



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2020 – 12:10 PM JST

PDB ID : 7CF6
Title : Crystal structure of Beta-aspartyl dipeptidase from thermophilic keratin degrading *Fervidobacterium islandicum* AW-1 in complex with beta-Asp-Leu dipeptide
Authors : Dhanasingh, I.; La, J.W.; Lee, D.W.; Lee, S.H.
Deposited on : 2020-06-24
Resolution : 2.75 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

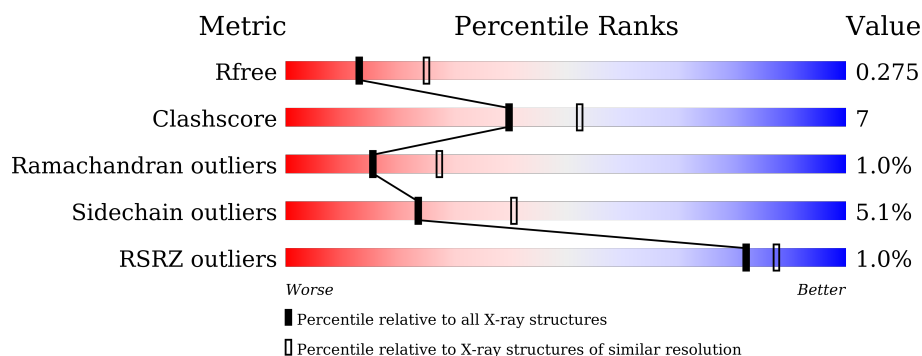
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	391	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	391	<div> <div></div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div>
1	C	391	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>.. 5%</div> </div> </div>
1	D	391	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>21%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11800 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 Isoaspartyl dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	372	Total	C	N	O	S	0	0	0
			2865	1833	479	544	9			
1	A	384	Total	C	N	O	S	0	0	0
			2954	1886	496	562	10			
1	C	371	Total	C	N	O	S	0	0	0
			2857	1827	478	543	9			
1	D	370	Total	C	N	O	S	0	0	0
			2845	1819	477	540	9			

There are 16 discrepancies between the modelled and reference sequences:

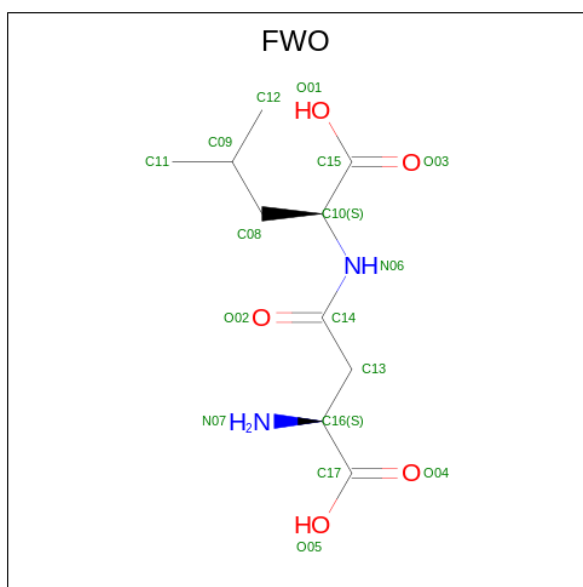
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	MET	-	initiating methionine	UNP A0A1B0VPV0
B	-2	ARG	-	expression tag	UNP A0A1B0VPV0
B	-1	GLY	-	expression tag	UNP A0A1B0VPV0
B	0	SER	-	expression tag	UNP A0A1B0VPV0
A	-3	MET	-	initiating methionine	UNP A0A1B0VPV0
A	-2	ARG	-	expression tag	UNP A0A1B0VPV0
A	-1	GLY	-	expression tag	UNP A0A1B0VPV0
A	0	SER	-	expression tag	UNP A0A1B0VPV0
C	-3	MET	-	initiating methionine	UNP A0A1B0VPV0
C	-2	ARG	-	expression tag	UNP A0A1B0VPV0
C	-1	GLY	-	expression tag	UNP A0A1B0VPV0
C	0	SER	-	expression tag	UNP A0A1B0VPV0
D	-3	MET	-	initiating methionine	UNP A0A1B0VPV0
D	-2	ARG	-	expression tag	UNP A0A1B0VPV0
D	-1	GLY	-	expression tag	UNP A0A1B0VPV0
D	0	SER	-	expression tag	UNP A0A1B0VPV0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is (2S)-2-[[[(3S)-3-azanyl-4-oxidanyl-4-oxidanylidene-butanoyl]amino]-4-methyl-pentanoic acid (three-letter code: FWO) (formula: C₁₀H₁₈N₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			17	10	2	5		
3	A	1	Total	C	N	O	0	0
			17	10	2	5		
3	C	1	Total	C	N	O	0	0
			17	10	2	5		
3	D	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

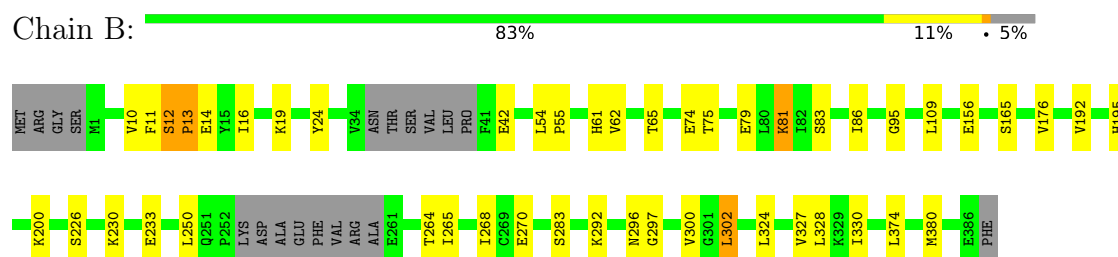
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	34	Total	O	0	0
			34	34		
6	A	27	Total	O	0	0
			27	27		
6	C	41	Total	O	0	0
			41	41		
6	D	21	Total	O	0	0
			21	21		

