WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 03:15 am GMT

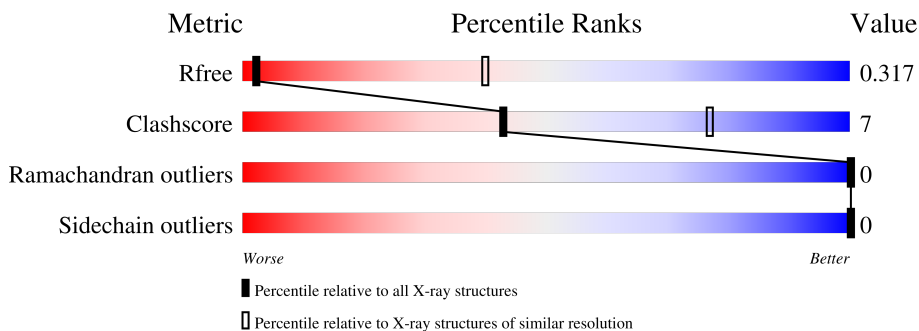|		
PDB ID	:	6S5G
Title	:	Non-square conformation of KtrA A80P mutant ring with bound ADP
Authors	:	Teixeira-Duarte, C.M.; Fonseca, F.; Morais-Cabral, J.H.
Deposited on	:	2019-07-01
Resolution	:	4.33 Å(reported)

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 4.33 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	Percentile Ranks	Value
Rfree		0.317
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		0

Worse — *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1018 (4.84-3.80)
Clashscore	141614	1081 (4.84-3.80)
Ramachandran outliers	138981	1033 (4.84-3.80)
Sidechain outliers	138945	1016 (4.84-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	222	83% 14% •
1	B	222	82% 15% •
1	C	222	79% 18% •
1	D	222	79% 18% •
1	E	222	82% 14% •
1	F	222	77% 20% •
1	G	222	82% 14% •

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Mol	Chain	Length	Quality of chain
1	H	222	

82%   15%   ·

2   Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 13744 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 Ktr system potassium uptake protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total 1691	C 1073	N 290	O 320	S 8	24	0	0
1	B	215	Total 1691	C 1073	N 290	O 320	S 8	24	0	0
1	C	215	Total 1691	C 1073	N 290	O 320	S 8	24	0	0
1	D	215	Total 1691	C 1073	N 290	O 320	S 8	24	0	0
1	E	215	Total 1691	C 1073	N 290	O 320	S 8	24	0	0
1	F	215	Total 1691	C 1073	N 290	O 320	S 8	24	0	0
1	G	215	Total 1691	C 1073	N 290	O 320	S 8	24	0	0
1	H	215	Total 1691	C 1073	N 290	O 320	S 8	24	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	PRO	ALA	engineered mutation	UNP O32080
B	80	PRO	ALA	engineered mutation	UNP O32080
C	80	PRO	ALA	engineered mutation	UNP O32080
D	80	PRO	ALA	engineered mutation	UNP O32080
E	80	PRO	ALA	engineered mutation	UNP O32080
F	80	PRO	ALA	engineered mutation	UNP O32080
G	80	PRO	ALA	engineered mutation	UNP O32080
H	80	PRO	ALA	engineered mutation	UNP O32080

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

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ADP

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

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. 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. 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.
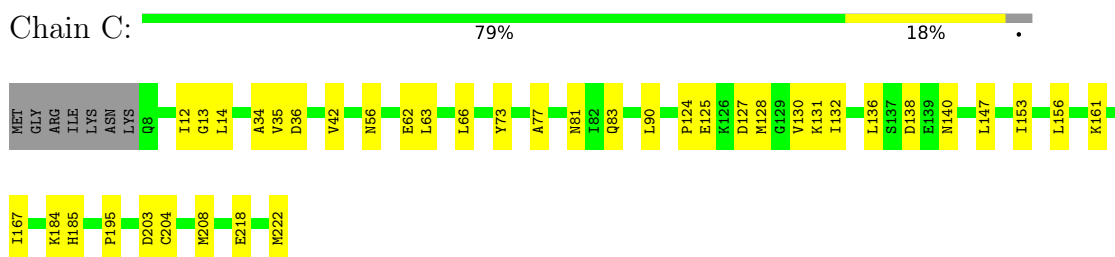
- Molecule 1: Ktr system potassium uptake protein A
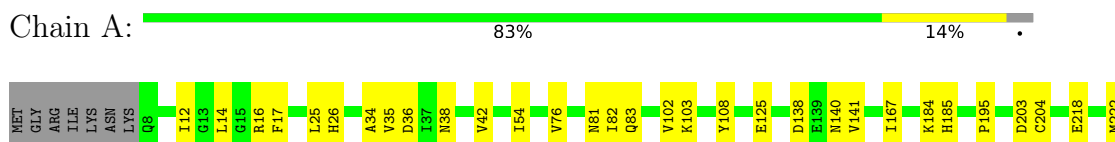
Chain A:

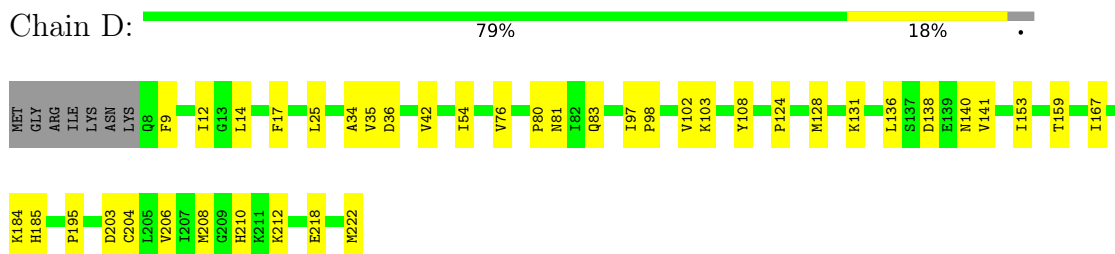
- Molecule 1: Ktr system potassium uptake protein A
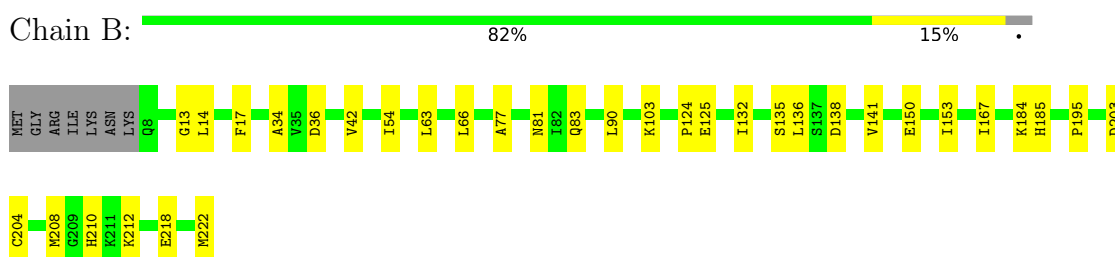
Chain B:

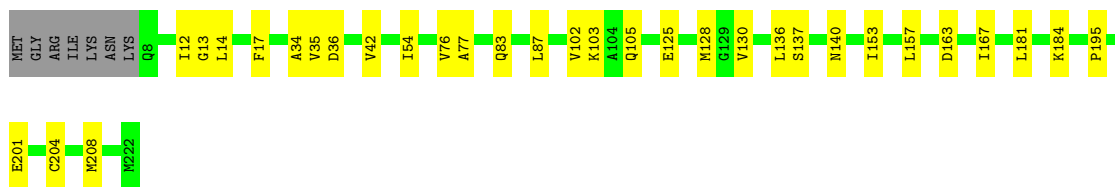- Molecule 1: Ktr system potassium uptake protein A

Chain C:

- Molecule 1: Ktr system potassium uptake protein A

Chain D:

- Molecule 1: Ktr system potassium uptake protein A

Chain E:

82%   14%

MET GLY ARG ILE LYS ASN LYS Q8 I12 G13 L14 F17 A34 V35 D36 V42 I54 V76 A77 Q83 L87 V102 K103 A104 Q105 E125 M128 G129 V130 L136 S137 N140 I153 L157 D163 I167 L181 K184 P195

E201 C204 M208 M222

• Molecule 1: Ktr system potassium uptake protein A

Chain F:

77%   20%

MET GLY ARG ILE LYS ASN LYS Q8 F9 I12 G13 L14 G15 R16 F17 G18 E24 L25 A34 V35 D36 V42 I54 L63 L66 E72 V76 A77 I78 I82 Q83 A84 L91 E94 P98 V102 K103 Y108 P124 E125 D138 V141

I153 I167 V172 R173 A174 I180 K184 H185 P195 D203 C204 M208 E218 M222
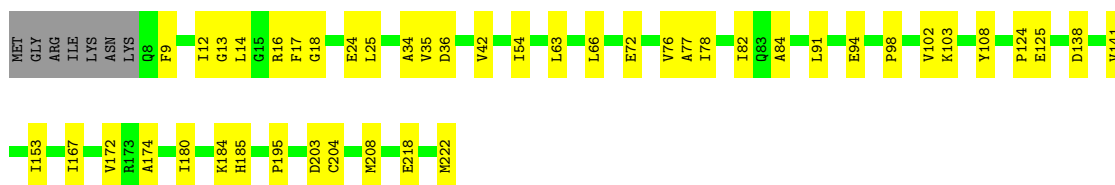
• Molecule 1: Ktr system potassium uptake protein A

Chain G:

82%   14%

MET GLY ARG ILE LYS ASN LYS Q8 I12 G13 L14 F17 A34 V35 D36 V42 I54 V76 I82 I100 W101 V102 K103 Y108 D119 E125 K126 D127 V130 L147 I153 I167 A182 I183 K184 H185 I189 P195 D203 C204 L205

V206 I207 M208 E218 M222

• Molecule 1: Ktr system potassium uptake protein A
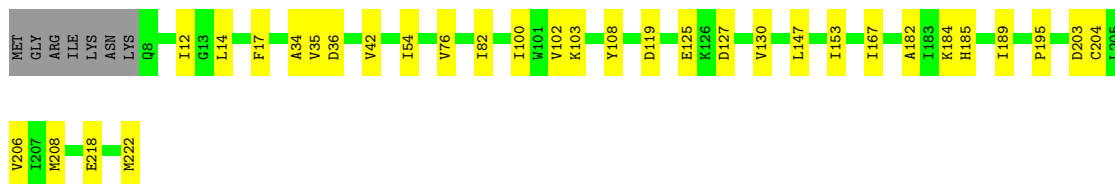
Chain H:

82%   15%

MET GLY ARG ILE LYS ASN LYS Q8 I12 G13 L14 G15 R16 F17 E24 A34 V35 D36 V42 I54 L63 L66 N81 I82 Q83 N99 D119 E125 D138 E139 N140 V141 L147 Y151 S152 I153 I167 A174 A182 I183 K184 P195

C204 L205 V206 I207 M208 E218 N219 E220 G221 M222

4 Data and refinement statistics (i)

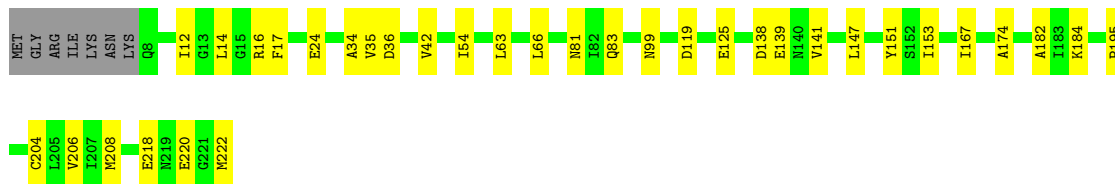| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.33Å　132.93Å　203.26Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	49.28 – 4.33 49.28 – 4.33	Depositor EDS
% Data completeness (in resolution range)	89.1 (49.28-4.33) 91.4 (49.28-4.33)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.254 , 0.314 0.257 , 0.317	Depositor DCC
R_{free} test set	1464 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	135.7	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 78.0	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	13744	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.22	0/1718	0.39	0/2322
1	B	0.22	0/1718	0.41	0/2322
1	C	0.22	0/1718	0.40	0/2322
1	D	0.21	0/1718	0.39	0/2322
1	E	0.22	0/1718	0.42	0/2322
1	F	0.22	0/1718	0.40	0/2322
1	G	0.22	0/1718	0.41	0/2322
1	H	0.21	0/1718	0.40	0/2322
All	All	0.22	0/13744	0.40	0/18576

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1691	0	1713	22	0
1	B	1691	0	1713	25	0
1	C	1691	0	1713	30	0
1	D	1691	0	1713	32	1
1	E	1691	0	1713	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1691	0	1713	32	1
1	G	1691	0	1713	23	0
1	H	1691	0	1713	26	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	2	0
2	E	27	0	12	1	0
2	F	27	0	12	2	0
2	G	27	0	12	1	0
2	H	27	0	12	1	0
All	All	13744	0	13800	184	1

