



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:43 PM UTC

PDB ID : 3GIG / pdb_00003gig
Title : Crystal structure of phosphorylated DesKC in complex with AMP-PCP
Authors : Trajtenberg, F.; Albanesi, D.; Alzari, P.M.; Buschiazzi, A.; de Mendoza, D.
Deposited on : 2009-03-05
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

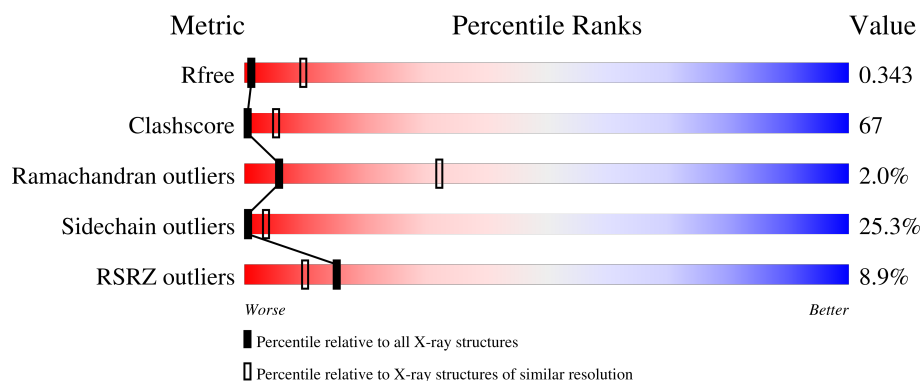
1 Overall quality at a glance

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	218	5% 29% 44% 19% 6%
2	B	218	12% 38% 40% 15% 6%

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	ACP	A	1303	-	-	X	-
3	ACP	B	1303	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3031 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 Sensor histidine kinase desK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1542	968	267	301	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	-	expression tag	UNP O34757

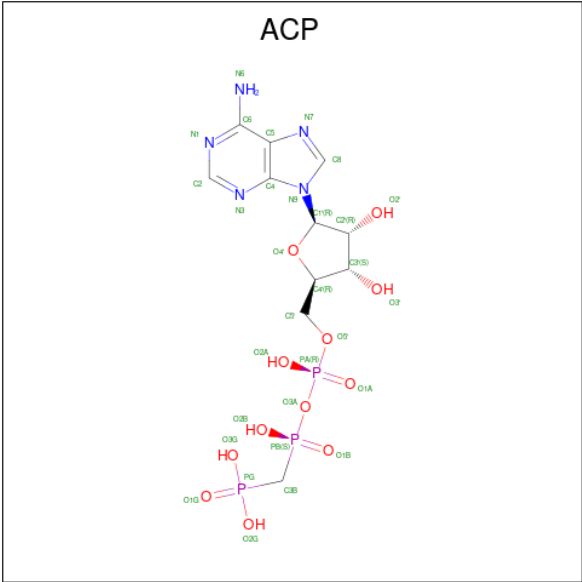
- Molecule 2 is a protein called Sensor histidine kinase desK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	B	205	Total	C	N	O	P	S	0	0	0
			1425	877	253	289	1	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	153	GLY	-	expression tag	UNP O34757

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

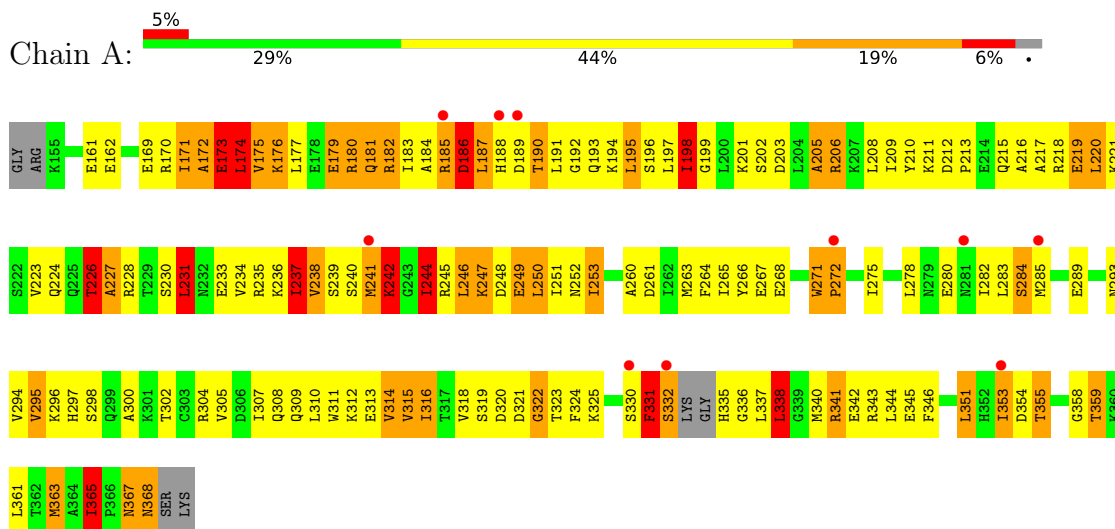
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

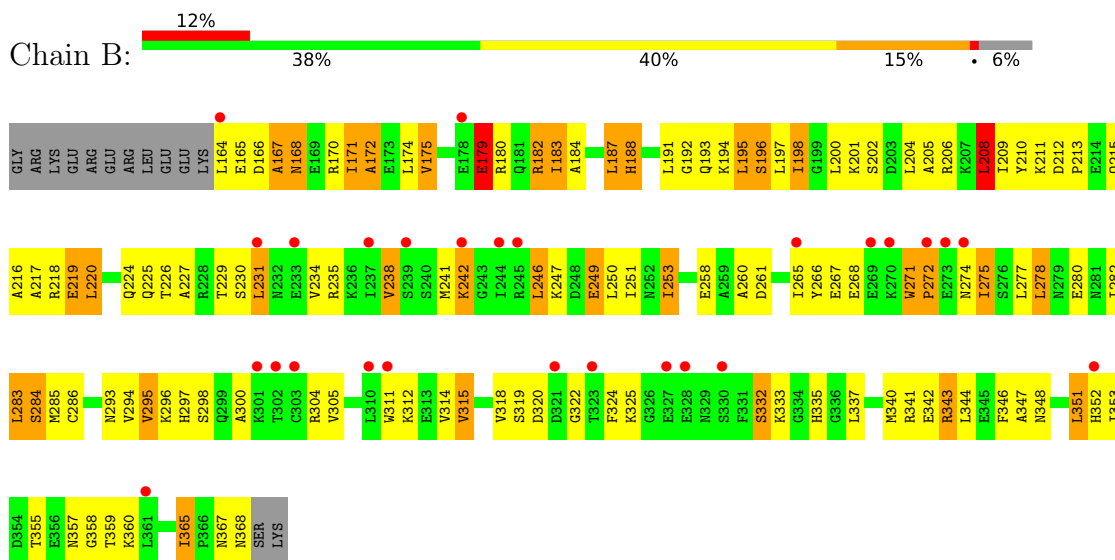
3 Residue-property plots

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: Sensor histidine kinase desK



• Molecule 2: Sensor histidine kinase desK



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.63Å 94.63Å 162.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.85 – 3.50 28.85 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.85-3.50) 99.2 (28.85-3.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 3.47Å)	Xtriage
Refinement program	PHENIX 2009_02_15_2320_3	Depositor
R, R_{free}	0.287 , 0.335 0.294 , 0.343	Depositor DCC
R_{free} test set	896 reflections (8.15%)	wwPDB-VP
Wilson B-factor (Å ²)	92.5	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 150.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3031	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: MG, ACP, NEP