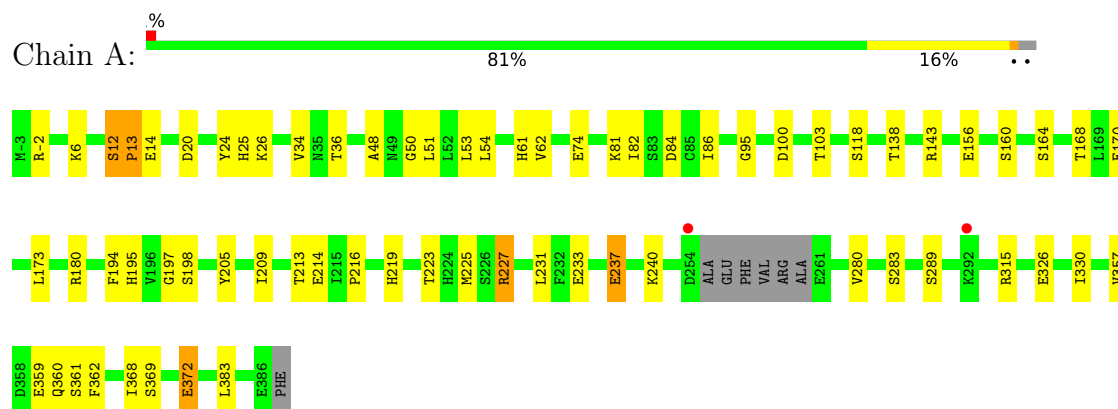
3 Residue-property plots

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

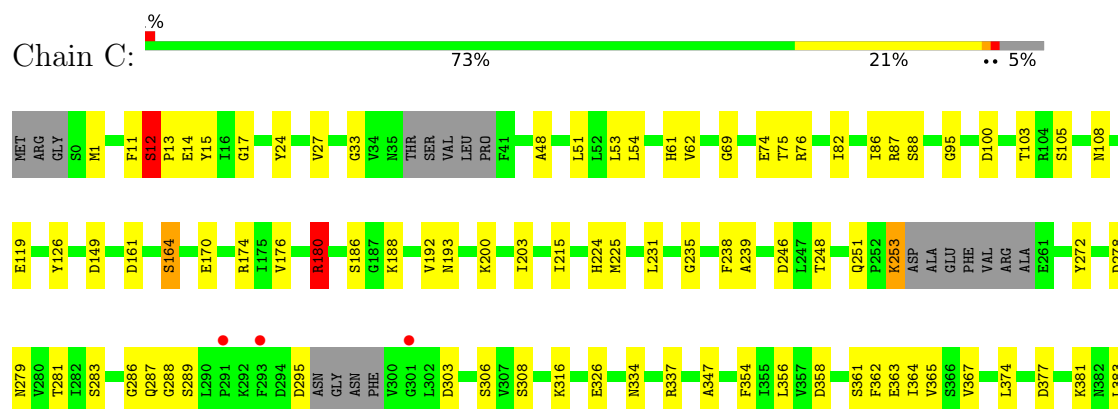
• Molecule 1: Isoaspartyl dipeptidase



• Molecule 1: Isoaspartyl dipeptidase

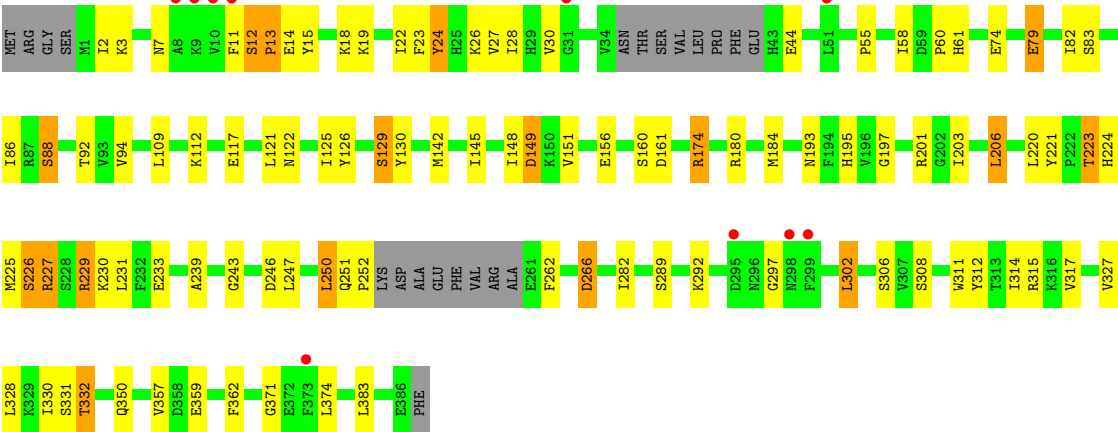


• Molecule 1: Isoaspartyl dipeptidase





● Molecule 1: Isoaspartyl dipeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.61Å 150.43Å 152.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 2.75 47.62 – 2.75	Depositor EDS
% Data completeness (in resolution range)	77.5 (47.66-2.75) 77.5 (47.62-2.75)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.196 , 0.278 0.197 , 0.275	Depositor DCC
R_{free} test set	1994 reflections (5.39%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11800	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: FWO, GOL, ZN, PEG

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	0.75	0/3005	0.86	0/4055
1	B	0.76	0/2914	0.85	0/3931
1	C	0.77	0/2904	0.88	1/3915 (0.0%)
1	D	0.77	0/2893	0.90	0/3903
All	All	0.76	0/11716	0.87	1/15804 (0.0%)

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
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	ARG	NE-CZ-NH1	6.19	123.40	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	SER	Peptide
1	B	12	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	12	SER	Peptide

