



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:22 AM UTC

PDB ID : 8F22 / pdb_00008f22
Title : HIV-CA Disulfide linked Hexamer bound to 11l capsid inhibitor.
Authors : Barnett, M.J.; Goldstone, D.C.
Deposited on : 2022-11-06
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

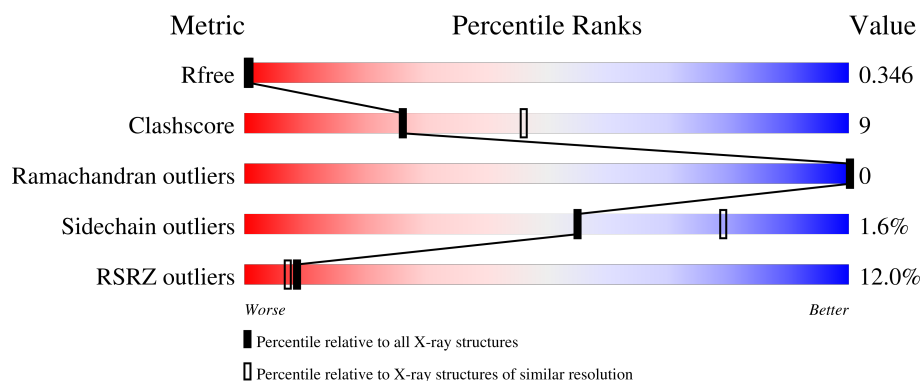
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	224	4% 73% 18% 8%
1	B	224	3% 75% 14% 11%
1	C	224	6% 74% 15% 10%
1	D	224	4% 78% 14% 8%
1	E	224	0% 73% 16% 11%

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Mol	Chain	Length	Quality of chain
1	F	224	
1	G	224	
1	H	224	
1	I	224	
1	J	224	
1	K	224	
1	L	224	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17342 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 Capsid protein p24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1589	1002	275	298	14			
1	B	200	Total	C	N	O	S	0	0	0
			1545	975	269	288	13			
1	C	201	Total	C	N	O	S	0	0	0
			1550	976	269	292	13			
1	D	205	Total	C	N	O	S	0	0	0
			1568	988	268	298	14			
1	E	199	Total	C	N	O	S	0	0	0
			1542	974	263	291	14			
1	F	203	Total	C	N	O	S	0	0	0
			1577	995	275	293	14			
1	G	168	Total	C	N	O	S	0	0	0
			1252	788	213	240	11			
1	H	177	Total	C	N	O	S	0	2	0
			1338	851	222	254	11			
1	I	169	Total	C	N	O	S	0	0	0
			1245	788	207	240	10			
1	J	171	Total	C	N	O	S	0	0	0
			1307	827	220	249	11			
1	K	171	Total	C	N	O	S	0	0	0
			1306	825	220	251	10			
1	L	164	Total	C	N	O	S	0	0	0
			1259	799	210	238	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	ALA	engineered mutation	UNP P12497
A	45	CYS	GLU	engineered mutation	UNP P12497
A	184	ALA	TRP	engineered mutation	UNP P12497
A	185	ALA	MET	engineered mutation	UNP P12497
B	14	CYS	ALA	engineered mutation	UNP P12497

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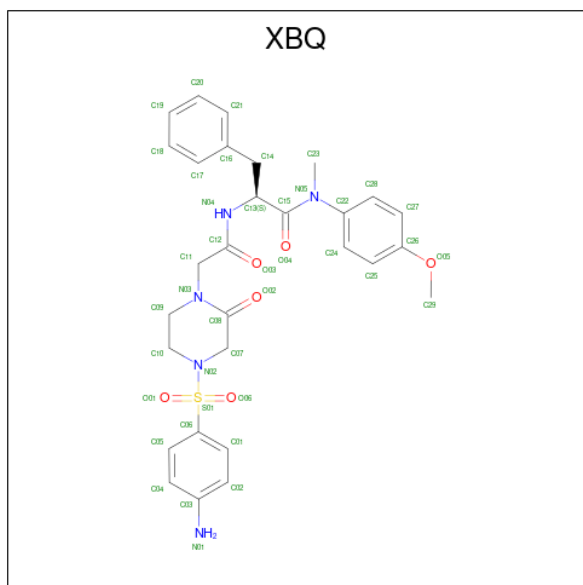
Chain	Residue	Modelled	Actual	Comment	Reference
B	45	CYS	GLU	engineered mutation	UNP P12497
B	184	ALA	TRP	engineered mutation	UNP P12497
B	185	ALA	MET	engineered mutation	UNP P12497
C	14	CYS	ALA	engineered mutation	UNP P12497
C	45	CYS	GLU	engineered mutation	UNP P12497
C	184	ALA	TRP	engineered mutation	UNP P12497
C	185	ALA	MET	engineered mutation	UNP P12497
D	14	CYS	ALA	engineered mutation	UNP P12497
D	45	CYS	GLU	engineered mutation	UNP P12497
D	184	ALA	TRP	engineered mutation	UNP P12497
D	185	ALA	MET	engineered mutation	UNP P12497
E	14	CYS	ALA	engineered mutation	UNP P12497
E	45	CYS	GLU	engineered mutation	UNP P12497
E	184	ALA	TRP	engineered mutation	UNP P12497
E	185	ALA	MET	engineered mutation	UNP P12497
F	14	CYS	ALA	engineered mutation	UNP P12497
F	45	CYS	GLU	engineered mutation	UNP P12497
F	184	ALA	TRP	engineered mutation	UNP P12497
F	185	ALA	MET	engineered mutation	UNP P12497
G	14	CYS	ALA	engineered mutation	UNP P12497
G	45	CYS	GLU	engineered mutation	UNP P12497
G	184	ALA	TRP	engineered mutation	UNP P12497
G	185	ALA	MET	engineered mutation	UNP P12497
H	14	CYS	ALA	engineered mutation	UNP P12497
H	45	CYS	GLU	engineered mutation	UNP P12497
H	184	ALA	TRP	engineered mutation	UNP P12497
H	185	ALA	MET	engineered mutation	UNP P12497
I	14	CYS	ALA	engineered mutation	UNP P12497
I	45	CYS	GLU	engineered mutation	UNP P12497
I	184	ALA	TRP	engineered mutation	UNP P12497
I	185	ALA	MET	engineered mutation	UNP P12497
J	14	CYS	ALA	engineered mutation	UNP P12497
J	45	CYS	GLU	engineered mutation	UNP P12497
J	184	ALA	TRP	engineered mutation	UNP P12497
J	185	ALA	MET	engineered mutation	UNP P12497
K	14	CYS	ALA	engineered mutation	UNP P12497
K	45	CYS	GLU	engineered mutation	UNP P12497
K	184	ALA	TRP	engineered mutation	UNP P12497
K	185	ALA	MET	engineered mutation	UNP P12497
L	14	CYS	ALA	engineered mutation	UNP P12497
L	45	CYS	GLU	engineered mutation	UNP P12497
L	184	ALA	TRP	engineered mutation	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
L	185	ALA	MET	engineered mutation	UNP P12497

- Molecule 2 is Nalpha-{[4-(4-aminobenzene-1-sulfonyl)-2-oxopiperazin-1-yl]acetyl}-N-(4-methoxyphenyl)-N-methyl-L-phenylalaninamide (CCD ID: XBQ) (formula: C₂₉H₃₃N₅O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			41	29	5	6	1		
2	B	1	Total	C	N	O	S	0	0
			41	29	5	6	1		
2	C	1	Total	C	N	O	S	0	0
			41	29	5	6	1		
2	D	1	Total	C	N	O	S	0	0
			41	29	5	6	1		
2	E	1	Total	C	N	O	S	0	0
			41	29	5	6	1		
2	F	1	Total	C	N	O	S	0	0
			41	29	5	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	3	Total	O	0	0
			3	3		

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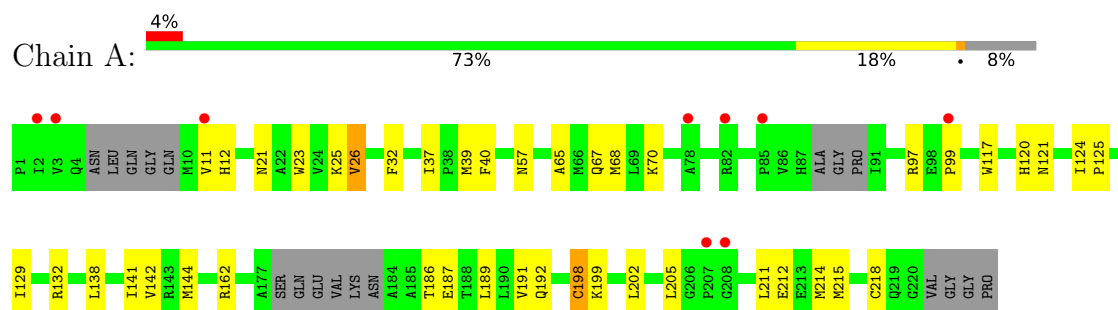
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	5	Total 5	O 5	0	0
3	D	4	Total 4	O 4	0	0
3	E	2	Total 2	O 2	0	0
3	F	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0

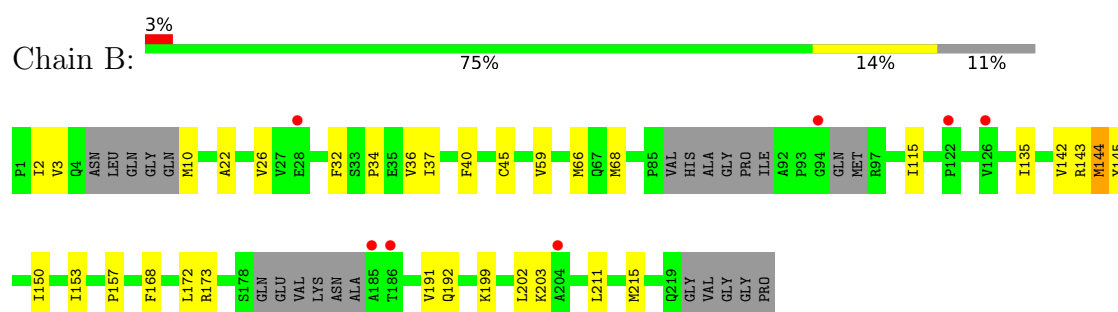
3 Residue-property plots [i](#)

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.

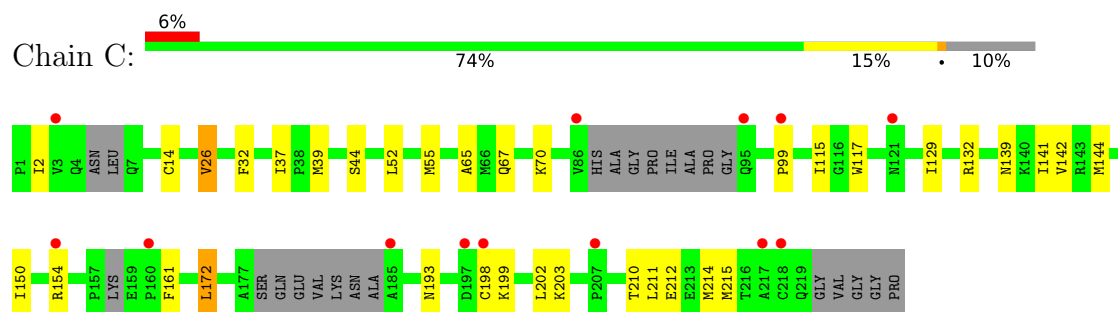
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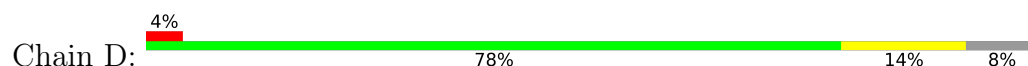
• Molecule 1: Capsid protein p24

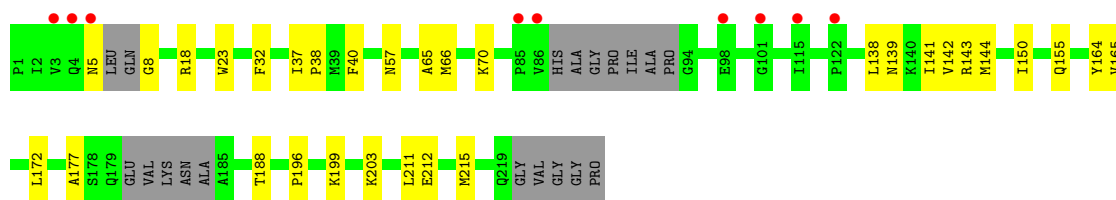


• Molecule 1: Capsid protein p24

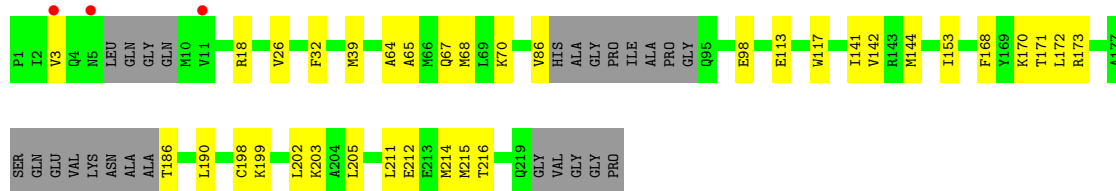
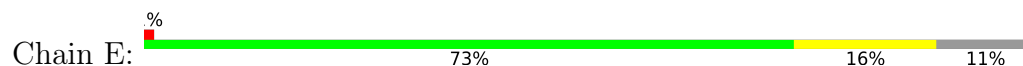