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	1.25	7/1557 (0.4%)	1.69	44/2112 (2.1%)
2	B	1.01	3/1421 (0.2%)	1.44	16/1936 (0.8%)
All	All	1.14	10/2978 (0.3%)	1.58	60/4048 (1.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	ARG	C-O	9.02	1.34	1.24
1	A	174	LEU	C-O	7.41	1.32	1.24
2	B	226	THR	C-O	6.74	1.31	1.24
1	A	186	ASP	C-O	6.72	1.31	1.24
2	B	171	ILE	CA-CB	6.25	1.63	1.54
1	A	190	THR	C-O	5.87	1.31	1.24
1	A	238	VAL	CA-CB	-5.70	1.46	1.54
1	A	250	LEU	CA-C	-5.60	1.45	1.52
1	A	185	ARG	C-O	5.14	1.30	1.24
2	B	179	GLU	C-O	-5.05	1.17	1.24

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	271	TRP	CA-C-N	15.95	136.17	119.90
2	B	271	TRP	C-N-CA	15.95	136.17	119.90
1	A	239	SER	N-CA-C	-15.46	95.27	114.75
1	A	271	TRP	CA-C-N	14.95	135.15	119.90
1	A	271	TRP	C-N-CA	14.95	135.15	119.90
1	A	242	LYS	N-CA-C	-9.33	101.11	111.28
1	A	180	ARG	N-CA-C	-8.87	101.61	111.28
1	A	250	LEU	N-CA-C	-8.80	101.64	111.14
1	A	226	THR	N-CA-C	8.77	120.45	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	CA-C-N	-7.67	110.19	120.54
1	A	185	ARG	C-N-CA	-7.67	110.19	120.54
1	A	365	ILE	CA-C-N	-7.42	111.97	119.99
1	A	365	ILE	C-N-CA	-7.42	111.97	119.99
2	B	365	ILE	CA-C-N	-7.34	112.07	119.99
2	B	365	ILE	C-N-CA	-7.34	112.07	119.99
1	A	367	ASN	CA-C-O	7.16	124.76	119.68
1	A	250	LEU	CA-C-N	-6.73	111.92	120.60
1	A	250	LEU	C-N-CA	-6.73	111.92	120.60
2	B	226	THR	N-CA-C	6.73	118.27	111.07
2	B	198	ILE	CB-CA-C	-6.63	103.49	111.97
1	A	367	ASN	CB-CA-C	-6.55	102.66	114.52
1	A	236	LYS	CA-C-N	-6.35	116.75	122.97
1	A	236	LYS	C-N-CA	-6.35	116.75	122.97
2	B	272	PRO	N-CA-C	6.32	121.13	111.15
1	A	249	GLU	CA-C-N	6.28	128.98	120.44
1	A	249	GLU	C-N-CA	6.28	128.98	120.44
1	A	181	GLN	N-CA-C	6.27	117.78	111.07
1	A	235	ARG	CB-CA-C	-6.27	100.02	110.68
1	A	235	ARG	N-CA-C	6.21	118.84	111.33
2	B	183	ILE	N-CA-C	-6.12	105.09	111.58
1	A	198	ILE	CB-CA-C	-6.05	104.22	111.97
1	A	174	LEU	N-CA-C	6.01	117.83	111.28
1	A	244	ILE	CB-CA-C	-6.00	102.99	111.21
2	B	315	VAL	CB-CA-C	-5.94	102.04	110.12
1	A	312	LYS	N-CA-C	-5.93	104.43	112.26
1	A	272	PRO	N-CA-C	5.88	120.44	111.15
2	B	277	LEU	N-CA-C	-5.85	104.98	111.71
1	A	315	VAL	N-CA-C	5.83	116.47	107.78
2	B	167	ALA	CA-C-O	5.59	126.89	120.90
2	B	187	LEU	CB-CA-C	-5.57	99.52	110.10
2	B	311	TRP	CB-CA-C	-5.48	110.23	116.54
1	A	173	GLU	CA-C-N	-5.45	112.97	120.28
1	A	173	GLU	C-N-CA	-5.45	112.97	120.28
1	A	249	GLU	N-CA-C	5.44	118.72	111.75
1	A	315	VAL	CB-CA-C	-5.40	102.78	110.12
2	B	208	LEU	N-CA-C	5.32	119.52	113.19
2	B	315	VAL	N-CA-C	5.31	115.69	107.78
1	A	205	ALA	CA-C-N	-5.31	113.17	120.28
1	A	205	ALA	C-N-CA	-5.31	113.17	120.28
1	A	237	ILE	N-CA-C	5.26	116.43	111.48
1	A	223	VAL	CB-CA-C	-5.26	104.97	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	LEU	CA-CB-CG	5.24	134.66	116.30
1	A	338	LEU	N-CA-C	-5.11	105.83	111.71
1	A	354	ASP	N-CA-C	5.08	116.70	108.26
1	A	186	ASP	N-CA-C	5.08	117.20	111.11
1	A	221	LYS	N-CA-C	-5.07	105.64	111.07
1	A	247	LYS	CB-CA-C	5.05	119.12	110.74
2	B	196	SER	N-CA-C	-5.02	105.27	111.40
1	A	314	VAL	CB-CA-C	-5.02	103.74	111.31
1	A	231	LEU	N-CA-CB	5.00	119.18	110.18

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	1542	0	1446	235	0
2	B	1425	0	1252	193	0
3	A	31	0	14	16	0
3	B	31	0	14	12	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	3031	0	2726	385	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 67.

