WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 07:50 PM EDT

PDB ID	:	3H06
Title	:	Crystal structure of the binding domain of the AMPA subunit GluR2 bound to the willardiine antagonist, UBP282
Authors	:	Ahmed, A.H.; Oswald, R.E.
Deposited on	:	2009-04-08
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

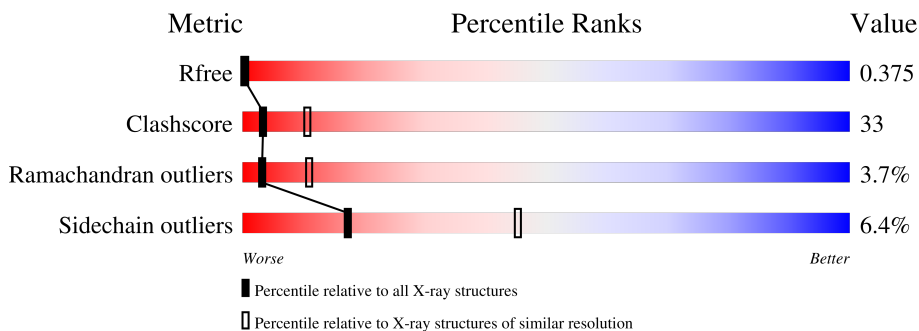|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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		0.375
Clashscore		33
Ramachandran outliers		3.7%
Sidechain outliers		6.4%

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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	B	258	53% 43% •
1	E	258	45% 48% 6%
1	G	258	57% 38% 5%
1	H	258	47% 45% 7%
1	J	258	51% 43% 5% •
1	L	258	48% 45% 6%
1	N	258	47% 45% 7%

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Mol	Chain	Length	Quality of chain
1	P	258	50% 43% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VBP	B	807	X	-	-	-
2	VBP	E	808	X	X	-	-
2	VBP	G	803	X	-	-	-
2	VBP	H	806	X	X	-	-
2	VBP	J	804	X	X	-	-
2	VBP	L	801	X	-	-	-
2	VBP	N	802	X	-	-	-
2	VBP	P	805	X	X	-	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 16564 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	B	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	E	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	H	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	J	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	L	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	N	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	P	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	118	GLY	-	LINKER	UNP P19491
G	119	THR	-	LINKER	UNP P19491
B	118	GLY	-	LINKER	UNP P19491
B	119	THR	-	LINKER	UNP P19491
E	118	GLY	-	LINKER	UNP P19491
E	119	THR	-	LINKER	UNP P19491
H	118	GLY	-	LINKER	UNP P19491
H	119	THR	-	LINKER	UNP P19491
J	118	GLY	-	LINKER	UNP P19491
J	119	THR	-	LINKER	UNP P19491
L	118	GLY	-	LINKER	UNP P19491
L	119	THR	-	LINKER	UNP P19491
N	118	GLY	-	LINKER	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
N	119	THR	-	LINKER	UNP P19491
P	118	GLY	-	LINKER	UNP P19491
P	119	THR	-	LINKER	UNP P19491

- Molecule 2 is 4-({3-[(2R)-2-amino-2-carboxyethyl]-2,6-dioxo-3,6-dihydropyrimidin-1(2H)-yl} methyl)benzoic acid (three-letter code: VBP) (formula: $C_{15}H_{15}N_3O_6$).
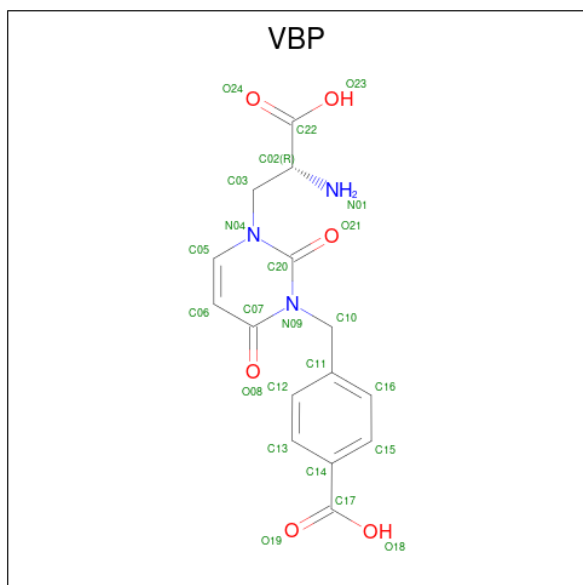
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			24	15	3	6		
2	B	1	Total	C	N	O	0	0
			24	15	3	6		
2	E	1	Total	C	N	O	0	0
			24	15	3	6		
2	H	1	Total	C	N	O	0	0
			24	15	3	6		
2	J	1	Total	C	N	O	0	0
			24	15	3	6		
2	L	1	Total	C	N	O	0	0
			24	15	3	6		
2	N	1	Total	C	N	O	0	0
			24	15	3	6		
2	P	1	Total	C	N	O	0	0
			24	15	3	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	39	Total 39	O 39	0	0
3	B	42	Total 42	O 42	0	0
3	E	30	Total 30	O 30	0	0
3	H	30	Total 30	O 30	0	0
3	J	43	Total 43	O 43	0	0
3	L	34	Total 34	O 34	0	0
3	N	39	Total 39	O 39	0	0
3	P	35	Total 35	O 35	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: Glutamate receptor 2

