



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:20 AM UTC

PDB ID : 4H82 / pdb_00004h82
Title : Crystal structure of mutant MMP-9 catalytic domain in complex with a twin inhibitor.
Authors : Antoni, C.; Stura, E.A.; Vera, L.; Cassar-Lajeunesse, E.; Nuti, E.; Dive, V.; Rossello, A.
Deposited on : 2012-09-21
Resolution : 1.90 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

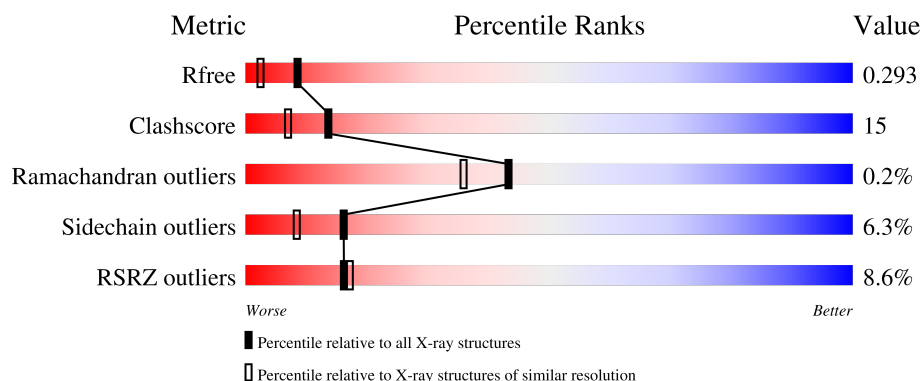
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	160	8% 62% 34% .
1	B	160	10% 71% 25% ..
1	C	160	8% 64% 32% ..
1	D	160	9% 66% 31% ..

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6145 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 Matrix metalloproteinase-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	4	0
			1313	846	224	241	2			
1	B	160	Total	C	N	O	S	0	3	0
			1305	841	225	236	3			
1	C	160	Total	C	N	O	S	0	2	0
			1295	835	221	237	2			
1	D	160	Total	C	N	O	S	0	3	0
			1305	841	225	236	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	GLN	GLU	engineered mutation	UNP P14780
B	227	GLN	GLU	engineered mutation	UNP P14780
C	227	GLN	GLU	engineered mutation	UNP P14780
D	227	GLN	GLU	engineered mutation	UNP P14780

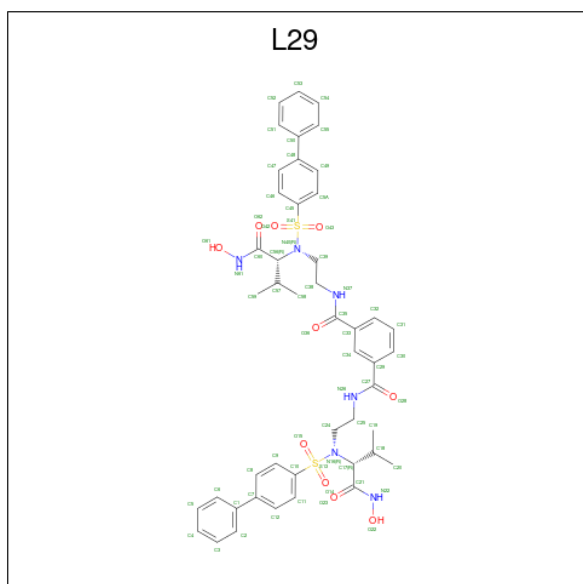
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Ca 3 3	0	0
3	B	3	Total Ca 3 3	0	0
3	C	3	Total Ca 3 3	0	0
3	D	3	Total Ca 3 3	0	0

- Molecule 4 is N,N'-bis(2-((biphenyl-4-ylsulfonyl)[(2R)-1-(hydroxyamino)-3-methyl-1-oxobutan-2-yl]amino)ethyl)benzene-1,3-dicarboxamide (non-preferred name) (CCD ID: L29) (formula: C₄₆H₅₂N₆O₁₀S₂).



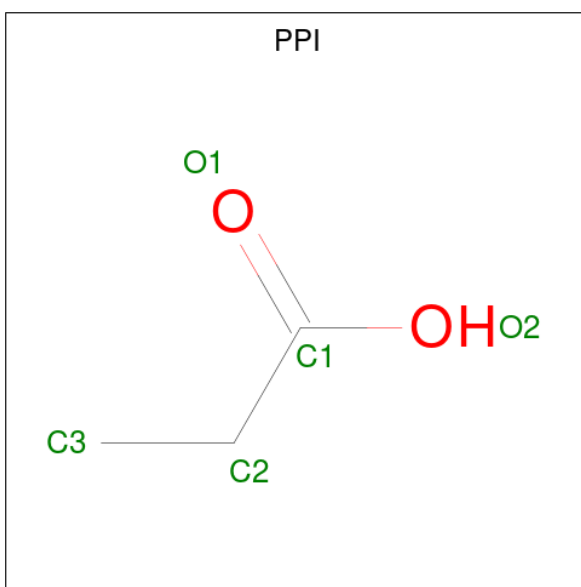
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 64 46 6 10 2	0	0
4	D	1	Total C N O S 64 46 6 10 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 6 is PROPANOIC ACID (CCD ID: PPI) (formula: $C_3H_6O_2$).



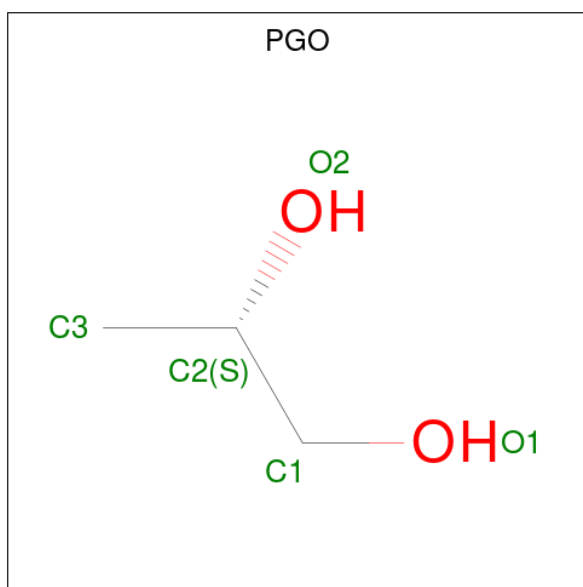
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			5	3	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			5	3	2		
8	D	1	Total	C	O	0	0
			5	3	2		
8	D	1	Total	C	O	0	0
			5	3	2		

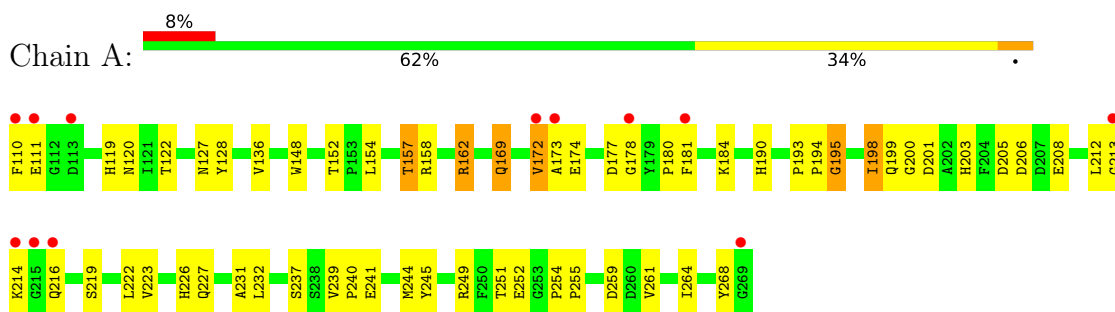
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	191	Total	O	0	1
			191	191		
9	B	187	Total	O	0	0
			187	187		
9	C	155	Total	O	0	0
			155	155		
9	D	171	Total	O	0	0
			171	171		