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	2954	0	3005	40	0
1	B	2865	0	2912	26	0
1	C	2857	0	2912	46	0
1	D	2845	0	2896	62	0
2	A	18	0	24	0	0
2	B	24	0	32	0	0
2	C	18	0	24	0	0
2	D	6	0	8	0	0
3	A	17	0	0	1	0
3	B	17	0	0	0	0
3	C	17	0	0	0	0
3	D	17	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	7	0	10	0	0
5	C	7	0	10	0	0
6	A	27	0	0	0	0
6	B	34	0	0	1	0
6	C	41	0	0	2	0
6	D	21	0	0	0	0
All	All	11800	0	11833	172	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 (172) 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:12:SER:O	1:A:14:GLU:N	1.96	0.97
1:D:282:ILE:HD11	1:D:331:SER:OG	1.70	0.90
1:D:328:LEU:O	1:D:332:THR:OG1	1.91	0.86
1:D:180:ARG:NH1	1:D:184:MET:SD	2.51	0.84
1:D:55:PRO:HG2	1:D:332:THR:HG21	1.57	0.84
1:B:83:SER:HA	1:B:380:MET:HE3	1.67	0.77
1:B:176:VAL:HG22	1:B:192:VAL:HG21	1.66	0.77
1:B:12:SER:O	1:B:14:GLU:N	2.19	0.75
1:C:365:VAL:HG22	1:C:377:ASP:HA	1.69	0.72
1:C:253:LYS:HD3	1:C:303:ASP:OD2	1.89	0.72
1:C:53:LEU:HD11	1:C:354:PHE:HB3	1.72	0.72
1:D:251:GLN:OE1	1:D:252:PRO:CD	2.38	0.71
1:C:176:VAL:HG12	1:C:192:VAL:HG21	1.71	0.71
1:B:83:SER:HA	1:B:380:MET:CE	2.20	0.71
1:D:251:GLN:OE1	1:D:252:PRO:HD2	1.91	0.71
1:A:225:MET:HE3	1:A:231:LEU:HG	1.70	0.71
1:C:69:GLY:HA2	1:C:75:THR:HB	1.75	0.69
1:C:278:ASP:O	1:C:334:ASN:ND2	2.28	0.67
1:D:203:ILE:HB	1:D:206:LEU:HD13	1.77	0.67
1:D:88:SER:HB3	1:D:308:SER:HA	1.77	0.66
1:D:58:ILE:HD13	1:D:92:THR:HB	1.77	0.65
1:C:82:ILE:HG21	1:C:383:LEU:HD22	1.79	0.64
1:D:282:ILE:O	1:D:282:ILE:HD12	1.96	0.64
3:A:405:FOW:O02	3:A:405:FOW:N07	2.31	0.63
1:C:278:ASP:O	1:C:337:ARG:NH2	2.30	0.62
1:D:314:ILE:O	1:D:317:VAL:HG12	1.99	0.62
1:A:214:GLU:OE2	1:D:160:SER:HA	2.00	0.62
1:C:61:HIS:HB3	1:C:283:SER:HB3	1.83	0.61
1:A:168:THR:HG22	1:A:170:GLU:H	1.66	0.61
1:C:356:LEU:O	1:C:365:VAL:HG12	2.01	0.60
1:A:61:HIS:HB3	1:A:283:SER:HB2	1.84	0.60
1:D:12:SER:O	1:D:13:PRO:C	2.40	0.60
1:C:12:SER:O	1:C:14:GLU:N	2.34	0.60
1:C:180:ARG:HG3	1:C:180:ARG:HH11	1.66	0.60
1:A:216:PRO:HG2	1:D:297:GLY:HA3	1.83	0.59
1:B:74:GLU:HG2	1:A:118:SER:OG	2.02	0.59
1:C:76:ARG:HG2	1:C:76:ARG:NH1	2.17	0.59
1:B:86:ILE:HD13	1:B:374:LEU:HB3	1.83	0.59
1:A:62:VAL:O	1:A:95:GLY:HA2	2.02	0.58
1:A:82:ILE:HG23	1:A:383:LEU:HD23	1.85	0.58
1:B:156:GLU:OE1	1:B:195:HIS:HB2	2.03	0.58
1:D:206:LEU:HD23	1:D:220:LEU:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HD21	1:A:209:ILE:HG12	1.86	0.58
1:B:16:ILE:O	1:B:19:LYS:NZ	2.26	0.58
1:C:100:ASP:OD2	1:C:103:THR:HB	2.04	0.57
1:D:82:ILE:HG23	1:D:383:LEU:HD13	1.84	0.57
1:D:109:LEU:HD21	1:D:125:ILE:HB	1.86	0.57
1:D:251:GLN:OE1	1:D:252:PRO:HG2	2.04	0.57
1:C:170:GLU:HG2	6:C:512:HOH:O	2.04	0.56
1:C:316:LYS:NZ	6:C:501:HOH:O	2.38	0.56
1:D:2:ILE:HD12	1:D:2:ILE:H	1.70	0.56
1:C:69:GLY:CA	1:C:75:THR:HB	2.35	0.56
1:C:76:ARG:HG2	1:C:76:ARG:HH11	1.71	0.55
1:C:358:ASP:HB3	1:C:361:SER:HB3	1.89	0.55
1:B:75:THR:HG23	1:B:302:LEU:HD13	1.89	0.55
1:A:280:VAL:HG23	1:A:330:ILE:HG22	1.88	0.55
1:D:174:ARG:HG2	1:D:174:ARG:NH1	2.22	0.55
1:D:223:THR:HG22	1:D:224:HIS:ND1	2.22	0.54
1:D:226:SER:CB	1:D:247:LEU:HD22	2.37	0.54
1:B:233:GLU:OE2	1:B:270:GLU:OE2	2.26	0.54
1:C:86:ILE:HD13	1:C:374:LEU:HB3	1.90	0.53
1:B:81:LYS:HE2	6:B:520:HOH:O	2.07	0.53
1:B:62:VAL:O	1:B:95:GLY:HA2	2.09	0.53
1:C:239:ALA:O	1:C:279:ASN:ND2	2.42	0.53
1:C:180:ARG:CG	1:C:180:ARG:HH11	2.22	0.52
1:C:27:VAL:HB	1:C:347:ALA:O	2.10	0.52
1:D:12:SER:O	1:D:14:GLU:N	2.43	0.52
1:D:251:GLN:OE1	1:D:252:PRO:CG	2.58	0.52
1:D:126:TYR:OH	1:D:193:ASN:ND2	2.41	0.51
1:A:6:LYS:HE2	1:A:20:ASP:OD2	2.09	0.51
1:D:156:GLU:OE1	1:D:195:HIS:HB2	2.11	0.51
1:C:186:SER:HB2	1:C:188:LYS:HD2	1.92	0.50
1:B:264:THR:O	1:B:268:ILE:HG13	2.12	0.50
1:A:48:ALA:HA	1:A:51:LEU:HD12	1.93	0.50
1:C:15:TYR:CZ	1:C:17:GLY:HA2	2.47	0.50
1:B:292:LYS:O	1:B:300:VAL:HB	2.11	0.49
1:D:289:SER:OG	1:D:302:LEU:HD11	2.12	0.49
1:A:34:VAL:O	1:A:36:THR:HG23	2.12	0.49
1:D:161:ASP:OD2	1:D:195:HIS:NE2	2.34	0.49
1:D:221:TYR:CE1	1:D:246:ASP:HB2	2.47	0.48
1:A:194:PHE:O	1:A:223:THR:HG22	2.13	0.48
1:C:86:ILE:O	1:C:367:VAL:HG21	2.13	0.48
1:D:149:ASP:OD1	1:D:149:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:C	1:A:54:LEU:HD12	2.33	0.48
1:D:266:ASP:N	1:D:266:ASP:OD1	2.45	0.48
1:A:6:LYS:HE3	1:A:36:THR:CG2	2.44	0.48
1:C:246:ASP:OD2	1:C:283:SER:OG	2.31	0.48
1:D:142:MET:O	1:D:145:ILE:HG22	2.14	0.47
1:C:62:VAL:O	1:C:95:GLY:HA2	2.14	0.47
1:C:235:GLY:O	1:C:238:PHE:HB3	2.14	0.47
1:A:357:VAL:CG1	1:A:362:PHE:HA	2.45	0.47
1:D:22:ILE:HD12	1:D:22:ILE:H	1.80	0.47
1:D:3:LYS:HE2	1:D:371:GLY:O	2.15	0.47
1:A:180:ARG:HG3	1:A:219:HIS:NE2	2.30	0.47
1:B:250:LEU:HD23	1:B:265:ILE:HD11	1.97	0.47
1:D:247:LEU:O	1:D:282:ILE:HA	2.15	0.47
1:D:19:LYS:CD	1:D:30:VAL:HG12	2.45	0.47
1:C:105:SER:HB3	1:C:108:ASN:CB	2.45	0.46
1:A:180:ARG:NH1	1:A:219:HIS:NE2	2.63	0.46
1:D:174:ARG:HG2	1:D:174:ARG:HH11	1.79	0.46
1:D:229:ARG:O	1:D:233:GLU:HG2	2.15	0.46
1:C:48:ALA:HA	1:C:51:LEU:HD12	1.98	0.46
1:A:100:ASP:OD2	1:A:103:THR:OG1	2.33	0.46
1:A:138:THR:OG1	1:A:143:ARG:HB2	2.16	0.46
1:B:327:VAL:O	1:B:330:ILE:HG12	2.16	0.46
1:A:6:LYS:HE3	1:A:36:THR:HG21	1.98	0.46
1:D:160:SER:OG	1:D:201:ARG:HB2	2.15	0.46
1:A:209:ILE:O	1:A:213:THR:OG1	2.24	0.45
1:C:278:ASP:C	1:C:334:ASN:HD21	2.19	0.45
1:D:250:LEU:HD23	1:D:312:TYR:HE2	1.81	0.45
1:D:225:MET:HA	1:D:231:LEU:HD23	1.98	0.45
1:B:11:PHE:CZ	1:B:324:LEU:HD23	2.52	0.44
1:D:117:GLU:HA	1:D:121:LEU:O	2.16	0.44
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.83	0.44
1:A:12:SER:O	1:A:13:PRO:C	2.52	0.44
1:B:12:SER:O	1:B:14:GLU:O	2.35	0.44
1:D:148:ILE:HB	1:D:151:VAL:HG23	1.99	0.44
1:C:76:ARG:CG	1:C:76:ARG:HH11	2.29	0.44
1:D:311:TRP:NE1	1:D:315:ARG:HD2	2.33	0.44
1:A:12:SER:C	1:A:14:GLU:N	2.69	0.44
1:A:74:GLU:H	1:A:74:GLU:HG2	1.67	0.44
1:C:161:ASP:O	1:C:164:SER:HB3	2.17	0.44
1:C:88:SER:OG	1:C:308:SER:HA	2.17	0.44
1:A:82:ILE:HG23	1:A:383:LEU:CD2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:GLU:O	1:C:381:LYS:NZ	2.51	0.44
1:D:129:SER:O	1:D:130:TYR:C	2.55	0.44
1:A:160:SER:O	1:A:197:GLY:HA3	2.18	0.43
1:D:229:ARG:HD3	1:D:262:PHE:CD2	2.53	0.43
1:C:286:GLY:C	1:C:288:GLY:H	2.21	0.43
1:C:76:ARG:NH1	1:C:103:THR:HG21	2.33	0.43
1:A:25:HIS:CE1	1:A:26:LYS:HG3	2.54	0.43
1:D:92:THR:HA	1:D:122:ASN:O	2.19	0.43
1:A:50:GLY:O	1:A:359:GLU:HB2	2.18	0.43
1:B:328:LEU:HA	1:B:328:LEU:HD23	1.90	0.43
1:C:11:PHE:HB2	1:C:54:LEU:HD23	1.99	0.43
1:C:272:TYR:CE1	1:C:326:GLU:HG2	2.53	0.43
1:D:282:ILE:HD11	1:D:331:SER:HG	1.77	0.43
1:D:315:ARG:HE	1:D:362:PHE:HB3	1.84	0.43
1:D:197:GLY:C	1:D:227:ARG:HH12	2.22	0.43
1:A:368:ILE:HA	1:A:372:GLU:O	2.19	0.43
1:B:11:PHE:HB2	1:B:54:LEU:HD23	2.01	0.43
1:B:13:PRO:HD3	1:B:55:PRO:CG	2.49	0.43
1:D:252:PRO:HD3	1:D:312:TYR:CZ	2.54	0.43
1:D:60:PRO:HA	1:D:94:VAL:HG23	2.01	0.43
1:A:156:GLU:OE1	1:A:195:HIS:HB2	2.19	0.42
1:B:10:VAL:HG21	1:B:19:LYS:HB2	2.02	0.42
1:C:246:ASP:HA	1:C:281:THR:HG23	2.02	0.42
1:D:86:ILE:HD13	1:D:374:LEU:HB3	2.02	0.42
1:A:82:ILE:O	1:A:86:ILE:HG13	2.20	0.42
1:D:79:GLU:OE2	1:D:112:LYS:HD3	2.20	0.42
1:A:227:ARG:HH11	1:A:227:ARG:CG	2.33	0.41
1:D:327:VAL:O	1:D:330:ILE:HG12	2.21	0.41
1:B:200:LYS:N	1:B:200:LYS:HD3	2.35	0.41
1:C:176:VAL:HG23	1:C:215:ILE:HD13	2.01	0.41
1:D:109:LEU:HD23	1:D:109:LEU:C	2.41	0.41
1:D:26:LYS:HB3	1:D:350:GLN:O	2.19	0.41
1:A:205:TYR:O	1:A:209:ILE:HG13	2.21	0.41
1:B:61:HIS:HB3	1:B:283:SER:HB2	2.02	0.41
1:D:61:HIS:CE1	1:D:156:GLU:OE2	2.73	0.41
1:D:23:PHE:HA	1:D:28:ILE:HG22	2.02	0.41
1:A:81:LYS:O	1:A:84:ASP:HB2	2.20	0.41
1:A:237:GLU:OE1	1:A:240:LYS:NZ	2.53	0.41
1:C:253:LYS:CD	1:C:303:ASP:OD2	2.63	0.41
1:B:65:THR:CG2	1:B:109:LEU:HA	2.51	0.41
1:D:311:TRP:CH2	1:D:357:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:TYR:CE2	1:C:193:ASN:HB2	2.56	0.40
1:C:203:ILE:CG2	1:C:225:MET:HE3	2.51	0.40
1:C:225:MET:HE2	1:C:231:LEU:HD21	2.02	0.40
1:D:239:ALA:HA	1:D:243:GLY:O	2.20	0.40
1:A:168:THR:HG22	1:A:170:GLU:N	2.34	0.40
1:B:83:SER:HA	1:B:380:MET:HE1	1.99	0.40
1:D:227:ARG:HD3	3:D:402:FOW:C11	2.52	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	380/391 (97%)	359 (94%)	20 (5%)	1 (0%)	41	60
1	B	366/391 (94%)	342 (93%)	20 (6%)	4 (1%)	14	25
1	C	363/391 (93%)	336 (93%)	22 (6%)	5 (1%)	11	19
1	D	364/391 (93%)	329 (90%)	30 (8%)	5 (1%)	11	19
All	All	1473/1564 (94%)	1366 (93%)	92 (6%)	15 (1%)	15	27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	PRO
1	B	42	GLU
1	B	296	ASN
1	A	13	PRO
1	C	13	PRO
1	D	359	GLU
1	C	33	GLY
1	D	18	LYS

