



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:35 PM UTC

PDB ID : 7KRW / pdb_00007krw
Title : Stimulating state of near full-length Hsp70 DnaK fused with a substrate peptide
Authors : Wang, W.; Hendrickson, W.A.
Deposited on : 2020-11-20
Resolution : 7.70 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

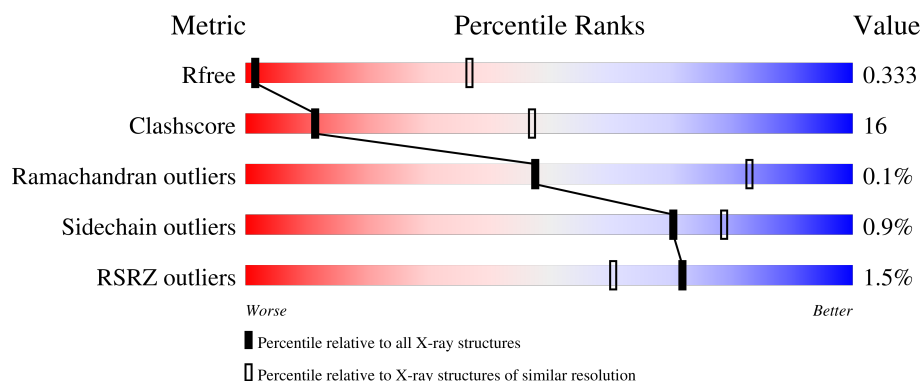
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.70 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	622	2% 70% 27% .
1	B	622	2% 59% 28% 13%
1	C	622	57% 29% 13%
1	D	622	2% 59% 28% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17034 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 Chaperone protein DnaK fused with substrate peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	541	Total	C	N	O	S	0	0	0
			4105	2557	712	823	13			
1	B	541	Total	C	N	O	S	0	0	0
			4105	2557	712	823	13			
1	A	608	Total	C	N	O	S	0	0	0
			4595	2857	799	924	15			
1	D	541	Total	C	N	O	S	0	0	0
			4105	2557	712	823	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	199	ALA	THR	engineered mutation	UNP A0A6D2W465
B	199	ALA	THR	engineered mutation	UNP A0A6D2W465
A	199	ALA	THR	engineered mutation	UNP A0A6D2W465
D	199	ALA	THR	engineered mutation	UNP A0A6D2W465

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

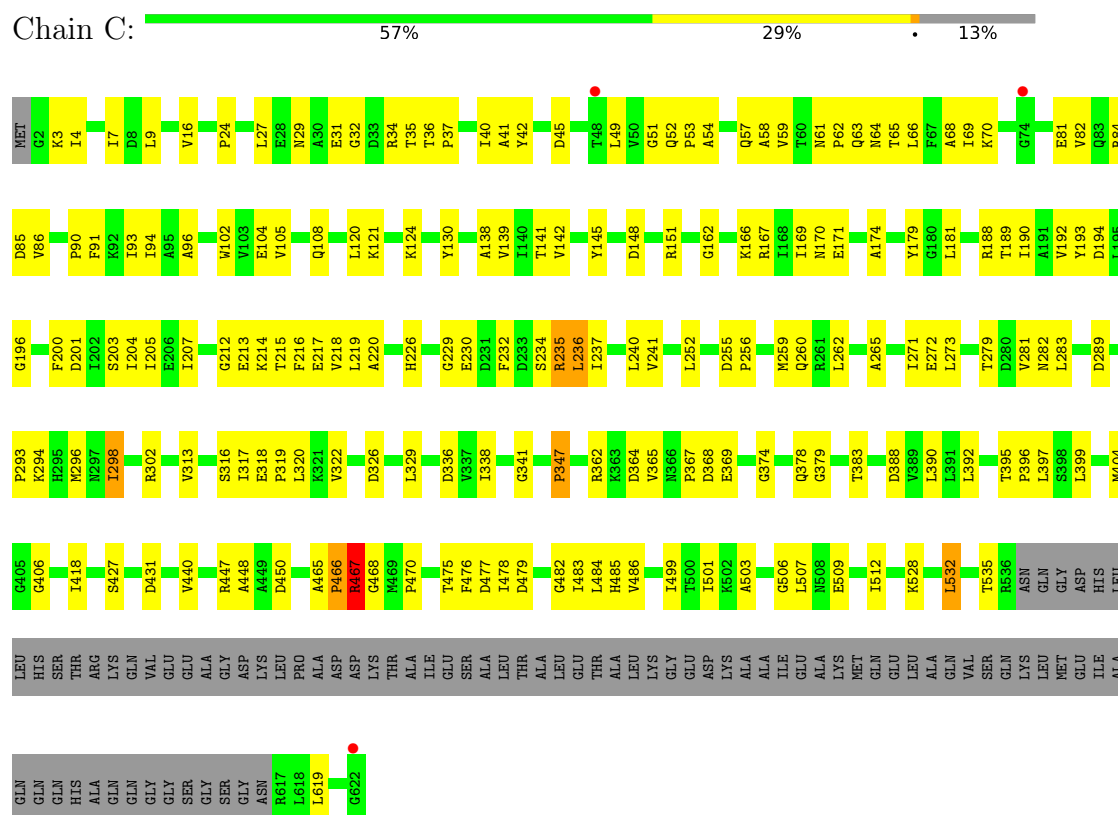


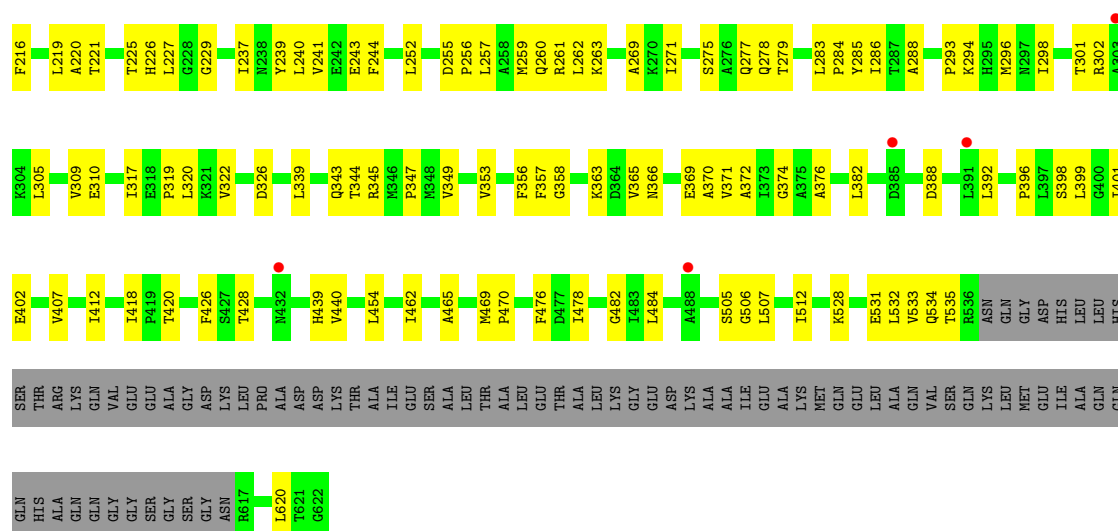
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

3 Residue-property plots

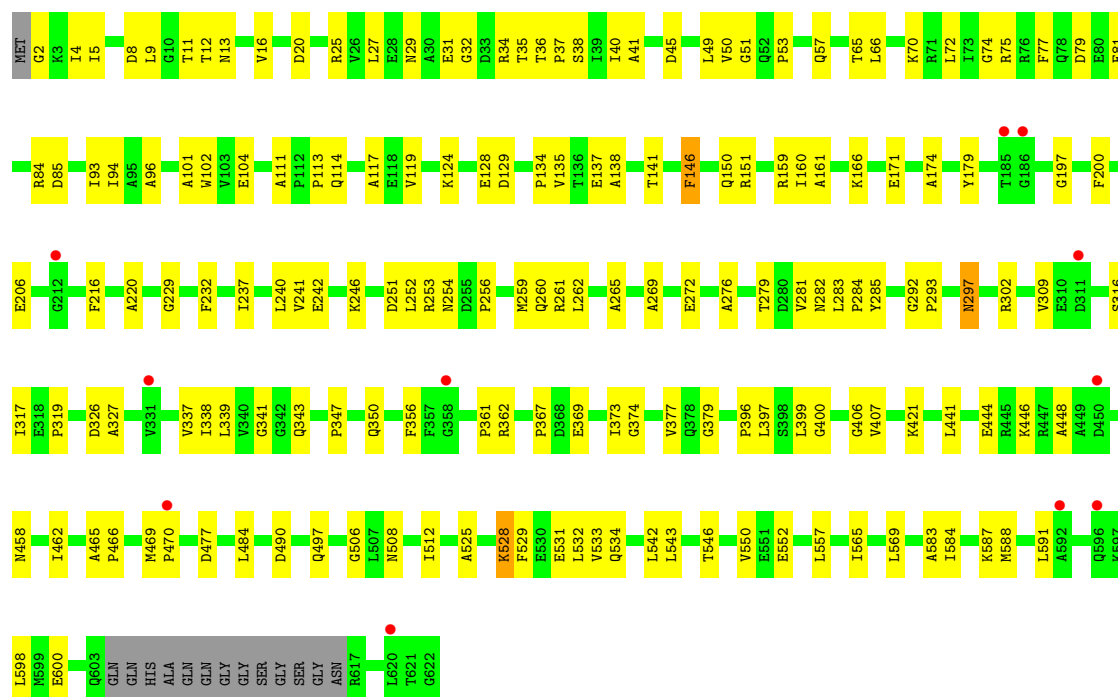
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Chaperone protein DnaK fused with substrate peptide

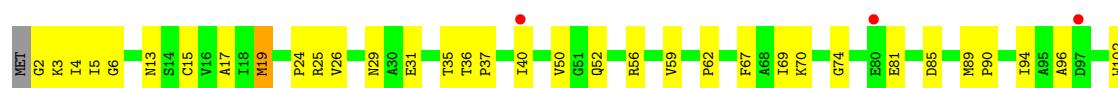




• Molecule 1: Chaperone protein DnaK fused with substrate peptide



• Molecule 1: Chaperone protein DnaK fused with substrate peptide



ILE	ALA	HIS	L1412	L308	L205	V103
	GLN	LEU	V309	V310	E206	E104
GLN	GLN	HIS	I4118	V313	D211	M110
GLN	GLN	THR	P419	V319	G212	I115
HIS	ALA	ARG	T420	P319	E217	V119
ALA	GLN	GLN	K421	L320	V218	L120
GLN	GLN	GLN	S427	L329	L219	L212
GLY	GLY	VAL	Q433	A327	A220	K121
GLY	GLY	GLU	V436	G328	T221	M123
SER	GLY	GLU	T437	L329	N222	K124
GLY	ALA	ALA	V437	V337	D231	K125
SER	GLY	GLY	I438	I338	E231	E128
SER	GLY	ASP	H439	R345	L236	D129
ASN	ASN	LEU	V440	K346	T237	E133
R617	L618	PRO	L441	P347	V241	P134
L619	L619	ALA	R467	M348	E242	V135
G622	G622	ASP	Q471	V353	E243	T136
		THR	T475	A354	F244	E137
		ALA	F476	E355	K245	A138
		ILE	D477	G358	K246	V139
		GLU	I478	K359	D247	I140
		SER	D479	E360	D251	T141
		ALA	LEU	P361	L252	V142
		LEU	ALA	V365	Q150	
		THR	I483	V366	P256	K155
		ALA	L484	E369	M259	R159
		LEU	H485	A372	Q260	T160
		GLU	V486	I373	L262	A161
		THR	S487	G374	K263	L163
		ALA	S493	A375	E264	E164
		LEU	G494	A376	V165	V165
		GLY	I499		K166	R167
		GLU	T500		L271	
		ASP		G380	S275	I168
		LYS	S505	V381	I169	
		ALA	G506	L382	Q278	M170
		ILE	L507	T383	E171	
		GLU	N508	G384	L283	A174
		ALA	Q513	D385	P284	
		LYS		V386	V285	
		MET	R517	K387	L286	
		GLN		D388		
		GLU	K528	V389	M296	V192
		LEU	F529		N297	L193
		LEU		T395	L195	D194
		GLN			L298	L195
		VAL	L532	S398	T301	G196
		SER	R536	I401	R302	
		GLN	ASN	E402	F200	F200
		LEU	GLN		D201	D201
		LEU	GLY		T202	T202
		MET	MET		E306	T204
		GLU	GLN		E307	

