



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:39 PM EDT

PDB ID : 4H2E / pdb_00004h2e
Title : Crystal structure of an MMP twin inhibitor complexing two MMP-9 catalytic domains
Authors : Stura, E.A.; Vera, L.; Cassar-Lajeunesse, E.; Nuti, E.; Catalani, M.P.; Dive, V.; Rossello, A.
Deposited on : 2012-09-12
Resolution : 2.90 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

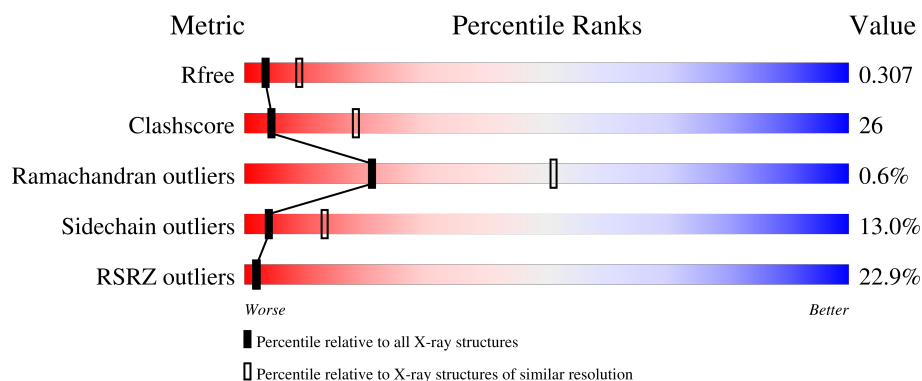
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	164	24% 55% 36% 9%
1	B	164	22% 56% 37% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCN	B	311	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 2977 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	164	Total	C	N	O	S	0	1	0
			1315	850	223	240	2			
1	B	164	Total	C	N	O	S	0	1	0
			1315	850	223	240	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	-	expression tag	UNP P14780
B	106	GLY	-	expression tag	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		

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

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



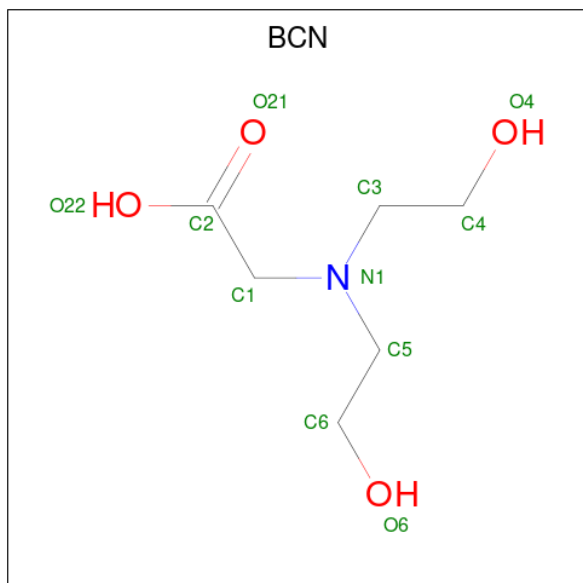
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



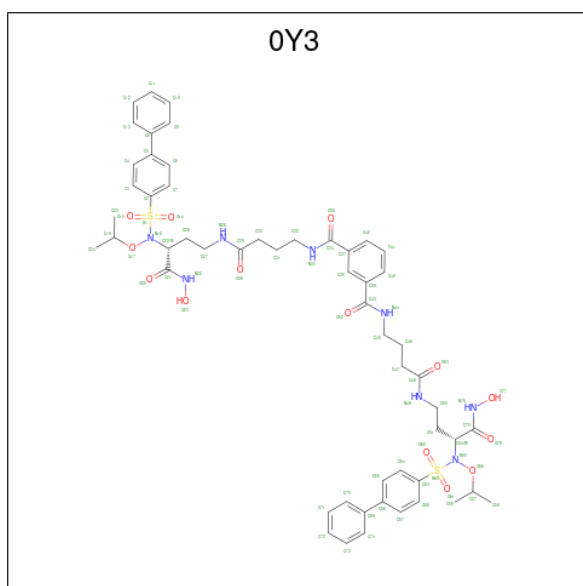
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is BICINE (CCD ID: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	6	1	4		
6	A	1	Total	C	N	O	0	0
			11	6	1	4		
6	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 7 is N,N'-bis(4-[[[(3R)-3-[(biphenyl-4-ylsulfonyl)(propan-2-yloxy)amino]-4-(hydroxyamino)-4-oxobutyl]amino]-4-oxobutyl]benzene-1,3-dicarboxamide (CCD ID: 0Y3) (formula: C₅₄H₆₆N₈O₁₄S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			78	54	8	14	2		