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 (184) 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:H:184:LYS:HB3	1:H:204:CYS:HB2	1.61	0.82
1:D:184:LYS:HB3	1:D:204:CYS:HB2	1.61	0.82
1:G:184:LYS:HB3	1:G:204:CYS:HB2	1.61	0.82
1:A:184:LYS:HB3	1:A:204:CYS:HB2	1.63	0.81
1:C:184:LYS:HB3	1:C:204:CYS:HB2	1.62	0.81
1:B:184:LYS:HB3	1:B:204:CYS:HB2	1.62	0.81
1:F:184:LYS:HB3	1:F:204:CYS:HB2	1.61	0.80
1:E:184:LYS:HB3	1:E:204:CYS:HB2	1.62	0.79
1:C:136:LEU:HD11	1:D:25:LEU:HD21	1.75	0.69
1:E:140:ASN:HA	1:E:157:LEU:HB3	1.75	0.68
1:A:81:ASN:OD1	1:A:83:GLN:HB3	1.93	0.68
1:A:25:LEU:HD21	1:B:136:LEU:HD11	1.75	0.67
1:D:42:VAL:HG21	1:D:54:ILE:HG13	1.77	0.67
1:E:42:VAL:HG21	1:E:54:ILE:HG13	1.78	0.65
1:B:42:VAL:HG21	1:B:54:ILE:HG13	1.77	0.65
1:C:131:LYS:HE3	1:D:131:LYS:NZ	2.11	0.65
1:G:42:VAL:HG21	1:G:54:ILE:HG13	1.79	0.64
1:D:81:ASN:OD1	1:D:83:GLN:HB3	1.96	0.64
1:A:42:VAL:HG21	1:A:54:ILE:HG13	1.79	0.64
1:A:103:LYS:HE2	2:A:601:ADP:O1B	1.97	0.64
1:F:42:VAL:HG21	1:F:54:ILE:HG13	1.80	0.63
1:C:125:GLU:HB3	1:D:17:PHE:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:GLU:HB3	1:F:17:PHE:HA	1.80	0.62
1:H:138:ASP:OD2	1:H:141:VAL:HG13	1.99	0.62
1:H:42:VAL:HG21	1:H:54:ILE:HG13	1.81	0.61
1:G:130:VAL:HA	1:H:24:GLU:HG2	1.81	0.61
1:F:103:LYS:HE2	2:F:601:ADP:O1B	2.00	0.61
1:A:138:ASP:OD2	1:A:141:VAL:HG13	2.02	0.60
1:D:210:HIS:HE1	1:D:212:LYS:HD2	1.66	0.59
1:C:124:PRO:HA	1:D:128:MET:HG2	1.87	0.56
1:E:103:LYS:HE2	2:E:601:ADP:O2B	2.05	0.56
1:G:17:PHE:HA	1:H:125:GLU:HB3	1.87	0.56
1:E:136:LEU:HD21	1:F:25:LEU:HD21	1.88	0.56
1:C:131:LYS:HE3	1:D:131:LYS:HZ1	1.70	0.55
1:G:125:GLU:HB3	1:H:17:PHE:HA	1.90	0.54
1:B:14:LEU:HD11	1:B:34:ALA:HB1	1.90	0.54
1:B:81:ASN:OD1	1:B:83:GLN:HB3	2.08	0.54
1:E:153:ILE:HG12	1:E:208:MET:HG3	1.90	0.53
1:C:167:ILE:HB	1:C:195:PRO:HA	1.89	0.53
1:E:17:PHE:HA	1:F:125:GLU:HB3	1.90	0.53
1:E:128:MET:HG3	1:F:124:PRO:HA	1.91	0.52
1:C:81:ASN:OD1	1:C:83:GLN:HB3	2.10	0.52
1:G:76:VAL:HB	1:G:102:VAL:HG13	1.91	0.52
1:F:218:GLU:HA	1:F:222:MET:HG2	1.92	0.51
1:F:63:LEU:HA	1:F:66:LEU:HD12	1.93	0.51
1:D:167:ILE:HB	1:D:195:PRO:HA	1.92	0.51
1:G:103:LYS:HE2	2:G:601:ADP:O1B	2.11	0.51
1:A:16:ARG:HB3	1:B:125:GLU:HG2	1.93	0.51
1:D:103:LYS:HE2	2:D:601:ADP:O2B	2.12	0.50
1:C:14:LEU:HD11	1:C:34:ALA:HB1	1.92	0.50
1:B:218:GLU:HA	1:B:222:MET:HG2	1.94	0.50
1:G:100:ILE:N	1:G:119:ASP:OD2	2.35	0.50
1:E:136:LEU:HD13	1:F:9:PHE:CE1	2.47	0.50
1:G:82:ILE:HG21	1:G:108:TYR:HE2	1.77	0.50
1:E:136:LEU:HD12	1:E:137:SER:N	2.27	0.50
1:F:78:ILE:HG21	1:F:84:ALA:HB3	1.94	0.50
1:G:14:LEU:HD11	1:G:34:ALA:HB1	1.94	0.50
1:H:167:ILE:HB	1:H:195:PRO:HA	1.94	0.50
1:A:125:GLU:HB3	1:B:17:PHE:HA	1.94	0.49
1:D:138:ASP:OD2	1:D:141:VAL:HG13	2.12	0.49
1:D:210:HIS:CE1	1:F:174:ALA:HB1	2.47	0.49
1:G:167:ILE:HB	1:G:195:PRO:HA	1.94	0.49
1:E:130:VAL:HA	1:F:24:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HB	1:A:195:PRO:HA	1.93	0.49
1:D:14:LEU:HD21	1:D:34:ALA:HB1	1.93	0.49
1:F:12:ILE:HA	1:F:35:VAL:HB	1.95	0.49
1:F:138:ASP:OD1	1:F:141:VAL:HG13	2.12	0.49
1:E:14:LEU:HD11	1:E:34:ALA:HB1	1.94	0.49
1:G:12:ILE:HA	1:G:35:VAL:HB	1.95	0.49
1:A:103:LYS:NZ	1:A:125:GLU:OE2	2.43	0.49
1:B:132:ILE:HG22	1:B:136:LEU:HD23	1.94	0.48
1:F:14:LEU:HD11	1:F:34:ALA:HB1	1.94	0.48
1:F:36:ASP:O	1:F:54:ILE:HA	2.13	0.48
1:H:14:LEU:HD12	1:H:36:ASP:HB2	1.95	0.48
1:D:14:LEU:HD11	1:D:34:ALA:HB1	1.94	0.48
1:H:16:ARG:N	2:H:601:ADP:O1B	2.46	0.48
1:F:167:ILE:HB	1:F:195:PRO:HA	1.94	0.48
1:H:14:LEU:HD11	1:H:34:ALA:HB1	1.95	0.48
1:E:167:ILE:HB	1:E:195:PRO:HA	1.95	0.48
1:H:139:GLU:OE2	1:H:139:GLU:HA	2.13	0.48
1:C:185:HIS:HD1	1:C:203:ASP:CG	2.16	0.48
1:D:185:HIS:HD1	1:D:203:ASP:CG	2.17	0.47
1:A:82:ILE:HG21	1:A:108:TYR:HE2	1.79	0.47
1:F:76:VAL:HB	1:F:102:VAL:HG13	1.96	0.47
1:H:14:LEU:HD21	1:H:34:ALA:HB1	1.96	0.47
1:C:56:ASN:HB2	1:C:62:GLU:OE2	2.14	0.47
1:C:153:ILE:HG12	1:C:208:MET:HG3	1.96	0.47
1:C:63:LEU:HA	1:C:66:LEU:HD12	1.95	0.47
1:E:13:GLY:HA3	1:E:77:ALA:O	2.15	0.47
1:H:99:ASN:HA	1:H:119:ASP:OD2	2.15	0.46
1:A:138:ASP:OD2	1:A:140:ASN:HB2	2.14	0.46
1:C:12:ILE:HA	1:C:35:VAL:HB	1.96	0.46
1:H:36:ASP:O	1:H:54:ILE:HA	2.16	0.46
1:E:12:ILE:HA	1:E:35:VAL:HB	1.97	0.46
1:B:185:HIS:HD1	1:B:203:ASP:CG	2.19	0.46
1:G:14:LEU:HD21	1:G:34:ALA:HB1	1.97	0.46
1:A:14:LEU:HD11	1:A:34:ALA:HB1	1.97	0.46
1:D:12:ILE:HA	1:D:35:VAL:HB	1.96	0.46
1:B:212:LYS:HZ2	1:H:220:GLU:HG3	1.81	0.46
1:C:14:LEU:HD21	1:C:34:ALA:HB1	1.97	0.46
1:D:76:VAL:HB	1:D:102:VAL:HG13	1.97	0.46
1:F:13:GLY:HA3	1:F:77:ALA:O	2.16	0.46
1:C:73:TYR:CD2	1:D:136:LEU:HD11	2.51	0.46
1:G:185:HIS:HD1	1:G:203:ASP:CG	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ASP:O	1:C:130:VAL:HG22	2.16	0.46
1:E:36:ASP:O	1:E:54:ILE:HA	2.16	0.45
1:A:185:HIS:HD1	1:A:203:ASP:CG	2.18	0.45
1:B:125:GLU:H	1:B:125:GLU:CD	2.20	0.45
1:G:153:ILE:HG12	1:G:208:MET:HG3	1.97	0.45
1:D:210:HIS:ND1	1:F:174:ALA:HB1	2.31	0.45
1:H:63:LEU:HA	1:H:66:LEU:HD12	1.97	0.45
1:A:218:GLU:HA	1:A:222:MET:HG2	1.98	0.45
1:D:138:ASP:OD2	1:D:140:ASN:HB3	2.17	0.45
1:D:218:GLU:HA	1:D:222:MET:HG2	1.97	0.45
1:A:12:ILE:HA	1:A:35:VAL:HB	1.98	0.45
1:G:182:ALA:HB2	1:H:208:MET:HE3	1.98	0.45
1:B:13:GLY:HA3	1:B:77:ALA:O	2.16	0.45
1:G:127:ASP:O	1:G:130:VAL:HG22	2.16	0.45
1:G:218:GLU:HA	1:G:222:MET:HG2	1.99	0.45
1:B:36:ASP:O	1:B:54:ILE:HA	2.17	0.45
1:B:153:ILE:HG12	1:B:208:MET:HG3	1.99	0.45
1:H:81:ASN:OD1	1:H:83:GLN:HB2	2.16	0.45
1:H:153:ILE:HG12	1:H:208:MET:HG3	1.99	0.45
1:A:14:LEU:HD21	1:A:34:ALA:HB1	1.99	0.44
1:F:153:ILE:HG12	1:F:208:MET:HG3	1.98	0.44
1:F:14:LEU:HD21	1:F:34:ALA:HB1	1.98	0.44
1:C:56:ASN:N	1:C:62:GLU:OE1	2.46	0.44
1:C:136:LEU:HD13	1:D:9:PHE:CE1	2.53	0.44
1:D:103:LYS:NZ	1:D:124:PRO:HG2	2.33	0.44
1:F:172:VAL:HG21	1:F:180:ILE:HG13	1.99	0.44
1:H:218:GLU:HA	1:H:222:MET:HG2	1.99	0.44
1:A:76:VAL:HB	1:A:102:VAL:HG13	2.00	0.44
1:C:218:GLU:HA	1:C:222:MET:HG2	2.00	0.43
1:D:153:ILE:HG12	1:D:208:MET:HG3	2.00	0.43
1:C:161:LYS:HB2	1:C:222:MET:HA	2.00	0.43
1:E:36:ASP:HB3	1:E:42:VAL:HG23	2.00	0.43
1:F:82:ILE:HG21	1:F:108:TYR:CE2	2.53	0.43
1:G:36:ASP:O	1:G:54:ILE:HA	2.19	0.43
1:C:140:ASN:OD1	1:C:156:LEU:HB3	2.18	0.43
1:G:147:LEU:HD22	1:H:206:VAL:HG21	2.01	0.43
1:G:208:MET:HE1	1:H:182:ALA:HB2	2.00	0.43
1:D:103:LYS:HZ2	1:D:124:PRO:HG2	1.83	0.43
1:C:13:GLY:HA3	1:C:77:ALA:O	2.18	0.43
1:A:36:ASP:OD2	1:A:38:ASN:HB3	2.17	0.43
1:B:63:LEU:HA	1:B:66:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ILE:HB	1:B:195:PRO:HA	2.00	0.43
1:C:14:LEU:HD12	1:C:36:ASP:HB2	2.01	0.43
1:C:138:ASP:N	1:C:138:ASP:OD1	2.48	0.43
1:F:13:GLY:O	1:F:18:GLY:HA3	2.19	0.43
1:B:14:LEU:HD21	1:B:34:ALA:HB1	1.99	0.43
1:F:36:ASP:OD2	2:F:601:ADP:H1'	2.18	0.43
1:B:103:LYS:HZ2	1:B:124:PRO:HG3	1.83	0.43
1:F:91:LEU:O	1:F:94:GLU:HB2	2.19	0.43
1:F:185:HIS:HD1	1:F:203:ASP:CG	2.22	0.43
1:B:150:GLU:HB3	1:B:210:HIS:CE1	2.53	0.43
1:B:138:ASP:HB3	1:B:141:VAL:HG22	2.00	0.42
1:A:17:PHE:HA	1:B:125:GLU:HB3	1.99	0.42
1:D:36:ASP:O	1:D:54:ILE:HA	2.19	0.42
1:C:132:ILE:HG22	1:C:136:LEU:HD23	2.01	0.42
1:D:140:ASN:HD21	1:D:159:THR:HG23	1.83	0.42
1:E:105:GLN:HE22	1:F:16:ARG:CZ	2.32	0.42
1:D:210:HIS:HE1	1:D:212:LYS:CD	2.30	0.42
1:E:163:ASP:HB2	1:E:201:GLU:HB3	2.01	0.42
1:C:36:ASP:HB3	1:C:42:VAL:HG23	2.02	0.42
1:C:147:LEU:HD22	1:D:206:VAL:HG21	2.01	0.42
1:E:76:VAL:HB	1:E:102:VAL:HG13	2.02	0.41
1:G:189:ILE:HG21	1:H:151:TYR:CD2	2.56	0.41
1:E:83:GLN:O	1:E:87:LEU:HG	2.20	0.41
1:E:181:LEU:HD11	1:E:208:MET:HB2	2.00	0.41
1:H:12:ILE:HA	1:H:35:VAL:HB	2.02	0.41
1:D:80:PRO:HD3	2:D:601:ADP:O2A	2.20	0.41
1:G:206:VAL:HG21	1:H:147:LEU:HD22	2.03	0.41
1:A:26:HIS:NE2	1:H:174:ALA:HB1	2.36	0.41
1:A:36:ASP:HB3	1:A:42:VAL:HG23	2.02	0.41
1:B:138:ASP:OD2	1:B:141:VAL:HG13	2.20	0.41
1:D:97:ILE:HA	1:D:98:PRO:HD3	1.93	0.41
1:F:82:ILE:HD12	1:F:82:ILE:H	1.85	0.41
1:B:135:SER:HA	1:B:141:VAL:HG23	2.03	0.41
1:F:72:GLU:HA	1:F:98:PRO:HG2	2.02	0.41
1:C:90:LEU:HD12	1:C:90:LEU:HA	1.80	0.41
1:E:36:ASP:HB3	1:E:42:VAL:CG2	2.51	0.41
1:B:90:LEU:HD12	1:B:90:LEU:HA	1.86	0.41
1:E:14:LEU:HD21	1:E:34:ALA:HB1	2.02	0.41
1:C:128:MET:O	1:C:132:ILE:HG12	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:TYR:OH	1:F:108:TYR:OH[3_444]	2.07	0.13

