CE1	1:A:185:LEU:HD23	2.51	0.45
1:A:143:ILE:O	1:A:147:ASN:ND2	2.42	0.45
1:B:32:ILE:N	1:B:33:PRO:CD	2.80	0.45
1:B:416:LEU:HD11	1:B:528:LEU:HD13	1.97	0.45
1:A:30:PHE:C	1:A:33:PRO:HD2	2.41	0.45
1:A:25:CYS:HB3	1:A:566:LEU:HD23	1.98	0.45
1:B:382:ILE:HD12	1:B:452:HIS:HD2	1.81	0.45
1:B:430:VAL:HG21	1:B:443:PRO:HG3	1.98	0.45
1:A:111:VAL:HG11	1:A:133:ILE:HG21	1.99	0.44
1:B:15:GLU:O	1:B:19:LEU:HB2	2.15	0.44
1:B:106:ASP:C	1:B:109:PRO:HD2	2.42	0.44
1:A:159:TYR:O	1:A:162:SER:OG	2.32	0.44
1:B:170:HIS:CG	1:B:173:HIS:HB2	2.52	0.44
1:A:166:LEU:O	1:A:177:LYS:NZ	2.30	0.44
1:A:321:LEU:O	1:A:325:LEU:HD12	2.17	0.44
1:B:306:LYS:HD3	1:B:362:GLU:HG2	2.00	0.44
1:A:416:LEU:O	1:A:420:ASP:HB2	2.17	0.44
1:B:525:LEU:HD23	1:B:525:LEU:HA	1.59	0.44
1:B:576:ARG:CD	1:B:577:GLN:N	2.80	0.44
1:A:30:PHE:HD1	1:A:121:ILE:HG21	1.83	0.44
1:A:529:MET:O	1:A:533:VAL:HG23	2.18	0.44
1:B:134:LEU:O	1:B:138:ARG:HG3	2.16	0.44
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.82	0.44
1:B:107:PHE:CE2	1:B:137:GLN:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:ARG:CG	1:B:577:GLN:N	2.80	0.44
1:A:37:LEU:HD11	1:A:64:MET:HE2	2.00	0.44
1:A:199:ALA:HA	1:A:272:ARG:O	2.17	0.44
1:A:230:GLN:HB3	1:A:231:PRO:HD3	1.99	0.44
1:B:416:LEU:O	1:B:420:ASP:HB2	2.17	0.44
1:B:496:GLU:O	1:B:500:ASN:OD1	2.35	0.44
1:B:147:ASN:CG	1:B:167:TRP:CZ3	2.96	0.44
1:B:261:ASP:O	1:B:262:ASN:C	2.60	0.44
1:A:7:ASP:HA	1:A:10:SER:HB2	1.99	0.43
1:A:307:ASN:O	1:A:362:GLU:HB2	2.18	0.43
1:B:153:ASP:OD1	1:B:153:ASP:N	2.50	0.43
1:B:428:ARG:O	1:B:432:SER:OG	2.25	0.43
1:A:399:GLN:NE2	1:A:517:ALA:O	2.52	0.43
1:A:545:LYS:C	1:A:546:GLN:HG2	2.43	0.43
1:B:412:ASP:OD1	1:B:522:ARG:NH1	2.52	0.43
1:A:79:ASP:O	1:A:80:ARG:HB3	2.18	0.43
1:A:70:ASP:O	1:A:71:GLN:HB2	2.17	0.43
1:A:293:LYS:HB3	1:A:367:ILE:HB	2.00	0.43
1:B:346:SER:HB2	1:B:361:ARG:HA	2.00	0.43