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Mol	Chain	Res	Type
1	D	24	TYR
1	C	12	SER
1	C	287	GLN
1	B	297	GLY
1	C	224	HIS
1	D	13	PRO
1	D	27	VAL

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	326/331 (98%)	312 (96%)	14 (4%)	29	48
1	B	315/331 (95%)	308 (98%)	7 (2%)	52	70
1	C	315/331 (95%)	296 (94%)	19 (6%)	19	33
1	D	313/331 (95%)	288 (92%)	25 (8%)	12	21
All	All	1269/1324 (96%)	1204 (95%)	65 (5%)	24	41

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	24	TYR
1	B	79	GLU
1	B	81	LYS
1	B	165	SER
1	B	226	SER
1	B	230	LYS
1	B	302	LEU
1	A	-2	ARG
1	A	24	TYR
1	A	164	SER
1	A	198	SER
1	A	227	ARG
1	A	233	GLU
1	A	237	GLU

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Mol	Chain	Res	Type
1	A	289	SER
1	A	315	ARG
1	A	326	GLU
1	A	360	GLN
1	A	361	SER
1	A	369	SER
1	A	372	GLU
1	C	1	MET
1	C	12	SER
1	C	24	TYR
1	C	74	GLU
1	C	87	ARG
1	C	149	ASP
1	C	164	SER
1	C	174	ARG
1	C	180	ARG
1	C	200	LYS
1	C	248	THR
1	C	251	GLN
1	C	253	LYS
1	C	289	SER
1	C	295	ASP
1	C	306	SER
1	C	362	PHE
1	C	363	GLU
1	C	364	ILE
1	D	7	ASN
1	D	11	PHE
1	D	12	SER
1	D	15	TYR
1	D	24	TYR
1	D	44	GLU
1	D	74	GLU
1	D	79	GLU
1	D	83	SER
1	D	88	SER
1	D	129	SER
1	D	149	ASP
1	D	174	ARG
1	D	206	LEU
1	D	223	THR
1	D	226	SER

