Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 – 02:26 am GMT

PDB ID	:	6S3T
Title	:	P46, an immunodominant surface protein from Mycoplasma hyopneumoniae
Authors	:	Guasch, A.; Gonzalez-Gonzalez, L.; Fita, I.
Deposited on	:	2019-06-26
Resolution	:	3.50 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 (i) 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 (i)) were used in the production of this report:

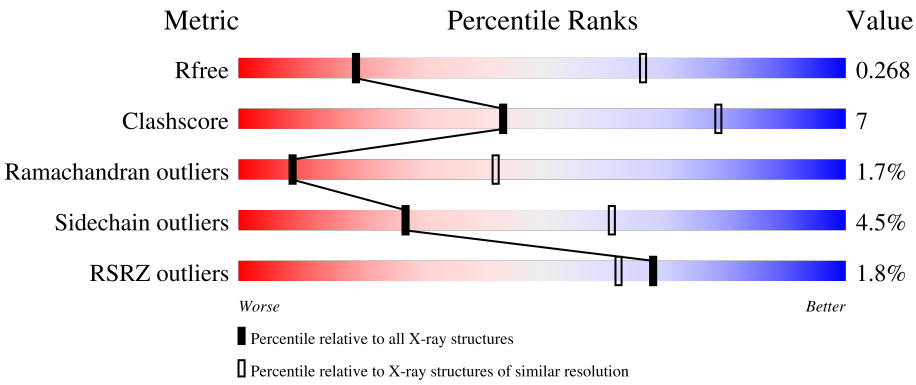
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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% 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	387	69% 24% • •
1	B	387	75% 17% 5% •
1	S	387	3% 78% 17% • •
1	T	387	3% 78% 17% • •
2	C	238	78% 11% • 9%

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Mol	Chain	Length	Quality of chain
2	I	238	3% 80% 8% • 9%
2	M	238	4% 75% 15% • 9%
2	Q	238	5% 80% 10% • 9%
3	D	474	35% 10% • 54%
3	E	474	39% 7% 54%
3	N	474	% 36% 9% • 54%
3	R	474	37% 9% • 54%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 24978 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 46 kDa surface antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	374	2894	1827	487	574	6	0	0	0
1	B	374	2894	1827	487	574	6	0	0	0
1	S	373	2887	1822	486	573	6	0	0	0
1	T	374	2895	1826	487	576	6	26	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	initiating methionine	UNP P0C0J8
B	32	MET	-	initiating methionine	UNP P0C0J8
S	32	MET	-	initiating methionine	UNP P0C0J8
T	32	MET	-	initiating methionine	UNP P0C0J8

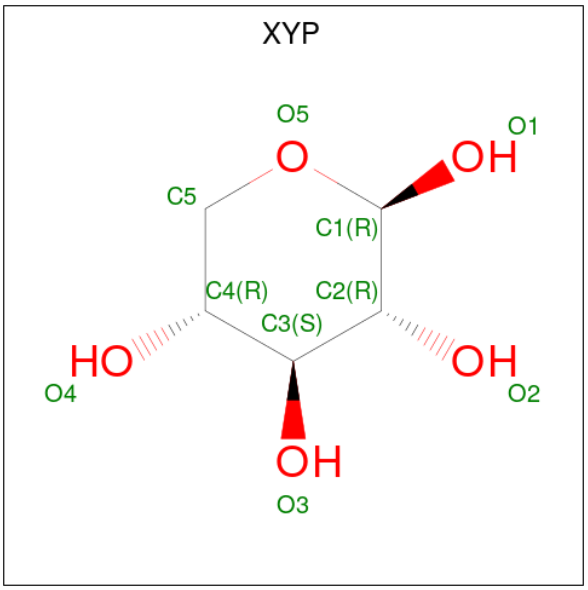
- Molecule 2 is a protein called Immunoglobulin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	216	1682	1051	284	341	6	0	0	0
2	I	216	1682	1051	284	341	6	0	0	0
2	M	216	1682	1051	284	341	6	0	0	0
2	Q	216	1682	1051	284	341	6	0	0	0

- Molecule 3 is a protein called Immunoglobulin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	219	1659	1049	269	333	8	0	0	0
3	E	219	1659	1049	269	333	8	0	0	0
3	N	219	1659	1049	269	333	8	0	0	0
3	R	219	1659	1049	269	333	8	4	0	0

- Molecule 4 is beta-D-xylopyranose (three-letter code: XYP) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	5	5	0	0
4	B	1	10	5	5	0	0
4	S	1	10	5	5	0	0
4	T	1	10	5	5	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	1	1	1	0	0

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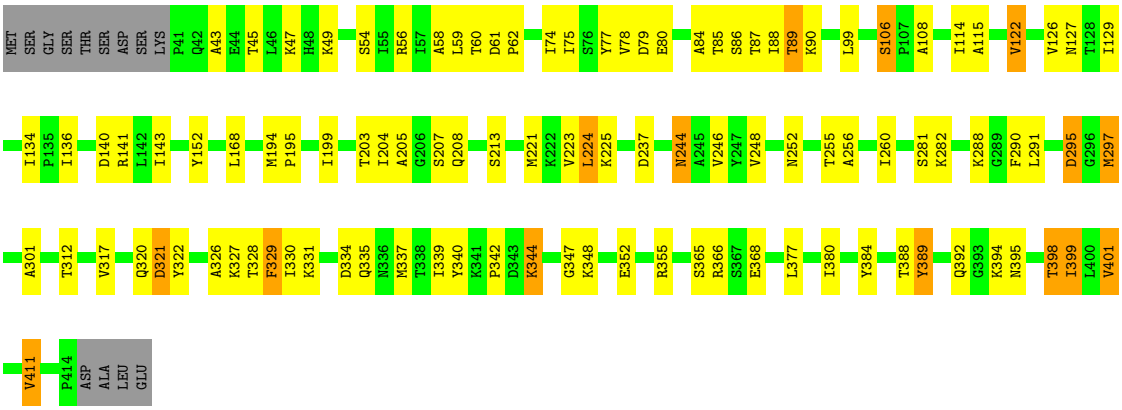
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	B	1	1	1	0	0
			Total	Na		
5	S	1	1	1	0	0
			Total	Na		
5	T	1	1	1	0	0

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.

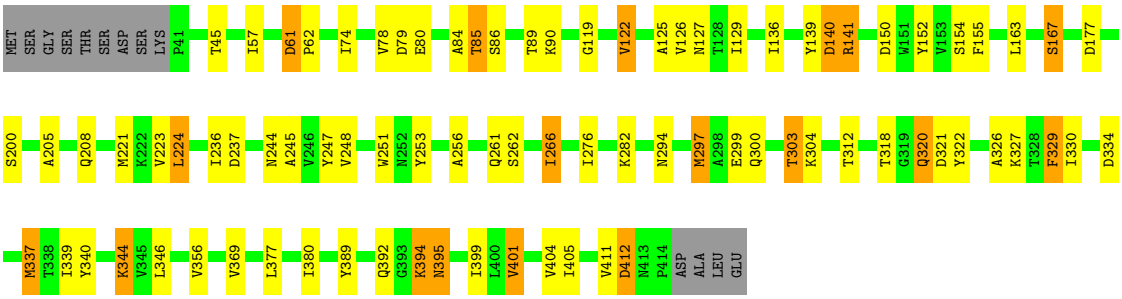
• Molecule 1: 46 kDa surface antigen

Chain A:



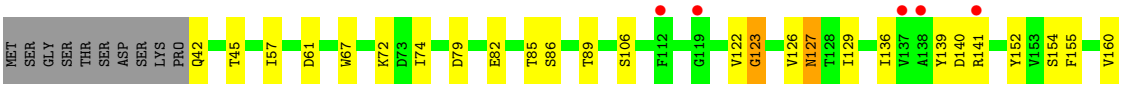
• Molecule 1: 46 kDa surface antigen

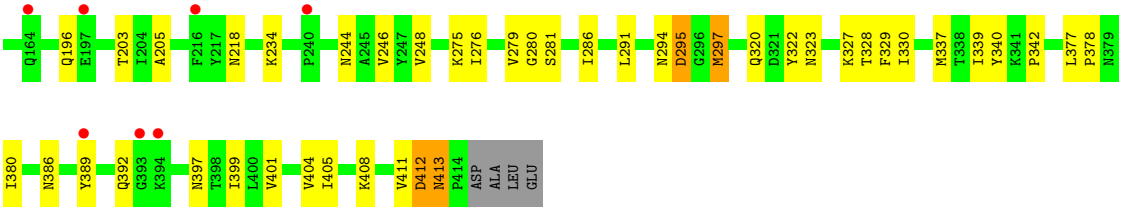
Chain B:



• Molecule 1: 46 kDa surface antigen

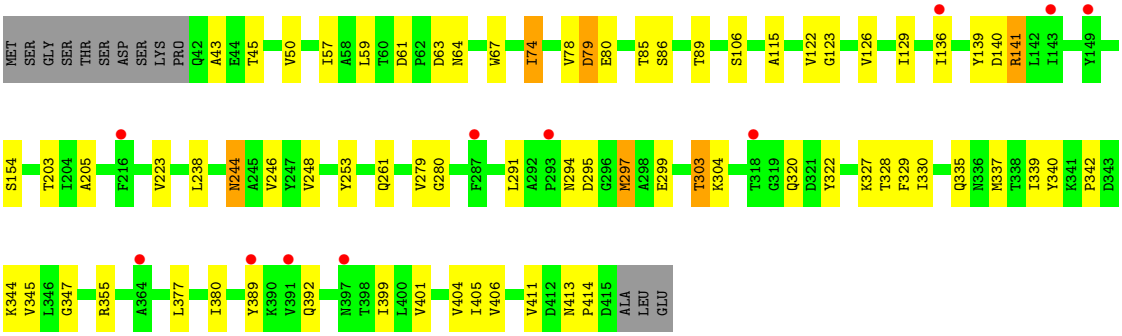
Chain S:





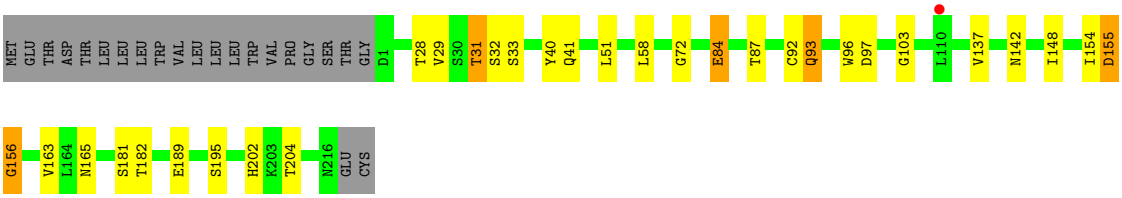
• Molecule 1: 46 kDa surface antigen

Chain T:



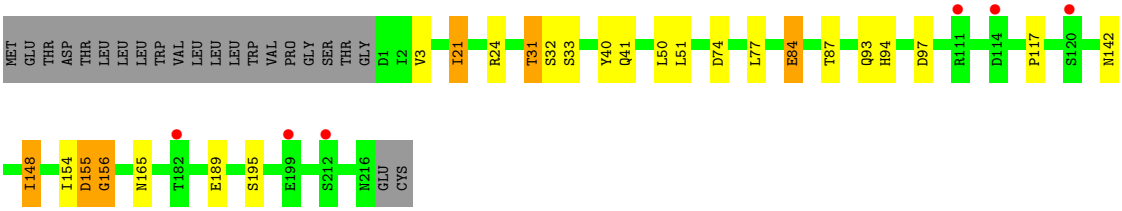
• Molecule 2: Immunoglobulin light chain

Chain C:



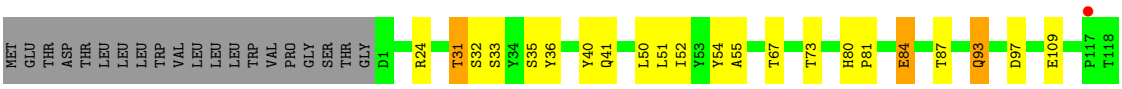
• Molecule 2: Immunoglobulin light chain

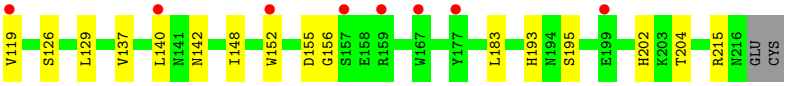
Chain I:



• Molecule 2: Immunoglobulin light chain

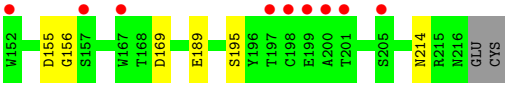
Chain M:





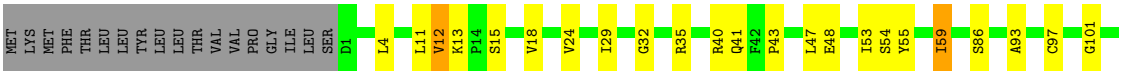
• Molecule 2: Immunoglobulin light chain

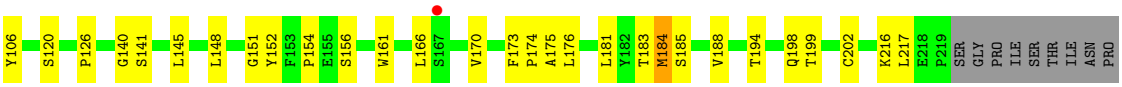
Chain Q:

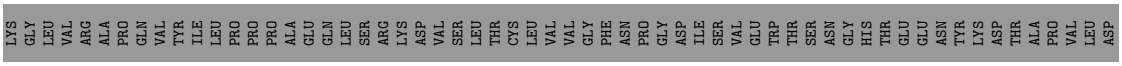


• Molecule 3: Immunoglobulin heavy chain

Chain D:

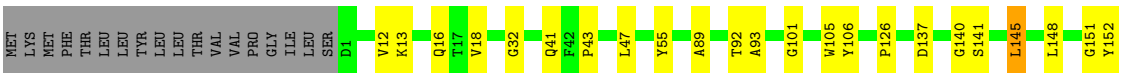


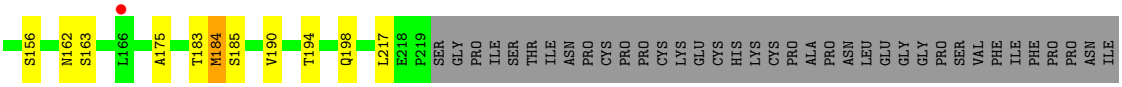




• Molecule 3: Immunoglobulin heavy chain

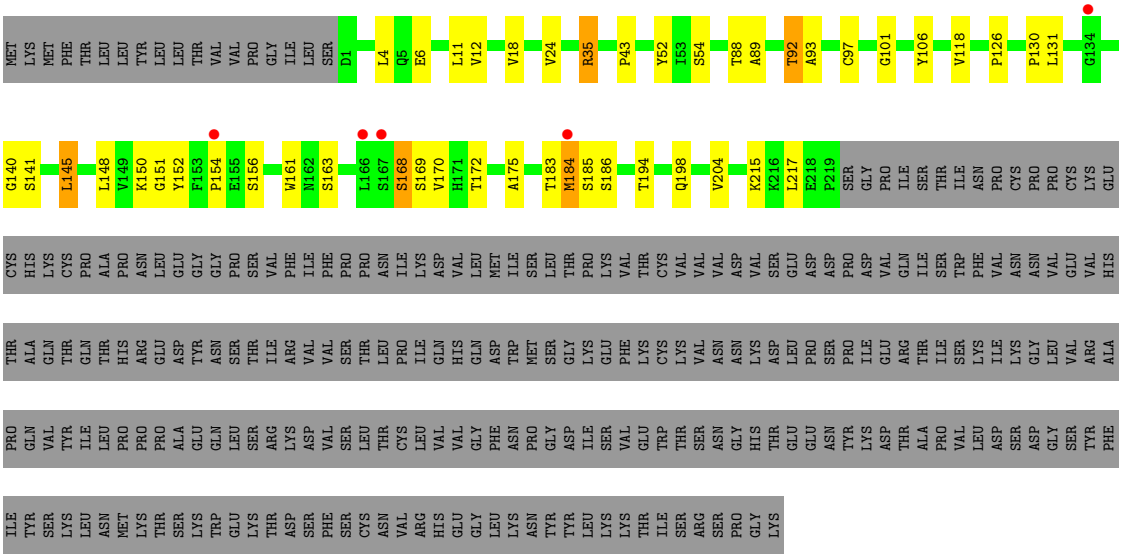
Chain E:





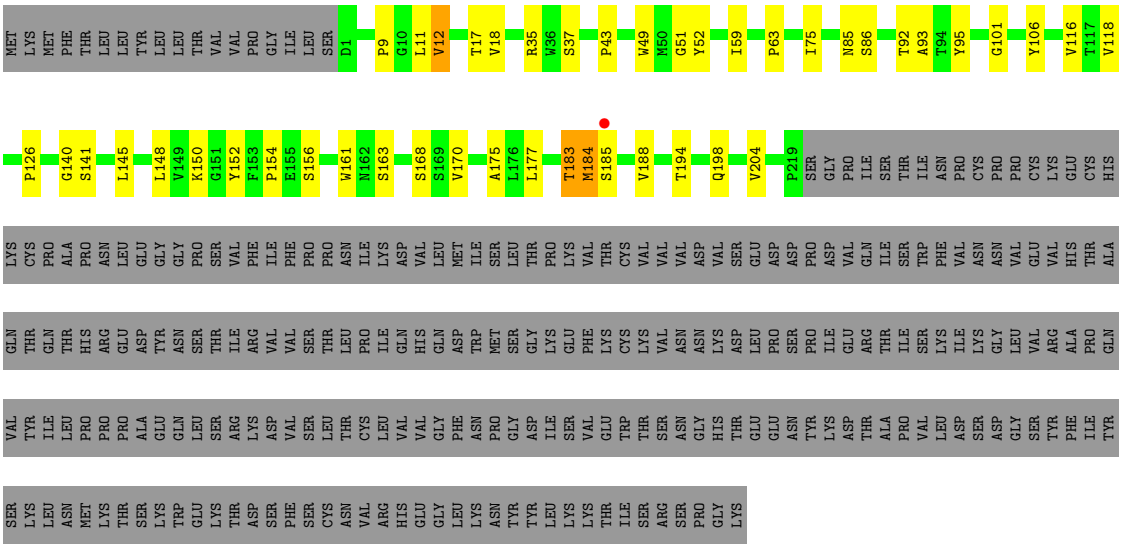
• Molecule 3: Immunoglobulin heavy chain

Chain N:



• Molecule 3: Immunoglobulin heavy chain

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	261.98Å 185.01Å 197.12Å 90.00° 134.43° 90.00°	Depositor
Resolution (Å)	29.00 – 3.50 98.30 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.00-3.50) 98.8 (98.30-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.17_3644, PHENIX 1.17_3644	Depositor
R, R_{free}	0.247 , 0.273 0.244 , 0.268	Depositor DCC
R_{free} test set	4665 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	99.0	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 71.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	24978	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, XYP

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	0.28	0/2946	0.47	0/3988
1	B	0.27	0/2946	0.46	0/3988
1	S	0.25	0/2938	0.44	0/3977
1	T	0.25	0/2946	0.44	0/3988
2	C	0.25	0/1725	0.44	0/2352
2	I	0.25	0/1725	0.44	0/2352
2	M	0.25	0/1725	0.45	0/2352
2	Q	0.25	0/1725	0.46	0/2352
3	D	0.26	0/1704	0.50	0/2341
3	E	0.26	0/1704	0.50	0/2341
3	N	0.25	0/1704	0.49	0/2341
3	R	0.26	0/1704	0.51	0/2341
All	All	0.26	0/25492	0.46	0/34713