1:A:193:GLU:H	1:A:193:GLU:CD	2.26	0.43
1:A:315:THR:HG23	1:A:341:GLU:OE1	2.19	0.43
1:A:453:GLN:O	1:A:454:GLN:HG3	2.18	0.43
1:B:36:TYR:HB3	1:B:67:GLY:O	2.18	0.43
1:B:360:PHE:C	1:B:362:GLU:H	2.26	0.43
1:B:401:PHE:HD2	1:B:402:LEU:HD23	1.84	0.43
1:A:37:LEU:C	1:A:37:LEU:HD23	2.43	0.43
1:B:329:HIS:O	1:B:333:LEU:HG	2.19	0.43
1:B:331:ASP:OD1	1:B:331:ASP:N	2.51	0.43
1:A:55:ASP:OD1	1:A:55:ASP:C	2.62	0.43
1:A:122:ALA:CB	1:A:570:LEU:HD23	2.49	0.43
1:B:23:LEU:C	1:B:27:ILE:HD12	2.43	0.43
1:A:345:VAL:O	1:A:345:VAL:HG13	2.18	0.42
1:A:422:TYR:CE2	1:A:450:LEU:HD13	2.54	0.42
1:A:515:ILE:O	1:A:516:LEU:C	2.62	0.42
1:A:309:TRP:CE2	1:A:358:HIS:CE1	3.07	0.42
1:A:410:LEU:HB3	1:A:414:ALA:HB3	2.01	0.42
1:A:550:GLU:CD	1:A:550:GLU:H	2.27	0.42
1:A:385:GLY:CA	1:A:445:LEU:HB3	2.49	0.42
1:B:40:GLU:O	1:B:65:MET:HG3	2.19	0.42
1:B:45:MET:O	1:B:46:LYS:C	2.62	0.42
1:B:82:ASP:OD2	1:B:86:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:THR:HB	1:B:584:PRO:O	2.19	0.42
1:B:245:GLN:OE1	1:B:296:LEU:CA	2.62	0.42
1:B:380:ARG:HG2	5:B:2029:HOH:O	2.19	0.42
1:A:32:ILE:N	1:A:33:PRO:CD	2.83	0.42
1:A:291:PHE:HB2	1:A:369:ARG:HB3	2.02	0.42
1:A:476:ILE:CD1	1:A:479:ILE:CD1	2.93	0.42
1:B:541:GLN:HA	1:B:544:LEU:CD1	2.47	0.42
1:A:230:GLN:C	1:A:232:ALA:H	2.28	0.42
1:B:49:PRO:O	1:B:50:PRO:C	2.59	0.42
1:B:438:GLY:HA3	1:B:475:GLY:H	1.85	0.42
1:B:381:SER:HA	1:B:450:LEU:O	2.20	0.42
1:B:501:ARG:O	1:B:502:ILE:C	2.60	0.42
4:B:1590:CIT:O1	4:B:1590:CIT:H41	2.19	0.42
1:A:313:GLU:O	1:A:316:VAL:HB	2.19	0.42
1:B:128:GLU:HG3	1:B:132:GLN:NE2	2.35	0.42
1:B:146:HIS:HD2	1:B:147:ASN:ND2	2.18	0.42
1:B:130:TYR:CE2	1:B:134:LEU:HD11	2.54	0.42
1:A:299:ARG:HB2	1:A:299:ARG:NH1	2.35	0.41
1:B:564:THR:CG2	1:B:581:VAL:HG22	2.50	0.41
1:A:213:GLY:O	1:A:343:GLY:HA2	2.20	0.41
1:A:359:TRP:O	1:A:363:GLN:HG2	2.20	0.41
1:B:218:THR:O	1:B:219:PRO:C	2.61	0.41