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	294.20Å 294.20Å 294.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.63 – 7.70 38.63 – 7.71	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.63-7.70) 94.6 (38.63-7.71)	Depositor EDS
R_{merge}	0.63	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 7.32Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.304 , 0.316 0.278 , 0.333	Depositor DCC
R_{free} test set	258 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	453.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 589.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.309 for -l,-k,-h	Xtriage
Reported twinning fraction	0.430 for -l,-k,-h	Depositor
Outliers	0 of 5015 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	17034	wwPDB-VP
Average B, all atoms (Å ²)	319.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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: ATP

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	0.45	0/4646	0.75	0/6281
1	B	0.47	0/4153	0.76	0/5616
1	C	0.47	0/4153	0.80	3/5616 (0.1%)
1	D	0.46	0/4153	0.76	1/5616 (0.0%)
All	All	0.46	0/17105	0.77	4/23129 (0.0%)

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	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	467	ARG	CB-CG-CD	7.88	129.41	111.30
1	D	388	ASP	N-CA-C	5.49	119.27	111.92
1	C	532	LEU	CA-CB-CG	5.19	134.46	116.30
1	C	347	PRO	N-CA-C	5.01	120.49	113.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	532	LEU	Peptide
1	C	466	PRO	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	4595	0	4641	131	0
1	B	4105	0	4153	145	0
1	C	4105	0	4153	164	0
1	D	4105	0	4153	147	0
2	A	31	0	12	2	0
2	B	31	0	12	3	0
2	C	31	0	12	1	0
2	D	31	0	12	5	0
All	All	17034	0	17148	551	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 16.

