



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:54 AM UTC

PDB ID : 6HQU / pdb_00006hqu
Title : Humanised RadA mutant HumRadA22 in complex with a recombined BRC repeat 8-2
Authors : Pantelejevs, T.; Lindenburg, L.; Hyvonen, M.; Hollfelder, F.
Deposited on : 2018-09-25
Resolution : 1.97 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

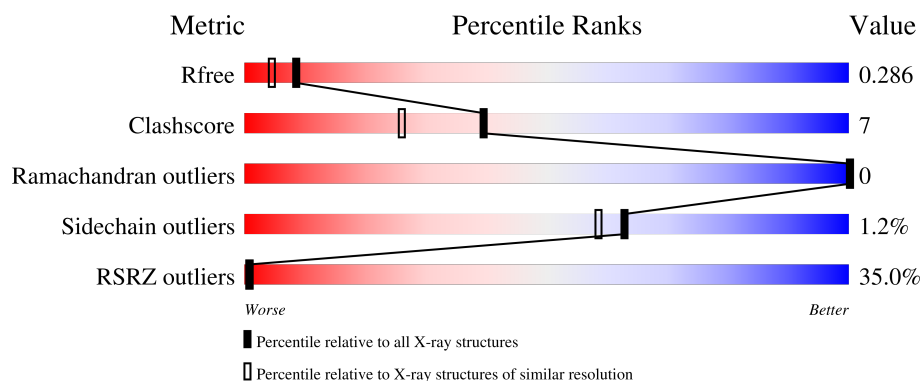
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	231	
1	B	231	
1	C	231	
1	D	231	
1	E	231	

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Mol	Chain	Length	Quality of chain
1	F	231	
1	G	231	
1	H	231	
2	I	38	
2	J	38	
2	K	38	
2	L	38	
2	M	38	
2	N	38	
2	O	38	

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
4	MG	H	402	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14419 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 repair and recombination protein RadA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1621	1015	292	308	6			
1	B	219	Total	C	N	O	S	0	0	0
			1704	1068	310	320	6			
1	C	210	Total	C	N	O	S	0	0	0
			1639	1027	298	308	6			
1	D	208	Total	C	N	O	S	0	0	0
			1615	1012	290	307	6			
1	E	212	Total	C	N	O	S	0	0	0
			1637	1023	296	312	6			
1	F	204	Total	C	N	O	S	0	0	0
			1578	987	285	300	6			
1	G	194	Total	C	N	O	S	0	0	0
			1534	965	273	290	6			
1	H	192	Total	C	N	O	S	0	0	0
			1440	901	257	276	6			

- Molecule 2 is a protein called Breast cancer type 2 susceptibility.

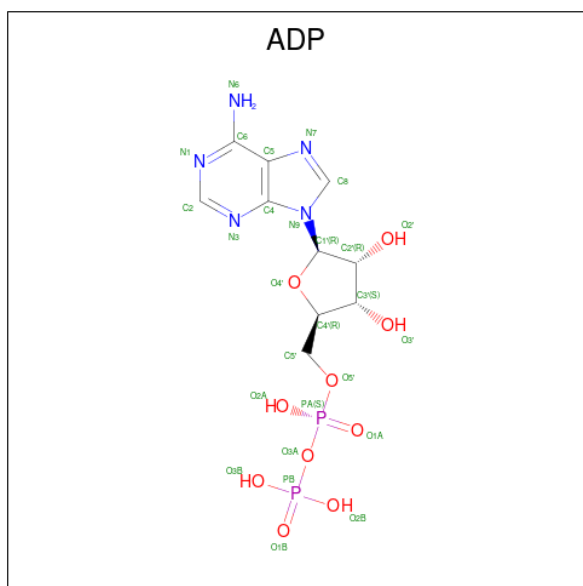
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	31	Total	C	N	O	0	0	0
			225	142	37	46			
2	J	31	Total	C	N	O	0	0	0
			225	142	37	46			
2	K	18	Total	C	N	O	0	0	0
			128	80	21	27			
2	L	31	Total	C	N	O	0	0	0
			225	142	37	46			
2	M	30	Total	C	N	O	0	0	0
			219	139	36	44			
2	N	12	Total	C	N	O	0	0	0
			84	53	15	16			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	15	Total	C	N	O	0	0	0
			107	68	18	21			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

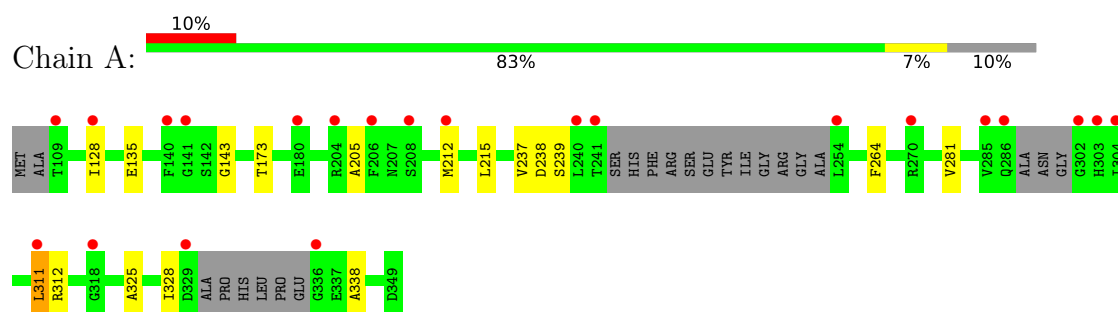
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	49	Total O 49 49	0	0
5	B	40	Total O 40 40	0	0
5	C	29	Total O 29 29	0	0
5	D	40	Total O 40 40	0	0
5	E	29	Total O 29 29	0	0
5	F	4	Total O 4 4	0	0
5	G	9	Total O 9 9	0	0
5	I	8	Total O 8 8	0	0
5	J	2	Total O 2 2	0	0
5	K	1	Total O 1 1	0	0
5	L	3	Total O 3 3	0	0

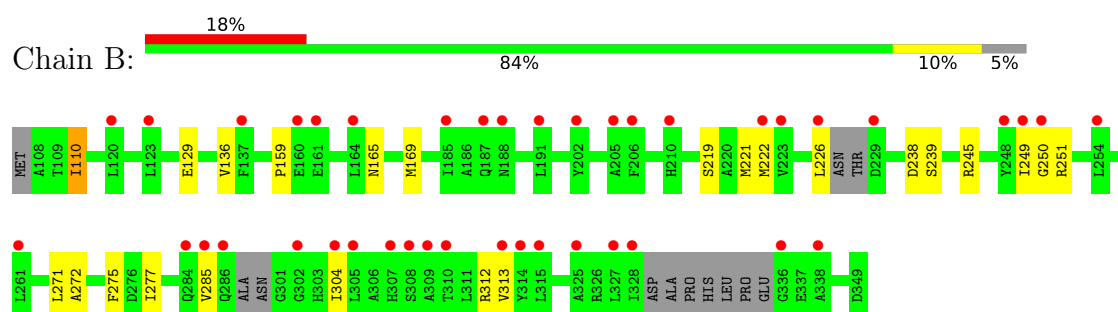
3 Residue-property plots [i](#)

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.

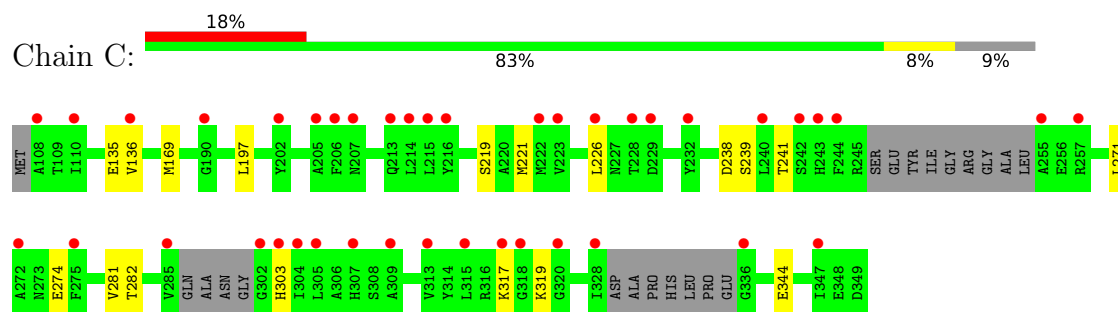
- Molecule 1: DNA repair and recombination protein RadA



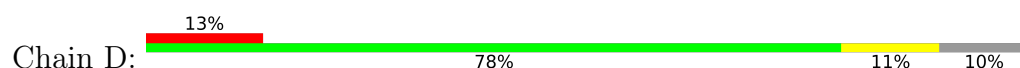
- Molecule 1: DNA repair and recombination protein RadA

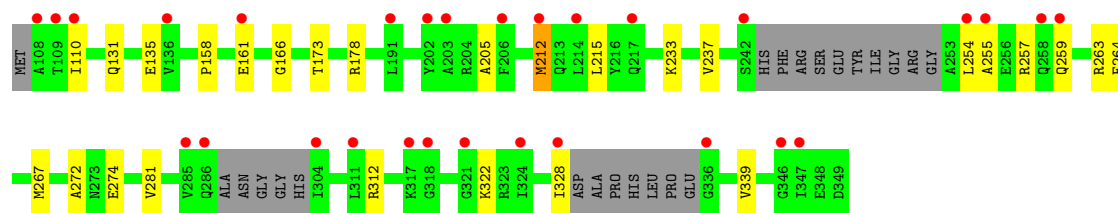


- Molecule 1: DNA repair and recombination protein RadA

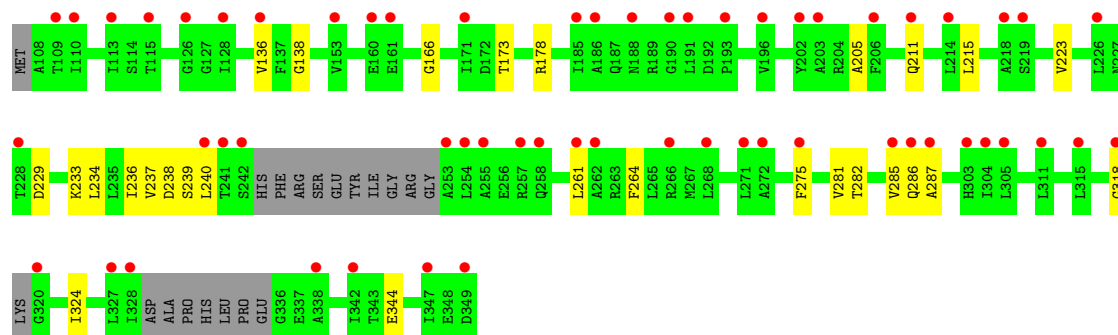
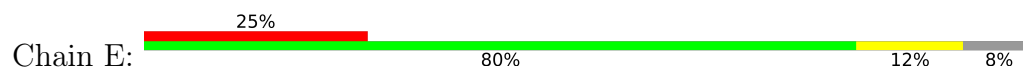


- Molecule 1: DNA repair and recombination protein RadA

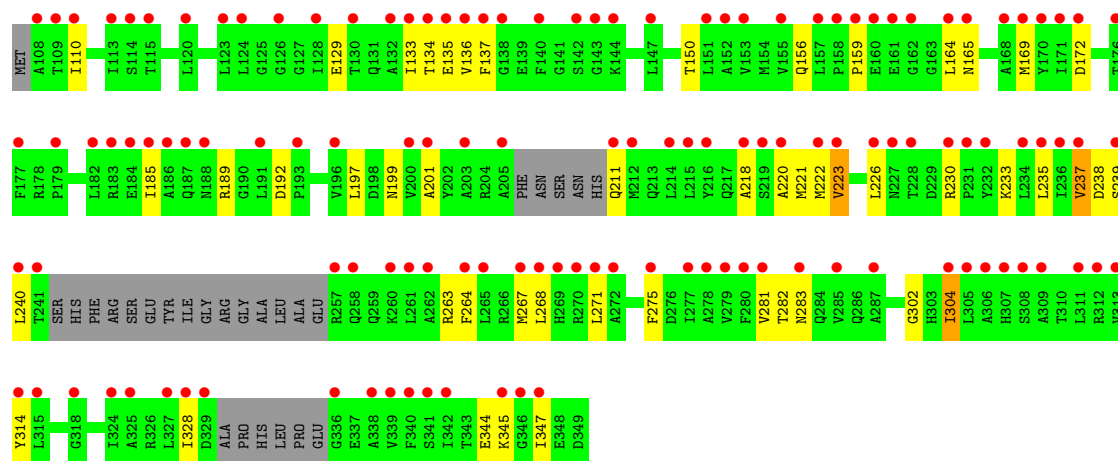




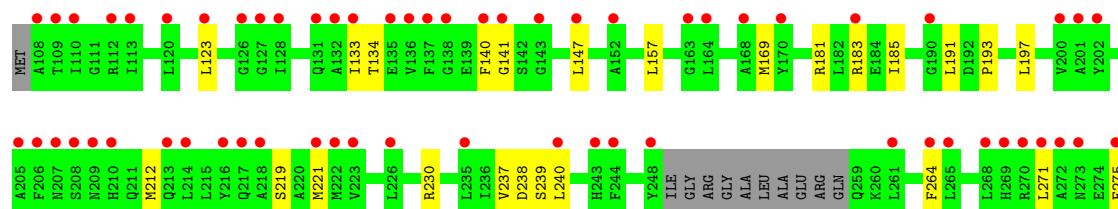
• Molecule 1: DNA repair and recombination protein RadA

