



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:45 AM UTC

PDB ID : 2IUT / pdb_00002iut
Title : P. aeruginosa FtsK motor domain, dimeric
Authors : Massey, T.H.; Mercoglian, C.P.; Yates, J.; Sherratt, D.J.; Lowe, J.
Deposited on : 2006-06-07
Resolution : 2.25 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

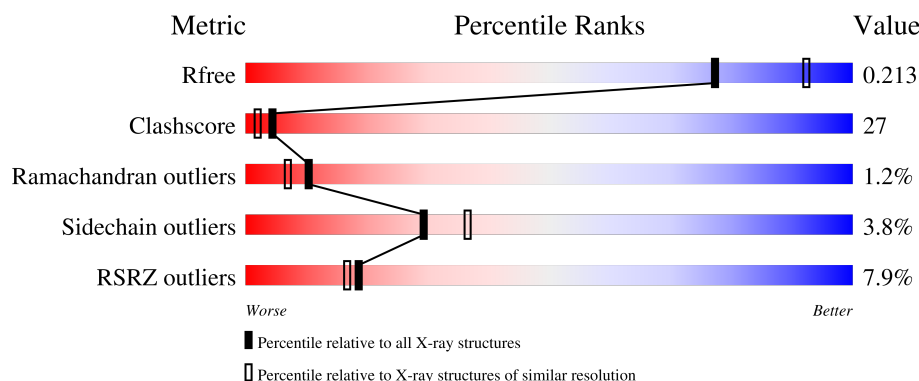
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	574	5% 41% 27% • 29%
1	B	574	6% 42% 26% • 29%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6673 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.

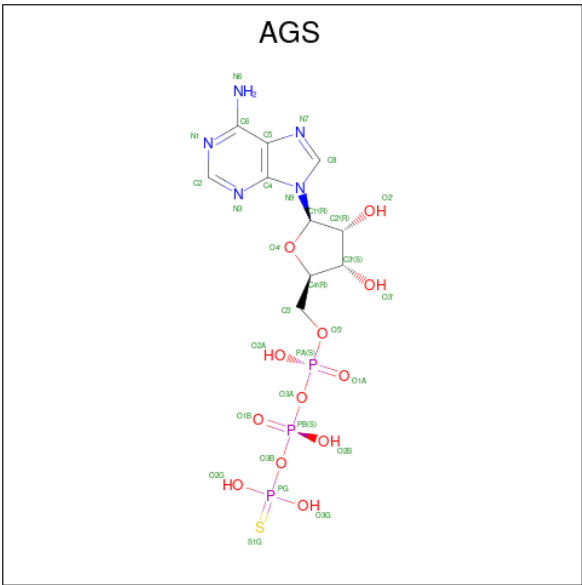
- Molecule 1 is a protein called DNA TRANSLOCASE FTSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	1
			3122	1983	541	583	15			
1	B	409	Total	C	N	O	S	0	0	1
			3122	1983	541	583	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	MET	-	expression tag	UNP Q9I0M3
A	812	LYS	-	expression tag	UNP Q9I0M3
A	813	LEU	-	expression tag	UNP Q9I0M3
A	814	HIS	-	expression tag	UNP Q9I0M3
A	815	HIS	-	expression tag	UNP Q9I0M3
A	816	HIS	-	expression tag	UNP Q9I0M3
A	817	HIS	-	expression tag	UNP Q9I0M3
A	818	HIS	-	expression tag	UNP Q9I0M3
A	819	HIS	-	expression tag	UNP Q9I0M3
B	246	MET	-	expression tag	UNP Q9I0M3
B	812	LYS	-	expression tag	UNP Q9I0M3
B	813	LEU	-	expression tag	UNP Q9I0M3
B	814	HIS	-	expression tag	UNP Q9I0M3
B	815	HIS	-	expression tag	UNP Q9I0M3
B	816	HIS	-	expression tag	UNP Q9I0M3
B	817	HIS	-	expression tag	UNP Q9I0M3
B	818	HIS	-	expression tag	UNP Q9I0M3
B	819	HIS	-	expression tag	UNP Q9I0M3

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

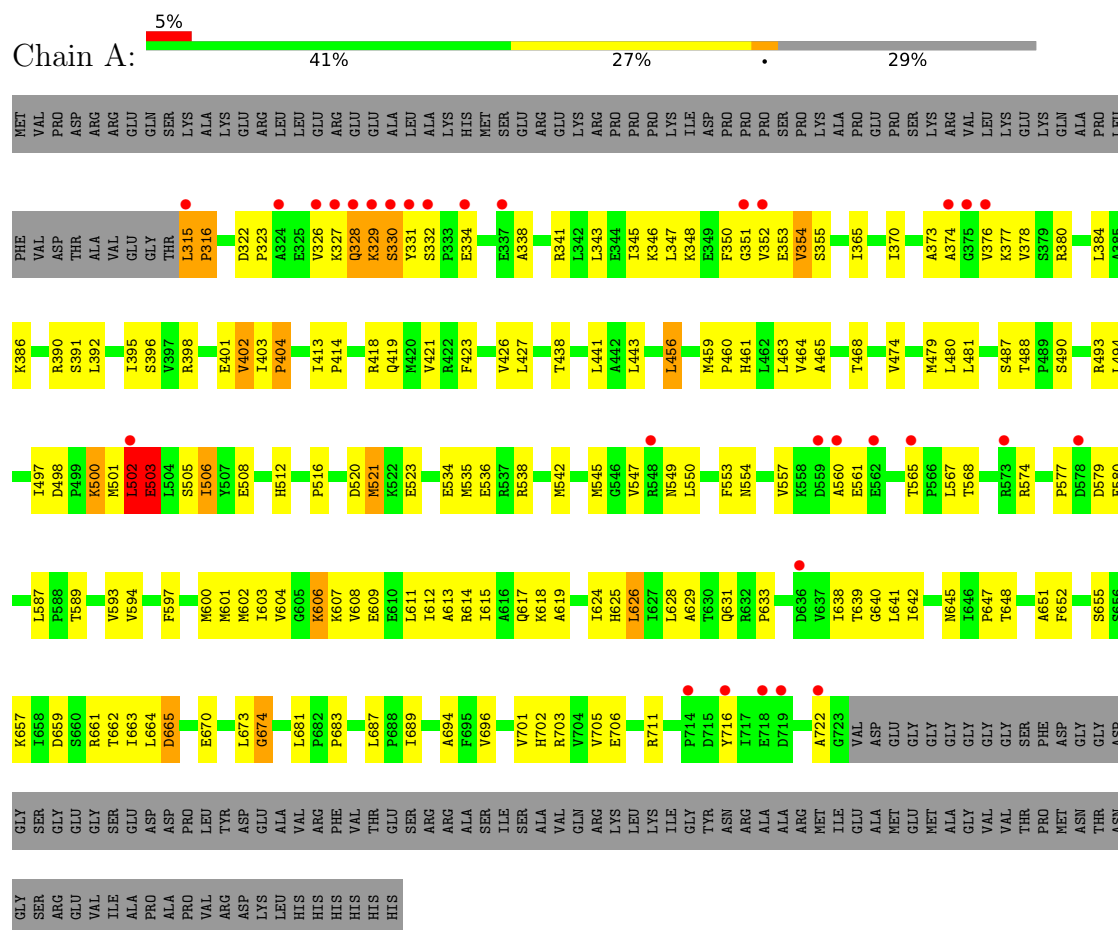
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	172	Total	O	0	0
			172	172		
4	B	193	Total	O	0	0
			193	193		