• Molecule 1: Capsid protein p24

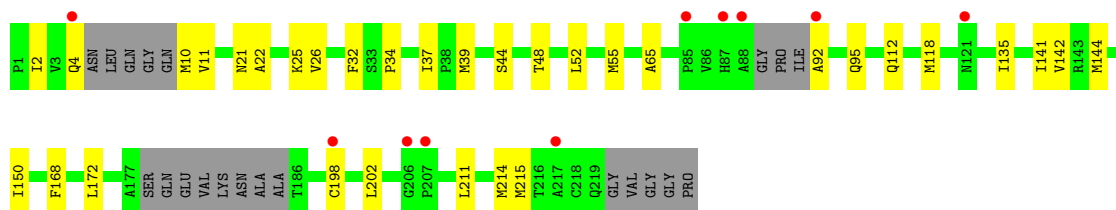
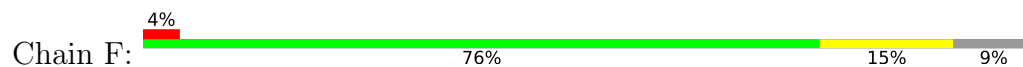




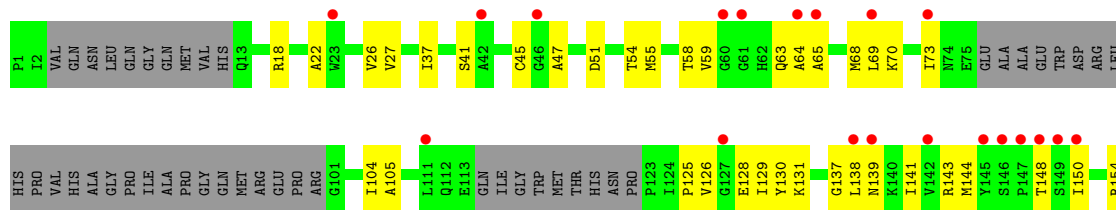
• Molecule 1: Capsid protein p24



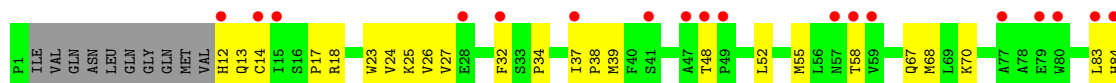
• Molecule 1: Capsid protein p24

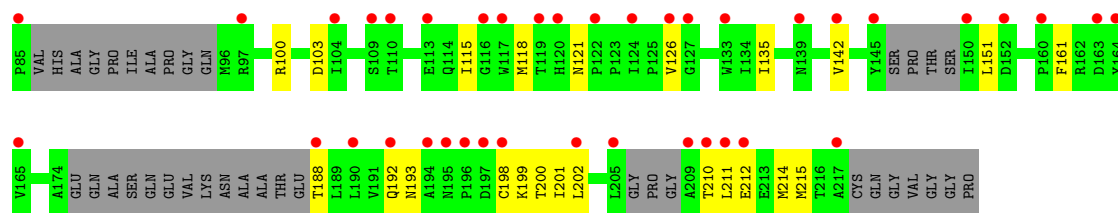


• Molecule 1: Capsid protein p24

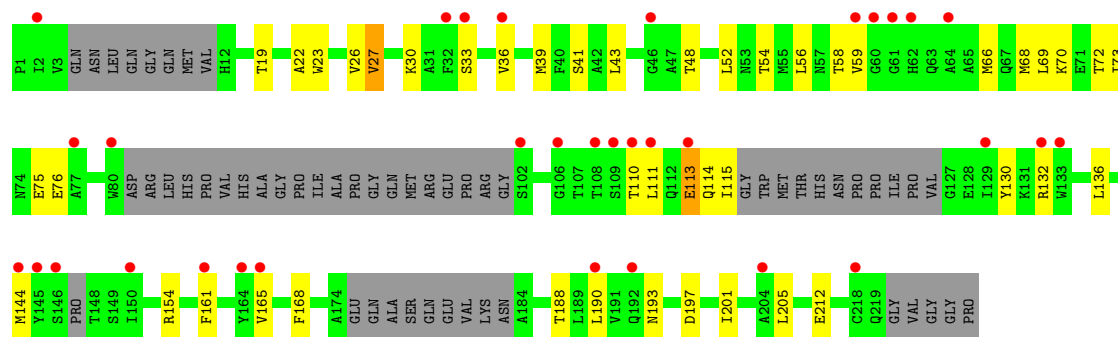


• Molecule 1: Capsid protein p24

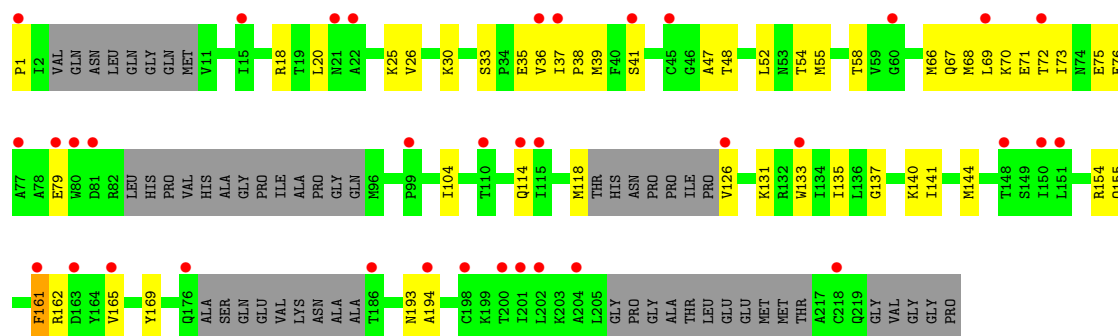




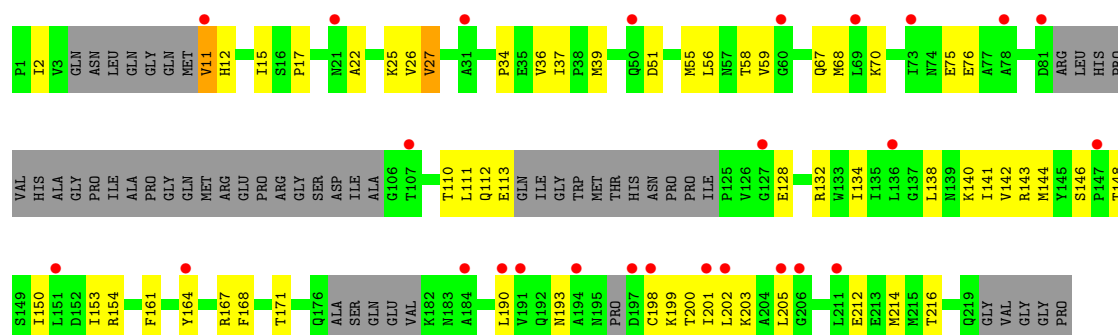
● Molecule 1: Capsid protein p24



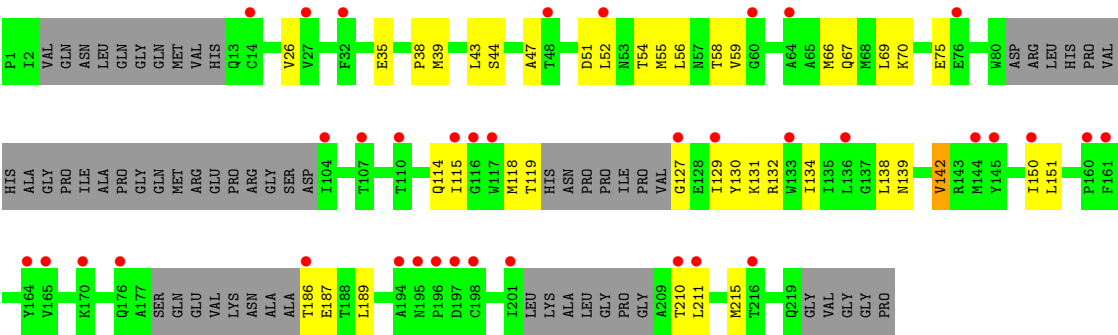
● Molecule 1: Capsid protein p24



● Molecule 1: Capsid protein p24



● Molecule 1: Capsid protein p24



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.95Å 91.19Å 116.27Å 87.17° 78.77° 60.37°	Depositor
Resolution (Å)	15.89 – 2.50 15.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.89-2.50) 96.6 (15.89-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.310 , 0.347 0.310 , 0.346	Depositor DCC
R_{free} test set	5353 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	17342	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.70% 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: XBQ

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	0.21	0/1622	0.51	0/2203
1	B	0.24	0/1576	0.48	1/2139 (0.0%)
1	C	0.21	0/1580	0.47	0/2144
1	D	0.20	0/1599	0.50	0/2172
1	E	0.20	0/1573	0.47	0/2137
1	F	0.19	0/1610	0.47	0/2186
1	G	0.17	0/1272	0.35	0/1727
1	H	0.29	0/1365	0.63	0/1858
1	I	0.12	0/1264	0.33	0/1718
1	J	0.14	0/1329	0.33	0/1801
1	K	0.14	0/1326	0.33	0/1796
1	L	0.15	0/1279	0.31	0/1734
All	All	0.20	0/17395	0.45	1/23615 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	MET	CB-CG-SD	5.21	128.34	112.70

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	1589	0	1573	28	0
1	B	1545	0	1539	25	0
1	C	1550	0	1524	25	0
1	D	1568	0	1538	26	0
1	E	1542	0	1527	25	0
1	F	1577	0	1573	29	0
1	G	1252	0	1215	41	0
1	H	1338	0	1273	34	0
1	I	1245	0	1183	26	0
1	J	1307	0	1262	32	0
1	K	1306	0	1284	36	0
1	L	1259	0	1235	23	0
2	A	41	0	0	1	0
2	B	41	0	0	0	0
2	C	41	0	0	1	0
2	D	41	0	0	1	0
2	E	41	0	0	0	0
2	F	41	0	0	1	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	17342	0	16726	320	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 9.