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2894	0	2887	65	0
1	B	2894	0	2887	54	0
1	S	2887	0	2879	39	0
1	T	2895	0	2883	39	0
2	C	1682	0	1603	14	0
2	I	1682	0	1603	15	0
2	M	1682	0	1603	18	0
2	Q	1682	0	1603	12	0
3	D	1659	0	1612	26	0
3	E	1659	0	1612	16	0
3	N	1659	0	1612	23	0
3	R	1659	0	1612	25	0
4	A	10	0	0	2	0
4	B	10	0	0	1	0
4	S	10	0	0	1	0
4	T	10	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	S	1	0	0	0	0
5	T	1	0	0	0	0
All	All	24978	0	24396	328	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (328) 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:A:290:PHE:HB3	1:A:317:VAL:HG12	1.62	0.82
1:B:61:ASP:OD1	1:B:141:ARG:NH2	2.20	0.75
1:A:141:ARG:NH1	4:A:501:XYP:O3	2.19	0.75
3:N:92:THR:HG22	3:N:118:VAL:H	1.51	0.74
2:C:31:THR:O	2:C:33:SER:N	2.25	0.70
2:Q:31:THR:O	2:Q:33:SER:N	2.23	0.70
3:E:43:PRO:HD3	3:E:93:ALA:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:31:THR:O	2:M:33:SER:N	2.24	0.68
3:E:12:VAL:HG21	3:E:18:VAL:HG12	1.76	0.67
1:A:312:THR:OG1	1:A:334:ASP:OD1	2.13	0.67
1:S:294:ASN:HB3	1:S:297:MET:HG3	1.76	0.66
1:B:299:GLU:O	1:B:303:THR:OG1	2.13	0.65
3:N:12:VAL:HG11	3:N:18:VAL:HG12	1.77	0.65
3:N:4:LEU:HD22	3:N:24:VAL:HG22	1.77	0.65
3:D:4:LEU:HD22	3:D:24:VAL:HG22	1.78	0.64
2:I:31:THR:O	2:I:33:SER:N	2.30	0.64
1:A:377:LEU:HB3	1:A:380:ILE:HD13	1.81	0.63
1:A:54:SER:O	1:A:56:ARG:NH1	2.33	0.62
1:A:59:LEU:HB2	1:A:88:ILE:HG12	1.80	0.62
1:A:203:THR:HG22	1:A:291:LEU:HB3	1.80	0.61
1:A:366:ARG:NH1	1:A:398:THR:OG1	2.34	0.61
1:B:321:ASP:OD1	4:B:501:XYP:O2	2.18	0.61
3:D:43:PRO:HD3	3:D:93:ALA:HA	1.83	0.61
1:B:256:ALA:HB3	1:B:297:MET:HE1	1.82	0.61
2:C:97:ASP:HB2	1:S:328:THR:HG21	1.83	0.60
1:S:42:GLN:HG3	1:S:72:LYS:HE3	1.82	0.60
3:D:12:VAL:HG11	3:D:18:VAL:HG12	1.84	0.60
1:B:340:TYR:HB3	1:B:405:ILE:HG23	1.83	0.60
1:B:377:LEU:HB3	1:B:380:ILE:HD13	1.83	0.60
3:D:145:LEU:HD13	3:D:217:LEU:HD22	1.84	0.59
3:D:24:VAL:HG21	3:D:29:ILE:HD11	1.84	0.58
2:M:155:ASP:HA	2:M:195:SER:HB3	1.84	0.58
3:R:43:PRO:HD3	3:R:93:ALA:HA	1.84	0.58
1:A:74:ILE:HG22	1:A:347:GLY:HA3	1.84	0.58
3:N:194:THR:O	3:N:198:GLN:N	2.34	0.58
1:A:152:TYR:HD1	1:A:399:ILE:HB	1.70	0.57
1:B:300:GLN:HE21	2:Q:33:SER:HB3	1.69	0.57
2:M:41:GLN:HB2	2:M:51:LEU:HD11	1.86	0.57
1:A:140:ASP:OD2	4:A:501:XYP:O2	2.23	0.57
3:D:174:PRO:O	3:D:184:MET:HG3	2.05	0.57
3:N:175:ALA:HA	3:N:184:MET:HB2	1.86	0.57
3:R:92:THR:HG22	3:R:118:VAL:H	1.68	0.57
1:A:61:ASP:OD1	1:A:141:ARG:NH2	2.37	0.57
3:R:12:VAL:HG23	3:R:118:VAL:HG22	1.86	0.57
3:D:194:THR:O	3:D:198:GLN:N	2.36	0.57
1:T:141:ARG:NH1	4:T:501:XYP:O3	2.37	0.56
1:A:49:LYS:HB3	2:C:163:VAL:HG13	1.87	0.56
1:B:399:ILE:HD12	1:B:401:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:41:GLN:HB2	2:I:51:LEU:HD11	1.86	0.56
3:E:148:LEU:HA	3:E:185:SER:HB3	1.87	0.56
1:S:61:ASP:HB2	1:S:67:TRP:CD1	2.41	0.56
1:T:377:LEU:HB3	1:T:380:ILE:HD13	1.87	0.56
1:B:57:ILE:HG21	1:B:74:ILE:HD12	1.88	0.56
3:E:194:THR:O	3:E:198:GLN:N	2.38	0.56
2:C:155:ASP:HA	2:C:195:SER:HB3	1.86	0.56
3:D:148:LEU:HA	3:D:185:SER:HB3	1.88	0.56
1:A:320:GLN:HA	1:A:339:ILE:HG12	1.87	0.55
3:D:11:LEU:HB2	3:D:154:PRO:HG3	1.89	0.55
3:E:101:GLY:N	3:E:106:TYR:O	2.38	0.55
1:A:237:ASP:O	1:A:282:LYS:NZ	2.40	0.55
3:N:92:THR:HG22	3:N:118:VAL:N	2.21	0.55
3:R:148:LEU:HA	3:R:185:SER:HB3	1.90	0.54
1:T:139:TYR:O	1:T:141:ARG:N	2.40	0.54
1:B:126:VAL:HG23	1:B:136:ILE:HD13	1.89	0.54
1:S:57:ILE:HG21	1:S:74:ILE:HD12	1.89	0.54
1:T:261:GLN:HB2	1:T:304:LYS:HD2	1.89	0.54
1:T:340:TYR:HB3	1:T:405:ILE:HG23	1.89	0.54
3:D:175:ALA:HA	3:D:184:MET:HB2	1.89	0.54
1:B:318:THR:HB	1:B:337:MET:HE2	1.90	0.54
2:C:29:VAL:HG13	2:C:96:TRP:HB2	1.89	0.54
2:I:97:ASP:HB2	1:T:328:THR:HG21	1.90	0.54
3:R:12:VAL:HG11	3:R:18:VAL:HG12	1.90	0.54
1:A:47:LYS:HB3	3:D:176:LEU:HD21	1.90	0.54
3:E:175:ALA:HA	3:E:184:MET:HB2	1.90	0.54
1:T:126:VAL:HG23	1:T:136:ILE:HD13	1.89	0.54
1:A:252:ASN:HB3	1:A:255:THR:HG22	1.90	0.53
3:D:101:GLY:N	3:D:106:TYR:O	2.39	0.53
1:A:256:ALA:HB3	1:A:297:MET:HE1	1.91	0.53
3:R:175:ALA:HA	3:R:184:MET:HB2	1.90	0.53
3:N:145:LEU:HD13	3:N:217:LEU:HD22	1.91	0.53
1:S:320:GLN:HA	1:S:339:ILE:HG12	1.90	0.53
1:T:339:ILE:HD12	1:T:404:VAL:HG11	1.91	0.53
1:S:196:GLN:O	1:S:234:LYS:NZ	2.42	0.53
1:A:85:THR:HG22	1:A:86:SER:H	1.73	0.52
3:N:126:PRO:HB3	3:N:152:TYR:HB3	1.91	0.52
2:M:40:TYR:HE2	2:M:93:GLN:HG2	1.74	0.52
2:Q:40:TYR:HE2	2:Q:93:GLN:HG2	1.75	0.52
1:S:340:TYR:CZ	1:S:342:PRO:HB3	2.44	0.52
1:B:244:ASN:HD21	1:B:247:TYR:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:294:ASN:ND2	4:S:501:XYP:O4	2.42	0.52
3:R:184:MET:CE	3:R:185:SER:H	2.23	0.52
1:B:200:SER:HB3	1:B:236:ILE:HG13	1.92	0.52
1:S:399:ILE:HD12	1:S:401:VAL:HG13	1.92	0.52
1:A:59:LEU:HA	1:A:115:ALA:HB3	1.92	0.52
1:T:43:ALA:O	1:T:86:SER:OG	2.24	0.52
3:N:151:GLY:H	3:N:183:THR:HG22	1.75	0.52
2:Q:41:GLN:HB2	2:Q:51:LEU:HD11	1.92	0.52
2:I:93:GLN:NE2	3:E:105:TRP:O	2.43	0.51
1:A:126:VAL:HG23	1:A:136:ILE:HD13	1.92	0.51
3:N:11:LEU:HB2	3:N:154:PRO:HG3	1.91	0.51
3:E:101:GLY:HA3	3:E:106:TYR:CE2	2.45	0.51
2:Q:117:PRO:HG3	2:Q:148:ILE:HD11	1.92	0.51
1:S:123:GLY:O	1:S:127:ASN:HB2	2.10	0.51
1:T:320:GLN:HA	1:T:339:ILE:HG12	1.93	0.51
1:S:412:ASP:O	1:S:413:ASN:ND2	2.41	0.51
1:B:412:ASP:HB2	2:I:3:VAL:HG11	1.91	0.51
1:A:205:ALA:O	1:A:248:VAL:HG12	2.11	0.51
2:I:155:ASP:HA	2:I:195:SER:HB3	1.92	0.50
1:A:194:MET:HE3	1:A:195:PRO:HD2	1.93	0.50
1:A:208:GLN:HB2	1:B:244:ASN:HB3	1.91	0.50
1:B:312:THR:OG1	1:B:334:ASP:OD1	2.30	0.50
1:S:45:THR:OG1	1:S:79:ASP:OD1	2.30	0.50
1:S:340:TYR:HB3	1:S:405:ILE:HG23	1.94	0.50
2:M:84:GLU:O	2:M:87:THR:HG22	2.12	0.50
1:T:205:ALA:O	1:T:248:VAL:HG12	2.11	0.50
1:T:253:TYR:HA	1:T:297:MET:HE1	1.93	0.50
1:A:62:PRO:HB3	1:A:88:ILE:HG22	1.93	0.50
3:R:184:MET:HE3	3:R:185:SER:H	1.76	0.50
1:B:139:TYR:O	1:B:141:ARG:N	2.45	0.50
1:T:85:THR:HG22	1:T:86:SER:H	1.76	0.50
1:S:152:TYR:HD1	1:S:399:ILE:HB	1.77	0.49
1:S:126:VAL:HG23	1:S:136:ILE:HD13	1.94	0.49
1:S:295:ASP:OD1	1:S:295:ASP:N	2.42	0.49
1:A:168:LEU:HD23	1:A:224:LEU:HD21	1.94	0.49
3:D:173:PHE:HB2	3:D:184:MET:SD	2.53	0.49
1:A:326:ALA:HA	1:A:329:PHE:HB2	1.94	0.49
2:I:97:ASP:CB	1:T:328:THR:HG21	2.43	0.49
1:B:205:ALA:O	1:B:248:VAL:HG12	2.13	0.49
1:B:237:ASP:O	1:B:282:LYS:NZ	2.46	0.49
1:B:389:TYR:CD2	1:B:399:ILE:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:117:PRO:HG3	2:I:148:ILE:HD11	1.96	0.48
1:T:339:ILE:HG22	1:T:406:VAL:HG23	1.96	0.48
2:M:202:HIS:CE1	2:M:204:THR:HG1	2.31	0.48
1:S:339:ILE:HD12	1:S:404:VAL:HG11	1.95	0.48
1:A:244:ASN:C	1:A:246:VAL:H	2.16	0.48
1:A:317:VAL:HG23	1:A:335:GLN:HA	1.95	0.48
1:B:152:TYR:HD1	1:B:399:ILE:HB	1.78	0.48
1:B:177:ASP:OD1	1:B:177:ASP:N	2.47	0.48
3:N:168:SER:OG	3:N:169:SER:N	2.46	0.48
1:A:317:VAL:CG2	1:A:335:GLN:HA	2.43	0.48
1:B:45:THR:HG21	1:B:84:ALA:H	1.79	0.48
3:R:101:GLY:HA3	3:R:106:TYR:CE2	2.49	0.48
3:D:32:GLY:HA2	3:D:55:TYR:CG	2.49	0.48
3:E:32:GLY:HA2	3:E:55:TYR:CG	2.47	0.48
1:S:205:ALA:O	1:S:248:VAL:HG12	2.13	0.48
1:A:108:ALA:HB1	1:A:134:ILE:HD11	1.95	0.48
2:I:154:ILE:O	2:I:156:GLY:N	2.47	0.48
3:R:17:THR:HG22	3:R:85:ASN:HA	1.95	0.48
1:B:320:GLN:HA	1:B:339:ILE:HG12	1.94	0.47
3:R:93:ALA:HB3	3:R:95:TYR:CE1	2.49	0.47
3:D:161:TRP:CZ3	3:D:202:CYS:HB3	2.48	0.47
1:A:295:ASP:OD1	1:A:320:GLN:N	2.45	0.47
2:C:40:TYR:HE2	2:C:93:GLN:HG2	1.80	0.47
2:C:154:ILE:O	2:C:156:GLY:N	2.48	0.47
3:D:151:GLY:HA2	3:D:181:LEU:HB3	1.97	0.47
2:M:126:SER:HA	2:M:129:LEU:HD12	1.96	0.47
2:Q:35:SER:HB2	2:Q:55:ALA:HB2	1.96	0.47
1:A:43:ALA:O	1:A:86:SER:OG	2.27	0.47
1:B:339:ILE:HD12	1:B:404:VAL:HG11	1.95	0.47
3:D:13:LYS:HG2	3:D:120:SER:HA	1.96	0.47
1:B:262:SER:O	1:B:266:ILE:HG23	2.15	0.47
3:E:13:LYS:O	3:E:16:GLN:HG2	2.14	0.47
2:M:36:TYR:HE2	2:M:54:TYR:HH	1.62	0.47
1:S:294:ASN:HB3	1:S:297:MET:CG	2.45	0.47