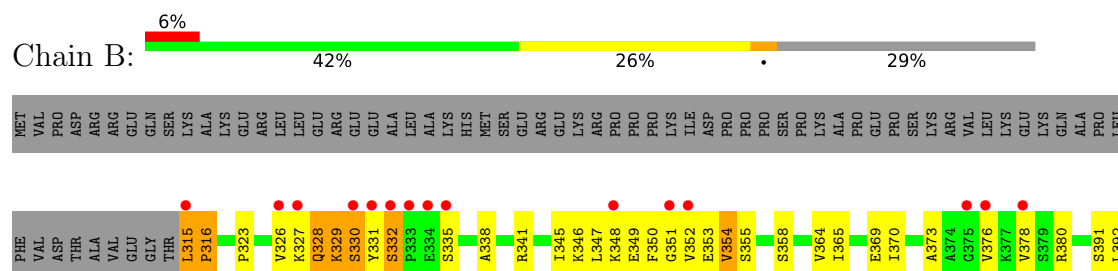
3 Residue-property plots

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: DNA TRANSLOCASE FTSK



• Molecule 1: DNA TRANSLOCASE FTSK



ALA	ASP	I663	V593	L594	I395
PRO	PRO	L664	V594	SS05	S396
VAL	LEU	D665	D595	IS06	V397
ARG	TYR	E670	E596	Y507	R398
ASP	ASP	E673	F597	E508	E401
LYS	GLU	L674	M600	H512	V402
LEU	ALA	G674	M601	P516	I403
HIS	VAL	L681	I603	T519	P404
HIS	PHE	P682	K606	D520	I413
HIS	THR	P683	E609	M521	P414
HIS	GLU	L687	E610	K522	D417
	SER	P698	L611	E523	R418
	ARG	I689	I612	A524	Q419
	ALA	R690	A613	E534	F423
	SER	V691	R614	M535	V426
	ILE	H692	I615	R538	E431
	SER	G693	A616	Y539	L441
	ALA	A694	Q617	M542	L456
	VAL	F695	K618	R545	M459
	GLN	V696	A619	V547	P460
	ARG	V701	R620	L550	H461
	LYS	H702	A621	F553	V464
	LEU	L705	I624	N554	A465
	LYS	G711	H625	R555	G466
	ILE	R711	L626	K556	T467
	GLY	Y716	A629	V557	T468
	TYR	I717	I630	A560	V474
	ASN	E718	Q631	E561	L480
	ARG	A722	R632	A562	L481
	MET	G723	P633	G564	L484
	ILE	VAL	S634	T565	S487
	GLU	ASP	V635	P566	T488
	ALA	GLU	D636	L567	P489
	MET	GLU	V637	T568	S490
	GLU	GLY	I638	R573	S499
	MET	GLY	L641	R574	R493
	ALA	GLY	T642	P577	M496
	GLY	GLY	K643	D578	I497
	VAL	GLY	A644	D579	D498
	THR	THR	N645	S655	P499
	PRO	PHE	R649	S656	K500
	MET	ASP	T650	K657	K501
	ASN	GLY	A651	I658	L502
	THR	GLY	F652	R661	E503
	ASN	GLY	GLY	T662	
	GLY	GLY	S655		
	SER	SER	S656		
	ARG	GLY	K657		
	GLU	GLU	I658		
	VAL	GLY	R661		
	ILE	SER			
	ALA	GLU			
	PRO	ASP			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.17Å 57.43Å 98.06Å 94.57° 93.80° 107.66°	Depositor
Resolution (Å)	100.00 – 2.25 97.30 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.8 (100.00-2.25) 93.8 (97.30-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 2.25Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.267 0.213 , 0.213	Depositor DCC
R_{free} test set	2278 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6673	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.21% 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: AGS, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	1/3178 (0.0%)	1.01	17/4314 (0.4%)
1	B	0.45	1/3178 (0.0%)	1.01	17/4314 (0.4%)
All	All	0.44	2/6356 (0.0%)	1.01	34/8628 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	722	ALA	C-N	-5.57	1.25	1.33
1	B	722	ALA	C-N	-5.57	1.25	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	502	LEU	N-CA-C	6.88	125.45	110.80
1	B	643	LYS	N-CA-C	6.42	118.27	111.28
1	B	655	SER	N-CA-C	6.17	120.07	112.54
1	A	665	ASP	N-CA-C	-6.12	105.40	112.86
1	A	502	LEU	N-CA-C	6.02	123.63	110.80
1	B	652	PHE	N-CA-C	-6.01	100.55	109.86
1	B	618	LYS	N-CA-C	5.94	121.87	113.02
1	A	674	GLY	N-CA-C	-5.93	103.87	112.17
1	A	655	SER	N-CA-C	5.88	120.18	112.89
1	B	474	VAL	N-CA-C	-5.85	104.81	110.72
1	B	579	ASP	N-CA-C	5.82	118.44	110.24
1	B	589	THR	N-CA-C	-5.76	101.10	110.20
1	A	395	ILE	N-CA-C	5.74	116.51	110.72
1	A	652	PHE	N-CA-C	-5.72	100.86	109.79
1	A	443	LEU	N-CA-C	5.64	117.51	111.36
1	B	487	SER	N-CA-C	5.63	118.58	109.40
1	B	503	GLU	N-CA-C	5.63	122.79	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	PRO	CA-C-N	5.62	125.55	119.76
1	A	316	PRO	C-N-CA	5.62	125.55	119.76
1	A	589	THR	N-CA-C	-5.61	101.34	110.20
1	B	316	PRO	CA-C-N	5.60	125.52	119.76
1	B	316	PRO	C-N-CA	5.60	125.52	119.76
1	A	500	LYS	N-CA-C	-5.54	103.39	110.53
1	A	503	GLU	N-CA-C	5.53	122.58	110.80
1	A	625	HIS	N-CA-C	5.51	118.39	109.40
1	B	500	LYS	N-CA-C	-5.39	102.92	110.35
1	B	401	GLU	N-CA-C	5.29	117.04	111.28
1	A	618	LYS	N-CA-C	5.28	120.52	112.54
1	A	579	ASP	N-CA-C	5.22	117.80	110.23
1	B	524	ALA	N-CA-C	-5.21	105.61	111.28
1	B	674	GLY	N-CA-C	-5.13	104.49	112.45
1	B	617	GLN	N-CA-C	5.07	116.80	111.28
1	A	487	SER	N-CA-C	5.02	117.58	109.40
1	A	506	ILE	N-CA-C	5.01	117.35	111.09

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	3122	0	3237	174	0
1	B	3122	0	3237	169	0
2	A	31	0	12	4	0
2	B	31	0	12	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	172	0	0	29	0
4	B	193	0	0	30	0
All	All	6673	0	6498	340	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 27.