All (320) 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:B:37:ILE:HD11	1:B:142:VAL:HG21	1.51	0.93
1:F:37:ILE:HD11	1:F:142:VAL:HG21	1.54	0.89
1:A:212:GLU:HB2	1:B:68:MET:HE3	1.54	0.88
1:A:202:LEU:HD22	1:A:214:MET:HG2	1.56	0.86
1:C:212:GLU:HG3	1:D:144:MET:HE1	1.63	0.80
1:G:27:VAL:HG11	1:G:59:VAL:HG22	1.67	0.77
1:K:110:THR:HG22	1:K:113:GLU:HG2	1.67	0.75
1:G:18:ARG:HD3	1:H:17:PRO:HB2	1.70	0.73
1:G:104:ILE:HG21	1:G:129:ILE:HG23	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:154:ARG:HA	1:J:193:ASN:HB3	1.70	0.73
1:G:150:ILE:HG12	1:G:186:THR:HG21	1.70	0.73
1:F:92:ALA:HB1	1:F:95:GLN:HB2	1.70	0.72
1:L:186:THR:OG1	1:L:187:GLU:N	2.22	0.71
1:H:192:GLN:HA	1:H:199:LYS:HE3	1.70	0.71
1:E:68:MET:HE1	1:E:144:MET:SD	2.30	0.71
1:H:212:GLU:HB2	1:I:68:MET:HE3	1.73	0.71
1:G:68:MET:HG3	1:L:211:LEU:HD23	1.72	0.71
1:D:150:ILE:HD12	1:D:172:LEU:HD13	1.71	0.70
1:F:52:LEU:HA	1:F:55:MET:HE2	1.75	0.69
1:D:212:GLU:HB2	1:E:68:MET:HE3	1.75	0.69
1:C:210:THR:O	1:C:214:MET:HG3	1.91	0.69
1:G:139:ASN:O	1:G:143:ARG:HG3	1.92	0.69
1:C:26:VAL:HG21	1:C:39:MET:HG2	1.75	0.69
1:L:26:VAL:HG21	1:L:39:MET:HG2	1.73	0.68
1:L:150:ILE:HD12	1:L:150:ILE:H	1.58	0.68
1:F:44:SER:HB3	1:F:55:MET:HE1	1.75	0.67
1:G:63:GLN:H	1:G:63:GLN:CD	2.03	0.67
1:F:4:GLN:HG3	1:F:10:MET:HE1	1.76	0.67
1:A:68:MET:HE1	1:A:144:MET:HE1	1.78	0.66
1:H:37:ILE:HD11	1:H:142:VAL:HG21	1.77	0.66
1:L:130:TYR:O	1:L:134:ILE:HG13	1.97	0.65
1:A:26:VAL:HG21	1:A:39:MET:HG2	1.79	0.63
1:I:56:LEU:HD22	1:I:66:MET:HE1	1.80	0.63
1:C:211:LEU:HG	1:C:215:MET:HE2	1.81	0.63
1:E:202:LEU:HD22	1:E:214:MET:HG2	1.79	0.63
1:I:132:ARG:O	1:I:136:LEU:HG	1.99	0.62
1:B:144:MET:HE3	1:B:145:TYR:HE1	1.63	0.62
1:G:47:ALA:HB1	1:G:51:ASP:HB2	1.80	0.62
1:K:56:LEU:HD11	1:K:134:ILE:HD13	1.81	0.62
1:I:110:THR:HG22	1:I:113:GLU:HB2	1.81	0.62
1:D:5:ASN:OD1	1:D:8:GLY:N	2.33	0.62
1:D:165:VAL:HG11	1:D:215:MET:HE2	1.81	0.62
1:L:129:ILE:HA	1:L:132:ARG:HD2	1.82	0.61
1:E:212:GLU:HG3	1:F:144:MET:HE1	1.81	0.61
1:F:65:ALA:HB1	1:F:141:ILE:HD13	1.82	0.61
1:L:118:MET:HE1	1:L:127:GLY:HA3	1.82	0.61
1:D:143:ARG:NE	1:D:177:ALA:O	2.32	0.60
1:B:59:VAL:HG11	1:B:66:MET:HE3	1.82	0.60
1:H:12:HIS:HB2	1:H:115:ILE:HD11	1.82	0.60
1:J:161:PHE:O	1:J:165:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:76:GLU:HG2	1:J:133:TRP:CD1	2.37	0.60
1:H:48:THR:O	1:H:52:LEU:HD12	2.00	0.60
1:J:162:ARG:HH21	1:K:144:MET:HE3	1.65	0.60
1:I:22:ALA:O	1:I:26:VAL:HG13	2.02	0.59
1:H:151:LEU:HA	1:H:193:ASN:HD21	1.67	0.59
1:F:202:LEU:HD22	1:F:214:MET:HG2	1.84	0.59
1:G:45:CYS:HB3	1:H:14:CYS:SG	2.43	0.59
1:A:192:GLN:O	1:A:199:LYS:NZ	2.36	0.59
1:A:212:GLU:CB	1:B:68:MET:HE3	2.30	0.58
1:A:11:VAL:HB	1:F:4:GLN:NE2	2.17	0.58
1:C:161:PHE:CD2	1:C:215:MET:HG2	2.39	0.58
1:I:33:SER:O	1:I:36:VAL:HG22	2.04	0.58
1:J:48:THR:HA	1:J:118:MET:HE1	1.86	0.58
1:I:76:GLU:HG3	1:I:136:LEU:HD12	1.86	0.58
1:B:153:ILE:HG21	1:B:168:PHE:HA	1.86	0.57
1:D:65:ALA:HB1	1:D:141:ILE:HD13	1.86	0.57
1:J:68:MET:O	1:J:72:THR:HG23	2.04	0.57
1:H:198:CYS:O	1:H:201:ILE:HG22	2.04	0.57
1:L:66:MET:O	1:L:70:LYS:HG2	2.04	0.57
1:B:37:ILE:HG23	1:B:135:ILE:HD12	1.85	0.57
1:H:118:MET:HG3	1:H:126:VAL:HG22	1.87	0.57
1:G:65:ALA:HB1	1:G:141:ILE:HD13	1.86	0.57
1:F:21:ASN:HD21	1:F:25:LYS:HE2	1.70	0.56
1:B:2:ILE:HD11	1:B:115:ILE:HG12	1.86	0.56
1:G:18:ARG:NE	1:H:18:ARG:HG2	2.20	0.56
1:G:186:THR:HG23	1:G:189:LEU:HD12	1.87	0.56
1:I:23:TRP:O	1:I:27:VAL:HG22	2.05	0.56
1:F:21:ASN:O	1:F:25:LYS:HG2	2.05	0.56
1:J:33:SER:O	1:J:36:VAL:HG12	2.06	0.56
1:J:114:GLN:O	1:J:118:MET:HG3	2.06	0.56
1:C:2:ILE:HD11	1:C:115:ILE:HG12	1.89	0.55
1:A:67:GLN:HA	1:A:70:LYS:HD2	1.88	0.55
1:G:137:GLY:O	1:G:141:ILE:HG13	2.06	0.55
1:I:39:MET:HE1	1:J:20:LEU:HD13	1.88	0.55
1:H:67:GLN:NE2	1:H:70:LYS:HB2	2.22	0.55
1:F:32:PHE:O	1:F:142:VAL:HG22	2.06	0.55
1:G:18:ARG:HE	1:H:18:ARG:HG2	1.73	0.54
1:G:69:LEU:O	1:G:73:ILE:HG23	2.08	0.54
1:H:211:LEU:O	1:H:215:MET:HG3	2.07	0.54
1:C:52:LEU:HA	1:C:55:MET:HE2	1.90	0.54
1:G:22:ALA:O	1:G:26:VAL:HG22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:LYS:O	1:K:203:LYS:N	2.41	0.54
1:D:211:LEU:O	1:D:215:MET:HG3	2.07	0.54
1:G:138:LEU:HD13	1:G:141:ILE:HD12	1.90	0.54
1:K:2:ILE:HD12	1:K:12:HIS:HA	1.89	0.54
1:L:67:GLN:HE22	1:L:70:LYS:HE2	1.72	0.53
1:H:188:THR:O	1:H:192:GLN:HG3	2.09	0.53
1:K:34:PRO:O	1:K:37:ILE:HD12	2.08	0.53
1:L:47:ALA:HB1	1:L:51:ASP:HB2	1.91	0.53
1:K:164:TYR:OH	1:K:190:LEU:O	2.22	0.53
1:H:32:PHE:O	1:H:142:VAL:HG22	2.08	0.53
1:D:32:PHE:O	1:D:142:VAL:HG22	2.09	0.52
1:H:161:PHE:CE1	1:H:202:LEU:HD11	2.44	0.52
1:D:23:TRP:CZ3	1:D:40:PHE:HB2	2.44	0.52
1:D:199:LYS:O	1:D:203:LYS:HG3	2.09	0.52
1:G:70:LYS:O	1:G:73:ILE:HG12	2.09	0.52
1:G:104:ILE:HG22	1:G:130:TYR:HB2	1.91	0.52
1:K:199:LYS:HE2	1:K:200:THR:N	2.24	0.52
1:L:52:LEU:HD21	1:L:131:LYS:HG3	1.91	0.52
1:I:52:LEU:HD12	1:I:130:TYR:CD2	2.45	0.52
1:K:212:GLU:O	1:K:216:THR:HG23	2.09	0.52
1:E:113:GLU:HB3	1:E:117:TRP:CZ3	2.45	0.51
1:I:69:LEU:O	1:I:73:ILE:HG23	2.09	0.51
1:C:161:PHE:HD2	1:C:215:MET:HG2	1.75	0.51
1:I:70:LYS:O	1:I:73:ILE:HG12	2.10	0.51
1:A:12:HIS:N	1:F:4:GLN:HE22	2.08	0.51
1:K:67:GLN:HA	1:K:70:LYS:HE2	1.93	0.51
1:J:54:THR:O	1:J:58:THR:HG23	2.10	0.51
1:F:48:THR:HG22	1:F:118:MET:SD	2.51	0.51
1:K:22:ALA:O	1:K:26:VAL:HG13	2.10	0.51
1:H:26:VAL:HG21	1:H:39:MET:HG2	1.93	0.51
1:A:129:ILE:O	1:A:132:ARG:HG2	2.11	0.51
1:L:44:SER:OG	1:L:131:LYS:HD3	2.11	0.50
1:K:154:ARG:HA	1:K:193:ASN:HB3	1.93	0.50
1:L:115:ILE:O	1:L:119:THR:HG23	2.11	0.50
1:F:22:ALA:O	1:F:26:VAL:HG13	2.11	0.50
1:B:157:PRO:HB3	1:H:121:ASN:HB2	1.94	0.50
1:C:32:PHE:O	1:C:142:VAL:HG22	2.11	0.50
1:I:212:GLU:HG2	1:J:144:MET:SD	2.51	0.50
1:J:69:LEU:O	1:J:73:ILE:HG23	2.10	0.50
1:E:86:VAL:HG13	1:E:98:GLU:HB2	1.94	0.50
1:G:201:ILE:HG21	1:G:217:ALA:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:GLU:HB2	1:H:68:MET:HE3	1.94	0.50
1:G:150:ILE:HD11	1:G:168:PHE:CZ	2.47	0.50
1:C:67:GLN:HA	1:C:70:LYS:HD2	1.94	0.49
1:H:83:LEU:HB3	1:H:84:HIS:CD2	2.46	0.49
1:D:155:GLN:HB3	1:D:164:TYR:CG	2.47	0.49
1:G:105:ALA:HA	1:G:130:TYR:CE2	2.47	0.49
1:A:57:ASN:OD1	2:A:300:XBQ:N04	2.45	0.49
1:C:65:ALA:HB1	1:C:141:ILE:HD13	1.94	0.49
1:J:1:PRO:HA	1:J:47:ALA:HA	1.94	0.49
1:D:37:ILE:HD12	1:D:138:LEU:HD13	1.94	0.49
1:G:41:SER:HA	1:G:131:LYS:HE3	1.94	0.49
1:G:125:PRO:HB2	1:G:128:GLU:HB3	1.95	0.49
1:K:68:MET:HB3	1:K:141:ILE:HD11	1.95	0.48
1:G:172:LEU:O	1:G:176:GLN:N	2.43	0.48
1:H:212:GLU:HG3	1:I:144:MET:SD	2.53	0.48
1:C:37:ILE:HD11	1:C:142:VAL:HG21	1.95	0.48
1:H:37:ILE:HG21	1:H:135:ILE:HG23	1.94	0.48
1:C:198:CYS:O	1:C:202:LEU:HG	2.13	0.48
1:K:198:CYS:O	1:K:202:LEU:N	2.44	0.48
1:C:44:SER:HB3	1:C:55:MET:HE1	1.96	0.48
1:F:150:ILE:HD11	1:F:168:PHE:CZ	2.49	0.48
1:B:32:PHE:O	1:B:142:VAL:HG22	2.13	0.48
1:B:191:VAL:HG22	1:B:202:LEU:HD13	1.96	0.48
1:C:99:PRO:HG3	1:C:117:TRP:CD2	2.49	0.48
1:G:54:THR:O	1:G:58:THR:HG23	2.14	0.48
1:K:110:THR:HG23	1:K:112:GLN:H	1.78	0.48
1:K:140:LYS:O	1:K:144:MET:HG2	2.14	0.48
1:A:97:ARG:O	1:A:117:TRP:NE1	2.37	0.48
1:F:34:PRO:O	1:F:37:ILE:HD12	2.14	0.48
1:I:54:THR:O	1:I:58:THR:HG23	2.14	0.48
1:B:199:LYS:O	1:B:203:LYS:HG3	2.14	0.47
1:E:153:ILE:HD11	1:E:171:THR:HG21	1.96	0.47
1:J:76:GLU:O	1:J:79:GLU:HG3	2.13	0.47
1:B:150:ILE:HG12	1:B:172:LEU:HD13	1.94	0.47
1:D:66:MET:O	1:D:70:LYS:HG3	2.14	0.47
1:D:212:GLU:HG3	1:E:144:MET:SD	2.54	0.47
1:C:52:LEU:HA	1:C:55:MET:CE	2.43	0.47
1:H:24:VAL:HG12	1:H:25:LYS:HE2	1.96	0.47
1:L:54:THR:O	1:L:58:THR:HG23	2.13	0.47
1:D:139:ASN:HB3	1:D:177:ALA:O	2.14	0.47
1:F:112:GLN:O	1:F:112:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:MET:HE2	1:E:68:MET:HB3	1.64	0.47
1:F:2:ILE:HA	1:F:11:VAL:O	2.15	0.47
1:G:125:PRO:O	1:G:129:ILE:HG22	2.15	0.47
1:J:104:ILE:HG12	1:J:126:VAL:HG12	1.97	0.47
1:D:215:MET:HE1	1:E:64:ALA:HB1	1.96	0.47
1:B:40:PHE:HD2	1:B:135:ILE:HD11	1.78	0.47
1:F:26:VAL:HG11	1:F:39:MET:HG2	1.97	0.47
1:L:56:LEU:O	1:L:59:VAL:HG22	2.15	0.47
1:E:65:ALA:HB1	1:E:141:ILE:HD13	1.95	0.46
1:B:34:PRO:O	1:B:37:ILE:HD12	2.16	0.46
1:A:65:ALA:HB1	1:A:141:ILE:HD13	1.97	0.46
1:D:150:ILE:HD12	1:D:172:LEU:CD1	2.43	0.46
1:J:37:ILE:HB	1:J:38:PRO:HD3	1.98	0.46
1:K:143:ARG:HA	1:K:146:SER:HB3	1.97	0.46
1:G:51:ASP:O	1:G:55:MET:HG3	2.15	0.46
1:J:71:GLU:O	1:J:75:GLU:HG3	2.15	0.46
1:J:155:GLN:HB3	1:J:194:ALA:HA	1.97	0.46
1:K:27:VAL:HG11	1:K:59:VAL:HG13	1.97	0.46
1:A:99:PRO:HG3	1:A:117:TRP:CD2	2.51	0.46
1:E:26:VAL:HG11	1:E:39:MET:HG2	1.97	0.46
1:K:15:ILE:HD11	1:K:51:ASP:HB3	1.97	0.46
1:K:153:ILE:HD12	1:K:167:ARG:NE	2.31	0.46
1:D:57:ASN:OD1	2:D:300:XBQ:N04	2.49	0.46
1:H:34:PRO:O	1:H:37:ILE:HD12	2.15	0.46
1:B:143:ARG:NH2	1:B:144:MET:HB2	2.31	0.46
1:G:154:ARG:O	1:G:167:ARG:NH2	2.49	0.46
1:H:25:LYS:HA	1:H:25:LYS:HD3	1.80	0.46
1:K:2:ILE:HD11	1:K:11:VAL:O	2.16	0.46
1:D:165:VAL:HG11	1:D:215:MET:CE	2.44	0.46
1:I:48:THR:O	1:I:52:LEU:HG	2.16	0.46
1:J:18:ARG:HG2	1:K:17:PRO:HB2	1.97	0.46
1:J:25:LYS:HD2	1:J:25:LYS:HA	1.75	0.45
1:A:32:PHE:O	1:A:142:VAL:HG22	2.16	0.45
1:C:129:ILE:HG12	1:C:132:ARG:HH12	1.80	0.45
1:A:186:THR:HG22	1:A:189:LEU:H	1.81	0.45
1:K:26:VAL:HG11	1:K:39:MET:HG2	1.99	0.45
1:A:198:CYS:O	1:A:202:LEU:HG	2.15	0.45
1:G:105:ALA:HA	1:G:130:TYR:CD2	2.51	0.45
1:E:170:LYS:HB3	1:E:170:LYS:HE2	1.81	0.45
1:E:212:GLU:HG3	1:F:144:MET:CE	2.46	0.45
1:B:3:VAL:O	1:B:10:MET:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:30:LYS:HD3	1:J:35:GLU:HG3	1.99	0.45
1:B:215:MET:HB2	1:C:144:MET:HE1	1.98	0.45
1:L:189:LEU:HD13	1:L:189:LEU:HA	1.84	0.45
1:K:153:ILE:HG21	1:K:168:PHE:HA	1.99	0.45
1:I:197:ASP:O	1:I:201:ILE:HD13	2.17	0.45
1:J:66:MET:O	1:J:70:LYS:HG3	2.17	0.45
1:F:150:ILE:HD13	1:F:172:LEU:HD13	1.99	0.45
1:G:155:GLN:HB3	1:G:195:ASN:H	1.82	0.45
1:J:52:LEU:HA	1:J:55:MET:HE3	1.99	0.45
1:E:32:PHE:O	1:E:142:VAL:HG22	2.17	0.44
1:L:138:LEU:O	1:L:142:VAL:HG13	2.17	0.44
1:B:22:ALA:O	1:B:26:VAL:HG22	2.16	0.44
1:B:45:CYS:HB3	1:C:14:CYS:SG	2.57	0.44
1:B:211:LEU:O	1:B:215:MET:HG3	2.17	0.44
1:E:211:LEU:O	1:E:215:MET:HG3	2.17	0.44
1:G:150:ILE:HD11	1:G:168:PHE:CE2	2.51	0.44
1:K:202:LEU:HD22	1:K:214:MET:HG2	1.99	0.44
1:L:43:LEU:HB3	1:L:55:MET:HE1	1.99	0.44
1:A:162:ARG:HA	1:A:215:MET:HE3	1.99	0.44
1:J:67:GLN:HA	1:J:70:LYS:HD2	1.99	0.44
1:G:211:LEU:HD12	1:G:211:LEU:HA	1.84	0.44
1:L:52:LEU:HD22	1:L:134:ILE:HD12	1.98	0.44
1:C:199:LYS:HG2	1:C:203:LYS:HE3	1.99	0.44
1:A:211:LEU:HA	1:A:214:MET:HE3	2.00	0.44
1:C:154:ARG:HG2	1:C:193:ASN:CG	2.43	0.44
1:D:18:ARG:NH1	1:E:18:ARG:HG2	2.33	0.44
1:I:59:VAL:HG11	1:I:66:MET:HG3	2.00	0.44
1:J:131:LYS:O	1:J:135:ILE:HG13	2.17	0.44
1:B:173:ARG:NE	2:C:300:XBQ:O02	2.51	0.43
1:E:168:PHE:CD2	1:E:190:LEU:HD13	2.53	0.43
1:K:25:LYS:HA	1:K:25:LYS:HD3	1.74	0.43
1:E:172:LEU:HD12	1:E:172:LEU:HA	1.89	0.43
1:C:44:SER:CB	1:C:55:MET:HE1	2.48	0.43
1:G:186:THR:CG2	1:G:189:LEU:HD12	2.48	0.43
1:I:168:PHE:HE2	1:I:190:LEU:HB2	1.83	0.43
1:G:144:MET:HB2	1:G:144:MET:HE2	1.57	0.43
1:H:55:MET:HE3	1:H:55:MET:HB3	1.88	0.43
1:I:30:LYS:HA	1:I:30:LYS:HD3	1.80	0.43
1:D:172:LEU:HD12	1:D:172:LEU:HA	1.90	0.43
1:H:100:ARG:HG2	1:H:103:ASP:OD2	2.19	0.43
1:J:169:TYR:CZ	1:K:67:GLN:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:55:MET:O	1:K:58:THR:HG22	2.19	0.43
1:F:211:LEU:O	1:F:215:MET:HG3	2.18	0.43
1:I:154:ARG:HA	1:I:193:ASN:HB3	2.01	0.43
1:I:111:LEU:O	1:I:114:GLN:HG2	2.19	0.43
1:G:68:MET:HE1	1:G:144:MET:HE1	2.01	0.43
1:K:212:GLU:OE1	1:K:212:GLU:N	2.42	0.43
1:A:120:HIS:CG	1:A:121:ASN:N	2.87	0.43
1:G:64:ALA:HB1	1:L:215:MET:CE	2.48	0.43
1:A:124:ILE:HA	1:A:125:PRO:HD3	1.87	0.42
1:A:12:HIS:O	1:F:4:GLN:NE2	2.51	0.42
1:I:39:MET:HE3	1:I:43:LEU:HG	2.00	0.42
1:L:35:GLU:O	1:L:38:PRO:HG2	2.20	0.42
1:E:198:CYS:O	1:E:202:LEU:HG	2.19	0.42
1:B:144:MET:HE3	1:B:145:TYR:CE1	2.48	0.42
1:A:187:GLU:O	1:A:191:VAL:HG23	2.19	0.42
1:D:144:MET:HE3	1:D:144:MET:HB2	1.63	0.42
1:B:192:GLN:HA	1:B:199:LYS:HE2	2.02	0.42
1:D:211:LEU:HD22	1:E:67:GLN:CG	2.50	0.42
1:J:68:MET:HE2	1:J:68:MET:HB2	1.86	0.42
1:K:128:GLU:O	1:K:132:ARG:HG3	2.20	0.42
1:E:212:GLU:O	1:E:216:THR:HG22	2.20	0.42
1:G:55:MET:O	1:G:58:THR:OG1	2.34	0.42
1:K:150:ILE:HD12	1:K:150:ILE:HA	1.93	0.42
1:A:37:ILE:HD12	1:A:138:LEU:HB3	2.01	0.42
1:A:144:MET:HB2	1:A:144:MET:HE2	1.55	0.42
1:D:37:ILE:N	1:D:38:PRO:HD2	2.35	0.42
1:H:23:TRP:O	1:H:27:VAL:HG23	2.20	0.42
1:J:140:LYS:O	1:J:144:MET:HG3	2.19	0.42
1:K:75:GLU:HG2	1:K:76:GLU:OE2	2.20	0.42
1:K:161:PHE:CZ	1:K:202:LEU:HD11	2.54	0.42
1:I:19:THR:HG23	1:I:43:LEU:HD22	2.02	0.42
1:E:199:LYS:O	1:E:203:LYS:HG3	2.20	0.41
1:G:37:ILE:HG12	1:G:138:LEU:HB3	2.02	0.41
1:K:138:LEU:O	1:K:142:VAL:HG23	2.20	0.41
1:D:196:PRO:HA	1:D:199:LYS:HB3	2.03	0.41
1:I:161:PHE:O	1:I:165:VAL:HG23	2.21	0.41
1:C:150:ILE:HG12	1:C:172:LEU:HD12	2.03	0.41
1:F:150:ILE:HD11	1:F:168:PHE:CE2	2.55	0.41
1:H:55:MET:O	1:H:58:THR:HG22	2.19	0.41
1:F:144:MET:HE2	1:F:144:MET:HB2	1.86	0.41
1:C:202:LEU:HD22	1:C:214:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:201:ILE:O	1:K:205:LEU:HD13	2.20	0.41
1:L:114:GLN:O	1:L:118:MET:HG2	2.21	0.41
1:B:143:ARG:NH1	1:B:144:MET:HA	2.35	0.41
1:F:21:ASN:ND2	1:F:25:LYS:HE2	2.35	0.41
1:J:26:VAL:HG11	1:J:39:MET:HE2	2.03	0.41
1:C:37:ILE:HD13	1:C:139:ASN:OD1	2.21	0.41
1:H:215:MET:HB3	1:H:215:MET:HE2	1.84	0.41
1:L:139:ASN:O	1:L:142:VAL:HG22	2.20	0.41
1:A:21:ASN:O	1:A:25:LYS:HG2	2.21	0.41
1:E:173:ARG:HA	2:F:300:XBQ:O01	2.21	0.41
1:G:215:MET:HE3	1:G:215:MET:HB2	2.01	0.41
1:J:137:GLY:O	1:J:141:ILE:HG12	2.21	0.41
1:K:150:ILE:HD13	1:K:171:THR:HB	2.03	0.41
1:E:205:LEU:HD23	1:E:205:LEU:HA	1.89	0.40
1:A:202:LEU:O	1:A:205:LEU:HB2	2.21	0.40
1:I:72:THR:O	1:I:75:GLU:HB2	2.21	0.40
1:F:37:ILE:HG21	1:F:135:ILE:HG23	2.03	0.40
1:F:198:CYS:O	1:F:202:LEU:HG	2.22	0.40
1:H:37:ILE:HB	1:H:38:PRO:HD3	2.03	0.40
1:H:210:THR:O	1:H:214[A]:MET:HE3	2.21	0.40
1:A:23:TRP:CZ3	1:A:40:PHE:HB2	2.56	0.40
1:J:41:SER:HB2	1:J:135:ILE:HD11	2.02	0.40
1:J:76:GLU:HG2	1:J:133:TRP:CG	2.55	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	198/224 (88%)	196 (99%)	2 (1%)	0	100	100
1	B	190/224 (85%)	188 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	191/224 (85%)	190 (100%)	1 (0%)	0	100	100
1	D	197/224 (88%)	197 (100%)	0	0	100	100
1	E	191/224 (85%)	190 (100%)	1 (0%)	0	100	100
1	F	195/224 (87%)	193 (99%)	2 (1%)	0	100	100
1	G	158/224 (70%)	154 (98%)	4 (2%)	0	100	100
1	H	166/224 (74%)	165 (99%)	1 (1%)	0	100	100
1	I	157/224 (70%)	150 (96%)	7 (4%)	0	100	100
1	J	159/224 (71%)	155 (98%)	4 (2%)	0	100	100
1	K	159/224 (71%)	153 (96%)	6 (4%)	0	100	100
1	L	152/224 (68%)	149 (98%)	3 (2%)	0	100	100
All	All	2113/2688 (79%)	2080 (98%)	33 (2%)	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	78
1	B	168/188 (89%)	167 (99%)	1 (1%)	78	91
1	C	167/188 (89%)	165 (99%)	2 (1%)	63	83
1	D	169/188 (90%)	168 (99%)	1 (1%)	78	91
1	E	169/188 (90%)	166 (98%)	3 (2%)	51	77
1	F	172/188 (92%)	172 (100%)	0	100	100
1	G	131/188 (70%)	129 (98%)	2 (2%)	57	80
1	H	139/188 (74%)	138 (99%)	1 (1%)	76	89
1	I	126/188 (67%)	120 (95%)	6 (5%)	23	46
1	J	138/188 (73%)	137 (99%)	1 (1%)	76	89
1	K	140/188 (74%)	135 (96%)	5 (4%)	31	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	134/188 (71%)	129 (96%)	5 (4%)	30 57
All	All	1825/2256 (81%)	1795 (98%)	30 (2%)	55 79