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	213/222 (96%)	207 (97%)	6 (3%)	0	100	100
1	B	213/222 (96%)	207 (97%)	6 (3%)	0	100	100
1	C	213/222 (96%)	207 (97%)	6 (3%)	0	100	100
1	D	213/222 (96%)	207 (97%)	6 (3%)	0	100	100
1	E	213/222 (96%)	207 (97%)	6 (3%)	0	100	100
1	F	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
1	G	213/222 (96%)	206 (97%)	7 (3%)	0	100	100
1	H	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
All	All	1704/1776 (96%)	1657 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	185/191 (97%)	185 (100%)	0	100	100
1	B	185/191 (97%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	185/191 (97%)	185 (100%)	0	100	100
1	D	185/191 (97%)	185 (100%)	0	100	100
1	E	185/191 (97%)	185 (100%)	0	100	100
1	F	185/191 (97%)	185 (100%)	0	100	100
1	G	185/191 (97%)	185 (100%)	0	100	100
1	H	185/191 (97%)	185 (100%)	0	100	100
All	All	1480/1528 (97%)	1480 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	210	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	ADP	F	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.44	4 (13%)
2	ADP	D	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.42	4 (13%)
2	ADP	E	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
2	ADP	A	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.46	4 (13%)
2	ADP	G	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.44	4 (13%)
2	ADP	B	601	-	24,29,29	0.97	1 (4%)	29,45,45	1.43	4 (13%)
2	ADP	C	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.44	4 (13%)
2	ADP	H	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)