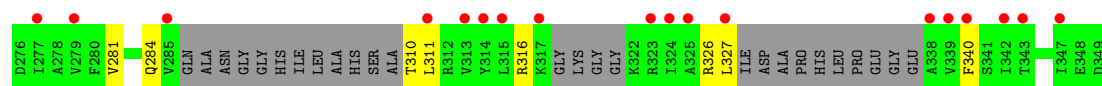


• Molecule 1: DNA repair and recombination protein RadA

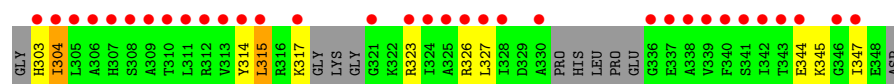
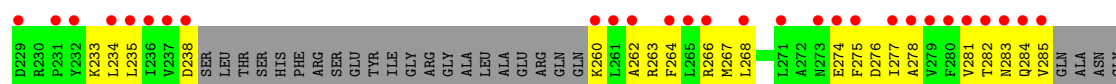
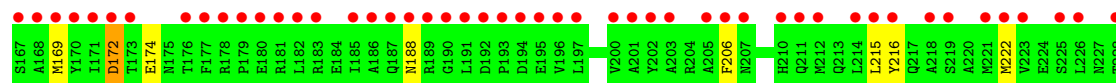
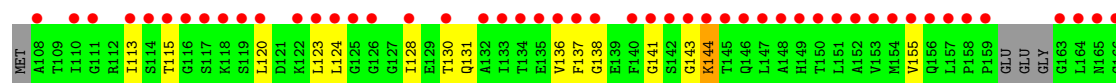


• Molecule 1: DNA repair and recombination protein RadA

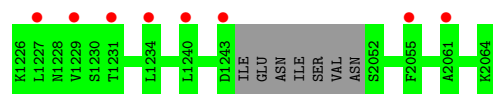
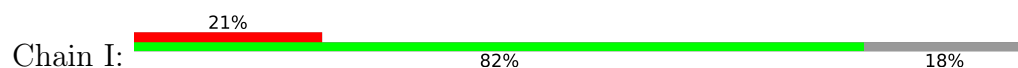




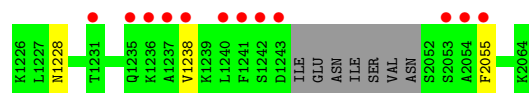
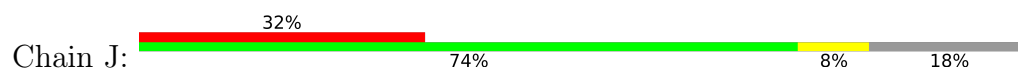
- Molecule 1: DNA repair and recombination protein RadA



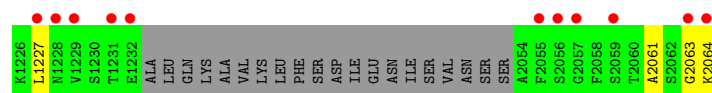
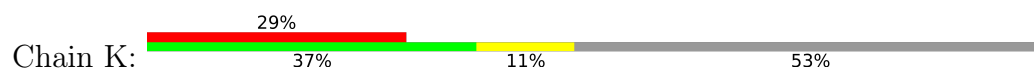
- Molecule 2: Breast cancer type 2 susceptibility



- Molecule 2: Breast cancer type 2 susceptibility

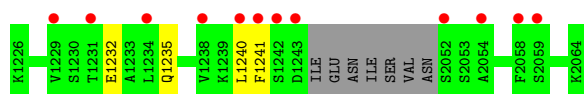


- Molecule 2: Breast cancer type 2 susceptibility

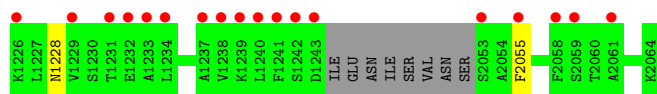
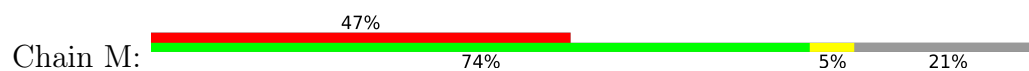


- Molecule 2: Breast cancer type 2 susceptibility

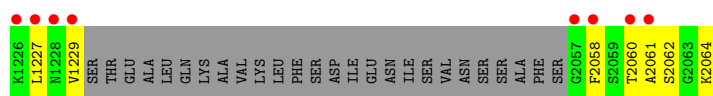




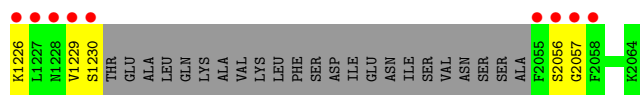
- Molecule 2: Breast cancer type 2 susceptibility



- Molecule 2: Breast cancer type 2 susceptibility



- Molecule 2: Breast cancer type 2 susceptibility



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.40Å 75.47Å 114.79Å 90.00° 97.06° 90.00°	Depositor
Resolution (Å)	85.87 – 1.97 85.87 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.7 (85.87-1.97) 99.7 (85.87-1.97)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.97Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.263 , 0.271 0.277 , 0.286	Depositor DCC
R_{free} test set	6853 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14419	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.54% 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: ADP, 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	0.66	0/1640	0.94	0/2203
1	B	0.69	0/1726	1.05	4/2316 (0.2%)
1	C	0.69	0/1660	0.95	2/2229 (0.1%)
1	D	0.64	0/1633	0.94	2/2194 (0.1%)
1	E	0.62	0/1656	1.03	2/2226 (0.1%)
1	F	0.63	0/1595	1.08	5/2142 (0.2%)
1	G	0.74	0/1553	0.94	1/2086 (0.0%)
1	H	0.59	0/1455	0.97	6/1959 (0.3%)
2	I	0.64	0/226	1.00	0/299
2	J	0.54	0/226	0.83	0/299
2	K	0.49	0/128	0.97	1/168 (0.6%)
2	L	0.47	0/226	0.87	0/299
2	M	0.53	0/220	0.89	0/291
2	N	0.49	0/83	0.71	0/107
2	O	0.59	0/107	0.92	1/139 (0.7%)
All	All	0.65	0/14134	0.98	24/18957 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	249	ILE	N-CA-C	7.96	118.76	110.72
1	C	241	THR	N-CA-C	6.88	121.84	113.17
1	B	250	GLY	N-CA-C	6.82	120.94	112.14
1	H	274	GLU	N-CA-C	6.48	118.42	111.36
2	K	2063	GLY	N-CA-C	6.08	123.70	115.32
1	B	110	ILE	N-CA-C	5.85	116.09	107.15
1	G	240	LEU	N-CA-C	5.72	117.60	111.36
2	O	2057	GLY	N-CA-C	-5.51	107.76	114.92
1	B	251	ARG	N-CA-C	-5.50	105.67	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	206	PHE	N-CA-C	5.50	117.36	111.36
1	F	230	ARG	CA-C-N	5.37	126.55	119.84
1	F	230	ARG	C-N-CA	5.37	126.55	119.84
1	C	274	GLU	N-CA-C	5.32	117.16	111.36
1	H	275	PHE	N-CA-C	5.23	118.97	112.59
1	H	234	LEU	N-CA-C	5.22	117.95	109.24
1	F	226	LEU	N-CA-C	5.21	116.96	111.28
1	F	192	ASP	CA-CB-CG	5.19	117.79	112.60
1	H	172	ASP	N-CA-C	5.19	117.36	108.90
1	H	143	GLY	N-CA-C	5.13	122.92	115.32
1	E	287	ALA	N-CA-C	5.13	115.82	108.74
1	E	286	GLN	N-CA-C	5.11	117.59	111.71
1	F	302	GLY	N-CA-C	5.08	122.91	115.08
1	D	178	ARG	CA-C-N	5.06	124.66	119.05
1	D	178	ARG	C-N-CA	5.06	124.66	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1621	0	1636	11	0
1	B	1704	0	1716	12	0
1	C	1639	0	1652	18	0
1	D	1615	0	1637	17	0
1	E	1637	0	1648	17	0
1	F	1578	0	1600	40	0
1	G	1534	0	1543	27	0
1	H	1440	0	1393	40	0
2	I	225	0	227	0	0
2	J	225	0	227	1	0
2	K	128	0	124	5	0
2	L	225	0	227	3	0
2	M	219	0	222	1	0
2	N	84	0	87	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	107	0	106	3	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
3	G	27	0	12	1	0
3	H	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	49	0	0	0	0
5	B	40	0	0	0	0
5	C	29	0	0	0	0
5	D	40	0	0	0	0
5	E	29	0	0	0	0
5	F	4	0	0	0	0
5	G	9	0	0	0	0
5	I	8	0	0	0	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
5	L	3	0	0	0	0
All	All	14419	0	14141	191	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 7.