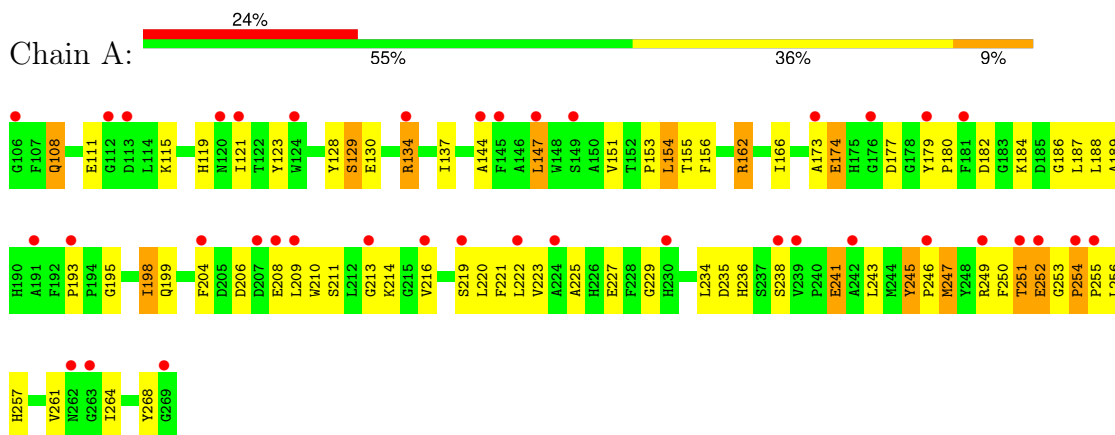
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	84	Total	O	0	0
			84	84		
8	B	64	Total	O	0	0
			64	64		

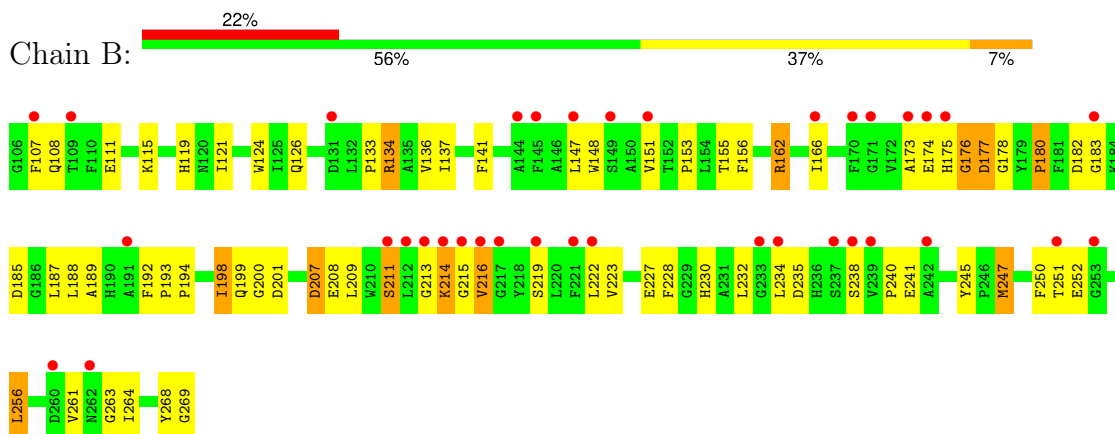
3 Residue-property plots

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: Matrix metalloproteinase-9



• Molecule 1: Matrix metalloproteinase-9



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.18Å 97.40Å 45.69Å 90.00° 111.99° 90.00°	Depositor
Resolution (Å)	38.85 – 2.90 38.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.85-2.90) 98.4 (38.85-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)/REFMAC	Depositor
R, R_{free}	0.277 , 0.311 0.279 , 0.307	Depositor DCC
R_{free} test set	358 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	2977	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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 47.35 % 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 1.0045e-04. 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: ACT, PEG, 0Y3, CA, ZN, BCN