All (551) 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:D:136:THR:O	1:D:164:GLU:N	1.96	0.99
1:B:31:GLU:HA	1:A:272:GLU:HG3	1.44	0.96
1:B:241:VAL:HG22	1:B:252:LEU:HB2	1.46	0.95
1:C:57:GLN:NE2	1:C:65:THR:OG1	2.07	0.87
1:B:26:VAL:HG21	1:B:369:GLU:HB3	1.55	0.87
1:C:59:VAL:HA	1:C:260:GLN:HB3	1.55	0.86
1:A:29:ASN:ND2	1:A:36:THR:OG1	2.09	0.85
1:D:220:ALA:HB2	1:D:327:ALA:HB2	1.58	0.85
1:C:40:ILE:O	1:C:66:LEU:N	2.10	0.85
1:C:326:ASP:HB3	1:C:506:GLY:HA3	1.60	0.84
1:A:237:ILE:HG21	1:A:259:MET:HE1	1.57	0.84
1:B:244:PHE:HB2	1:B:296:MET:HE2	1.59	0.84
1:A:241:VAL:HG21	1:A:253:ARG:HG3	1.61	0.83
1:C:281:VAL:HA	1:D:56:ARG:HH12	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:ASP:O	1:C:485:HIS:N	2.12	0.82
1:C:142:VAL:O	1:C:171:GLU:N	2.12	0.81
1:D:62:PRO:HB3	1:D:260:GLN:HG3	1.63	0.81
1:C:241:VAL:HG22	1:C:252:LEU:HB2	1.61	0.81
1:B:237:ILE:HG23	1:B:262:LEU:HD23	1.62	0.80
1:A:34:ARG:NE	1:A:369:GLU:OE2	2.15	0.80
1:B:72:LEU:HD22	1:B:82:VAL:HG22	1.65	0.79
1:C:404:MET:HB2	1:C:619:LEU:HB2	1.63	0.78
1:C:29:ASN:ND2	1:C:36:THR:OG1	2.17	0.77
1:D:244:PHE:CE2	1:D:296:MET:HA	2.19	0.76
1:D:271:ILE:HG23	2:D:701:ATP:N1	2.01	0.76
1:C:479:ASP:OD2	1:C:485:HIS:NE2	2.18	0.76
1:C:94:ILE:HD13	1:C:104:GLU:HB2	1.67	0.76
1:C:194:ASP:HB3	1:C:201:ASP:HB3	1.66	0.76
1:B:146:PHE:HB3	1:B:151:ARG:HG3	1.67	0.76
1:D:242:GLU:O	1:D:246:LYS:N	2.17	0.76
1:A:242:GLU:OE2	1:A:253:ARG:NH2	2.19	0.76
1:C:139:VAL:HG22	1:C:167:ARG:HB2	1.67	0.75
1:C:338:ILE:HG23	1:C:365:VAL:HG21	1.68	0.75
1:B:56:ARG:HB3	1:A:282:ASN:HB3	1.68	0.75
1:C:532:LEU:HA	1:C:535:THR:HB	1.69	0.75
1:C:81:GLU:OE2	1:C:226:HIS:NE2	2.20	0.74
1:A:128:GLU:HG2	1:A:134:PRO:HA	1.69	0.74
1:C:42:TYR:HB2	1:C:64:ASN:HB3	1.69	0.74
1:C:200:PHE:HE1	1:C:319:PRO:HB2	1.51	0.74
1:B:74:GLY:HA3	1:B:150:GLN:HA	1.70	0.74
1:A:40:ILE:O	1:A:66:LEU:N	2.21	0.74
1:C:31:GLU:HA	1:D:345:ARG:NH1	2.03	0.74
1:C:120:LEU:O	1:C:124:LYS:N	2.20	0.73
1:A:13:ASN:HB3	1:A:35:THR:HB	1.69	0.73
1:A:546:THR:O	1:A:550:VAL:N	2.21	0.73
1:D:206:GLU:N	1:D:217:GLU:O	2.18	0.73
1:B:142:VAL:O	1:B:171:GLU:N	2.19	0.73
1:C:31:GLU:HA	1:D:345:ARG:HH12	1.52	0.72
1:B:142:VAL:HG21	1:B:151:ARG:HG2	1.71	0.71
1:B:220:ALA:HA	1:B:506:GLY:HA2	1.71	0.71
1:B:399:LEU:HD13	1:B:484:LEU:HD22	1.72	0.71
1:D:59:VAL:HA	1:D:260:GLN:HB3	1.71	0.71
1:B:56:ARG:HH12	1:A:281:VAL:HA	1.55	0.71
1:C:362:ARG:NH2	1:C:364:ASP:OD2	2.20	0.71
1:D:2:GLY:N	1:D:137:GLU:OE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:LEU:HB2	1:D:296:MET:HB3	1.73	0.70
1:B:345:ARG:HH12	1:A:31:GLU:HA	1.56	0.69
1:A:406:GLY:O	1:A:448:ALA:N	2.21	0.69
1:C:190:ILE:HD13	1:C:207:ILE:HD11	1.75	0.69
1:B:62:PRO:HB3	1:B:260:GLN:HG3	1.75	0.69
1:B:128:GLU:HG2	1:B:134:PRO:HA	1.74	0.69
1:C:188:ARG:NE	1:C:336:ASP:OD2	2.23	0.69
1:C:477:ASP:HB3	1:C:485:HIS:HB2	1.75	0.68
1:D:29:ASN:ND2	1:D:36:THR:OG1	2.19	0.68
1:B:167:ARG:HG3	1:B:382:LEU:HD11	1.75	0.68
1:B:418:ILE:HG21	1:B:482:GLY:HA2	1.75	0.68
1:B:71:ARG:NH1	1:B:198:GLY:O	2.27	0.67
1:B:345:ARG:NH1	1:A:31:GLU:HA	2.08	0.67
1:D:70:LYS:NZ	2:D:701:ATP:O3G	2.25	0.67
1:B:345:ARG:NH2	1:A:31:GLU:O	2.28	0.67
1:C:66:LEU:HB3	1:C:69:ILE:HD11	1.77	0.66
1:A:552:GLU:HA	1:D:532:LEU:HB3	1.78	0.66
1:C:273:LEU:O	1:C:302:ARG:NH2	2.28	0.66
1:C:477:ASP:N	1:C:485:HIS:O	2.28	0.66
1:B:275:SER:OG	1:A:53:PRO:HB3	1.96	0.66
1:B:243:GLU:HB3	1:B:298:ILE:HD13	1.77	0.66
1:B:284:PRO:HG2	1:A:285:TYR:CD1	2.31	0.66
1:D:204:ILE:O	1:D:219:LEU:N	2.27	0.66
1:C:62:PRO:HB2	1:C:90:PRO:HB2	1.78	0.65
1:B:81:GLU:OE2	1:B:225:THR:OG1	2.14	0.65
1:D:467:ARG:HH22	1:D:619:LEU:HD13	1.61	0.65
1:A:528:LYS:HA	1:A:531:GLU:HG2	1.77	0.65
1:B:237:ILE:HG12	1:B:262:LEU:HG	1.78	0.64
1:C:404:MET:SD	1:C:619:LEU:HD12	2.37	0.64
1:C:465:ALA:HB3	1:C:470:PRO:HD3	1.79	0.64
1:C:271:ILE:HG23	2:C:701:ATP:N6	2.11	0.64
1:B:136:THR:O	1:B:164:GLU:N	2.21	0.64
1:B:339:LEU:HD21	1:B:353:VAL:HG21	1.79	0.64
1:A:41:ALA:HB3	1:A:49:LEU:HB2	1.79	0.64
1:B:261:ARG:NH1	1:B:286:ILE:HA	2.13	0.64
1:C:404:MET:N	1:C:619:LEU:O	2.32	0.63
1:D:174:ALA:O	1:D:374:GLY:HA3	1.98	0.63
1:B:200:PHE:HE1	1:B:319:PRO:HB2	1.63	0.63
1:C:162:GLY:HA2	1:B:358:GLY:HA2	1.80	0.63
1:A:220:ALA:HB2	1:A:327:ALA:HB2	1.80	0.63
1:A:341:GLY:O	1:A:367:PRO:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PHE:CE2	1:B:263:LYS:HE3	2.33	0.62
1:D:338:ILE:HG23	1:D:365:VAL:HG21	1.79	0.62
1:A:41:ALA:HA	1:A:65:THR:HA	1.80	0.62
1:D:220:ALA:HA	1:D:506:GLY:HA2	1.81	0.62
1:D:278:GLN:HA	1:D:301:THR:HA	1.80	0.62
1:D:467:ARG:NH2	1:D:619:LEU:HD13	2.14	0.62
1:C:3:LYS:HA	1:C:383:THR:HG21	1.80	0.62
1:B:144:ALA:HA	1:B:170:ASN:HB2	1.81	0.61
1:D:159:ARG:HG3	1:D:165:VAL:HG23	1.82	0.61
1:B:31:GLU:OE2	1:B:53:PRO:HD3	2.01	0.61
1:A:160:ILE:O	1:D:355:GLU:HG2	2.00	0.61
1:D:19:MET:HE3	1:D:19:MET:HA	1.83	0.61
1:D:337:VAL:HG11	1:D:353:VAL:HG11	1.82	0.61
1:D:479:ASP:OD2	1:D:485:HIS:NE2	2.24	0.61
1:C:166:LYS:O	1:C:167:ARG:NH2	2.30	0.61
1:A:241:VAL:HG22	1:A:252:LEU:HB2	1.83	0.61
1:C:37:PRO:O	1:C:51:GLY:HA2	2.00	0.61
1:B:407:VAL:HG21	1:B:533:VAL:HG11	1.82	0.61
1:A:72:LEU:HD22	1:A:101:ALA:HB1	1.81	0.60
1:B:151:ARG:HH12	1:B:170:ASN:HB3	1.65	0.60
1:C:200:PHE:CE1	1:C:319:PRO:HB2	2.33	0.60
1:A:12:THR:O	1:A:38:SER:N	2.29	0.60
1:A:531:GLU:HA	1:A:534:GLN:HB3	1.83	0.60
1:C:204:ILE:O	1:C:219:LEU:N	2.34	0.60
1:C:108:GLN:HE22	1:B:310:GLU:CD	2.10	0.60
1:A:232:PHE:CD2	1:A:309:VAL:HG11	2.36	0.60
1:D:142:VAL:O	1:D:171:GLU:N	2.30	0.59
1:B:239:TYR:O	1:B:243:GLU:N	2.21	0.59
1:B:420:THR:HG22	1:B:478:ILE:HB	1.85	0.59
1:C:81:GLU:O	1:C:85:ASP:N	2.33	0.59
1:B:322:VAL:O	1:B:326:ASP:N	2.35	0.59
1:D:313:VAL:HG21	1:D:348:MET:HE3	1.83	0.59
1:D:243:GLU:O	1:D:247:ASP:N	2.31	0.59
1:B:179:TYR:CD1	1:B:365:VAL:HG22	2.36	0.59
1:D:26:VAL:HG21	1:D:369:GLU:HB3	1.85	0.59
1:A:8:ASP:HA	1:A:141:THR:OG1	2.03	0.59
1:D:74:GLY:HA3	1:D:150:GLN:HA	1.84	0.59
1:D:200:PHE:HE1	1:D:319:PRO:HB2	1.69	0.58
1:D:120:LEU:O	1:D:124:LYS:N	2.32	0.58
1:A:77:PHE:HE1	1:A:93:ILE:HG22	1.67	0.58
1:D:167:ARG:HG2	1:D:382:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:PHE:HB2	1:D:296:MET:HE2	1.84	0.58
1:B:86:VAL:HG22	1:B:93:ILE:HB	1.85	0.58
1:B:196:GLY:O	1:B:229:GLY:N	2.28	0.58
1:C:484:LEU:N	1:C:501:ILE:O	2.34	0.57
1:A:41:ALA:O	1:A:49:LEU:N	2.33	0.57
1:B:366:ASN:ND2	1:A:32:GLY:O	2.38	0.57
1:D:354:ALA:HA	1:D:359:LYS:O	2.04	0.57
1:A:256:PRO:O	1:A:260:GLN:N	2.35	0.57
1:A:557:LEU:HD21	1:A:565:ILE:HD12	1.85	0.57
1:C:53:PRO:HB3	1:D:275:SER:OG	2.05	0.57
1:B:155:LYS:HG2	1:B:165:VAL:HG11	1.86	0.57
1:A:2:GLY:N	1:A:137:GLU:OE2	2.38	0.57
1:D:477:ASP:HB3	1:D:485:HIS:HB2	1.85	0.57
1:B:56:ARG:CZ	1:A:282:ASN:H	2.17	0.57
1:D:241:VAL:HG22	1:D:252:LEU:HB2	1.87	0.57
1:C:9:LEU:O	1:C:70:LYS:NZ	2.35	0.57
1:D:471:GLN:HE22	1:D:617:ARG:HH11	1.53	0.57
1:D:244:PHE:HE2	1:D:296:MET:HA	1.66	0.56
1:C:237:ILE:HG21	1:C:259:MET:HE1	1.88	0.56
1:D:241:VAL:HG13	1:D:251:ASP:HA	1.86	0.56
1:A:114:GLN:HA	1:A:160:ILE:HG21	1.88	0.56
1:A:584:ILE:O	1:A:588:MET:N	2.32	0.56
1:D:59:VAL:HG12	1:D:260:GLN:O	2.06	0.56
1:D:62:PRO:HB3	1:D:260:GLN:CG	2.35	0.56
1:D:242:GLU:OE1	1:D:245:LYS:HD3	2.06	0.56
1:A:421:LYS:HD3	1:A:477:ASP:OD2	2.05	0.56
1:C:237:ILE:CG2	1:C:259:MET:HE1	2.37	0.55
1:C:240:LEU:HD11	1:C:262:LEU:HD11	1.88	0.55
1:A:174:ALA:O	1:A:374:GLY:HA3	2.05	0.55
1:C:205:ILE:HG12	1:C:218:VAL:HG22	1.88	0.55
1:A:220:ALA:HA	1:A:506:GLY:HA2	1.87	0.55
1:A:37:PRO:O	1:A:51:GLY:HA2	2.06	0.55
1:B:143:PRO:HD2	1:B:146:PHE:CD2	2.41	0.55
1:B:174:ALA:O	1:B:374:GLY:HA3	2.06	0.55
1:A:396:PRO:HB2	1:A:512:ILE:HG21	1.88	0.55
1:D:155:LYS:HG2	1:D:165:VAL:HG11	1.89	0.55
1:D:529:PHE:O	1:D:532:LEU:HG	2.06	0.55
1:C:64:ASN:OD1	1:C:105:VAL:HG13	2.06	0.55
1:C:192:VAL:HG21	1:C:205:ILE:HD12	1.87	0.55
1:A:197:GLY:O	1:A:229:GLY:N	2.40	0.55
1:C:41:ALA:HA	1:C:65:THR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:VAL:O	1:C:86:VAL:N	2.36	0.55
1:A:146:PHE:HB3	1:A:151:ARG:HG3	1.88	0.55
1:A:341:GLY:HA2	2:A:701:ATP:O2A	2.07	0.55
1:A:16:VAL:HG13	1:A:27:LEU:HB2	1.88	0.55
1:A:94:ILE:HD13	1:A:104:GLU:HB2	1.88	0.54
1:B:71:ARG:O	1:B:75:ARG:NE	2.39	0.54
1:A:20:ASP:OD2	1:A:25:ARG:HD2	2.06	0.54
1:C:31:GLU:OE1	1:C:52:GLN:HG2	2.07	0.54
1:C:240:LEU:HD22	1:C:262:LEU:HD21	1.89	0.54
1:B:143:PRO:HB3	1:B:145:TYR:CE2	2.42	0.54
1:D:402:GLU:HB2	1:D:441:LEU:HD11	1.88	0.54
1:A:240:LEU:HD13	1:A:262:LEU:HD11	1.90	0.54