All (191) 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:G:169:MET:CE	1:G:221:MET:HE2	1.94	0.97
1:G:169:MET:HE3	1:G:221:MET:HE2	1.55	0.87
1:C:169:MET:HE3	1:C:221:MET:HE1	1.63	0.78
1:C:169:MET:HE3	1:C:221:MET:CE	2.13	0.78
1:H:131:GLN:HG2	1:H:276:ASP:HA	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:VAL:HB	1:F:281:VAL:HG12	1.68	0.74
1:H:315:LEU:HD12	1:H:315:LEU:N	2.03	0.73
1:B:219:SER:HB2	1:B:271:LEU:HD21	1.71	0.71
1:A:237:VAL:HB	1:A:281:VAL:HG12	1.73	0.70
1:G:169:MET:HE1	1:G:221:MET:HE2	1.75	0.68
1:C:169:MET:CE	1:C:221:MET:CE	2.72	0.66
1:G:169:MET:HE3	1:G:221:MET:CE	2.23	0.66
1:H:304:ILE:HD12	1:H:304:ILE:N	2.12	0.65
1:F:263:ARG:HG2	1:F:267:MET:HE3	1.79	0.64
1:H:136:VAL:CG2	1:H:315:LEU:HD11	2.28	0.63
1:F:135:GLU:HB3	1:F:281:VAL:HG23	1.82	0.62
1:E:237:VAL:HB	1:E:281:VAL:HG12	1.81	0.62
1:B:219:SER:HA	1:B:222:MET:HE3	1.81	0.62
1:A:311:LEU:N	1:A:311:LEU:HD22	2.14	0.62
1:F:328:ILE:O	1:F:328:ILE:HG22	2.00	0.61
1:H:314:TYR:CD2	1:H:326:ARG:NH1	2.69	0.60
1:G:212:MET:HE2	1:G:264:PHE:HB2	1.83	0.60
1:C:169:MET:CE	1:C:221:MET:HE2	2.33	0.59
1:D:166:GLY:HA3	1:D:233:LYS:HG3	1.86	0.58
1:H:120:LEU:O	1:H:124:LEU:HG	2.03	0.58
1:G:134:THR:HG23	1:G:311:LEU:HD23	1.85	0.57
1:F:197:LEU:HB3	2:N:2062:SER:HB3	1.87	0.57
1:B:272:ALA:HA	1:B:277:ILE:HG12	1.87	0.57
1:E:136:VAL:CG2	1:E:282:THR:HG22	2.34	0.56
2:K:2064:LYS:O	2:K:2064:LYS:HG3	2.03	0.56
1:D:254:LEU:HD23	1:D:257:ARG:HH21	1.69	0.56
1:G:183:ARG:HG2	1:G:193:PRO:HB2	1.87	0.56
1:B:245:ARG:HH12	1:B:285:VAL:HB	1.71	0.56
2:O:1229:VAL:HG12	2:O:2056:SER:HB3	1.87	0.55
1:G:316:ARG:HH22	1:G:326:ARG:HD2	1.71	0.55
1:D:212:MET:HG2	1:D:263:ARG:HH21	1.72	0.55
1:H:174:GLU:HA	1:H:174:GLU:OE1	2.06	0.55
1:G:141:GLY:HA2	3:G:401:ADP:H5'1	1.88	0.55
1:F:221:MET:HE1	2:N:1227:LEU:HD13	1.88	0.54
1:D:173:THR:HG22	1:D:205:ALA:HB3	1.90	0.54
1:G:140:PHE:HD2	1:G:284:GLN:HE22	1.54	0.54
1:A:312:ARG:HB2	1:A:328:ILE:HB	1.90	0.54
1:F:223:VAL:HG22	1:F:275:PHE:HE1	1.72	0.54
1:H:123:LEU:HD12	1:H:123:LEU:O	2.08	0.54
1:D:110:ILE:H	1:D:110:ILE:HD12	1.73	0.53
1:H:123:LEU:HD11	1:H:327:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:277:ILE:HG13	1:H:277:ILE:O	2.08	0.53
1:H:169:MET:HB3	1:H:235:LEU:HD13	1.89	0.53
1:G:316:ARG:NH2	1:G:326:ARG:HD2	2.23	0.53
1:F:223:VAL:HG22	1:F:275:PHE:CE1	2.44	0.52
1:G:183:ARG:HG2	1:G:193:PRO:CB	2.39	0.52
1:C:169:MET:HE3	1:C:221:MET:HE2	1.89	0.52
2:O:1229:VAL:HG22	2:O:1230:SER:N	2.23	0.52
1:G:237:VAL:HB	1:G:281:VAL:HG12	1.91	0.52
1:H:128:ILE:O	1:H:128:ILE:HG13	2.09	0.52
1:H:315:LEU:N	1:H:315:LEU:CD1	2.72	0.52
1:C:169:MET:CE	1:C:221:MET:HE1	2.37	0.51
1:F:344:GLU:H	1:F:344:GLU:CD	2.17	0.51
1:E:229:ASP:OD1	1:E:229:ASP:N	2.40	0.51
1:H:123:LEU:HD11	1:H:327:LEU:CD1	2.41	0.51
1:H:215:LEU:HD22	1:H:264:PHE:CE1	2.45	0.51
1:D:312:ARG:HB2	1:D:328:ILE:HB	1.93	0.51
1:A:173:THR:HG22	1:A:205:ALA:HB3	1.92	0.51
1:G:133:ILE:HB	1:G:310:THR:HG22	1.91	0.51
1:C:344:GLU:H	1:C:344:GLU:CD	2.19	0.51
1:F:221:MET:CE	2:N:1227:LEU:HD22	2.41	0.51
1:E:223:VAL:HG22	1:E:275:PHE:CZ	2.46	0.50
1:H:113:ILE:HD13	1:H:155:VAL:HB	1.94	0.50
1:F:110:ILE:CG2	1:F:129:GLU:HB2	2.41	0.50
1:G:275:PHE:N	1:G:275:PHE:CD2	2.80	0.50
1:C:226:LEU:HD12	1:C:226:LEU:O	2.12	0.49
1:F:169:MET:HB2	1:F:235:LEU:HD13	1.93	0.49
2:L:1232:GLU:HA	2:L:1235:GLN:HE21	1.77	0.49
1:H:136:VAL:HG23	1:H:315:LEU:HD11	1.93	0.49
1:H:138:GLY:HA2	1:H:314:TYR:CE1	2.47	0.49
1:D:135:GLU:HG2	1:D:281:VAL:CG2	2.43	0.49
1:G:123:LEU:HG	1:G:327:LEU:HD21	1.95	0.49
1:E:344:GLU:H	1:E:344:GLU:CD	2.21	0.49
1:A:143:GLY:HA2	3:A:401:ADP:H5'1	1.95	0.48
1:G:219:SER:HB2	1:G:271:LEU:HD21	1.95	0.48
1:D:131:GLN:HA	1:D:272:ALA:O	2.13	0.48
1:B:226:LEU:HD13	1:B:275:PHE:HD1	1.78	0.48
1:E:166:GLY:HA3	1:E:233:LYS:HG3	1.95	0.48
1:E:173:THR:HG22	1:E:205:ALA:HB3	1.96	0.48
1:F:220:ALA:HB3	2:N:1229:VAL:HG21	1.95	0.48
1:B:110:ILE:HG22	1:B:110:ILE:O	2.13	0.48
1:H:137:PHE:CE1	1:H:283:ASN:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:PRO:HD2	1:D:161:GLU:HB2	1.96	0.47
1:F:211:GLN:HG2	1:F:264:PHE:CE2	2.49	0.47
1:B:136:VAL:HG12	1:B:313:VAL:HB	1.97	0.47
1:H:136:VAL:O	1:H:136:VAL:HG13	2.15	0.47
1:B:245:ARG:NH1	1:B:285:VAL:HB	2.28	0.47
1:C:219:SER:HB2	1:C:271:LEU:HD21	1.96	0.47
2:J:1228:ASN:HD22	2:J:2055:PHE:HA	1.80	0.47
1:H:262:ALA:O	1:H:266:ARG:HG3	2.15	0.47
1:H:344:GLU:H	1:H:344:GLU:CD	2.23	0.46
1:D:237:VAL:HB	1:D:281:VAL:HG12	1.98	0.46
1:H:345:LYS:O	1:H:345:LYS:HG2	2.16	0.46
1:F:137:PHE:CD1	1:F:283:ASN:HB2	2.51	0.46
1:F:156:GLN:CD	1:F:199:ASN:HB2	2.41	0.46
1:F:218:ALA:O	1:F:222:MET:HG3	2.16	0.46
1:H:130:THR:HA	1:H:278:ALA:HB2	1.98	0.46
1:H:215:LEU:HD12	1:H:215:LEU:HA	1.71	0.46
1:E:318:GLY:HA3	1:E:324:ILE:HD11	1.97	0.46
1:F:134:THR:O	1:F:134:THR:HG23	2.15	0.45
1:G:183:ARG:HG3	1:G:197:LEU:HD11	1.97	0.45
1:D:267:MET:HE3	2:L:1241:PHE:CD2	2.50	0.45
1:B:169:MET:HE1	1:B:221:MET:SD	2.56	0.45
1:H:215:LEU:HD11	1:H:268:LEU:HD21	1.98	0.45
1:C:238:ASP:HA	1:C:239:SER:HA	1.60	0.45
1:D:274:GLU:HG2	2:L:1240:LEU:HD11	1.99	0.45
1:A:238:ASP:HA	1:A:239:SER:HA	1.65	0.45
1:C:135:GLU:HG2	1:C:281:VAL:CG2	2.46	0.45
2:O:1226:LYS:HE3	2:O:1226:LYS:HB2	1.70	0.45
1:E:173:THR:HG21	1:E:211:GLN:HE21	1.81	0.45
1:H:188:ASN:ND2	1:H:344:GLU:HB2	2.32	0.45
1:G:219:SER:CB	1:G:271:LEU:HD21	2.46	0.44
1:C:197:LEU:HA	2:K:2061:ALA:HB3	1.98	0.44
1:F:136:VAL:CG2	1:F:282:THR:HG22	2.48	0.44
1:B:238:ASP:HA	1:B:239:SER:HA	1.81	0.44
1:F:159:PRO:HD3	1:F:165:ASN:HB2	1.98	0.44
1:B:245:ARG:HH12	1:B:285:VAL:CA	2.31	0.44
1:F:169:MET:HA	1:F:201:ALA:HB3	1.99	0.44
1:F:314:TYR:HB2	1:F:328:ILE:CD1	2.48	0.44
1:F:172:ASP:HA	1:F:238:ASP:O	2.18	0.44
1:E:138:GLY:C	1:E:285:VAL:HG12	2.43	0.44
1:F:150:THR:OG1	1:F:347:ILE:HG12	2.18	0.44
1:F:164:LEU:CB	1:F:233:LYS:HG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:238:ASP:HA	1:G:239:SER:HA	1.65	0.44
1:A:311:LEU:N	1:A:311:LEU:CD2	2.80	0.43
1:F:185:ILE:HG23	1:F:345:LYS:O	2.18	0.43
1:F:197:LEU:HA	2:N:2061:ALA:HB3	2.00	0.43
2:K:1227:LEU:HD21	2:K:2064:LYS:HE3	2.00	0.43
1:H:131:GLN:CG	1:H:276:ASP:HA	2.44	0.43
1:F:133:ILE:HD11	1:F:268:LEU:HB3	2.00	0.43
1:G:157:LEU:HD21	1:G:191:LEU:HD11	2.00	0.43
1:H:141:GLY:O	1:H:317:LYS:HE3	2.19	0.43
1:A:325:ALA:HB3	1:A:338:ALA:HB3	1.99	0.42
1:C:197:LEU:HD22	2:K:2061:ALA:HB1	2.00	0.42
1:D:255:ALA:O	1:D:259:GLN:HG2	2.20	0.42
1:E:215:LEU:HD22	1:E:264:PHE:CE1	2.54	0.42
1:E:223:VAL:HG22	1:E:275:PHE:HZ	1.84	0.42
1:E:238:ASP:HA	1:E:239:SER:HA	1.65	0.42
1:F:185:ILE:O	1:F:189:ARG:HG3	2.18	0.42
1:H:216:TYR:CE2	1:H:267:MET:HE1	2.53	0.42
1:A:135:GLU:HG2	1:A:281:VAL:CG2	2.50	0.42
1:C:197:LEU:CA	2:K:2061:ALA:HB3	2.50	0.42
1:F:314:TYR:HB2	1:F:328:ILE:HG13	2.01	0.42
1:D:110:ILE:HD12	1:D:110:ILE:N	2.34	0.42
1:A:215:LEU:HD22	1:A:264:PHE:CE1	2.54	0.42
1:C:319:LYS:H	1:C:319:LYS:HG3	1.64	0.42
1:F:238:ASP:HA	1:F:239:SER:HA	1.56	0.42
1:G:340:PHE:CD1	1:G:340:PHE:C	2.98	0.42
1:G:147:LEU:HD12	1:G:147:LEU:O	2.20	0.42
1:F:304:ILE:HD12	1:F:304:ILE:HA	1.88	0.41
1:G:212:MET:HE2	1:G:264:PHE:HD1	1.85	0.41
1:G:271:LEU:HD23	1:G:271:LEU:HA	1.87	0.41
1:B:159:PRO:HD3	1:B:165:ASN:ND2	2.35	0.41
1:C:317:LYS:HE2	1:C:317:LYS:HB2	1.78	0.41
1:H:144:LYS:HG3	1:H:282:THR:HB	2.02	0.41
1:F:271:LEU:N	1:F:271:LEU:CD1	2.82	0.41
1:E:240:LEU:HG	1:E:261:LEU:HD11	2.03	0.41
1:F:345:LYS:HE2	1:F:345:LYS:HB3	1.92	0.41
2:M:1228:ASN:HD22	2:M:2055:PHE:HA	1.85	0.41
1:C:303:HIS:CD2	1:C:303:HIS:N	2.85	0.41
1:E:173:THR:HG21	1:E:211:GLN:NE2	2.36	0.41
1:C:136:VAL:CG2	1:C:282:THR:HG22	2.50	0.41
1:F:169:MET:SD	1:F:222:MET:HE2	2.60	0.41
1:H:115:THR:HB	1:H:120:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:LEU:HB3	1:F:233:LYS:HG2	2.02	0.41
1:D:254:LEU:HD23	1:D:257:ARG:NH2	2.34	0.41
1:H:233:LYS:HA	1:H:233:LYS:HD3	1.63	0.41
1:F:201:ALA:HB1	2:N:2058:PHE:CD2	2.56	0.41
1:G:230:ARG:O	1:G:230:ARG:HG3	2.20	0.41
1:F:220:ALA:CB	2:N:1229:VAL:HG21	2.51	0.40
1:H:136:VAL:HG12	1:H:282:THR:HA	2.03	0.40
1:H:172:ASP:HA	1:H:238:ASP:O	2.22	0.40
1:F:221:MET:HE1	2:N:1227:LEU:HB3	2.03	0.40
1:H:222:MET:CE	1:H:277:ILE:HD13	2.51	0.40
1:H:260:LYS:HD3	1:H:260:LYS:HA	1.79	0.40
1:H:303:HIS:N	1:H:304:ILE:HD12	2.36	0.40
2:N:2060:THR:CG2	2:N:2064:LYS:HB2	2.51	0.40
1:D:322:LYS:HD3	1:D:339:VAL:HG11	2.02	0.40
1:E:178:ARG:HD3	1:E:178:ARG:HA	1.87	0.40
1:E:234:LEU:HD21	1:E:236:ILE:HD11	2.03	0.40
1:F:240:LEU:HD12	1:F:240:LEU:HA	1.89	0.40
1:G:181:ARG:CZ	1:G:185:ILE:HD11	2.51	0.40
1:A:135:GLU:HG2	1:A:281:VAL:HG23	2.04	0.40
1:D:215:LEU:HD22	1:D:264:PHE:CE1	2.56	0.40
1:H:263:ARG:HA	1:H:266:ARG:CZ	2.51	0.40
1:H:323:ARG:NH2	3:H:401:ADP:H4'	2.36	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	200/231 (87%)	200 (100%)	0	0	100	100
1	B	211/231 (91%)	208 (99%)	3 (1%)	0	100	100
1	C	202/231 (87%)	201 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	200/231 (87%)	198 (99%)	2 (1%)	0	100	100
1	E	204/231 (88%)	201 (98%)	3 (2%)	0	100	100
1	F	196/231 (85%)	190 (97%)	6 (3%)	0	100	100
1	G	184/231 (80%)	182 (99%)	2 (1%)	0	100	100
1	H	180/231 (78%)	178 (99%)	2 (1%)	0	100	100
2	I	27/38 (71%)	27 (100%)	0	0	100	100
2	J	27/38 (71%)	27 (100%)	0	0	100	100
2	K	14/38 (37%)	14 (100%)	0	0	100	100
2	L	27/38 (71%)	27 (100%)	0	0	100	100
2	M	26/38 (68%)	26 (100%)	0	0	100	100
2	N	8/38 (21%)	8 (100%)	0	0	100	100
2	O	11/38 (29%)	11 (100%)	0	0	100	100
All	All	1717/2114 (81%)	1698 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	172/188 (92%)	169 (98%)	3 (2%)	53	48
1	B	178/188 (95%)	175 (98%)	3 (2%)	53	48
1	C	173/188 (92%)	173 (100%)	0	100	100
1	D	171/188 (91%)	170 (99%)	1 (1%)	78	76
1	E	172/188 (92%)	172 (100%)	0	100	100
1	F	166/188 (88%)	163 (98%)	3 (2%)	51	46
1	G	165/188 (88%)	165 (100%)	0	100	100
1	H	143/188 (76%)	136 (95%)	7 (5%)	22	10
2	I	25/32 (78%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	25/32 (78%)	24 (96%)	1 (4%)	28	17
2	K	14/32 (44%)	14 (100%)	0	100	100
2	L	25/32 (78%)	25 (100%)	0	100	100
2	M	24/32 (75%)	24 (100%)	0	100	100
2	N	9/32 (28%)	9 (100%)	0	100	100
2	O	12/32 (38%)	12 (100%)	0	100	100
All	All	1474/1728 (85%)	1456 (99%)	18 (1%)	63	58

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ILE
1	A	212	MET
1	A	311	LEU
1	B	129	GLU
1	B	304	ILE
1	B	312	ARG
1	D	212	MET
1	F	223	VAL
1	F	237	VAL
1	F	304	ILE
1	H	144	LYS
1	H	281	VAL
1	H	284	GLN
1	H	285	VAL
1	H	304	ILE
1	H	315	LEU
1	H	347	ILE
2	J	1238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	211	GLN
1	B	165	ASN
1	B	187	GLN
1	C	131	GLN
1	D	188	ASN

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Mol	Chain	Res	Type
1	E	211	GLN
1	E	258	GLN
1	F	175	ASN
1	G	209	ASN
1	G	217	GLN
1	G	273	ASN
1	G	283	ASN
1	H	188	ASN
1	H	283	ASN
1	H	307	HIS
2	J	1228	ASN
2	L	1228	ASN
2	L	1235	GLN
2	M	1228	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](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	ADP	F	401	4	28,29,29	1.37	5 (17%)	43,45,45	1.81	9 (20%)
3	ADP	G	401	4	28,29,29	1.38	5 (17%)	43,45,45	1.81	9 (20%)
3	ADP	C	401	4	28,29,29	1.42	5 (17%)	43,45,45	1.81	7 (16%)
3	ADP	B	401	4	28,29,29	1.36	5 (17%)	43,45,45	1.77	9 (20%)
3	ADP	A	401	4	28,29,29	1.41	4 (14%)	43,45,45	1.83	10 (23%)
3	ADP	D	401	4	28,29,29	1.40	5 (17%)	43,45,45	1.87	10 (23%)
3	ADP	H	401	4	28,29,29	1.44	5 (17%)	43,45,45	1.80	11 (25%)
3	ADP	E	401	4	28,29,29	1.43	5 (17%)	43,45,45	1.86	10 (23%)