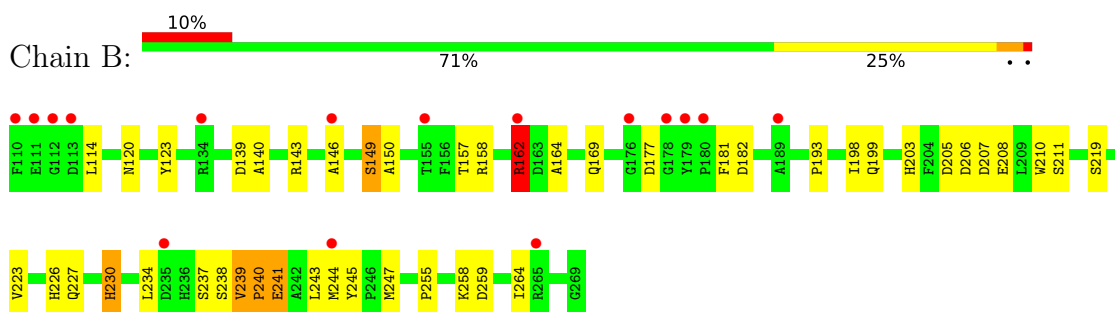
3 Residue-property plots [i](#)

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.

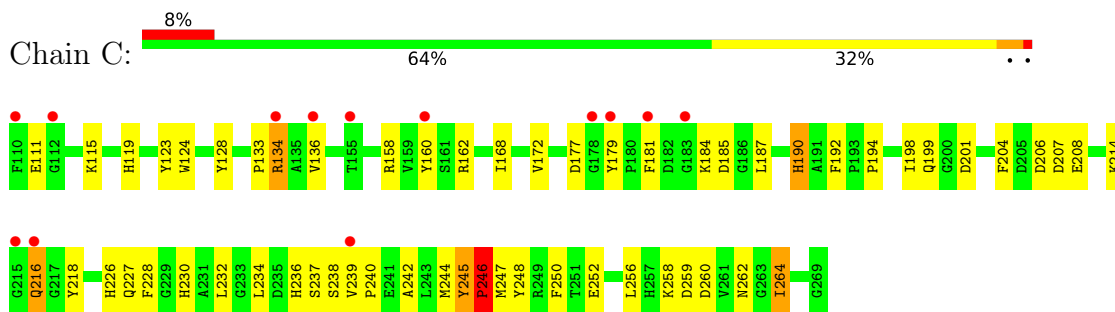
• Molecule 1: Matrix metalloproteinase-9



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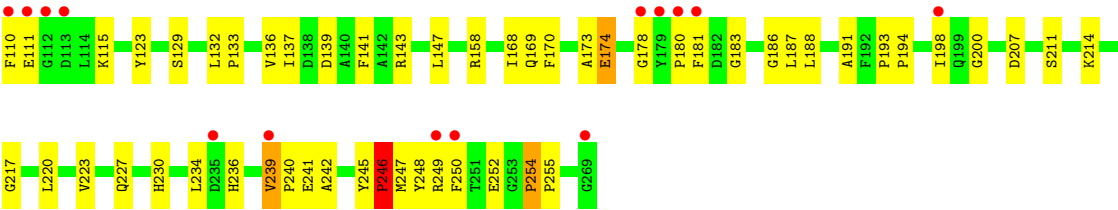


• Molecule 1: Matrix metalloproteinase-9



• Molecule 1: Matrix metalloproteinase-9





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	39.90Å 98.86Å 47.13Å 90.03° 111.95° 89.98°	Depositor
Resolution (Å)	33.46 – 1.90 33.46 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.0 (33.46-1.90) 87.0 (33.46-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.207 , 0.241 (Not available) , 0.293	Depositor DCC
R_{free} test set	2281 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.448 for -h,k,-l	Xtriage
Reported twinning fraction	0.480 for -h,k,-l	Depositor
Outliers	0 of 45613 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6145	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4757e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: L29, PPI, PEG, CA, ZN, GOL, PGO

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	0.48	0/1360	0.85	3/1850 (0.2%)
1	B	0.52	0/1352	0.91	3/1839 (0.2%)
1	C	0.55	1/1342 (0.1%)	0.93	5/1827 (0.3%)
1	D	0.54	1/1352 (0.1%)	0.87	2/1839 (0.1%)
All	All	0.52	2/5406 (0.0%)	0.89	13/7355 (0.2%)

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	B	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	246	PRO	N-CD	5.24	1.55	1.47
1	D	246	PRO	N-CD	5.22	1.55	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	254	PRO	CA-C-N	7.16	126.41	118.97
1	D	254	PRO	C-N-CA	7.16	126.41	118.97
1	C	179	TYR	CA-C-N	6.36	126.12	119.76
1	C	179	TYR	C-N-CA	6.36	126.12	119.76
1	C	190	HIS	N-CA-C	5.86	117.87	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	GLY	CA-C-N	5.63	125.60	120.03
1	A	195	GLY	C-N-CA	5.63	125.60	120.03
1	B	239	VAL	CA-C-N	5.31	126.47	119.84
1	B	239	VAL	C-N-CA	5.31	126.47	119.84
1	A	173	ALA	CB-CA-C	-5.24	110.52	116.54
1	C	245	TYR	CA-C-N	-5.12	113.43	119.84
1	C	245	TYR	C-N-CA	-5.12	113.43	119.84
1	B	140	ALA	N-CA-C	-5.03	105.69	111.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	162[A]	ARG	Mainchain
1	C	134	ARG	Sidechain

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	1313	0	1207	41	0
1	B	1305	0	1205	32	0
1	C	1295	0	1190	44	2
1	D	1305	0	1205	36	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	64	0	50	2	0
4	D	64	0	50	7	0
5	C	42	0	60	2	0
5	D	7	0	10	0	0
6	C	5	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	6	0	8	2	0
8	D	15	0	24	2	0
9	A	191	0	0	5	0
9	B	187	0	0	5	1
9	C	155	0	0	13	0
9	D	171	0	0	2	2
All	All	6145	0	5014	153	3

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 15.