1:A:316:SER:C	1:A:319:PRO:HD2	2.33	0.54
1:C:431:ASP:OD2	1:C:467:ARG:HG3	2.08	0.54
1:B:271:ILE:HG23	2:B:701:ATP:C6	2.43	0.54
1:C:41:ALA:HB3	1:C:49:LEU:HB2	1.89	0.54
1:B:283:LEU:HB2	1:B:296:MET:HB3	1.90	0.54
1:B:200:PHE:HB3	1:B:227:LEU:HB2	1.90	0.54
1:B:261:ARG:HH12	1:B:286:ILE:HA	1.71	0.54
1:D:206:GLU:HB3	1:D:217:GLU:HB3	1.89	0.54
1:C:16:VAL:HG13	1:C:27:LEU:HB2	1.90	0.53
1:B:244:PHE:CE2	1:B:296:MET:HA	2.43	0.53
1:A:74:GLY:HA3	1:A:150:GLN:HA	1.90	0.53
1:B:175:ALA:HB2	1:B:371:VAL:HG22	1.90	0.53
1:B:317:ILE:HG23	1:B:356:PHE:CE1	2.43	0.53
1:A:543:LEU:HD12	1:A:569:LEU:HD22	1.90	0.53
1:D:202:ILE:HD13	1:D:320:LEU:HD22	1.91	0.53
1:D:244:PHE:CD2	1:D:296:MET:HG3	2.43	0.53
1:B:178:ALA:HB2	1:B:374:GLY:N	2.24	0.53
1:A:339:LEU:HD11	1:A:350:GLN:HG2	1.90	0.53
1:D:477:ASP:O	1:D:485:HIS:N	2.24	0.53
1:D:231:ASP:O	1:D:235:ARG:HG2	2.08	0.53
1:C:196:GLY:O	1:C:229:GLY:N	2.36	0.53
1:B:221:THR:N	1:B:505:SER:O	2.30	0.53
1:B:428:THR:HG21	1:B:462:ILE:HG21	1.91	0.53
1:D:139:VAL:HG22	1:D:167:ARG:HB2	1.90	0.53
1:C:58:ALA:HB2	1:C:65:THR:HG21	1.90	0.53
1:A:102:TRP:CZ2	1:A:111:ALA:HB2	2.44	0.53
1:A:583:ALA:O	1:A:587:LYS:HG2	2.09	0.53
1:C:86:VAL:HA	1:C:93:ILE:HD12	1.89	0.52
1:B:401:ILE:HD11	1:B:426:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ASP:OD2	1:C:485:HIS:CE1	2.62	0.52
1:C:316:SER:O	1:C:320:LEU:HG	2.09	0.52
1:D:125:LYS:HD2	1:D:128:GLU:HB2	1.91	0.52
1:C:7:ILE:HD13	1:C:120:LEU:HD22	1.91	0.52
1:B:241:VAL:HG13	1:B:252:LEU:H	1.74	0.52
1:C:256:PRO:HA	1:C:259:MET:HB2	1.92	0.52
1:D:85:ASP:OD1	1:D:89:MET:HE3	2.09	0.52
1:C:241:VAL:HG13	1:C:252:LEU:H	1.74	0.52
1:C:265:ALA:HB2	1:C:283:LEU:HD11	1.92	0.52
1:C:397:LEU:HD21	1:C:512:ILE:HG23	1.90	0.52
1:B:90:PRO:HB3	1:B:256:PRO:HB3	1.90	0.52
1:D:401:ILE:HA	1:D:439:HIS:O	2.10	0.52
1:B:269:ALA:HB1	1:B:279:THR:HG21	1.92	0.52
1:B:339:LEU:HD13	1:B:344:THR:HB	1.90	0.52
1:B:402:GLU:OE1	1:B:439:HIS:ND1	2.42	0.52
1:A:341:GLY:N	1:A:367:PRO:O	2.39	0.52
1:D:137:GLU:HG2	1:D:166:LYS:HD3	1.90	0.52
1:D:4:ILE:HG12	1:D:137:GLU:HB3	1.91	0.52
1:D:271:ILE:HG23	2:D:701:ATP:C6	2.45	0.52
1:B:244:PHE:HE2	1:B:296:MET:HA	1.74	0.52
1:B:396:PRO:HB2	1:B:512:ILE:HD13	1.92	0.52
1:A:458:ASN:O	1:A:497:GLN:HG3	2.09	0.52
1:C:42:TYR:N	1:C:64:ASN:O	2.39	0.52
1:B:277:GLN:HB2	1:A:45:ASP:CG	2.35	0.52
1:D:328:GLY:HA3	1:D:508:ASN:ND2	2.25	0.52
1:C:121:LYS:HA	1:C:124:LYS:HB3	1.92	0.51
1:D:90:PRO:HG3	1:D:260:GLN:OE1	2.09	0.51
1:C:4:ILE:O	1:C:379:GLY:HA3	2.10	0.51
1:B:277:GLN:O	1:B:302:ARG:N	2.28	0.51
1:B:240:LEU:HB3	1:B:296:MET:HE1	1.93	0.51
1:D:395:THR:HG22	1:D:418:ILE:HD11	1.93	0.51
1:C:70:LYS:NZ	1:C:171:GLU:OE2	2.35	0.51
1:C:212:GLY:O	1:C:388:ASP:HB3	2.11	0.51
1:B:26:VAL:HG21	1:B:369:GLU:CB	2.35	0.51
1:C:296:MET:HG3	1:C:298:ILE:HD11	1.92	0.51
1:B:219:LEU:HA	1:B:507:LEU:HB3	1.92	0.51
1:C:138:ALA:O	1:C:166:LYS:N	2.44	0.51
1:C:447:ARG:HD2	1:C:450:ASP:OD2	2.11	0.51
1:C:484:LEU:O	1:C:501:ILE:N	2.32	0.51
1:B:302:ARG:HH12	1:B:347:PRO:HG2	1.75	0.51
1:D:94:ILE:HD13	1:D:104:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:VAL:CG1	1:D:389:VAL:HB	2.41	0.51
1:D:204:ILE:HG21	1:D:329:LEU:HD12	1.93	0.50
1:C:256:PRO:O	1:C:260:GLN:HG2	2.11	0.50
1:B:90:PRO:CB	1:B:256:PRO:HB3	2.41	0.50
1:A:341:GLY:C	1:A:367:PRO:HB2	2.36	0.50
1:C:139:VAL:HG21	1:C:378:GLN:HG3	1.93	0.50
1:A:400:GLY:O	1:A:441:LEU:N	2.33	0.50
1:D:69:ILE:HG13	1:D:115:ILE:HG21	1.94	0.50
1:C:215:THR:HG22	1:C:390:LEU:HD23	1.93	0.50
1:C:484:LEU:HB3	1:C:501:ILE:HB	1.93	0.50
1:B:469:MET:HB3	1:B:470:PRO:HD3	1.92	0.50
1:C:440:VAL:HG11	1:C:501:ILE:CD1	2.42	0.50
1:A:338:ILE:HD13	1:A:362:ARG:HB2	1.93	0.50
1:C:174:ALA:O	1:C:374:GLY:HA3	2.11	0.49
1:A:9:LEU:O	1:A:70:LYS:NZ	2.40	0.49
1:A:81:GLU:O	1:A:85:ASP:N	2.45	0.49
1:D:125:LYS:HA	1:D:128:GLU:HB2	1.94	0.49
1:C:34:ARG:NE	1:C:369:GLU:OE2	2.31	0.49
1:C:81:GLU:HA	1:C:84:ARG:HB3	1.94	0.49
1:A:282:ASN:ND2	1:A:297:ASN:OD1	2.45	0.49
1:A:399:LEU:HD13	1:A:484:LEU:HD22	1.94	0.49
1:B:206:GLU:HB2	1:B:219:LEU:HD11	1.93	0.49
1:B:353:VAL:HG13	1:B:357:PHE:CD2	2.48	0.49
1:D:420:THR:HG22	1:D:478:ILE:HD12	1.93	0.49
1:A:407:VAL:HA	1:A:446:LYS:O	2.12	0.49
1:D:243:GLU:HA	1:D:246:LYS:HB2	1.94	0.49
1:C:289:ASP:OD1	1:C:294:LYS:NZ	2.42	0.49
1:B:200:PHE:HE1	1:B:319:PRO:CB	2.26	0.49
1:A:261:ARG:NH1	1:A:284:PRO:O	2.42	0.49
1:C:42:TYR:O	1:C:61:ASN:ND2	2.46	0.49
1:D:243:GLU:HG2	1:D:298:ILE:HG23	1.94	0.49
1:D:477:ASP:N	1:D:485:HIS:O	2.36	0.49
1:A:302:ARG:NH1	1:A:347:PRO:HG2	2.27	0.49
1:D:433:GLN:NE2	1:D:436:VAL:HG12	2.28	0.49
1:C:61:ASN:HD21	1:C:64:ASN:HB2	1.78	0.49
1:C:145:TYR:HD2	1:C:201:ASP:OD1	1.96	0.49
1:C:193:TYR:CE2	1:C:320:LEU:HD21	2.48	0.49
1:B:121:LYS:HG2	1:B:161:ALA:HA	1.94	0.49
1:C:41:ALA:HB1	1:C:57:GLN:NE2	2.28	0.48
1:A:13:ASN:HA	1:A:36:THR:O	2.13	0.48
1:A:138:ALA:O	1:A:166:LYS:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:PRO:O	1:B:57:GLN:HG3	2.13	0.48
1:B:344:THR:HA	1:B:349:VAL:HG11	1.95	0.48
1:A:407:VAL:HG22	1:A:529:PHE:CE2	2.48	0.48
1:B:212:GLY:O	1:B:388:ASP:HB3	2.13	0.48
1:A:269:ALA:HB1	1:A:279:THR:HG21	1.95	0.48
1:D:302:ARG:HH12	1:D:347:PRO:HG2	1.79	0.48
1:C:440:VAL:HG11	1:C:501:ILE:HD13	1.95	0.48
1:A:343:GLN:HA	2:A:701:ATP:N3	2.29	0.48
1:D:19:MET:HE3	1:D:24:PRO:HB3	1.96	0.48
1:C:90:PRO:HG3	1:C:260:GLN:OE1	2.13	0.48
1:B:124:LYS:HD3	1:B:161:ALA:O	2.13	0.48
1:C:141:THR:HA	1:C:169:ILE:O	2.14	0.48
1:A:141:THR:HB	1:A:171:GLU:HG3	1.96	0.48
1:A:466:PRO:HD2	1:A:469:MET:SD	2.54	0.48
1:D:401:ILE:HG22	1:D:440:VAL:HA	1.96	0.48
1:C:59:VAL:HA	1:C:260:GLN:CB	2.37	0.48
1:A:117:ALA:CB	1:A:160:ILE:HG22	2.44	0.48
1:D:136:THR:HA	1:D:163:LEU:HD23	1.96	0.48
1:D:244:PHE:CE1	1:D:250:ILE:HD12	2.48	0.48
1:C:142:VAL:HG21	1:C:151:ARG:HG2	1.95	0.47
1:C:272:GLU:OE2	1:C:279:THR:HB	2.13	0.47
1:C:399:LEU:CD1	1:C:478:ILE:HD11	2.44	0.47
1:B:4:ILE:HG12	1:B:137:GLU:HB3	1.96	0.47
1:D:221:THR:N	1:D:505:SER:O	2.34	0.47
1:C:49:LEU:C	1:C:54:ALA:HB2	2.38	0.47
1:B:195:LEU:HD23	1:B:343:GLN:HB3	1.95	0.47
1:B:216:PHE:O	1:B:392:LEU:HB3	2.14	0.47
1:D:244:PHE:HE1	1:D:250:ILE:HD12	1.79	0.47
1:C:220:ALA:HA	1:C:506:GLY:HA2	1.96	0.47
1:C:298:ILE:N	1:C:298:ILE:HD12	2.30	0.47
1:A:206:GLU:O	1:A:216:PHE:HA	2.13	0.47
1:D:353:VAL:HG11	1:D:361:PRO:HG3	1.94	0.47
1:C:94:ILE:CD1	1:C:104:GLU:HB2	2.43	0.47
1:C:240:LEU:CD1	1:C:262:LEU:HD11	2.44	0.47
1:C:475:THR:O	1:C:486:VAL:HA	2.14	0.47
1:A:256:PRO:HA	1:A:259:MET:HB2	1.96	0.47
1:D:103:VAL:HG22	1:D:110:MET:O	2.15	0.47
1:C:313:VAL:O	1:C:317:ILE:HG12	2.15	0.47
1:B:155:LYS:HE3	1:B:165:VAL:CG1	2.45	0.47
1:D:167:ARG:CG	1:D:382:LEU:HD11	2.44	0.47
1:B:285:TYR:CZ	1:A:292:GLY:HA2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:VAL:CG2	1:D:369:GLU:HB3	2.44	0.47
1:C:232:PHE:O	1:C:236:LEU:HD22	2.15	0.47
1:B:58:ALA:CB	1:B:65:THR:HG21	2.45	0.47
1:A:242:GLU:O	1:A:246:LYS:N	2.46	0.47
1:A:465:ALA:HB1	1:A:469:MET:SD	2.55	0.47
1:D:124:LYS:HD3	1:D:161:ALA:O	2.15	0.47
1:D:427:SER:HB2	1:D:617:ARG:HG2	1.96	0.47
1:B:29:ASN:ND2	1:B:36:THR:OG1	2.45	0.47
1:C:32:GLY:HA3	1:D:366:ASN:ND2	2.30	0.46
1:D:17:ALA:HB3	1:D:372:ALA:C	2.39	0.46
1:C:194:ASP:N	1:C:201:ASP:O	2.36	0.46
1:C:318:GLU:O	1:C:322:VAL:HG23	2.15	0.46
1:B:296:MET:SD	1:B:298:ILE:HD12	2.55	0.46
1:D:15:CYS:SG	1:D:26:VAL:HG13	2.55	0.46
1:D:283:LEU:HD13	1:D:286:ILE:HD13	1.96	0.46
1:C:281:VAL:HA	1:D:56:ARG:NH1	2.21	0.46
1:A:337:VAL:HB	1:A:361:PRO:HA	1.97	0.46
1:D:204:ILE:HG22	1:D:219:LEU:HB2	1.97	0.46
1:C:45:ASP:HB3	1:D:278:GLN:HG2	1.98	0.46
1:C:139:VAL:HG11	1:C:378:GLN:HG2	1.98	0.46
1:B:30:ALA:O	1:A:276:ALA:HB2	2.16	0.46
1:B:208:ASP:O	1:B:215:THR:N	2.41	0.46
1:A:397:LEU:HD22	1:A:444:GLU:HG2	1.98	0.46
1:D:476:PHE:CE1	1:D:486:VAL:HG13	2.50	0.46
1:C:396:PRO:HG3	1:C:507:LEU:HG	1.98	0.46
1:A:41:ALA:HB2	1:A:65:THR:HG23	1.98	0.46
1:A:160:ILE:HA	1:D:355:GLU:O	2.14	0.46
1:A:326:ASP:O	1:A:508:ASN:HB2	2.16	0.46
1:A:531:GLU:HA	1:A:534:GLN:CB	2.46	0.46
1:C:63:GLN:HA	1:C:91:PHE:HB3	1.98	0.46
1:A:531:GLU:O	1:A:534:GLN:HB3	2.16	0.46
1:C:255:ASP:O	1:C:259:MET:HG2	2.15	0.46
1:D:59:VAL:HG11	1:D:264:GLU:OE1	2.15	0.46
1:D:141:THR:HA	1:D:169:ILE:O	2.15	0.46
1:C:509:GLU:HA	1:C:512:ILE:HB	1.98	0.45
1:B:54:ALA:O	1:B:58:ALA:N	2.49	0.45
1:D:31:GLU:OE1	1:D:52:GLN:HG2	2.16	0.45
1:D:37:PRO:HG2	1:D:52:GLN:OE1	2.17	0.45
1:A:159:ARG:O	1:D:358:GLY:HA2	2.16	0.45
1:C:139:VAL:HG21	1:C:378:GLN:CG	2.46	0.45