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	ADP	F	401	4	-	3/16/32/32	0/3/3/3
3	ADP	G	401	4	-	6/16/32/32	0/3/3/3
3	ADP	C	401	4	-	2/16/32/32	0/3/3/3
3	ADP	B	401	4	-	4/16/32/32	0/3/3/3
3	ADP	A	401	4	-	0/16/32/32	0/3/3/3
3	ADP	D	401	4	-	3/16/32/32	0/3/3/3
3	ADP	H	401	4	-	3/16/32/32	0/3/3/3
3	ADP	E	401	4	-	2/16/32/32	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	401	ADP	C5-C4	4.70	1.47	1.39
3	F	401	ADP	C5-C4	4.47	1.47	1.39
3	E	401	ADP	C5-C4	4.38	1.46	1.39
3	G	401	ADP	C5-C4	4.35	1.46	1.39
3	B	401	ADP	C5-C4	4.29	1.46	1.39
3	D	401	ADP	C5-C4	4.24	1.46	1.39
3	A	401	ADP	C5-C4	4.15	1.46	1.39
3	C	401	ADP	C5-C4	4.14	1.46	1.39
3	C	401	ADP	C5-N7	-2.70	1.34	1.39
3	E	401	ADP	C5-C6	2.70	1.48	1.41
3	G	401	ADP	C5-C6	2.67	1.48	1.41
3	H	401	ADP	C5-C6	2.66	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	C5-N7	-2.65	1.34	1.39
3	F	401	ADP	C5-C6	2.57	1.48	1.41
3	D	401	ADP	C5-C6	2.57	1.48	1.41
3	D	401	ADP	C5-N7	-2.51	1.34	1.39
3	B	401	ADP	C5-C6	2.50	1.47	1.41
3	B	401	ADP	C5-N7	-2.49	1.34	1.39
3	A	401	ADP	C5-C6	2.48	1.47	1.41
3	F	401	ADP	C5-N7	-2.40	1.34	1.39
3	C	401	ADP	C5-C6	2.37	1.47	1.41
3	A	401	ADP	C4-N9	-2.36	1.32	1.37
3	E	401	ADP	C5-N7	-2.35	1.34	1.39
3	C	401	ADP	C4-N9	-2.34	1.32	1.37
3	G	401	ADP	C8-N7	2.31	1.36	1.31
3	G	401	ADP	C5-N7	-2.30	1.34	1.39
3	H	401	ADP	C8-N7	2.30	1.36	1.31
3	H	401	ADP	C5-N7	-2.23	1.35	1.39
3	B	401	ADP	C4-N9	-2.23	1.33	1.37
3	E	401	ADP	C8-N7	2.22	1.35	1.31
3	D	401	ADP	C4-N9	-2.21	1.33	1.37
3	E	401	ADP	C4-N9	-2.19	1.33	1.37
3	D	401	ADP	C8-N7	2.16	1.35	1.31
3	F	401	ADP	C8-N7	2.13	1.35	1.31
3	G	401	ADP	C4-N9	-2.07	1.33	1.37
3	F	401	ADP	C4-N9	-2.05	1.33	1.37
3	H	401	ADP	C4-N9	-2.04	1.33	1.37
3	C	401	ADP	C8-N9	-2.03	1.34	1.37
3	B	401	ADP	C8-N7	2.03	1.35	1.31

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ADP	C5-C4-N3	-5.69	118.88	126.72
3	F	401	ADP	C5-C4-N3	-5.65	118.94	126.72
3	D	401	ADP	C5-C4-N3	-5.61	119.00	126.72
3	G	401	ADP	C5-C4-N3	-5.59	119.02	126.72
3	E	401	ADP	C5-C4-N3	-5.57	119.05	126.72
3	A	401	ADP	C5-C4-N3	-5.47	119.19	126.72
3	H	401	ADP	C5-C4-N3	-5.43	119.24	126.72
3	B	401	ADP	C5-C4-N3	-5.42	119.25	126.72
3	C	401	ADP	N3-C4-N9	4.76	135.27	127.17
3	F	401	ADP	N3-C4-N9	4.59	134.97	127.17
3	D	401	ADP	N3-C4-N9	4.53	134.87	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	N3-C4-N9	4.47	134.77	127.17
3	B	401	ADP	N3-C4-N9	4.45	134.74	127.17
3	E	401	ADP	N3-C4-N9	4.39	134.63	127.17
3	H	401	ADP	N3-C4-N9	4.39	134.63	127.17
3	G	401	ADP	N3-C4-N9	4.38	134.61	127.17
3	E	401	ADP	C2-N3-C4	3.81	121.14	111.83
3	D	401	ADP	C2-N3-C4	3.78	121.06	111.83
3	D	401	ADP	N3-C2-N1	-3.78	122.86	128.58
3	E	401	ADP	N3-C2-N1	-3.73	122.94	128.58
3	A	401	ADP	C2-N3-C4	3.69	120.84	111.83
3	F	401	ADP	C2-N3-C4	3.65	120.74	111.83
3	G	401	ADP	C2-N3-C4	3.64	120.72	111.83
3	C	401	ADP	C2-N3-C4	3.60	120.62	111.83
3	E	401	ADP	C4-C5-N7	-3.59	106.48	110.58
3	B	401	ADP	C2-N3-C4	3.57	120.54	111.83
3	H	401	ADP	C2-N3-C4	3.55	120.51	111.83
3	G	401	ADP	C4-C5-N7	-3.54	106.54	110.58
3	D	401	ADP	C4-C5-N7	-3.42	106.67	110.58
3	A	401	ADP	N3-C2-N1	-3.35	123.51	128.58
3	B	401	ADP	N3-C2-N1	-3.34	123.53	128.58
3	H	401	ADP	N3-C2-N1	-3.33	123.54	128.58
3	A	401	ADP	C4-C5-N7	-3.31	106.80	110.58
3	H	401	ADP	C4-C5-N7	-3.26	106.86	110.58
3	F	401	ADP	N3-C2-N1	-3.25	123.66	128.58
3	F	401	ADP	C4-C5-N7	-3.23	106.89	110.58
3	G	401	ADP	N3-C2-N1	-3.22	123.70	128.58
3	B	401	ADP	C4-C5-N7	-3.21	106.91	110.58
3	C	401	ADP	N3-C2-N1	-3.16	123.81	128.58
3	D	401	ADP	C4-N9-C8	3.14	109.03	105.74
3	C	401	ADP	C4-C5-N7	-3.11	107.02	110.58
3	A	401	ADP	C4-N9-C8	3.06	108.95	105.74
3	E	401	ADP	C4-N9-C8	3.04	108.93	105.74
3	C	401	ADP	C4-N9-C8	2.98	108.87	105.74
3	B	401	ADP	C4-N9-C8	2.96	108.85	105.74
3	G	401	ADP	C4-N9-C8	2.92	108.81	105.74
3	H	401	ADP	C4-N9-C8	2.83	108.71	105.74
3	F	401	ADP	C4-N9-C8	2.79	108.66	105.74
3	E	401	ADP	C5-N7-C8	2.69	107.67	103.45
3	D	401	ADP	C5-N7-C8	2.66	107.63	103.45
3	G	401	ADP	C5-N7-C8	2.61	107.55	103.45
3	A	401	ADP	C5-N7-C8	2.54	107.44	103.45
3	F	401	ADP	C5-N7-C8	2.43	107.27	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	N9-C8-N7	-2.40	110.53	113.94
3	B	401	ADP	C5-N7-C8	2.39	107.21	103.45
3	H	401	ADP	C5-N7-C8	2.39	107.21	103.45
3	E	401	ADP	N9-C8-N7	-2.35	110.60	113.94
3	C	401	ADP	C5-N7-C8	2.34	107.13	103.45
3	E	401	ADP	C6-C5-N7	2.33	136.59	132.09
3	A	401	ADP	C6-C5-N7	2.32	136.55	132.09
3	G	401	ADP	C6-C5-N7	2.31	136.53	132.09
3	G	401	ADP	N9-C8-N7	-2.26	110.73	113.94
3	A	401	ADP	N9-C8-N7	-2.23	110.77	113.94
3	D	401	ADP	C2-N1-C6	2.22	122.38	118.73
3	D	401	ADP	C6-C5-N7	2.20	136.34	132.09
3	E	401	ADP	C2-N1-C6	2.19	122.33	118.73
3	H	401	ADP	C2-N1-C6	2.10	122.19	118.73
3	B	401	ADP	C6-C5-N7	2.09	136.11	132.09
3	B	401	ADP	N9-C8-N7	-2.06	111.02	113.94
3	H	401	ADP	C6-C5-N7	2.03	136.00	132.09
3	H	401	ADP	C3'-C2'-C1'	2.03	105.30	101.46
3	A	401	ADP	O3B-PB-O2B	2.02	115.39	107.80
3	F	401	ADP	N9-C8-N7	-2.01	111.08	113.94
3	F	401	ADP	C6-C5-N7	2.00	135.95	132.09
3	H	401	ADP	N9-C8-N7	-2.00	111.10	113.94

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	ADP	PA-O3A-PB-O2B
3	B	401	ADP	C5'-O5'-PA-O2A
3	C	401	ADP	C5'-O5'-PA-O1A
3	D	401	ADP	C5'-O5'-PA-O2A
3	E	401	ADP	PA-O3A-PB-O3B
3	F	401	ADP	C5'-O5'-PA-O2A
3	G	401	ADP	PA-O3A-PB-O2B
3	G	401	ADP	PA-O3A-PB-O3B
3	G	401	ADP	C3'-C4'-C5'-O5'
3	G	401	ADP	O4'-C4'-C5'-O5'
3	H	401	ADP	O4'-C4'-C5'-O5'
3	H	401	ADP	C3'-C4'-C5'-O5'
3	B	401	ADP	C5'-O5'-PA-O3A
3	D	401	ADP	C5'-O5'-PA-O3A
3	F	401	ADP	C5'-O5'-PA-O1A

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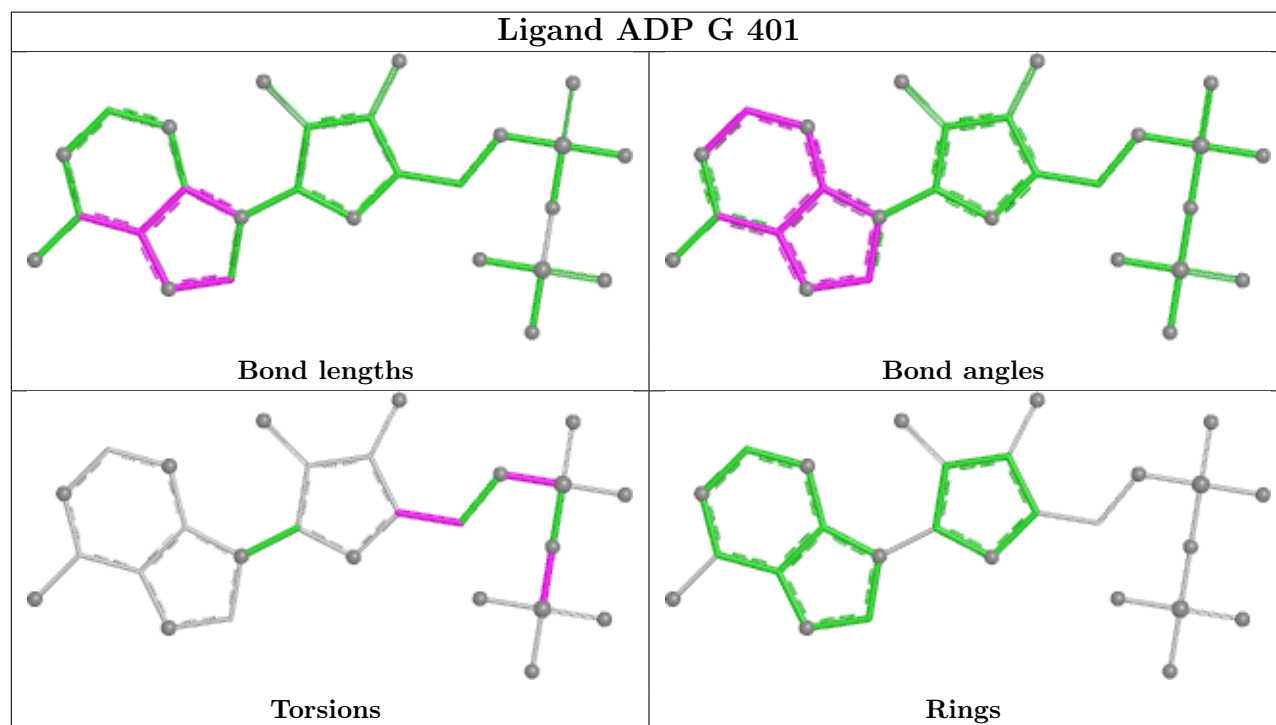
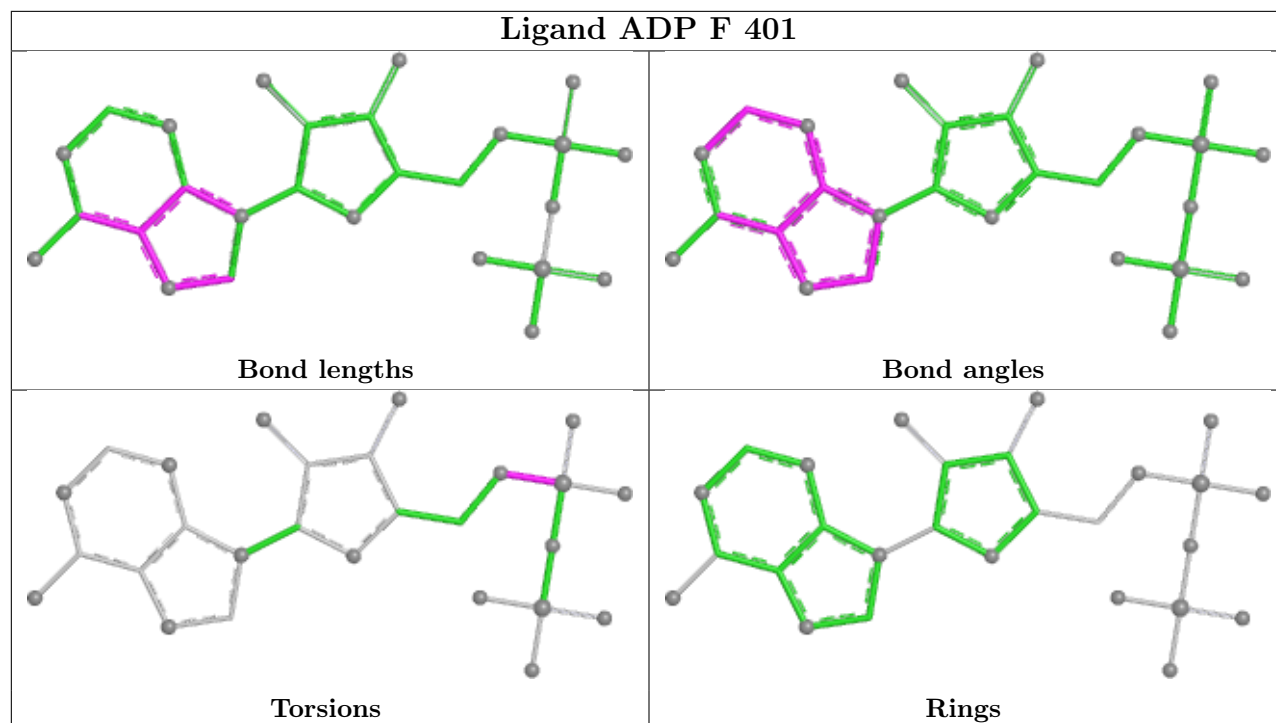
Mol	Chain	Res	Type	Atoms
3	F	401	ADP	C5'-O5'-PA-O3A
3	G	401	ADP	C5'-O5'-PA-O1A
3	D	401	ADP	PA-O3A-PB-O1B
3	E	401	ADP	PA-O3A-PB-O1B
3	C	401	ADP	PA-O3A-PB-O3B
3	B	401	ADP	PA-O3A-PB-O1B
3	G	401	ADP	PA-O3A-PB-O1B
3	H	401	ADP	C2'-C1'-N9-C8