All (153) 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:C:214:LYS:HG3	7:C:312:GOL:H11	1.46	0.94
8:D:301:PGO:H31	9:D:558:HOH:O	1.80	0.81
1:A:136:VAL:HG13	1:A:212:LEU:HD11	1.69	0.75
4:D:303:L29:H17	4:D:303:L29:H22	1.68	0.75
1:C:187:LEU:HD11	9:D:447:HOH:O	1.88	0.73
1:D:174:GLU:HG3	1:D:180:PRO:HB3	1.74	0.69
1:C:239:VAL:HG12	9:C:527:HOH:O	1.92	0.68
1:C:239:VAL:CG1	9:C:527:HOH:O	2.42	0.67
1:A:120:ASN:OD1	1:A:157:THR:OG1	2.13	0.67
1:A:237:SER:OG	1:A:259:ASP:OD2	2.08	0.66
1:B:237:SER:OG	1:B:259:ASP:OD2	2.10	0.65
1:D:173:ALA:O	1:D:181:PHE:N	2.28	0.64
1:A:213:GLY:O	1:A:214:LYS:HB3	1.99	0.63
1:A:148:TRP:O	1:A:152:THR:OG1	2.14	0.62
1:A:169:GLN:NE2	9:A:465:HOH:O	2.32	0.62
1:A:205:ASP:HB3	1:A:208:GLU:HG2	1.82	0.62
1:C:234:LEU:HD11	1:C:264:ILE:HG12	1.81	0.61
1:C:240:PRO:HA	1:C:245:TYR:CD1	2.34	0.61
1:A:122:THR:HG22	1:A:157:THR:HB	1.81	0.61
1:C:236:HIS:CG	1:C:246:PRO:HB3	2.35	0.60
1:C:124:TRP:CD1	1:C:160:TYR:HA	2.37	0.60
1:A:128:TYR:OH	1:A:158:ARG:NH2	2.34	0.60
1:C:244:MET:HA	1:C:244:MET:HE2	1.84	0.59
1:C:240:PRO:HA	1:C:245:TYR:CE1	2.39	0.58
1:D:132:LEU:HD21	1:D:211:SER:HA	1.85	0.58
1:C:258:LYS:HG3	9:C:457:HOH:O	2.05	0.57
1:C:230:HIS:ND1	1:C:234:LEU:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ASN:HB3	9:B:424:HOH:O	2.04	0.57
1:A:222:LEU:HD11	1:A:251:THR:HG22	1.88	0.56
1:B:239:VAL:HG12	1:B:241:GLU:HG2	1.88	0.56
1:A:249[A]:ARG:NH2	9:A:540:HOH:O	2.39	0.55
1:D:248:TYR:O	1:D:249:ARG:HG2	2.08	0.54
1:C:192:PHE:HB2	1:C:199:GLN:HA	1.89	0.54
1:A:214:LYS:O	1:A:214:LYS:HG3	2.08	0.53
1:C:214:LYS:N	1:C:250:PHE:CZ	2.77	0.53
1:D:248:TYR:C	1:D:249:ARG:HG2	2.33	0.53
1:A:178:GLY:O	1:A:180:PRO:HD3	2.09	0.53
1:A:136:VAL:CG1	1:A:212:LEU:HD11	2.38	0.53
1:D:239:VAL:HG22	1:D:242:ALA:H	1.74	0.53
1:D:230:HIS:ND1	1:D:234:LEU:O	2.34	0.53
1:C:184:LYS:HE2	9:C:550:HOH:O	2.09	0.52
1:D:214:LYS:HG3	1:D:250:PHE:CE1	2.44	0.52
1:C:123:TYR:CZ	1:C:158:ARG:HB2	2.46	0.51
1:C:177:ASP:HB2	1:C:198:ILE:HD11	1.91	0.51
1:B:169:GLN:HG2	1:B:203:HIS:CD2	2.46	0.50
1:D:193:PRO:O	1:D:200:GLY:N	2.44	0.50
1:A:223:VAL:O	1:A:227:GLN:HG2	2.12	0.50
1:B:114:LEU:HD12	1:B:193:PRO:HB2	1.95	0.49
1:A:190:HIS:HB3	4:A:306:L29:H17	1.94	0.49
1:D:183:GLY:HA2	1:D:207:ASP:OD2	2.12	0.49
1:D:178:GLY:O	1:D:180:PRO:HD3	2.13	0.49
1:D:236:HIS:CE1	1:D:246:PRO:HB3	2.47	0.49
1:A:219:SER:HB3	1:A:222:LEU:HB2	1.93	0.49
1:D:236:HIS:NE2	1:D:246:PRO:HB3	2.28	0.49
1:C:237:SER:OG	1:C:259:ASP:OD2	2.28	0.48
1:B:211:SER:O	1:B:219:SER:HA	2.13	0.48
1:C:237:SER:OG	5:C:313:PEG:H12	2.14	0.48
1:A:194:PRO:HG3	1:A:231:ALA:O	2.13	0.47
1:D:115:LYS:HA	1:D:194:PRO:HG2	1.96	0.47
1:A:177:ASP:HB3	1:A:198:ILE:CD1	2.44	0.47
1:C:236:HIS:ND1	1:C:246:PRO:HB3	2.28	0.47
1:D:139:ASP:O	1:D:143:ARG:HG3	2.13	0.47
1:C:128:TYR:OH	1:C:158:ARG:NH2	2.48	0.46
1:C:242:ALA:N	9:C:527:HOH:O	2.47	0.46
1:A:190:HIS:CB	4:A:306:L29:H17	2.46	0.46
1:C:198:ILE:O	1:C:201:ASP:HB2	2.16	0.46
1:B:238:SER:O	1:B:240:PRO:HD3	2.16	0.46
1:A:240:PRO:HA	1:A:245:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ALA:HA	1:B:149:SER:OG	2.16	0.46
1:B:258:LYS:HG3	9:B:417:HOH:O	2.15	0.45
1:D:137:ILE:HG23	1:D:220:LEU:HD21	1.97	0.45
1:A:198:ILE:HA	1:A:201:ASP:OD2	2.16	0.45
1:D:188:LEU:N	4:D:303:L29:O43	2.42	0.45
9:C:469:HOH:O	1:D:187:LEU:HD21	2.16	0.45
1:A:178:GLY:C	1:A:180:PRO:HD3	2.41	0.45
1:C:226:HIS:O	1:C:244:MET:HE1	2.16	0.45
1:C:216:GLN:HA	9:C:540:HOH:O	2.16	0.45
1:B:123:TYR:CZ	1:B:158:ARG:HB2	2.51	0.45
1:B:169:GLN:NE2	9:B:473:HOH:O	2.44	0.45
1:A:240:PRO:HA	1:A:245:TYR:CG	2.52	0.45
1:A:162:ARG:NH1	9:A:548:HOH:O	2.48	0.44
1:B:210:TRP:CH2	1:B:223:VAL:HG11	2.52	0.44