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	0.35	0/1363	0.91	6/1856 (0.3%)
1	B	0.40	0/1363	0.96	5/1856 (0.3%)
All	All	0.38	0/2726	0.94	11/3712 (0.3%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	GLY	N-CA-C	11.68	126.75	112.73
1	A	252	GLU	N-CA-C	-9.09	102.36	112.72
1	B	216	VAL	CB-CA-C	-7.25	102.43	112.36
1	A	254	PRO	CA-C-N	7.16	126.65	118.85
1	A	254	PRO	C-N-CA	7.16	126.65	118.85
1	A	245	TYR	CA-C-N	6.44	126.13	119.82
1	A	245	TYR	C-N-CA	6.44	126.13	119.82
1	B	215	GLY	N-CA-C	6.43	123.57	115.21
1	B	177	ASP	N-CA-C	6.05	120.69	112.88
1	B	173	ALA	CB-CA-C	-5.45	110.31	116.63
1	A	251	THR	N-CA-C	5.34	118.31	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1315	0	1211	60	0
1	B	1315	0	1211	78	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
4	A	42	0	60	3	0
4	B	21	0	30	2	0
5	A	12	0	9	0	0
5	B	4	0	3	0	0
6	A	22	0	24	3	0
6	B	11	0	12	7	0
7	B	78	0	64	12	0
8	A	84	0	0	1	0
8	B	64	0	0	0	0
All	All	2977	0	2624	144	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 26.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LYS:HE2	1:B:214:LYS:HA	1.21	1.11
1:B:174:GLU:HB3	6:B:311:BCN:H12	1.04	1.04
1:B:177:ASP:HB3	1:B:198:ILE:HD11	1.42	1.02
1:B:216:VAL:HG12	1:B:216:VAL:O	1.60	1.01
1:B:174:GLU:HB3	6:B:311:BCN:C1	1.91	0.99
1:B:174:GLU:CB	6:B:311:BCN:H12	1.96	0.96
1:B:214:LYS:HE2	1:B:214:LYS:CA	1.93	0.95
1:B:177:ASP:HB3	1:B:198:ILE:CD1	1.99	0.92
1:B:137:ILE:HG22	1:B:141:PHE:CE2	2.09	0.88
1:A:257:HIS:O	1:A:261:VAL:HG23	1.79	0.82
1:A:213:GLY:HA3	1:A:250:PHE:CE2	2.15	0.82
1:B:214:LYS:HA	1:B:214:LYS:CE	2.08	0.81
1:A:119:HIS:NE2	1:A:153:PRO:HB2	1.96	0.81
1:A:219:SER:HB3	1:A:222:LEU:HB2	1.66	0.76
1:A:222:LEU:HD11	1:A:251:THR:HG22	1.68	0.76
1:B:107:PHE:O	7:B:306:OY3:H42	1.88	0.74
4:A:306:PEG:H31	4:B:308:PEG:H22	1.71	0.73
1:B:175:HIS:CD2	1:B:176:GLY:H	2.05	0.73
6:B:311:BCN:O21	6:B:311:BCN:H31	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:VAL:O	1:B:216:VAL:CG1	2.35	0.70
1:B:209:LEU:HD23	1:B:216:VAL:O	1.92	0.69
1:B:227:GLU:OE1	1:B:227:GLU:HA	1.92	0.69
1:B:137:ILE:HG22	1:B:141:PHE:HE2	1.57	0.68
1:A:189:ALA:O	7:B:306:OY3:H56	1.95	0.67
1:A:119:HIS:CD2	1:A:153:PRO:HB2	2.30	0.66
1:A:108:GLN:OE1	1:B:107:PHE:CD2	2.49	0.65
6:A:315:BCN:O21	6:A:315:BCN:H31	1.96	0.65
1:A:245:TYR:CD2	1:A:247:MET:HB3	2.33	0.64
1:A:129:SER:HB3	1:A:206:ASP:OD1	1.99	0.63
1:B:134[A]:ARG:HB3	1:B:134[A]:ARG:CZ	2.28	0.63
1:B:148:TRP:CZ3	1:B:264:ILE:HG21	2.34	0.62
1:B:192:PHE:HB3	1:B:199:GLN:HA	1.82	0.61
1:B:198:ILE:O	1:B:201:ASP:HB2	2.01	0.60
1:B:177:ASP:CB	1:B:198:ILE:HD11	2.24	0.60
1:A:119:HIS:HD2	1:A:154:LEU:HD23	1.67	0.60
1:A:241:GLU:OE2	4:A:306:PEG:H22	2.03	0.59
1:B:119:HIS:CD2	1:B:153:PRO:HB2	2.37	0.59
1:A:123:TYR:HA	1:A:166:ILE:O	2.03	0.59
1:B:189:ALA:O	7:B:306:OY3:H11	2.03	0.59
1:B:230:HIS:CD2	7:B:306:OY3:O77	2.56	0.58
1:A:162:ARG:HB3	1:A:162:ARG:NH1	2.19	0.58
1:B:209:LEU:CD2	1:B:216:VAL:O	2.52	0.57
1:B:175:HIS:CG	1:B:176:GLY:H	2.20	0.57
1:B:247:MET:HB2	7:B:306:OY3:H63	1.85	0.57
1:B:245:TYR:CE2	1:B:247:MET:HB3	2.39	0.57
1:B:183:GLY:HA2	1:B:207:ASP:CB	2.35	0.56
1:B:134[A]:ARG:NH2	1:B:134[A]:ARG:HB2	2.19	0.56
1:B:134[A]:ARG:CZ	1:B:134[A]:ARG:CB	2.83	0.56
1:B:107:PHE:CE2	1:B:235:ASP:OD2	2.58	0.56
1:A:137:ILE:HG23	1:A:220:LEU:HD21	1.87	0.56
1:A:147:LEU:HD13	1:A:256:LEU:HG	1.88	0.56
1:A:173:ALA:HB1	4:A:309:PEG:H41	1.87	0.55
1:A:252:GLU:OE1	1:A:252:GLU:HA	2.05	0.55
1:B:214:LYS:HE3	1:B:250:PHE:CE1	2.42	0.55
1:A:235:ASP:CG	1:A:236:HIS:H	2.15	0.55
1:B:166:ILE:HG12	1:B:200:GLY:O	2.07	0.55
1:A:144:ALA:HA	1:A:221:PHE:HE1	1.71	0.54
1:B:178:GLY:O	4:B:309:PEG:H22	2.08	0.54
1:A:193:PRO:O	1:A:199:GLN:HB3	2.08	0.54
1:A:222:LEU:O	7:B:306:OY3:H66	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASP:OD2	7:B:306:OY3:H41	2.08	0.52
1:A:210:TRP:HZ3	1:A:223:VAL:HG21	1.75	0.52
1:A:162:ARG:HB3	1:A:162:ARG:HH11	1.74	0.51
1:B:211:SER:O	1:B:219:SER:HA	2.09	0.51
1:B:245:TYR:CD2	1:B:247:MET:HB3	2.45	0.51