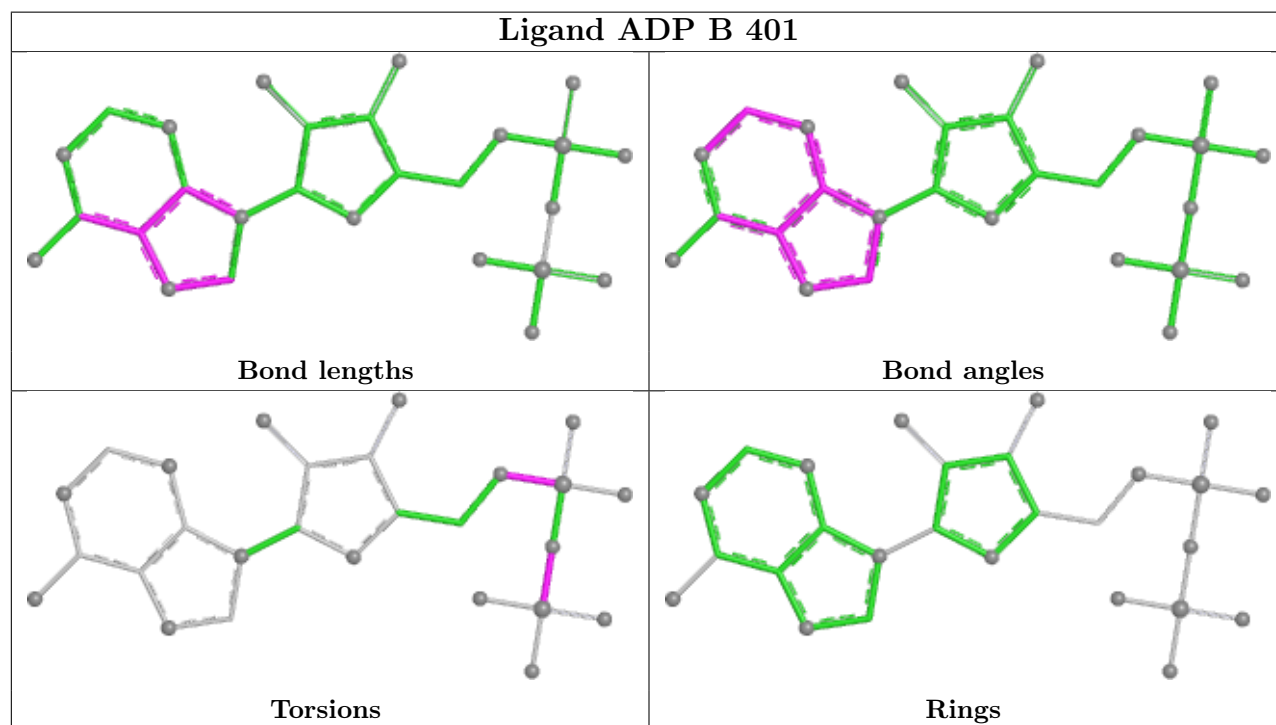
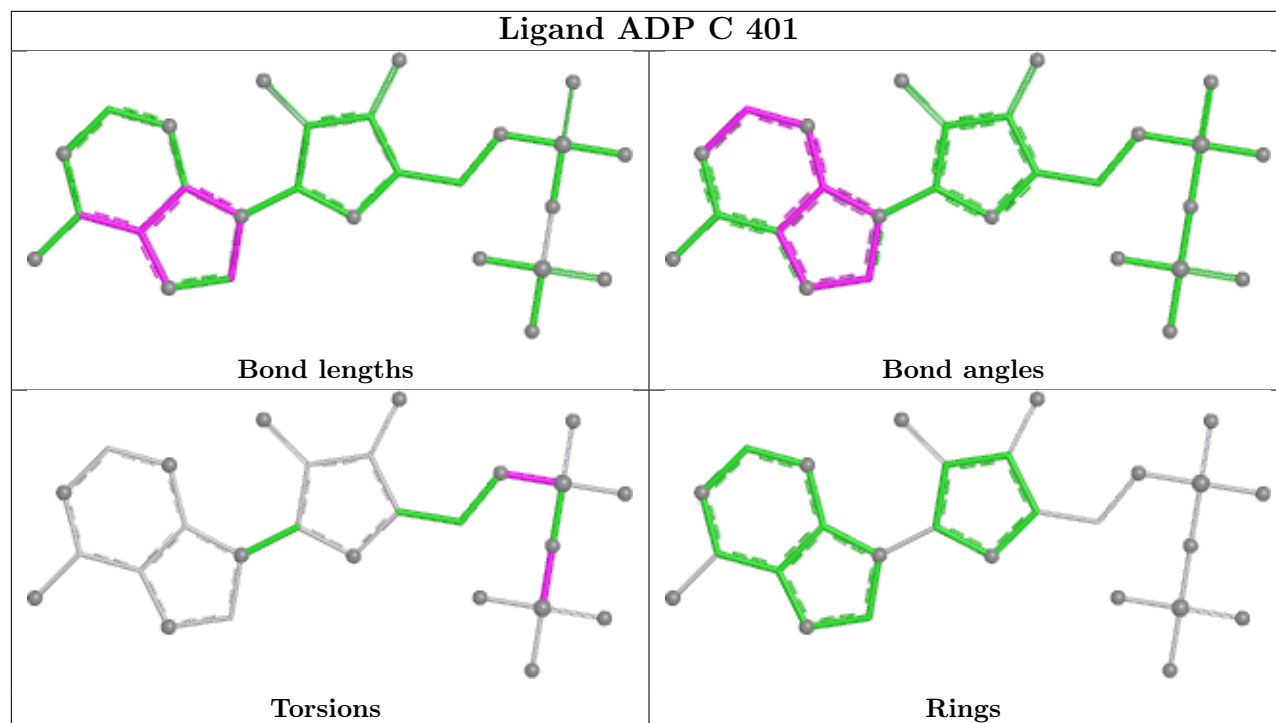
There are no ring outliers.

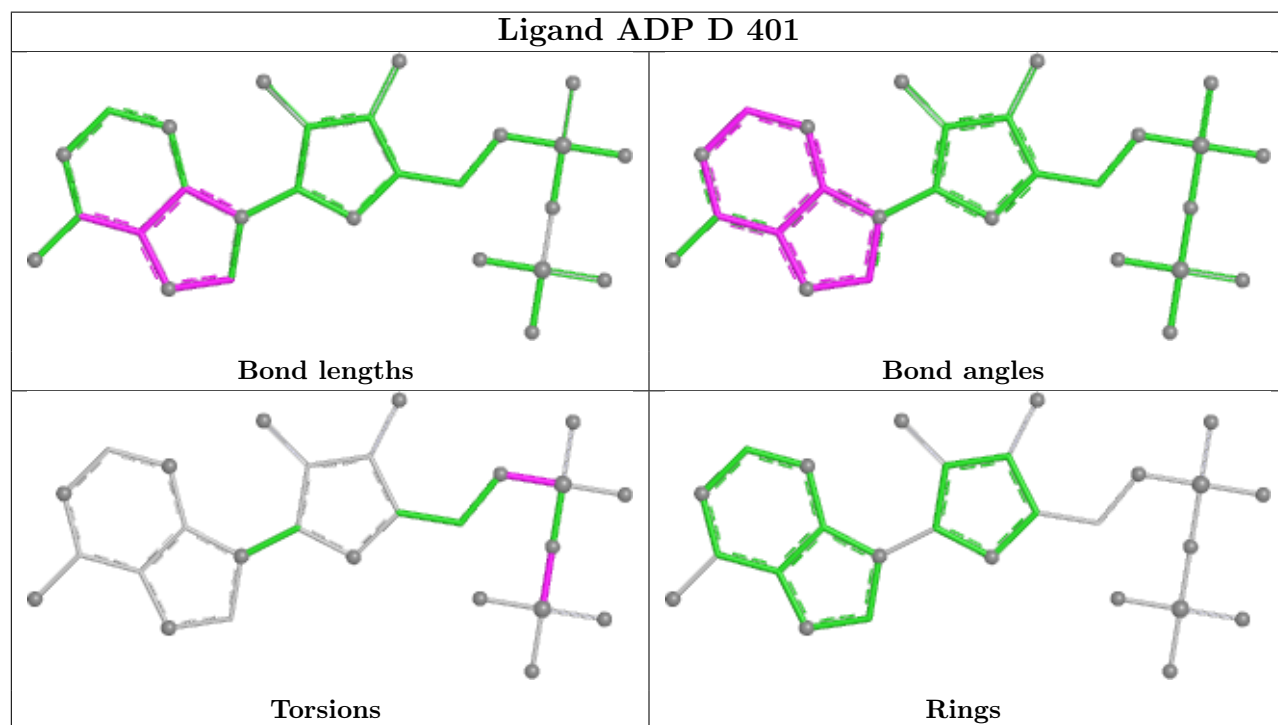
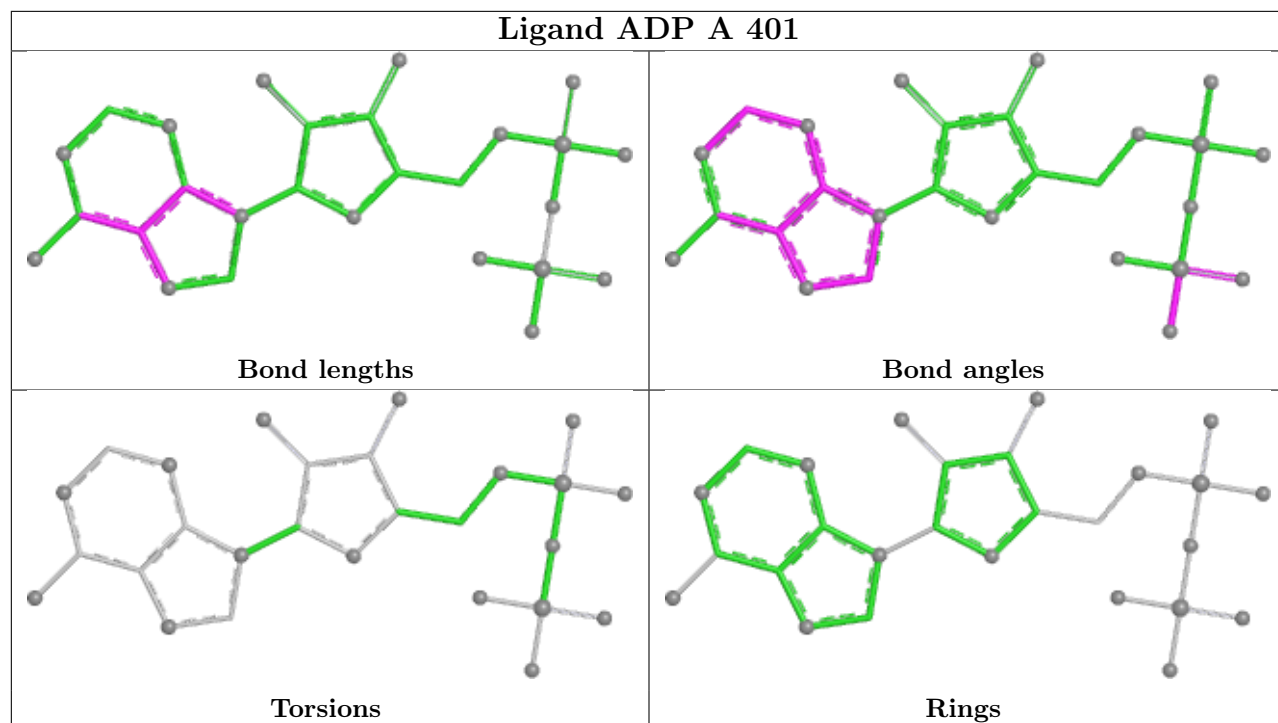
3 monomers are involved in 3 short contacts:

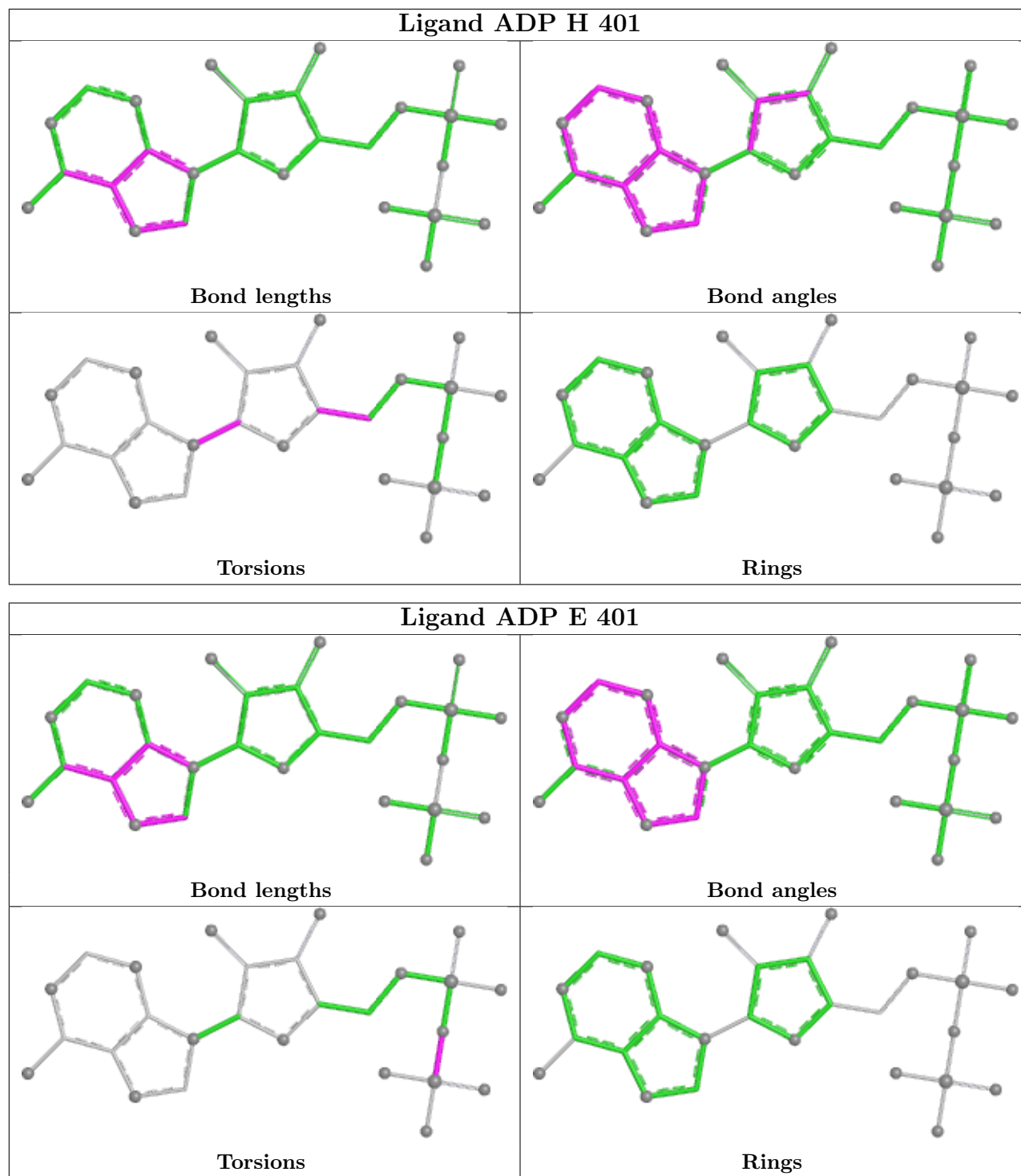
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	ADP	1	0
3	A	401	ADP	1	0
3	H	401	ADP	1	0

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.









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	208/231 (90%)	0.96	22 (10%) 11 15	33, 47, 69, 96	0
1	B	219/231 (94%)	1.28	41 (18%) 3 4	37, 53, 76, 104	0
1	C	210/231 (90%)	1.34	41 (19%) 3 3	36, 58, 86, 101	0
1	D	208/231 (90%)	1.15	29 (13%) 6 9	38, 53, 75, 99	0
1	E	212/231 (91%)	1.60	58 (27%) 1 1	43, 61, 85, 98	0
1	F	204/231 (88%)	2.46	129 (63%) 0 0	54, 78, 101, 117	0
1	G	194/231 (83%)	1.96	79 (40%) 0 0	54, 75, 97, 111	0
1	H	192/231 (83%)	3.57	159 (82%) 0 0	107, 107, 107, 107	0
2	I	31/38 (81%)	1.52	8 (25%) 1 2	41, 60, 76, 89	0
2	J	31/38 (81%)	1.64	12 (38%) 1 0	43, 64, 80, 98	0
2	K	18/38 (47%)	2.16	11 (61%) 0 0	53, 72, 88, 120	0
2	L	31/38 (81%)	1.90	12 (38%) 1 0	57, 67, 81, 109	0
2	M	30/38 (78%)	2.30	18 (60%) 0 0	66, 90, 104, 124	0
2	N	12/38 (31%)	2.88	8 (66%) 0 0	98, 101, 113, 124	0
2	O	15/38 (39%)	2.19	9 (60%) 0 0	73, 81, 97, 116	0
All	All	1815/2114 (85%)	1.78	636 (35%) 1 1	33, 64, 107, 124	0

All (636) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	147	LEU	9.6
1	H	143	GLY	9.6
1	H	196	VAL	7.8
1	H	153	VAL	7.7
1	H	151	LEU	7.6
1	H	285	VAL	7.4
1	H	280	PHE	7.1