1:T:342:PRO:HG2	1:T:345:VAL:HG22	1.97	0.47
1:S:129:ILE:HG13	1:S:136:ILE:HD11	1.97	0.47
1:A:328:THR:HG21	2:M:97:ASP:CB	2.44	0.47
1:S:377:LEU:HB3	1:S:380:ILE:HD13	1.98	0.46
1:T:399:ILE:HD12	1:T:401:VAL:HG13	1.96	0.46
2:Q:31:THR:O	2:Q:31:THR:OG1	2.28	0.46
1:T:299:GLU:O	1:T:303:THR:OG1	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:151:GLY:H	3:E:183:THR:HG22	1.80	0.46
2:M:40:TYR:CE1	2:M:50:LEU:HD12	2.50	0.46
2:C:41:GLN:HB2	2:C:51:LEU:HD11	1.97	0.46
3:R:9:PRO:O	3:R:116:VAL:HG12	2.16	0.46
1:T:129:ILE:HG13	1:T:136:ILE:HD11	1.97	0.46
1:T:74:ILE:HG22	1:T:347:GLY:HA3	1.97	0.46
3:N:43:PRO:HD3	3:N:93:ALA:HA	1.97	0.46
1:T:330:ILE:HA	1:T:335:GLN:O	2.16	0.46
1:A:384:TYR:HE1	1:A:398:THR:HG22	1.81	0.46
1:B:344:LYS:HE3	1:B:344:LYS:H	1.80	0.46
3:N:148:LEU:HA	3:N:185:SER:HB3	1.97	0.46
3:R:11:LEU:HB2	3:R:154:PRO:HG3	1.98	0.46
3:R:194:THR:O	3:R:198:GLN:N	2.47	0.46
1:A:75:ILE:HD11	1:A:86:SER:HB3	1.97	0.46
2:C:28:THR:HG23	2:C:72:GLY:HA2	1.98	0.46
2:I:84:GLU:O	2:I:87:THR:HG22	2.16	0.46
3:R:92:THR:HG22	3:R:118:VAL:N	2.31	0.46
1:A:260:ILE:HD13	1:A:301:ALA:HA	1.97	0.45
1:S:154:SER:OG	1:S:155:PHE:N	2.49	0.45
3:R:161:TRP:CD2	3:R:188:VAL:HG21	2.51	0.45
2:C:84:GLU:O	2:C:87:THR:HG22	2.16	0.45
1:T:322:TYR:CZ	1:T:327:LYS:HD3	2.51	0.45
2:Q:24:ARG:HG3	2:Q:73:THR:HG23	1.99	0.45
3:R:101:GLY:N	3:R:106:TYR:O	2.47	0.45
1:T:115:ALA:HB2	1:T:139:TYR:HB3	1.97	0.45
2:M:137:VAL:HG21	3:N:131:LEU:HD13	1.99	0.45
3:R:35:ARG:HD3	3:R:52:TYR:CE1	2.52	0.45
1:B:154:SER:OG	1:B:155:PHE:N	2.49	0.45
2:C:97:ASP:CB	1:S:328:THR:HG21	2.45	0.45
1:S:389:TYR:CD2	1:S:399:ILE:HD13	2.52	0.45
1:B:221:MET:HA	1:B:224:LEU:HB2	1.98	0.45
1:S:139:TYR:O	1:S:141:ARG:N	2.50	0.45
1:A:330:ILE:HA	1:A:335:GLN:O	2.16	0.45
1:B:140:ASP:HA	1:B:154:SER:HB2	1.98	0.45
2:I:24:ARG:HH12	2:Q:98:ILE:HG13	1.81	0.45
3:D:126:PRO:HB3	3:D:152:TYR:HB3	1.99	0.45
2:Q:155:ASP:HA	2:Q:195:SER:HB3	1.98	0.45
1:S:330:ILE:HD13	1:S:408:LYS:O	2.17	0.45
1:B:154:SER:O	1:B:401:VAL:HA	2.17	0.44
1:B:251:TRP:HZ3	1:B:294:ASN:HB2	1.82	0.44
3:D:170:VAL:HG13	3:D:188:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:294:ASN:OD1	1:T:295:ASP:N	2.50	0.44
1:B:62:PRO:HD2	1:B:90:LYS:HB2	1.99	0.44
1:S:203:THR:HG22	1:S:291:LEU:HB3	1.98	0.44
1:T:203:THR:HG22	1:T:291:LEU:HB3	1.98	0.44
1:A:340:TYR:CZ	1:A:342:PRO:HB3	2.52	0.44
3:N:150:LYS:HD2	3:N:183:THR:HB	1.98	0.44
1:A:77:TYR:CD1	1:A:348:LYS:HG2	2.52	0.44
1:S:85:THR:HG22	1:S:86:SER:H	1.82	0.44
1:A:62:PRO:HD2	1:A:90:LYS:HB2	2.00	0.44
2:M:35:SER:HB2	2:M:55:ALA:HB2	1.99	0.44
2:Q:84:GLU:O	2:Q:87:THR:HG22	2.18	0.44
3:D:35:ARG:HA	3:D:54:SER:HA	1.99	0.44
3:N:35:ARG:HD2	3:N:52:TYR:CE1	2.53	0.44
1:T:238:LEU:HD22	1:T:279:VAL:HG21	1.98	0.44
1:B:326:ALA:HA	1:B:329:PHE:HB2	2.00	0.44
3:R:37:SER:HA	3:R:52:TYR:HA	1.99	0.44
3:R:126:PRO:HB3	3:R:152:TYR:HB3	1.99	0.43
1:T:59:LEU:HD11	1:T:74:ILE:HD11	2.00	0.43
3:D:161:TRP:CH2	3:D:202:CYS:HB3	2.53	0.43
2:I:21:ILE:HG23	2:I:77:LEU:HB3	2.00	0.43
1:A:122:VAL:O	1:A:126:VAL:HG12	2.18	0.43
1:T:57:ILE:HG21	1:T:74:ILE:HD12	1.99	0.43
2:M:152:TRP:CG	2:M:183:LEU:HD12	2.54	0.43
3:N:88:THR:OG1	3:N:89:ALA:N	2.52	0.43
1:B:327:LYS:O	1:B:330:ILE:HG13	2.19	0.43
1:B:394:LYS:O	1:B:394:LYS:HG2	2.19	0.43
2:I:93:GLN:HG2	2:I:94:HIS:N	2.32	0.43
1:T:340:TYR:CZ	1:T:342:PRO:HB3	2.53	0.43
1:A:58:ALA:HB2	1:A:99:LEU:HD21	2.00	0.43
2:C:137:VAL:HG12	2:C:182:THR:HG23	2.01	0.43
1:S:339:ILE:O	1:S:339:ILE:HG13	2.18	0.43
1:T:389:TYR:CD2	1:T:399:ILE:HD13	2.53	0.43
1:A:321:ASP:OD1	1:A:321:ASP:N	2.50	0.43
1:B:78:VAL:C	1:B:80:GLU:H	2.22	0.43
1:A:344:LYS:HE3	1:A:344:LYS:H	1.84	0.42
3:D:53:ILE:HG13	3:D:59:ILE:HG22	2.01	0.42
3:E:184:MET:HE3	3:E:185:SER:H	1.83	0.42
1:S:160:VAL:HG23	1:S:404:VAL:HG21	2.01	0.42
1:B:119:GLY:O	1:B:122:VAL:HG23	2.18	0.42
1:B:356:VAL:HG21	1:B:369:VAL:HG12	2.00	0.42
1:A:221:MET:HB3	1:A:225:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:CE1	1:B:346:LEU:HD22	2.54	0.42
3:R:49:TRP:CZ2	3:R:51:GLY:HA2	2.54	0.42
1:S:279:VAL:O	1:S:281:SER:N	2.52	0.42
1:A:322:TYR:CZ	1:A:327:LYS:HD3	2.55	0.42
1:B:155:PHE:HB3	1:B:404:VAL:HG22	2.01	0.42
3:N:130:PRO:HD3	3:N:215:LYS:HG2	2.01	0.42
1:T:45:THR:OG1	1:T:79:ASP:OD1	2.38	0.42
1:S:275:LYS:HA	1:S:286:ILE:HA	2.01	0.42
1:B:85:THR:OG1	1:B:86:SER:N	2.53	0.42
3:D:41:GLN:HB2	3:D:47:LEU:HD13	2.02	0.42
1:S:322:TYR:CZ	1:S:327:LYS:HD3	2.54	0.42
3:D:199:THR:HB	3:D:216:LYS:HE3	2.01	0.42
2:M:24:ARG:HG3	2:M:73:THR:HG23	2.01	0.42
1:T:78:VAL:C	1:T:80:GLU:H	2.23	0.42
1:A:204:ILE:HD11	1:A:297:MET:HB3	2.01	0.42
1:B:163:LEU:O	1:B:167:SER:OG	2.35	0.42
2:I:40:TYR:CE2	2:I:50:LEU:HD12	2.55	0.42
3:E:89:ALA:O	3:E:92:THR:HG22	2.20	0.42
3:N:6:GLU:OE1	3:N:6:GLU:N	2.53	0.42
1:S:295:ASP:HB2	1:S:323:ASN:ND2	2.34	0.42
1:A:352:GLU:HA	1:A:355:ARG:HB2	2.00	0.41
1:B:125:ALA:O	1:B:129:ILE:HG23	2.19	0.41
1:T:63:ASP:OD1	1:T:64:ASN:N	2.53	0.41
1:A:199:ILE:HD13	1:A:288:LYS:HD3	2.03	0.41
1:A:207:SER:O	1:A:213:SER:OG	2.37	0.41
3:N:172:THR:HG22	3:N:186:SER:OG	2.21	0.41
1:S:294:ASN:OD1	1:S:295:ASP:N	2.53	0.41
1:T:61:ASP:HB2	1:T:67:TRP:CD1	2.55	0.41
1:B:253:TYR:HA	1:B:297:MET:HE1	2.02	0.41
1:B:320:GLN:O	1:B:322:TYR:N	2.53	0.41
1:T:244:ASN:C	1:T:246:VAL:H	2.21	0.41
1:A:399:ILE:HD12	1:A:401:VAL:HG13	2.03	0.41
2:C:92:CYS:O	2:C:103:GLY:N	2.53	0.41
1:A:45:THR:CG2	1:A:84:ALA:H	2.34	0.41
1:A:60:THR:HA	1:A:89:THR:O	2.20	0.41
1:A:78:VAL:C	1:A:80:GLU:H	2.24	0.41
2:I:24:ARG:NH2	3:R:63:PRO:HG2	2.36	0.41
2:M:193:HIS:O	2:M:215:ARG:NH1	2.54	0.41
3:N:35:ARG:HA	3:N:54:SER:HA	2.02	0.41
3:R:150:LYS:HD2	3:R:183:THR:OG1	2.20	0.41
1:S:397:ASN:O	1:S:399:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:HIS:CE1	2:C:204:THR:HG1	2.37	0.41
3:N:101:GLY:N	3:N:106:TYR:O	2.40	0.41
3:E:145:LEU:HD13	3:E:217:LEU:HD22	2.01	0.41
3:R:93:ALA:HB3	3:R:95:TYR:HE1	1.85	0.41
1:A:208:GLN:HE22	1:B:208:GLN:NE2	2.18	0.41
1:A:281:SER:HB2	1:B:395:ASN:N	2.36	0.41
1:A:368:GLU:OE1	1:A:368:GLU:N	2.53	0.41
1:B:45:THR:CG2	1:B:84:ALA:H	2.33	0.41
3:D:40:ARG:HD2	3:D:48:GLU:OE1	2.21	0.41
1:B:78:VAL:O	1:B:80:GLU:N	2.53	0.41
3:E:126:PRO:HB3	3:E:152:TYR:HB3	2.02	0.41
3:N:12:VAL:HG23	3:N:118:VAL:HG22	2.03	0.41
1:A:45:THR:HG21	1:A:84:ALA:H	1.86	0.40
1:A:60:THR:OG1	1:A:61:ASP:N	2.54	0.40
1:B:253:TYR:HA	1:B:297:MET:CE	2.51	0.40
3:D:15:SER:O	3:D:86:SER:HA	2.20	0.40
1:A:114:ILE:HB	1:A:143:ILE:HD11	2.03	0.40
1:A:328:THR:HA	1:A:331:LYS:HB2	2.03	0.40
1:B:261:GLN:HB2	1:B:304:LYS:HD2	2.03	0.40
1:S:386:ASN:OD1	1:S:386:ASN:N	2.53	0.40
1:A:389:TYR:CD2	1:A:399:ILE:HD13	2.57	0.40
1:A:389:TYR:HB2	1:A:399:ILE:HG21	2.04	0.40
2:M:93:GLN:HE21	2:M:93:GLN:HB2	1.59	0.40
3:R:75:ILE:HG21	1:T:50:VAL:HB	2.02	0.40
1:S:244:ASN:C	1:S:246:VAL:H	2.22	0.40
1:T:85:THR:HG22	1:T:86:SER:N	2.37	0.40
1:T:154:SER:O	1:T:401:VAL:HA	2.21	0.40
1:A:365:SER:HB3	1:A:368:GLU:CD	2.41	0.40
2:M:80:HIS:HA	2:M:81:PRO:HA	1.95	0.40
1:B:244:ASN:HD22	1:B:245:ALA:N	2.20	0.40
1:B:300:GLN:NE2	2:Q:33:SER:HB3	2.35	0.40
3:E:41:GLN:HB2	3:E:47:LEU:HD23	2.03	0.40
2:M:119:VAL:HG13	2:M:140:LEU:HG	2.03	0.40
1:T:294:ASN:HB3	1:T:297:MET:HG3	2.03	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	372/387 (96%)	326 (88%)	41 (11%)	5 (1%)	12	48
1	B	372/387 (96%)	333 (90%)	34 (9%)	5 (1%)	12	48
1	S	371/387 (96%)	334 (90%)	32 (9%)	5 (1%)	12	48
1	T	372/387 (96%)	336 (90%)	30 (8%)	6 (2%)	9	43
2	C	214/238 (90%)	192 (90%)	18 (8%)	4 (2%)	8	40
2	I	214/238 (90%)	194 (91%)	16 (8%)	4 (2%)	8	40
2	M	214/238 (90%)	193 (90%)	18 (8%)	3 (1%)	11	46
2	Q	214/238 (90%)	193 (90%)	18 (8%)	3 (1%)	11	46
3	D	217/474 (46%)	197 (91%)	17 (8%)	3 (1%)	11	46
3	E	217/474 (46%)	199 (92%)	13 (6%)	5 (2%)	6	36
3	N	217/474 (46%)	196 (90%)	15 (7%)	6 (3%)	5	32
3	R	217/474 (46%)	194 (89%)	17 (8%)	6 (3%)	5	32
All	All	3211/4396 (73%)	2887 (90%)	269 (8%)	55 (2%)	9	42