1:A:151:VAL:CG2	1:A:264:ILE:HD12	2.41	0.50
1:A:245:TYR:HD2	1:A:247:MET:HB3	1.74	0.50
1:B:175:HIS:CG	1:B:176:GLY:N	2.79	0.50
1:B:213:GLY:HA3	1:B:219:SER:HB2	1.93	0.50
1:B:227:GLU:OE2	7:B:306:OY3:N76	2.45	0.49
1:B:174:GLU:CG	1:B:174:GLU:O	2.60	0.49
1:A:245:TYR:CE2	1:A:247:MET:HB3	2.47	0.49
6:B:311:BCN:O21	6:B:311:BCN:C3	2.57	0.49
1:A:115:LYS:HB2	1:A:268:TYR:CE1	2.48	0.49
1:B:183:GLY:HA2	1:B:207:ASP:CG	2.37	0.48
1:B:137:ILE:CG2	1:B:141:PHE:CE2	2.92	0.48
1:A:204:PHE:HB3	1:A:210:TRP:CZ2	2.49	0.48
1:B:134[A]:ARG:NH2	1:B:134[A]:ARG:CB	2.77	0.48
1:A:151:VAL:HG21	1:A:264:ILE:CD1	2.44	0.48
1:A:195:GLY:C	1:A:199:GLN:HB2	2.39	0.48
1:A:261:VAL:HA	1:A:264:ILE:HG12	1.96	0.48
1:B:252:GLU:HA	1:B:252:GLU:OE1	2.14	0.47
1:B:162:ARG:NH1	1:B:162:ARG:HB3	2.29	0.47
1:B:174:GLU:HA	1:B:180:PRO:HB3	1.96	0.47
1:A:225:ALA:HB1	1:A:243:LEU:HD21	1.97	0.46
1:B:192:PHE:CB	1:B:199:GLN:HA	2.46	0.46
1:A:227:GLU:HA	1:A:227:GLU:OE1	2.15	0.46
1:B:240:PRO:HA	1:B:245:TYR:CD1	2.51	0.46
1:A:211:SER:O	1:A:219:SER:HA	2.16	0.46
1:B:234:LEU:HD21	1:B:263:GLY:HA3	1.98	0.46
6:B:311:BCN:H51	6:B:311:BCN:H42	1.57	0.46
1:B:174:GLU:HB3	6:B:311:BCN:C2	2.43	0.45
1:A:134[A]:ARG:HE	1:A:134[A]:ARG:HB2	1.53	0.45
1:A:182:ASP:OD1	1:A:186:GLY:HA3	2.15	0.45
1:A:213:GLY:HA3	1:A:250:PHE:HE2	1.77	0.45
1:B:182:ASP:OD2	1:B:182:ASP:N	2.47	0.45
1:A:216:VAL:O	1:A:216:VAL:HG12	2.15	0.45
1:B:175:HIS:CD2	1:B:176:GLY:N	2.81	0.45
1:A:151:VAL:CG2	1:A:264:ILE:CD1	2.95	0.45
1:B:134[A]:ARG:HB2	1:B:134[A]:ARG:HH21	1.82	0.45
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:VAL:HA	1:B:264:ILE:HG12	1.98	0.45
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.83	0.45
1:A:174:GLU:O	1:A:174:GLU:HG2	2.16	0.44
1:A:253:GLY:HA2	1:A:254:PRO:C	2.42	0.44
1:B:121:ILE:HB	1:B:156:PHE:CD1	2.52	0.44
1:A:209:LEU:HD23	1:A:216:VAL:O	2.17	0.44
1:B:185:ASP:N	1:B:208:GLU:OE2	2.50	0.44
1:B:121:ILE:O	1:B:156:PHE:HA	2.18	0.44
1:A:261:VAL:HA	1:A:264:ILE:CG1	2.48	0.44
1:B:223:VAL:HA	7:B:306:OY3:H14	2.00	0.44
1:B:115:LYS:HA	1:B:194:PRO:HG2	2.00	0.43
1:B:214:LYS:HE2	1:B:214:LYS:C	2.42	0.43
1:A:147:LEU:C	1:A:147:LEU:HD12	2.42	0.43
1:A:210:TRP:CZ3	1:A:223:VAL:HG21	2.53	0.43
1:A:254:PRO:HA	1:A:255:PRO:HD3	1.67	0.43
1:B:124:TRP:CH2	1:B:126:GLN:HG3	2.54	0.43
1:B:183:GLY:C	1:B:207:ASP:HB3	2.43	0.43
1:B:147:LEU:HG	1:B:256:LEU:HD13	2.00	0.43
1:B:148:TRP:CE3	1:B:264:ILE:HG21	2.54	0.43
1:A:177:ASP:HB3	1:A:198:ILE:HD11	2.01	0.42
1:B:133:PRO:O	1:B:136:VAL:N	2.53	0.42
6:A:315:BCN:O21	6:A:315:BCN:C3	2.65	0.42
1:A:179:TYR:HA	1:A:180:PRO:HD3	1.84	0.42
1:A:238:SER:HB3	8:A:476:HOH:O	2.20	0.42
1:B:268:TYR:HA	1:B:269:GLY:C	2.44	0.42
1:A:182:ASP:HA	6:A:314:BCN:H31	2.01	0.42
1:A:245:TYR:HA	1:A:246:PRO:HD2	1.79	0.42
1:B:133:PRO:O	1:B:134[A]:ARG:C	2.62	0.42
1:B:193:PRO:O	1:B:199:GLN:HB3	2.20	0.42
1:B:250:PHE:CG	1:B:251:THR:N	2.88	0.42
1:A:219:SER:O	1:A:223:VAL:HG23	2.20	0.41
1:A:229:GLY:O	1:A:234:LEU:HB2	2.19	0.41
1:B:250:PHE:CE2	1:B:251:THR:HG23	2.55	0.41
1:B:183:GLY:HA2	1:B:207:ASP:OD1	2.21	0.41
1:A:121:ILE:O	1:A:156:PHE:HA	2.20	0.41
1:A:235:ASP:CG	1:A:236:HIS:N	2.78	0.41
1:B:222:LEU:O	7:B:306:OY3:H15	2.21	0.41
1:A:128:TYR:HD2	1:A:137:ILE:HD12	1.86	0.41
1:A:223:VAL:HA	7:B:306:OY3:H5	2.02	0.41
1:B:192:PHE:HA	1:B:193:PRO:HD3	1.94	0.40
1:B:228:PHE:O	1:B:232:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:306:OY3:H59	7:B:306:OY3:O15	2.22	0.40
1:A:252:GLU:OE1	1:A:252:GLU:CA	2.67	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	163/164 (99%)	160 (98%)	3 (2%)	0	100	100
1	B	163/164 (99%)	154 (94%)	6 (4%)	3 (2%)	6	25
All	All	326/328 (99%)	314 (96%)	9 (3%)	3 (1%)	21	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134[A]	ARG
1	B	134[B]	ARG
1	B	180	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	132/131 (101%)	112 (85%)	20 (15%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	132/131 (101%)	117 (89%)	15 (11%)	5	18
All	All	264/262 (101%)	229 (87%)	35 (13%)	4	12