All (340) 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:329:LYS:H	1:A:329:LYS:HD3	1.20	1.06
1:A:329:LYS:HG2	1:A:330:SER:H	1.23	1.04
1:B:329:LYS:H	1:B:329:LYS:HD3	1.21	1.03
1:B:329:LYS:HG2	1:B:330:SER:H	1.21	1.03
1:A:554:ASN:HD21	1:A:587:LEU:H	1.04	1.01
1:B:554:ASN:HD21	1:B:587:LEU:H	1.11	0.96
1:A:601:MET:HE1	1:A:609:GLU:HG2	1.53	0.91
1:A:497:ILE:HG21	1:A:600:MET:HE2	1.54	0.89
1:B:545:MET:HE1	1:B:567:LEU:HD13	1.55	0.88
1:B:369:GLU:HB2	4:B:2017:HOH:O	1.75	0.87
1:B:601:MET:HE1	1:B:609:GLU:HG2	1.55	0.86
4:A:2029:HOH:O	2:B:1724:AGS:S1G	2.33	0.85
1:B:497:ILE:HG21	1:B:600:MET:HE2	1.58	0.84
1:A:545:MET:HE1	1:A:567:LEU:HD13	1.62	0.81
1:A:378:VAL:HG12	1:A:401:GLU:HG2	1.61	0.80
1:B:365:ILE:HG12	4:B:2165:HOH:O	1.82	0.79
1:A:500:LYS:HD2	4:B:2029:HOH:O	1.81	0.79
1:A:557:VAL:HB	4:A:2097:HOH:O	1.84	0.77
1:B:358:SER:N	4:B:2017:HOH:O	2.17	0.76
1:A:329:LYS:H	1:A:329:LYS:CD	1.98	0.75
1:A:647:PRO:HG2	4:A:2127:HOH:O	1.87	0.75
1:A:347:LEU:HD22	1:A:352:VAL:HG21	1.70	0.74
1:B:613:ALA:O	1:B:617:GLN:HG3	1.88	0.73
2:A:1723:AGS:S1G	4:B:2032:HOH:O	2.47	0.73
1:B:373:ALA:O	1:B:376:VAL:HG12	1.89	0.73
1:B:329:LYS:H	1:B:329:LYS:CD	1.99	0.73
1:A:538:ARG:O	1:A:542:MET:HG3	1.89	0.72
1:A:373:ALA:O	1:A:376:VAL:HG12	1.89	0.72
1:B:378:VAL:HG12	1:B:401:GLU:HG2	1.71	0.72
1:B:315:LEU:N	1:B:316:PRO:HD2	2.04	0.72
1:A:617:GLN:HG2	1:A:645:ASN:ND2	2.06	0.71
1:A:329:LYS:HD3	1:A:329:LYS:N	2.01	0.71
1:A:554:ASN:ND2	1:A:587:LEU:H	1.87	0.70
1:B:329:LYS:HD3	1:B:329:LYS:N	2.02	0.69
1:B:347:LEU:HD22	1:B:352:VAL:HG21	1.74	0.69
1:A:315:LEU:N	1:A:316:PRO:HD2	2.06	0.69
1:B:329:LYS:HB2	1:B:331:TYR:CE1	2.28	0.69
1:A:329:LYS:HG2	1:A:330:SER:N	2.04	0.69
1:B:468:THR:HG23	1:B:631:GLN:OE1	1.94	0.68
1:A:355:SER:HB2	4:A:2012:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:MET:HE3	1:A:521:MET:HA	1.74	0.68
1:B:329:LYS:HG2	1:B:330:SER:N	2.03	0.68
1:A:554:ASN:HD21	1:A:587:LEU:N	1.86	0.68
1:B:467:THR:HG22	4:B:2133:HOH:O	1.92	0.68
1:A:580:GLU:HG2	4:A:2103:HOH:O	1.94	0.67
1:A:391:SER:O	1:B:502:LEU:HD11	1.95	0.67
1:B:338:ALA:O	1:B:341:ARG:HB3	1.95	0.67
1:B:521:MET:HE3	1:B:521:MET:HA	1.78	0.66
1:A:613:ALA:O	1:A:617:GLN:HG3	1.94	0.66
1:A:392:LEU:C	1:B:502:LEU:HD13	2.21	0.66
1:A:351:GLY:HA3	1:A:380:ARG:NH1	2.11	0.66
1:A:614:ARG:HG2	1:A:614:ARG:HH21	1.61	0.66
1:B:617:GLN:HG2	1:B:645:ASN:ND2	2.12	0.65
1:A:396:SER:HA	4:A:2032:HOH:O	1.97	0.65
1:B:554:ASN:ND2	1:B:587:LEU:H	1.90	0.65
1:B:351:GLY:HA3	1:B:380:ARG:NH1	2.12	0.65
1:B:335:SER:HB2	4:B:2008:HOH:O	1.96	0.64
1:A:468:THR:HG23	1:A:631:GLN:OE1	1.98	0.64
1:A:329:LYS:HB2	1:A:331:TYR:CE1	2.33	0.63
1:A:377:LYS:HG2	4:A:2019:HOH:O	1.97	0.63
1:A:465:ALA:CB	1:A:663:ILE:HG21	2.28	0.63
1:B:315:LEU:HB3	1:B:711:ARG:HE	1.63	0.63
1:A:465:ALA:HB3	1:A:663:ILE:HG21	1.81	0.63
1:B:341:ARG:O	1:B:345:ILE:HG12	1.99	0.62
1:A:315:LEU:HB3	1:A:711:ARG:HE	1.64	0.62
1:B:560:ALA:HB1	1:B:565:THR:O	1.99	0.62
1:A:516:PRO:HG3	1:A:716:TYR:CE1	2.34	0.62
1:A:560:ALA:HB1	1:A:565:THR:O	1.99	0.62
1:A:617:GLN:HG2	1:A:645:ASN:CG	2.24	0.61
1:B:465:ALA:CB	1:B:663:ILE:HG21	2.29	0.61
1:A:601:MET:HE1	1:A:609:GLU:CG	2.29	0.61
1:A:480:LEU:HD21	1:A:593:VAL:HG11	1.82	0.61
1:A:703:ARG:HA	4:A:2162:HOH:O	1.99	0.61
1:B:614:ARG:HG2	1:B:614:ARG:HH21	1.66	0.61
1:B:617:GLN:HG2	1:B:645:ASN:CG	2.26	0.60
1:A:503:GLU:OE2	2:A:1723:AGS:S1G	2.59	0.60
1:B:341:ARG:HG2	4:B:2012:HOH:O	2.00	0.60
1:B:493:ARG:HD2	1:B:512:HIS:O	2.01	0.60
1:A:488:THR:HG23	1:A:490:SER:H	1.65	0.60
1:B:465:ALA:HB3	1:B:663:ILE:HG21	1.84	0.60
1:A:545:MET:CE	1:A:567:LEU:HD13	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:LYS:NZ	1:B:606:LYS:HB3	2.17	0.59
1:B:625:HIS:ND1	4:B:2118:HOH:O	2.30	0.59
1:B:683:PRO:HA	4:B:2160:HOH:O	2.03	0.59
1:A:547:VAL:HG11	1:A:553:PHE:N	2.17	0.59
1:A:493:ARG:HD2	1:A:512:HIS:O	2.03	0.59
1:A:502:LEU:HD13	1:B:392:LEU:C	2.28	0.58
1:A:597:PHE:HZ	1:A:638:ILE:HD13	1.67	0.58
1:A:341:ARG:O	1:A:345:ILE:HG12	2.04	0.58
1:B:506:ILE:HD12	4:B:2108:HOH:O	2.04	0.57
1:B:597:PHE:HZ	1:B:638:ILE:HD13	1.69	0.57
1:B:545:MET:CE	1:B:567:LEU:HD13	2.30	0.57
1:B:690:ARG:CZ	4:B:2165:HOH:O	2.51	0.57
1:A:657:LYS:HE3	4:A:2139:HOH:O	2.04	0.57
1:A:338:ALA:O	1:A:341:ARG:HB3	2.06	0.56
1:B:547:VAL:HG11	1:B:553:PHE:N	2.20	0.56
1:B:315:LEU:N	4:B:2001:HOH:O	2.38	0.56
1:B:550:LEU:HD21	1:B:587:LEU:HB2	1.86	0.56
1:B:594:VAL:HG11	1:B:597:PHE:HB3	1.87	0.56
1:A:606:LYS:HB3	1:A:606:LYS:NZ	2.21	0.56
1:A:631:GLN:C	1:A:633:PRO:HD3	2.31	0.56
1:B:329:LYS:CG	1:B:330:SER:H	1.99	0.56
1:A:593:VAL:O	1:A:593:VAL:HG23	2.06	0.56
1:A:594:VAL:HG11	1:A:597:PHE:HB3	1.88	0.55
1:B:347:LEU:HB3	1:B:352:VAL:HG23	1.87	0.55
1:A:689:ILE:O	1:A:689:ILE:HG13	2.06	0.55
1:A:347:LEU:HB3	1:A:352:VAL:HG23	1.88	0.55
1:A:465:ALA:HB1	1:A:633:PRO:HG3	1.88	0.55
1:A:506:ILE:HD11	1:A:702:HIS:HA	1.89	0.55
1:B:327:LYS:O	1:B:329:LYS:N	2.40	0.55
1:B:538:ARG:O	1:B:542:MET:HG3	2.07	0.54
1:B:615:ILE:HG21	1:B:626:LEU:HD13	1.88	0.54
1:B:414:PRO:CG	1:B:673:LEU:HD21	2.38	0.54
1:A:601:MET:CE	1:A:609:GLU:HG2	2.33	0.54
1:B:464:VAL:O	1:B:629:ALA:HA	2.07	0.54