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	156	SER
3	E	156	SER
3	N	156	SER
3	N	168	SER
2	Q	32	SER
3	R	156	SER
1	A	392	GLN
1	B	392	GLN
1	B	395	ASN
2	I	32	SER
2	M	32	SER
3	N	92	THR

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Mol	Chain	Res	Type
1	S	123	GLY
1	S	280	GLY
1	S	392	GLN
1	T	123	GLY
1	T	140	ASP
1	T	392	GLN
1	A	395	ASN
2	C	32	SER
2	C	155	ASP
3	D	141	SER
2	I	155	ASP
3	N	141	SER
3	N	163	SER
3	R	141	SER
3	R	163	SER
3	R	168	SER
1	S	140	ASP
1	T	414	PRO
1	A	79	ASP
1	B	79	ASP
1	B	320	GLN
2	C	142	ASN
2	I	142	ASN
3	E	141	SER
3	E	162	ASN
3	E	163	SER
1	T	280	GLY
1	A	389	TYR
2	M	142	ASN
2	Q	142	ASN
1	B	140	ASP
2	M	156	GLY
2	Q	156	GLY
3	R	86	SER
1	T	79	ASP
2	C	156	GLY
2	I	156	GLY
1	A	411	VAL
3	E	140	GLY
3	N	140	GLY
3	R	140	GLY
3	D	140	GLY

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Mol	Chain	Res	Type
1	S	378	PRO

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	316/327 (97%)	295 (93%)	21 (7%)	16	49
1	B	316/327 (97%)	295 (93%)	21 (7%)	16	49
1	S	315/327 (96%)	301 (96%)	14 (4%)	28	62
1	T	316/327 (97%)	301 (95%)	15 (5%)	26	60
2	C	192/212 (91%)	184 (96%)	8 (4%)	30	63
2	I	192/212 (91%)	185 (96%)	7 (4%)	35	66
2	M	192/212 (91%)	185 (96%)	7 (4%)	35	66
2	Q	192/212 (91%)	184 (96%)	8 (4%)	30	63
3	D	193/431 (45%)	187 (97%)	6 (3%)	40	70
3	E	193/431 (45%)	189 (98%)	4 (2%)	53	79
3	N	193/431 (45%)	186 (96%)	7 (4%)	35	66
3	R	193/431 (45%)	185 (96%)	8 (4%)	30	63
All	All	2803/3880 (72%)	2677 (96%)	126 (4%)	27	61

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	THR
1	A	89	THR
1	A	106	SER
1	A	122	VAL
1	A	127	ASN
1	A	129	ILE
1	A	223	VAL
1	A	224	LEU
1	A	244	ASN

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Mol	Chain	Res	Type
1	A	295	ASP
1	A	297	MET
1	A	321	ASP
1	A	329	PHE
1	A	337	MET
1	A	344	LYS
1	A	388	THR
1	A	394	LYS
1	A	398	THR
1	A	399	ILE
1	A	401	VAL
1	A	411	VAL
1	B	61	ASP
1	B	85	THR
1	B	89	THR
1	B	122	VAL
1	B	127	ASN
1	B	141	ARG
1	B	150	ASP
1	B	167	SER
1	B	223	VAL
1	B	224	LEU
1	B	266	ILE
1	B	276	ILE
1	B	297	MET
1	B	303	THR
1	B	329	PHE
1	B	337	MET
1	B	344	LYS
1	B	394	LYS
1	B	401	VAL
1	B	411	VAL
1	B	412	ASP
2	C	31	THR
2	C	58	LEU
2	C	84	GLU
2	C	93	GLN
2	C	148	ILE
2	C	165	ASN
2	C	181	SER
2	C	189	GLU
3	D	12	VAL

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Mol	Chain	Res	Type
3	D	59	ILE
3	D	97	CYS
3	D	166	LEU
3	D	183	THR
3	D	184	MET
2	I	21	ILE
2	I	31	THR
2	I	74	ASP
2	I	84	GLU
2	I	148	ILE
2	I	165	ASN
2	I	189	GLU
3	E	137	ASP
3	E	145	LEU
3	E	184	MET
3	E	190	VAL
2	M	31	THR
2	M	52	ILE
2	M	67	THR
2	M	84	GLU
2	M	93	GLN
2	M	109	GLU
2	M	148	ILE
3	N	35	ARG
3	N	97	CYS
3	N	145	LEU
3	N	161	TRP
3	N	170	VAL
3	N	184	MET
3	N	204	VAL
2	Q	1	ASP
2	Q	31	THR
2	Q	52	ILE
2	Q	74	ASP
2	Q	148	ILE
2	Q	169	ASP
2	Q	189	GLU
2	Q	214	ASN
3	R	12	VAL
3	R	59	ILE
3	R	145	LEU
3	R	170	VAL