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Mol	Chain	Res	Type	RSRZ
1	H	339	VAL	7.0
1	B	226	LEU	6.9
1	H	145	THR	6.8
1	E	253	ALA	6.8
1	H	201	ALA	6.7
1	H	342	ILE	6.7
1	H	234	LEU	6.7
1	E	286	GLN	6.1
1	H	152	ALA	6.1
1	H	136	VAL	6.1
1	G	205	ALA	6.0
1	H	305	LEU	6.0
1	H	146	GLN	6.0
1	G	261	LEU	5.8
1	F	268	LEU	5.8
1	H	113	ILE	5.8
1	H	324	ILE	5.7
1	F	157	LEU	5.6
1	G	327	LEU	5.6
1	H	148	ALA	5.6
1	H	176	THR	5.5
1	H	200	VAL	5.5
1	H	313	VAL	5.5
1	H	197	LEU	5.5
1	H	205	ALA	5.4
1	H	237	VAL	5.3
1	H	128	ILE	5.2
1	H	321	GLY	5.2
1	H	170	TYR	5.2
1	G	285	VAL	5.2
2	N	2061	ALA	5.1
1	H	167	SER	5.1
1	H	283	ASN	5.1
1	H	150	THR	5.1
1	H	171	ILE	5.1
1	H	119	SER	5.1
1	H	235	LEU	5.1
1	F	309	ALA	5.0
1	E	271	LEU	5.0
1	F	261	LEU	5.0
1	B	249	ILE	5.0
1	F	188	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	H	115	THR	4.9
1	H	261	LEU	4.9
1	C	285	VAL	4.9
1	H	311	LEU	4.9
2	N	1229	VAL	4.9
1	H	340	PHE	4.8
1	F	113	ILE	4.8
1	H	304	ILE	4.8
2	M	1238	VAL	4.8
1	H	271	LEU	4.8
1	H	149	HIS	4.8
1	H	182	LEU	4.8
1	G	340	PHE	4.7
1	B	328	ILE	4.7
1	H	278	ALA	4.7
1	H	281	VAL	4.7
1	H	144	LYS	4.7
1	H	158	PRO	4.7
1	A	254	LEU	4.7
1	F	161	GLU	4.6
1	F	304	ILE	4.6
1	E	254	LEU	4.6
1	H	177	PHE	4.6
1	H	185	ILE	4.6
1	F	306	ALA	4.6
1	H	140	PHE	4.6
1	H	347	ILE	4.6
1	F	313	VAL	4.5
1	D	328	ILE	4.5
1	G	271	LEU	4.5
1	G	347	ILE	4.5
1	H	226	LEU	4.5
1	E	196	VAL	4.4
1	H	179	PRO	4.4
1	C	244	PHE	4.4
1	H	157	LEU	4.4
1	F	128	ILE	4.4
1	F	134	THR	4.4
1	G	214	LEU	4.3
1	G	120	LEU	4.3
1	H	327	LEU	4.3
1	F	205	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	223	VAL	4.3
1	H	193	PRO	4.3
1	F	241	THR	4.2
2	L	1240	LEU	4.2
1	F	262	ALA	4.2
1	H	191	LEU	4.2
1	C	328	ILE	4.2
1	H	141	GLY	4.2
1	H	232	TYR	4.2
1	E	285	VAL	4.1
1	H	236	ILE	4.1
2	N	1227	LEU	4.1
1	H	137	PHE	4.1
1	F	171	ILE	4.1
1	F	216	TYR	4.1
1	H	314	TYR	4.1
1	F	315	LEU	4.1
1	G	128	ILE	4.1
1	H	277	ILE	4.1
1	E	255	ALA	4.1
1	E	202	TYR	4.1
1	F	124	LEU	4.1
1	F	237	VAL	4.0
1	G	110	ILE	4.0
1	G	206	PHE	4.0
1	H	108	ALA	4.0
1	F	110	ILE	4.0
1	F	285	VAL	4.0
1	H	142	SER	4.0
1	H	228	THR	4.0
2	O	1230	SER	4.0
1	F	138	GLY	4.0
1	H	190	GLY	4.0
1	F	226	LEU	4.0
1	E	349	ASP	4.0
1	H	159	PRO	4.0
1	H	268	LEU	4.0
1	H	315	LEU	4.0
2	M	1243	ASP	4.0
1	G	123	LEU	3.9
1	E	262	ALA	3.9
1	H	262	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	328	ILE	3.9
1	G	339	VAL	3.9
2	N	2057	GLY	3.9
1	H	306	ALA	3.9
1	H	325	ALA	3.9
1	C	302	GLY	3.9
1	H	155	VAL	3.9
1	E	242	SER	3.9
1	B	302	GLY	3.9
1	F	280	PHE	3.9
1	G	268	LEU	3.8
2	L	1231	THR	3.8
1	C	255	ALA	3.8
1	H	303	HIS	3.8
1	C	206	PHE	3.8
1	H	188	ASN	3.8
1	F	240	LEU	3.8
1	D	259	GLN	3.8
2	M	2058	PHE	3.8
1	A	302	GLY	3.8
1	D	304	ILE	3.8
1	E	287	ALA	3.7
1	H	168	ALA	3.7
1	C	304	ILE	3.7
1	H	312	ARG	3.7
1	B	206	PHE	3.7
1	B	161	GLU	3.7
1	F	346	GLY	3.7
1	H	163	GLY	3.7
1	H	346	GLY	3.7
1	H	118	LYS	3.7
1	G	272	ALA	3.7
1	G	325	ALA	3.7
1	H	279	VAL	3.7
1	E	190	GLY	3.7
1	F	193	PRO	3.7
1	E	327	LEU	3.7
1	F	235	LEU	3.6
1	F	152	ALA	3.6
1	H	202	TYR	3.6
1	E	110	ILE	3.6
1	F	126	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	275	PHE	3.6
1	F	275	PHE	3.6
1	H	282	THR	3.6
1	F	308	SER	3.6
1	H	218	ALA	3.6
1	F	347	ILE	3.6
1	G	133	ILE	3.6
2	N	2058	PHE	3.6
1	F	265	LEU	3.6
1	H	338	ALA	3.6
1	E	206	PHE	3.6
1	F	264	PHE	3.6
1	E	272	ALA	3.5
1	F	215	LEU	3.6
1	H	126	GLY	3.5
1	H	212	MET	3.5
1	H	133	ILE	3.5
1	H	343	THR	3.5
1	H	264	PHE	3.5
1	D	255	ALA	3.5
1	H	173	THR	3.5
1	F	133	ILE	3.5
1	F	177	PHE	3.5
1	G	244	PHE	3.5
1	H	206	PHE	3.5
1	H	164	LEU	3.5
1	F	170	TYR	3.5
1	G	202	TYR	3.5
1	G	248	TYR	3.5
1	F	176	THR	3.5
1	H	134	THR	3.5
1	H	231	PRO	3.5
1	F	184	GLU	3.5
1	H	344	GLU	3.5
1	H	211	GLN	3.5
1	H	154	MET	3.5
1	B	123	LEU	3.5
1	C	309	ALA	3.5
2	M	2061	ALA	3.5
1	E	318	GLY	3.5
1	A	241	THR	3.4
2	I	1243	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	202	TYR	3.4
1	G	324	ILE	3.4
1	H	223	VAL	3.4
1	F	108	ALA	3.4
1	D	311	LEU	3.4
1	F	191	LEU	3.4
1	F	311	LEU	3.4
1	H	207	ASN	3.4
1	G	113	ILE	3.4
1	F	200	VAL	3.4
1	G	126	GLY	3.3
1	D	206	PHE	3.3
1	H	138	GLY	3.3
1	F	342	ILE	3.3
1	B	223	VAL	3.3
1	C	226	LEU	3.3
1	E	261	LEU	3.3
2	L	1234	LEU	3.3
1	F	143	GLY	3.3
1	H	110	ILE	3.3
1	H	308	SER	3.3
1	B	286	GLN	3.2
1	F	279	VAL	3.2
2	M	1240	LEU	3.2
1	B	137	PHE	3.2
1	H	210	HIS	3.2
1	H	216	TYR	3.2
2	L	1243	ASP	3.2
1	B	313	VAL	3.2
1	H	214	LEU	3.2
1	D	258	GLN	3.2
1	H	330	ALA	3.2
1	F	136	VAL	3.2
2	J	1242	SER	3.2
1	F	278	ALA	3.1
1	G	152	ALA	3.1
1	E	258	GLN	3.1
1	E	191	LEU	3.1
1	G	313	VAL	3.1
2	J	1238	VAL	3.1
1	G	143	GLY	3.1
1	G	275	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	160	GLU	3.1
1	A	286	GLN	3.1
1	H	156	GLN	3.1
1	D	109	THR	3.1
1	H	328	ILE	3.1
1	C	320	GLY	3.1
1	H	125	GLY	3.1
1	H	124	LEU	3.1
2	O	1229	VAL	3.1
1	H	275	PHE	3.1
2	O	1228	ASN	3.1
1	F	203	ALA	3.1
1	F	287	ALA	3.1
1	F	277	ILE	3.1
1	G	135	GLU	3.1
1	F	211	GLN	3.1
2	M	1231	THR	3.1
1	F	236	ILE	3.0
1	F	328	ILE	3.0
1	F	120	LEU	3.0
1	F	271	LEU	3.0
1	F	305	LEU	3.0
1	G	200	VAL	3.0
2	K	1229	VAL	3.0
1	C	243	HIS	3.0
1	F	142	SER	3.0
1	H	130	THR	3.0
2	I	1231	THR	3.0
2	K	1231	THR	3.0
1	B	185	ILE	3.0
1	G	342	ILE	3.0
1	B	285	VAL	3.0
1	C	216	TYR	3.0
2	M	1241	PHE	3.0
1	H	166	GLY	3.0
1	A	180	GLU	3.0
1	C	315	LEU	3.0
1	G	269	HIS	3.0
1	H	260	LYS	3.0
1	G	190	GLY	3.0
1	H	111	GLY	3.0
1	H	169	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	201	ALA	3.0
1	H	114	SER	2.9
1	F	109	THR	2.9
1	H	132	ALA	2.9
1	C	305	LEU	2.9
1	E	240	LEU	2.9
1	F	114	SER	2.9
1	F	144	LYS	2.9
1	H	238	ASP	2.9
1	G	279	VAL	2.9
1	A	212	MET	2.9
1	B	250	GLY	2.9
2	K	1232	GLU	2.9
2	O	2057	GLY	2.9
1	F	258	GLN	2.9
1	H	117	SER	2.9
1	H	225	SER	2.9
1	B	254	LEU	2.9
1	F	115	THR	2.9
1	F	137	PHE	2.9
2	J	1241	PHE	2.9
1	G	201	ALA	2.9
1	E	347	ILE	2.9
1	F	214	LEU	2.9
1	F	324	ILE	2.9
1	G	265	LEU	2.9
1	C	303	HIS	2.8
1	D	203	ALA	2.8
1	F	218	ALA	2.8
2	O	2058	PHE	2.8
1	H	172	ASP	2.8
1	E	304	ILE	2.8
1	F	123	LEU	2.8
1	D	318	GLY	2.8
1	D	317	LYS	2.8
1	A	329	ASP	2.8
1	E	186	ALA	2.8
1	G	338	ALA	2.8
1	F	283	ASN	2.8
1	B	336	GLY	2.8
1	F	234	LEU	2.8
1	G	213	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	317	LYS	2.8
1	F	196	VAL	2.8
1	B	248	TYR	2.8
1	G	314	TYR	2.8
1	A	140	PHE	2.8
1	B	188	ASN	2.8
1	H	165	ASN	2.8
1	H	183	ARG	2.8
1	H	266	ARG	2.8
1	B	120	LEU	2.8
1	E	241	THR	2.8
1	G	343	THR	2.8
1	H	265	LEU	2.8
1	C	205	ALA	2.7
1	D	191	LEU	2.7
1	H	186	ALA	2.7
1	F	307	HIS	2.7
2	L	2058	PHE	2.7
1	G	109	THR	2.7
1	G	222	MET	2.7
1	F	147	LEU	2.7
1	H	178	ARG	2.7
1	B	325	ALA	2.7
1	D	321	GLY	2.7
1	E	115	THR	2.7
1	H	310	THR	2.7
1	G	217	GLN	2.7
1	H	341	SER	2.7
1	G	317	LYS	2.7
1	H	221	MET	2.6
1	D	202	TYR	2.6
1	H	181	ARG	2.6
1	G	208	SER	2.6
1	B	327	LEU	2.6
1	F	164	LEU	2.6
2	K	1227	LEU	2.6
1	E	113	ILE	2.6
1	G	136	VAL	2.6
1	H	323	ARG	2.6
1	G	207	ASN	2.6
2	O	2055	PHE	2.6
1	G	210	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	270	ARG	2.6
1	C	222	MET	2.6
1	G	112	ARG	2.6
1	G	132	ALA	2.6
2	I	1229	VAL	2.6
2	M	1237	ALA	2.6
1	F	345	LYS	2.6
2	J	1236	LYS	2.6
1	A	109	THR	2.6
1	F	314	TYR	2.6
2	J	2055	PHE	2.6
1	F	182	LEU	2.6
1	C	110	ILE	2.6
1	E	161	GLU	2.6
2	K	2057	GLY	2.6
1	F	168	ALA	2.6
1	D	242	SER	2.6
2	L	1242	SER	2.6
1	E	275	PHE	2.5
1	A	304	ILE	2.5
1	F	272	ALA	2.5
2	L	2052	SER	2.5
1	G	315	LEU	2.5
1	E	188	ASN	2.5
1	F	269	HIS	2.5
1	F	130	THR	2.5
1	F	160	GLU	2.5
1	E	193	PRO	2.5
1	F	329	ASP	2.5
1	F	151	LEU	2.5
1	G	164	LEU	2.5
1	G	240	LEU	2.5
2	M	1234	LEU	2.5
2	O	1227	LEU	2.5
1	E	257	ARG	2.5
1	H	189	ARG	2.5
1	E	185	ILE	2.5
2	M	1242	SER	2.5
2	M	2059	SER	2.5
1	D	161	GLU	2.5
1	F	230	ARG	2.4
1	G	216	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	340	PHE	2.4
2	I	1240	LEU	2.4
2	J	1240	LEU	2.4
1	H	195	GLU	2.4
1	C	228	THR	2.4
1	C	214	LEU	2.4
1	H	215	LEU	2.4
1	H	219	SER	2.4
2	K	2056	SER	2.4
1	C	317	LYS	2.4
1	D	324	ILE	2.4
1	B	205	ALA	2.4
1	C	108	ALA	2.4
1	F	257	ARG	2.4
1	C	223	VAL	2.4
1	B	187	GLN	2.4
2	J	1235	GLN	2.4
1	C	318	GLY	2.4
1	D	212	MET	2.4
1	F	169	MET	2.4
2	O	2056	SER	2.4
1	E	315	LEU	2.4
1	F	232	TYR	2.4
2	M	2055	PHE	2.4
1	F	312	ARG	2.4
1	H	326	ARG	2.4
1	E	203	ALA	2.4
1	H	203	ALA	2.4
1	G	243	HIS	2.4
1	C	336	GLY	2.4
1	H	116	GLY	2.4
2	K	2063	GLY	2.4
1	C	240	LEU	2.3
1	H	123	LEU	2.3
1	B	314	TYR	2.3
1	E	228	THR	2.3
1	C	213	GLN	2.3
1	B	304	ILE	2.3
1	B	338	ALA	2.3
1	E	218	ALA	2.3
1	F	325	ALA	2.3
2	M	1233	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	231	PRO	2.3
1	H	307	HIS	2.3
1	G	141	GLY	2.3
2	N	1226	LYS	2.3
1	F	239	SER	2.3
1	G	223	VAL	2.3
2	L	1238	VAL	2.3
1	H	135	GLU	2.3
1	H	337	GLU	2.3
1	A	240	LEU	2.3
1	D	254	LEU	2.3
1	D	286	GLN	2.3
1	G	235	LEU	2.3
1	F	140	PHE	2.3
2	K	2055	PHE	2.3
1	C	207	ASN	2.3
1	E	303	HIS	2.3
1	E	338	ALA	2.3
1	F	220	ALA	2.3
1	A	141	GLY	2.3
1	A	336	GLY	2.3
1	C	242	SER	2.3
2	J	2053	SER	2.3
1	F	153	VAL	2.3
1	H	194	ASP	2.3
1	H	284	GLN	2.3
1	B	210	HIS	2.3
1	F	228	THR	2.3
2	N	1228	ASN	2.3
2	M	1239	LYS	2.3
2	O	1226	LYS	2.3
1	F	158	PRO	2.3
1	F	159	PRO	2.3
1	F	186	ALA	2.3
1	D	336	GLY	2.3
1	F	162	GLY	2.3
1	F	135	GLU	2.3
1	H	192	ASP	2.3
2	J	1243	ASP	2.3
1	B	284	GLN	2.3
2	L	1229	VAL	2.3
1	B	315	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	226	LEU	2.3
1	G	311	LEU	2.3
1	H	120	LEU	2.3
1	B	309	ALA	2.2
1	G	108	ALA	2.2
1	D	347	ILE	2.2
1	F	339	VAL	2.2
1	C	307	HIS	2.2
1	H	273	ASN	2.2
1	F	260	LYS	2.2
1	G	323	ARG	2.2
1	B	305	LEU	2.2
1	C	215	LEU	2.2
1	A	208	SER	2.2
1	F	341	SER	2.2
2	J	1237	ALA	2.2
2	J	2054	ALA	2.2
2	L	2054	ALA	2.2
1	E	342	ILE	2.2
1	F	185	ILE	2.2
1	F	183	ARG	2.2
1	G	183	ARG	2.2
1	E	268	LEU	2.2
1	E	126	GLY	2.2
1	F	172	ASP	2.2
1	G	138	GLY	2.2
1	H	229	ASP	2.2
2	M	2053	SER	2.2
2	I	2061	ALA	2.2
1	G	140	PHE	2.2
2	K	2064	LYS	2.2
2	M	1226	LYS	2.2
1	H	180	GLU	2.2
1	D	136	VAL	2.2
1	F	155	VAL	2.2
1	G	131	GLN	2.2
1	H	187	GLN	2.2
1	B	229	ASP	2.2
1	E	305	LEU	2.2
1	F	327	LEU	2.2
1	G	127	GLY	2.2
1	G	163	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	1227	LEU	2.2
1	F	338	ALA	2.2
1	B	307	HIS	2.1
1	C	257	ARG	2.2
1	F	267	MET	2.1
1	E	160	GLU	2.1
1	H	274	GLU	2.1
2	L	1241	PHE	2.1
1	C	347	ILE	2.1
1	F	187	GLN	2.1
1	E	136	VAL	2.1
2	M	1229	VAL	2.1
1	D	346	GLY	2.1
1	B	191	LEU	2.1
1	F	179	PRO	2.1
1	H	122	LYS	2.1
1	C	272	ALA	2.1
1	F	165	ASN	2.1
1	G	168	ALA	2.1
1	H	309	ALA	2.1
1	A	206	PHE	2.1
1	G	277	ILE	2.1
1	E	219	SER	2.1
2	J	1231	THR	2.1
2	K	2059	SER	2.1
2	N	2060	THR	2.1
1	C	313	VAL	2.1
1	E	266	ARG	2.1
1	F	318	GLY	2.1
1	H	336	GLY	2.1
1	F	222	MET	2.1
1	G	221	MET	2.1
1	H	222	MET	2.1
1	B	164	LEU	2.1
1	E	214	LEU	2.1
1	G	147	LEU	2.1
1	G	226	LEU	2.1
1	D	108	ALA	2.1
1	G	218	ALA	2.1
1	E	128	ILE	2.1
1	G	270	ARG	2.1
2	L	2059	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	320	GLY	2.1
1	A	285	VAL	2.1
1	F	227	ASN	2.1
1	F	281	VAL	2.1
1	G	273	ASN	2.1
2	K	1228	ASN	2.1
1	B	261	LEU	2.1
1	E	311	LEU	2.1
1	C	229	ASP	2.1
1	F	270	ARG	2.1
1	G	264	PHE	2.0
2	I	2055	PHE	2.0
2	M	1232	GLU	2.0
1	B	308	SER	2.0
1	B	310	THR	2.0
1	E	109	THR	2.0
1	A	303	HIS	2.0
1	A	318	GLY	2.0
1	C	190	GLY	2.0
1	D	217	GLN	2.0
1	E	211	GLN	2.0
1	A	311	LEU	2.0
1	D	214	LEU	2.0
2	I	1234	LEU	2.0
1	F	132	ALA	2.0
1	F	219	SER	2.0
1	B	222	MET	2.0
1	F	212	MET	2.0
1	A	128	ILE	2.0
1	D	110	ILE	2.0
1	E	171	ILE	2.0
1	G	137	PHE	2.0
1	F	336	GLY	2.0
1	B	202	TYR	2.0
1	C	232	TYR	2.0
1	G	170	TYR	2.0
1	G	209	ASN	2.0
1	A	204	ARG	2.0
1	C	136	VAL	2.0
1	D	285	VAL	2.0
1	E	153	VAL	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](#)