1:B:402:VAL:HG22	1:B:687:LEU:CD1	2.37	0.54
1:A:327:LYS:O	1:A:329:LYS:N	2.40	0.54
1:B:611:LEU:O	1:B:615:ILE:HG12	2.08	0.53
1:A:683:PRO:HB3	4:A:2127:HOH:O	2.08	0.53
1:A:521:MET:HE2	1:A:600:MET:HG3	1.90	0.53
1:A:315:LEU:N	4:A:2001:HOH:O	2.42	0.53
1:B:315:LEU:N	1:B:316:PRO:CD	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:MET:HE2	1:B:600:MET:HG3	1.90	0.53
1:A:706:GLU:HB2	4:A:2162:HOH:O	2.07	0.53
1:B:619:ALA:HB1	1:B:624:ILE:HB	1.91	0.53
1:B:631:GLN:C	1:B:633:PRO:HD3	2.34	0.53
1:A:329:LYS:CG	1:A:330:SER:H	2.00	0.53
1:B:341:ARG:HB2	4:B:2010:HOH:O	2.09	0.53
1:B:593:VAL:HG23	1:B:593:VAL:O	2.07	0.53
1:B:601:MET:HE1	1:B:609:GLU:CG	2.33	0.52
1:A:550:LEU:C	1:A:550:LEU:HD13	2.35	0.52
1:A:657:LYS:NZ	1:A:661:ARG:HH12	2.07	0.52
1:B:426:VAL:HG21	1:B:694:ALA:HB2	1.92	0.52
1:B:535:MET:HE1	1:B:614:ARG:NH2	2.23	0.52
1:A:402:VAL:HG22	1:A:687:LEU:CD1	2.40	0.52
1:B:349:GLU:HB3	4:B:2015:HOH:O	2.10	0.52
1:A:502:LEU:HD11	1:B:391:SER:O	2.09	0.52
1:B:315:LEU:HD22	1:B:711:ARG:HE	1.73	0.52
1:B:612:ILE:HG21	1:B:642:ILE:HD12	1.92	0.52
1:A:651:ALA:CB	1:A:663:ILE:HD12	2.40	0.52
1:B:516:PRO:HG3	1:B:716:TYR:CE1	2.45	0.51
1:B:601:MET:CE	1:B:609:GLU:HG2	2.33	0.51
1:B:508:GLU:HA	1:B:508:GLU:OE1	2.10	0.51
1:A:464:VAL:O	1:A:629:ALA:HA	2.10	0.51
1:A:506:ILE:HG22	4:A:2083:HOH:O	2.10	0.51
1:B:378:VAL:HG21	4:B:2040:HOH:O	2.10	0.51
1:B:521:MET:HE2	1:B:600:MET:CG	2.41	0.51
1:A:535:MET:HE1	1:A:614:ARG:NH2	2.26	0.50
1:B:506:ILE:HD11	1:B:702:HIS:HA	1.92	0.50
1:B:594:VAL:HG11	1:B:600:MET:HE3	1.94	0.50
1:A:611:LEU:O	1:A:615:ILE:HG12	2.11	0.50
1:B:441:LEU:HD11	1:B:456:LEU:HG	1.92	0.50
1:B:460:PRO:O	1:B:625:HIS:HD2	1.95	0.50
1:B:692:HIS:HE1	4:B:2165:HOH:O	1.93	0.50
1:B:465:ALA:HB1	1:B:633:PRO:HG3	1.92	0.50
1:A:521:MET:HG2	1:A:603:ILE:HB	1.94	0.50
1:B:480:LEU:HD21	1:B:593:VAL:HG11	1.93	0.50
1:B:589:THR:HG22	4:B:2118:HOH:O	2.12	0.50
1:A:418:ARG:NH2	4:A:2049:HOH:O	2.38	0.49
1:A:516:PRO:HG3	1:A:716:TYR:CD1	2.47	0.49
1:A:681:LEU:C	1:A:681:LEU:HD23	2.37	0.49
1:B:557:VAL:O	1:B:561:GLU:HG3	2.11	0.49
1:A:441:LEU:HD12	1:A:459:MET:HE1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LYS:N	4:B:2006:HOH:O	2.45	0.49
1:A:423:PHE:CE1	1:A:427:LEU:HD11	2.47	0.49
1:A:550:LEU:HD21	1:A:587:LEU:HB2	1.94	0.49
1:B:460:PRO:HG2	1:B:461:HIS:CD2	2.47	0.49
1:A:315:LEU:N	1:A:316:PRO:CD	2.73	0.49
1:B:521:MET:HG2	1:B:603:ILE:HB	1.94	0.49
1:A:534:GLU:O	1:A:538:ARG:HG3	2.13	0.49
1:B:488:THR:HG23	1:B:490:SER:H	1.78	0.49
1:B:689:ILE:O	1:B:689:ILE:HG13	2.10	0.49
1:A:498:ASP:O	1:A:500:LYS:O	2.31	0.48
1:B:574:ARG:NH1	1:B:577:PRO:HA	2.28	0.48
1:A:378:VAL:CG1	1:A:401:GLU:HG2	2.39	0.48
1:A:547:VAL:HG13	4:A:2093:HOH:O	2.13	0.48
1:B:554:ASN:HA	1:B:557:VAL:HG12	1.95	0.48
1:A:315:LEU:HD22	1:A:711:ARG:HE	1.78	0.48
1:A:615:ILE:HG21	1:A:626:LEU:HD13	1.94	0.48
1:B:327:LYS:HG2	4:B:2006:HOH:O	2.13	0.48
1:A:474:VAL:CG2	2:A:1723:AGS:H5'2	2.44	0.48
1:A:554:ASN:HA	1:A:557:VAL:HG12	1.96	0.48
1:B:480:LEU:O	1:B:484:LEU:HG	2.14	0.48
1:A:474:VAL:HG23	2:A:1723:AGS:H5'2	1.95	0.48
1:B:520:ASP:OD2	1:B:523:GLU:HG3	2.13	0.48
1:B:354:VAL:HG13	1:B:370:ILE:HB	1.95	0.47
1:B:614:ARG:HG2	1:B:614:ARG:NH2	2.29	0.47
1:A:421:VAL:HG22	4:A:2051:HOH:O	2.14	0.47
1:A:502:LEU:HB2	4:A:2079:HOH:O	2.14	0.47
1:A:557:VAL:O	1:A:561:GLU:HG3	2.15	0.47
1:B:403:ILE:O	1:B:404:PRO:C	2.58	0.47
1:B:414:PRO:HG3	1:B:673:LEU:HD21	1.95	0.47
1:B:539:TYR:OH	1:B:621:ALA:HB3	2.14	0.47
1:A:614:ARG:HG2	1:A:614:ARG:NH2	2.27	0.47
1:B:326:VAL:HG12	1:B:327:LYS:N	2.29	0.47
1:A:327:LYS:O	1:A:328:GLN:C	2.57	0.47
1:A:501:MET:O	1:A:505:SER:HB3	2.15	0.47
1:A:550:LEU:HD13	1:A:550:LEU:O	2.15	0.47
1:A:497:ILE:HG21	1:A:600:MET:CE	2.35	0.47
1:A:506:ILE:HD11	1:A:702:HIS:CA	2.44	0.47
1:A:607:LYS:HG3	4:A:2110:HOH:O	2.14	0.47
1:A:326:VAL:HG12	1:A:327:LYS:N	2.30	0.47
1:A:441:LEU:HD22	1:A:479:MET:HB3	1.96	0.47
1:A:638:ILE:HB	1:A:662:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ASP:OD2	1:A:523:GLU:HG3	2.15	0.47
1:A:386:LYS:HA	4:A:2025:HOH:O	2.15	0.47
1:A:414:PRO:CG	1:A:673:LEU:HD21	2.44	0.47
1:B:681:LEU:HD23	1:B:682:PRO:O	2.14	0.47
1:A:441:LEU:HD11	1:A:456:LEU:HG	1.97	0.46
1:A:674:GLY:HA2	4:A:2145:HOH:O	2.15	0.46
1:B:556:LYS:HD2	4:B:2103:HOH:O	2.14	0.46
1:B:348:LYS:O	1:B:350:PHE:O	2.33	0.46
1:B:474:VAL:HG23	2:B:1724:AGS:H5'2	1.96	0.46
1:A:346:LYS:HE3	1:A:391:SER:O	2.16	0.46
1:B:547:VAL:HG12	1:B:549:ASN:H	1.81	0.46
1:A:327:LYS:O	1:A:327:LYS:HG3	2.14	0.46
1:A:426:VAL:HG21	1:A:694:ALA:HB2	1.96	0.46
1:A:612:ILE:HG21	1:A:642:ILE:HD12	1.97	0.46
1:B:481:LEU:HD22	1:B:696:VAL:HG21	1.98	0.46
1:A:328:GLN:HE22	1:B:323:PRO:HD2	1.80	0.46
1:B:402:VAL:HG22	1:B:687:LEU:HD13	1.97	0.46
1:B:661:ARG:O	1:B:665:ASP:N	2.45	0.46
1:B:701:VAL:O	1:B:705:VAL:HG23	2.16	0.46
1:B:711:ARG:HH21	1:B:711:ARG:HG3	1.80	0.46
1:B:638:ILE:HB	1:B:662:THR:HG22	1.97	0.46
1:B:690:ARG:NE	4:B:2165:HOH:O	2.49	0.46
1:A:460:PRO:HG2	1:A:461:HIS:CD2	2.50	0.45
1:B:498:ASP:O	1:B:500:LYS:O	2.33	0.45
1:A:604:VAL:CG1	1:A:608:VAL:HG23	2.47	0.45
1:A:327:LYS:HB2	1:A:419:GLN:OE1	2.17	0.45
1:A:354:VAL:CG1	1:A:355:SER:N	2.76	0.45