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Mol	Chain	Res	Type
1	D	227	ARG
1	D	229	ARG
1	D	230	LYS
1	D	250	LEU
1	D	266	ASP
1	D	292	LYS
1	D	302	LEU
1	D	306	SER
1	D	332	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	C	334	ASN
1	D	193	ASN
1	D	382	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 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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$
2	GOL	C	403	-	5,5,5	0.13	0	5,5,5	0.32	0
3	FWO	B	405	4	10,16,16	2.64	3 (30%)	12,21,21	1.34	2 (16%)
3	FWO	A	405	-	10,16,16	2.06	1 (10%)	12,21,21	0.84	0
3	FWO	D	402	4	10,16,16	2.61	2 (20%)	12,21,21	2.32	3 (25%)
2	GOL	B	402	-	5,5,5	0.13	0	5,5,5	0.38	0
2	GOL	A	404	-	5,5,5	0.16	0	5,5,5	0.50	0
2	GOL	C	404	-	5,5,5	0.17	0	5,5,5	0.42	0
5	PEG	A	402	-	6,6,6	0.61	0	5,5,5	0.77	0
5	PEG	C	402	-	6,6,6	0.68	0	5,5,5	0.73	0
2	GOL	A	401	-	5,5,5	0.32	0	5,5,5	0.68	0
2	GOL	D	401	-	5,5,5	0.13	0	5,5,5	0.35	0
2	GOL	C	401	-	5,5,5	0.15	0	5,5,5	0.39	0
3	FWO	C	405	-	10,16,16	2.62	4 (40%)	12,21,21	1.75	3 (25%)
2	GOL	B	401	-	5,5,5	0.16	0	5,5,5	0.40	0
2	GOL	A	403	-	5,5,5	0.16	0	5,5,5	0.35	0
2	GOL	B	403	-	5,5,5	0.21	0	5,5,5	0.42	0
2	GOL	B	404	-	5,5,5	0.08	0	5,5,5	0.25	0

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	GOL	C	403	-	-	2/4/4/4	-
3	FWO	B	405	4	-	2/12/20/20	-
3	FWO	A	405	-	-	6/12/20/20	-
3	FWO	D	402	4	-	4/12/20/20	-
2	GOL	B	402	-	-	4/4/4/4	-
2	GOL	A	404	-	-	1/4/4/4	-
2	GOL	C	404	-	-	2/4/4/4	-
5	PEG	A	402	-	-	2/4/4/4	-
5	PEG	C	402	-	-	4/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	D	401	-	-	2/4/4/4	-
2	GOL	C	401	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FWO	C	405	-	-	2/12/20/20	-
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	A	403	-	-	3/4/4/4	-
2	GOL	B	403	-	-	0/4/4/4	-
2	GOL	B	404	-	-	4/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	FWO	C14-N06	7.16	1.49	1.34
3	B	405	FWO	C14-N06	6.68	1.48	1.34
3	C	405	FWO	C14-N06	6.65	1.48	1.34
3	A	405	FWO	C14-N06	6.10	1.47	1.34
3	B	405	FWO	C08-C10	3.74	1.57	1.53
3	C	405	FWO	C08-C10	3.35	1.56	1.53
3	D	402	FWO	C10-N06	2.66	1.50	1.46
3	B	405	FWO	C10-N06	2.43	1.49	1.46
3	C	405	FWO	C10-N06	2.15	1.49	1.46
3	C	405	FWO	O02-C14	-2.01	1.19	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	FWO	C13-C14-N06	6.19	124.43	116.33
3	C	405	FWO	C13-C14-N06	4.60	122.35	116.33
3	D	402	FWO	O02-C14-C13	-3.44	116.45	121.50
3	B	405	FWO	C10-N06-C14	2.82	127.82	123.33
3	B	405	FWO	C08-C10-N06	2.63	114.49	109.80
3	D	402	FWO	O02-C14-N06	-2.28	119.11	122.95
3	C	405	FWO	O02-C14-N06	-2.21	119.23	122.95
3	C	405	FWO	O02-C14-C13	-2.10	118.42	121.50

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	403	GOL	C1-C2-C3-O3
3	B	405	FWO	C09-C08-C10-C15
3	D	402	FWO	C14-C13-C16-N07
2	C	401	GOL	O1-C1-C2-C3

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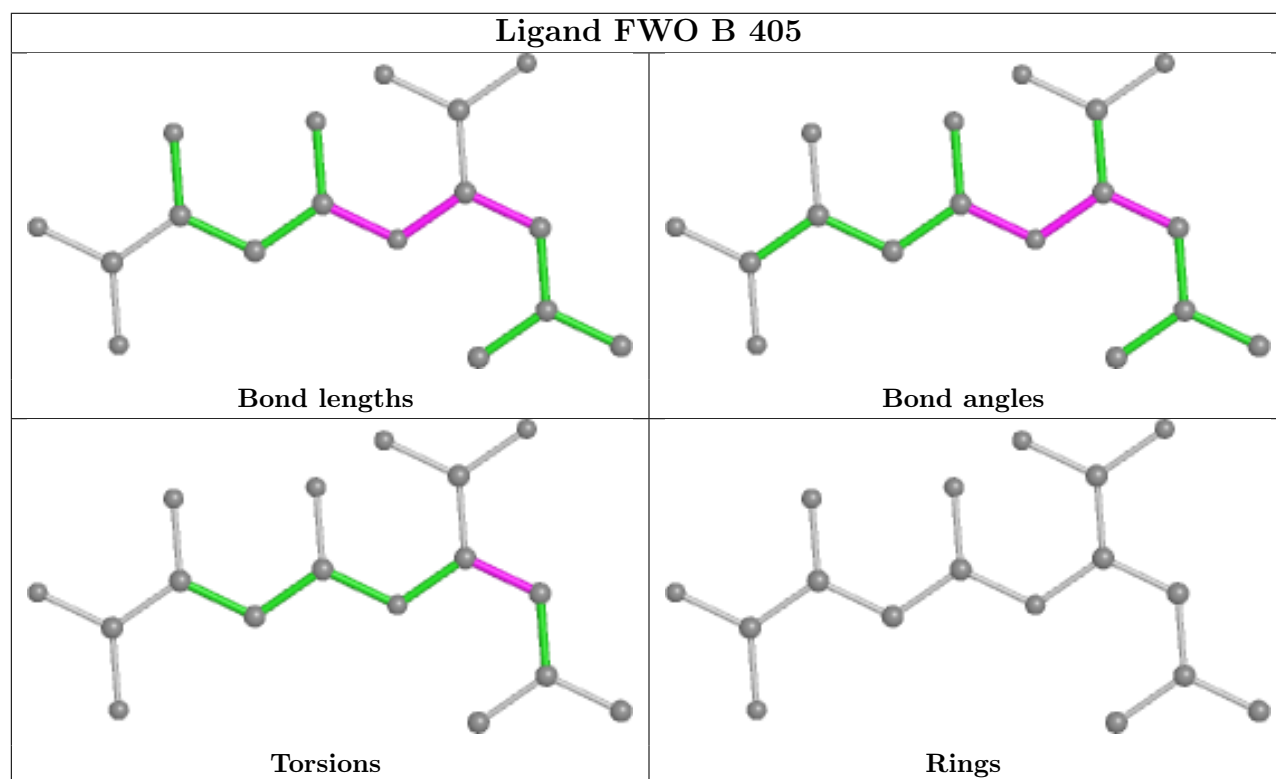
Mol	Chain	Res	Type	Atoms
3	C	405	FWO	C09-C08-C10-C15
2	D	401	GOL	O1-C1-C2-O2
2	D	401	GOL	O1-C1-C2-C3
2	C	404	GOL	C1-C2-C3-O3
2	C	404	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-C3
3	A	405	FWO	C09-C08-C10-C15
3	A	405	FWO	C14-C13-C16-C17
3	A	405	FWO	C14-C13-C16-N07
2	B	404	GOL	O1-C1-C2-C3
2	B	404	GOL	C1-C2-C3-O3
2	A	403	GOL	C1-C2-C3-O3
2	B	401	GOL	O1-C1-C2-O2
2	B	401	GOL	O1-C1-C2-C3
3	B	405	FWO	C09-C08-C10-N06
3	D	402	FWO	C10-C08-C09-C12
3	D	402	FWO	C10-C08-C09-C11
2	C	401	GOL	O1-C1-C2-O2
5	C	402	PEG	O2-C3-C4-O4
3	C	405	FWO	C09-C08-C10-N06
2	B	402	GOL	C1-C2-C3-O3
2	C	401	GOL	C1-C2-C3-O3
2	C	403	GOL	O2-C2-C3-O3
2	B	402	GOL	O2-C2-C3-O3
2	C	401	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	B	404	GOL	O1-C1-C2-O2
2	B	404	GOL	O2-C2-C3-O3
5	A	402	PEG	O2-C3-C4-O4
3	A	405	FWO	C10-C08-C09-C12
3	A	405	FWO	C10-C08-C09-C11
3	A	405	FWO	C09-C08-C10-N06
3	D	402	FWO	C14-C13-C16-C17
2	A	403	GOL	O2-C2-C3-O3
5	A	402	PEG	O1-C1-C2-O2
5	C	402	PEG	O1-C1-C2-O2
5	C	402	PEG	C1-C2-O2-C3
2	B	402	GOL	O1-C1-C2-C3
2	B	402	GOL	O1-C1-C2-O2
2	A	403	GOL	O1-C1-C2-C3
2	A	404	GOL	O2-C2-C3-O3
5	C	402	PEG	C4-C3-O2-C2