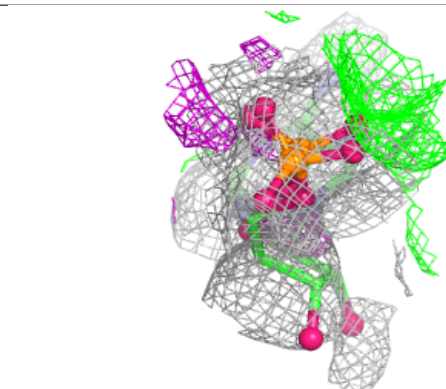
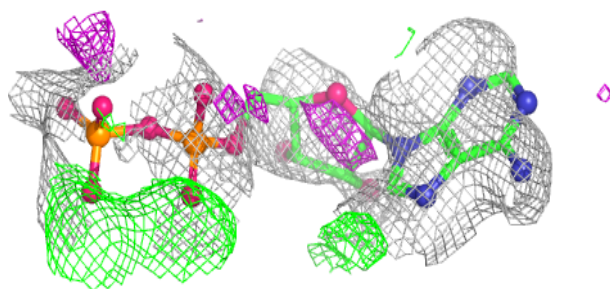
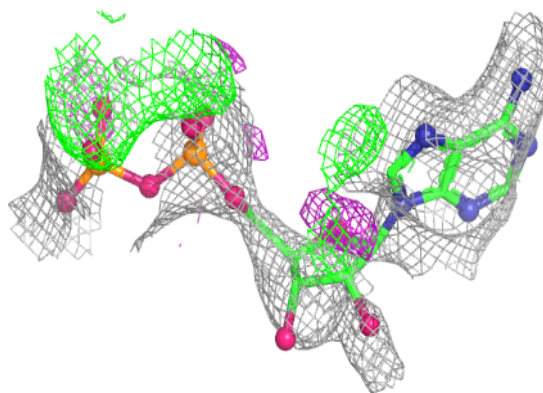
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	MG	G	402	1/1	0.34	0.33	97,97,97,97	0
3	ADP	H	401	27/27	0.49	0.19	100,102,103,104	0
4	MG	F	402	1/1	0.74	0.28	59,59,59,59	0
4	MG	H	402	1/1	0.74	0.41	66,66,66,66	0
3	ADP	F	401	27/27	0.85	0.12	50,56,57,57	0
3	ADP	G	401	27/27	0.85	0.12	66,78,84,84	0
3	ADP	D	401	27/27	0.94	0.08	39,49,54,56	0
3	ADP	C	401	27/27	0.94	0.08	41,44,47,49	0
4	MG	C	402	1/1	0.94	0.14	41,41,41,41	0
3	ADP	B	401	27/27	0.95	0.09	43,50,55,60	0
4	MG	A	402	1/1	0.95	0.12	40,40,40,40	0
3	ADP	E	401	27/27	0.95	0.09	49,54,57,60	0
4	MG	B	402	1/1	0.96	0.07	53,53,53,53	0
3	ADP	A	401	27/27	0.96	0.08	38,43,51,53	0
4	MG	D	402	1/1	0.96	0.06	44,44,44,44	0
4	MG	E	402	1/1	0.98	0.06	45,45,45,45	0

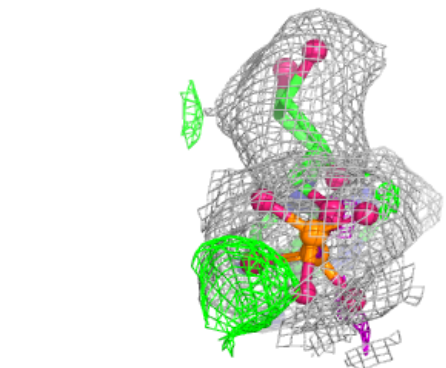
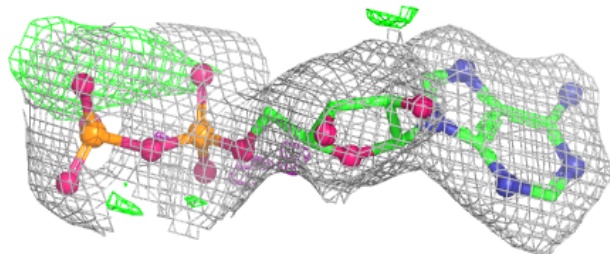
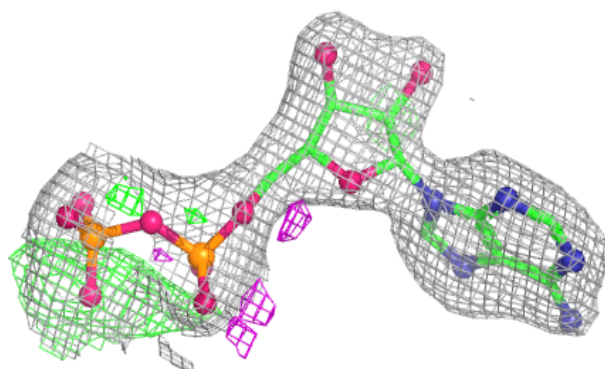
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP H 401:

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

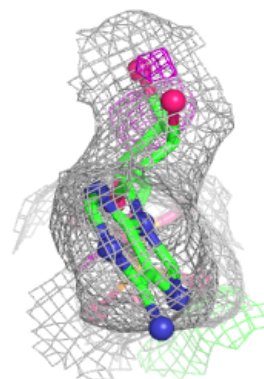
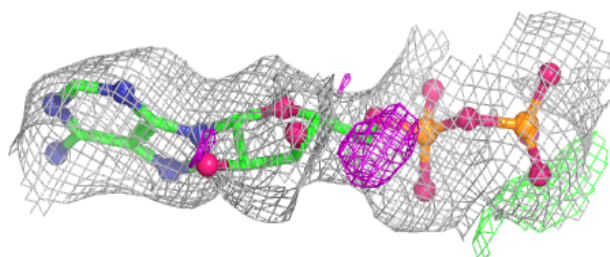
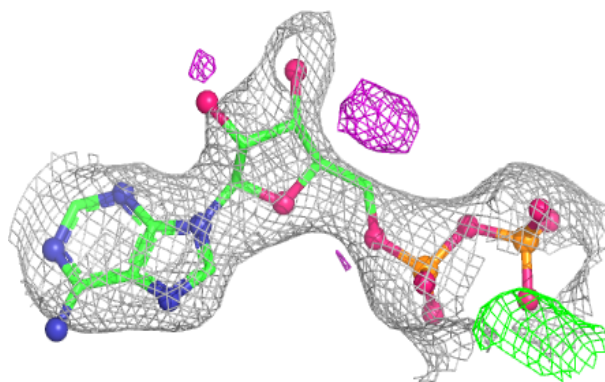
**Electron density around ADP F 401:**

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

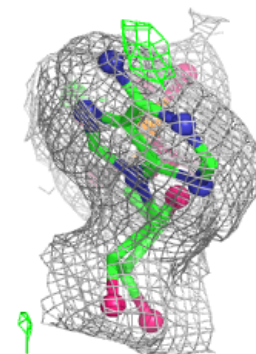
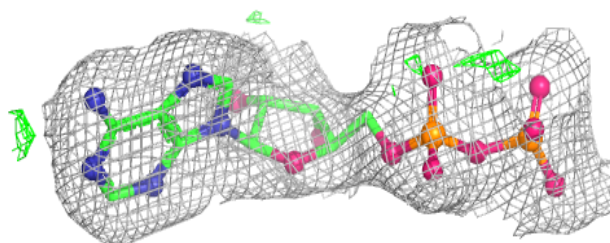
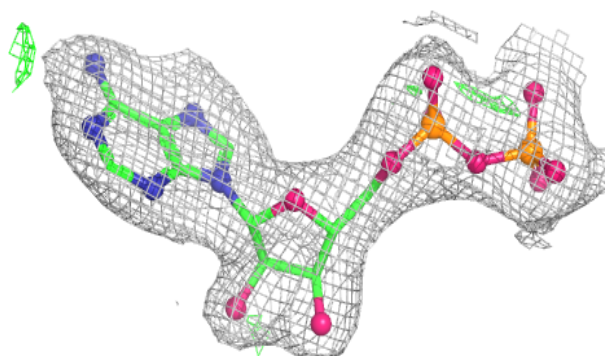


Electron density around ADP G 401:

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

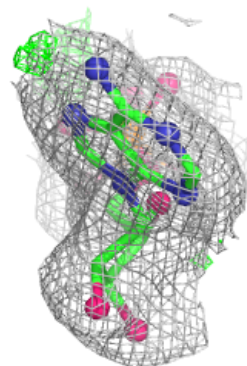
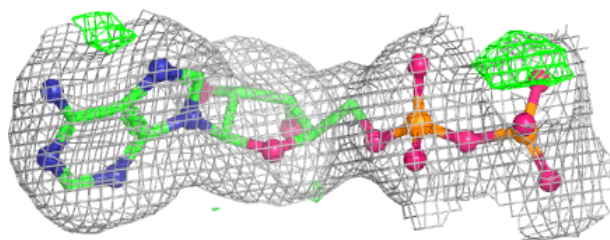
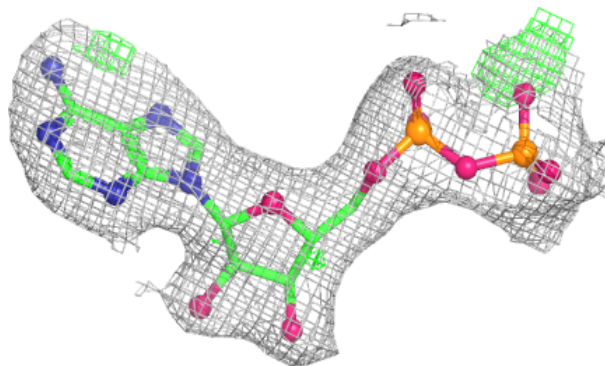
**Electron density around ADP D 401:**

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

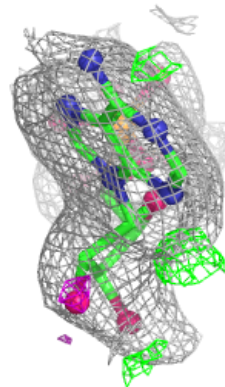
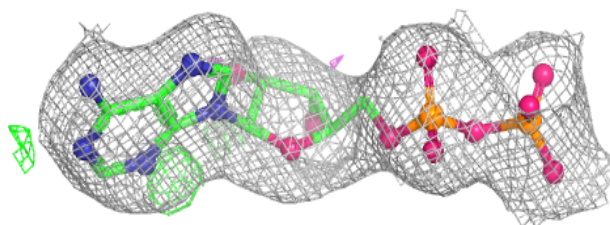
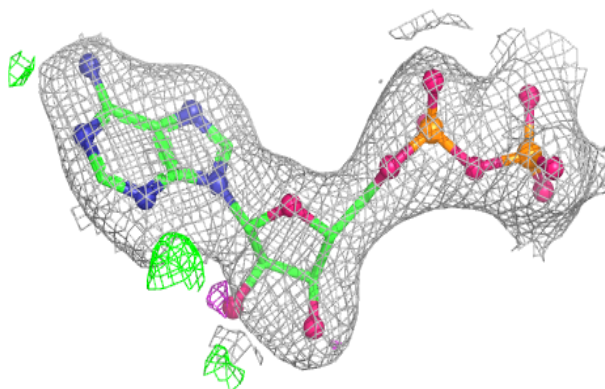


Electron density around ADP C 401:

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

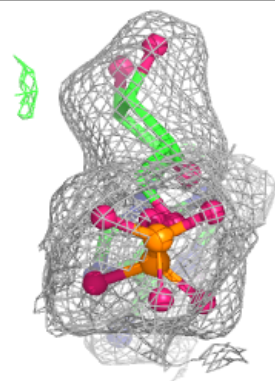
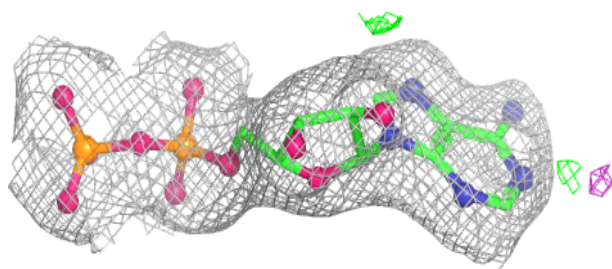
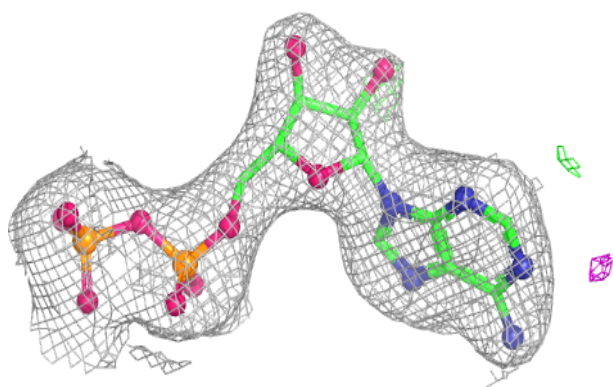
**Electron density around ADP B 401:**

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

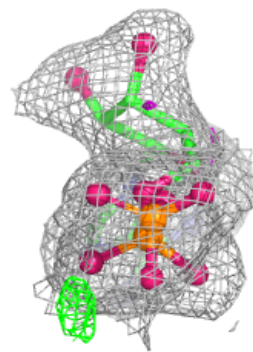
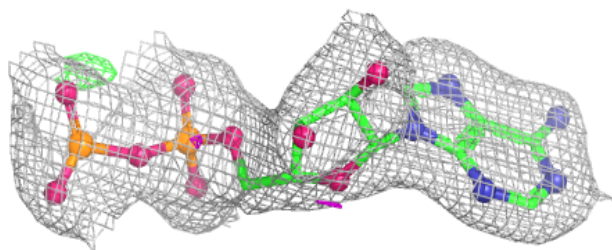
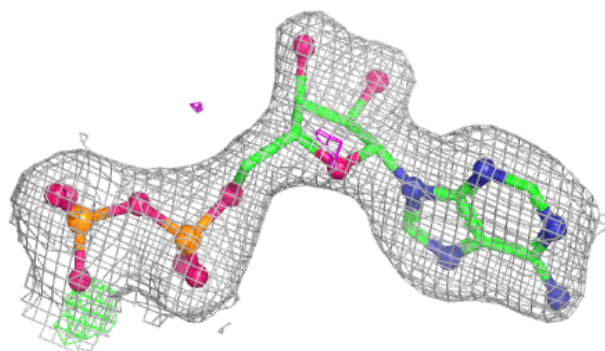


Electron density around ADP E 401:

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

**Electron density around ADP A 401:**

$2mF_o-DF_c$ (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.