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	111	GLU
1	A	129	SER
1	A	130	GLU
1	A	134[A]	ARG
1	A	134[B]	ARG
1	A	147	LEU
1	A	154	LEU
1	A	155	THR
1	A	162	ARG
1	A	174	GLU
1	A	184	LYS
1	A	187	LEU
1	A	188	LEU
1	A	198	ILE
1	A	208	GLU
1	A	214	LYS
1	A	241	GLU
1	A	247	MET
1	A	249	ARG
1	B	108	GLN
1	B	111	GLU
1	B	151	VAL
1	B	155	THR
1	B	162	ARG
1	B	187	LEU
1	B	188	LEU
1	B	198	ILE
1	B	207	ASP
1	B	211	SER
1	B	214	LYS
1	B	238	SER
1	B	241	GLU
1	B	247	MET
1	B	256	LEU

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

Mol	Chain	Res	Type
1	A	108	GLN
1	A	119	HIS
1	A	199	GLN
1	B	119	HIS
1	B	169	GLN
1	B	175	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 26 ligands modelled in this entry, 9 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	$\# Z > 2$
4	PEG	A	309	-	6,6,6	0.45	0	5,5,5	0.32	0
6	BCN	B	311	-	10,10,10	0.68	0	11,11,11	1.99	3 (27%)
4	PEG	B	308	-	6,6,6	0.35	0	5,5,5	0.19	0
5	ACT	A	312	-	3,3,3	0.83	0	3,3,3	1.36	0
4	PEG	A	306	-	6,6,6	0.55	0	5,5,5	0.32	0
4	PEG	A	305	-	6,6,6	0.48	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	313	-	3,3,3	0.80	0	3,3,3	1.36	0
6	BCN	A	314	-	10,10,10	0.71	0	11,11,11	1.95	3 (27%)
4	PEG	A	310	-	6,6,6	0.40	0	5,5,5	0.23	0
6	BCN	A	315	-	10,10,10	0.70	0	11,11,11	1.98	3 (27%)
4	PEG	B	309	-	6,6,6	0.42	0	5,5,5	0.33	0
5	ACT	B	310	-	3,3,3	0.80	0	3,3,3	1.29	0
4	PEG	A	308	-	6,6,6	0.52	0	5,5,5	0.33	0
4	PEG	A	307	-	6,6,6	0.49	0	5,5,5	0.17	0
5	ACT	A	311	-	3,3,3	0.83	0	3,3,3	1.34	0
7	0Y3	B	306	2	80,82,82	2.16	6 (7%)	92,112,112	1.70	8 (8%)
4	PEG	B	307	-	6,6,6	0.56	0	5,5,5	0.26	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	PEG	A	309	-	-	3/4/4/4	-
6	BCN	B	311	-	-	4/10/10/10	-
4	PEG	B	308	-	-	3/4/4/4	-
6	BCN	A	315	-	-	4/10/10/10	-
4	PEG	A	306	-	-	1/4/4/4	-
4	PEG	A	305	-	-	2/4/4/4	-
6	BCN	A	314	-	-	3/10/10/10	-
7	0Y3	B	306	2	-	8/82/94/94	0/5/5/5
4	PEG	A	310	-	-	1/4/4/4	-
4	PEG	B	309	-	-	2/4/4/4	-
4	PEG	A	308	-	-	2/4/4/4	-
4	PEG	A	307	-	-	3/4/4/4	-
4	PEG	B	307	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	306	0Y3	C2-S1	-9.19	1.64	1.76
7	B	306	0Y3	C63-S60	-8.99	1.64	1.76
7	B	306	0Y3	O56-N55	-8.47	1.28	1.42
7	B	306	0Y3	O17-N16	-8.33	1.28	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	306	0Y3	S1-N16	-2.88	1.56	1.70
7	B	306	0Y3	S60-N55	-2.80	1.57	1.70