1:C:193:TYR:HE2	1:C:320:LEU:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:VAL:HB	1:C:499:ILE:CG1	2.46	0.45
1:A:75:ARG:HD3	1:A:79:ASP:OD1	2.17	0.45
1:D:119:VAL:O	1:D:123:MET:HG2	2.16	0.45
1:D:401:ILE:HD13	1:D:438:ILE:HG23	1.99	0.45
1:C:31:GLU:O	1:D:345:ARG:NH2	2.46	0.45
1:C:193:TYR:CD2	1:C:320:LEU:HD21	2.51	0.45
1:B:72:LEU:CD2	1:B:82:VAL:HG22	2.42	0.45
1:C:234:SER:C	1:C:236:LEU:H	2.25	0.45
1:C:282:ASN:H	1:D:56:ARG:CZ	2.30	0.45
1:C:406:GLY:O	1:C:448:ALA:N	2.45	0.45
1:B:262:LEU:HD13	1:B:283:LEU:HD11	1.99	0.45
1:B:428:THR:CG2	1:B:462:ILE:HD13	2.47	0.45
1:C:217:GLU:HB2	1:C:392:LEU:HD23	1.99	0.45
1:A:265:ALA:HB2	1:A:283:LEU:HD21	1.98	0.45
1:D:483:ILE:HG21	1:D:500:THR:HG23	1.98	0.45
1:B:243:GLU:HG2	1:B:298:ILE:CG2	2.47	0.45
1:B:353:VAL:HG13	1:B:357:PHE:CE2	2.51	0.45
1:D:128:GLU:HG2	1:D:133:GLU:O	2.16	0.45
1:B:202:ILE:HG12	1:B:320:LEU:HA	1.99	0.44
1:D:200:PHE:HE1	1:D:319:PRO:CB	2.30	0.44
1:D:237:ILE:HG23	1:D:262:LEU:HD23	1.99	0.44
1:A:546:THR:O	1:A:550:VAL:HG23	2.17	0.44
1:D:67:PHE:CZ	1:D:263:LYS:HE3	2.51	0.44
1:D:235:ARG:NH1	1:D:308:LEU:O	2.46	0.44
1:C:41:ALA:HB1	1:C:57:GLN:CD	2.42	0.44
1:B:4:ILE:HA	1:B:137:GLU:O	2.18	0.44
1:C:213:GLU:OE1	1:C:390:LEU:HB2	2.17	0.44
1:B:57:GLN:HB3	1:A:282:ASN:ND2	2.31	0.44
1:B:532:LEU:HA	1:B:535:THR:HB	2.00	0.44
1:A:81:GLU:O	1:A:85:ASP:HB2	2.18	0.44
1:A:200:PHE:CE1	1:A:319:PRO:HB2	2.52	0.44
1:A:542:LEU:HG	1:A:591:LEU:HD23	1.99	0.44
1:C:397:LEU:HD11	1:C:512:ILE:HG12	2.00	0.44
1:B:243:GLU:HG2	1:B:298:ILE:HG23	1.98	0.44
1:A:5:ILE:HG12	1:A:137:GLU:O	2.18	0.44
1:A:81:GLU:HA	1:A:84:ARG:HB3	1.98	0.44
1:A:200:PHE:HE1	1:A:319:PRO:HB2	1.83	0.44
1:D:244:PHE:CB	1:D:296:MET:HE2	2.48	0.44
1:A:160:ILE:HG23	1:D:355:GLU:HB3	1.99	0.44
1:D:222:ASN:ND2	1:D:319:PRO:O	2.46	0.44
1:D:302:ARG:NH1	1:D:347:PRO:HG2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:TYR:CD2	1:C:105:VAL:HG11	2.53	0.44
1:C:192:VAL:HB	1:C:203:SER:HB2	2.00	0.44
1:C:476:PHE:CD2	1:C:484:LEU:HD11	2.53	0.44
1:C:235:ARG:O	1:C:236:LEU:HD13	2.18	0.44
1:B:17:ALA:HB2	1:B:26:VAL:HG22	2.00	0.44
1:C:81:GLU:O	1:C:84:ARG:HB3	2.18	0.43
1:A:317:ILE:HG23	1:A:356:PHE:CE1	2.53	0.43
1:D:31:GLU:OE2	1:D:52:GLN:HB3	2.17	0.43
1:D:136:THR:HA	1:D:163:LEU:HA	2.00	0.43
1:C:341:GLY:C	1:C:367:PRO:HB2	2.42	0.43
1:C:427:SER:OG	1:C:468:GLY:HA2	2.18	0.43
1:D:40:ILE:HD13	1:D:115:ILE:HG22	2.01	0.43
1:D:200:PHE:CE1	1:D:319:PRO:HB2	2.51	0.43
1:D:271:ILE:HG12	2:D:701:ATP:C2	2.51	0.43
1:C:68:ALA:HB2	1:C:230:GLU:OE2	2.18	0.43
1:C:478:ILE:HA	1:C:483:ILE:O	2.18	0.43
1:C:483:ILE:HG12	1:C:503:ALA:H	1.83	0.43
1:B:4:ILE:HG21	1:B:139:VAL:HG23	1.99	0.43
1:B:11:THR:OG1	1:B:70:LYS:HB3	2.19	0.43
1:B:278:GLN:HA	1:B:301:THR:HA	2.01	0.43
1:D:5:ILE:HD13	1:D:135:VAL:HG11	2.00	0.43
1:D:256:PRO:HA	1:D:259:MET:HB2	2.01	0.43
1:C:24:PRO:HD3	1:C:181:LEU:HD13	1.98	0.43
1:D:196:GLY:HA3	2:D:701:ATP:O3B	2.19	0.43
1:D:398:SER:HA	1:D:412:ILE:O	2.19	0.43
1:C:3:LYS:HA	1:C:383:THR:CG2	2.45	0.43
1:B:305:LEU:O	1:B:309:VAL:HG22	2.18	0.43
1:D:475:THR:HB	1:D:487:SER:OG	2.17	0.43
1:C:96:ALA:HB2	1:C:102:TRP:CD1	2.53	0.43
1:C:179:TYR:HE1	1:C:362:ARG:CZ	2.31	0.43
1:B:155:LYS:HE3	1:B:165:VAL:HG11	2.01	0.43
1:B:288:ALA:HA	1:B:293:PRO:HA	2.01	0.43
1:D:513:GLN:O	1:D:517:ARG:HG3	2.18	0.43
1:C:27:LEU:HD22	1:C:130:TYR:CZ	2.54	0.43
1:C:194:ASP:O	1:C:201:ASP:N	2.47	0.43
1:C:200:PHE:HE1	1:C:319:PRO:CB	2.27	0.43
1:C:379:GLY:O	1:C:383:THR:HG23	2.19	0.43
1:B:255:ASP:O	1:B:259:MET:HG2	2.19	0.43
1:C:418:ILE:HG21	1:C:482:GLY:HA2	2.00	0.42
1:B:119:VAL:O	1:B:123:MET:HG2	2.18	0.42
1:A:101:ALA:C	1:A:102:TRP:HD1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:PHE:O	1:C:392:LEU:HB3	2.18	0.42
1:A:241:VAL:HG13	1:A:252:LEU:H	1.83	0.42
1:A:466:PRO:HG2	1:A:469:MET:HE3	1.99	0.42
1:D:241:VAL:O	1:D:245:LYS:HB2	2.19	0.42
1:C:70:LYS:HZ1	1:C:171:GLU:CD	2.22	0.42
1:A:11:THR:O	1:A:38:SER:HB2	2.18	0.42
1:D:244:PHE:HB2	1:D:298:ILE:HD11	2.01	0.42
1:D:475:THR:O	1:D:486:VAL:HA	2.19	0.42
1:B:17:ALA:HB3	1:B:372:ALA:C	2.44	0.42
1:A:124:LYS:HG3	1:A:135:VAL:O	2.19	0.42
1:D:337:VAL:HG11	1:D:353:VAL:CG1	2.49	0.42
1:D:380:GLY:O	1:D:384:GLY:N	2.51	0.42
1:D:486:VAL:HB	1:D:499:ILE:CG1	2.49	0.42
1:C:395:THR:HG22	1:C:418:ILE:HD11	2.02	0.42
1:C:35:THR:HG21	1:C:368:ASP:HB3	2.00	0.42
1:B:86:VAL:HA	1:B:93:ILE:HD12	2.01	0.42
1:B:418:ILE:HG12	1:B:478:ILE:HG21	2.01	0.42
1:C:293:PRO:HD3	1:D:285:TYR:CE1	2.55	0.42
1:B:73:ILE:O	1:B:150:GLN:HG2	2.19	0.42
1:B:398:SER:HA	1:B:412:ILE:O	2.19	0.42
1:D:421:LYS:HD3	1:D:477:ASP:OD2	2.20	0.42
1:B:19:MET:HG2	1:B:376:ALA:O	2.19	0.42
1:B:56:ARG:NH1	1:A:282:ASN:H	2.17	0.42
1:B:196:GLY:HA3	2:B:701:ATP:O3B	2.19	0.42
1:B:167:ARG:CG	1:B:382:LEU:HD11	2.47	0.42
1:B:363:LYS:HD2	1:A:129:ASP:OD2	2.19	0.42
1:B:465:ALA:HB3	1:B:470:PRO:HG3	2.02	0.42
1:D:6:GLY:HA3	1:D:376:ALA:N	2.34	0.42
1:C:142:VAL:O	1:C:170:ASN:HA	2.19	0.42
1:B:58:ALA:HB1	1:B:65:THR:HG21	2.02	0.42
1:A:50:VAL:HG13	1:A:119:VAL:HG22	2.01	0.42
1:A:96:ALA:HB2	1:A:102:TRP:CD2	2.54	0.42
1:C:61:ASN:ND2	1:C:64:ASN:HB2	2.35	0.41
1:A:160:ILE:HA	1:D:355:GLU:HA	2.01	0.41
1:A:12:THR:O	1:A:37:PRO:HA	2.20	0.41
1:A:373:ILE:O	1:A:377:VAL:HG23	2.20	0.41
1:D:306:GLU:O	1:D:310:GLU:HB2	2.19	0.41
1:C:96:ALA:HB2	1:C:102:TRP:CE2	2.55	0.41
1:A:179:TYR:OH	1:A:362:ARG:NH1	2.52	0.41
1:C:96:ALA:HB2	1:C:102:TRP:CD2	2.55	0.41
1:C:162:GLY:HA2	1:B:358:GLY:CA	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:LEU:HD13	1:C:484:LEU:HD22	2.02	0.41
1:B:412:ILE:HD11	1:B:476:PHE:HB3	2.02	0.41
1:A:272:GLU:OE2	1:A:279:THR:OG1	2.36	0.41
1:B:12:THR:HB	2:B:701:ATP:H3'	2.02	0.41
1:B:531:GLU:O	1:B:534:GLN:HB3	2.19	0.41
1:A:4:ILE:HB	1:A:379:GLY:CA	2.51	0.41
1:D:96:ALA:HB2	1:D:102:TRP:CE2	2.55	0.41
1:C:262:LEU:HD12	1:C:262:LEU:HA	1.85	0.41
1:B:15:CYS:HB2	1:B:35:THR:HG22	2.02	0.41
1:B:75:ARG:HH22	1:B:225:THR:HG21	1.86	0.41
1:B:82:VAL:O	1:B:86:VAL:HG23	2.20	0.41
1:A:49:LEU:HD12	1:A:57:GLN:HG2	2.03	0.41
1:D:50:VAL:HG12	1:D:122:LYS:HD3	2.01	0.41
1:C:302:ARG:HH12	1:C:347:PRO:HD2	1.85	0.41
1:B:178:ALA:HB2	1:B:370:ALA:O	2.20	0.41
1:B:285:TYR:CG	1:A:293:PRO:HD3	2.55	0.41
1:A:117:ALA:HA	1:A:161:ALA:HB2	2.02	0.41
1:A:302:ARG:HH12	1:A:347:PRO:HG2	1.84	0.41
1:D:241:VAL:O	1:D:245:LYS:N	2.43	0.41
1:C:189:THR:HG21	1:C:329:LEU:CD1	2.50	0.41
1:A:34:ARG:NH2	1:A:369:GLU:OE1	2.54	0.41
1:B:81:GLU:OE2	1:B:226:HIS:NE2	2.54	0.41
1:A:525:ALA:O	1:A:528:LYS:HG3	2.21	0.41
1:D:3:LYS:O	1:D:137:GLU:HB2	2.21	0.41
1:C:40:ILE:HB	1:C:66:LEU:HB2	2.02	0.41
1:B:440:VAL:HG12	1:B:454:LEU:HD12	2.03	0.41
1:A:469:MET:HB3	1:A:470:PRO:HD3	2.02	0.41
1:D:81:GLU:O	1:D:85:ASP:HB2	2.21	0.41
1:B:283:LEU:HD13	1:B:286:ILE:HD13	2.03	0.40
1:A:113:PRO:HB2	1:A:160:ILE:HD12	2.03	0.40
1:A:462:ILE:HG12	1:A:490:ASP:OD2	2.21	0.40
1:D:13:ASN:HB3	1:D:35:THR:HB	2.04	0.40
1:B:396:PRO:CB	1:B:512:ILE:HD13	2.50	0.40
1:B:426:PHE:HB3	1:B:620:LEU:HG	2.03	0.40
1:A:251:ASP:O	1:A:254:ASN:ND2	2.54	0.40
1:A:281:VAL:O	1:A:297:ASN:HA	2.21	0.40
1:D:529:PHE:HA	1:D:532:LEU:CD2	2.50	0.40
1:C:192:VAL:CG2	1:C:205:ILE:HD12	2.50	0.40
1:C:214:LYS:HG2	1:C:216:PHE:CE1	2.56	0.40
1:B:52:GLN:O	1:B:56:ARG:HG3	2.21	0.40
1:B:62:PRO:HG3	1:B:257:LEU:HD23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:GLU:HB2	1:D:219:LEU:HD21	2.03	0.40
1:B:294:LYS:HA	1:B:294:LYS:HD3	1.88	0.40
1:B:428:THR:HG22	1:B:462:ILE:HD13	2.03	0.40
1:D:26:VAL:HG21	1:D:369:GLU:OE1	2.22	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	604/622 (97%)	597 (99%)	6 (1%)	1 (0%)	43	78
1	B	537/622 (86%)	532 (99%)	5 (1%)	0	100	100
1	C	537/622 (86%)	528 (98%)	8 (2%)	1 (0%)	43	78
1	D	537/622 (86%)	532 (99%)	5 (1%)	0	100	100
All	All	2215/2488 (89%)	2189 (99%)	24 (1%)	2 (0%)	48	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	VAL
1	C	235	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/506 (97%)	487 (99%)	5 (1%)	68	78
1	B	443/506 (88%)	441 (100%)	2 (0%)	81	83
1	C	443/506 (88%)	438 (99%)	5 (1%)	65	76
1	D	443/506 (88%)	438 (99%)	5 (1%)	65	76
All	All	1821/2024 (90%)	1804 (99%)	17 (1%)	70	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	236	LEU
1	C	298	ILE
1	C	466	PRO
1	C	467	ARG
1	C	528	LYS
1	B	209	GLU
1	B	528	LYS
1	A	146	PHE
1	A	297	ASN
1	A	528	LYS
1	A	598	LEU
1	A	600	GLU
1	D	19	MET
1	D	25	ARG
1	D	129	ASP
1	D	385	ASP
1	D	528	LYS