All (385) 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)
2:B:246:LEU:HB3	2:B:271:TRP:CH2	1.46	1.47
1:A:241:MET:HG2	2:B:180:ARG:CD	1.47	1.45
2:B:231:LEU:HD12	2:B:235:ARG:NE	1.13	1.40
2:B:231:LEU:O	2:B:235:ARG:HG2	1.21	1.28
2:B:242:LYS:HD3	2:B:242:LYS:N	1.44	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:MET:CG	2:B:180:ARG:HD2	1.72	1.20
1:A:188:HIS:CE1	2:B:235:ARG:HH12	1.60	1.18
1:A:188:HIS:CE1	2:B:235:ARG:NH1	2.12	1.18
2:B:231:LEU:CD1	2:B:235:ARG:NE	2.10	1.15
2:B:246:LEU:CB	2:B:271:TRP:CH2	2.33	1.10
1:A:179:GLU:OE1	1:A:179:GLU:HA	1.52	1.07
1:A:241:MET:HG2	2:B:180:ARG:HD2	1.07	1.06
2:B:242:LYS:H	2:B:242:LYS:CD	1.67	1.06
1:A:245:ARG:HH11	1:A:245:ARG:HB2	1.20	1.04
1:A:171:ILE:O	1:A:175:VAL:HG23	1.60	1.01
1:A:180:ARG:O	1:A:183:ILE:HG12	1.57	1.01
2:B:225:GLN:O	2:B:229:THR:HG23	1.63	0.97
1:A:331:PHE:HD1	1:A:338:LEU:HD23	1.30	0.96
2:B:182:ARG:O	2:B:182:ARG:HD3	1.63	0.96
1:A:188:HIS:ND1	2:B:235:ARG:NH1	2.15	0.95
1:A:346:PHE:HD2	2:B:174:LEU:HD12	1.29	0.95
1:A:245:ARG:HB2	1:A:245:ARG:NH1	1.82	0.94
1:A:322:GLY:O	1:A:358:GLY:HA2	1.70	0.91
1:A:245:ARG:NH1	1:A:245:ARG:CB	2.33	0.91
2:B:246:LEU:HB3	2:B:271:TRP:HH2	0.83	0.91
2:B:351:LEU:C	2:B:351:LEU:HD23	1.96	0.91
2:B:246:LEU:CB	2:B:271:TRP:HH2	1.77	0.91
1:A:171:ILE:HA	1:A:174:LEU:HD12	1.52	0.91
1:A:188:HIS:HE1	2:B:235:ARG:HH12	1.13	0.91
1:A:241:MET:HG2	2:B:180:ARG:HD3	1.52	0.90
1:A:195:LEU:HD22	2:B:227:ALA:O	1.71	0.90
1:A:271:TRP:CG	1:A:272:PRO:HD2	2.04	0.90
1:A:316:ILE:HB	1:A:363:MET:CE	2.01	0.90
2:B:231:LEU:HD12	2:B:235:ARG:CZ	2.01	0.90
2:B:300:ALA:HB2	2:B:322:GLY:H	1.37	0.89
1:A:300:ALA:HB2	1:A:322:GLY:H	1.37	0.89
1:A:351:LEU:C	1:A:351:LEU:HD23	1.99	0.88
2:B:231:LEU:O	2:B:235:ARG:CG	2.17	0.87
2:B:271:TRP:CG	2:B:272:PRO:HD2	2.10	0.87
1:A:209:ILE:O	1:A:213:PRO:HG3	1.76	0.86
1:A:250:LEU:O	1:A:253:ILE:HG12	1.76	0.85
2:B:231:LEU:CD1	2:B:235:ARG:HE	1.77	0.85
1:A:192:GLY:HA2	2:B:231:LEU:HD21	1.58	0.85
1:A:240:SER:O	1:A:241:MET:HB2	1.74	0.85
1:A:307:ILE:HG12	1:A:316:ILE:HG23	1.58	0.85
2:B:231:LEU:HD12	2:B:235:ARG:CD	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:LEU:HD12	2:B:351:LEU:HB2	1.56	0.84
2:B:322:GLY:O	2:B:358:GLY:HA2	1.77	0.84
2:B:182:ARG:HD3	2:B:182:ARG:C	2.02	0.84
2:B:215:GLN:NE2	2:B:218:ARG:HH11	1.76	0.84
1:A:231:LEU:H	1:A:231:LEU:HD12	1.45	0.82
2:B:231:LEU:C	2:B:235:ARG:HG2	2.05	0.82
1:A:195:LEU:HD23	2:B:227:ALA:HB1	1.63	0.81
1:A:215:GLN:NE2	1:A:218:ARG:HH11	1.79	0.81
1:A:297:HIS:CD2	3:A:1303:ACP:H2'	2.16	0.81
1:A:241:MET:HG2	2:B:180:ARG:CG	2.11	0.80
2:B:183:ILE:O	2:B:187:LEU:HD23	1.82	0.80
1:A:176:LYS:HB3	1:A:176:LYS:HZ2	1.45	0.79
1:A:335:HIS:HB3	3:A:1303:ACP:O2A	1.81	0.79
2:B:247:LYS:O	2:B:251:ILE:HG13	1.83	0.78
1:A:181:GLN:HB3	2:B:241:MET:SD	2.24	0.78
1:A:346:PHE:CD2	2:B:174:LEU:HD12	2.17	0.78
1:A:314:VAL:HG23	1:A:367:ASN:HB2	1.66	0.78
1:A:227:ALA:O	1:A:231:LEU:HD12	1.85	0.77
1:A:249:GLU:O	1:A:253:ILE:HG23	1.84	0.77
1:A:250:LEU:HA	1:A:253:ILE:CD1	2.15	0.77
1:A:187:LEU:HD23	1:A:187:LEU:H	1.50	0.76
1:A:181:GLN:CG	2:B:241:MET:SD	2.74	0.76
1:A:173:GLU:O	1:A:177:LEU:HG	1.86	0.76
1:A:176:LYS:HB3	1:A:176:LYS:NZ	2.00	0.76
1:A:346:PHE:CE2	2:B:171:ILE:HG23	2.20	0.76
2:B:335:HIS:HB3	3:B:1303:ACP:O2A	1.84	0.75
2:B:246:LEU:CB	2:B:271:TRP:CZ2	2.69	0.75
1:A:344:LEU:HD12	1:A:351:LEU:HB2	1.67	0.75
1:A:246:LEU:O	1:A:247:LYS:C	2.30	0.74
2:B:346:PHE:O	2:B:346:PHE:HD1	1.68	0.74
1:A:179:GLU:OE1	1:A:179:GLU:CA	2.31	0.74
1:A:265:ILE:HB	1:A:304:ARG:HA	1.71	0.73
2:B:182:ARG:C	2:B:182:ARG:CD	2.59	0.73
2:B:231:LEU:HD12	2:B:235:ARG:HE	0.92	0.73
2:B:351:LEU:HD23	2:B:351:LEU:O	1.87	0.73
1:A:331:PHE:CD1	1:A:338:LEU:HD23	2.21	0.73
1:A:341:ARG:CZ	1:A:345:GLU:CB	2.67	0.72
1:A:324:PHE:CD2	1:A:355:THR:HG21	2.24	0.72
1:A:337:LEU:CD1	3:A:1303:ACP:H5'1	2.20	0.72
1:A:245:ARG:CZ	1:A:245:ARG:HB3	2.20	0.72
1:A:337:LEU:HD11	3:A:1303:ACP:H5'1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:O	1:A:195:LEU:HB2	1.90	0.71
1:A:309:GLN:HE22	1:A:367:ASN:ND2	1.87	0.71
2:B:300:ALA:HB2	2:B:322:GLY:N	2.05	0.71
1:A:245:ARG:HH11	1:A:245:ARG:CB	1.93	0.71
2:B:265:ILE:HB	2:B:304:ARG:HA	1.73	0.71
1:A:245:ARG:NH1	1:A:245:ARG:HB3	2.06	0.71
2:B:246:LEU:HB3	2:B:271:TRP:CZ2	2.21	0.71
1:A:245:ARG:NH1	1:A:280:GLU:OE2	2.22	0.70
1:A:241:MET:CG	2:B:180:ARG:CD	2.39	0.70
2:B:312:LYS:O	2:B:367:ASN:CB	2.40	0.70
1:A:224:GLN:O	1:A:228:ARG:HG3	1.92	0.70
1:A:316:ILE:HB	1:A:363:MET:HE3	1.71	0.70
2:B:191:LEU:O	2:B:195:LEU:HB2	1.92	0.70
1:A:245:ARG:NH1	1:A:280:GLU:CD	2.50	0.69
1:A:245:ARG:NH1	1:A:280:GLU:OE1	2.25	0.69
2:B:242:LYS:N	2:B:242:LYS:CD	2.35	0.69
1:A:195:LEU:HD21	2:B:227:ALA:HA	1.74	0.69
1:A:300:ALA:HB2	1:A:322:GLY:N	2.07	0.69
1:A:351:LEU:HD23	1:A:351:LEU:O	1.92	0.69
2:B:192:GLY:O	2:B:193:GLN:C	2.36	0.69
1:A:245:ARG:HH12	1:A:280:GLU:CD	2.01	0.68
2:B:337:LEU:CD1	3:B:1303:ACP:H5'1	2.23	0.68
1:A:238:VAL:HG13	2:B:184:ALA:HB1	1.75	0.67
1:A:181:GLN:HG2	2:B:241:MET:SD	2.35	0.66
1:A:195:LEU:CD2	2:B:227:ALA:O	2.43	0.66
1:A:224:GLN:HG3	2:B:202:SER:HB3	1.77	0.66
2:B:191:LEU:HD21	2:B:230:SER:HB3	1.77	0.66
1:A:271:TRP:CD2	1:A:272:PRO:HD2	2.30	0.66
2:B:337:LEU:HG	3:B:1303:ACP:O2A	1.95	0.66
1:A:187:LEU:HD23	1:A:187:LEU:N	2.10	0.66
2:B:209:ILE:O	2:B:213:PRO:HG3	1.96	0.65
1:A:294:VAL:HG22	3:A:1303:ACP:HN62	1.60	0.65
2:B:215:GLN:HE22	2:B:218:ARG:HH11	1.42	0.65
2:B:246:LEU:HB2	2:B:271:TRP:CZ2	2.31	0.65
2:B:242:LYS:HD3	2:B:242:LYS:H	0.72	0.64
2:B:324:PHE:CD2	2:B:355:THR:HG21	2.32	0.64
2:B:164:LEU:O	2:B:168:ASN:HB2	1.98	0.64
2:B:260:ALA:O	2:B:261:ASP:HB2	1.98	0.64
1:A:215:GLN:HE22	1:A:218:ARG:HH11	1.44	0.64
1:A:228:ARG:HA	1:A:231:LEU:CD1	2.27	0.64
2:B:297:HIS:HB2	3:B:1303:ACP:C2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:O	1:A:183:ILE:CG1	2.41	0.64