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	306	0Y3	O61-S60-O62	-9.36	104.98	119.59
7	B	306	0Y3	O15-S1-O14	-8.91	105.68	119.59
6	A	314	BCN	C1-N1-C5	4.54	122.86	111.91
6	A	315	BCN	C1-N1-C3	4.05	121.69	111.91
6	B	311	BCN	C1-N1-C3	3.83	121.16	111.91
6	A	314	BCN	C1-N1-C3	3.48	120.31	111.91
6	B	311	BCN	C5-N1-C3	3.32	119.36	111.44
6	A	315	BCN	C5-N1-C3	3.30	119.31	111.44
6	B	311	BCN	C1-N1-C5	3.14	119.48	111.91
7	B	306	0Y3	C37-C34-N33	3.08	123.52	117.12
6	A	315	BCN	C1-N1-C5	2.94	118.99	111.91
7	B	306	0Y3	C27-N28-C29	2.70	127.84	122.82
7	B	306	0Y3	C63-S60-N55	2.33	114.57	104.35
6	A	314	BCN	C5-N1-C3	2.26	116.82	111.44
7	B	306	0Y3	C50-N49-C48	2.25	127.01	122.82
7	B	306	0Y3	C45-N44-C43	2.17	127.02	122.11
7	B	306	0Y3	O35-C34-C37	-2.03	116.88	120.90

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	314	BCN	C4-C3-N1-C1
6	A	314	BCN	C6-C5-N1-C1
6	A	315	BCN	C2-C1-N1-C3
6	B	311	BCN	C2-C1-N1-C3
6	B	311	BCN	C4-C3-N1-C5
6	B	311	BCN	C6-C5-N1-C1
6	B	311	BCN	N1-C3-C4-O4
7	B	306	0Y3	C50-C51-C54-C75
7	B	306	0Y3	O56-N55-S60-O62
7	B	306	0Y3	O56-N55-S60-O61
7	B	306	0Y3	N49-C50-C51-C54
7	B	306	0Y3	C21-C20-C26-C27
4	B	307	PEG	C1-C2-O2-C3
7	B	306	0Y3	C30-C31-C32-N33

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Mol	Chain	Res	Type	Atoms
4	A	307	PEG	O2-C3-C4-O4
4	A	309	PEG	O1-C1-C2-O2
4	B	308	PEG	O1-C1-C2-O2
4	A	306	PEG	O2-C3-C4-O4
4	A	308	PEG	O2-C3-C4-O4
4	B	307	PEG	O1-C1-C2-O2
4	B	309	PEG	O1-C1-C2-O2
4	A	308	PEG	O1-C1-C2-O2
4	B	309	PEG	O2-C3-C4-O4
4	B	308	PEG	C4-C3-O2-C2
4	A	309	PEG	C1-C2-O2-C3
4	B	308	PEG	C1-C2-O2-C3
4	B	307	PEG	C4-C3-O2-C2
4	A	305	PEG	O1-C1-C2-O2
4	B	307	PEG	O2-C3-C4-O4
4	A	307	PEG	C4-C3-O2-C2
4	A	305	PEG	C4-C3-O2-C2
7	B	306	0Y3	N44-C45-C46-C47
7	B	306	0Y3	C20-C26-C27-N28
4	A	310	PEG	O2-C3-C4-O4
6	A	314	BCN	N1-C3-C4-O4
4	A	309	PEG	C4-C3-O2-C2
6	A	315	BCN	N1-C3-C4-O4
4	A	307	PEG	C1-C2-O2-C3
6	A	315	BCN	C4-C3-N1-C1
6	A	315	BCN	C6-C5-N1-C3