Chain G:

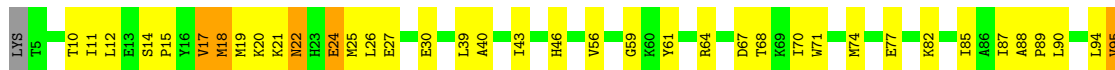

- Molecule 1: Glutamate receptor 2
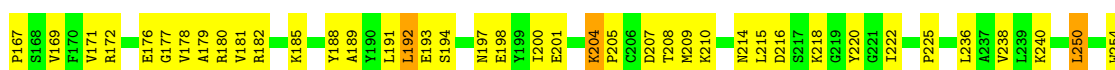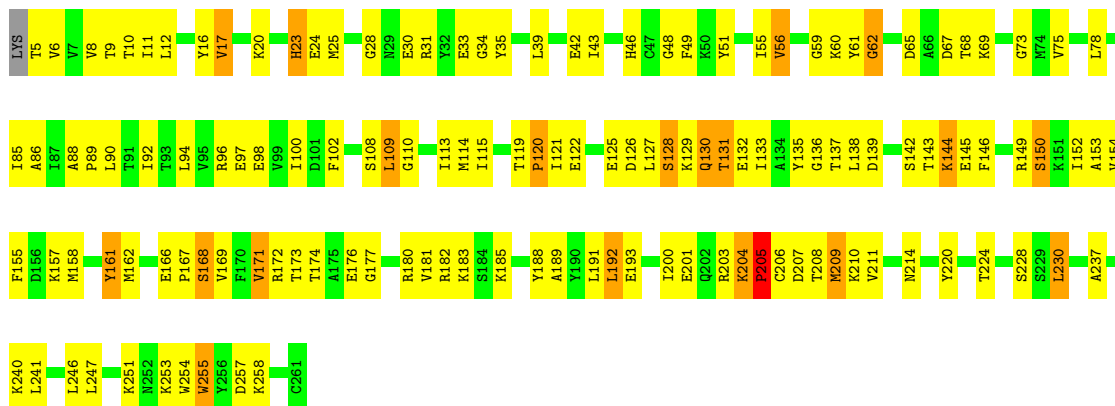
Chain B:

- Molecule 1: Glutamate receptor 2

Chain E:

M162 R163 S164 A165 E166 P167 S168 V169 F170 V171 R172 T173 E176 R180 V181 R182 K183 S184 K185 G186 K187 Y188 A189 Y190 L191 L192 E193 S194 T195 M196 N197 E198 Y199 R203 K204 P205 C206 D207 K210 N214 L215 D216 S217 K218 G219 Y220 G221 I222 A223 T224 P225 K226 G227 S228 S229

L230 A233 V234 A237 V238 L241 Q244 G245 L246 L247 L250 K251 W255 C261

• Molecule 1: Glutamate receptor 2

Chain H:

47%   45%   7%

LYS T5 T10 I11 L12 E13 S14 P15 Y16 V17 M18 M19 K20 K21 N22 H23 E24 M25 L26 E27 E30 L39 A40 I43 H46 V56 G59 K60 Y61 R64 D67 T68 K69 I70 W71 M74 E77 K82 I85 A86 I87 A88 P89 L90 L94 V95

R96 E97 E98 V99 I100 D101 F102 F106 M107 S108 L109 I115 K116 K117 G118 T119 P120 I121 F122 E125 D126 L127 Q130 T131 E132 I133 A134 Y135 G136 T137 L138 G141 S142 T143 K144 E145 F146 F147 R148 A153 V154 F155 D156 K157 T160 Y161 M162 R163 E166 P167 S168 V169

F170 V171 R172 T173 T174 A175 E176 R180 V181 R182 K183 S184 K185 G186 K187 Y188 A189 Y190 L191 L192 E193 S194 T195 M196 N197 E198 Y199 I200 E201 Q202 R203 K204 M209 K210 V211 N214 L215 I222 A223 T224 P225 K226 L230 V234 V238 L241 N242 E243 Q244 G245 L246

K249 L250 K251 N252 K253 Y256 D257 E260 C261

• Molecule 1: Glutamate receptor 2

Chain J:

51%   43%   5% •

LYS T5 V6 V7 V8 I11 L12 Y16 V17 K20 K21 E24 M25 L26 E27 R31 G34 Y35 H46 Y51 V56 G57 D58 G59 K60 Y61 G62 A63 R64 D65 T68 K69 I70 G73 M74 V75 G76 E77 L78 D84 A88 P89 L90 T93 L94 V95

R96 E97 E98 V99 I100 D101 F102 P105 L109 G110 I113 M114 I115 K116 K117 G118 T119 P120 I121 E122 E125 D126 L127 S128 K129 Q130 T131 E132 I133 A134 Y135 G136 T137 L138 T143 K144 E145 F146 F147 R148 R149 S150 K151 I152 A153 V154 F155 D156 K157 M158 W159 R163 E166