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

Mol	Chain	Res	Type
1	C	13	ASN
1	C	29	ASN
1	C	108	GLN
1	C	152	GLN
1	C	432	ASN
1	C	451	ASN
1	C	463	ASN
1	B	170	ASN
1	B	343	GLN
1	B	451	ASN

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Mol	Chain	Res	Type
1	A	29	ASN
1	A	64	ASN
1	A	108	GLN
1	A	282	ASN
1	A	422	HIS
1	A	497	GLN
1	A	513	GLN
1	D	114	GLN
1	D	248	GLN
1	D	422	HIS
1	D	451	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	ATP	D	701	-	32,33,33	2.07	5 (15%)	48,52,52	1.91	10 (20%)
2	ATP	B	701	-	32,33,33	2.00	7 (21%)	48,52,52	2.14	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	A	701	-	32,33,33	1.94	7 (21%)	48,52,52	1.80	11 (22%)
2	ATP	C	701	-	32,33,33	2.34	8 (25%)	48,52,52	2.10	12 (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	ATP	D	701	-	-	0/22/38/38	0/3/3/3
2	ATP	B	701	-	-	1/22/38/38	0/3/3/3
2	ATP	A	701	-	-	0/22/38/38	0/3/3/3
2	ATP	C	701	-	-	1/22/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	ATP	PB-O3B	6.97	1.67	1.59
2	C	701	ATP	PB-O3B	6.58	1.66	1.59
2	C	701	ATP	C5-C4	6.58	1.50	1.39
2	B	701	ATP	C5-C4	5.49	1.48	1.39
2	A	701	ATP	C5-C4	5.37	1.48	1.39
2	B	701	ATP	PB-O3B	5.35	1.65	1.59
2	D	701	ATP	C5-C4	5.22	1.48	1.39
2	A	701	ATP	PB-O3B	5.19	1.65	1.59
2	B	701	ATP	PA-O3A	4.95	1.64	1.59
2	C	701	ATP	PA-O3A	4.91	1.64	1.59
2	A	701	ATP	PA-O3A	4.50	1.64	1.59
2	C	701	ATP	C5-C6	3.90	1.51	1.41
2	D	701	ATP	PA-O3A	3.69	1.63	1.59
2	D	701	ATP	C5-C6	3.56	1.50	1.41
2	C	701	ATP	PB-O3A	3.41	1.63	1.59
2	A	701	ATP	C5-C6	3.27	1.50	1.41
2	B	701	ATP	C5-C6	3.24	1.50	1.41
2	B	701	ATP	C8-N7	3.08	1.37	1.31
2	C	701	ATP	C8-N7	3.01	1.37	1.31
2	A	701	ATP	PB-O3A	2.73	1.62	1.59
2	D	701	ATP	C8-N7	2.69	1.36	1.31
2	A	701	ATP	C8-N7	2.69	1.36	1.31
2	B	701	ATP	C1'-N9	2.35	1.52	1.46
2	B	701	ATP	C5-N7	-2.23	1.35	1.39
2	C	701	ATP	C2-N1	2.21	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	ATP	C4-N3	2.03	1.38	1.34
2	A	701	ATP	C5-N7	-2.03	1.35	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	ATP	C5-C4-N3	-7.46	116.44	126.72
2	D	701	ATP	C5-C4-N3	-5.75	118.79	126.72
2	A	701	ATP	C5-C4-N3	-5.68	118.89	126.72
2	C	701	ATP	C5-C4-N3	-5.65	118.94	126.72
2	B	701	ATP	O2B-PB-O3A	-5.29	92.99	107.27
2	C	701	ATP	N3-C2-N1	-5.02	120.98	128.58
2	B	701	ATP	N3-C4-N9	4.71	135.18	127.17
2	C	701	ATP	N3-C4-N9	4.63	135.04	127.17
2	B	701	ATP	C4-C5-N7	-4.56	105.37	110.58
2	D	701	ATP	C4-C5-N7	-4.40	105.55	110.58
2	C	701	ATP	C2-N1-C6	4.39	125.94	118.73
2	B	701	ATP	C2-N3-C4	4.29	122.31	111.83
2	A	701	ATP	N3-C4-N9	4.23	134.37	127.17
2	A	701	ATP	C4-C5-N7	-4.09	105.91	110.58
2	C	701	ATP	C2-N3-C4	4.04	121.70	111.83
2	D	701	ATP	N3-C4-N9	3.99	133.96	127.17
2	D	701	ATP	C2-N3-C4	3.77	121.03	111.83
2	A	701	ATP	C2-N3-C4	3.75	120.98	111.83
2	C	701	ATP	O2B-PB-O3A	-3.68	97.33	107.27
2	C	701	ATP	C4-C5-N7	-3.66	106.40	110.58
2	A	701	ATP	N3-C2-N1	-3.56	123.20	128.58
2	D	701	ATP	N3-C2-N1	-3.38	123.46	128.58
2	B	701	ATP	O2A-PA-O5'	3.35	122.73	107.57
2	D	701	ATP	C5-N7-C8	3.10	108.33	103.45
2	D	701	ATP	O2B-PB-O3A	-3.06	99.00	107.27
2	B	701	ATP	N3-C2-N1	-3.03	124.00	128.58
2	C	701	ATP	O2B-PB-O3B	2.97	115.31	107.27
2	C	701	ATP	C5-N7-C8	2.87	107.96	103.45
2	D	701	ATP	O2A-PA-O5'	2.81	120.30	107.57
2	A	701	ATP	C5-N7-C8	2.80	107.85	103.45
2	D	701	ATP	C2-N1-C6	2.77	123.28	118.73
2	A	701	ATP	O2A-PA-O3A	2.74	114.67	107.27
2	B	701	ATP	C5-N7-C8	2.69	107.67	103.45
2	C	701	ATP	O2A-PA-O3A	2.65	114.45	107.27
2	A	701	ATP	C2-N1-C6	2.64	123.07	118.73
2	A	701	ATP	C6-C5-N7	2.57	137.04	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	ATP	C6-C5-N7	2.49	136.89	132.09
2	C	701	ATP	C4-N9-C8	2.41	108.27	105.74
2	B	701	ATP	C5-C4-N9	2.34	108.36	105.81
2	C	701	ATP	O3'-C3'-C2'	-2.29	104.47	111.82
2	A	701	ATP	O2B-PB-O3B	2.18	113.15	107.27
2	A	701	ATP	C4-N9-C8	2.16	108.00	105.74
2	B	701	ATP	C6-C5-N7	2.11	136.17	132.09
2	B	701	ATP	C4'-O4'-C1'	2.08	114.05	109.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