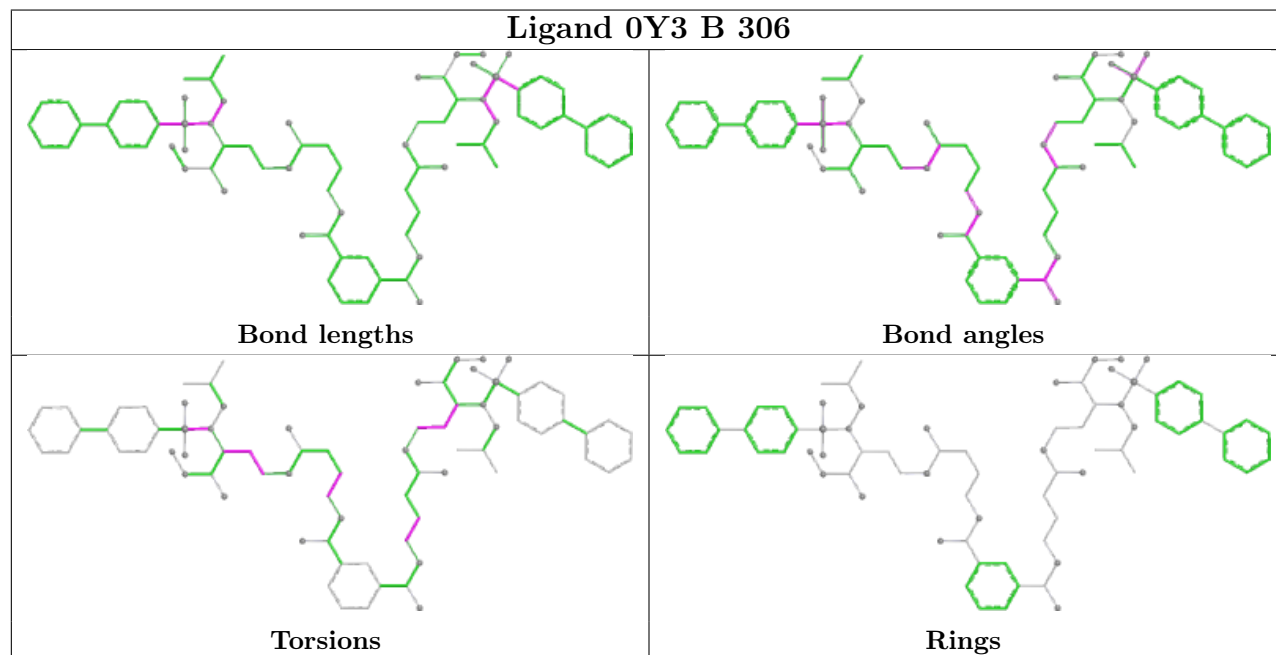
There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	309	PEG	1	0
6	B	311	BCN	7	0
4	B	308	PEG	1	0
4	A	306	PEG	2	0
6	A	314	BCN	1	0
6	A	315	BCN	2	0
4	B	309	PEG	1	0
7	B	306	0Y3	12	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	164/164 (100%)	1.53	39 (23%) 2 2	1, 15, 35, 49	1 (0%)
1	B	164/164 (100%)	1.38	36 (21%) 2 2	0, 14, 31, 42	1 (0%)
All	All	328/328 (100%)	1.45	75 (22%) 2 2	0, 15, 35, 49	2 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	SER	4.8
1	A	149	SER	4.6
1	B	242	ALA	4.4
1	B	215	GLY	4.2
1	A	176	GLY	4.2
1	A	147	LEU	3.8
1	A	213	GLY	3.8
1	B	251	THR	3.8
1	B	238	SER	3.7
1	B	213	GLY	3.6
1	B	147	LEU	3.6
1	A	191	ALA	3.6
1	A	112	GLY	3.6
1	A	262	ASN	3.4
1	B	183	GLY	3.4
1	A	106	GLY	3.4
1	B	216	VAL	3.3
1	B	214	LYS	3.3
1	A	251	THR	3.2
1	A	242	ALA	3.2
1	A	239	VAL	3.1
1	A	230	HIS	3.1
1	B	174	GLU	3.0
1	A	121	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	120	ASN	3.0
1	A	252	GLU	2.9
1	B	107	PHE	2.9
1	A	269	GLY	2.9
1	A	173	ALA	2.8
1	A	209	LEU	2.8
1	A	249	ARG	2.7
1	A	207	ASP	2.7
1	B	151	VAL	2.7
1	A	179	TYR	2.6
1	B	191	ALA	2.6
1	A	238	SER	2.6
1	A	145	PHE	2.5
1	A	263	GLY	2.5
1	A	224	ALA	2.5
1	B	212	LEU	2.5
1	B	260	ASP	2.5
1	B	144	ALA	2.5
1	B	171	GLY	2.4
1	B	217	GLY	2.4
1	A	124	TRP	2.4
1	A	219	SER	2.4
1	B	234	LEU	2.4
1	A	255	PRO	2.4
1	A	134[A]	ARG	2.4
1	A	222	LEU	2.4
1	A	216	VAL	2.3
1	B	233	GLY	2.3
1	A	204	PHE	2.3
1	A	144	ALA	2.3
1	B	219	SER	2.3
1	A	246	PRO	2.3
1	B	175	HIS	2.3
1	B	166	ILE	2.3
1	B	211	SER	2.3
1	B	145	PHE	2.2
1	B	253	GLY	2.2
1	B	173	ALA	2.2
1	B	239	VAL	2.1
1	B	131	ASP	2.1
1	A	254	PRO	2.1
1	A	181	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	170	PHE	2.1
1	B	149	SER	2.1
1	A	193	PRO	2.1
1	B	222	LEU	2.1
1	B	221	PHE	2.1
1	A	113	ASP	2.1
1	B	109	THR	2.1
1	B	262	ASN	2.0
1	A	208	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BCN	A	315	11/11	0.61	0.20	41,41,41,41	0
5	ACT	B	310	4/4	0.69	0.17	10,10,10,10	0
4	PEG	B	307	7/7	0.69	0.17	20,20,20,20	0
4	PEG	A	307	7/7	0.70	0.14	24,24,24,24	0
4	PEG	A	305	7/7	0.73	0.14	16,17,18,18	0
4	PEG	A	306	7/7	0.74	0.14	23,23,23,24	0
7	0Y3	B	306	78/78	0.74	0.23	32,38,49,50	0
6	BCN	B	311	11/11	0.75	0.15	38,38,38,38	0
4	PEG	A	309	7/7	0.75	0.15	29,29,30,30	0
6	BCN	A	314	11/11	0.76	0.13	17,18,18,18	0
3	CA	B	305	1/1	0.81	0.13	51,51,51,51	0
4	PEG	A	308	7/7	0.82	0.13	13,13,14,14	0
4	PEG	A	310	7/7	0.85	0.11	2,2,2,3	0
4	PEG	B	308	7/7	0.86	0.13	5,5,6,6	0