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	198	CYS
1	A	218	CYS
1	B	36	VAL
1	C	26	VAL
1	C	172	LEU
1	D	188	THR
1	E	3	VAL
1	E	70	LYS
1	E	186	THR
1	G	126	VAL
1	G	148	THR
1	H	13	GLN
1	I	27	VAL
1	I	41	SER
1	I	113	GLU
1	I	115	ILE
1	I	188	THR
1	I	205	LEU
1	J	161	PHE
1	K	11	VAL
1	K	27	VAL
1	K	36	VAL
1	K	111	LEU
1	K	148	THR
1	L	69	LEU
1	L	75	GLU
1	L	142	VAL
1	L	151	LEU
1	L	210	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN

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Mol	Chain	Res	Type
1	A	84	HIS
1	A	193	ASN
1	B	21	ASN
1	B	84	HIS
1	C	12	HIS
1	C	21	ASN
1	C	62	HIS
1	C	63	GLN
1	C	112	GLN
1	D	63	GLN
1	D	67	GLN
1	D	112	GLN
1	E	4	GLN
1	E	12	HIS
1	F	4	GLN
1	F	21	ASN
1	F	84	HIS
1	G	155	GLN
1	G	195	ASN
1	H	67	GLN
1	J	112	GLN
1	J	155	GLN
1	K	74	ASN
1	L	67	GLN
1	L	155	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

6 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	XBQ	F	300	-	44,44,44	1.94	3 (6%)	60,62,62	1.09	3 (5%)
2	XBQ	B	300	-	44,44,44	1.92	3 (6%)	60,62,62	1.63	4 (6%)
2	XBQ	D	300	-	44,44,44	1.94	3 (6%)	60,62,62	1.59	5 (8%)
2	XBQ	C	300	-	44,44,44	1.95	3 (6%)	60,62,62	0.67	1 (1%)
2	XBQ	E	300	-	44,44,44	1.95	3 (6%)	60,62,62	0.71	1 (1%)
2	XBQ	A	300	-	44,44,44	1.97	3 (6%)	60,62,62	0.80	2 (3%)