1:B:150:ALA:N	9:B:573:HOH:O	2.45	0.44
1:D:230:HIS:CD2	4:D:303:L29:O61	2.70	0.44
1:A:110:PHE:N	9:A:525:HOH:O	2.51	0.44
1:A:249[A]:ARG:NH1	1:B:182:ASP:OD2	2.51	0.44
1:C:115:LYS:HA	1:C:194:PRO:HG2	1.98	0.44
1:D:191:ALA:HB2	1:D:227:GLN:HB3	2.00	0.44
1:A:226:HIS:CE1	1:A:244:MET:HA	2.53	0.44
1:B:223:VAL:O	1:B:227:GLN:HG2	2.17	0.44
1:D:133:PRO:HB2	1:D:136:VAL:HG23	2.00	0.44
1:A:193:PRO:O	1:A:200:GLY:N	2.51	0.44
1:B:230:HIS:ND1	1:B:234:LEU:O	2.49	0.44
1:B:243:LEU:HB2	1:B:255:PRO:O	2.18	0.44
1:C:216:GLN:NE2	9:C:535:HOH:O	2.51	0.43
1:A:172:VAL:HG12	1:A:206:ASP:HB3	2.00	0.43
1:C:228:PHE:O	1:C:232:LEU:HG	2.19	0.43
1:A:127:ASN:OD1	1:A:127:ASN:N	2.50	0.43
1:C:214:LYS:HG3	7:C:312:GOL:C1	2.34	0.43
1:D:223:VAL:HG22	4:D:303:L29:H52	2.00	0.43
1:C:245:TYR:CD2	1:C:247:MET:HB3	2.54	0.43
1:A:232:LEU:O	1:A:268:TYR:OH	2.32	0.43
1:A:249[A]:ARG:NH2	1:B:182:ASP:OD2	2.51	0.42
1:C:133:PRO:O	1:C:136:VAL:HG22	2.19	0.42
1:C:208:GLU:HG3	9:C:503:HOH:O	2.19	0.42
1:D:129:SER:HB2	1:D:170:PHE:CD1	2.54	0.42
1:A:119:HIS:ND1	1:A:154:LEU:HD23	2.34	0.42
1:B:162[A]:ARG:C	1:B:164:ALA:H	2.27	0.42
1:C:239:VAL:HG11	9:C:527:HOH:O	2.15	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162[A]:ARG:H	1:B:162[A]:ARG:HG2	1.61	0.42
1:D:123:TYR:CZ	1:D:158:ARG:HB2	2.54	0.42
1:D:223:VAL:HG13	4:D:303:L29:H46	2.02	0.42
1:D:240:PRO:HA	1:D:245:TYR:CG	2.55	0.42
1:C:181:PHE:CE1	1:C:190:HIS:CE1	3.07	0.42
5:C:313:PEG:H42	9:C:509:HOH:O	2.20	0.42
1:A:169:GLN:O	1:A:203:HIS:HA	2.20	0.42
1:A:239:VAL:HA	1:A:240:PRO:HD3	1.91	0.42
4:D:303:L29:C46	4:D:303:L29:H33	2.50	0.42
1:B:139:ASP:O	1:B:143:ARG:HG3	2.20	0.42
1:B:206:ASP:C	1:B:208:GLU:H	2.27	0.42
1:B:255:PRO:HA	9:B:508:HOH:O	2.18	0.42
1:B:207:ASP:CG	1:C:162:ARG:HH12	2.27	0.42
1:C:218:TYR:HD1	1:C:248:TYR:CE2	2.38	0.42
1:C:226:HIS:HA	1:C:244:MET:CE	2.50	0.42
1:C:247:MET:HE2	1:D:186:GLY:HA2	2.01	0.42
1:A:111[B]:GLU:HG3	9:A:587:HOH:O	2.19	0.41
1:A:181:PHE:HB3	1:A:205:ASP:OD2	2.20	0.41
1:D:147:LEU:HD21	1:D:255:PRO:HD2	2.02	0.41
1:B:226:HIS:HD1	1:B:244[B]:MET:HA	1.84	0.41
1:B:193:PRO:O	1:B:199:GLN:HB3	2.20	0.41
1:D:254:PRO:HA	1:D:255:PRO:HD3	1.72	0.41
1:A:195:GLY:C	1:A:199:GLN:HB2	2.46	0.41
1:C:185:ASP:N	1:C:208:GLU:OE2	2.54	0.41
1:D:240:PRO:HB2	1:D:241:GLU:OE1	2.20	0.41
1:A:254:PRO:HA	1:A:255:PRO:HD3	1.82	0.41
1:B:237:SER:O	1:B:245:TYR:HD1	2.03	0.41
1:D:239:VAL:HG22	1:D:241:GLU:H	1.85	0.41
1:B:226:HIS:HD2	1:B:227:GLN:NE2	2.18	0.41
1:D:141:PHE:CE2	1:D:168:ILE:HG21	2.56	0.41
1:A:261:VAL:O	1:A:264:ILE:HG22	2.20	0.41
1:C:192:PHE:CB	1:C:199:GLN:HA	2.51	0.41
1:D:217:GLY:O	8:D:310:PGO:H11	2.21	0.41
1:B:245:TYR:CE2	1:B:247:MET:HE3	2.56	0.40
1:C:134:ARG:NH1	9:C:536:HOH:O	2.54	0.40
1:B:177:ASP:HB2	1:B:198:ILE:HD11	2.03	0.40
1:C:168:ILE:HG23	1:C:204:PHE:HE1	1.86	0.40
1:D:115:LYS:HE3	1:D:115:LYS:HB2	1.87	0.40
1:B:181:PHE:HB3	1:B:205:ASP:OD2	2.21	0.40
1:D:246:PRO:CG	4:D:303:L29:C34	2.99	0.40
1:B:240:PRO:HA	1:B:245:TYR:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:HIS:CE1	9:C:530:HOH:O	2.74	0.40
1:C:172:VAL:CG1	1:C:206:ASP:HB3	2.52	0.40
1:D:110:PHE:HB3	1:D:111:GLU:H	1.78	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:GLU:O	9:D:435:HOH:O[1_556]	2.00	0.20
9:B:472:HOH:O	9:B:513:HOH:O[1_655]	2.06	0.14
1:C:262:ASN:O	9:D:431:HOH:O[1_656]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/160 (101%)	145 (90%)	17 (10%)	0	100	100
1	B	161/160 (101%)	145 (90%)	15 (9%)	1 (1%)	21	13
1	C	160/160 (100%)	151 (94%)	9 (6%)	0	100	100
1	D	161/160 (101%)	153 (95%)	8 (5%)	0	100	100
All	All	644/640 (101%)	594 (92%)	49 (8%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	240	PRO