1:A:403:ILE:O	1:A:404:PRO:C	2.59	0.45
1:B:610:GLU:HG3	4:B:2122:HOH:O	2.16	0.45
1:B:651:ALA:CB	1:B:663:ILE:HD12	2.47	0.45
1:A:463:LEU:HD23	1:A:628:LEU:HB2	1.98	0.45
1:A:574:ARG:NH1	1:A:577:PRO:HA	2.31	0.45
1:B:554:ASN:HA	1:B:557:VAL:CG1	2.45	0.45
1:A:536:GLU:OE2	1:A:614:ARG:NH1	2.50	0.45
1:A:557:VAL:HA	1:A:567:LEU:HD12	1.99	0.45
1:A:647:PRO:HD2	4:A:2066:HOH:O	2.16	0.45
1:B:493:ARG:NE	4:B:2079:HOH:O	2.40	0.45
1:B:499:PRO:O	1:B:519:THR:HG23	2.17	0.45
1:B:506:ILE:HG22	4:B:2085:HOH:O	2.15	0.45
1:B:596:GLU:HB2	4:B:2081:HOH:O	2.15	0.45
1:B:327:LYS:O	1:B:328:GLN:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLY:O	1:A:380:ARG:CZ	2.64	0.45
1:A:413:ILE:HA	1:A:414:PRO:HD3	1.86	0.45
1:A:547:VAL:HG12	1:A:549:ASN:H	1.82	0.45
1:B:501:MET:O	1:B:505:SER:HB3	2.16	0.45
1:A:657:LYS:HG2	1:A:670:GLU:CD	2.42	0.44
1:A:348:LYS:O	1:A:350:PHE:O	2.36	0.44
1:A:398:ARG:NH1	4:A:2037:HOH:O	2.46	0.44
1:B:503:GLU:HB2	1:B:595:ASP:OD1	2.17	0.44
1:B:331:TYR:O	1:B:332:SER:C	2.60	0.44
1:A:374:ALA:N	4:A:2015:HOH:O	2.50	0.44
1:B:657:LYS:NZ	1:B:661:ARG:HH12	2.16	0.44
1:A:459:MET:SD	1:A:648:THR:HG21	2.58	0.44
4:A:2010:HOH:O	1:B:501:MET:HB3	2.16	0.44
1:B:606:LYS:HB3	1:B:606:LYS:HZ2	1.82	0.44
1:B:657:LYS:HG2	1:B:670:GLU:CD	2.42	0.44
1:A:380:ARG:O	1:A:384:LEU:HD13	2.18	0.44
1:B:351:GLY:O	1:B:380:ARG:CZ	2.66	0.44
1:A:481:LEU:HD22	1:A:696:VAL:HG21	1.99	0.43
1:B:315:LEU:N	4:B:2002:HOH:O	2.51	0.43
1:B:554:ASN:HD21	1:B:587:LEU:N	1.94	0.43
1:B:353:GLU:O	1:B:354:VAL:HG23	2.18	0.43
1:B:634:SER:OG	1:B:637:VAL:HG23	2.18	0.43
1:A:631:GLN:O	1:A:631:GLN:HG2	2.19	0.43
1:B:354:VAL:CG1	1:B:355:SER:N	2.80	0.43
1:B:631:GLN:O	1:B:631:GLN:HG2	2.17	0.43
1:B:557:VAL:HA	1:B:567:LEU:HD12	1.99	0.43
1:B:594:VAL:CG1	1:B:600:MET:HE3	2.49	0.43
1:A:354:VAL:HG13	1:A:355:SER:N	2.34	0.43
1:A:351:GLY:O	1:A:352:VAL:CG1	2.67	0.42
1:A:659:ASP:O	1:A:663:ILE:HG12	2.19	0.42
1:B:592:VAL:HB	1:B:626:LEU:HD12	2.00	0.42
1:A:331:TYR:O	1:A:332:SER:C	2.61	0.42
1:A:354:VAL:HG13	1:A:370:ILE:HB	2.01	0.42
1:A:353:GLU:O	1:A:354:VAL:HG23	2.19	0.42
1:A:402:VAL:HG22	1:A:687:LEU:HD13	2.00	0.42
1:B:649:ARG:HH21	1:B:649:ARG:HG3	1.84	0.42
1:B:681:LEU:HD23	1:B:681:LEU:C	2.44	0.42
1:B:364:VAL:HB	1:B:692:HIS:CE1	2.54	0.42
1:B:593:VAL:O	1:B:593:VAL:CG2	2.67	0.42
1:A:373:ALA:HB1	4:A:2015:HOH:O	2.18	0.42
1:A:554:ASN:HA	1:A:557:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:THR:HG22	2:B:1724:AGS:O2G	2.19	0.42
1:A:322:ASP:HA	1:A:323:PRO:HD3	1.89	0.42
1:A:365:ILE:C	1:A:365:ILE:HD12	2.45	0.42
1:A:390:ARG:HG2	1:A:390:ARG:HH21	1.84	0.42
1:B:346:LYS:HD2	1:B:391:SER:HB2	2.02	0.42
1:A:594:VAL:CG1	1:A:600:MET:HE3	2.50	0.42
1:A:639:THR:OG1	1:A:642:ILE:HG12	2.20	0.42
1:A:640:GLY:N	4:A:2123:HOH:O	2.52	0.42
1:A:663:ILE:HB	4:A:2067:HOH:O	2.18	0.42
1:B:550:LEU:HD13	1:B:550:LEU:C	2.45	0.42
1:B:395:ILE:HG23	1:B:396:SER:N	2.35	0.42
1:B:414:PRO:HG2	1:B:673:LEU:HD21	2.00	0.42
1:B:506:ILE:HD11	1:B:702:HIS:CA	2.50	0.42
1:B:534:GLU:O	1:B:538:ARG:HG3	2.20	0.42
1:A:351:GLY:C	1:A:352:VAL:HG13	2.45	0.42
1:A:506:ILE:HD11	1:A:702:HIS:HB2	2.02	0.42
1:A:354:VAL:N	4:A:2011:HOH:O	2.53	0.41
1:A:503:GLU:N	4:A:2079:HOH:O	2.53	0.41
1:A:508:GLU:OE1	1:A:508:GLU:HA	2.20	0.41
1:B:398:ARG:NH1	4:B:2037:HOH:O	2.51	0.41
1:B:516:PRO:HG3	1:B:716:TYR:CD1	2.55	0.41
1:B:696:VAL:HG13	1:B:696:VAL:O	2.20	0.41
1:B:413:ILE:HA	1:B:414:PRO:HD3	1.87	0.41
1:B:474:VAL:CG2	2:B:1724:AGS:H5'2	2.51	0.41
1:B:625:HIS:HE1	4:B:2132:HOH:O	2.02	0.41
1:B:329:LYS:HB2	1:B:331:TYR:CZ	2.53	0.41
1:B:351:GLY:C	1:B:352:VAL:HG13	2.46	0.41
1:A:351:GLY:O	1:A:352:VAL:HG13	2.20	0.41
1:A:535:MET:CE	1:A:614:ARG:HH22	2.32	0.41
1:A:631:GLN:O	1:A:633:PRO:HD3	2.20	0.41
1:B:315:LEU:HB3	1:B:711:ARG:NE	2.34	0.41
1:B:327:LYS:HB2	1:B:419:GLN:OE1	2.20	0.41
1:A:315:LEU:HD23	1:A:711:ARG:HH11	1.85	0.41
1:A:332:SER:C	1:A:334:GLU:N	2.78	0.41
1:A:593:VAL:O	1:A:593:VAL:CG2	2.67	0.41
1:A:664:LEU:O	1:A:665:ASP:HB2	2.20	0.41
1:A:657:LYS:HB3	1:A:661:ARG:HH22	1.85	0.41
1:B:423:PHE:HE1	1:B:481:LEU:HB3	1.86	0.41
1:A:414:PRO:HG3	1:A:673:LEU:HD21	2.02	0.41
1:A:651:ALA:HB2	1:A:663:ILE:HD12	2.01	0.41
1:B:589:THR:CG2	4:B:2118:HOH:O	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:VAL:O	1:A:696:VAL:HG13	2.19	0.41
1:B:597:PHE:CZ	1:B:638:ILE:HD13	2.52	0.41
1:A:594:VAL:HG11	1:A:600:MET:HE3	2.02	0.40
1:A:459:MET:N	1:A:460:PRO:HA	2.36	0.40
1:B:496:MET:HE1	1:B:507:TYR:CG	2.56	0.40
1:A:651:ALA:HB1	1:A:663:ILE:HD12	2.02	0.40
1:B:354:VAL:HG13	1:B:355:SER:N	2.37	0.40
1:B:459:MET:N	1:B:460:PRO:HA	2.36	0.40
1:A:619:ALA:HB1	1:A:624:ILE:HB	2.03	0.40
1:A:701:VAL:O	1:A:705:VAL:HG23	2.21	0.40
1:B:467:THR:HG21	1:B:655:SER:OG	2.21	0.40
1:A:657:LYS:HB3	1:A:657:LYS:HE2	1.89	0.40
1:B:354:VAL:HG21	1:B:370:ILE:HD12	2.02	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	407/574 (71%)	389 (96%)	13 (3%)	5 (1%)	10	7
1	B	407/574 (71%)	387 (95%)	15 (4%)	5 (1%)	10	7
All	All	814/1148 (71%)	776 (95%)	28 (3%)	10 (1%)	10	7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	LEU
1	B	502	LEU
1	A	328	GLN
1	B	328	GLN
1	A	503	GLU