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	XBQ	F	300	-	-	11/38/51/51	0/3/4/4
2	XBQ	B	300	-	-	4/38/51/51	0/3/4/4
2	XBQ	D	300	-	-	10/38/51/51	0/3/4/4
2	XBQ	C	300	-	-	11/38/51/51	0/4/4/4
2	XBQ	E	300	-	-	10/38/51/51	0/3/4/4
2	XBQ	A	300	-	-	11/38/51/51	0/3/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	XBQ	C08-N03	9.50	1.46	1.34
2	E	300	XBQ	C08-N03	9.41	1.46	1.34
2	C	300	XBQ	C08-N03	9.32	1.46	1.34
2	F	300	XBQ	C08-N03	9.21	1.46	1.34
2	D	300	XBQ	C08-N03	9.16	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	XBQ	C08-N03	8.93	1.46	1.34
2	C	300	XBQ	O02-C08	8.39	1.41	1.23
2	B	300	XBQ	O02-C08	8.39	1.41	1.23
2	D	300	XBQ	O02-C08	8.39	1.41	1.23
2	A	300	XBQ	O02-C08	8.38	1.41	1.23
2	F	300	XBQ	O02-C08	8.38	1.41	1.23
2	E	300	XBQ	O02-C08	8.36	1.41	1.23
2	D	300	XBQ	C07-C08	2.98	1.57	1.51
2	F	300	XBQ	C07-C08	2.90	1.56	1.51
2	B	300	XBQ	C07-C08	2.89	1.56	1.51
2	E	300	XBQ	C07-C08	2.87	1.56	1.51
2	A	300	XBQ	C07-C08	2.83	1.56	1.51
2	C	300	XBQ	C07-C08	2.74	1.56	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	300	XBQ	C11-N03-C08	8.97	130.74	118.66
2	B	300	XBQ	C11-N03-C08	8.59	130.22	118.66
2	B	300	XBQ	C09-N03-C08	-6.99	116.20	123.60
2	D	300	XBQ	C09-N03-C08	-6.79	116.42	123.60
2	F	300	XBQ	C11-N03-C08	6.54	127.47	118.66
2	B	300	XBQ	C07-C08-N03	-4.49	111.61	118.20
2	A	300	XBQ	C11-N03-C08	4.11	124.20	118.66
2	E	300	XBQ	C11-N03-C08	4.11	124.20	118.66
2	F	300	XBQ	C09-N03-C08	-3.16	120.26	123.60
2	C	300	XBQ	C11-N03-C08	3.02	122.73	118.66
2	D	300	XBQ	C07-C08-N03	-2.96	113.85	118.20
2	A	300	XBQ	C15-C13-N04	-2.84	101.61	108.97
2	B	300	XBQ	O02-C08-C07	2.77	124.34	118.26
2	D	300	XBQ	C07-N02-S01	2.41	121.94	117.06
2	F	300	XBQ	C10-N02-S01	2.37	121.47	117.06
2	D	300	XBQ	O02-C08-C07	2.08	122.81	118.26

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	300	XBQ	C10-N02-S01-C06
2	E	300	XBQ	C10-N02-S01-C06
2	B	300	XBQ	C27-C26-O05-C29
2	C	300	XBQ	C27-C26-O05-C29

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Mol	Chain	Res	Type	Atoms
2	C	300	XBQ	C10-N02-S01-O01
2	B	300	XBQ	C25-C26-O05-C29
2	C	300	XBQ	C25-C26-O05-C29
2	E	300	XBQ	C25-C26-O05-C29
2	E	300	XBQ	C27-C26-O05-C29
2	A	300	XBQ	C10-N02-S01-O01
2	E	300	XBQ	C10-N02-S01-O06
2	F	300	XBQ	C25-C26-O05-C29
2	F	300	XBQ	C27-C26-O05-C29
2	D	300	XBQ	C25-C26-O05-C29
2	F	300	XBQ	C07-N02-S01-O01
2	D	300	XBQ	C05-C06-S01-N02
2	D	300	XBQ	C27-C26-O05-C29
2	D	300	XBQ	C01-C06-S01-N02
2	C	300	XBQ	C10-N02-S01-O06
2	E	300	XBQ	C10-N02-S01-O01
2	E	300	XBQ	C07-N02-S01-O01
2	F	300	XBQ	C07-N02-S01-O06
2	A	300	XBQ	C10-N02-S01-C06
2	A	300	XBQ	O03-C12-N04-C13
2	A	300	XBQ	N04-C13-C14-C16
2	A	300	XBQ	C10-N02-S01-O06
2	F	300	XBQ	C07-N02-S01-C06
2	F	300	XBQ	C01-C06-S01-N02
2	C	300	XBQ	C07-N02-S01-O01
2	F	300	XBQ	C05-C06-S01-N02
2	A	300	XBQ	C11-C12-N04-C13
2	E	300	XBQ	C07-N02-S01-C06
2	C	300	XBQ	C07-N02-S01-C06
2	D	300	XBQ	C05-C06-S01-O01
2	C	300	XBQ	N04-C13-C14-C16
2	F	300	XBQ	C05-C06-S01-O06
2	F	300	XBQ	C01-C06-S01-O06
2	D	300	XBQ	C01-C06-S01-O01
2	E	300	XBQ	N03-C11-C12-O03
2	F	300	XBQ	C10-N02-S01-O01
2	C	300	XBQ	N03-C11-C12-N04
2	D	300	XBQ	N03-C11-C12-N04
2	E	300	XBQ	N03-C11-C12-N04
2	A	300	XBQ	C25-C26-O05-C29
2	C	300	XBQ	N03-C11-C12-O03
2	D	300	XBQ	N03-C11-C12-O03

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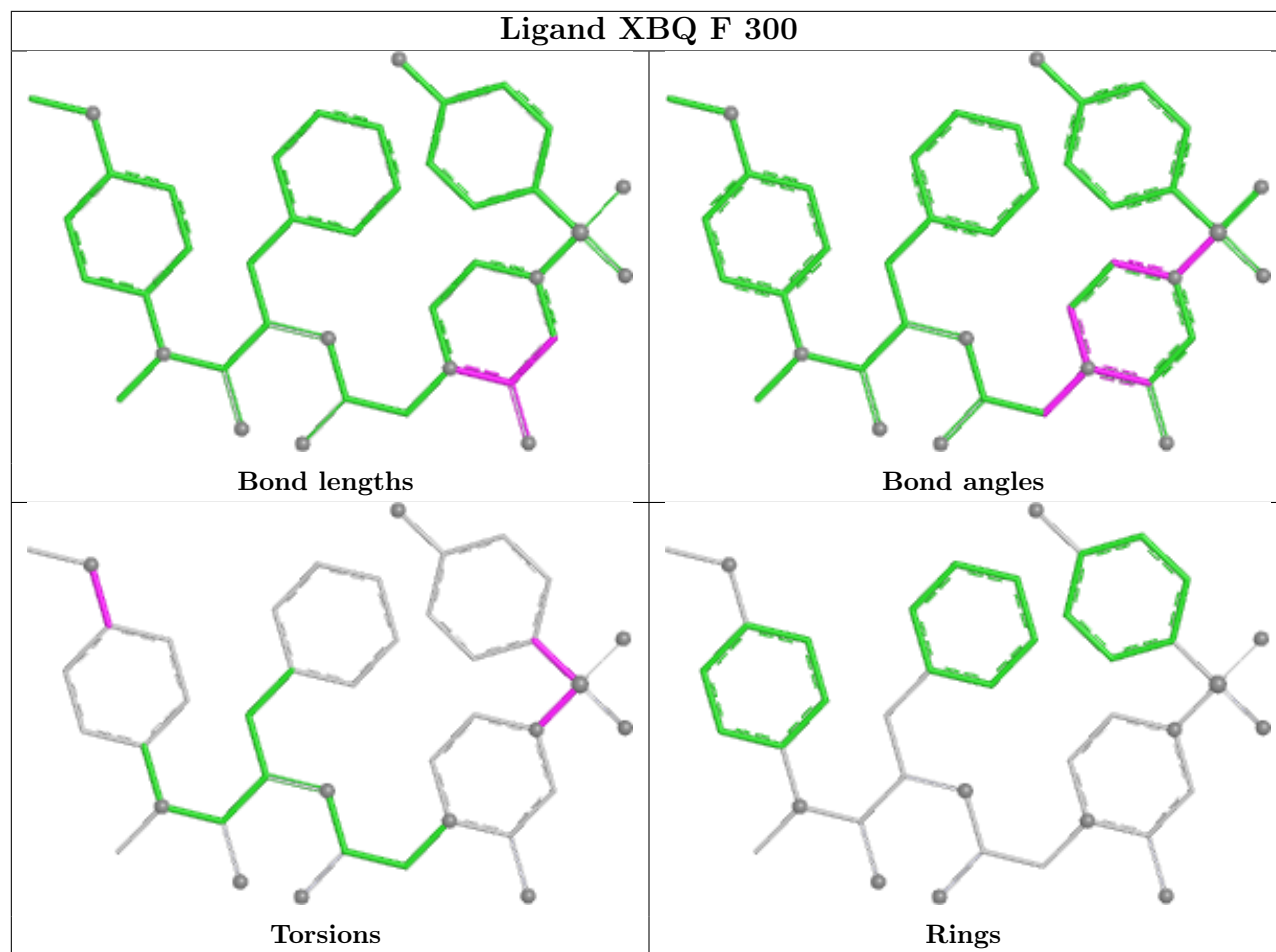
Mol	Chain	Res	Type	Atoms
2	A	300	XBQ	C27-C26-O05-C29
2	A	300	XBQ	C15-C13-C14-C16
2	D	300	XBQ	C10-N02-S01-O06
2	B	300	XBQ	C10-N02-S01-O06
2	E	300	XBQ	C07-N02-S01-O06
2	B	300	XBQ	C10-N02-S01-O01
2	D	300	XBQ	C10-N02-S01-O01
2	A	300	XBQ	C07-N02-S01-O06
2	F	300	XBQ	C10-N02-S01-C06
2	A	300	XBQ	C07-N02-S01-O01
2	C	300	XBQ	C15-C13-C14-C16

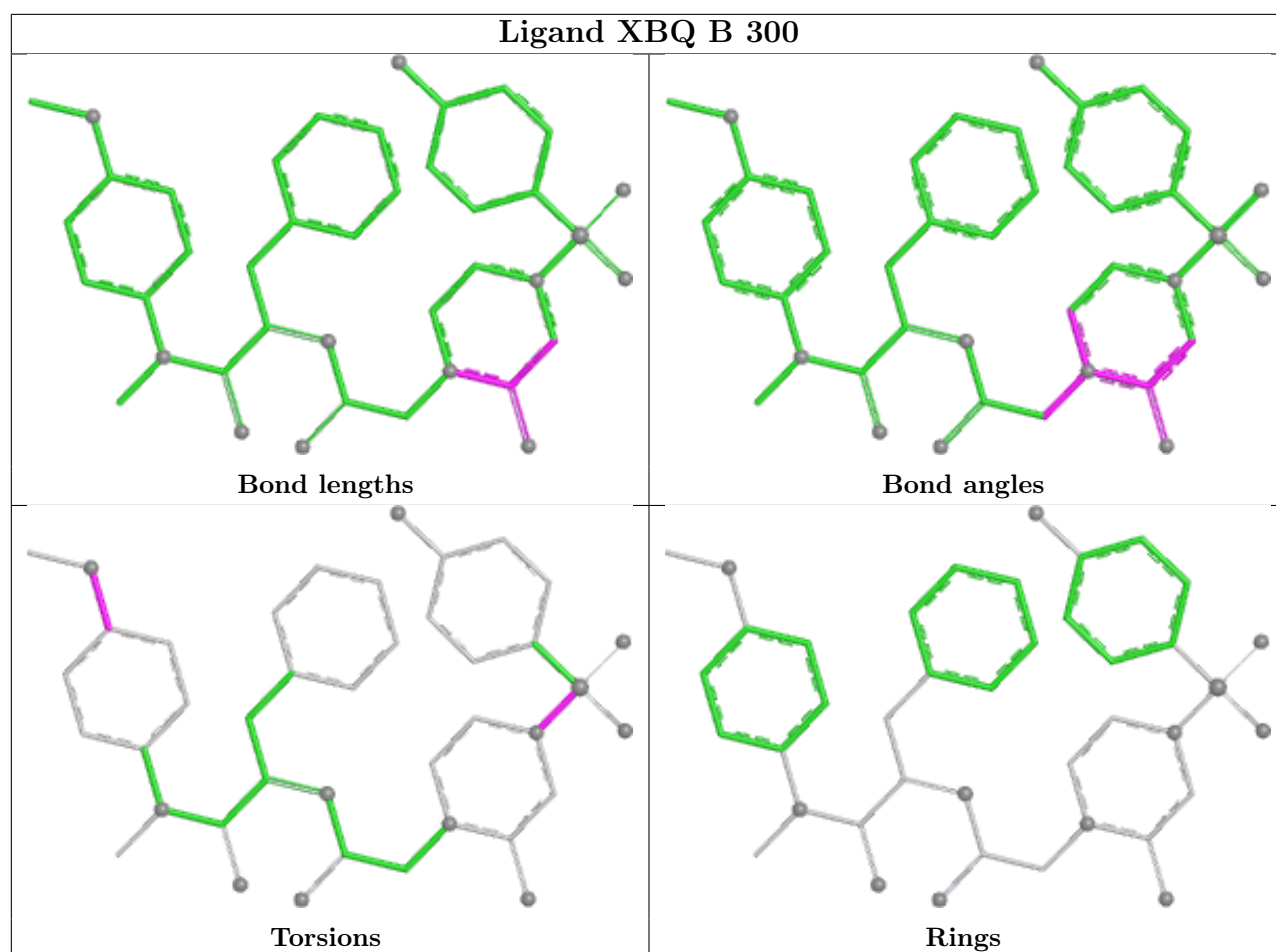
There are no ring outliers.