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	127/128 (99%)	116 (91%)	11 (9%)	9	4
1	B	131/128 (102%)	124 (95%)	7 (5%)	20	12
1	C	130/128 (102%)	121 (93%)	9 (7%)	14	7
1	D	131/128 (102%)	124 (95%)	7 (5%)	20	12
All	All	519/512 (101%)	485 (93%)	34 (7%)	16	8

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	THR
1	A	162	ARG
1	A	169	GLN
1	A	172	VAL
1	A	174	GLU
1	A	184	LYS
1	A	198	ILE
1	A	216	GLN
1	A	241[A]	GLU
1	A	241[B]	GLU
1	A	252	GLU
1	B	149	SER
1	B	157	THR
1	B	162[A]	ARG
1	B	162[B]	ARG
1	B	230	HIS
1	B	241	GLU
1	B	264	ILE
1	C	111	GLU
1	C	207	ASP
1	C	216	GLN
1	C	227	GLN
1	C	238	SER
1	C	246	PRO

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Mol	Chain	Res	Type
1	C	256	LEU
1	C	260	ASP
1	C	264	ILE
1	D	169	GLN
1	D	174	GLU
1	D	198	ILE
1	D	239	VAL
1	D	246	PRO
1	D	247	MET
1	D	252	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	120	ASN
1	B	199	GLN
1	C	169	GLN
1	C	190	HIS
1	C	266	HIS
1	D	236	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 20 are monoatomic - leaving 14 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	L29	A	306	2	64,68,68	6.42	34 (53%)	90,96,96	1.90	23 (25%)
5	PEG	C	310	-	6,6,6	0.74	0	5,5,5	1.21	0
8	PGO	D	310	-	4,4,4	0.77	0	4,4,4	0.43	0
5	PEG	C	311	-	6,6,6	0.51	0	5,5,5	0.75	0
5	PEG	C	306	-	6,6,6	0.43	0	5,5,5	0.11	0
6	PPI	C	308	-	4,4,4	1.00	0	4,4,4	0.90	0
8	PGO	D	308	-	4,4,4	0.60	0	4,4,4	0.78	0
5	PEG	C	307	-	6,6,6	0.76	0	5,5,5	1.45	0
4	L29	D	303	2	64,68,68	6.41	35 (54%)	90,96,96	2.39	26 (28%)
5	PEG	C	313	-	6,6,6	0.66	0	5,5,5	1.43	0
5	PEG	D	309	-	6,6,6	0.59	0	5,5,5	1.21	1 (20%)
7	GOL	C	312	-	5,5,5	0.73	0	5,5,5	0.77	0
8	PGO	D	301	-	4,4,4	0.61	0	4,4,4	0.91	0
5	PEG	C	309	-	6,6,6	0.55	0	5,5,5	1.58	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
4	L29	A	306	2	-	6/80/80/80	0/5/5/5
5	PEG	C	310	-	-	1/4/4/4	-
8	PGO	D	310	-	-	0/2/2/2	-
5	PEG	C	311	-	-	2/4/4/4	-
5	PEG	C	306	-	-	2/4/4/4	-
6	PPI	C	308	-	-	0/2/2/2	-
8	PGO	D	308	-	-	2/2/2/2	-
5	PEG	C	307	-	-	2/4/4/4	-
4	L29	D	303	2	-	9/80/80/80	0/5/5/5
5	PEG	C	313	-	-	1/4/4/4	-
5	PEG	D	309	-	-	3/4/4/4	-
7	GOL	C	312	-	-	0/4/4/4	-
8	PGO	D	301	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	C	309	-	-	3/4/4/4	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	306	L29	O15-S13	22.32	1.67	1.43
4	D	303	L29	O43-S41	21.73	1.66	1.43
4	D	303	L29	O15-S13	21.57	1.66	1.43
4	A	306	L29	O43-S41	21.08	1.66	1.43
4	A	306	L29	O14-S13	19.53	1.64	1.43
4	D	303	L29	O42-S41	19.48	1.64	1.43
4	D	303	L29	O14-S13	19.43	1.64	1.43
4	A	306	L29	O42-S41	19.07	1.63	1.43
4	D	303	L29	C34-C29	10.26	1.54	1.39
4	A	306	L29	C34-C29	9.54	1.53	1.39
4	A	306	L29	C5A-C45	8.52	1.52	1.38
4	D	303	L29	C5A-C45	8.43	1.52	1.38
4	D	303	L29	C3-C2	8.17	1.52	1.38
4	A	306	L29	C3-C2	8.03	1.52	1.38
4	D	303	L29	C31-C32	7.98	1.52	1.38
4	A	306	L29	C31-C30	7.36	1.51	1.38
4	A	306	L29	C31-C32	7.35	1.51	1.38
4	A	306	L29	C27-N26	7.24	1.49	1.33
4	D	303	L29	C31-C30	7.14	1.51	1.38
4	A	306	L29	C8-C7	7.06	1.53	1.39
4	A	306	L29	S41-N40	7.05	1.73	1.63
4	D	303	L29	C27-N26	7.03	1.49	1.33
4	D	303	L29	S41-N40	6.87	1.73	1.63
4	D	303	L29	C8-C7	6.70	1.52	1.39
4	A	306	L29	C10-S13	6.62	1.85	1.76
4	A	306	L29	C47-C46	6.54	1.49	1.38
4	D	303	L29	C45-S41	6.39	1.85	1.76
4	A	306	L29	C12-C11	6.37	1.49	1.38
4	A	306	L29	C35-N37	6.34	1.47	1.33
4	D	303	L29	C47-C46	6.25	1.48	1.38
4	A	306	L29	C45-S41	6.09	1.84	1.76
4	D	303	L29	C11-C10	6.06	1.48	1.38
4	A	306	L29	C11-C10	6.06	1.48	1.38
4	D	303	L29	C12-C11	5.94	1.48	1.38
4	D	303	L29	C35-N37	5.92	1.46	1.33
4	D	303	L29	C10-S13	5.83	1.84	1.76
4	A	306	L29	C9-C10	4.57	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	303	L29	C34-C33	4.55	1.46	1.39
4	A	306	L29	S13-N16	-4.55	1.56	1.63
4	D	303	L29	C5-C6	4.40	1.46	1.38
4	A	306	L29	C5-C6	4.34	1.46	1.38
4	D	303	L29	C9-C10	4.28	1.45	1.38
4	D	303	L29	C47-C48	4.21	1.47	1.39
4	A	306	L29	C55-C50	4.15	1.47	1.39
4	D	303	L29	C55-C50	4.00	1.47	1.39
4	A	306	L29	C34-C33	3.86	1.45	1.39
4	D	303	L29	C5A-C49	3.74	1.44	1.38
4	A	306	L29	C47-C48	3.74	1.46	1.39
4	A	306	L29	C5A-C49	3.62	1.44	1.38
4	A	306	L29	C52-C51	3.48	1.44	1.38
4	D	303	L29	C52-C51	3.42	1.44	1.38
4	A	306	L29	C1-C7	2.98	1.56	1.49
4	A	306	L29	C9-C8	2.98	1.43	1.38
4	D	303	L29	S13-N16	-2.95	1.58	1.63
4	A	306	L29	C49-C48	2.92	1.45	1.39
4	D	303	L29	C1-C7	2.80	1.55	1.49
4	D	303	L29	C50-C48	2.79	1.55	1.49
4	D	303	L29	C49-C48	2.60	1.44	1.39
4	D	303	L29	C33-C35	2.55	1.55	1.50
4	D	303	L29	O23-C21	-2.44	1.18	1.23
4	A	306	L29	C50-C48	2.43	1.54	1.49
4	D	303	L29	C9-C8	2.42	1.42	1.38
4	A	306	L29	C53-C52	2.32	1.43	1.38
4	A	306	L29	C51-C50	-2.29	1.34	1.39
4	A	306	L29	O23-C21	-2.25	1.19	1.23
4	D	303	L29	C51-C50	-2.13	1.35	1.39
4	D	303	L29	C29-C27	2.12	1.54	1.50
4	A	306	L29	C29-C27	2.08	1.54	1.50
4	D	303	L29	C53-C52	2.06	1.42	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	303	L29	O42-S41-O43	-9.21	105.22	119.59
4	D	303	L29	O14-S13-C10	-9.11	96.78	108.10
4	A	306	L29	O42-S41-O43	-6.48	109.48	119.59
4	D	303	L29	O14-S13-N16	6.27	117.94	106.97
4	A	306	L29	O15-S13-C10	-6.09	100.53	108.10
4	A	306	L29	O15-S13-N16	5.85	117.21	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	303	L29	C39-N40-S41	-5.63	105.53	118.43
4	D	303	L29	O15-S13-N16	4.73	115.24	106.97
4	D	303	L29	C38-N37-C35	-4.40	112.15	122.11
4	D	303	L29	C9-C10-S13	-4.30	115.47	119.73
4	D	303	L29	C25-C24-N16	4.02	119.90	112.49
4	A	306	L29	C25-C24-N16	3.88	119.64	112.49
4	D	303	L29	C11-C10-S13	3.72	123.43	119.73
4	A	306	L29	O14-S13-C10	-3.71	103.49	108.10
4	A	306	L29	O43-S41-C45	3.56	112.53	108.10
4	D	303	L29	C60-C56-N40	3.56	119.13	109.56
4	D	303	L29	O43-S41-N40	3.48	113.05	106.97
4	D	303	L29	O15-S13-C10	-3.26	104.05	108.10
4	A	306	L29	C38-C39-N40	3.18	118.35	112.49
4	A	306	L29	C60-C56-N40	3.04	117.73	109.56
4	A	306	L29	C17-N16-S13	-3.03	112.23	118.39
4	D	303	L29	C59-C57-C56	2.86	118.11	110.77
4	A	306	L29	O14-S13-N16	2.84	111.93	106.97
4	A	306	L29	C19-C18-C17	2.82	118.00	110.77
4	A	306	L29	C56-N40-S41	-2.80	112.70	118.39
4	A	306	L29	O62-C60-C56	2.68	125.35	120.95
4	A	306	L29	C32-C33-C34	2.65	122.31	119.25
4	A	306	L29	C56-C60-N61	2.61	120.44	115.50
4	D	303	L29	O14-S13-O15	-2.55	115.62	119.59
4	D	303	L29	C30-C29-C34	2.50	122.14	119.25
4	A	306	L29	C31-C32-C33	-2.50	117.91	120.36
4	D	303	L29	C10-S13-N16	-2.47	103.05	107.36
4	D	303	L29	C21-C17-N16	2.43	116.10	109.56
4	D	303	L29	C31-C30-C29	-2.37	118.03	120.36
4	D	303	L29	C20-C18-C17	2.36	116.83	110.77
4	A	306	L29	C30-C29-C34	2.23	121.83	119.25
4	D	303	L29	C58-C57-C56	2.22	116.45	110.77
4	A	306	L29	C38-N37-C35	-2.17	117.19	122.11
4	D	303	L29	C24-C25-N26	2.14	115.69	111.56
4	A	306	L29	C18-C17-N16	2.13	116.46	112.83
5	D	309	PEG	O1-C1-C2	2.12	124.29	111.82
4	D	303	L29	C46-C45-S41	2.11	121.83	119.73
4	D	303	L29	C45-S41-N40	2.10	111.03	107.36
4	A	306	L29	O14-S13-O15	-2.08	116.34	119.59
4	D	303	L29	C31-C32-C33	-2.08	118.32	120.36
4	D	303	L29	C39-C38-N37	2.04	115.49	111.56
4	A	306	L29	C21-C17-N16	2.02	115.01	109.56
4	D	303	L29	C8-C7-C1	-2.02	117.77	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	306	L29	C39-C38-N37	2.02	115.46	111.56
4	A	306	L29	C20-C18-C17	2.02	115.94	110.77