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Mol	Chain	Res	Type
3	R	177	LEU
3	R	183	THR
3	R	184	MET
3	R	204	VAL
1	S	82	GLU
1	S	89	THR
1	S	106	SER
1	S	122	VAL
1	S	127	ASN
1	S	218	ASN
1	S	276	ILE
1	S	295	ASP
1	S	297	MET
1	S	329	PHE
1	S	337	MET
1	S	411	VAL
1	S	412	ASP
1	S	413	ASN
1	T	74	ILE
1	T	89	THR
1	T	106	SER
1	T	122	VAL
1	T	141	ARG
1	T	223	VAL
1	T	244	ASN
1	T	297	MET
1	T	303	THR
1	T	329	PHE
1	T	337	MET
1	T	344	LYS
1	T	355	ARG
1	T	411	VAL
1	T	413	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	371	ASN
1	B	300	GLN
2	Q	93	GLN
1	T	371	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	XYP	B	501	-	10,10,10	2.31	3 (30%)	14,14,14	1.17	1 (7%)
4	XYP	A	501	-	10,10,10	2.14	2 (20%)	14,14,14	1.11	2 (14%)
4	XYP	S	501	-	10,10,10	2.00	2 (20%)	14,14,14	1.14	2 (14%)
4	XYP	T	501	-	10,10,10	2.09	2 (20%)	14,14,14	1.00	1 (7%)

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
4	XYP	B	501	-	-	-	0/1/1/1
4	XYP	A	501	-	-	-	0/1/1/1
4	XYP	S	501	-	-	-	0/1/1/1
4	XYP	T	501	-	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	XYP	O5-C1	5.71	1.51	1.43
4	A	501	XYP	O5-C1	5.23	1.50	1.43
4	T	501	XYP	O5-C1	5.19	1.50	1.43
4	S	501	XYP	O5-C1	4.95	1.49	1.43
4	A	501	XYP	O5-C5	3.32	1.49	1.43
4	B	501	XYP	O5-C5	3.21	1.48	1.43
4	T	501	XYP	O5-C5	3.09	1.48	1.43
4	S	501	XYP	O5-C5	2.88	1.48	1.43
4	B	501	XYP	C4-C3	-2.38	1.49	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	501	XYP	C5-C4-C3	3.11	113.49	109.67
4	B	501	XYP	O5-C1-C2	3.05	113.97	109.43
4	A	501	XYP	C5-C4-C3	2.95	113.29	109.67
4	A	501	XYP	O5-C5-C4	2.32	114.35	110.77
4	T	501	XYP	C5-C4-C3	2.16	112.33	109.67
4	S	501	XYP	O5-C5-C4	2.11	114.03	110.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

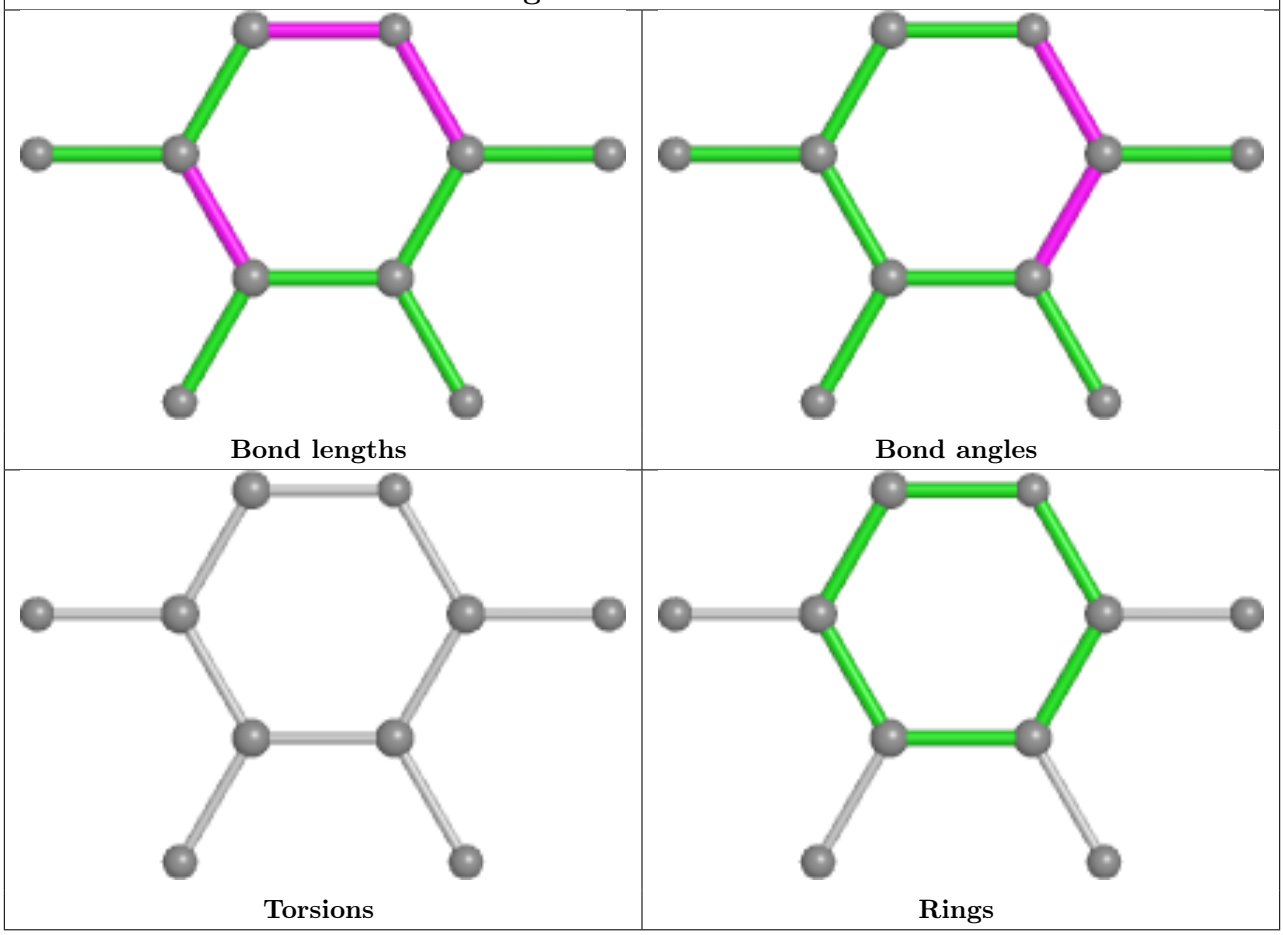
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	XYP	1	0
4	A	501	XYP	2	0
4	S	501	XYP	1	0
4	T	501	XYP	1	0

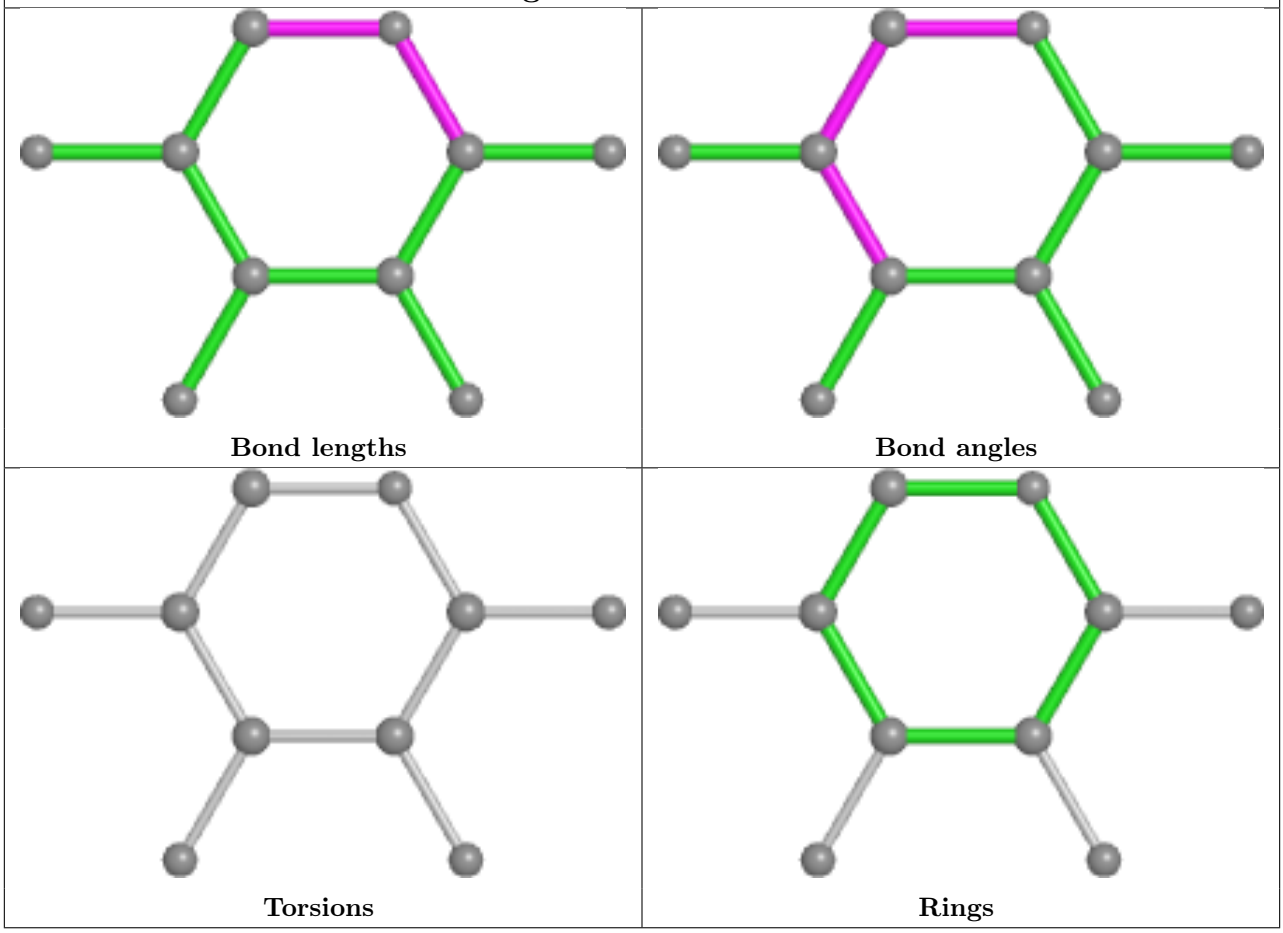
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