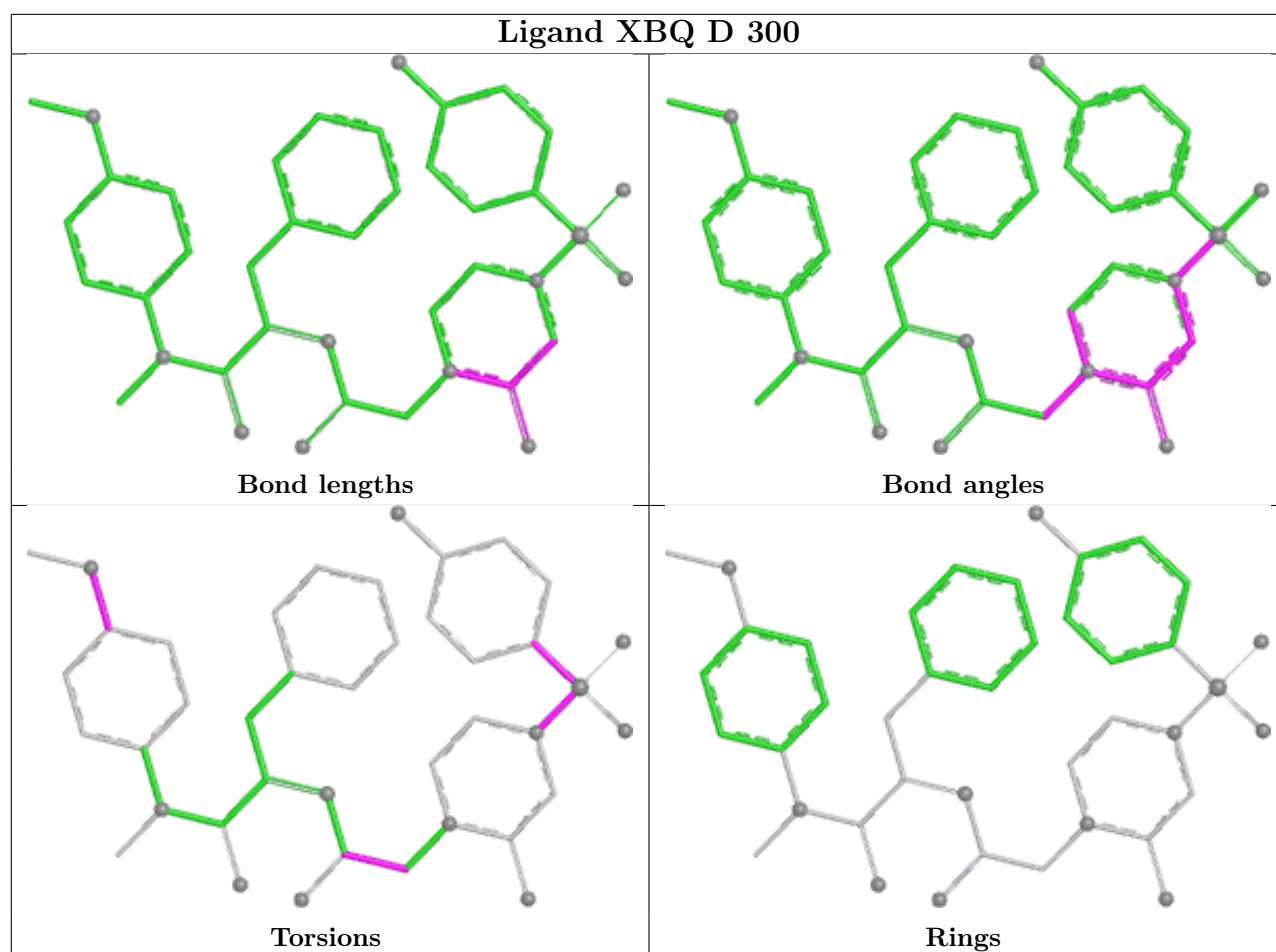
4 monomers are involved in 4 short contacts:

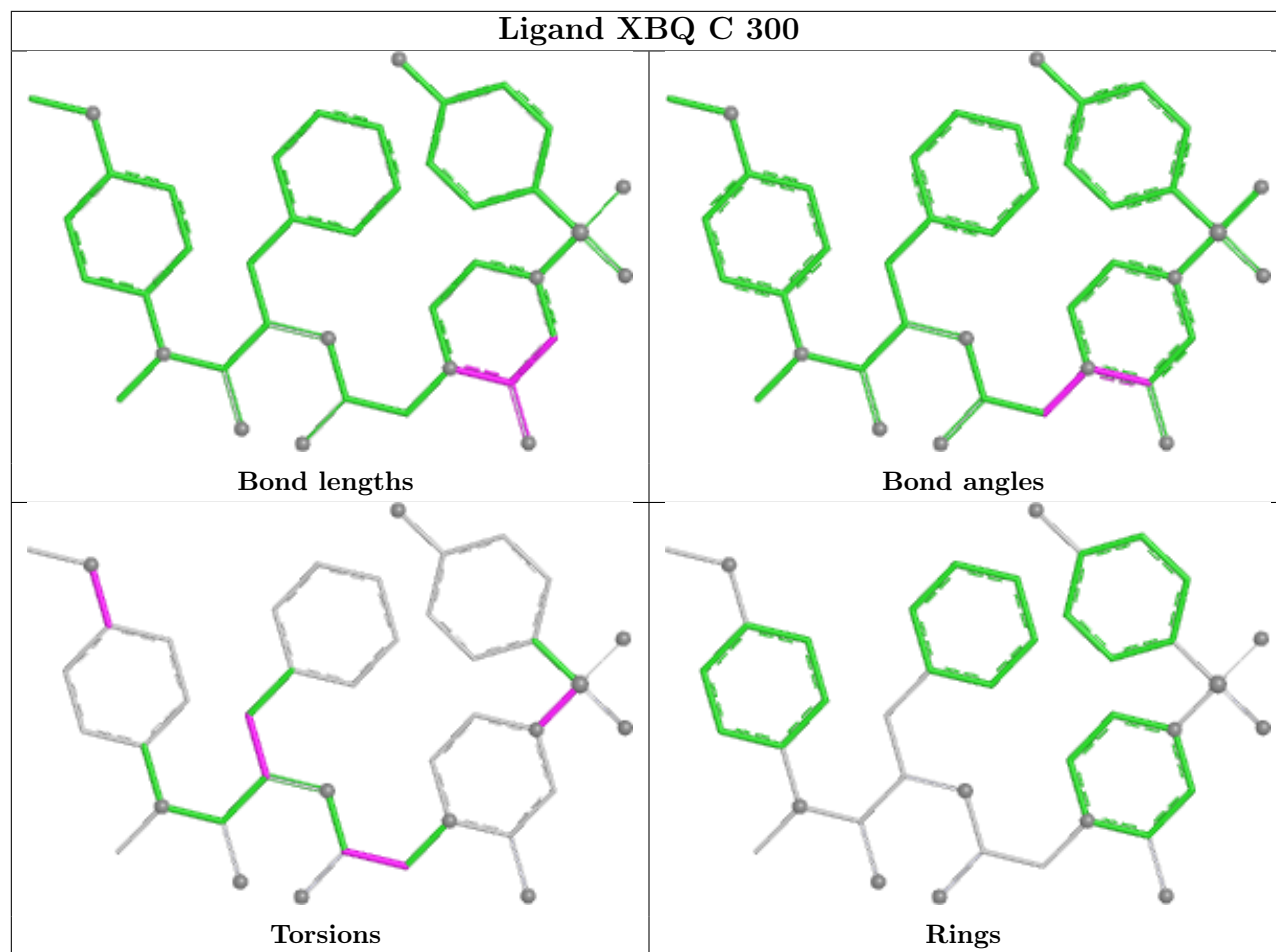
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	300	XBQ	1	0
2	D	300	XBQ	1	0
2	C	300	XBQ	1	0
2	A	300	XBQ	1	0

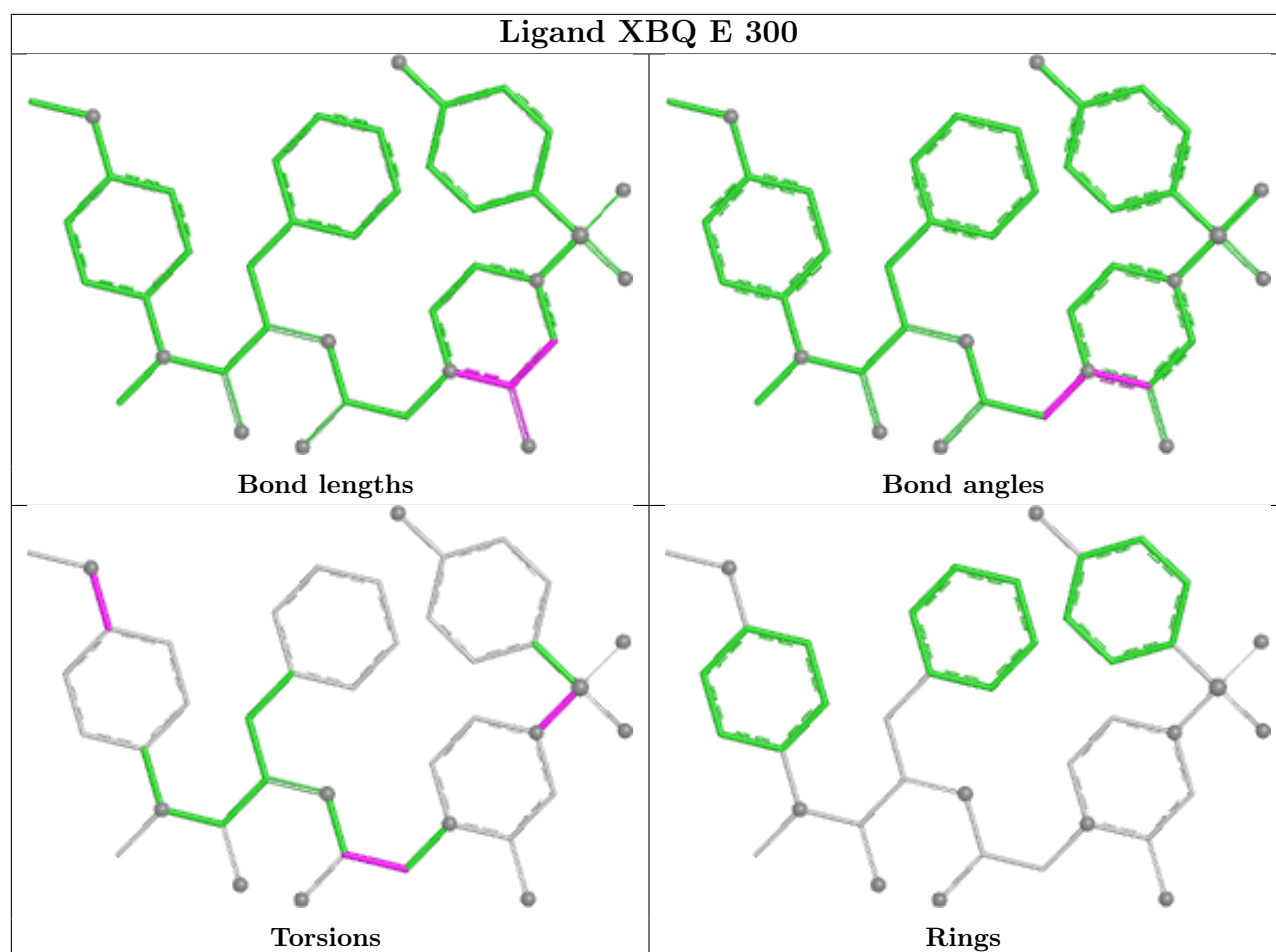
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