1:A:181:GLN:NE2	2:B:241:MET:SD	2.71	0.63
1:A:298:SER:HB3	3:A:1303:ACP:N1	2.12	0.63
1:A:203:ASP:HA	2:B:224:GLN:NE2	2.14	0.63
1:A:305:VAL:HG22	1:A:318:VAL:HG22	1.80	0.63
2:B:234:VAL:O	2:B:238:VAL:HG23	1.99	0.63
1:A:169:GLU:O	1:A:172:ALA:HB3	1.97	0.63
2:B:295:VAL:HG12	2:B:295:VAL:O	1.99	0.63
1:A:271:TRP:CG	1:A:272:PRO:CD	2.82	0.63
1:A:172:ALA:O	1:A:173:GLU:C	2.42	0.62
2:B:337:LEU:HD12	3:B:1303:ACP:H5'1	1.82	0.62
1:A:245:ARG:CB	1:A:245:ARG:CZ	2.75	0.62
1:A:231:LEU:HD12	1:A:231:LEU:N	2.14	0.62
1:A:353:ILE:HG13	1:A:361:LEU:HD23	1.81	0.61
1:A:181:GLN:O	1:A:182:ARG:C	2.43	0.61
1:A:298:SER:HA	3:A:1303:ACP:H2	1.82	0.61
2:B:215:GLN:NE2	2:B:215:GLN:HA	2.14	0.61
1:A:181:GLN:CB	2:B:241:MET:SD	2.89	0.61
1:A:250:LEU:HA	1:A:253:ILE:HD11	1.82	0.61
1:A:295:VAL:HG12	1:A:295:VAL:O	2.01	0.61
1:A:297:HIS:HB2	3:A:1303:ACP:N3	2.16	0.60
1:A:264:PHE:CZ	1:A:266:TYR:HB2	2.36	0.60
1:A:341:ARG:O	1:A:342:GLU:C	2.43	0.60
2:B:166:ASP:OD1	2:B:166:ASP:O	2.20	0.60
1:A:322:GLY:O	1:A:358:GLY:CA	2.46	0.59
1:A:298:SER:HB2	1:A:320:ASP:OD1	2.01	0.59
2:B:271:TRP:CD2	2:B:272:PRO:HD2	2.37	0.59
2:B:351:LEU:C	2:B:351:LEU:CD2	2.70	0.59
1:A:202:SER:CB	2:B:224:GLN:HG3	2.32	0.59
1:A:297:HIS:O	1:A:325:LYS:NZ	2.36	0.59
2:B:215:GLN:HA	2:B:215:GLN:HE21	1.65	0.59
1:A:346:PHE:O	1:A:346:PHE:CD1	2.56	0.59
1:A:245:ARG:HB2	1:A:280:GLU:OE1	2.02	0.59
2:B:201:LYS:HD2	2:B:219:GLU:HG3	1.85	0.59
1:A:293:ASN:ND2	3:A:1303:ACP:O1A	2.29	0.58
1:A:337:LEU:HD11	3:A:1303:ACP:C5'	2.33	0.58
1:A:187:LEU:N	1:A:187:LEU:CD2	2.65	0.58
1:A:332:SER:O	1:A:335:HIS:HB2	2.02	0.58
1:A:246:LEU:HB3	1:A:271:TRP:HH2	1.68	0.58
2:B:205:ALA:CB	2:B:220:LEU:HD21	2.33	0.58
1:A:190:THR:OG1	1:A:191:LEU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ALA:O	2:B:171:ILE:CD1	2.52	0.58
1:A:227:ALA:O	1:A:228:ARG:C	2.47	0.57
1:A:250:LEU:HA	1:A:253:ILE:HD13	1.86	0.57
1:A:179:GLU:O	1:A:180:ARG:C	2.45	0.57
1:A:187:LEU:O	1:A:188:HIS:C	2.45	0.57
1:A:227:ALA:O	1:A:231:LEU:CD1	2.53	0.57
1:A:266:TYR:CD2	1:A:267:GLU:N	2.72	0.57
1:A:309:GLN:HE22	1:A:367:ASN:HD22	1.51	0.57
2:B:322:GLY:O	2:B:358:GLY:CA	2.53	0.57
1:A:294:VAL:C	1:A:296:LYS:H	2.13	0.56
2:B:182:ARG:O	2:B:182:ARG:CD	2.47	0.56
2:B:294:VAL:C	2:B:296:LYS:H	2.13	0.56
1:A:201:LYS:HD2	1:A:219:GLU:HG3	1.87	0.56
1:A:215:GLN:NE2	1:A:215:GLN:HA	2.19	0.56
1:A:247:LYS:HG2	1:A:271:TRP:CZ2	2.39	0.56
1:A:231:LEU:HG	2:B:195:LEU:HD22	1.88	0.56
2:B:271:TRP:CG	2:B:272:PRO:CD	2.87	0.56
1:A:195:LEU:CD2	2:B:227:ALA:HA	2.36	0.56
1:A:351:LEU:C	1:A:351:LEU:CD2	2.70	0.56
1:A:215:GLN:NE2	1:A:218:ARG:NH1	2.53	0.56
2:B:179:GLU:HG2	2:B:182:ARG:HG2	1.88	0.55
2:B:335:HIS:CE1	3:B:1303:ACP:H3B1	2.40	0.55
2:B:346:PHE:CD1	2:B:346:PHE:C	2.82	0.55
1:A:246:LEU:HB3	1:A:271:TRP:CH2	2.41	0.55
2:B:249:GLU:O	2:B:253:ILE:HG23	2.06	0.55
1:A:250:LEU:HD21	1:A:266:TYR:CE1	2.41	0.55
2:B:167:ALA:O	2:B:171:ILE:HD13	2.05	0.55
2:B:266:TYR:CD2	2:B:267:GLU:N	2.74	0.55
2:B:346:PHE:HD1	2:B:346:PHE:C	2.15	0.55
1:A:177:LEU:N	1:A:177:LEU:HD23	2.20	0.55
1:A:181:GLN:CD	2:B:241:MET:SD	2.89	0.55
1:A:283:LEU:CD2	1:A:316:ILE:HG13	2.37	0.55
1:A:215:GLN:HA	1:A:215:GLN:HE21	1.71	0.55
1:A:195:LEU:CD2	2:B:227:ALA:CA	2.85	0.55
2:B:337:LEU:HD11	3:B:1303:ACP:H5'1	1.88	0.55
1:A:206:ARG:HG3	2:B:217:ALA:HA	1.89	0.54
1:A:264:PHE:CE1	1:A:266:TYR:HB2	2.42	0.54
1:A:346:PHE:O	1:A:346:PHE:HD1	1.90	0.54
1:A:241:MET:HG3	2:B:180:ARG:HD2	1.81	0.54
2:B:282:ILE:O	2:B:285:MET:HB2	2.07	0.54
1:A:228:ARG:HA	1:A:231:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:TRP:CD1	2:B:271:TRP:C	2.85	0.54
1:A:234:VAL:HA	1:A:237:ILE:HB	1.89	0.54
1:A:294:VAL:HG22	3:A:1303:ACP:N6	2.22	0.54
1:A:300:ALA:CB	1:A:322:GLY:H	2.14	0.54
2:B:298:SER:HB2	2:B:320:ASP:OD1	2.07	0.54
2:B:341:ARG:O	2:B:342:GLU:C	2.51	0.54
2:B:215:GLN:NE2	2:B:218:ARG:NH1	2.49	0.53
2:B:274:ASN:OD1	2:B:274:ASN:O	2.26	0.53
2:B:205:ALA:HB1	2:B:220:LEU:HD21	1.89	0.53
1:A:245:ARG:O	1:A:246:LEU:C	2.51	0.53
2:B:187:LEU:N	2:B:187:LEU:CD2	2.72	0.53
2:B:305:VAL:HG22	2:B:318:VAL:HG22	1.91	0.53
1:A:314:VAL:CG2	1:A:367:ASN:HD22	2.21	0.53
1:A:340:MET:O	1:A:344:LEU:HG	2.08	0.53
2:B:346:PHE:O	2:B:346:PHE:CD1	2.57	0.53
1:A:188:HIS:O	1:A:189:ASP:C	2.50	0.53
1:A:283:LEU:HD22	1:A:316:ILE:HD11	1.91	0.52
1:A:195:LEU:HD13	2:B:231:LEU:HD23	1.91	0.52
2:B:210:TYR:O	2:B:213:PRO:HD3	2.09	0.52
1:A:199:GLY:O	1:A:202:SER:HB2	2.10	0.52
1:A:220:LEU:N	1:A:220:LEU:HD23	2.24	0.52
2:B:179:GLU:HG2	2:B:182:ARG:CG	2.40	0.52
1:A:324:PHE:CD2	1:A:355:THR:CG2	2.93	0.51
2:B:266:TYR:CE2	2:B:268:GLU:N	2.78	0.51
2:B:347:ALA:O	2:B:348:ASN:HB2	2.09	0.51
1:A:193:GLN:O	1:A:194:LYS:C	2.54	0.51
2:B:278:LEU:HD12	2:B:278:LEU:O	2.10	0.51
2:B:220:LEU:N	2:B:220:LEU:HD23	2.24	0.51
2:B:208:LEU:N	2:B:208:LEU:HD23	2.25	0.51
1:A:209:ILE:CG2	2:B:213:PRO:HB3	2.40	0.51
1:A:241:MET:HG2	2:B:180:ARG:HG2	1.93	0.51
1:A:246:LEU:O	1:A:249:GLU:N	2.43	0.51
2:B:210:TYR:O	2:B:211:LYS:C	2.53	0.50
1:A:195:LEU:HD23	2:B:227:ALA:CB	2.39	0.50
2:B:278:LEU:HD12	2:B:278:LEU:C	2.35	0.50
2:B:351:LEU:C	2:B:352:HIS:ND1	2.70	0.50
1:A:316:ILE:HB	1:A:363:MET:HE2	1.88	0.50
2:B:340:MET:O	2:B:344:LEU:HG	2.12	0.50
1:A:246:LEU:HD12	1:A:284:SER:OG	2.12	0.49
2:B:271:TRP:CD1	2:B:272:PRO:N	2.79	0.49
1:A:330:SER:O	1:A:332:SER:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ILE:O	2:B:175:VAL:HG22	2.11	0.49
1:A:210:TYR:O	1:A:213:PRO:HD3	2.13	0.49
2:B:208:LEU:O	2:B:209:ILE:C	2.54	0.49
1:A:202:SER:HB3	2:B:224:GLN:HG3	1.95	0.49
1:A:208:LEU:O	1:A:209:ILE:C	2.56	0.49
1:A:298:SER:CB	3:A:1303:ACP:N1	2.75	0.49
2:B:188:NEP:ND1	2:B:188:NEP:C	2.76	0.49
1:A:266:TYR:CE2	1:A:268:GLU:N	2.81	0.49
1:A:337:LEU:HG	3:A:1303:ACP:PA	2.53	0.48