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Mol	Chain	Res	Type
1	B	330	SER
1	A	330	SER
1	B	404	PRO
1	A	404	PRO
1	B	332	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/481 (72%)	332 (96%)	14 (4%)	28	34
1	B	346/481 (72%)	334 (96%)	12 (4%)	32	39
All	All	692/962 (72%)	666 (96%)	26 (4%)	29	36

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	LEU
1	A	329	LYS
1	A	343	LEU
1	A	354	VAL
1	A	402	VAL
1	A	438	THR
1	A	456	LEU
1	A	494	LEU
1	A	521	MET
1	A	568	THR
1	A	602	MET
1	A	606	LYS
1	A	626	LEU
1	A	641	LEU
1	B	315	LEU
1	B	329	LYS
1	B	354	VAL
1	B	402	VAL

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Mol	Chain	Res	Type
1	B	404	PRO
1	B	456	LEU
1	B	521	MET
1	B	568	THR
1	B	602	MET
1	B	606	LYS
1	B	626	LEU
1	B	641	LEU

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	415	ASN
1	A	554	ASN
1	A	583	GLN
1	A	617	GLN
1	A	645	ASN
1	A	666	GLN
1	B	415	ASN
1	B	554	ASN
1	B	583	GLN
1	B	625	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
2	AGS	B	1724	3	32,33,33	2.61	10 (31%)	45,52,52	1.50	8 (17%)
2	AGS	A	1723	3	32,33,33	2.56	10 (31%)	45,52,52	1.44	7 (15%)

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	AGS	B	1724	3	-	5/21/38/38	0/3/3/3
2	AGS	A	1723	3	-	5/21/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1724	AGS	PB-O3A	-8.55	1.50	1.59
2	A	1723	AGS	PB-O3A	-6.79	1.52	1.59
2	A	1723	AGS	PA-O3A	6.40	1.66	1.59
2	B	1724	AGS	PG-S1G	-6.23	1.77	1.90
2	A	1723	AGS	C6-N6	5.12	1.47	1.34
2	A	1723	AGS	PG-S1G	-5.01	1.79	1.90
2	B	1724	AGS	C6-N6	4.57	1.45	1.34
2	B	1724	AGS	PA-O3A	4.30	1.64	1.59
2	B	1724	AGS	C4-N3	3.70	1.41	1.34
2	A	1723	AGS	C4-N3	3.58	1.41	1.34
2	A	1723	AGS	C2-N1	3.36	1.39	1.33
2	A	1723	AGS	C5-C4	3.33	1.45	1.39
2	B	1724	AGS	C5-C4	3.13	1.44	1.39
2	B	1724	AGS	C2-N1	2.95	1.39	1.33
2	A	1723	AGS	C2-N3	2.28	1.38	1.33
2	A	1723	AGS	PG-O2G	-2.22	1.47	1.54
2	B	1724	AGS	PG-O2G	-2.22	1.47	1.54
2	B	1724	AGS	O5'-C5'	-2.14	1.36	1.44
2	B	1724	AGS	C1'-N9	2.09	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1723	AGS	C1'-N9	2.06	1.52	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1723	AGS	N9-C8-N7	4.20	119.89	113.94
2	B	1724	AGS	N9-C8-N7	4.10	119.75	113.94
2	B	1724	AGS	C4-N9-C8	-3.73	101.82	105.74
2	A	1723	AGS	C4-N9-C8	-3.63	101.93	105.74
2	B	1724	AGS	O3A-PB-O1B	-3.07	101.47	110.70
2	A	1723	AGS	O3A-PB-O1B	-3.03	101.59	110.70
2	B	1724	AGS	PB-O3B-PG	-2.36	124.52	133.17
2	A	1723	AGS	PB-O3B-PG	-2.25	124.93	133.17
2	B	1724	AGS	O2A-PA-O1A	2.22	122.76	112.44
2	B	1724	AGS	O3G-PG-O3B	2.16	111.84	104.64
2	B	1724	AGS	C5-N7-C8	-2.13	100.11	103.45
2	A	1723	AGS	C5-N7-C8	-2.12	100.12	103.45
2	A	1723	AGS	O2G-PG-O3B	-2.06	97.75	104.64
2	A	1723	AGS	O2A-PA-O1A	2.04	121.93	112.44
2	B	1724	AGS	C4-C5-N7	2.02	112.89	110.58