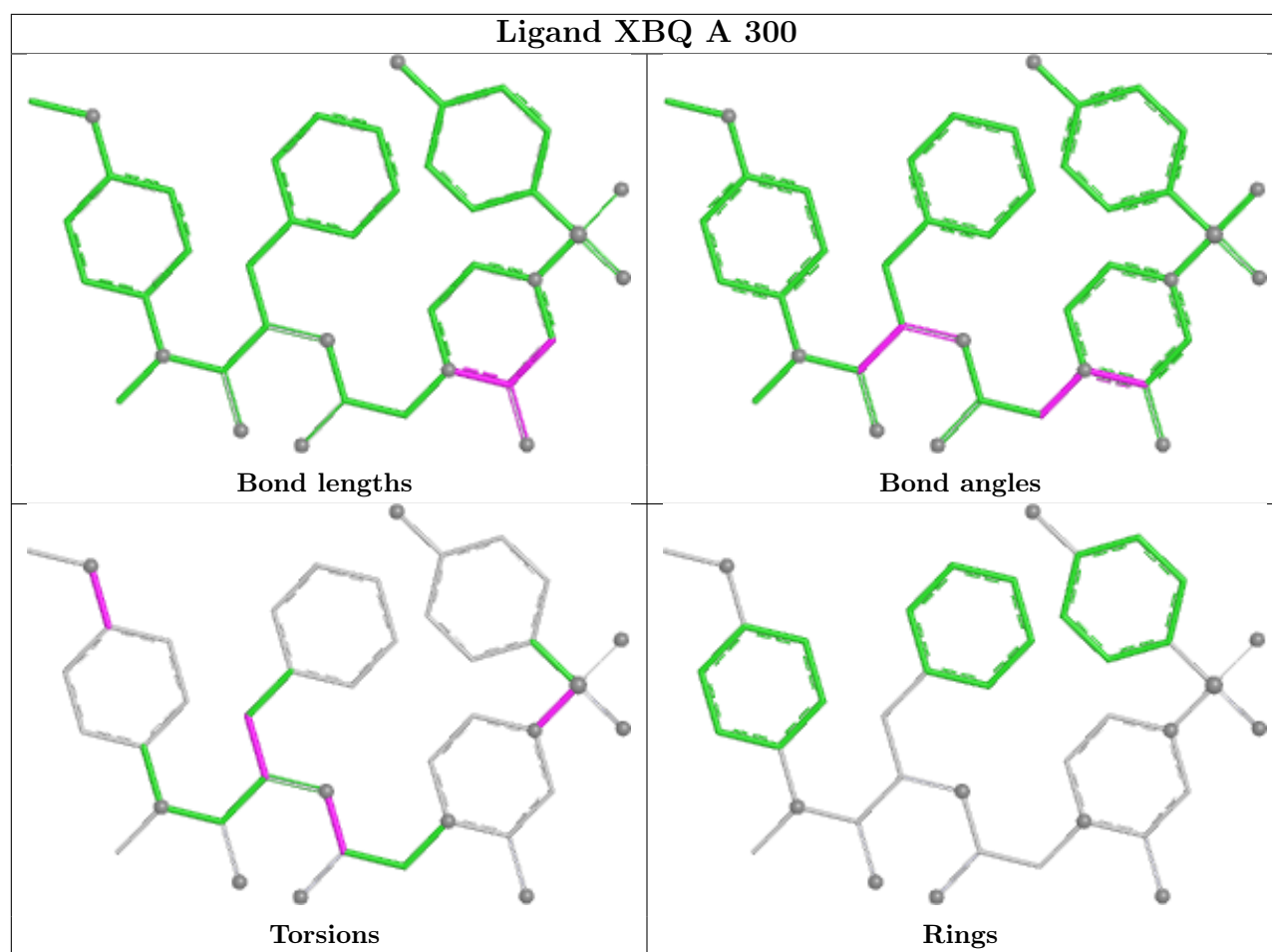












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	206/224 (91%)	0.40	9 (4%) 39 34	10, 33, 61, 81	0
1	B	200/224 (89%)	0.36	7 (3%) 47 42	9, 30, 55, 84	0
1	C	201/224 (89%)	0.56	13 (6%) 25 22	7, 33, 66, 86	0
1	D	205/224 (91%)	0.43	9 (4%) 39 34	10, 33, 61, 85	0
1	E	199/224 (88%)	0.38	3 (1%) 72 68	12, 34, 63, 76	0
1	F	203/224 (90%)	0.37	10 (4%) 35 31	8, 30, 61, 84	0
1	G	168/224 (75%)	1.23	29 (17%) 4 3	43, 62, 83, 94	0
1	H	177/224 (79%)	1.58	57 (32%) 1 1	44, 67, 89, 105	0
1	I	169/224 (75%)	1.28	33 (19%) 3 2	44, 65, 82, 90	0
1	J	171/224 (76%)	1.36	36 (21%) 2 2	45, 65, 84, 93	0
1	K	171/224 (76%)	1.28	26 (15%) 5 4	46, 66, 80, 96	0
1	L	164/224 (73%)	1.29	37 (22%) 2 2	43, 62, 87, 97	0
All	All	2234/2688 (83%)	0.84	269 (12%) 9 7	7, 52, 80, 105	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	127	GLY	6.3
1	C	86	VAL	5.0
1	H	150	ILE	4.6
1	F	92	ALA	4.6
1	G	46	GLY	4.5
1	H	104	ILE	4.4
1	J	114	GLN	4.4
1	H	28	GLU	4.3
1	G	148	THR	4.3
1	H	83	LEU	4.2
1	L	116	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	217	ALA	4.0
1	H	124	ILE	3.9
1	H	198	CYS	3.9
1	E	5	ASN	3.8
1	H	195	ASN	3.8
1	L	160	PRO	3.8
1	L	117	TRP	3.7
1	C	3	VAL	3.7
1	J	69	LEU	3.7
1	H	117	TRP	3.6
1	L	129	ILE	3.6
1	J	99	PRO	3.6
1	B	185	ALA	3.5
1	H	217	ALA	3.5
1	I	60	GLY	3.5
1	G	185	ALA	3.5
1	I	111	LEU	3.4
1	G	65	ALA	3.4
1	I	32	PHE	3.4
1	I	161	PHE	3.4
1	H	192	GLN	3.4
1	K	60	GLY	3.4
1	L	196	PRO	3.3
1	A	82	ARG	3.3
1	H	41	SER	3.3
1	L	194	ALA	3.3
1	H	120	HIS	3.2
1	J	165	VAL	3.2
1	K	197	ASP	3.2
1	G	60	GLY	3.2
1	J	202	LEU	3.2
1	E	11	VAL	3.2
1	I	110	THR	3.2
1	L	64	ALA	3.1
1	I	109	SER	3.1
1	J	81	ASP	3.1
1	K	202	LEU	3.1
1	K	191	VAL	3.1
1	L	136	LEU	3.1
1	B	94	GLY	3.1
1	H	97	ARG	3.1
1	I	64	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	163	ASP	3.1
1	I	33	SER	3.0
1	D	101	GLY	3.0
1	L	115	ILE	3.0
1	H	113	GLU	3.0
1	F	207	PRO	3.0
1	H	202	LEU	3.0
1	I	59	VAL	3.0
1	L	176	GLN	3.0
1	D	3	VAL	2.9
1	H	194	ALA	2.9
1	B	122	PRO	2.9
1	I	150	ILE	2.9
1	J	150	ILE	2.9
1	H	197	ASP	2.9
1	H	212	GLU	2.9
1	B	204	ALA	2.9
1	K	206	GLY	2.9
1	I	218	CYS	2.9
1	J	80	TRP	2.9
1	G	61	GLY	2.9
1	K	127	GLY	2.9
1	K	198	CYS	2.8
1	G	146	SER	2.8
1	H	126	VAL	2.8
1	J	186	THR	2.8
1	H	127	GLY	2.8
1	G	184	ALA	2.8
1	I	190	LEU	2.8
1	I	204	ALA	2.8
1	K	107	THR	2.8
1	K	190	LEU	2.8
1	L	145	TYR	2.8
1	I	102	SER	2.8
1	H	210	THR	2.8
1	J	77	ALA	2.8
1	K	205	LEU	2.7
1	C	218	CYS	2.7
1	G	150	ILE	2.7
1	H	205	LEU	2.7
1	J	72	THR	2.7
1	J	163	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	81	ASP	2.7
1	D	85	PRO	2.7
1	H	188	THR	2.7
1	K	50	GLN	2.7
1	H	211	LEU	2.6
1	G	145	TYR	2.6
1	J	110	THR	2.6
1	I	144	MET	2.6
1	L	195	ASN	2.6
1	I	36	VAL	2.6
1	K	11	VAL	2.6
1	H	48	THR	2.6
1	L	48	THR	2.6
1	H	164	TYR	2.6
1	L	60	GLY	2.6
1	C	121	ASN	2.6
1	F	121	ASN	2.6
1	G	212	GLU	2.6
1	B	186	THR	2.6
1	I	77	ALA	2.6
1	H	84	HIS	2.6
1	J	200	THR	2.6
1	L	164	TYR	2.6
1	A	208	GLY	2.6
1	L	197	ASP	2.6
1	L	14	CYS	2.6
1	I	62	HIS	2.6
1	I	146	SER	2.6
1	K	31	ALA	2.6
1	K	184	ALA	2.6
1	G	162	ARG	2.5
1	I	129	ILE	2.5
1	K	211	LEU	2.5
1	C	185	ALA	2.5
1	G	42	ALA	2.5
1	G	194	ALA	2.5
1	H	110	THR	2.5
1	G	147	PRO	2.5
1	J	115	ILE	2.5
1	J	133	TRP	2.5
1	J	201	ILE	2.5
1	K	136	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	164	TYR	2.5
1	L	201	ILE	2.5
1	J	161	PHE	2.5
1	I	192	GLN	2.5
1	J	22	ALA	2.5
1	D	122	PRO	2.5
1	F	206	GLY	2.5
1	I	46	GLY	2.5
1	I	61	GLY	2.5
1	I	145	TYR	2.5
1	L	161	PHE	2.5
1	C	198	CYS	2.4
1	H	85	PRO	2.4
1	K	147	PRO	2.4
1	A	3	VAL	2.4
1	H	58	THR	2.4
1	L	210	THR	2.4
1	H	190	LEU	2.4
1	H	59	VAL	2.4
1	A	78	ALA	2.4
1	K	78	ALA	2.4
1	H	109	SER	2.4
1	J	41	SER	2.4
1	J	15	ILE	2.4
1	A	11	VAL	2.4
1	L	27	VAL	2.4
1	C	207	PRO	2.4
1	H	196[A]	PRO	2.4
1	I	106	GLY	2.4
1	J	60	GLY	2.4
1	D	115	ILE	2.4
1	G	111	LEU	2.4
1	J	151	LEU	2.4
1	L	198	CYS	2.4
1	H	32	PHE	2.4
1	J	36	VAL	2.4
1	I	108	THR	2.3
1	H	15	ILE	2.3
1	J	37	ILE	2.3
1	C	197	ASP	2.3
1	H	37	ILE	2.3
1	L	150	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	218	CYS	2.3
1	G	164	TYR	2.3
1	H	145	TYR	2.3
1	H	79	GLU	2.3
1	H	57	ASN	2.3
1	J	1	PRO	2.3
1	K	194	ALA	2.3
1	G	200	THR	2.3
1	J	126	VAL	2.3
1	H	49	PRO	2.3
1	J	21	ASN	2.3
1	F	4	GLN	2.3
1	G	127	GLY	2.3
1	K	69	LEU	2.3
1	D	4	GLN	2.2
1	K	201	ILE	2.2
1	H	133	TRP	2.2
1	E	3	VAL	2.2
1	H	165	VAL	2.2
1	L	144	MET	2.2
1	L	211	LEU	2.2
1	F	217	ALA	2.2
1	G	204	ALA	2.2
1	C	95	GLN	2.2
1	H	14	CYS	2.2
1	D	98	GLU	2.2
1	C	154	ARG	2.2
1	D	5	ASN	2.2
1	H	139	ASN	2.2
1	H	209	ALA	2.2
1	J	194	ALA	2.2
1	F	198	CYS	2.2
1	G	149	SER	2.2
1	H	152	ASP	2.2
1	A	85	PRO	2.2
1	H	160	PRO	2.2
1	L	170	LYS	2.2
1	H	142	VAL	2.1
1	G	64	ALA	2.1
1	J	204	ALA	2.1
1	L	107	THR	2.1
1	L	110	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	216	THR	2.1
1	I	2	ILE	2.1
1	K	73	ILE	2.1
1	B	28	GLU	2.1
1	C	99	PRO	2.1
1	I	80	TRP	2.1
1	I	133	TRP	2.1
1	J	148	THR	2.1
1	A	2	ILE	2.1
1	G	73	ILE	2.1
1	J	79	GLU	2.1
1	A	99	PRO	2.1
1	B	126	VAL	2.1
1	H	80	TRP	2.1
1	L	133	TRP	2.1
1	G	139	ASN	2.1
1	K	21	ASN	2.1
1	K	151	LEU	2.1
1	L	52	LEU	2.1
1	G	210	THR	2.1
1	H	119	THR	2.1
1	I	113	GLU	2.1
1	J	198	CYS	2.1
1	A	207	PRO	2.1
1	C	160	PRO	2.1
1	I	165	VAL	2.1
1	L	32	PHE	2.1
1	H	47	ALA	2.1
1	L	186	THR	2.1
1	J	176	GLN	2.0
1	D	86	VAL	2.0
1	G	142	VAL	2.0
1	I	132	ARG	2.0
1	G	69	LEU	2.0
1	G	23	TRP	2.0
1	H	116	GLY	2.0
1	L	76	GLU	2.0
1	L	104	ILE	2.0
1	I	164	TYR	2.0
1	H	12	HIS	2.0
1	J	45	CYS	2.0
1	L	165	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	88	ALA	2.0
1	G	138	LEU	2.0
1	H	77	ALA	2.0
1	F	85	PRO	2.0
1	H	122	PRO	2.0
1	F	87	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

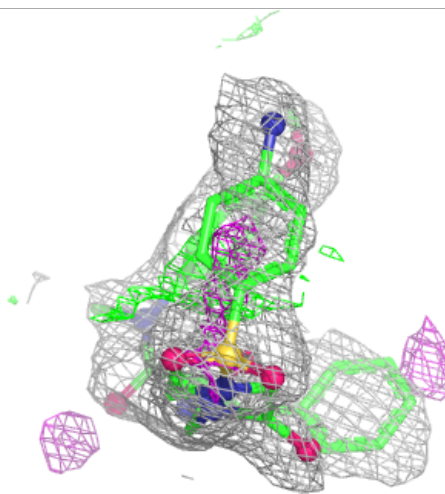
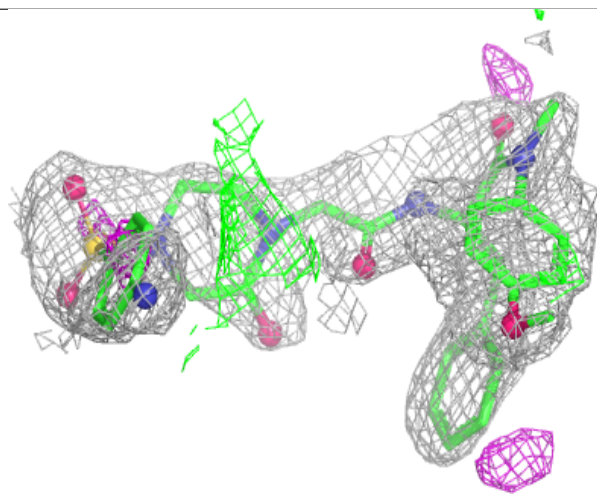
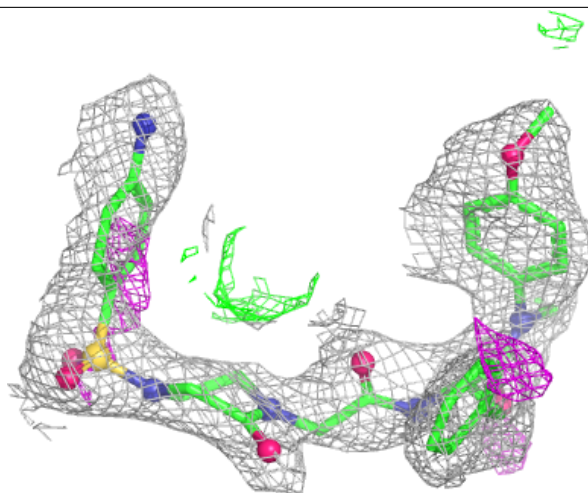
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XBQ	B	300	41/41	0.83	0.15	48,48,48,48	0
2	XBQ	A	300	41/41	0.84	0.13	42,42,42,42	0
2	XBQ	F	300	41/41	0.84	0.13	39,39,39,39	0
2	XBQ	E	300	41/41	0.85	0.13	42,42,42,42	0
2	XBQ	C	300	41/41	0.89	0.10	32,32,32,32	0
2	XBQ	D	300	41/41	0.89	0.10	31,31,31,31	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.