1:A:170:ARG:O	1:A:174:LEU:HG	2.12	0.48
1:A:250:LEU:HD11	1:A:271:TRP:CZ3	2.48	0.48
1:A:271:TRP:CD1	1:A:272:PRO:N	2.82	0.48
1:A:181:GLN:O	1:A:184:ALA:N	2.47	0.48
1:A:263:MET:CB	1:A:302:THR:HG23	2.44	0.48
1:A:264:PHE:CD1	1:A:264:PHE:C	2.90	0.48
1:A:210:TYR:O	1:A:211:LYS:C	2.57	0.48
1:A:335:HIS:C	1:A:337:LEU:H	2.22	0.48
2:B:297:HIS:HB2	3:B:1303:ACP:N3	2.29	0.48
1:A:271:TRP:CD1	1:A:271:TRP:C	2.92	0.48
2:B:333:LYS:C	2:B:335:HIS:H	2.22	0.48
1:A:346:PHE:CD1	1:A:346:PHE:C	2.90	0.48
2:B:250:LEU:O	2:B:253:ILE:HG12	2.14	0.48
1:A:238:VAL:HG12	1:A:242:LYS:HG3	1.96	0.48
2:B:171:ILE:O	2:B:175:VAL:CG2	2.62	0.48
2:B:293:ASN:ND2	3:B:1303:ACP:O1A	2.46	0.48
2:B:305:VAL:HG22	2:B:318:VAL:HA	1.94	0.47
1:A:308:GLN:HB2	1:A:310:LEU:HD11	1.96	0.47
1:A:216:ALA:O	1:A:217:ALA:C	2.57	0.47
1:A:353:ILE:HD11	1:A:359:THR:HG22	1.95	0.47
2:B:172:ALA:O	2:B:174:LEU:N	2.47	0.47
1:A:202:SER:HB2	2:B:224:GLN:HG3	1.95	0.47
2:B:192:GLY:O	2:B:195:LEU:N	2.47	0.47
2:B:231:LEU:CD1	2:B:235:ARG:CD	2.80	0.47
2:B:274:ASN:OD1	2:B:274:ASN:C	2.58	0.47
2:B:300:ALA:CB	2:B:322:GLY:H	2.19	0.47
1:A:234:VAL:HG12	1:A:238:VAL:HG23	1.96	0.47
1:A:300:ALA:HB1	1:A:321:ASP:OD1	2.15	0.47
1:A:305:VAL:HG22	1:A:318:VAL:HA	1.95	0.47
2:B:216:ALA:O	2:B:217:ALA:C	2.55	0.47
1:A:226:THR:O	1:A:227:ALA:C	2.57	0.47
1:A:250:LEU:O	1:A:251:ILE:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ARG:HD3	2:B:343:ARG:HA	1.81	0.47
1:A:230:SER:O	1:A:233:GLU:N	2.47	0.47
1:A:205:ALA:HB3	2:B:220:LEU:CD1	2.44	0.47
2:B:332:SER:O	2:B:335:HIS:HB2	2.14	0.47
1:A:245:ARG:O	1:A:248:ASP:N	2.47	0.46
2:B:166:ASP:OD1	2:B:170:ARG:CB	2.63	0.46
2:B:235:ARG:HA	2:B:238:VAL:HG23	1.96	0.46
1:A:250:LEU:HD21	1:A:266:TYR:HE1	1.81	0.46
1:A:247:LYS:HE2	1:A:271:TRP:CE2	2.51	0.46
1:A:305:VAL:CG2	1:A:318:VAL:HG22	2.46	0.46
1:A:212:ASP:OD1	1:A:212:ASP:C	2.58	0.46
1:A:185:ARG:O	1:A:186:ASP:C	2.55	0.46
1:A:298:SER:O	1:A:325:LYS:NZ	2.48	0.46
1:A:282:ILE:O	1:A:285:MET:HB2	2.15	0.46
2:B:335:HIS:C	2:B:337:LEU:H	2.24	0.45
1:A:205:ALA:HB3	2:B:220:LEU:HD12	1.99	0.45
1:A:251:ILE:O	1:A:252:ASN:C	2.59	0.45
1:A:367:ASN:HB3	1:A:368:ASN:H	1.60	0.45
2:B:231:LEU:CD1	2:B:235:ARG:CZ	2.80	0.45
1:A:266:TYR:OH	1:A:268:GLU:HG3	2.17	0.45
1:A:338:LEU:HD22	1:A:338:LEU:HA	1.73	0.45
1:A:278:LEU:HD12	1:A:278:LEU:C	2.42	0.45
2:B:212:ASP:C	2:B:212:ASP:OD1	2.60	0.45
2:B:234:VAL:O	2:B:238:VAL:CG2	2.65	0.45
2:B:187:LEU:HA	2:B:187:LEU:HD22	1.74	0.44
1:A:215:GLN:HE21	1:A:215:GLN:CA	2.27	0.44
1:A:278:LEU:HD12	1:A:278:LEU:O	2.17	0.44
1:A:314:VAL:HG12	1:A:315:VAL:N	2.32	0.44
1:A:335:HIS:O	1:A:337:LEU:N	2.51	0.44
1:A:341:ARG:O	1:A:343:ARG:N	2.51	0.44
1:A:314:VAL:HG22	1:A:367:ASN:HD22	1.82	0.44
1:A:324:PHE:CB	1:A:355:THR:HG22	2.48	0.44
2:B:215:GLN:HE21	2:B:215:GLN:CA	2.26	0.43
2:B:335:HIS:O	2:B:337:LEU:N	2.50	0.43
1:A:228:ARG:CA	1:A:231:LEU:CD1	2.94	0.43
1:A:250:LEU:CD2	1:A:266:TYR:CE1	3.01	0.43
2:B:286:CYS:HB3	2:B:340:MET:SD	2.58	0.43
2:B:300:ALA:CB	2:B:322:GLY:N	2.80	0.43
1:A:337:LEU:HD12	3:A:1303:ACP:H5'1	2.00	0.43
1:A:318:VAL:O	1:A:318:VAL:HG12	2.19	0.43
1:A:353:ILE:HG13	1:A:361:LEU:CD2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:VAL:C	2:B:296:LYS:N	2.77	0.43
2:B:166:ASP:OD1	2:B:166:ASP:C	2.62	0.43
2:B:202:SER:O	2:B:205:ALA:HB3	2.19	0.43
2:B:325:LYS:H	3:B:1303:ACP:H2	1.83	0.43
2:B:367:ASN:O	2:B:368:ASN:CB	2.67	0.43
1:A:289:GLU:OE2	1:A:336:GLY:HA3	2.19	0.42
2:B:314:VAL:HG12	2:B:315:VAL:N	2.35	0.42
2:B:167:ALA:O	2:B:171:ILE:HD12	2.18	0.42
1:A:172:ALA:O	1:A:176:LYS:HG2	2.19	0.42
1:A:324:PHE:CG	1:A:355:THR:HG22	2.54	0.42
2:B:164:LEU:O	2:B:165:GLU:C	2.63	0.42
2:B:193:GLN:O	2:B:194:LYS:C	2.62	0.42
2:B:335:HIS:ND1	3:B:1303:ACP:O3A	2.53	0.42
1:A:344:LEU:N	1:A:344:LEU:HD23	2.33	0.42
1:A:242:LYS:NZ	1:A:242:LYS:HB3	2.30	0.42
2:B:353:ILE:HA	2:B:360:LYS:O	2.20	0.42
1:A:208:LEU:N	1:A:208:LEU:HD23	2.34	0.42
2:B:275:ILE:HD11	2:B:280:GLU:N	2.35	0.42
1:A:300:ALA:CB	1:A:322:GLY:N	2.80	0.41
2:B:204:LEU:HD23	2:B:219:GLU:HG2	2.01	0.41
2:B:231:LEU:C	2:B:235:ARG:CG	2.83	0.41
2:B:266:TYR:OH	2:B:268:GLU:HG3	2.21	0.41
2:B:166:ASP:O	2:B:167:ALA:C	2.63	0.41
2:B:224:GLN:O	2:B:225:GLN:C	2.63	0.41
2:B:341:ARG:O	2:B:343:ARG:N	2.53	0.41
1:A:161:GLU:O	1:A:162:GLU:C	2.63	0.41
1:A:260:ALA:O	1:A:261:ASP:CB	2.68	0.41
2:B:260:ALA:O	2:B:261:ASP:CB	2.68	0.41
1:A:337:LEU:HG	3:A:1303:ACP:O1A	2.20	0.41
1:A:228:ARG:HA	1:A:231:LEU:HD11	2.02	0.41
1:A:244:ILE:HD13	1:A:244:ILE:N	2.36	0.41
1:A:304:ARG:O	1:A:305:VAL:HG23	2.21	0.41
1:A:363:MET:HE3	1:A:363:MET:HB2	1.78	0.41
1:A:341:ARG:NH2	1:A:345:GLU:CB	2.84	0.41
1:A:271:TRP:HA	1:A:272:PRO:HD3	1.70	0.41
2:B:200:LEU:HD23	2:B:200:LEU:HA	1.84	0.41
2:B:249:GLU:HG2	2:B:284:SER:OG	2.21	0.41
2:B:283:LEU:O	2:B:284:SER:C	2.63	0.41
2:B:294:VAL:HG13	2:B:298:SER:OG	2.20	0.41
1:A:183:ILE:CG1	1:A:184:ALA:N	2.84	0.40
2:B:191:LEU:HD23	2:B:191:LEU:HA	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:CD2	2:B:227:ALA:C	2.94	0.40
1:A:205:ALA:CB	1:A:220:LEU:HD21	2.51	0.40
1:A:298:SER:HA	3:A:1303:ACP:C2	2.49	0.40
1:A:313:GLU:HG3	1:A:365:ILE:O	2.21	0.40
2:B:250:LEU:HA	2:B:253:ILE:CD1	2.51	0.40
2:B:335:HIS:ND1	3:B:1303:ACP:H3B1	2.36	0.40
1:A:198:ILE:O	1:A:199:GLY:C	2.61	0.40
1:A:294:VAL:C	1:A:296:LYS:N	2.76	0.40
2:B:179:GLU:O	2:B:182:ARG:HG3	2.21	0.40
2:B:179:GLU:O	2:B:183:ILE:HG13	2.21	0.40
1:A:346:PHE:CD2	2:B:171:ILE:HG23	2.55	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	208/218 (95%)	168 (81%)	35 (17%)	5 (2%)	4	29
2	B	202/218 (93%)	161 (80%)	38 (19%)	3 (2%)	8	37
All	All	410/436 (94%)	329 (80%)	73 (18%)	8 (2%)	6	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	PHE
2	B	168	ASN
1	A	172	ALA
1	A	227	ALA
1	A	295	VAL
2	B	295	VAL
2	B	172	ALA