There are no chirality outliers.

All (33) torsion outliers are listed below:

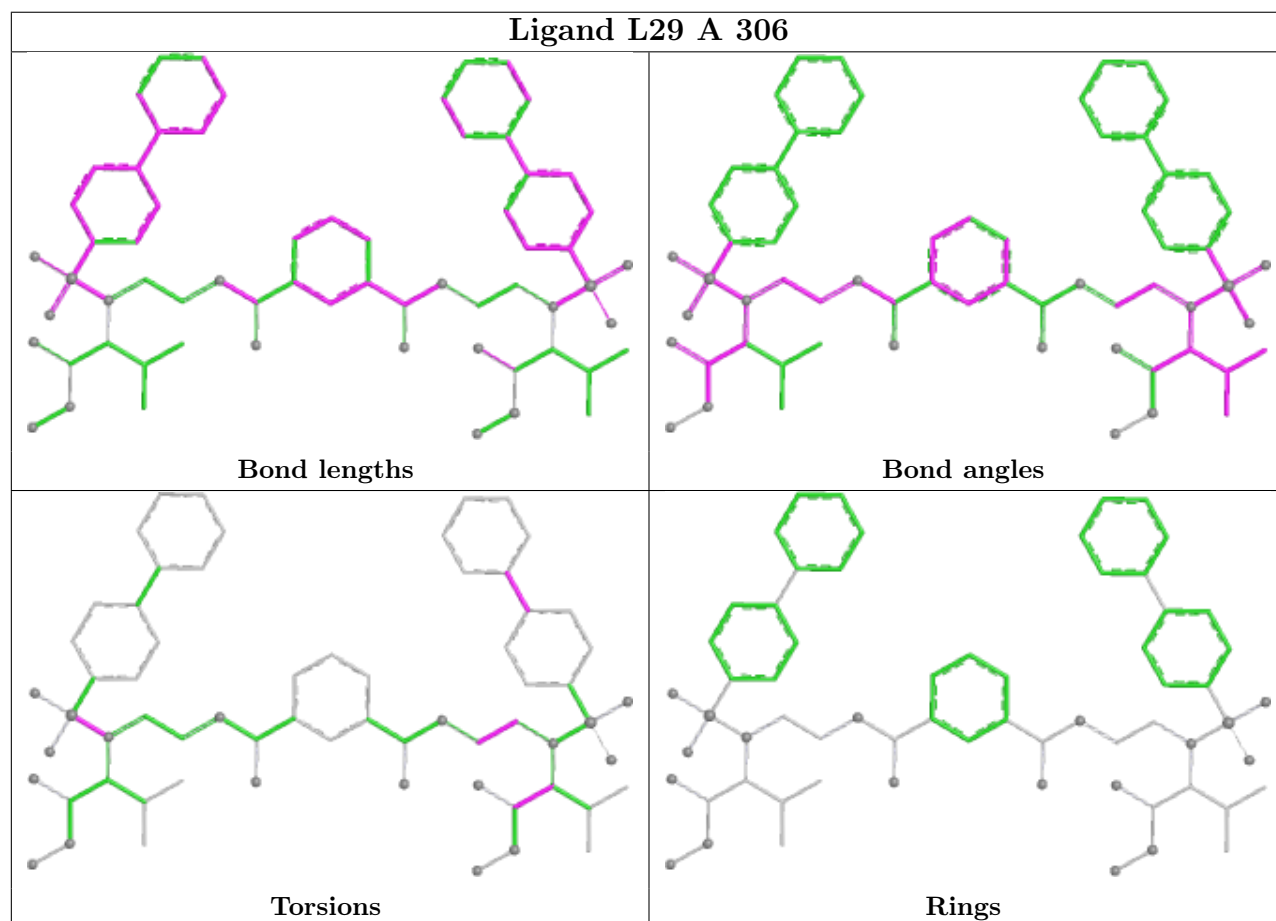
Mol	Chain	Res	Type	Atoms
4	D	303	L29	N40-C56-C57-C58
4	D	303	L29	N40-C56-C57-C59
4	D	303	L29	C60-C56-C57-C58
4	D	303	L29	C56-C60-N61-O61
8	D	301	PGO	O1-C1-C2-C3
8	D	308	PGO	O1-C1-C2-C3
8	D	308	PGO	O1-C1-C2-O2
5	C	313	PEG	C4-C3-O2-C2
4	D	303	L29	C60-C56-C57-C59
5	C	307	PEG	C4-C3-O2-C2
5	C	311	PEG	O1-C1-C2-O2
4	A	306	L29	C39-N40-S41-O42
5	C	306	PEG	O2-C3-C4-O4
5	C	309	PEG	O1-C1-C2-O2
5	C	310	PEG	O1-C1-C2-O2
5	D	309	PEG	C4-C3-O2-C2
5	C	309	PEG	C1-C2-O2-C3
4	A	306	L29	C6-C1-C7-C8
5	D	309	PEG	C1-C2-O2-C3
8	D	301	PGO	O1-C1-C2-O2
5	C	306	PEG	C4-C3-O2-C2
4	D	303	L29	C39-N40-S41-O42
5	D	309	PEG	O2-C3-C4-O4
4	A	306	L29	C6-C1-C7-C12
5	C	309	PEG	C4-C3-O2-C2
5	C	307	PEG	C1-C2-O2-C3
4	D	303	L29	C57-C56-C60-N61
5	C	311	PEG	C4-C3-O2-C2
4	A	306	L29	N16-C24-C25-N26
4	A	306	L29	C18-C17-C21-N22
4	D	303	L29	C38-C39-N40-C56
4	D	303	L29	C18-C17-C21-O23
4	A	306	L29	C39-N40-S41-C45