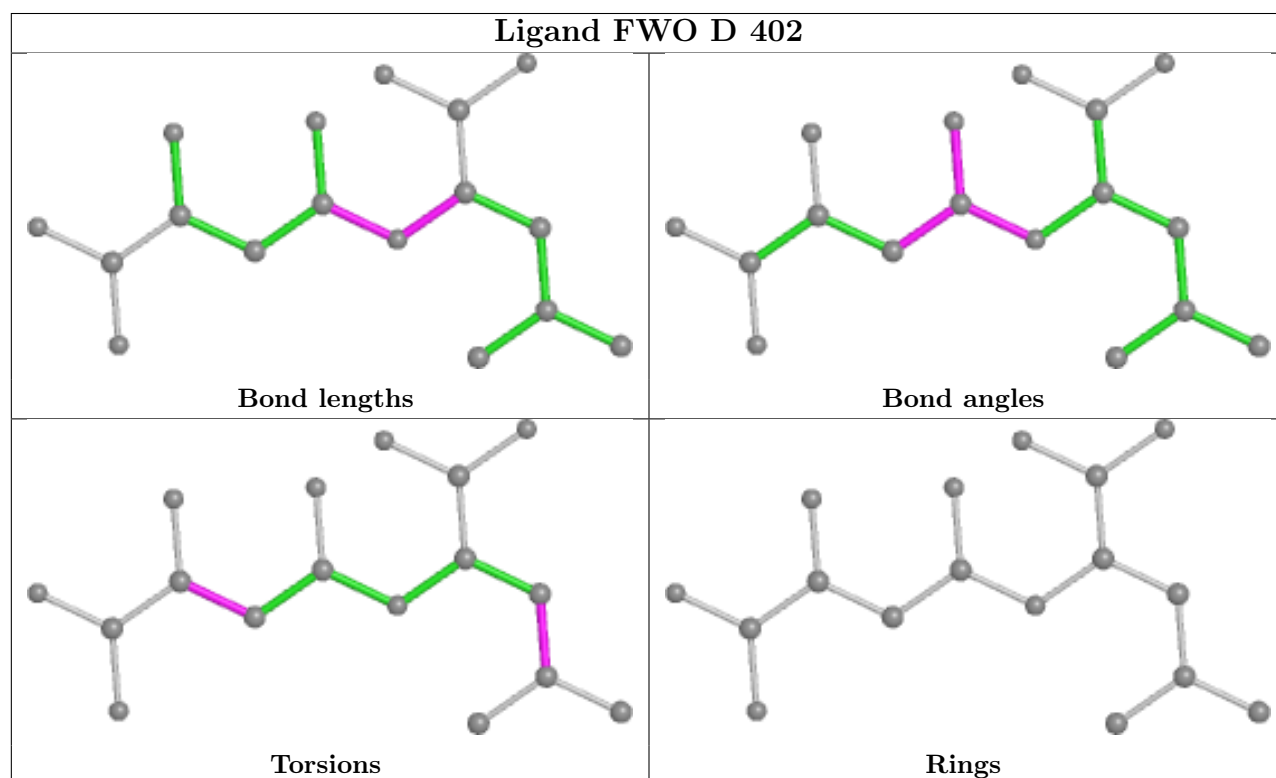
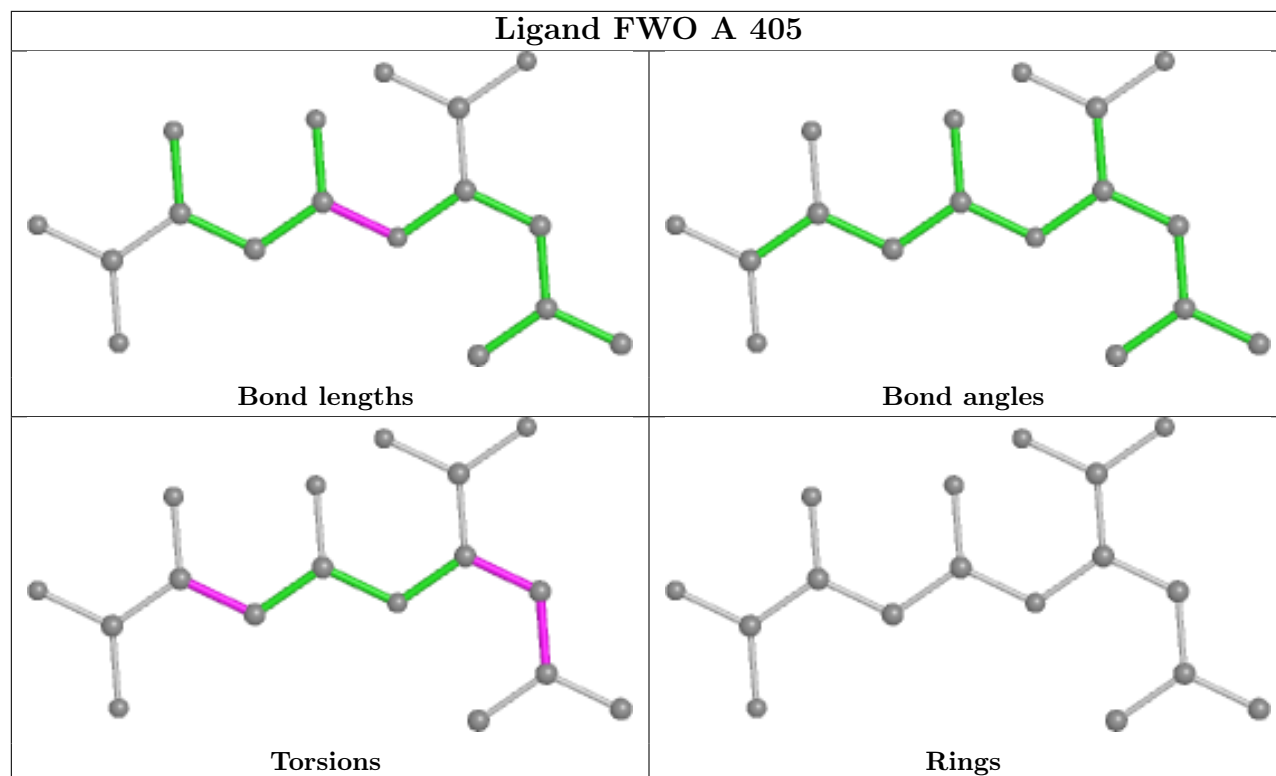
There are no ring outliers.