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Mol	Chain	Res	Type
1	A	322	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	148/194 (76%)	108 (73%)	40 (27%)	0	3
2	B	125/193 (65%)	96 (77%)	29 (23%)	1	5
All	All	273/387 (70%)	204 (75%)	69 (25%)	0	3

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	ILE
1	A	173	GLU
1	A	174	LEU
1	A	175	VAL
1	A	176	LYS
1	A	179	GLU
1	A	186	ASP
1	A	187	LEU
1	A	195	LEU
1	A	196	SER
1	A	197	LEU
1	A	198	ILE
1	A	206	ARG
1	A	219	GLU
1	A	220	LEU
1	A	226	THR
1	A	231	LEU
1	A	237	ILE
1	A	241	MET
1	A	242	LYS
1	A	244	ILE
1	A	246	LEU

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Mol	Chain	Res	Type
1	A	253	ILE
1	A	275	ILE
1	A	284	SER
1	A	311	TRP
1	A	316	ILE
1	A	319	SER
1	A	323	THR
1	A	331	PHE
1	A	332	SER
1	A	338	LEU
1	A	341	ARG
1	A	351	LEU
1	A	353	ILE
1	A	355	THR
1	A	359	THR
1	A	363	MET
1	A	365	ILE
1	A	368	ASN
2	B	175	VAL
2	B	179	GLU
2	B	182	ARG
2	B	195	LEU
2	B	196	SER
2	B	197	LEU
2	B	198	ILE
2	B	206	ARG
2	B	208	LEU
2	B	219	GLU
2	B	220	LEU
2	B	231	LEU
2	B	238	VAL
2	B	242	LYS
2	B	246	LEU
2	B	249	GLU
2	B	253	ILE
2	B	258	GLU
2	B	275	ILE
2	B	278	LEU
2	B	283	LEU
2	B	284	SER
2	B	319	SER
2	B	332	SER

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Mol	Chain	Res	Type
2	B	343	ARG
2	B	351	LEU
2	B	357	ASN
2	B	359	THR
2	B	365	ILE

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

Mol	Chain	Res	Type
1	A	188	HIS
1	A	215	GLN
1	A	279	ASN
1	A	367	ASN
1	A	368	ASN
2	B	215	GLN
2	B	297	HIS
2	B	357	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NEP	B	188	2	11,14,15	1.63	1 (9%)	8,20,22	1.64	2 (25%)