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1723	AGS	C5'-O5'-PA-O1A
2	B	1724	AGS	C5'-O5'-PA-O1A
2	B	1724	AGS	PA-O3A-PB-O2B
2	A	1723	AGS	O4'-C4'-C5'-O5'
2	A	1723	AGS	C3'-C4'-C5'-O5'
2	A	1723	AGS	PA-O3A-PB-O2B
2	B	1724	AGS	O4'-C4'-C5'-O5'
2	B	1724	AGS	C3'-C4'-C5'-O5'
2	A	1723	AGS	PA-O3A-PB-O1B
2	B	1724	AGS	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 8 short contacts:

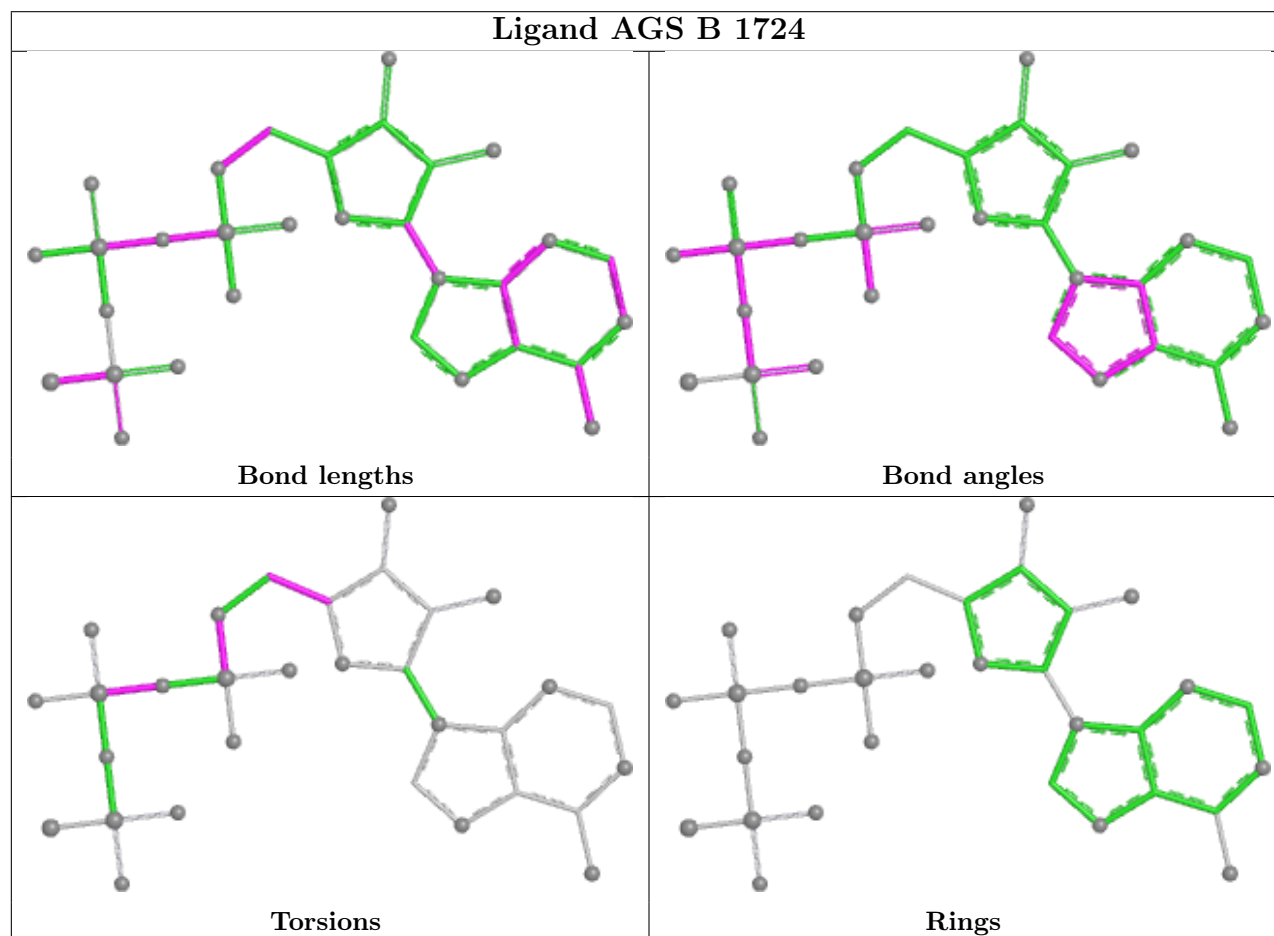
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1724	AGS	4	0