1:B:437:HIS:O	1:B:475:GLY:HA2	2.19	0.41
1:A:386:THR:O	1:A:387:LEU:C	2.63	0.41
1:B:16:LYS:HE3	1:B:20:HIS:CE1	2.55	0.41
1:B:119:GLU:HG2	1:B:125:LYS:HA	2.02	0.41
1:B:360:PHE:O	1:B:362:GLU:N	2.53	0.41
1:A:201:HIS:HA	1:A:269:GLN:HA	2.03	0.41
1:B:129:LEU:HD22	1:B:569:ARG:HB2	2.01	0.41
1:B:251:GLN:NE2	5:B:2015:HOH:O	2.38	0.41
1:A:318:ILE:HG23	1:A:322:PHE:HE2	1.86	0.41
1:B:503:MET:CE	1:B:561:ALA:CB	2.98	0.41
1:A:318:ILE:CG2	1:A:322:PHE:CE2	3.04	0.41
1:B:463:ARG:O	1:B:464:ASP:CB	2.69	0.41
1:A:508:ILE:HD13	1:A:583:LEU:HD12	2.03	0.41
1:A:104:CYS:HA	1:A:105:PRO:HD2	1.90	0.41
1:A:109:PRO:O	1:A:113:ARG:HB2	2.20	0.41
1:A:476:ILE:HD13	1:A:492:LEU:HD13	2.01	0.41
1:B:230:GLN:O	1:B:232:ALA:N	2.54	0.41
1:B:293:LYS:HB3	1:B:367:ILE:HB	2.01	0.41
1:B:433:LEU:HD22	1:B:439:VAL:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:HG3	1:A:46:LYS:H	1.86	0.41
1:A:69:PRO:HD2	1:A:121:ILE:HD11	2.02	0.41
1:B:27:ILE:HA	1:B:31:ALA:HB3	2.03	0.41
1:B:349:PRO:O	1:B:350:ALA:C	2.64	0.41
1:B:442:GLU:HG3	1:B:501:ARG:HH11	1.86	0.41
1:B:199:ALA:HA	1:B:273:VAL:HA	2.02	0.41
1:A:182:PRO:HB3	1:A:184:HIS:ND1	2.36	0.40
1:A:541:GLN:HB2	1:A:551:LEU:CD2	2.51	0.40
1:B:154:ALA:N	1:B:155:PRO:CD	2.84	0.40
1:B:534:GLN:NE2	1:B:555:ILE:O	2.54	0.40
1:A:267:LEU:H	1:A:267:LEU:HG	1.61	0.40
1:A:321:LEU:HD11	1:A:478:TYR:CB	2.51	0.40
1:A:384:ALA:O	1:A:387:LEU:N	2.54	0.40
1:B:232:ALA:HB2	1:B:238:ILE:HG13	2.03	0.40
1:B:435:PHE:HB2	1:B:544:LEU:HD22	2.03	0.40
1:B:534:GLN:HG3	1:B:587:TRP:CE2	2.56	0.40
1:A:321:LEU:HD11	1:A:478:TYR:HB3	2.04	0.40
1:B:369:ARG:NH2	3:B:1589:SO4:O2	2.53	0.40
1:A:133:ILE:HG12	1:A:174:PRO:O	2.22	0.40
1:A:442:GLU:HG3	1:A:501:ARG:HH11	1.86	0.40
1:B:78:VAL:HG11	1:B:87:GLN:HG3	2.02	0.40
1:B:141:SER:O	1:B:142:ALA:C	2.64	0.40
1:B:360:PHE:O	1:B:361:ARG:C	2.64	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	568/620 (92%)	501 (88%)	59 (10%)	8 (1%)	9	24