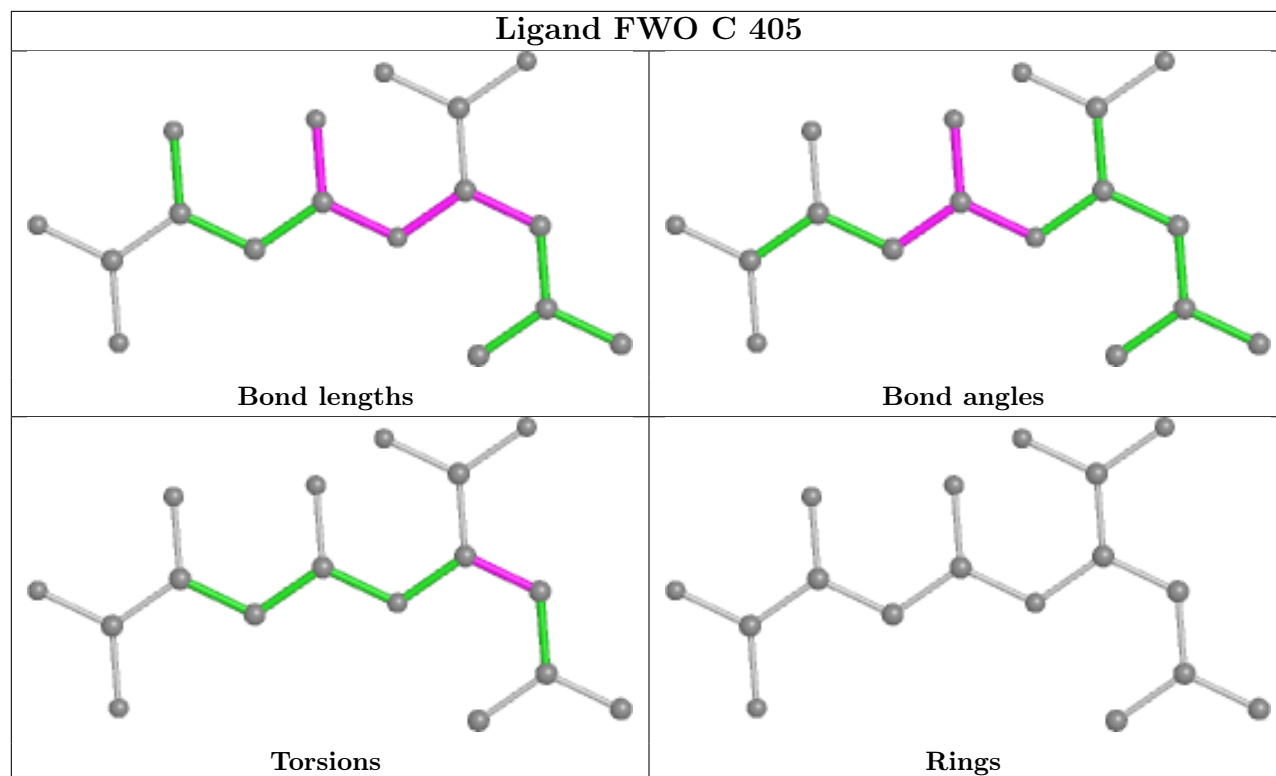
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	FWO	1	0
3	D	402	FWO	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 [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	384/391 (98%)	-0.48	2 (0%) 91 94	26, 43, 76, 102	0
1	B	372/391 (95%)	-0.60	0 100 100	25, 39, 67, 91	0
1	C	371/391 (94%)	-0.38	3 (0%) 86 90	27, 48, 79, 128	0
1	D	370/391 (94%)	-0.08	10 (2%) 54 63	34, 61, 89, 119	0
All	All	1497/1564 (95%)	-0.39	15 (1%) 82 87	25, 46, 81, 128	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	GLY	4.1
1	D	299	PHE	3.3
1	C	293	PHE	3.3
1	D	31	GLY	3.3
1	D	10	VAL	3.1
1	D	295	ASP	2.8
1	C	291	PRO	2.5
1	D	8	ALA	2.2
1	D	9	LYS	2.2
1	D	11	PHE	2.2
1	A	292	LYS	2.2
1	D	373	PHE	2.2
1	D	298	ASN	2.1
1	A	254	ASP	2.0
1	D	51	LEU	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

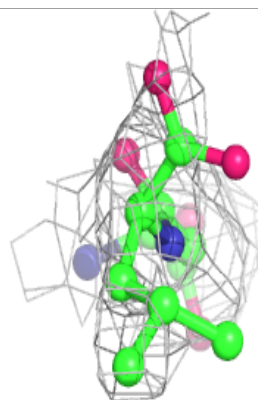
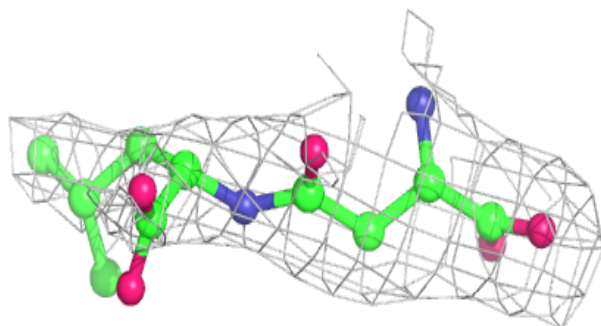
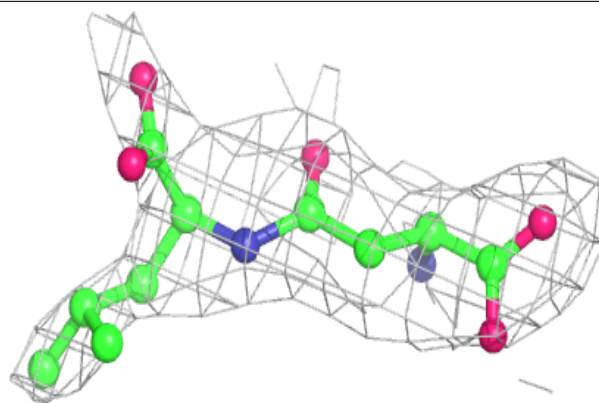
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	D	401	6/6	0.68	0.30	66,79,82,83	0
2	GOL	B	402	6/6	0.74	0.36	63,73,78,86	0
2	GOL	B	404	6/6	0.74	0.36	85,91,96,107	0
2	GOL	B	403	6/6	0.75	0.22	60,79,80,83	0
2	GOL	B	401	6/6	0.80	0.38	74,77,79,82	0
2	GOL	C	404	6/6	0.82	0.21	63,68,73,76	0
2	GOL	C	401	6/6	0.83	0.27	67,74,76,76	0
3	FWO	C	405	17/17	0.84	0.24	66,82,101,112	0
3	FWO	D	402	17/17	0.86	0.22	70,88,113,118	0
4	ZN	B	407	1/1	0.86	0.06	105,105,105,105	0
2	GOL	A	403	6/6	0.87	0.22	60,72,73,75	0
5	PEG	C	402	7/7	0.88	0.22	47,55,66,67	0
3	FWO	B	405	17/17	0.90	0.18	38,66,86,93	0
3	FWO	A	405	17/17	0.92	0.22	49,85,116,119	0
2	GOL	A	404	6/6	0.92	0.26	56,61,64,70	0
2	GOL	C	403	6/6	0.92	0.15	58,61,65,70	0
5	PEG	A	402	7/7	0.93	0.18	44,45,47,48	0
2	GOL	A	401	6/6	0.93	0.25	47,55,56,60	0
4	ZN	D	403	1/1	0.94	0.10	123,123,123,123	0
4	ZN	A	407	1/1	0.95	0.07	74,74,74,74	0
4	ZN	D	404	1/1	0.97	0.10	66,66,66,66	0
4	ZN	C	406	1/1	0.98	0.05	88,88,88,88	0
4	ZN	B	406	1/1	0.99	0.08	49,49,49,49	0
4	ZN	A	406	1/1	0.99	0.11	48,48,48,48	0
4	ZN	C	407	1/1	1.00	0.07	52,52,52,52	0