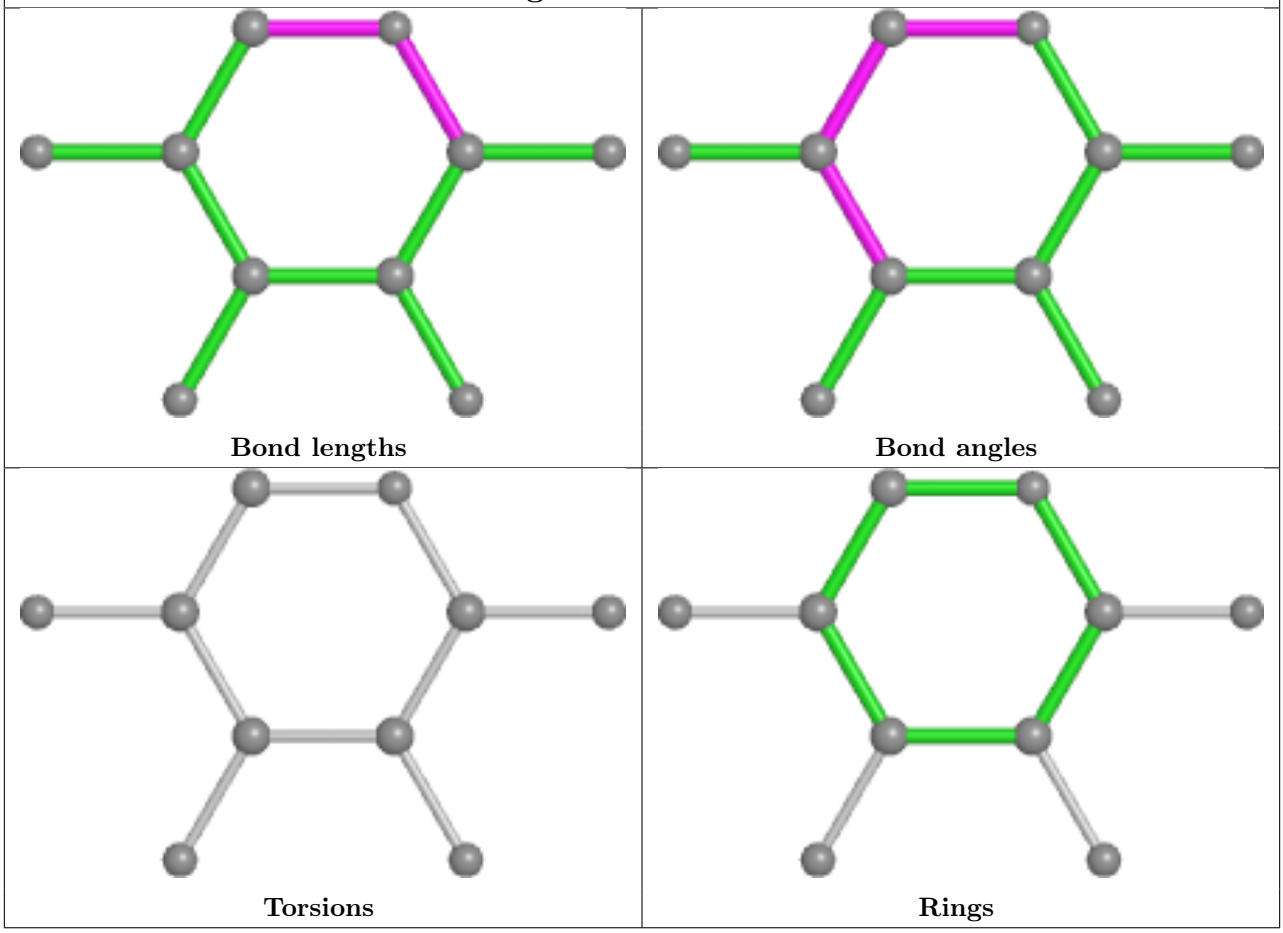
Ligand XYP B 501

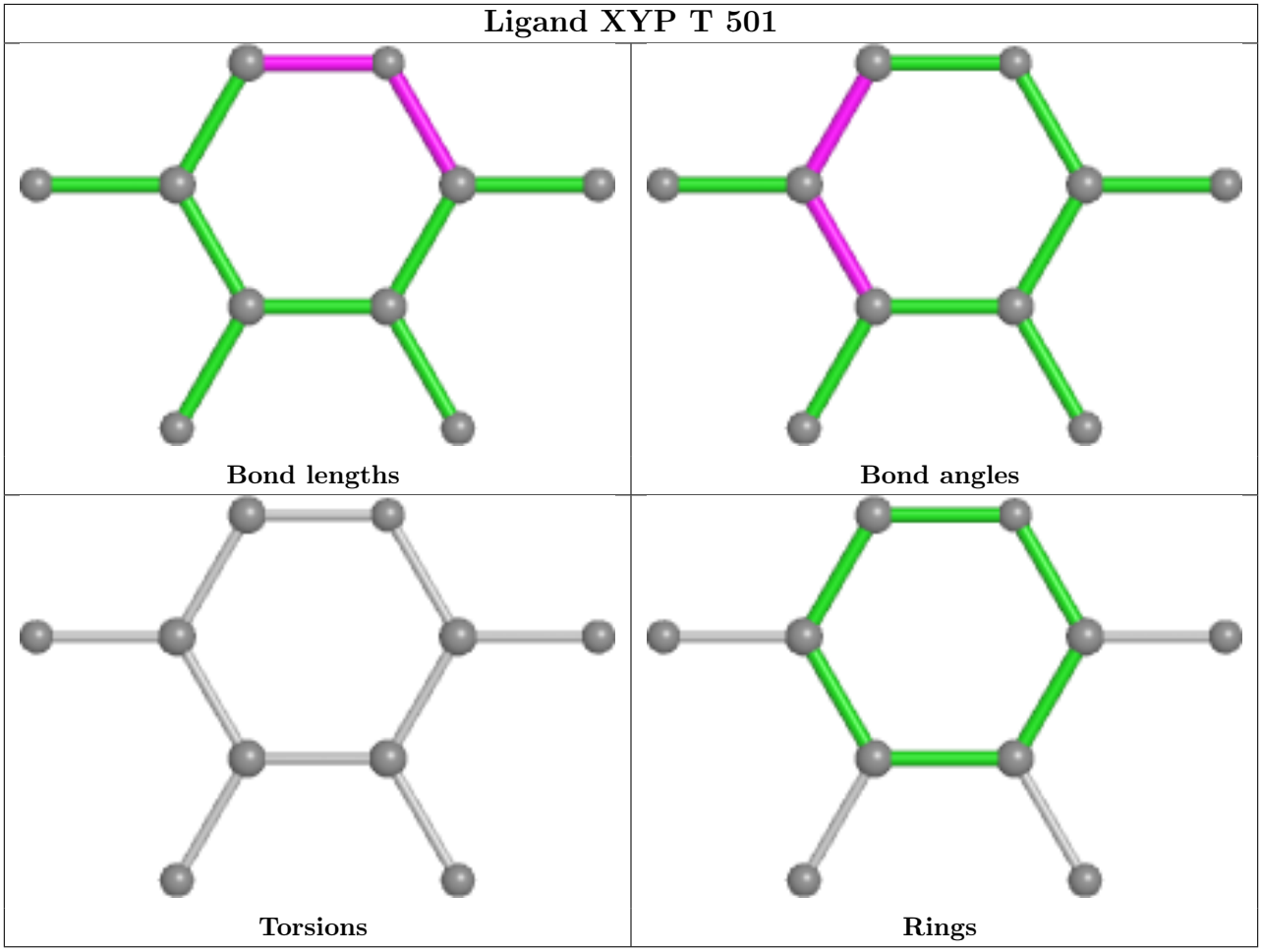


Ligand XYP A 501



Ligand XYP S 501





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 (i)

6.1 Protein, DNA and RNA chains (i)

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	374/387 (96%)	0.04	0	100	100	47, 72, 113, 131	0
1	B	374/387 (96%)	0.07	0	100	100	51, 74, 110, 133	0
1	S	373/387 (96%)	0.39	12 (3%)	47	42	80, 119, 149, 161	0
1	T	370/387 (95%)	0.40	11 (2%)	50	44	74, 125, 155, 168	0
2	C	216/238 (90%)	0.29	1 (0%)	91	88	76, 105, 130, 136	0
2	I	216/238 (90%)	0.34	6 (2%)	53	47	72, 108, 133, 140	0
2	M	216/238 (90%)	0.50	9 (4%)	36	32	62, 116, 155, 174	0
2	Q	216/238 (90%)	0.52	12 (5%)	24	22	58, 121, 155, 175	0
3	D	219/474 (46%)	0.23	1 (0%)	91	88	69, 96, 144, 176	0
3	E	219/474 (46%)	0.20	1 (0%)	91	88	66, 99, 146, 173	0
3	N	219/474 (46%)	0.34	5 (2%)	60	54	60, 100, 140, 168	0
3	R	218/474 (45%)	0.32	1 (0%)	91	88	60, 104, 140, 170	0
All	All	3230/4396 (73%)	0.29	59 (1%)	68	62	47, 102, 147, 176	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	394	LYS	5.0
3	D	167	SER	4.3
2	M	152	TRP	4.0
3	N	184	MET	3.9
1	S	138	ALA	3.9
1	S	389	TYR	3.8
1	T	136	ILE	3.8
1	T	364	ALA	3.6
3	N	167	SER	3.3
3	E	166	LEU	3.3
1	S	137	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	I	182	THR	3.1
2	Q	112	ARG	3.0
1	S	393	GLY	2.8
2	M	159	ARG	2.8
1	T	318	THR	2.7
1	T	389	TYR	2.7
2	M	199	GLU	2.7
2	M	117	PRO	2.7
1	T	216	PHE	2.7
2	Q	139	PHE	2.6
1	T	143	ILE	2.6
2	Q	152	TRP	2.6
3	N	166	LEU	2.5
2	C	110	LEU	2.5
2	Q	201	THR	2.5
1	T	391	VAL	2.4
1	S	141	ARG	2.4
1	T	293	PRO	2.4
2	M	167	TRP	2.4
2	Q	199	GLU	2.4
1	S	112	PHE	2.4
2	Q	200	ALA	2.4
1	S	197	GLU	2.3
2	Q	167	TRP	2.3
1	S	164	GLN	2.3
1	S	216	PHE	2.3
2	I	114	ASP	2.3
2	M	157	SER	2.3
1	S	240	PRO	2.2
2	Q	157	SER	2.2
2	Q	140	LEU	2.1
1	T	287	PHE	2.1
1	S	119	GLY	2.1
3	R	185	SER	2.1
2	Q	197	THR	2.1
2	I	199	GLU	2.1
2	M	119	VAL	2.1
2	Q	198	CYS	2.1
3	N	154	PRO	2.1
1	T	149	TYR	2.0
2	I	120	SER	2.0
2	M	177	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	Q	205	SER	2.0
1	T	397	ASN	2.0
2	M	140	LEU	2.0
2	I	212	SER	2.0
2	I	111	ARG	2.0
3	N	134	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