1	B	571/620 (92%)	494 (86%)	65 (11%)	12 (2%)	5	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1139/1240 (92%)	995 (87%)	124 (11%)	20 (2%)	6	19

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	ASP
1	B	351	ALA
1	B	482	ASP
1	A	464	ASP
1	A	515	ILE
1	A	516	LEU
1	B	141	SER
1	B	464	ASP
1	B	516	LEU
1	A	378	ALA
1	B	142	ALA
1	B	228	ASP
1	B	399	GLN
1	B	556	ALA
1	A	316	VAL
1	A	231	PRO
1	B	123	GLY
1	B	231	PRO
1	B	515	ILE
1	A	123	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	485/522 (93%)	467 (96%)	18 (4%)	30	55
1	B	487/522 (93%)	464 (95%)	23 (5%)	23	49
All	All	972/1044 (93%)	931 (96%)	41 (4%)	26	53

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	70	ASP
1	A	113	ARG
1	A	150	GLN
1	A	180	LEU
1	A	193	GLU
1	A	217	LEU
1	A	254	ARG
1	A	260	ARG
1	A	281	ARG
1	A	286	ASP
1	A	305	ARG
1	A	477	ARG
1	A	480	ASP
1	A	483	ILE
1	A	496	GLU
1	A	508	ILE
1	A	568	VAL
1	B	8	VAL
1	B	114	LEU
1	B	115	LEU
1	B	146	HIS
1	B	180	LEU
1	B	230	GLN
1	B	255	VAL
1	B	265	ARG
1	B	272	ARG
1	B	280	ILE
1	B	300	ILE
1	B	362	GLU
1	B	383	MET
1	B	392	VAL
1	B	474	LEU
1	B	481	ASP
1	B	540	ILE
1	B	541	GLN
1	B	548	SER
1	B	569	ARG
1	B	570	LEU
1	B	576	ARG
1	B	582	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	87	GLN
1	A	97	GLN
1	A	132	GLN
1	A	195	GLN
1	A	220	GLN
1	A	395	GLN
1	B	20	HIS
1	B	87	GLN
1	B	132	GLN
1	B	137	GLN
1	B	187	GLN
1	B	256	GLN
1	B	269	GLN
1	B	288	HIS
1	B	302	ASN
1	B	307	ASN
1	B	329	HIS
1	B	405	HIS
1	B	423	GLN
1	B	577	GLN

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 oligosaccharides 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
3	SO4	A	1589	-	4,4,4	0.33	0	6,6,6	0.56	0
2	ADN	B	1588	-	21,21,21	1.25	3 (14%)	31,31,31	2.00	7 (22%)
4	CIT	B	1590	-	12,12,12	1.32	1 (8%)	17,17,17	1.73	4 (23%)
3	SO4	B	1589	-	4,4,4	0.43	0	6,6,6	0.54	0