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	ADP	F	601	-	-	2/12/32/32	0/3/3/3
2	ADP	D	601	-	-	2/12/32/32	0/3/3/3
2	ADP	E	601	-	-	7/12/32/32	0/3/3/3
2	ADP	A	601	-	-	2/12/32/32	0/3/3/3
2	ADP	G	601	-	-	4/12/32/32	0/3/3/3
2	ADP	B	601	-	-	2/12/32/32	0/3/3/3
2	ADP	C	601	-	-	4/12/32/32	0/3/3/3
2	ADP	H	601	-	-	6/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	C5-C4	2.51	1.47	1.40
2	C	601	ADP	C5-C4	2.50	1.47	1.40
2	E	601	ADP	C5-C4	2.50	1.47	1.40
2	G	601	ADP	C5-C4	2.49	1.47	1.40
2	H	601	ADP	C5-C4	2.49	1.47	1.40
2	F	601	ADP	C5-C4	2.48	1.47	1.40
2	D	601	ADP	C5-C4	2.46	1.47	1.40
2	A	601	ADP	C5-C4	2.44	1.47	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	601	ADP	PA-O3A-PB	-3.37	121.28	132.83
2	B	601	ADP	PA-O3A-PB	-3.35	121.33	132.83
2	A	601	ADP	PA-O3A-PB	-3.34	121.36	132.83
2	F	601	ADP	PA-O3A-PB	-3.32	121.44	132.83
2	D	601	ADP	PA-O3A-PB	-3.32	121.44	132.83
2	G	601	ADP	PA-O3A-PB	-3.29	121.53	132.83
2	C	601	ADP	PA-O3A-PB	-3.28	121.58	132.83
2	E	601	ADP	N3-C2-N1	-3.20	123.67	128.68
2	A	601	ADP	N3-C2-N1	-3.20	123.67	128.68
2	B	601	ADP	N3-C2-N1	-3.20	123.67	128.68
2	F	601	ADP	N3-C2-N1	-3.18	123.70	128.68
2	H	601	ADP	N3-C2-N1	-3.18	123.71	128.68
2	C	601	ADP	N3-C2-N1	-3.16	123.75	128.68
2	G	601	ADP	N3-C2-N1	-3.15	123.76	128.68
2	D	601	ADP	N3-C2-N1	-3.11	123.82	128.68
2	E	601	ADP	PA-O3A-PB	-3.09	122.21	132.83
2	A	601	ADP	C3'-C2'-C1'	3.07	105.60	100.98
2	H	601	ADP	C3'-C2'-C1'	3.06	105.59	100.98
2	C	601	ADP	C3'-C2'-C1'	3.05	105.57	100.98
2	G	601	ADP	C3'-C2'-C1'	3.03	105.53	100.98
2	F	601	ADP	C3'-C2'-C1'	2.95	105.42	100.98
2	B	601	ADP	C3'-C2'-C1'	2.94	105.40	100.98
2	E	601	ADP	C3'-C2'-C1'	2.87	105.30	100.98
2	D	601	ADP	C3'-C2'-C1'	2.80	105.20	100.98
2	D	601	ADP	C4-C5-N7	-2.75	106.53	109.40
2	G	601	ADP	C4-C5-N7	-2.75	106.54	109.40
2	A	601	ADP	C4-C5-N7	-2.73	106.55	109.40
2	C	601	ADP	C4-C5-N7	-2.73	106.56	109.40
2	B	601	ADP	C4-C5-N7	-2.72	106.57	109.40
2	F	601	ADP	C4-C5-N7	-2.69	106.60	109.40
2	H	601	ADP	C4-C5-N7	-2.68	106.61	109.40
2	E	601	ADP	C4-C5-N7	-2.65	106.64	109.40