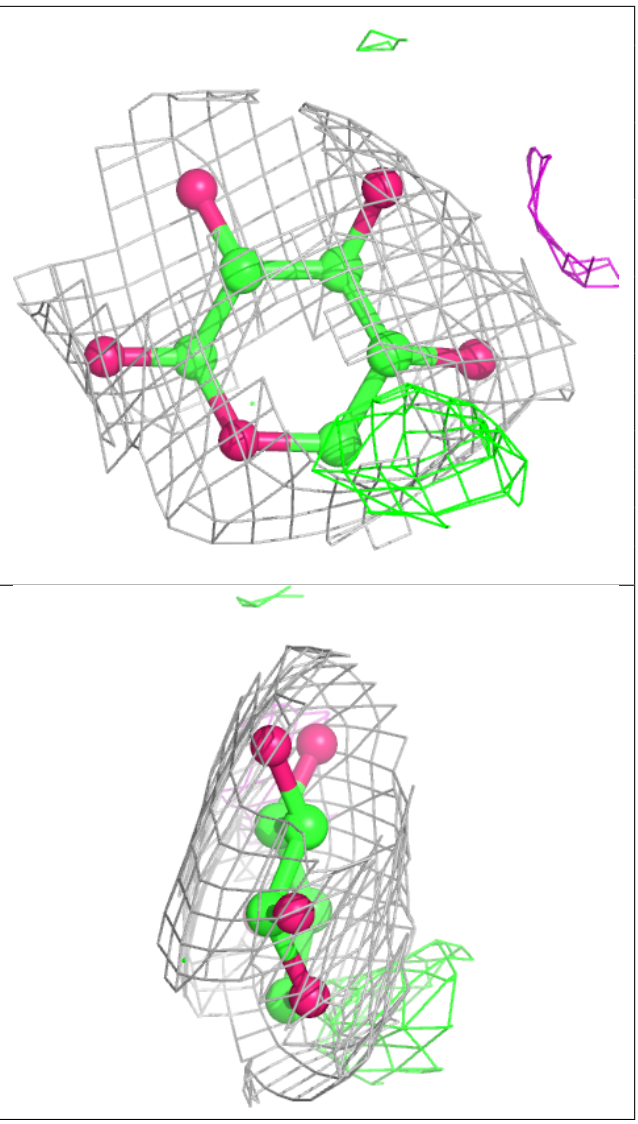
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	B	502	1/1	0.79	0.14	75,75,75,75	0
5	NA	S	502	1/1	0.79	0.16	95,95,95,95	0
4	XYP	S	501	10/10	0.92	0.31	108,112,114,114	0
5	NA	A	502	1/1	0.92	0.17	45,45,45,45	0
4	XYP	T	501	10/10	0.94	0.29	100,110,114,115	0
4	XYP	B	501	10/10	0.95	0.32	57,64,71,73	0
4	XYP	A	501	10/10	0.97	0.25	55,60,63,66	0
5	NA	T	502	1/1	0.97	0.11	91,91,91,91	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.

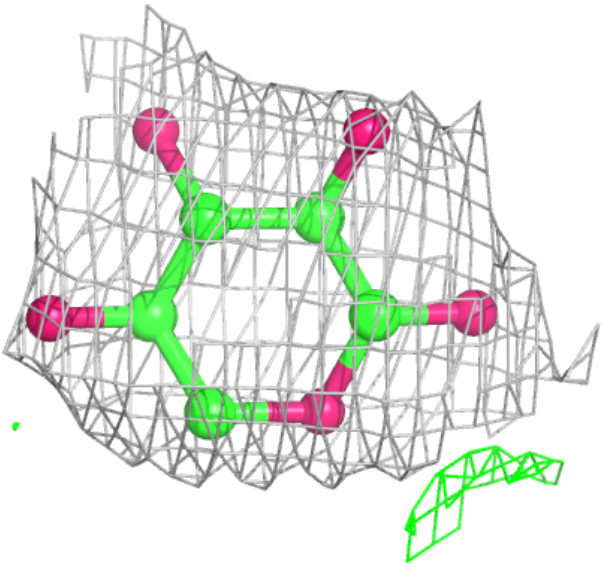
Electron density around XYP S 501:

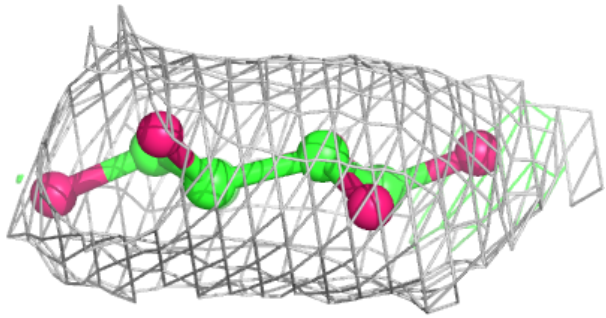
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

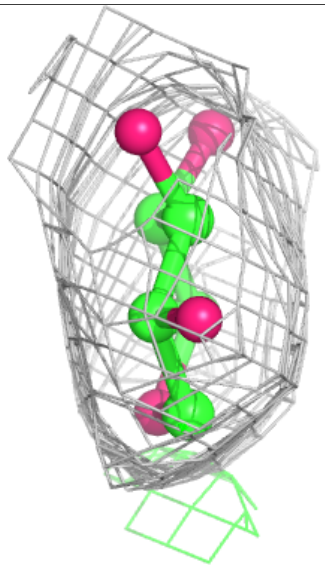


Electron density around XYP T 501:

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

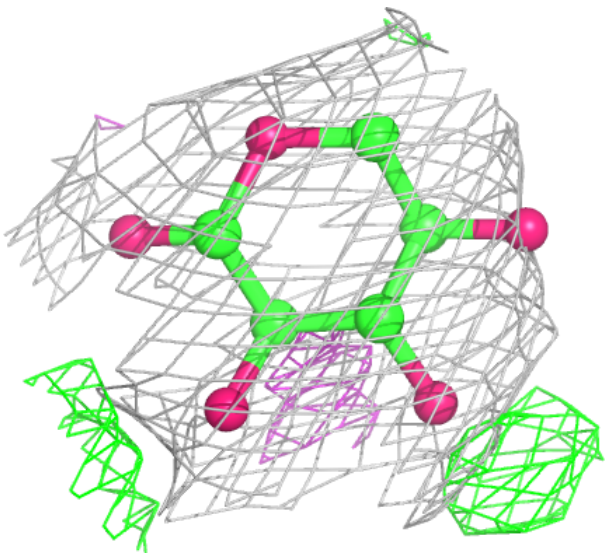


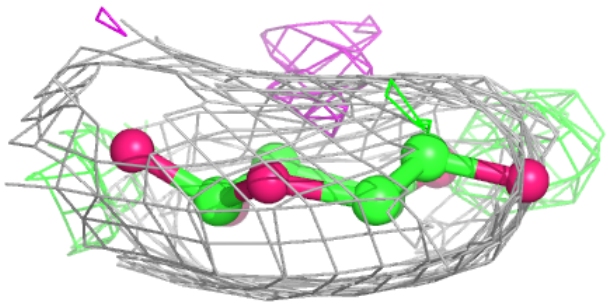


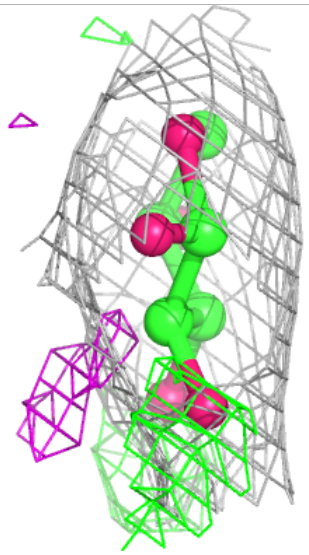


Electron density around XYP B 501:

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

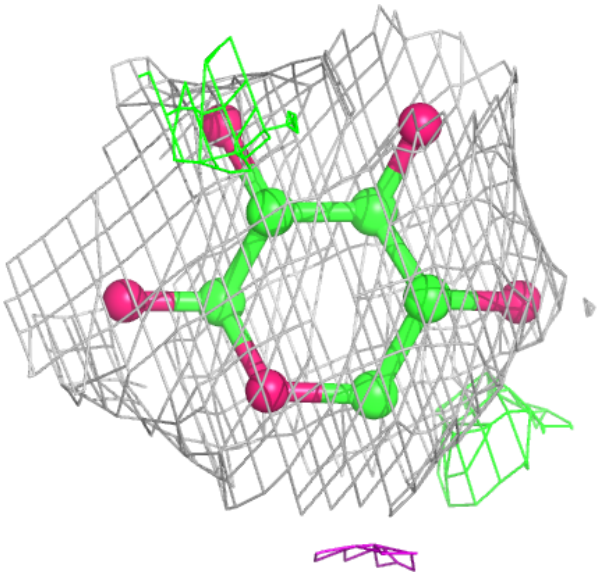


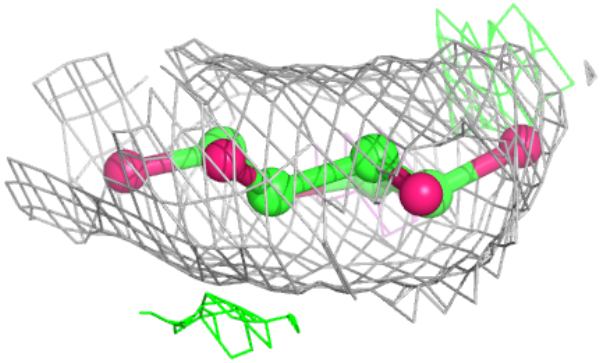


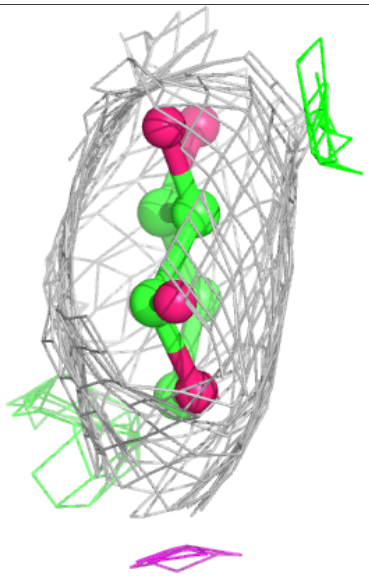


Electron density around XYP A 501:

$2mF_o$-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.