2	ADN	A	1588	-	21,21,21	1.30	3 (14%)	31,31,31	2.02	7 (22%)

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	ADN	B	1588	-	-	2/6/22/22	0/3/3/3
4	CIT	B	1590	-	-	8/16/16/16	-
2	ADN	A	1588	-	-	3/6/22/22	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1588	ADN	C5-N7	-3.60	1.32	1.39
2	A	1588	ADN	C5-N7	-3.21	1.33	1.39
2	B	1588	ADN	C8-N9	-2.53	1.33	1.37
2	A	1588	ADN	C1'-N9	2.23	1.52	1.46
2	A	1588	ADN	C8-N9	-2.15	1.33	1.37
2	B	1588	ADN	C1'-N9	2.05	1.52	1.46
4	B	1590	CIT	O7-C3	2.02	1.47	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1588	ADN	C5-C4-N3	-5.87	118.63	126.72
2	B	1588	ADN	C5-C4-N3	-5.51	119.12	126.72
2	A	1588	ADN	N3-C2-N1	-4.35	122.00	128.58
2	B	1588	ADN	N3-C4-N9	4.29	134.46	127.17
2	A	1588	ADN	N3-C4-N9	4.11	134.16	127.17
2	B	1588	ADN	N3-C2-N1	-4.11	122.36	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1588	ADN	C2-N3-C4	3.65	120.73	111.83
4	B	1590	CIT	O6-C6-C3	3.54	119.93	113.14
2	B	1588	ADN	C2-N3-C4	3.29	119.87	111.83
2	A	1588	ADN	C5-N7-C8	2.90	108.00	103.45
4	B	1590	CIT	O7-C3-C6	-2.77	105.03	108.96
2	A	1588	ADN	N9-C8-N7	-2.77	110.01	113.94
2	B	1588	ADN	C5-N7-C8	2.73	107.74	103.45
2	A	1588	ADN	C4-C5-N7	-2.72	107.48	110.58
2	B	1588	ADN	N9-C8-N7	-2.70	110.11	113.94
4	B	1590	CIT	O4-C5-O3	-2.33	117.34	123.33
2	B	1588	ADN	C4-C5-N7	-2.24	108.02	110.58
4	B	1590	CIT	O2-C1-O1	-2.15	117.81	123.33

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1590	CIT	C2-C3-C4-C5
4	B	1590	CIT	O7-C3-C4-C5
4	B	1590	CIT	C6-C3-C4-C5
4	B	1590	CIT	C2-C3-C6-O5
4	B	1590	CIT	C2-C3-C6-O6
4	B	1590	CIT	O7-C3-C6-O5
4	B	1590	CIT	O7-C3-C6-O6
2	B	1588	ADN	O4'-C4'-C5'-O5'
2	A	1588	ADN	C3'-C4'-C5'-O5'
2	B	1588	ADN	C3'-C4'-C5'-O5'
2	A	1588	ADN	O4'-C4'-C5'-O5'
4	B	1590	CIT	C1-C2-C3-O7
2	A	1588	ADN	O4'-C1'-N9-C8

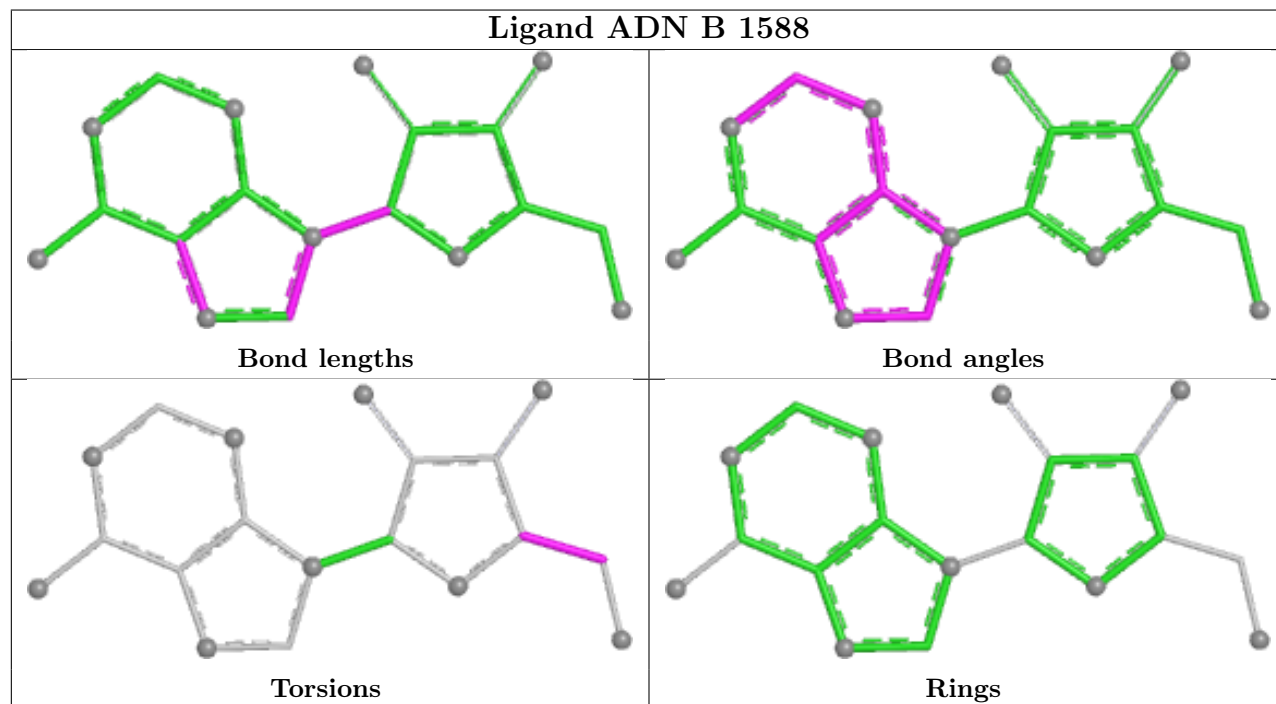
There are no ring outliers.