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ADP	O4'-C4'-C5'-O5'
2	E	601	ADP	C5'-O5'-PA-O2A
2	H	601	ADP	C5'-O5'-PA-O1A
2	H	601	ADP	C5'-O5'-PA-O2A
2	H	601	ADP	O4'-C4'-C5'-O5'
2	H	601	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	601	ADP	O4'-C4'-C5'-O5'
2	B	601	ADP	C3'-C4'-C5'-O5'
2	C	601	ADP	O4'-C4'-C5'-O5'
2	D	601	ADP	O4'-C4'-C5'-O5'
2	E	601	ADP	O4'-C4'-C5'-O5'
2	E	601	ADP	C3'-C4'-C5'-O5'
2	G	601	ADP	O4'-C4'-C5'-O5'
2	G	601	ADP	C3'-C4'-C5'-O5'
2	A	601	ADP	C3'-C4'-C5'-O5'
2	D	601	ADP	C3'-C4'-C5'-O5'
2	C	601	ADP	C3'-C4'-C5'-O5'
2	E	601	ADP	C5'-O5'-PA-O3A
2	H	601	ADP	C5'-O5'-PA-O3A
2	C	601	ADP	PB-O3A-PA-O2A
2	E	601	ADP	PB-O3A-PA-O1A
2	E	601	ADP	C5'-O5'-PA-O1A
2	F	601	ADP	O4'-C4'-C5'-O5'
2	G	601	ADP	PB-O3A-PA-O2A
2	C	601	ADP	PB-O3A-PA-O1A
2	E	601	ADP	PB-O3A-PA-O2A
2	F	601	ADP	PB-O3A-PA-O2A
2	G	601	ADP	PB-O3A-PA-O1A
2	H	601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	ADP	2	0
2	D	601	ADP	2	0
2	E	601	ADP	1	0
2	A	601	ADP	1	0
2	G	601	ADP	1	0
2	H	601	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 then 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 ADP F 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP G 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP H 601

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.
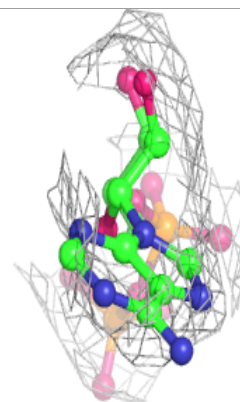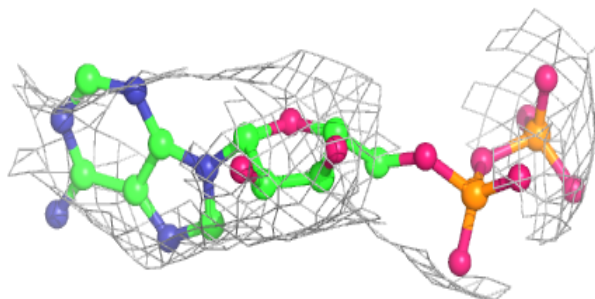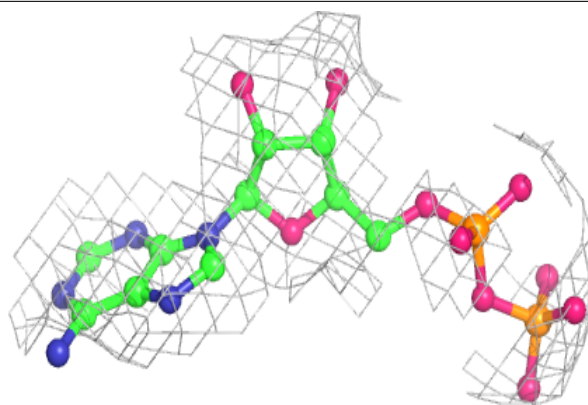
Electron density around ADP A 601:

$2mF_o$-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 601:

$2mF_o$-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 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
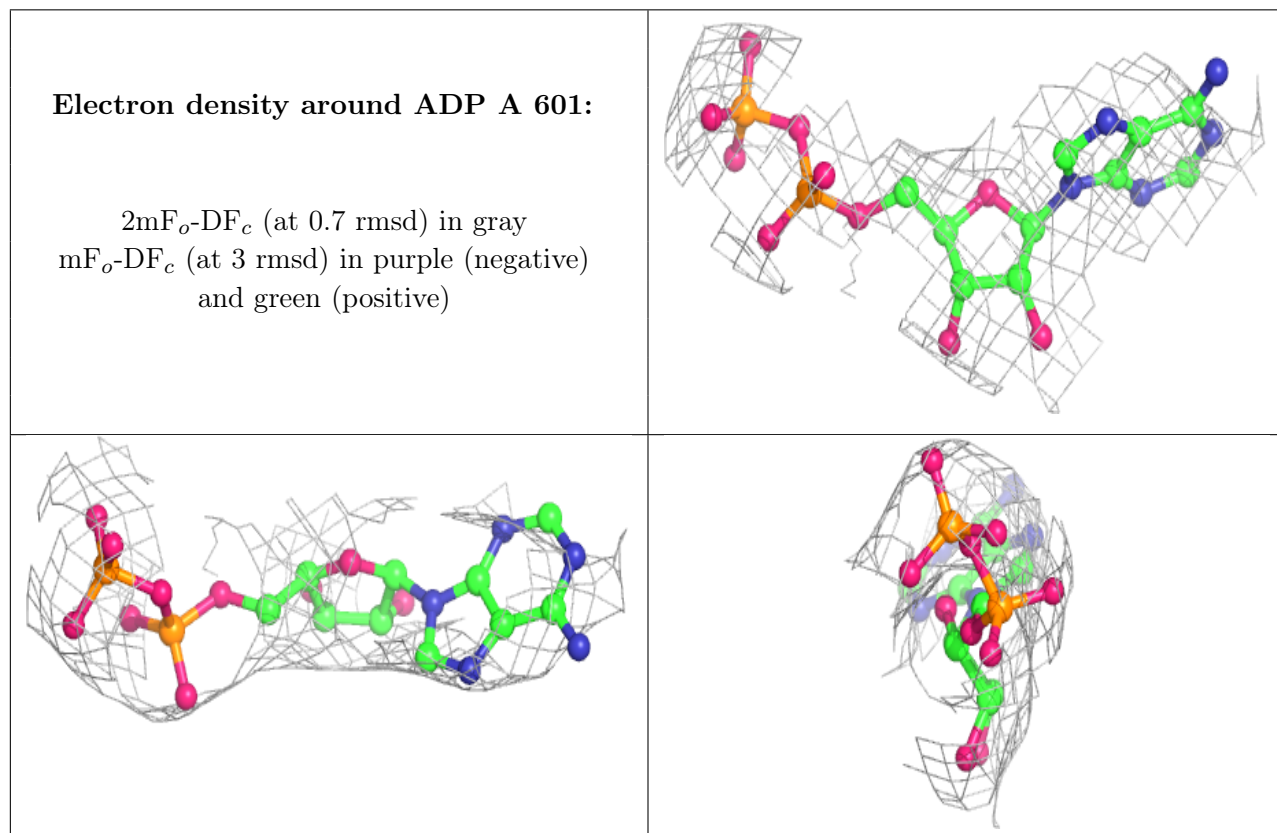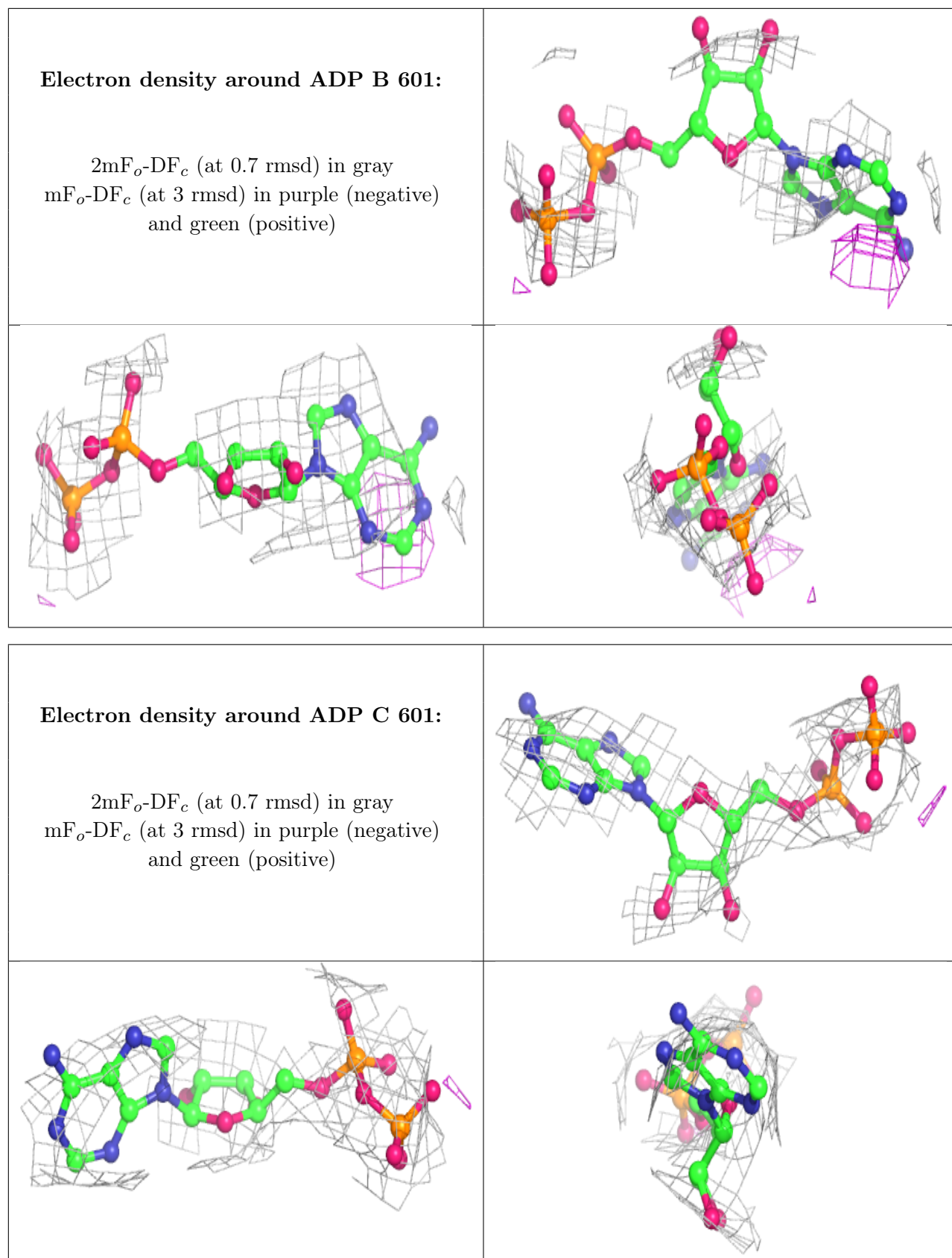
Electron density around ADP D 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
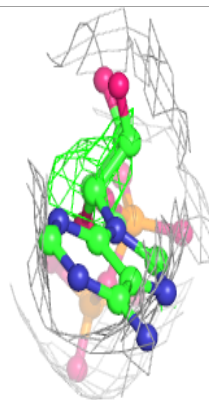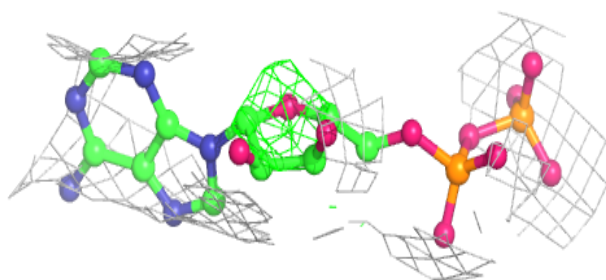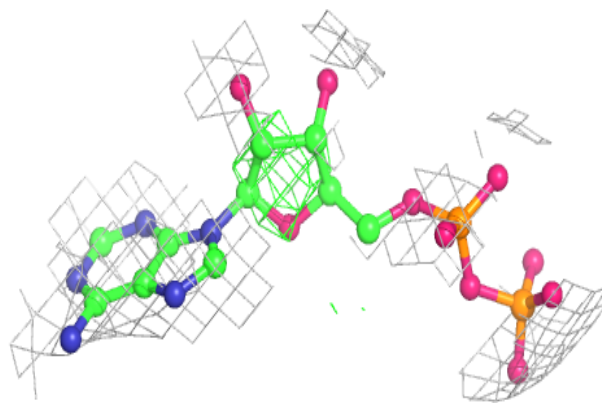
Electron density around ADP E 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
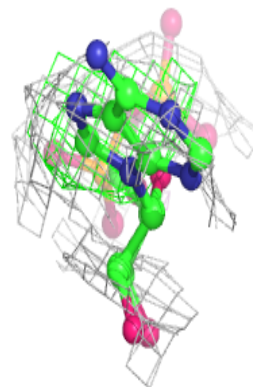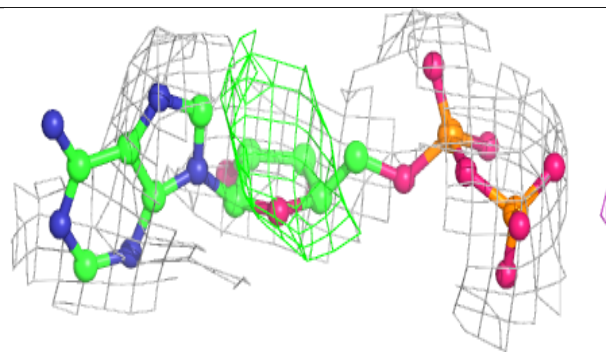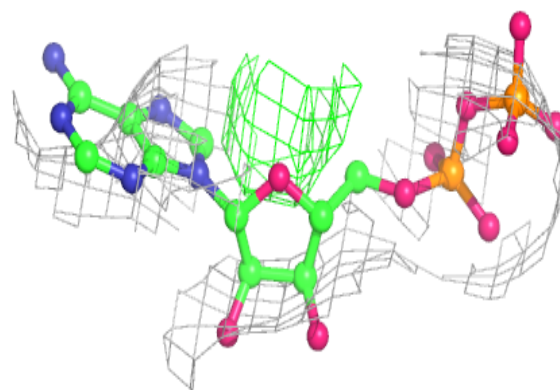
Electron density around ADP F 601:

$2mF_o$-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 601:

$2mF_o$-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 H 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
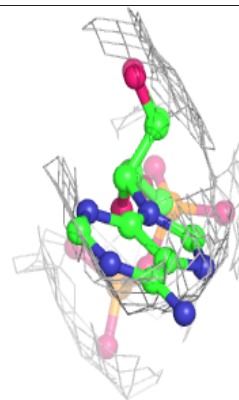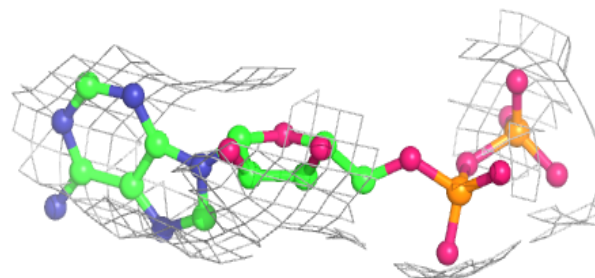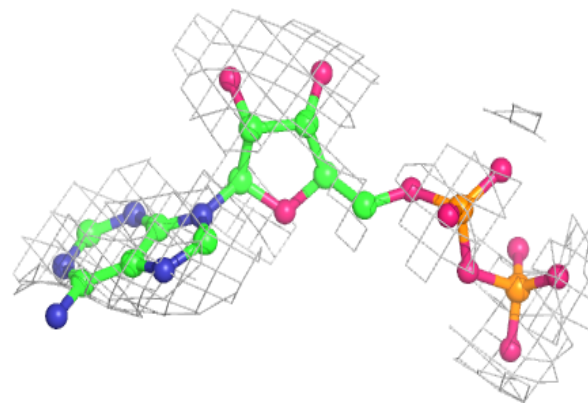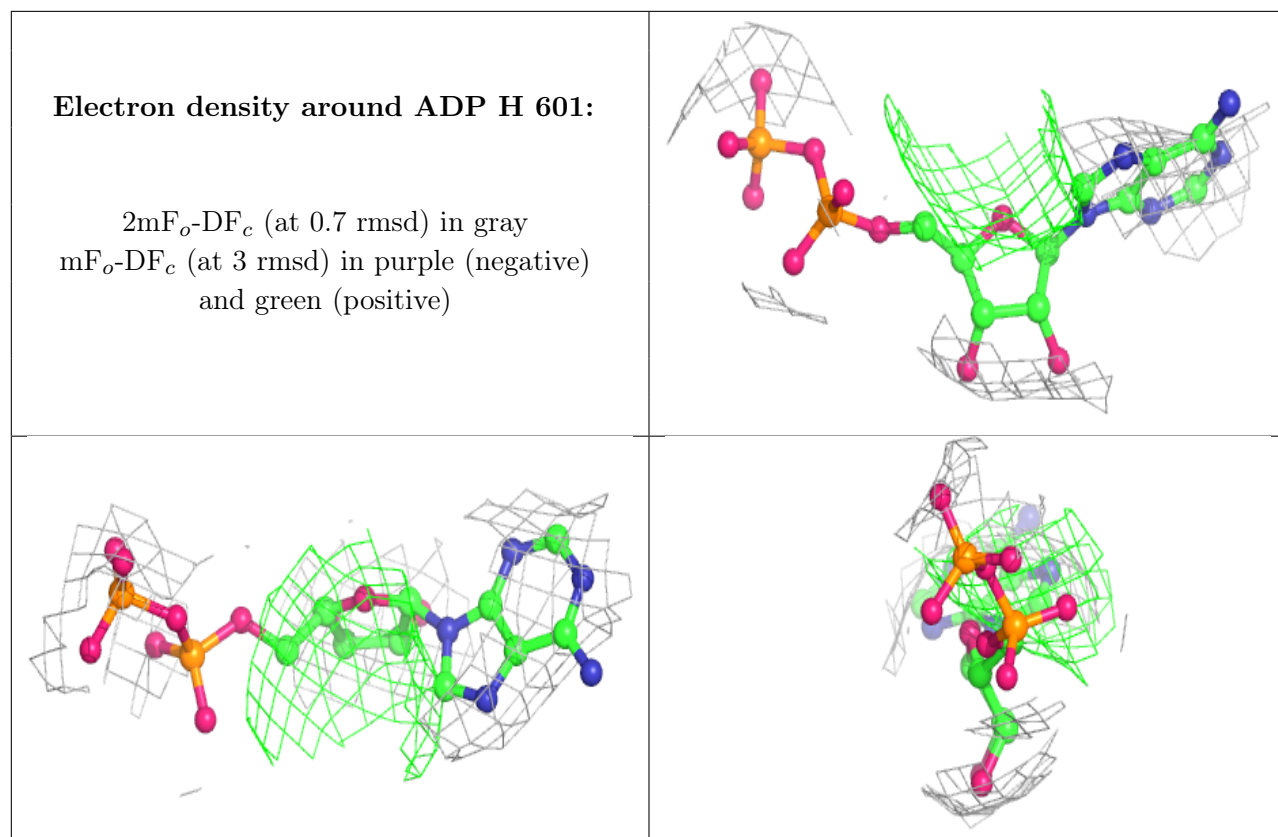
6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.