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	NEP	B	188	2	-	3/5/12/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	188	NEP	P-O3P	3.62	1.51	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	188	NEP	CE1-ND1-CG	2.50	109.81	105.80
2	B	188	NEP	CA-CB-CG	-2.04	108.75	113.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	188	NEP	CA-CB-CG-ND1
2	B	188	NEP	CA-CB-CG-CD2
2	B	188	NEP	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	188	NEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ACP	B	1303	4	31,33,33	1.63	6 (19%)	47,52,52	2.14	15 (31%)
3	ACP	A	1303	4	31,33,33	1.61	8 (25%)	47,52,52	2.06	13 (27%)

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	ACP	B	1303	4	-	3/19/38/38	0/3/3/3
3	ACP	A	1303	4	-	3/19/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1303	ACP	C5-C4	4.60	1.47	1.39
3	A	1303	ACP	C5-C4	4.14	1.46	1.39
3	B	1303	ACP	PB-O3A	3.46	1.62	1.58
3	B	1303	ACP	C5-C6	3.21	1.49	1.41
3	A	1303	ACP	C5-N7	-3.14	1.33	1.39
3	A	1303	ACP	PA-O3A	2.94	1.62	1.59
3	B	1303	ACP	PA-O3A	2.82	1.62	1.59
3	A	1303	ACP	PB-O3A	2.64	1.61	1.58
3	A	1303	ACP	C8-N7	2.41	1.36	1.31
3	B	1303	ACP	C8-N7	2.33	1.36	1.31
3	A	1303	ACP	PB-O2B	-2.31	1.50	1.56
3	B	1303	ACP	PB-O2B	-2.31	1.50	1.56
3	A	1303	ACP	C5-C6	2.28	1.47	1.41
3	A	1303	ACP	C4-N9	-2.10	1.33	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1303	ACP	C5-C4-N3	-7.15	116.88	126.72
3	B	1303	ACP	C5-C4-N3	-6.41	117.90	126.72
3	B	1303	ACP	N3-C4-N9	4.85	135.42	127.17
3	B	1303	ACP	C4-C5-N7	-4.77	105.13	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1303	ACP	N3-C4-N9	4.52	134.85	127.17
3	A	1303	ACP	C4-C5-N7	-4.25	105.72	110.58
3	B	1303	ACP	C2-N3-C4	3.85	121.24	111.83
3	A	1303	ACP	C2-N3-C4	3.81	121.14	111.83
3	B	1303	ACP	C5-N7-C8	3.62	109.14	103.45
3	B	1303	ACP	O1G-PG-C3B	-3.61	103.51	111.37
3	B	1303	ACP	C4-N9-C8	3.38	109.28	105.74
3	A	1303	ACP	PB-O3A-PA	-3.08	122.31	132.37
3	A	1303	ACP	O2B-PB-O1B	3.08	119.98	109.95
3	B	1303	ACP	N9-C8-N7	-2.94	109.76	113.94
3	A	1303	ACP	O1G-PG-C3B	-2.84	105.19	111.37
3	B	1303	ACP	N3-C2-N1	-2.82	124.31	128.58
3	A	1303	ACP	O4'-C1'-N9	2.79	113.45	108.09
3	B	1303	ACP	C3'-C2'-C1'	2.71	106.58	101.46
3	B	1303	ACP	C6-C5-N7	2.66	137.22	132.09
3	A	1303	ACP	C5-N7-C8	2.60	107.54	103.45
3	B	1303	ACP	PB-O3A-PA	-2.56	124.00	132.37
3	B	1303	ACP	O2B-PB-O1B	2.54	118.20	109.95
3	A	1303	ACP	C3'-C2'-C1'	2.29	105.79	101.46
3	A	1303	ACP	C5-C4-N9	2.26	108.27	105.81
3	B	1303	ACP	O3G-PG-O2G	2.23	114.32	107.96
3	A	1303	ACP	N3-C2-N1	-2.21	125.23	128.58
3	B	1303	ACP	O2A-PA-O1A	2.16	122.51	112.44
3	A	1303	ACP	C2'-C3'-C4'	2.01	106.50	102.61

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1303	ACP	C5'-O5'-PA-O2A
3	B	1303	ACP	PB-C3B-PG-O1G
3	B	1303	ACP	PB-C3B-PG-O2G
3	B	1303	ACP	PB-C3B-PG-O3G
3	A	1303	ACP	C5'-O5'-PA-O1A
3	A	1303	ACP	C5'-O5'-PA-O3A

There are no ring outliers.

2 monomers are involved in 28 short contacts:

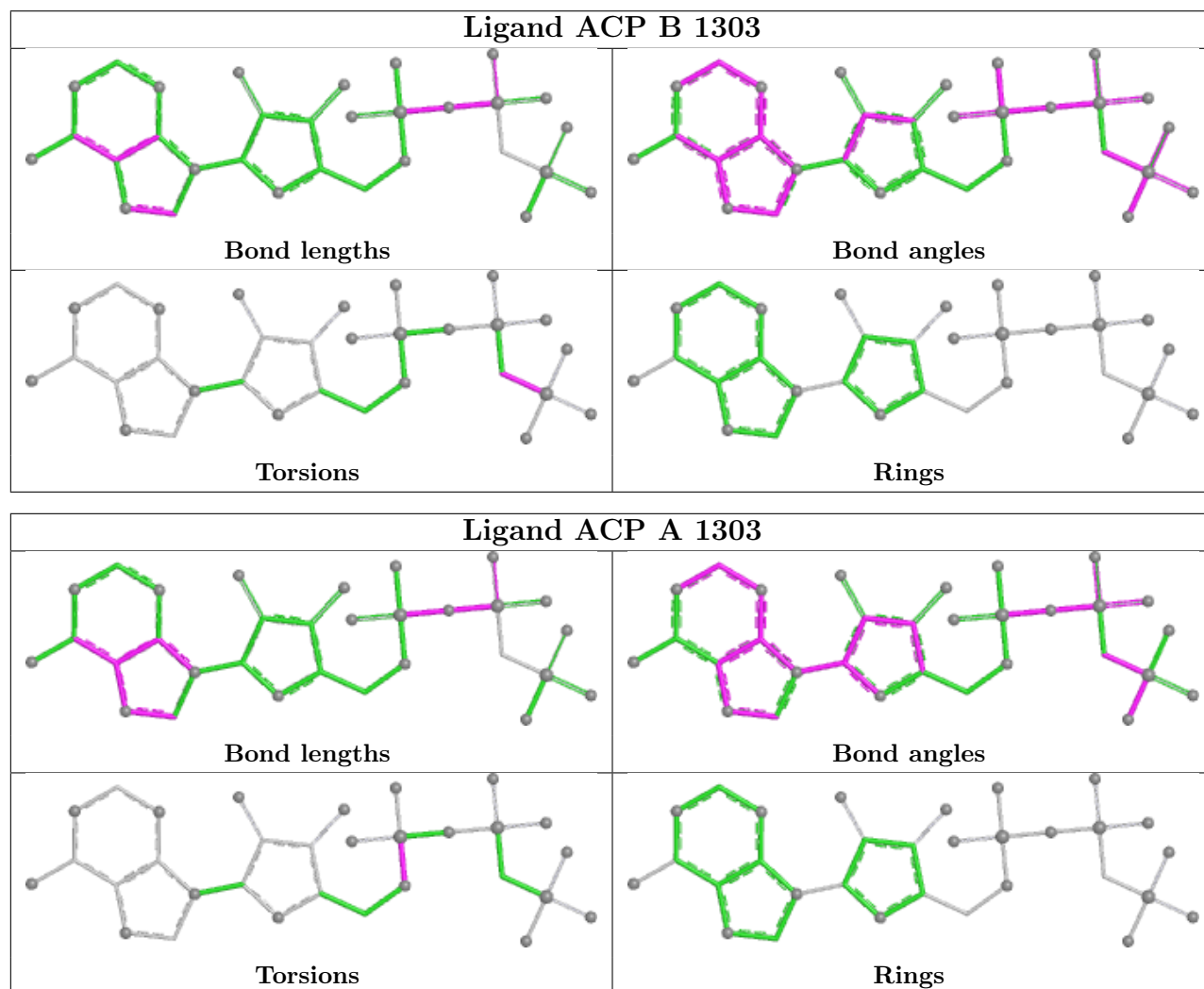
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1303	ACP	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1303	ACP	16	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