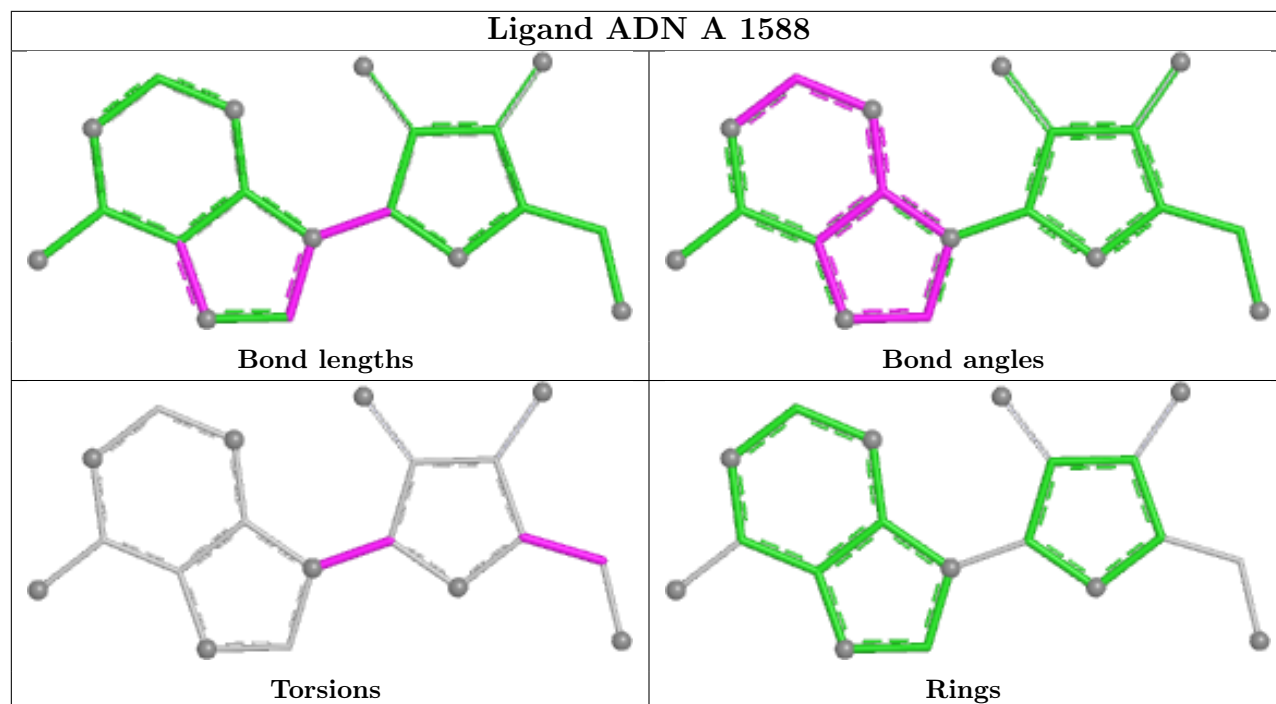
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1588	ADN	4	0
4	B	1590	CIT	1	0
3	B	1589	SO4	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	574/620 (92%)	-0.14	6 (1%) 79 74	8, 20, 31, 38	0
1	B	577/620 (93%)	-0.03	9 (1%) 70 63	6, 20, 31, 46	2 (0%)
All	All	1151/1240 (92%)	-0.08	15 (1%) 75 69	6, 20, 31, 46	2 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	571	ALA	6.3
1	B	304	VAL	5.9
1	B	144	VAL	5.4
1	A	571	ALA	4.5
1	A	482	ASP	4.2
1	B	69	PRO	3.4
1	A	69	PRO	3.0
1	A	98	ALA	2.7
1	A	135	GLN	2.4
1	B	417	TYR	2.3
1	B	127	PRO	2.3
1	A	480	ASP	2.2
1	B	581	VAL	2.1
1	B	481	ASP	2.1