P167 S168 V169 F170 V171 R172 E176 G177 V178 A179 R180 V181 R182 K185 Y188 A189 Y190 L191 L192 E193 S194 N197 E198 Y199 I200 E201 K204 P205 C206 D207 T208 M209 K210 N214 L215 D216 S217 K218 G219 Y220 G221 I222 P225 L236 A237 V238 L239 K240 L250 W254

W255 C261

• Molecule 1: Glutamate receptor 2

Chain L:

48%   45%   6%

LYS T5 V8 T9 T10 I11 P15 Y16 V17 K20 K21 N22 H23 E24 M25 L26 E27 Q28 N29 E30 R31 Y35 C36 V37 H46 Y51 K52 L53 T54 J55 V56 G57 D58 G59 K60 Y61 G62 A63 R64 W71 V75 L78 V79 Y80 A83 D84 I85 A88 P89

L90 E97 I100 D101 F102 S103 K104 P105 L109 G110 I111 I115 K116 K117 G118 T119 P120 I121 E122 S123 A124 E125 D126 L127 S128 K129 Q130 T131 E132 I133 A134 Y135 G136 T137 G141 S142 T143 K144 E145 F147 R148 R149 S150 K151 I152 A153 V154 F155 D156 K157 M158 W159 T160 Y161

M162 R163 S164 A165 E166 P167 S168 V169 R172 T173 R180 K183 S184 K185 G186 K187 Y188 L191 L192 E193 S194 T195 M196 N197 E198 Y199 I200 R203 K204 P205 C206 D207 K210 V211 L215 D216 S217 K218 G219 Y220 Q231 V234 N235 L236 A237 V238 L239 K240 Q244 G245

L246 L247 D248 K251 N252 K253 W254 W255 Y256 D257 E260 C261

• Molecule 1: Glutamate receptor 2

Chain N:

47%   45%   7%

LYS T5 V6 V7 V8 T9 T10 I11 L12 Y16 V17 K20 H23 E24 M25 G28 N29 E30 R31 Y32 E33 G34 Y35 L39 E42 I43 H46 C47 G48 F49 K50 Y51 I55 V56 G59 K60 Y61 G62 D65 A66 D67 T68 K69 G73 M74 V75 L78

I85 A86 I87 A88 P89 L90 T91 I92 T93 L94 V95 R96 E97 E98 V99 I100 D101 F102 S108 L109 G110 I113 M114 I115 T119 P120 I121 E122 E125 D126 L127 S128 K129 Q130 T131 E132 I133 A134 Y135 G136 T137 L138 D139 S142 T143 K144 E145 F146 R149 S150 K151 I152 A153 V154

F155 D156 K157 M158 Y161 M162 E166 P167 S168 V169 F170 V171 R172 T173 T174 A175 E176 G177 R180 V181 R182 K183 S184 K185 Y188 A189 Y190 L191 L192 E193 I200 E201 Q202 R203 K204 P205 C206 D207 T208 M209 K210 V211 N214 Y220 T224 S228 S229 L230 A237

K240 L241 L246 L247 K251 N252 K253 W254 W255 Y256 D257 K258 C261

• Molecule 1: Glutamate receptor 2

Chain P:

50%   43%   6%

LYS T5 V6 V7 V8 I11 L12 Y16 V17 M18 M19 K20 E24 G28 N29 E30 R31 C36 V37 D38 L39 I43 H46 Y51 K52 L53 T54 I55 V56 G57 D58 G59 K60 Y61 G62 A63 R64 D65 T68 K69 N72 V75 V79 K82 I85

A88 P89 L90 L94 V95 R96 E97 E98 V99 I100 L109 I113 M114 I115 K116 T119 P120 I121 E125 D126 L127 S128 K129 Q130 T131 E132 I133 A134 Y135 G136 T137 L138 D139 S140 G141 S142 T143 K144 R149 S150 K151 I152 A153 V154 K157 M158 W159 T160 Y161 M162 A165 E166

P167 S168 V169 F170 V171 R172 T173 T174 A175 E176 G177 V178 A179 R180 V181 R182 K183 S184 K185 G186 K187 Y188 L191 L192 E193 S194 T195 M196 N197 E198 Y199 I200 E201 Q202 R203 K204 P205 C206 D207 T208 M209 K210 V211 D216 S217 G219 Y220 Q231 N232 K240 Q244 L247

L250 E260 C261

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	91.01Å 90.92Å 92.51Å 85.61° 85.52° 72.40°	Depositor
Resolution (Å)	39.71 – 2.80 39.71 – 2.78	Depositor EDS
% Data completeness (in resolution range)	93.5 (39.71-2.80) 90.8 (39.71-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	64.73 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.295 0.375 , 0.375	Depositor DCC
R_{free} test set	3259 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 16.7	EDS
L-test for twinning[2]	$< |L| > = 0.62, < L^2 > = 0.49$	Xtriage
Estimated twinning fraction	0.349 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	16564	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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: VBP