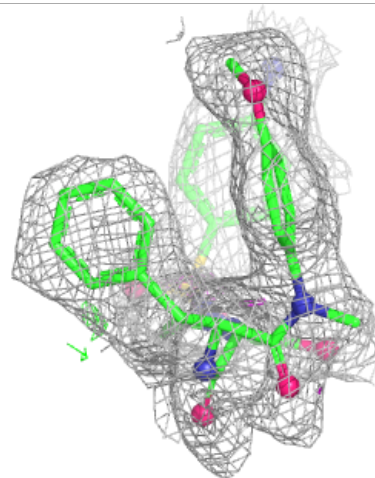
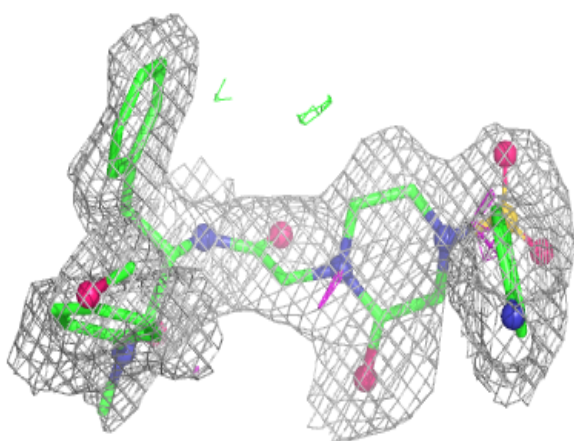
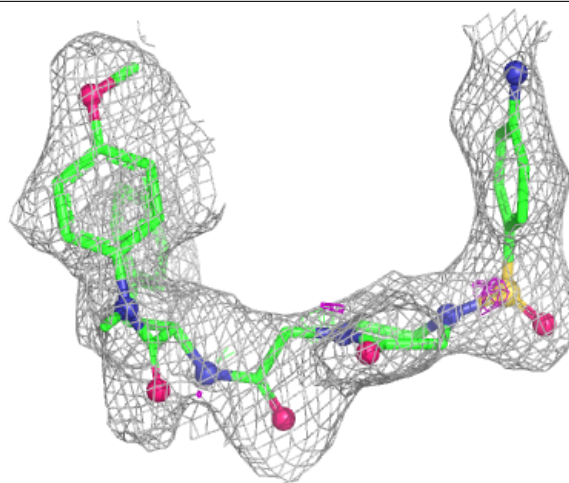
Electron density around XBQ B 300:

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



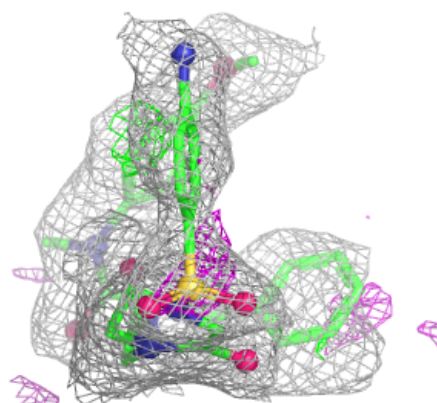
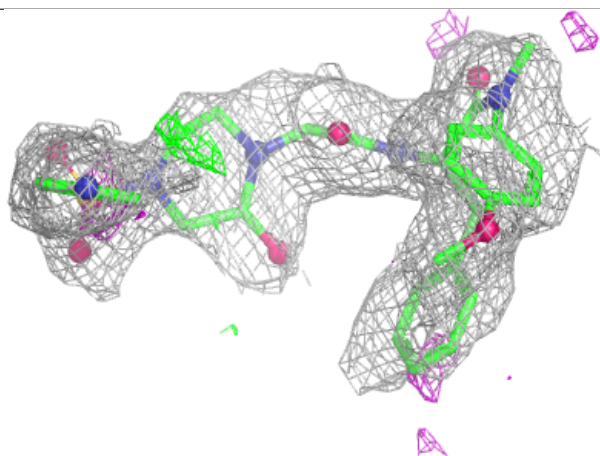
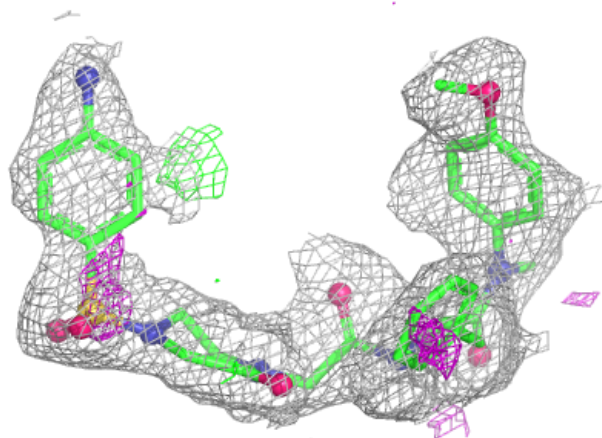
Electron density around XBQ A 300:

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



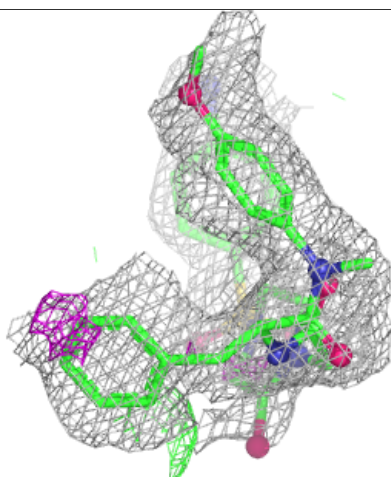
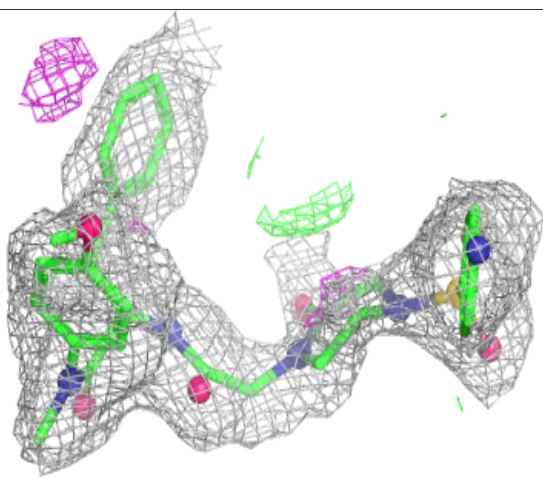
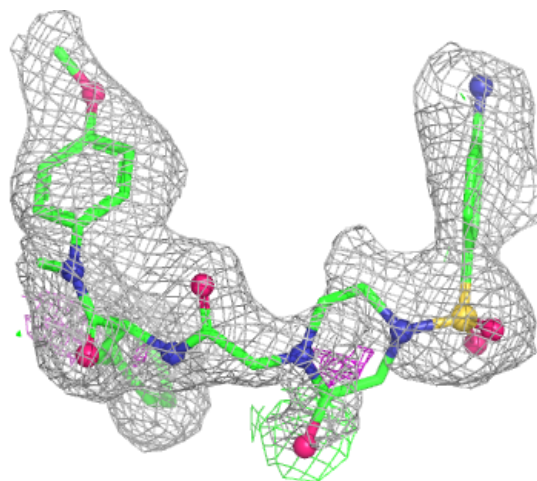
Electron density around XBQ F 300:

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



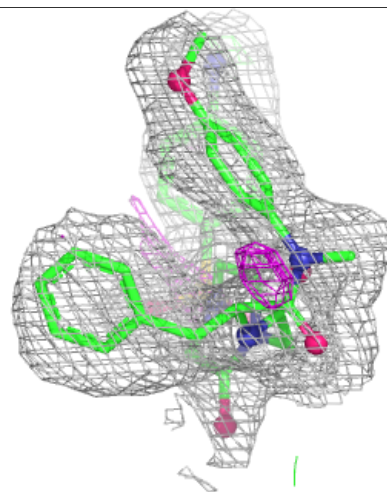
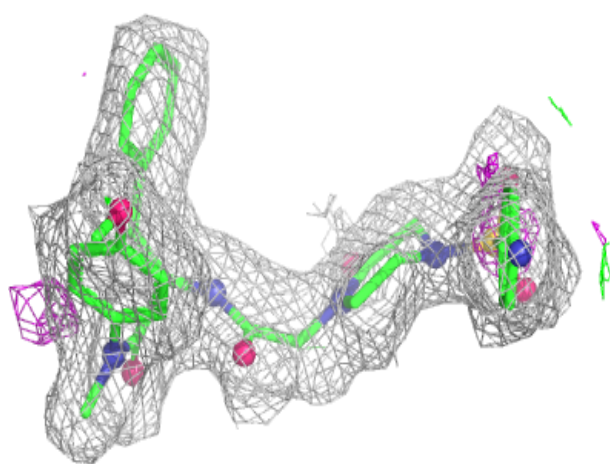
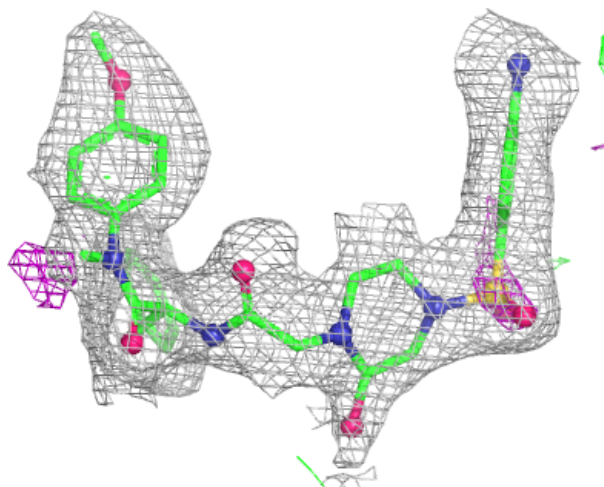
Electron density around XBQ E 300:

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



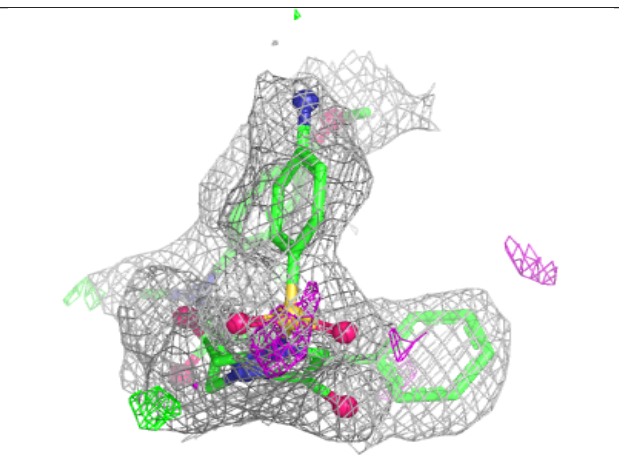
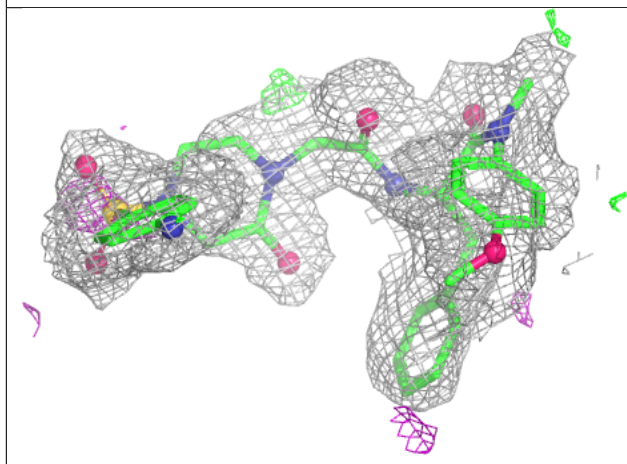
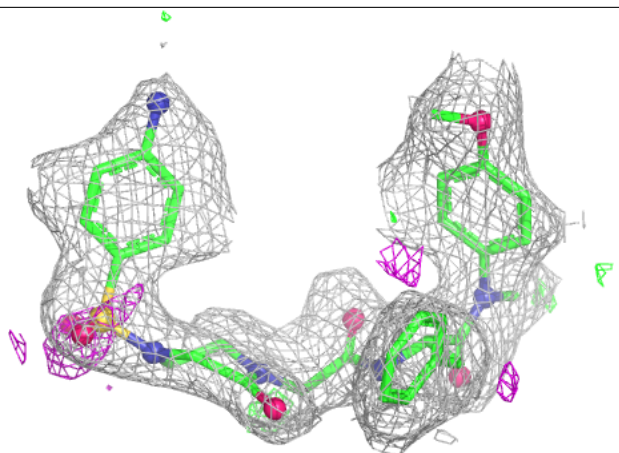
Electron density around XBQ C 300:

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



Electron density around XBQ D 300:

$2mF_o - DF_c$ (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.