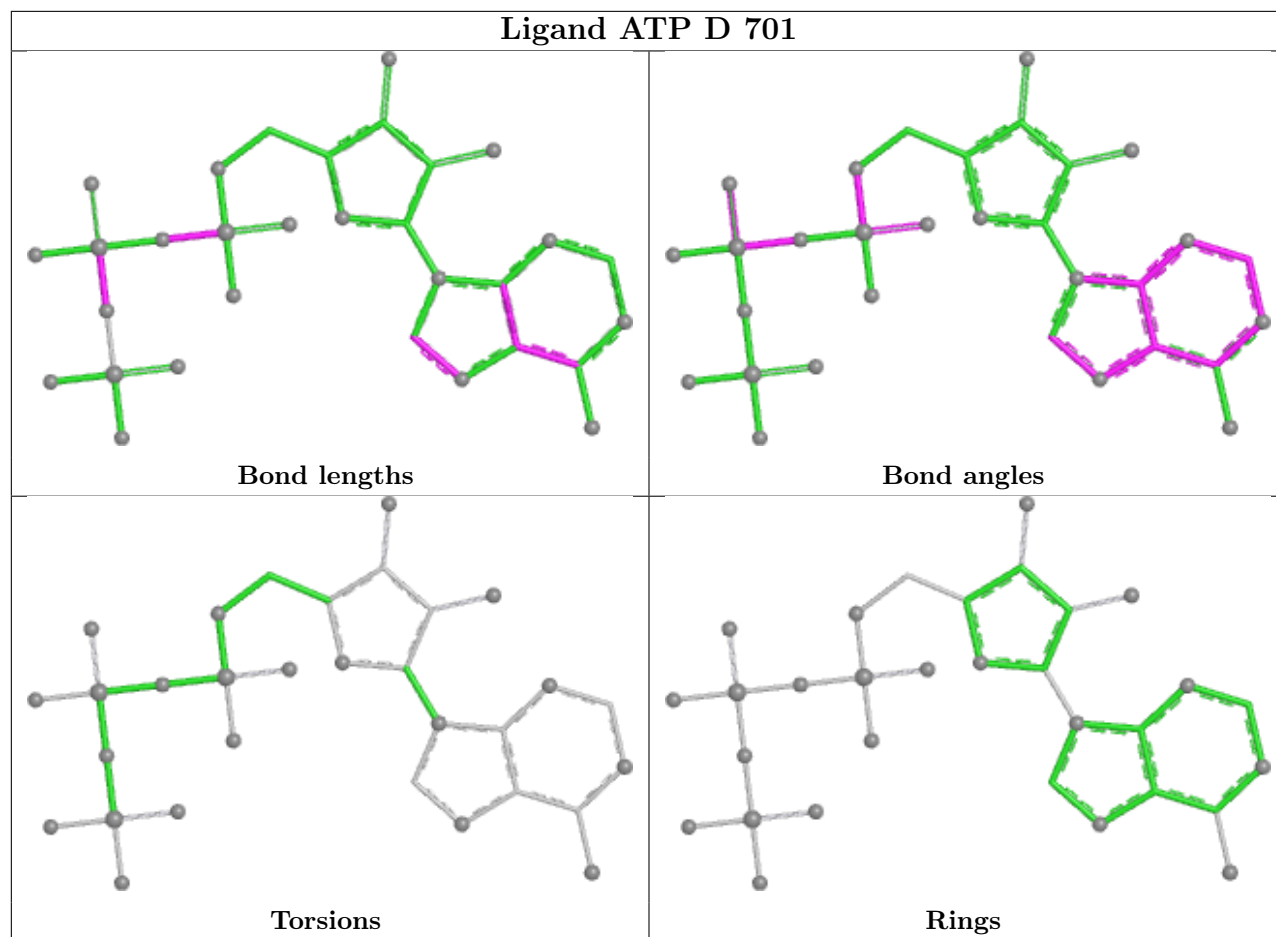
Mol	Chain	Res	Type	Atoms
2	C	701	ATP	PG-O3B-PB-O2B
2	B	701	ATP	PG-O3B-PB-O2B

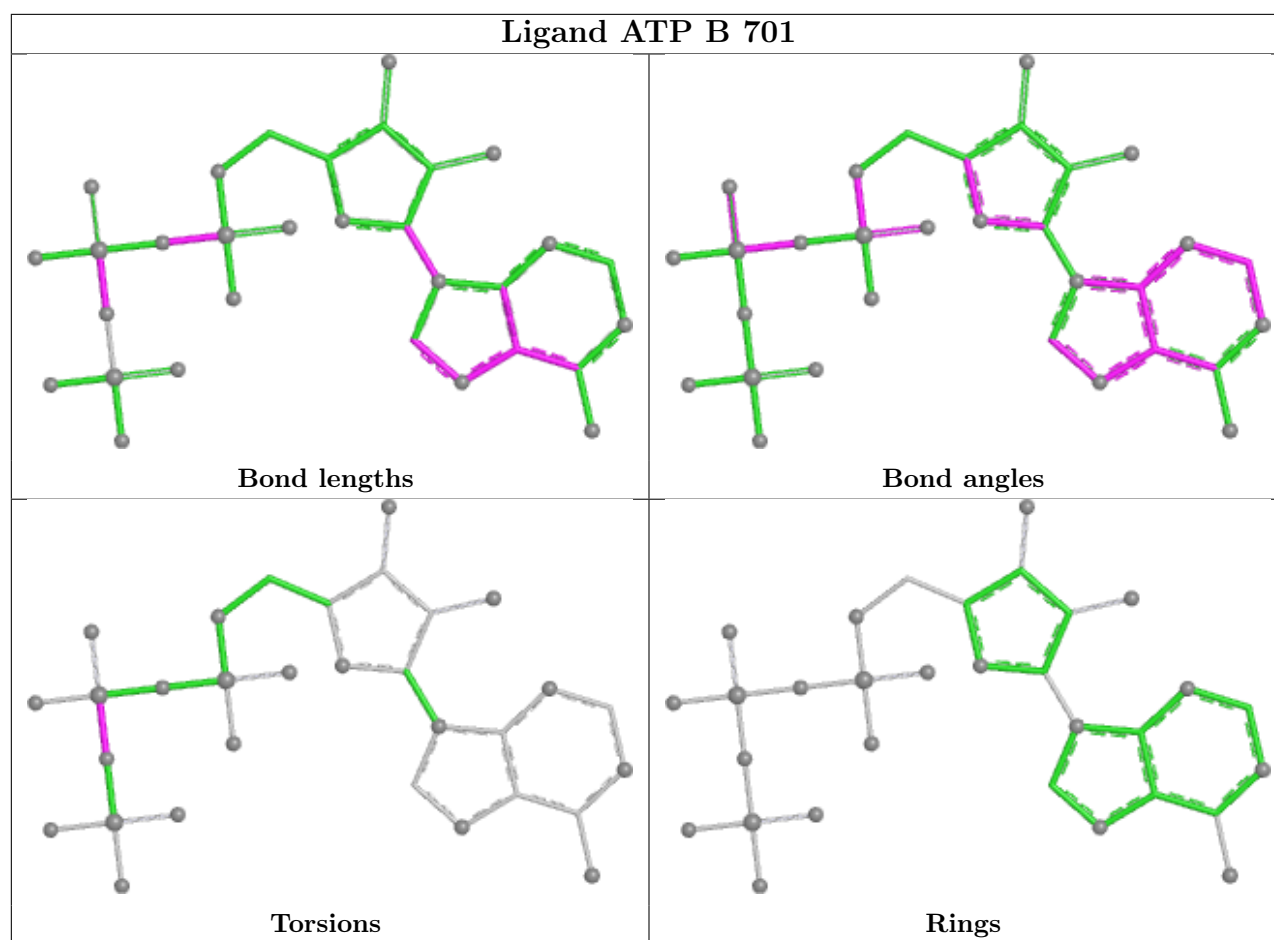
There are no ring outliers.

4 monomers are involved in 11 short contacts:

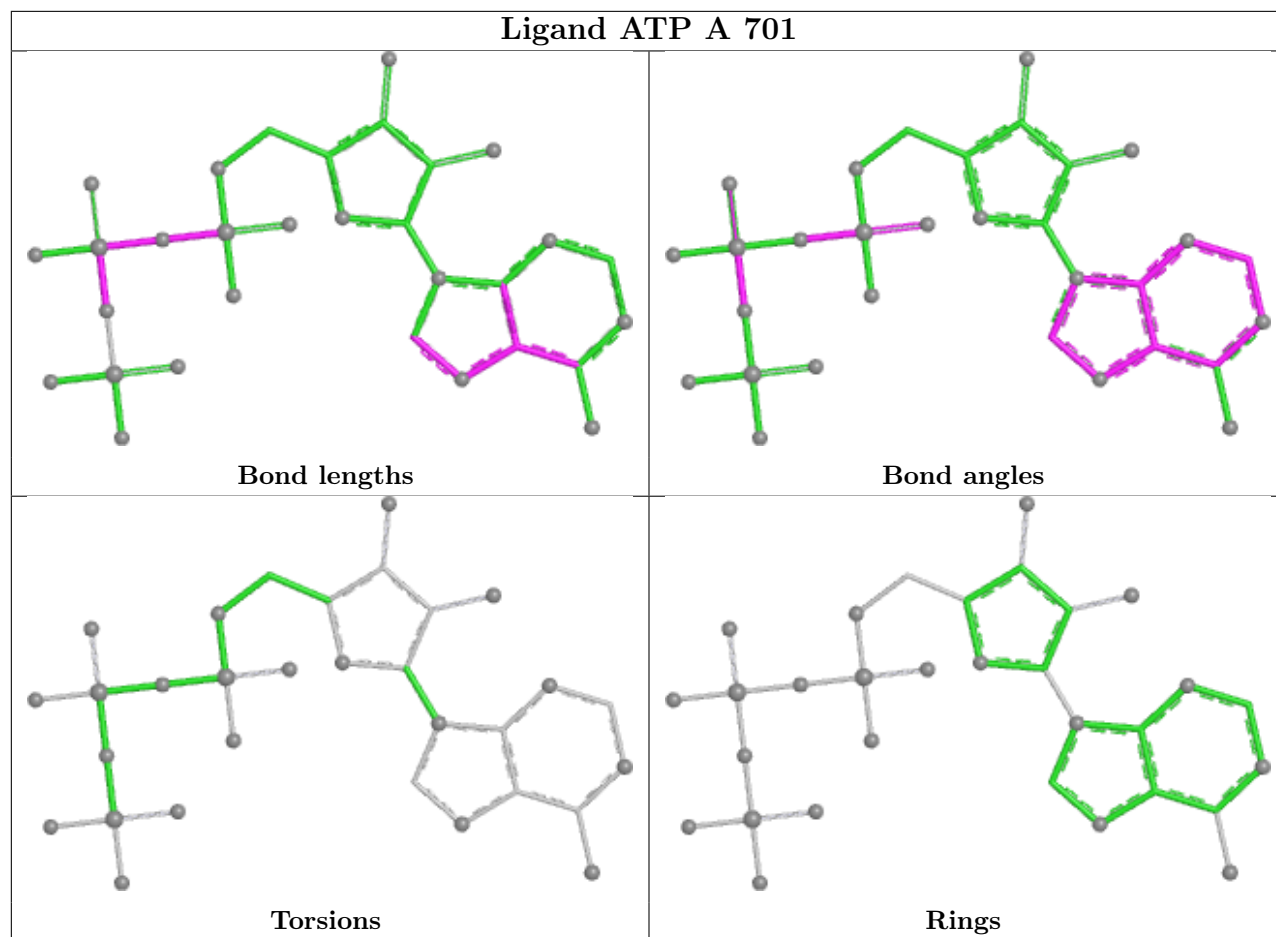
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	ATP	5	0
2	B	701	ATP	3	0
2	A	701	ATP	2	0
2	C	701	ATP	1	0