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	B	0.41	0/2046	0.64	0/2751
1	E	0.41	0/2046	0.63	0/2751
1	G	0.41	0/2046	0.65	0/2751
1	H	0.41	0/2046	0.61	0/2751
1	J	0.40	0/2046	0.62	0/2751
1	L	0.41	0/2046	0.62	0/2751
1	N	0.39	0/2046	0.62	0/2751
1	P	0.40	0/2046	0.64	0/2751
All	All	0.40	0/16368	0.63	0/22008

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	B	2010	0	2037	133	0
1	E	2010	0	2037	140	0
1	G	2010	0	2037	116	0
1	H	2010	0	2037	139	0
1	J	2010	0	2037	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2010	0	2037	137	0
1	N	2010	0	2037	129	0
1	P	2010	0	2037	155	0
2	B	24	0	13	3	0
2	E	24	0	13	4	0
2	G	24	0	13	5	0
2	H	24	0	13	3	0
2	J	24	0	13	4	0
2	L	24	0	13	2	0
2	N	24	0	13	3	0
2	P	24	0	13	5	0
3	B	42	0	0	8	0
3	E	30	0	0	6	0
3	G	39	0	0	4	0
3	H	30	0	0	6	0
3	J	43	0	0	9	0
3	L	34	0	0	1	0
3	N	39	0	0	7	0
3	P	35	0	0	10	0
All	All	16564	0	16400	1065	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 33.

The worst 5 of 1065 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:E:204:LYS:HB3	1:E:205:PRO:HD2	1.12	1.11
1:L:204:LYS:HB3	1:L:205:PRO:HD2	1.09	1.09
1:P:204:LYS:HB3	1:P:205:PRO:HD2	1.31	1.09
1:H:173:THR:HG23	1:H:176:GLU:HB2	1.36	1.07
1:G:204:LYS:HB3	1:G:205:PRO:HD2	1.11	1.06

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	B	255/258 (99%)	227 (89%)	23 (9%)	5 (2%)	7	24
1	E	255/258 (99%)	222 (87%)	20 (8%)	13 (5%)	2	6
1	G	255/258 (99%)	223 (88%)	27 (11%)	5 (2%)	7	24
1	H	255/258 (99%)	211 (83%)	35 (14%)	9 (4%)	3	12
1	J	255/258 (99%)	228 (89%)	19 (8%)	8 (3%)	4	14
1	L	255/258 (99%)	212 (83%)	32 (12%)	11 (4%)	2	8
1	N	255/258 (99%)	220 (86%)	23 (9%)	12 (5%)	2	7
1	P	255/258 (99%)	206 (81%)	37 (14%)	12 (5%)	2	7
All	All	2040/2064 (99%)	1749 (86%)	216 (11%)	75 (4%)	3	11

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	205	PRO
1	G	206	CYS
1	B	163	ARG
1	E	14	SER
1	E	185	LYS

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	B	216/217 (100%)	206 (95%)	10 (5%)	27	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	216/217 (100%)	207 (96%)	9 (4%)	30	63
1	G	216/217 (100%)	201 (93%)	15 (7%)	15	41
1	H	216/217 (100%)	199 (92%)	17 (8%)	12	34
1	J	216/217 (100%)	203 (94%)	13 (6%)	19	48
1	L	216/217 (100%)	200 (93%)	16 (7%)	13	37
1	N	216/217 (100%)	198 (92%)	18 (8%)	11	32
1	P	216/217 (100%)	204 (94%)	12 (6%)	21	51
All	All	1728/1736 (100%)	1618 (94%)	110 (6%)	17	45

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	125	GLU
1	L	144	LYS
1	P	232	ASN
1	P	18	MET
1	J	148	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	244	GLN
1	L	197	ASN
1	P	130	GLN
1	L	130	GLN
1	L	252	ASN

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	VBP	H	806	-	24,25,25	6.53	19 (79%)	28,35,35	2.57	10 (35%)
2	VBP	L	801	-	24,25,25	6.69	19 (79%)	28,35,35	2.51	8 (28%)
2	VBP	B	807	-	24,25,25	6.68	19 (79%)	28,35,35	2.41	8 (28%)
2	VBP	G	803	-	24,25,25	6.73	19 (79%)	28,35,35	2.49	8 (28%)
2	VBP	J	804	-	24,25,25	6.69	19 (79%)	28,35,35	2.39	8 (28%)
2	VBP	E	808	-	24,25,25	6.81	19 (79%)	28,35,35	2.58	8 (28%)
2	VBP	N	802	-	24,25,25	6.52	19 (79%)	28,35,35	2.29	8 (28%)
2	VBP	P	805	-	24,25,25	6.85	20 (83%)	28,35,35	2.38	8 (28%)

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	VBP	H	806	-	1/1/3/3	4/16/16/16	0/2/2/2
2	VBP	L	801	-	1/1/3/3	4/16/16/16	0/2/2/2
2	VBP	B	807	-	1/1/3/3	4/16/16/16	0/2/2/2
2	VBP	G	803	-	1/1/3/3	4/16/16/16	0/2/2/2
2	VBP	J	804	-	1/1/3/3	6/16/16/16	0/2/2/2
2	VBP	E	808	-	1/1/3/3	5/16/16/16	0/2/2/2
2	VBP	N	802	-	1/1/3/3	4/16/16/16	0/2/2/2
2	VBP	P	805	-	1/1/3/3	4/16/16/16	0/2/2/2