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	212/218 (97%)	0.35	10 (4%) 36 20	57, 128, 221, 262	0
2	B	204/218 (93%)	0.77	27 (13%) 7 6	62, 144, 326, 380	0
All	All	416/436 (95%)	0.56	37 (8%) 15 10	57, 134, 283, 380	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	302	THR	4.2
2	B	273	GLU	3.9
2	B	244	ILE	3.6
2	B	303	CYS	3.6
2	B	231	LEU	3.6
2	B	269	GLU	3.5
2	B	327	GLU	3.2
1	A	189	ASP	3.0
1	A	272	PRO	3.0
2	B	272	PRO	3.0
2	B	239	SER	3.0
2	B	245	ARG	3.0
2	B	270	LYS	2.9
2	B	311	TRP	2.9
1	A	241	MET	2.8
2	B	265	ILE	2.8
2	B	242	LYS	2.8
2	B	328	GLU	2.8
2	B	361	LEU	2.7
2	B	330	SER	2.7
1	A	185	ARG	2.5
1	A	332	SER	2.5
2	B	352	HIS	2.5
1	A	188	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	310	LEU	2.4
2	B	164	LEU	2.3
1	A	353	ILE	2.3
2	B	301	LYS	2.2
2	B	233	GLU	2.1
1	A	281	ASN	2.1
1	A	285	MET	2.1
1	A	330	SER	2.1
2	B	321	ASP	2.1
2	B	178	GLU	2.1
2	B	323	THR	2.1
2	B	274	ASN	2.1
2	B	237	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	NEP	B	188	14/15	0.84	0.11	111,177,198,202	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

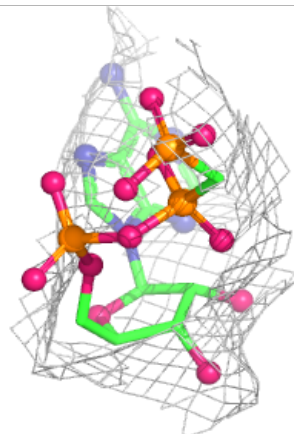
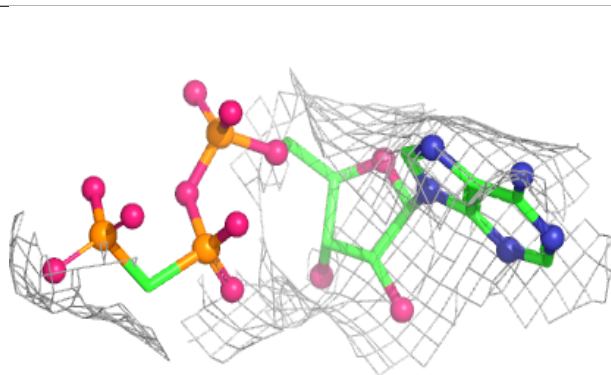
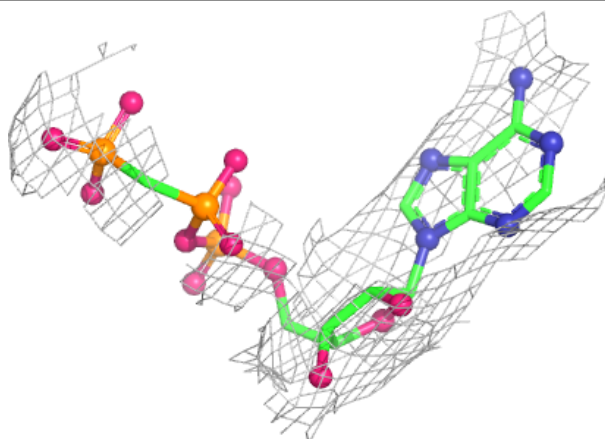
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

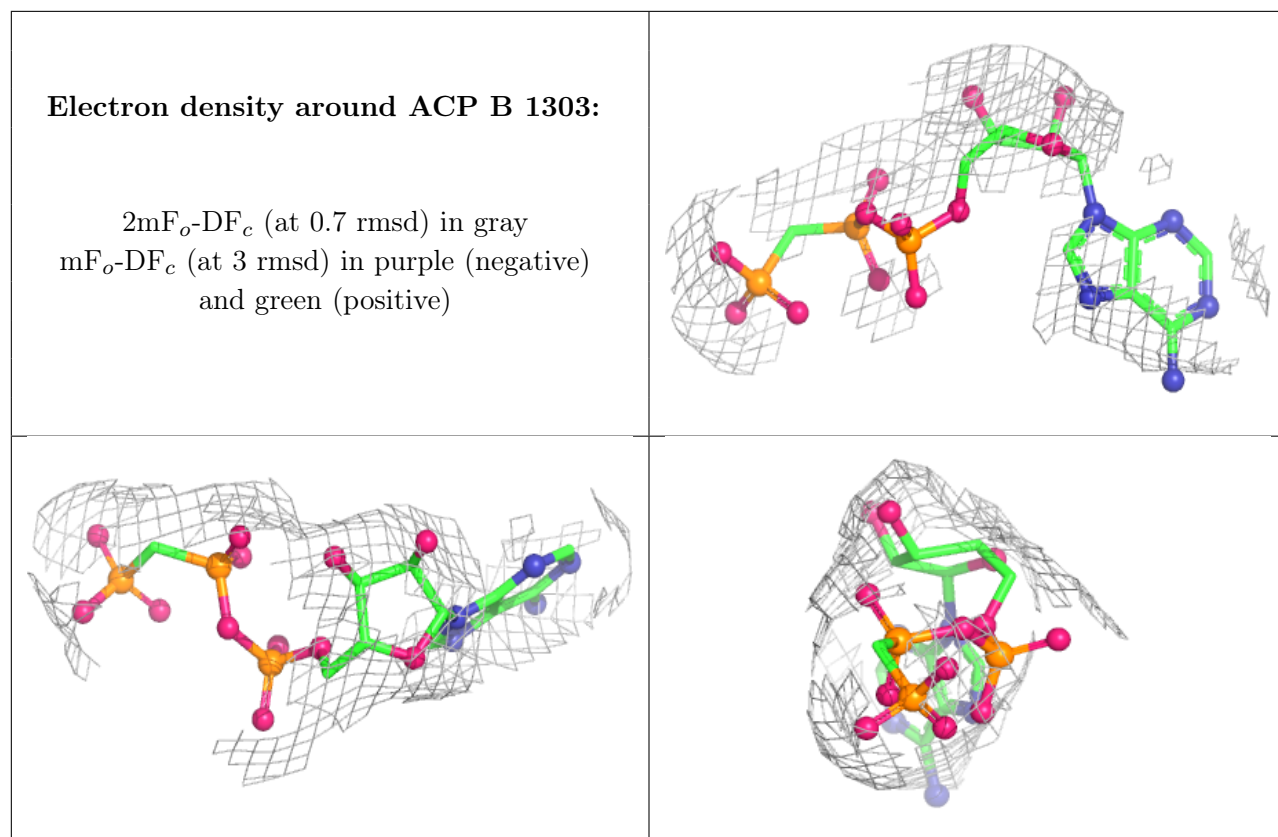
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACP	A	1303	31/31	0.91	0.09	122,149,183,215	0
3	ACP	B	1303	31/31	0.91	0.09	147,169,195,243	0
4	MG	B	1	1/1	0.98	0.04	108,108,108,108	0
4	MG	A	1	1/1	0.99	0.03	160,160,160,160	0

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 ACP A 1303:

$2mF_o-DF_c$ (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.