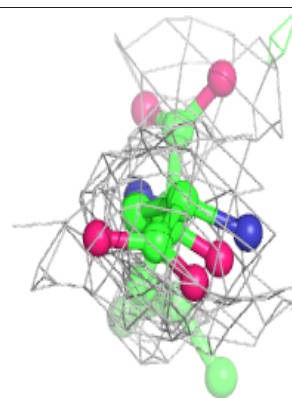
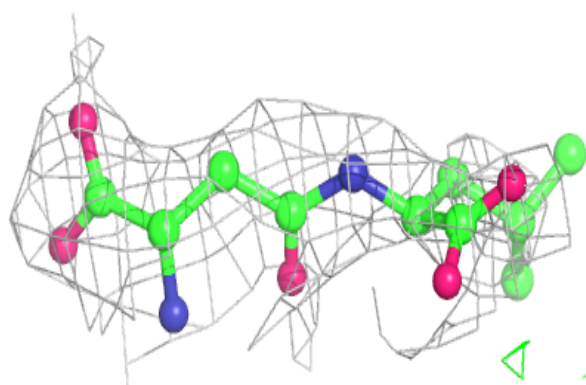
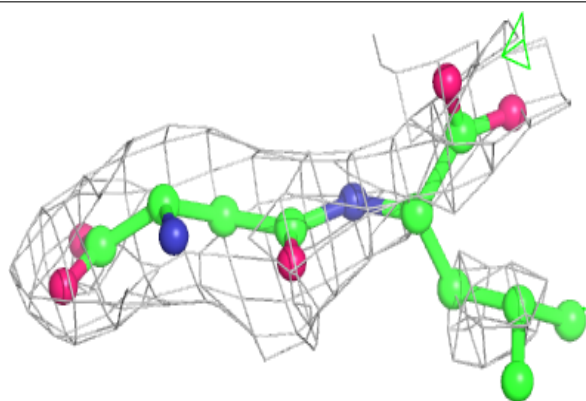
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FWO C 405:

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

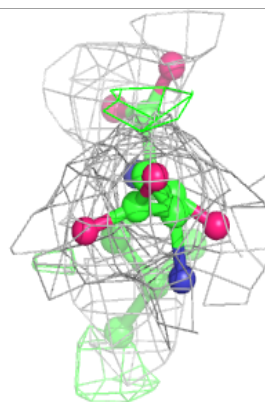
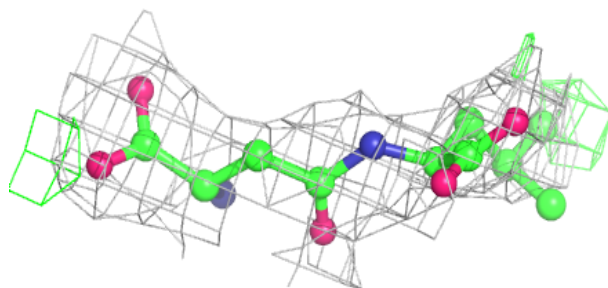
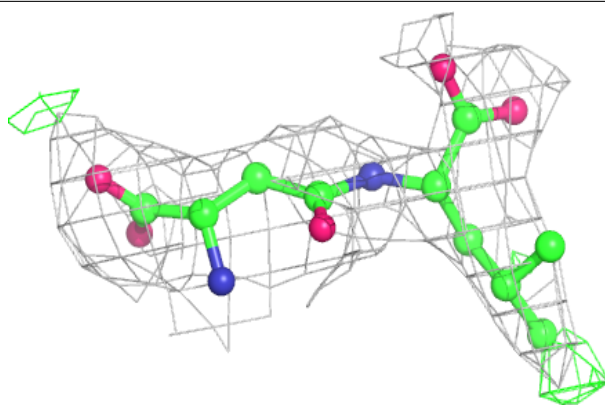
**Electron density around FWO D 402:**

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

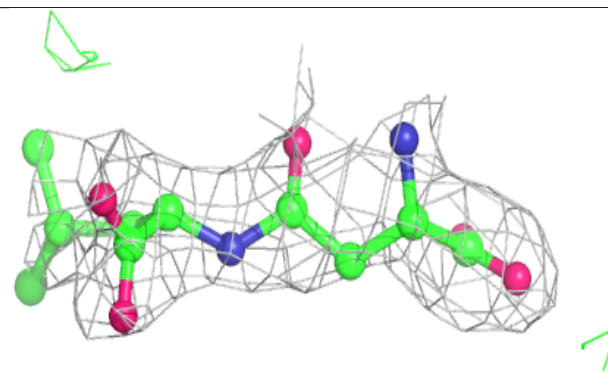
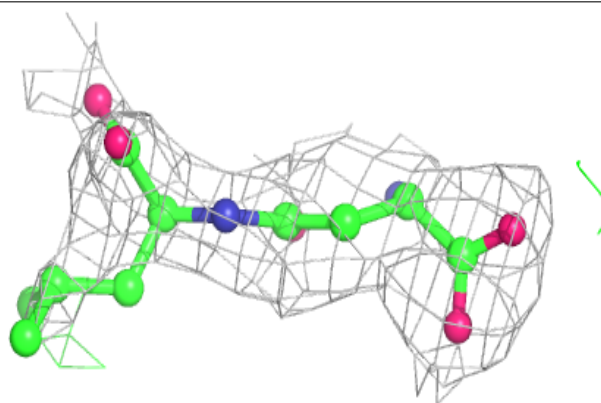


Electron density around FWO B 405:

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

**Electron density around FWO A 405:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.