The worst 5 of 153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	805	VBP	C16-C15	11.12	1.56	1.38
2	P	805	VBP	C15-C14	10.96	1.56	1.39
2	E	808	VBP	C15-C14	10.88	1.55	1.39
2	G	803	VBP	C15-C14	10.56	1.55	1.39
2	H	806	VBP	C15-C14	10.51	1.55	1.39

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	808	VBP	O23-C22-O24	-6.38	109.61	124.08
2	H	806	VBP	O23-C22-O24	-6.32	109.73	124.08
2	J	804	VBP	O23-C22-O24	-6.25	109.90	124.08
2	G	803	VBP	O23-C22-O24	-6.22	109.97	124.08
2	B	807	VBP	O23-C22-O24	-6.19	110.04	124.08

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	803	VBP	C02
2	B	807	VBP	C02
2	E	808	VBP	C02
2	H	806	VBP	C02
2	J	804	VBP	C02

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	803	VBP	C13-C14-C17-O18
2	G	803	VBP	C15-C14-C17-O19
2	G	803	VBP	C15-C14-C17-O18
2	G	803	VBP	C13-C14-C17-O19
2	E	808	VBP	C13-C14-C17-O19

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	806	VBP	3	0
2	L	801	VBP	2	0
2	B	807	VBP	3	0
2	G	803	VBP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	804	VBP	4	0
2	E	808	VBP	4	0
2	N	802	VBP	3	0
2	P	805	VBP	5	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 VBP H 806

Bond lengths

Bond angles

Torsions

Rings

Ligand VBP L 801

Bond lengths

Bond angles

Torsions

Rings

Ligand VBP B 807

Bond lengths

Bond angles

Torsions

Rings

Ligand VBP G 803

Bond lengths

Bond angles

Torsions

Rings

Ligand VBP J 804

Bond lengths

Bond angles

Torsions

Rings

Ligand VBP E 808

Bond lengths

Bond angles

Torsions

Rings

Ligand VBP N 802

Bond lengths

Bond angles

Torsions

Rings

Ligand VBP P 805

Bond lengths

Bond angles

Torsions

Rings

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 ⓘ

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.
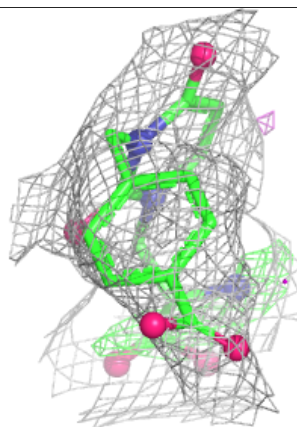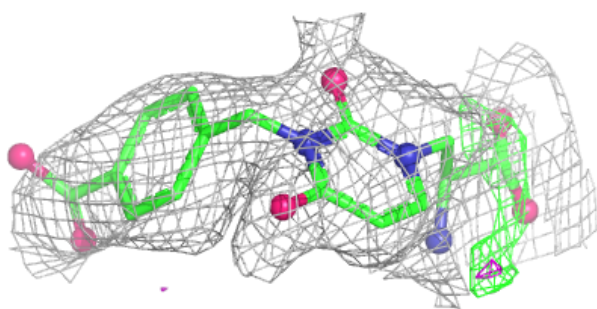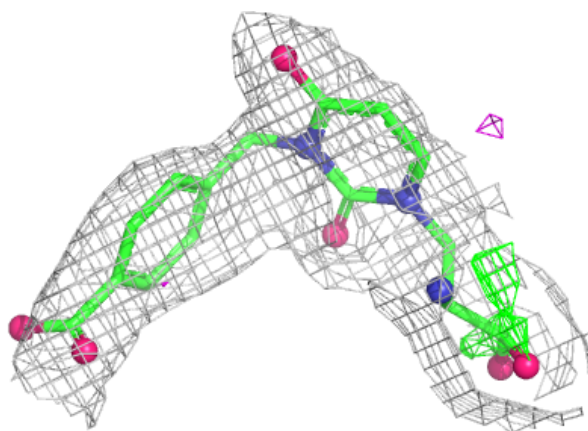

Electron density around VBP G 803:

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

Electron density around VBP B 807:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
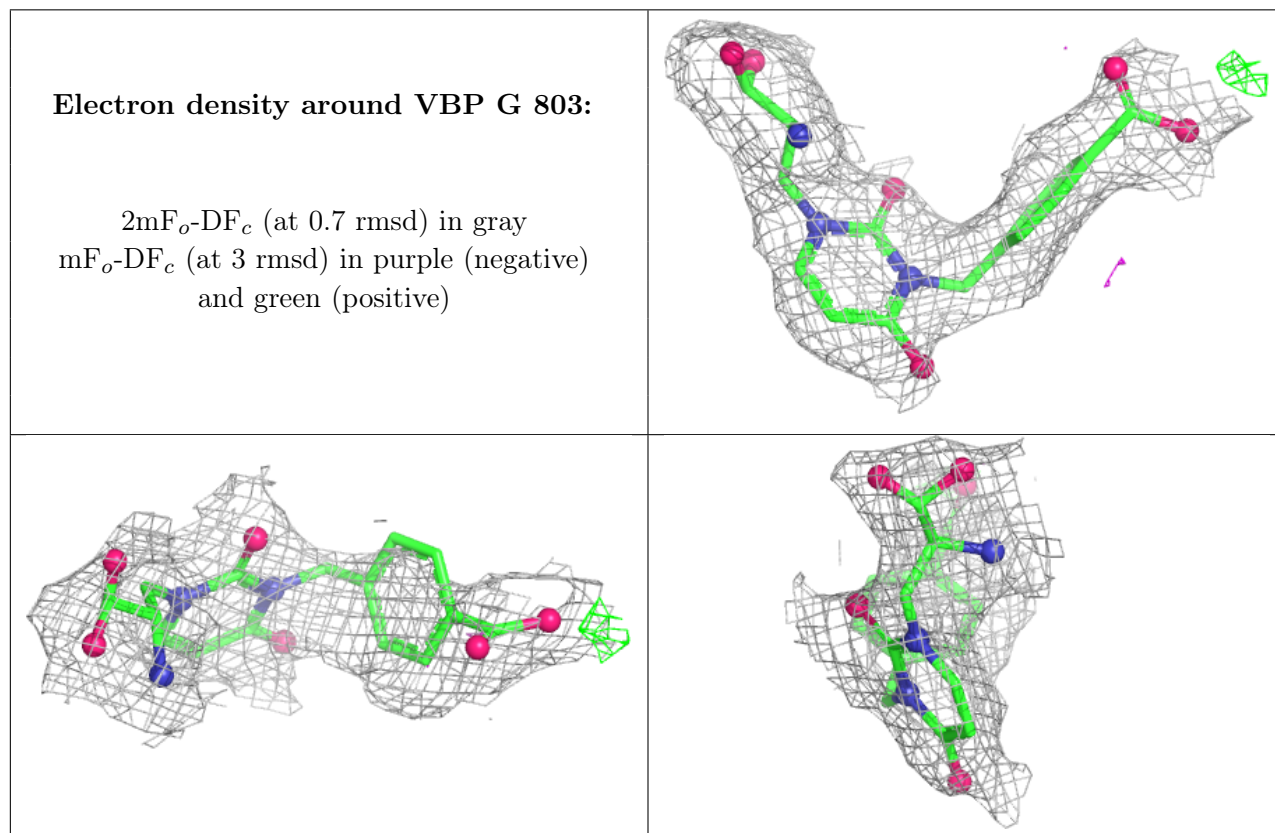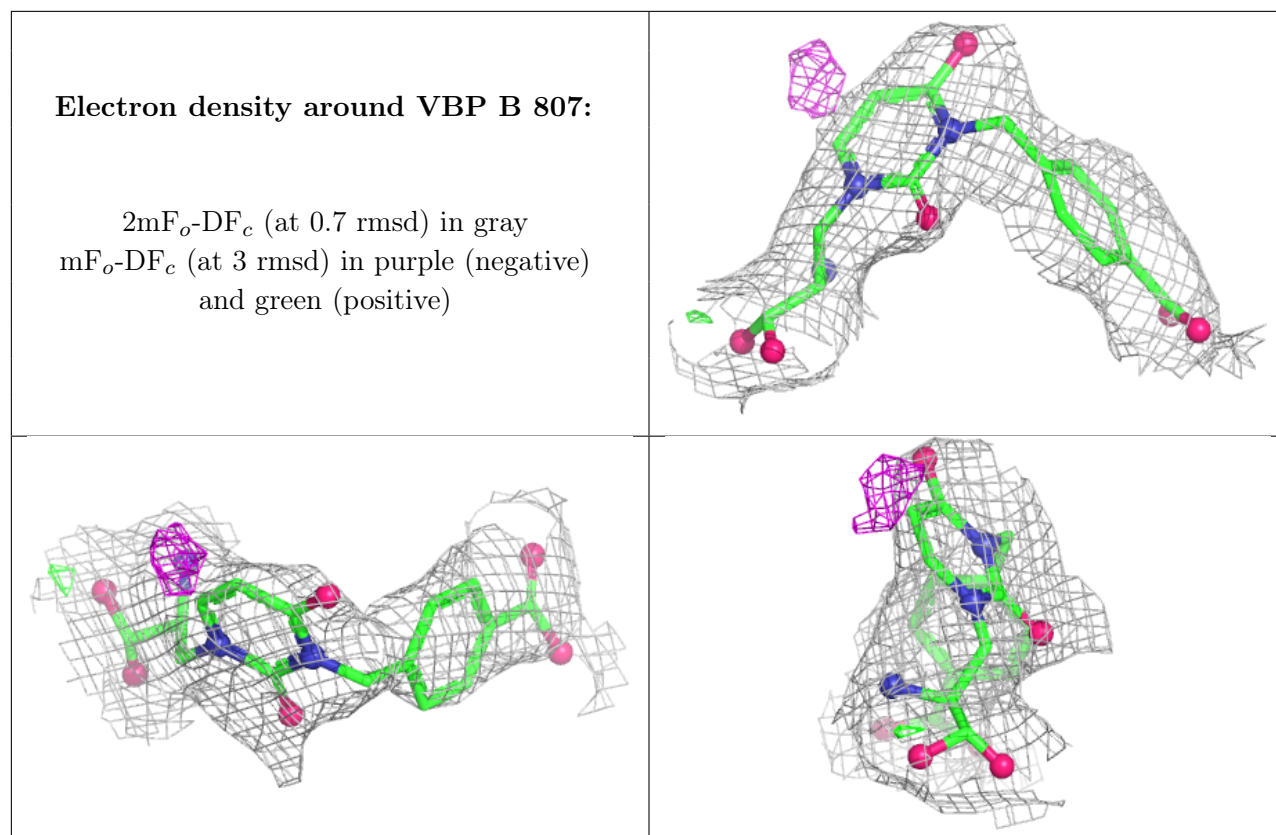
Electron density around VBP E 808:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
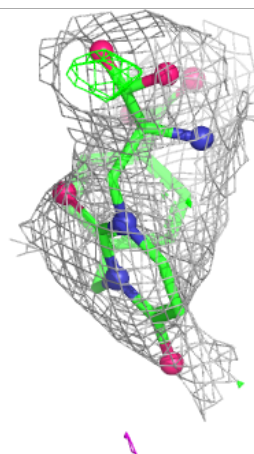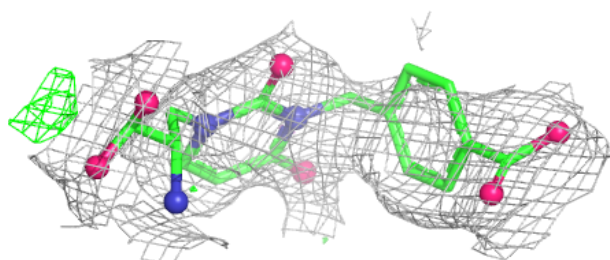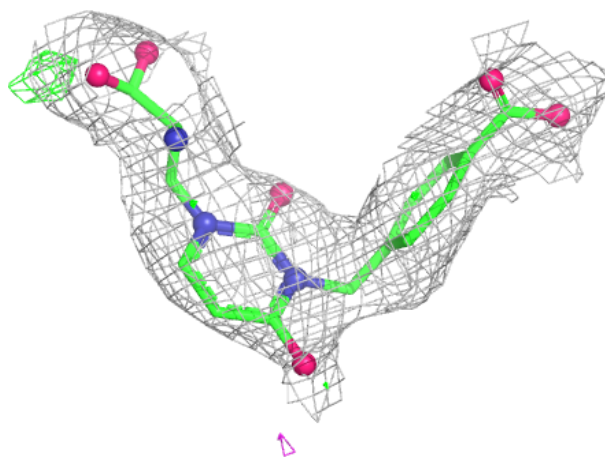
Electron density around VBP H 806:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