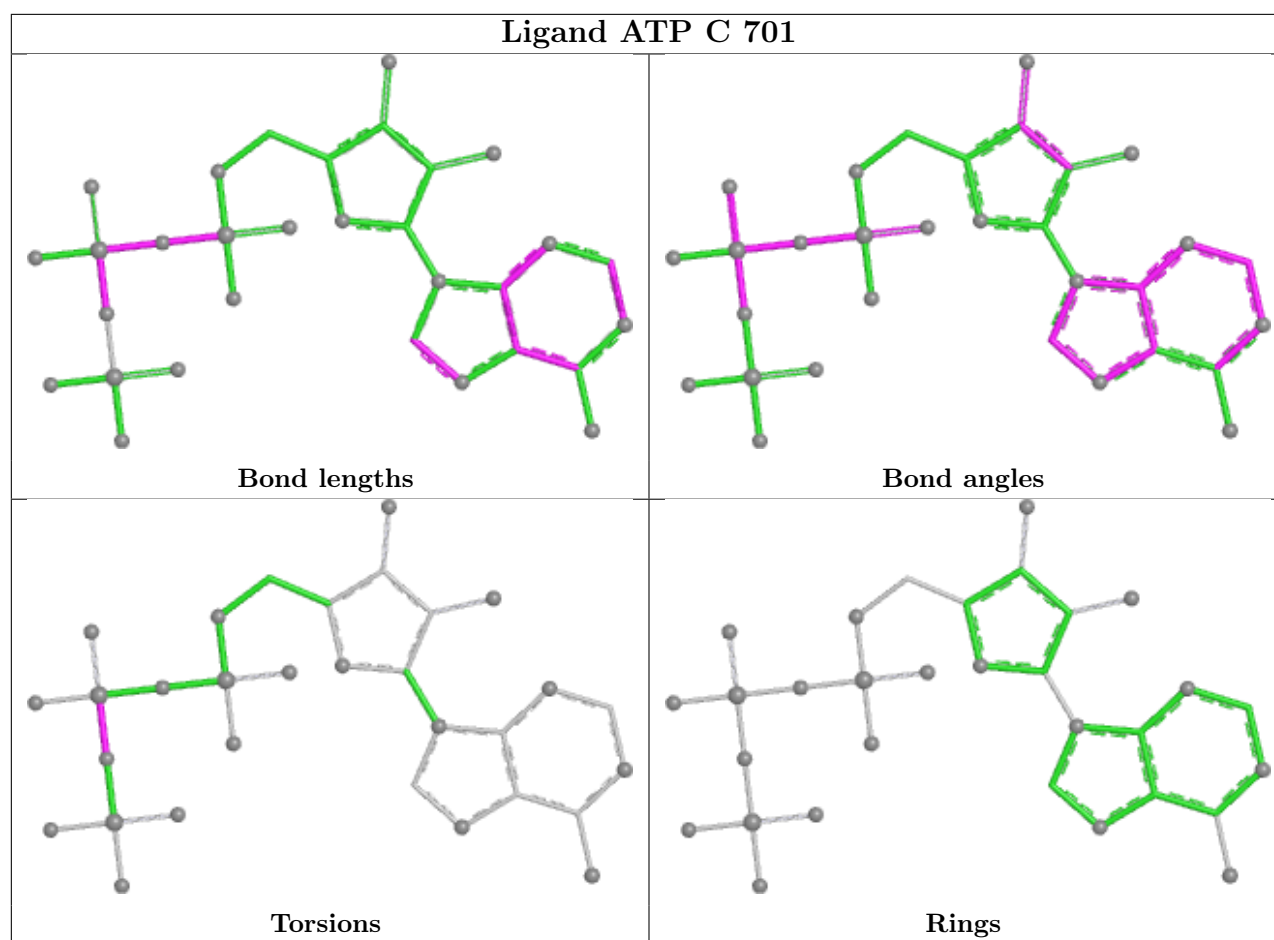
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





Ligand ATP A 701





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	608/622 (97%)	-0.52	11 (1%) 67 58	320, 320, 320, 320	0
1	B	541/622 (86%)	-0.47	10 (1%) 67 58	320, 320, 320, 320	0
1	C	541/622 (86%)	-0.51	3 (0%) 85 76	320, 320, 320, 320	0
1	D	541/622 (86%)	-0.41	10 (1%) 67 58	320, 320, 320, 320	0
All	All	2231/2488 (89%)	-0.48	34 (1%) 72 60	320, 320, 320, 320	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	ALA	5.9
1	B	211	ASP	5.7
1	A	186	GLY	5.2
1	D	194	ASP	4.3
1	A	212	GLY	4.1
1	D	211	ASP	4.0
1	A	450	ASP	3.9
1	D	40	ILE	3.8
1	A	620	LEU	3.5
1	D	212	GLY	3.3
1	B	385	ASP	3.1
1	B	391	LEU	3.1
1	C	74	GLY	3.0
1	A	311	ASP	2.9
1	A	185	THR	2.8
1	B	432	ASN	2.7
1	D	80	GLU	2.7
1	D	493	SER	2.7
1	D	494	GLY	2.7
1	A	596	GLN	2.6
1	B	99	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	622	GLY	2.5
1	D	405	GLY	2.5
1	A	358	GLY	2.5
1	B	191	ALA	2.5
1	B	162	GLY	2.4
1	A	331	VAL	2.3
1	A	470	PRO	2.3
1	C	48	THR	2.2
1	B	303	ALA	2.1
1	D	192	VAL	2.1
1	D	97	ASP	2.1
1	A	592	ALA	2.1
1	B	203	SER	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](#)

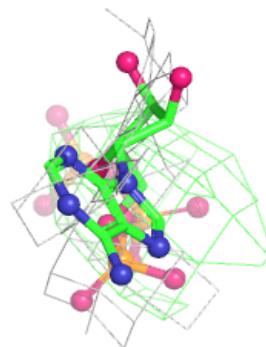
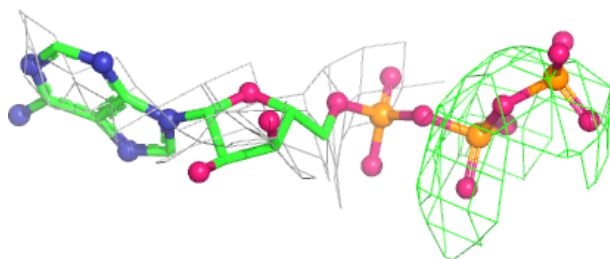
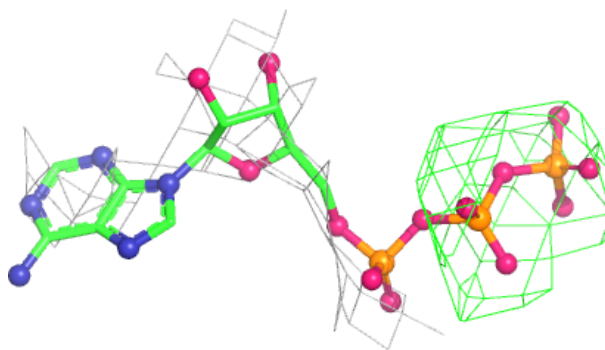
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ATP	C	701	31/31	0.97	0.09	320,320,320,320	0
2	ATP	D	701	31/31	0.98	0.08	319,319,319,319	0
2	ATP	A	701	31/31	0.99	0.08	319,319,319,319	0
2	ATP	B	701	31/31	0.99	0.06	319,319,319,319	0

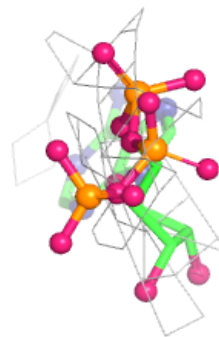
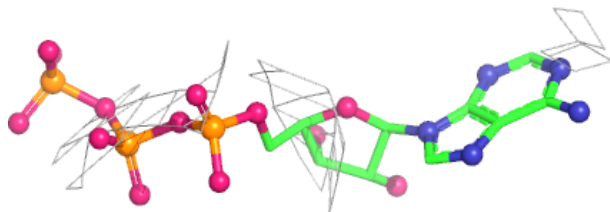
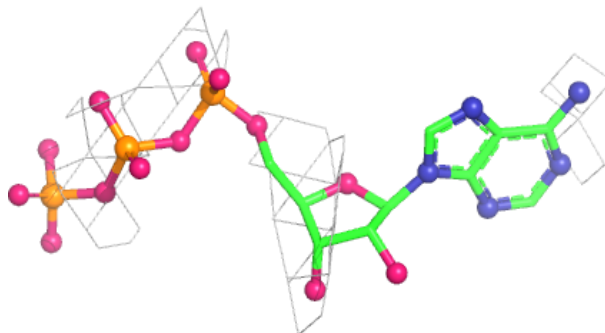
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 701:

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

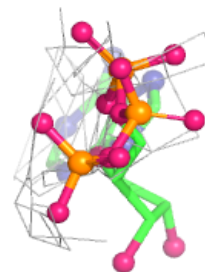
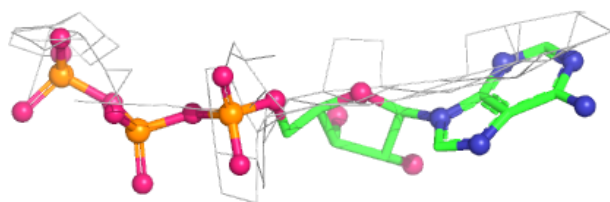
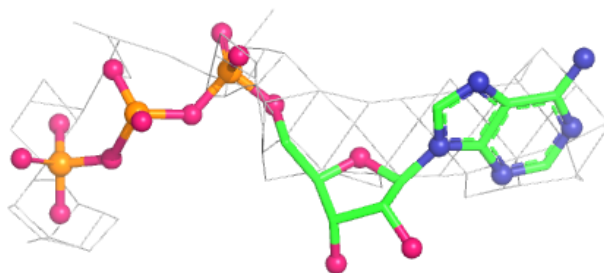
**Electron density around ATP D 701:**

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

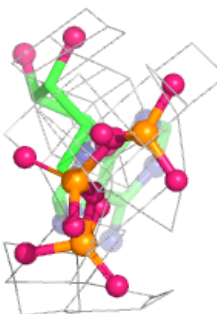
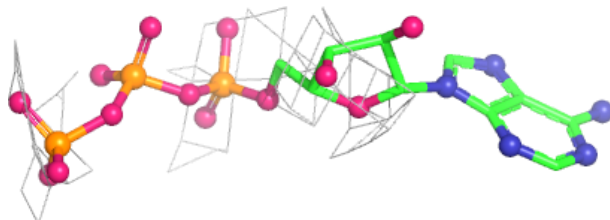
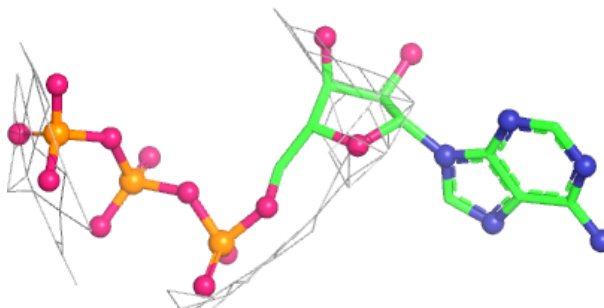


Electron density around ATP A 701:

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

**Electron density around ATP B 701:**

$2mF_o - DF_c$ (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.