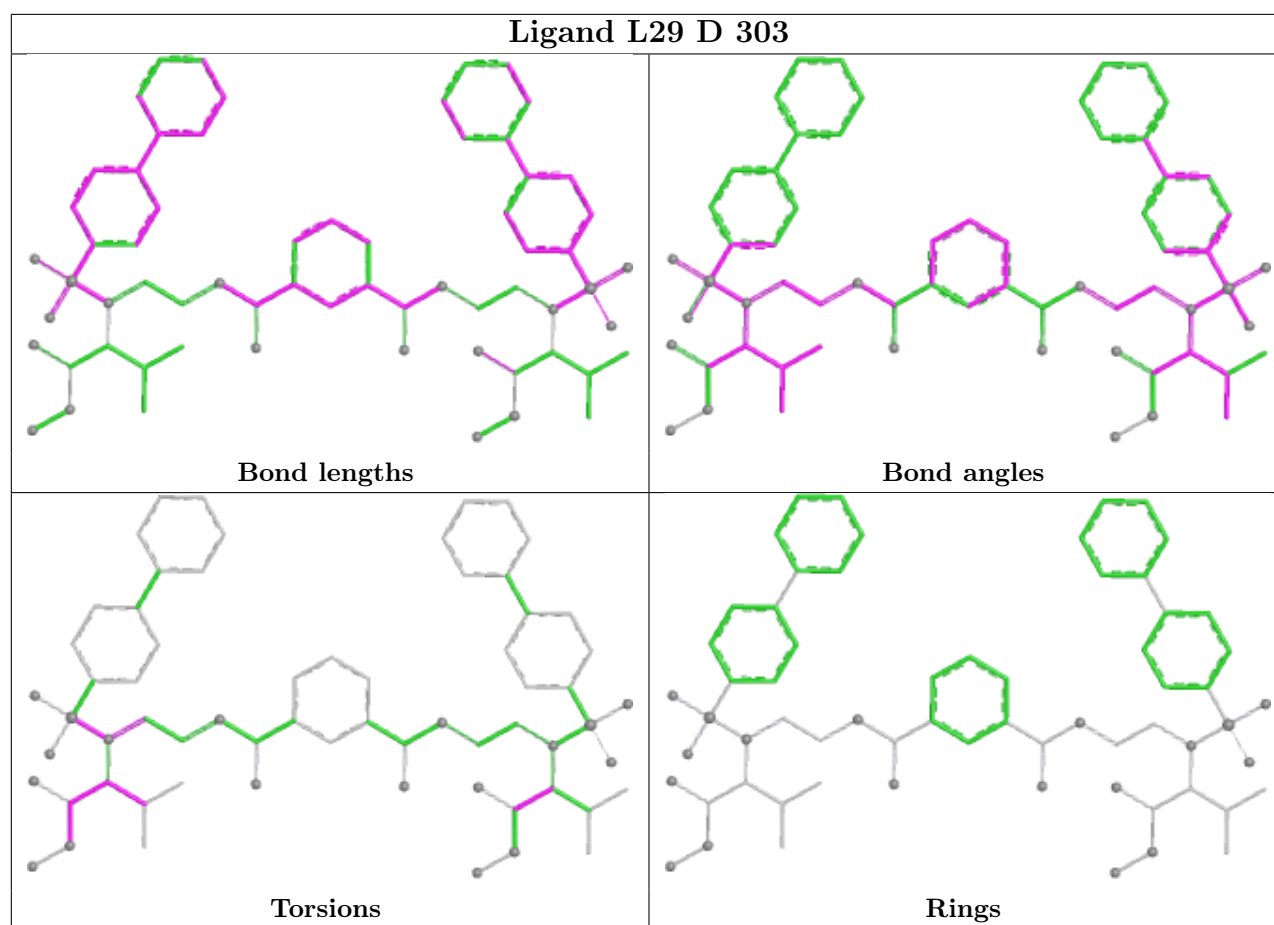
There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	306	L29	2	0
8	D	310	PGO	1	0
4	D	303	L29	7	0
5	C	313	PEG	2	0
7	C	312	GOL	2	0
8	D	301	PGO	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	160/160 (100%)	0.93	12 (7%)	20 21	3, 12, 26, 44	4 (2%)
1	B	160/160 (100%)	1.00	16 (10%)	12 13	5, 12, 25, 68	3 (1%)
1	C	160/160 (100%)	0.92	13 (8%)	18 19	6, 12, 26, 44	2 (1%)
1	D	160/160 (100%)	0.88	14 (8%)	15 16	4, 11, 22, 76	3 (1%)
All	All	640/640 (100%)	0.93	55 (8%)	16 17	3, 12, 26, 76	12 (1%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162[A]	ARG	9.0
1	D	110	PHE	5.2
1	D	112	GLY	4.7
1	B	110	PHE	4.4
1	B	112	GLY	4.3
1	B	265[A]	ARG	4.1
1	C	215	GLY	3.8
1	A	269	GLY	3.6
1	A	110	PHE	3.3
1	A	113	ASP	3.2
1	D	111	GLU	3.1
1	A	215	GLY	3.1
1	D	180	PRO	3.0
1	A	181	PHE	3.0
1	D	249	ARG	2.9
1	A	216	GLN	2.9
1	B	113	ASP	2.9
1	C	216	GLN	2.9
1	D	113	ASP	2.9
1	D	235	ASP	2.8
1	B	178	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	269	GLY	2.7
1	B	179	TYR	2.5
1	A	213	GLY	2.5
1	D	239	VAL	2.5
1	B	235	ASP	2.4
1	C	110	PHE	2.4
1	C	112	GLY	2.4
1	C	179	TYR	2.4
1	A	172	VAL	2.4
1	A	178	GLY	2.4
1	B	134	ARG	2.3
1	C	181	PHE	2.3
1	B	189	ALA	2.3
1	C	136	VAL	2.3
1	B	146	ALA	2.2
1	C	183	GLY	2.2
1	B	111	GLU	2.2
1	D	198	ILE	2.2
1	C	239	VAL	2.2
1	B	176	GLY	2.2
1	A	214	LYS	2.2
1	A	173	ALA	2.2
1	C	160	TYR	2.1
1	D	179	TYR	2.1
1	C	134	ARG	2.1
1	D	178	GLY	2.1
1	D	181	PHE	2.0
1	B	244[A]	MET	2.0
1	C	155	THR	2.0
1	C	178	GLY	2.0
1	B	180	PRO	2.0
1	A	111[A]	GLU	2.0
1	D	250	PHE	2.0
1	B	155	THR	2.0