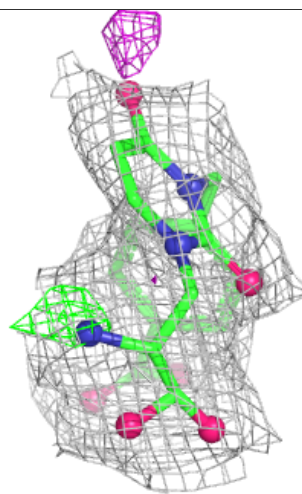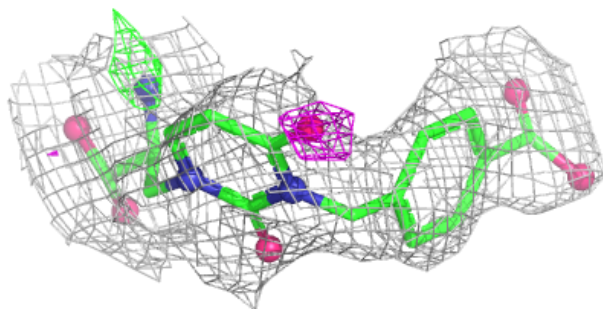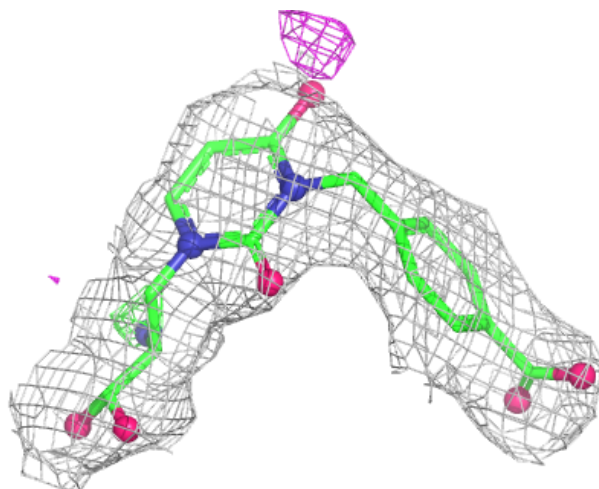
Electron density around VBP J 804:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
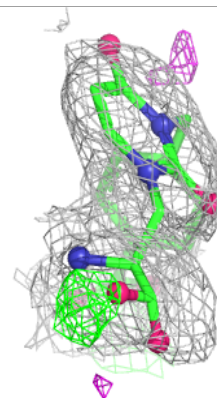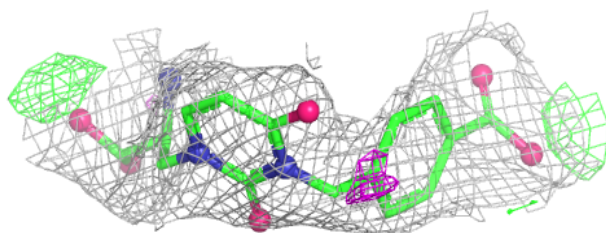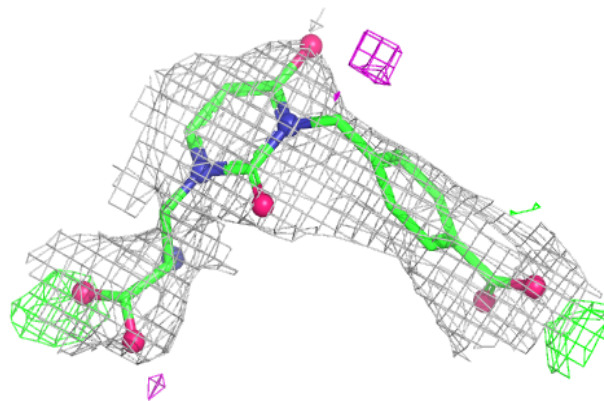
Electron density around VBP L 801:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
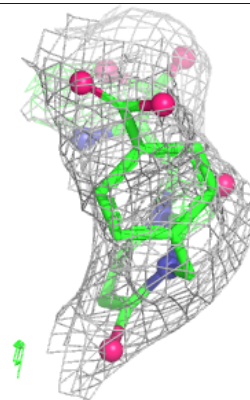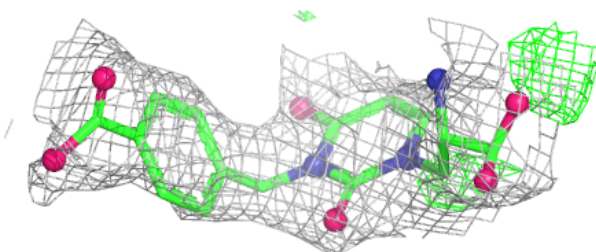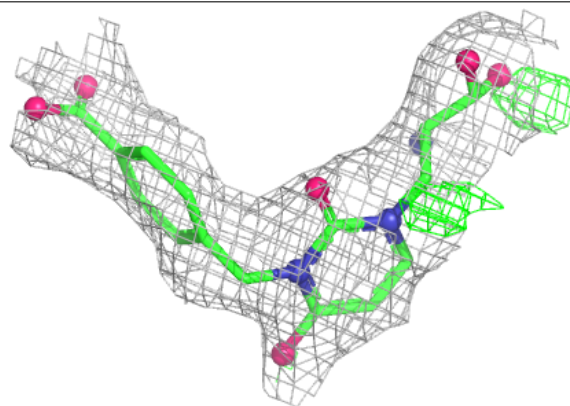
Electron density around VBP N 802:

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

Electron density around VBP P 805:

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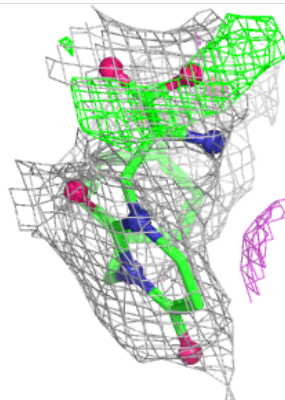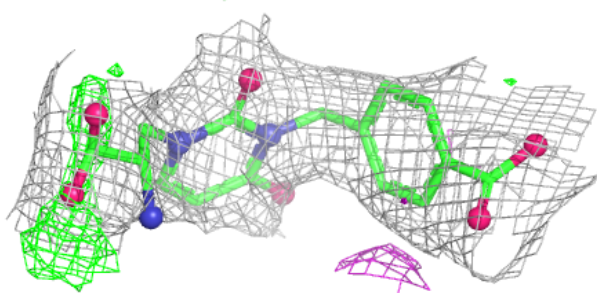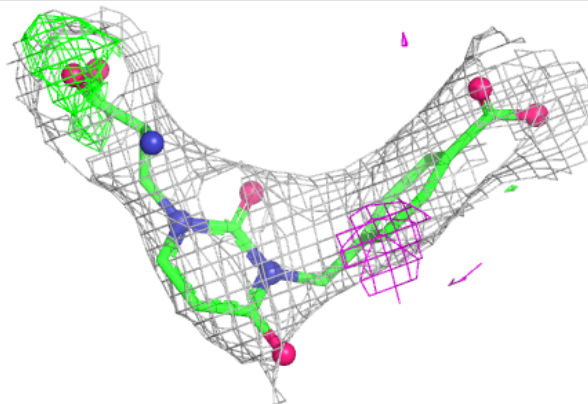
6.5 Other polymers (i)

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