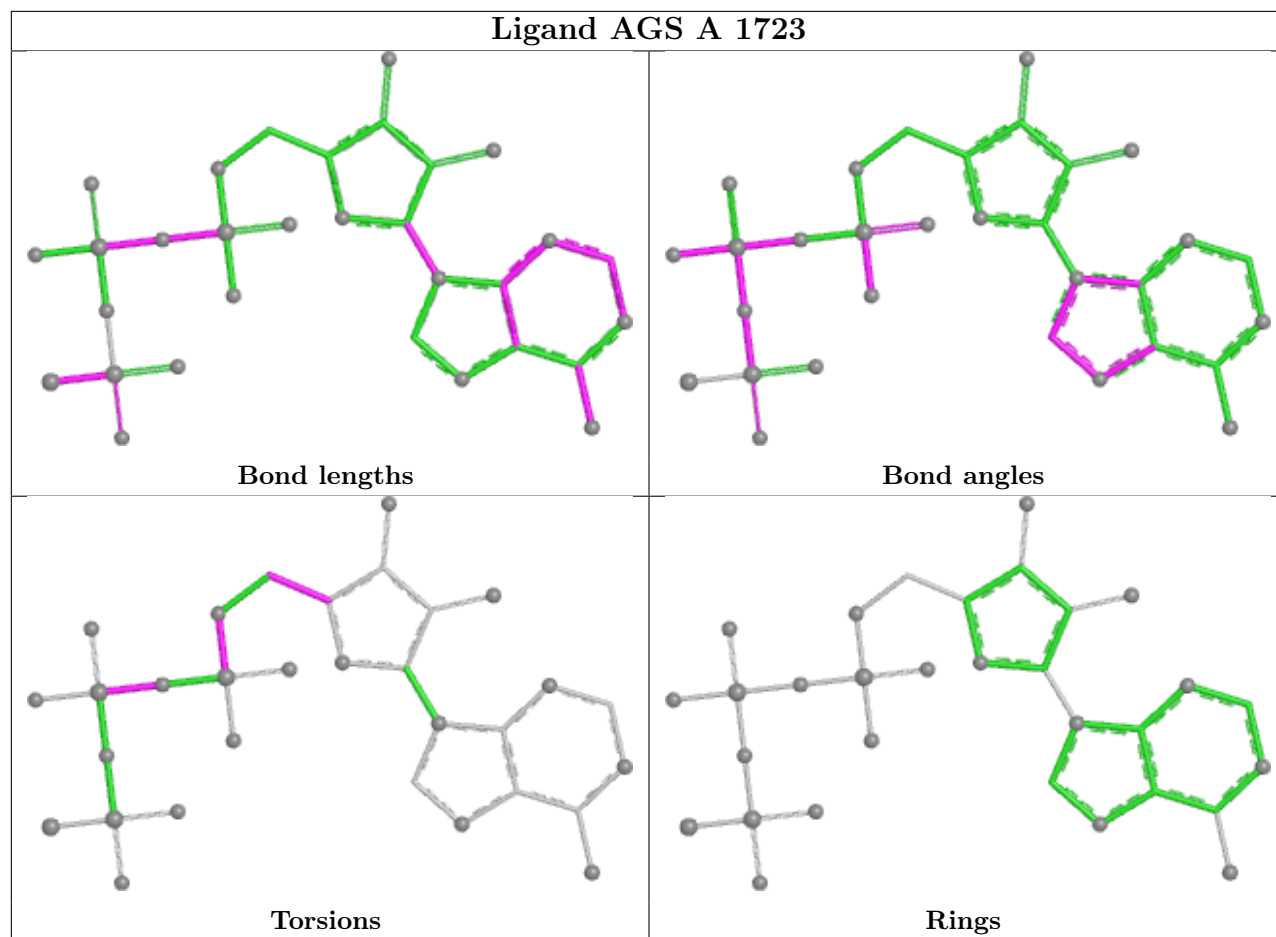
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1723	AGS	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	409/574 (71%)	0.43	30 (7%) 21 19	10, 30, 57, 97	0
1	B	409/574 (71%)	0.38	35 (8%) 16 15	11, 30, 57, 97	0
All	All	818/1148 (71%)	0.40	65 (7%) 18 17	10, 30, 57, 97	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	TYR	7.5
1	A	375	GLY	5.2
1	A	718	GLU	4.3
1	A	327	LYS	4.3
1	A	331	TYR	4.3
1	A	326	VAL	4.2
1	B	326	VAL	4.2
1	B	351	GLY	4.1
1	A	351	GLY	4.0
1	A	330	SER	3.8
1	A	328	GLN	3.6
1	B	332	SER	3.5
1	B	501	MET	3.4
1	A	352	VAL	3.3
1	B	352	VAL	3.3
1	B	636	ASP	3.3
1	A	376	VAL	3.2
1	B	333	PRO	3.1
1	B	502	LEU	3.1
1	A	332	SER	3.1
1	B	718	GLU	3.0
1	B	563	ALA	2.9
1	B	610	GLU	2.9
1	A	560	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	315	LEU	2.9
1	B	315	LEU	2.9
1	A	565	THR	2.8
1	B	500	LYS	2.7
1	A	716	TYR	2.7
1	B	375	GLY	2.7
1	B	378	VAL	2.6
1	A	329	LYS	2.6
1	A	334	GLU	2.6
1	A	719	ASP	2.5
1	B	330	SER	2.5
1	B	658	ILE	2.5
1	B	557	VAL	2.5
1	A	559	ASP	2.5
1	A	324	ALA	2.4
1	B	335	SER	2.4
1	B	419	GLN	2.4
1	A	374	ALA	2.4
1	B	376	VAL	2.4
1	B	327	LYS	2.3
1	B	560	ALA	2.3
1	B	334	GLU	2.3
1	A	714	PRO	2.3
1	B	565	THR	2.3
1	B	348	LYS	2.2
1	A	573	ARG	2.2
1	A	337	GLU	2.2
1	B	573	ARG	2.1
1	A	502	LEU	2.1
1	A	636	ASP	2.1
1	A	562	GLU	2.1
1	B	431	GLU	2.1
1	B	562	GLU	2.1
1	B	564	GLY	2.1
1	B	548	ARG	2.1
1	A	722	ALA	2.1
1	B	722	ALA	2.1
1	A	548	ARG	2.1
1	B	417	ASP	2.0
1	B	555	ARG	2.0
1	A	578	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

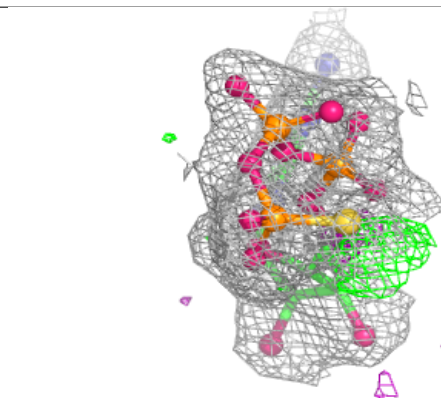
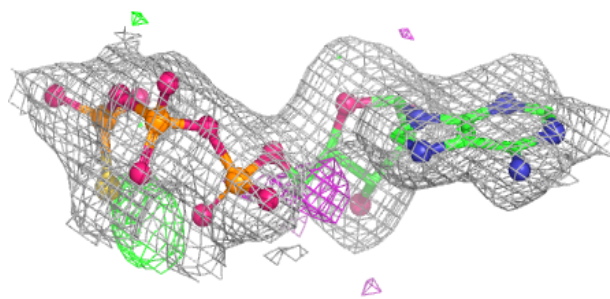
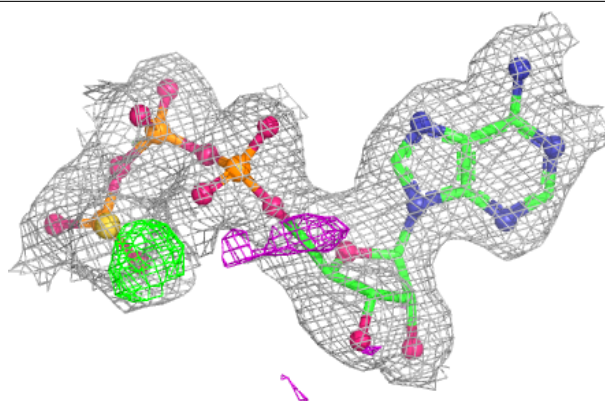
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AGS	A	1723	31/31	0.95	0.08	8,21,28,33	0
2	AGS	B	1724	31/31	0.97	0.07	4,19,26,32	0
3	MG	A	1724	1/1	0.99	0.02	1,1,1,1	0
3	MG	B	1723	1/1	0.99	0.03	2,2,2,2	0

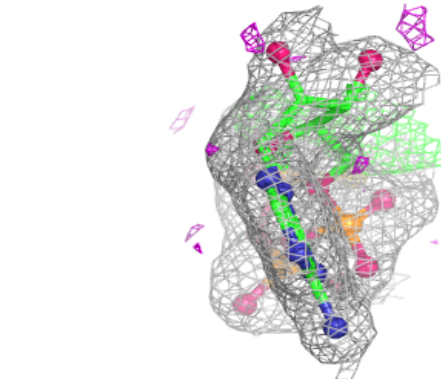
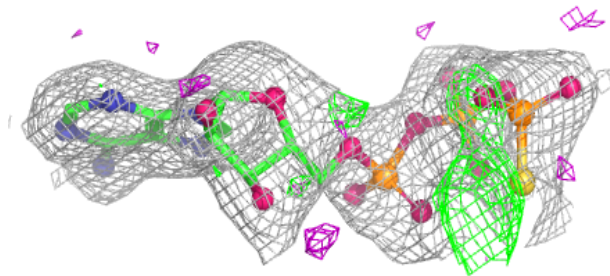
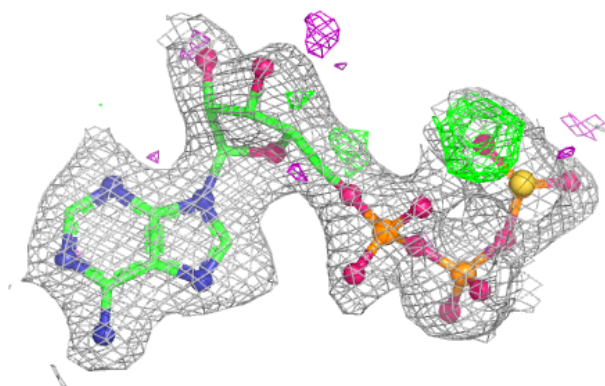
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AGS A 1723:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around AGS B 1724:**

$2mF_o-DF_c$ (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.