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

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(Å ²)	Q<0.9
3	CA	B	304	1/1	0.57	0.18	36,36,36,36	0
8	PGO	D	308	5/5	0.71	0.15	5,7,9,12	0
8	PGO	D	301	5/5	0.74	0.14	15,16,26,30	0
5	PEG	C	311	7/7	0.76	0.13	8,19,23,27	0
8	PGO	D	310	5/5	0.76	0.14	6,13,19,24	0
5	PEG	D	309	7/7	0.77	0.14	16,19,24,29	0
5	PEG	C	307	7/7	0.77	0.12	7,9,18,21	0
5	PEG	C	313	7/7	0.78	0.12	6,8,18,25	0
5	PEG	C	310	7/7	0.79	0.12	10,15,17,24	0
3	CA	C	305	1/1	0.80	0.13	27,27,27,27	0
3	CA	A	304	1/1	0.82	0.07	25,25,25,25	0
5	PEG	C	309	7/7	0.82	0.10	8,14,18,18	0
6	PPI	C	308	5/5	0.82	0.10	6,7,8,12	0
3	CA	A	305	1/1	0.84	0.07	39,39,39,39	0
3	CA	D	305	1/1	0.84	0.09	15,15,15,15	0
7	GOL	C	312	6/6	0.86	0.16	7,17,24,27	0
3	CA	A	303	1/1	0.86	0.06	9,9,9,9	0
3	CA	C	304	1/1	0.88	0.08	10,10,10,10	0
3	CA	C	303	1/1	0.88	0.05	8,8,8,8	0
4	L29	D	303	64/64	0.89	0.10	1,10,21,26	0
4	L29	A	306	64/64	0.89	0.10	3,9,18,24	0
5	PEG	C	306	7/7	0.91	0.07	2,5,16,26	0
3	CA	D	306	1/1	0.91	0.12	22,22,22,22	0
3	CA	B	303	1/1	0.93	0.04	12,12,12,12	0
2	ZN	B	300	1/1	0.94	0.06	10,10,10,10	0
2	ZN	A	302	1/1	0.95	0.04	17,17,17,17	0
2	ZN	A	301	1/1	0.96	0.05	12,12,12,12	0
2	ZN	D	304	1/1	0.96	0.05	8,8,8,8	0
3	CA	D	307	1/1	0.97	0.06	13,13,13,13	0
2	ZN	D	302	1/1	0.97	0.03	13,13,13,13	0
2	ZN	C	302	1/1	0.97	0.04	13,13,13,13	0
2	ZN	B	301	1/1	0.98	0.05	22,22,22,22	0

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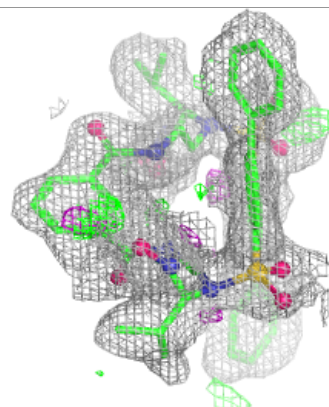
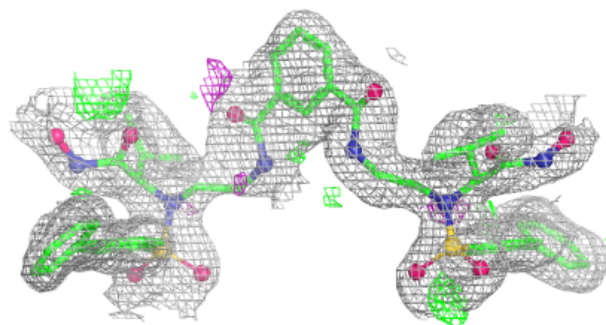
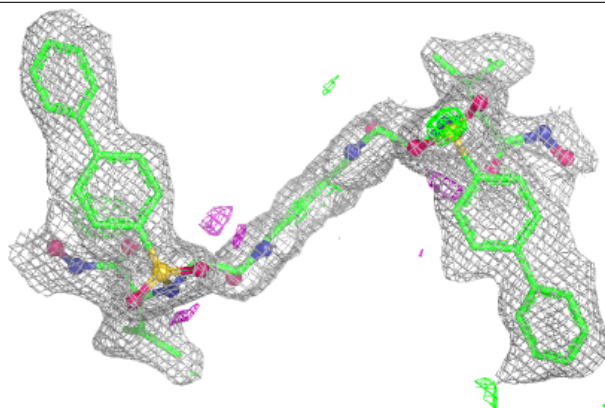
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	B	302	1/1	0.98	0.03	4,4,4,4	0
2	ZN	C	301	1/1	0.99	0.04	11,11,11,11	0

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.

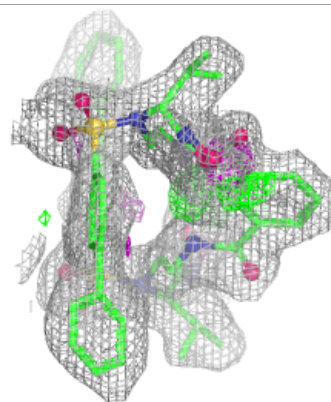
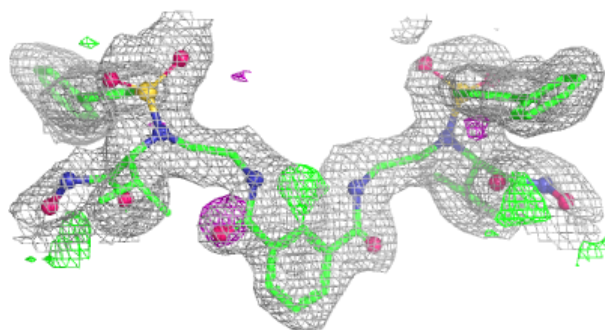
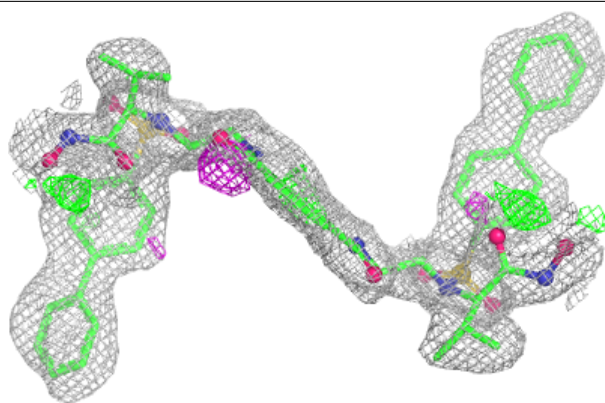
Electron density around L29 D 303:

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 L29 A 306:

$2mF_o-DF_c$ (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.