1	B	98	ALA	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](#)

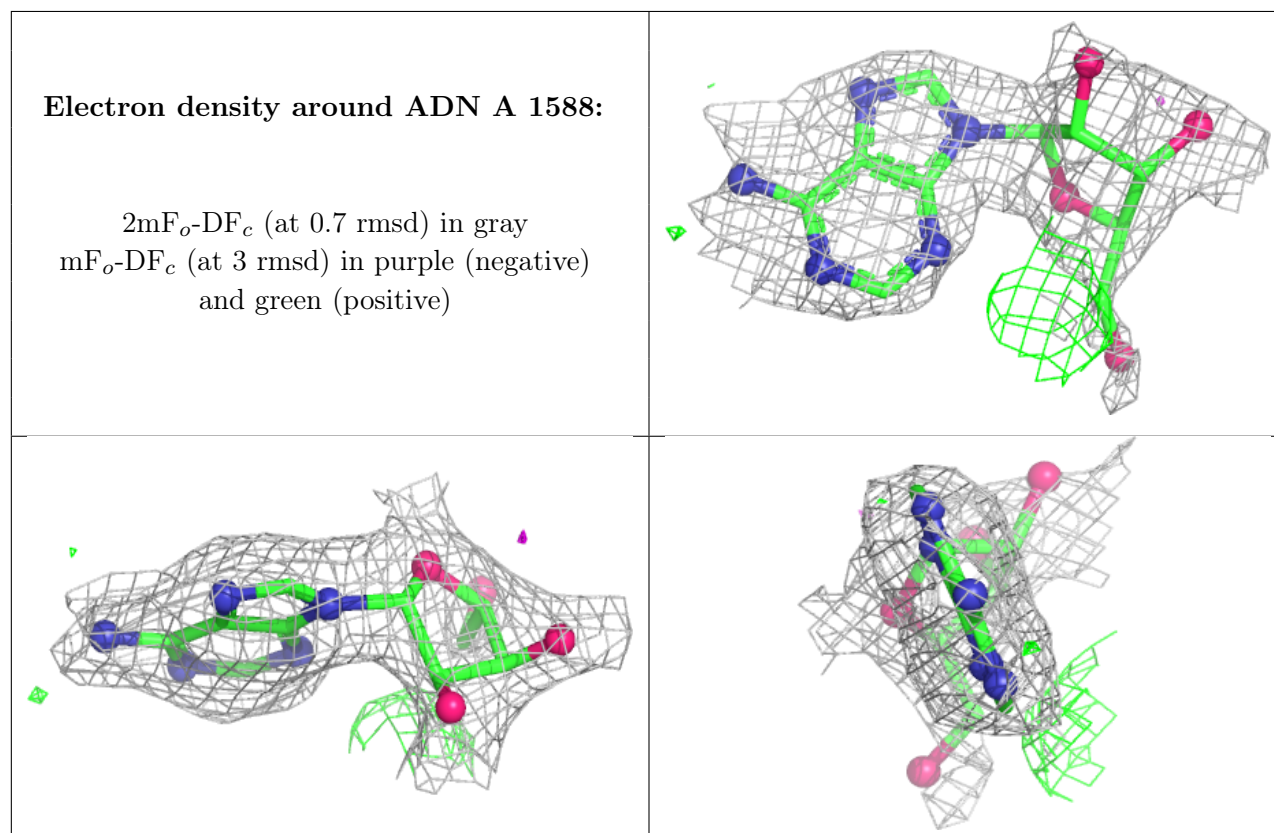
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

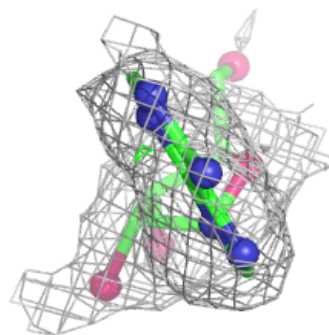
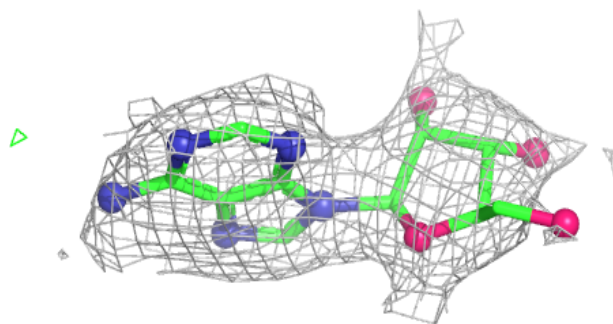
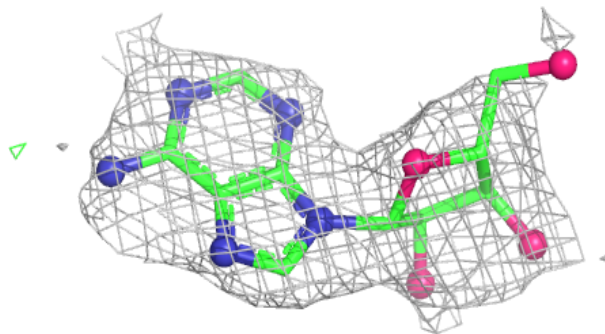
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADN	A	1588	19/19	0.86	0.12	42,43,45,46	0
2	ADN	B	1588	19/19	0.93	0.09	30,31,36,38	0
4	CIT	B	1590	13/13	0.93	0.08	16,29,32,33	0
3	SO4	A	1589	5/5	0.97	0.07	19,24,25,25	0
3	SO4	B	1589	5/5	0.98	0.06	18,21,22,22	0

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 ADN B 1588:

$2mF_o-DF_c$ (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.