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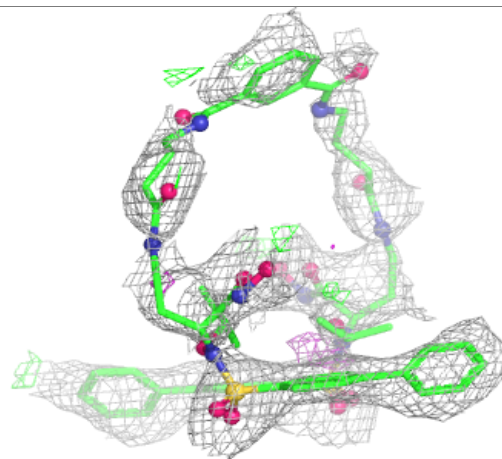
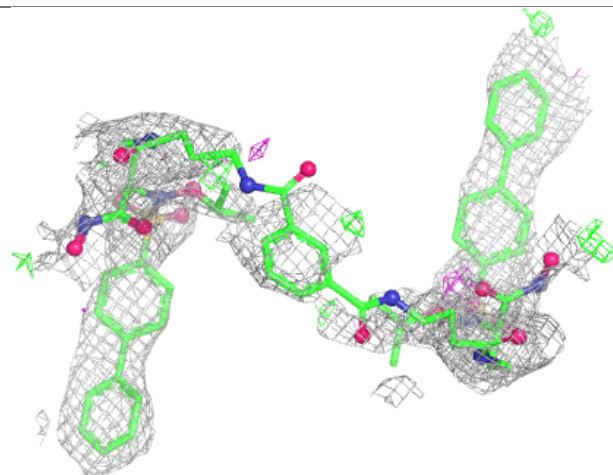
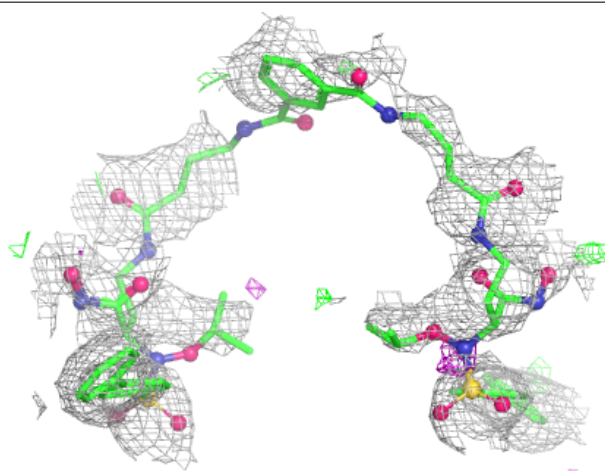
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	A	312	4/4	0.89	0.10	17,17,17,17	0
5	ACT	A	311	4/4	0.90	0.14	5,5,5,5	0
5	ACT	A	313	4/4	0.91	0.08	6,6,6,6	0
4	PEG	B	309	7/7	0.91	0.10	3,3,3,3	0
3	CA	A	303	1/1	0.93	0.04	15,15,15,15	0
3	CA	A	304	1/1	0.96	0.05	21,21,21,21	0
2	ZN	B	301	1/1	0.97	0.05	17,17,17,17	0
3	CA	B	304	1/1	0.97	0.04	25,25,25,25	0
3	CA	B	303	1/1	0.98	0.06	13,13,13,13	0
2	ZN	A	301	1/1	0.99	0.05	16,16,16,16	0
2	ZN	B	302	1/1	0.99	0.03	13,13,13,13	0
2	ZN	A	302	1/1	1.00	0.01	15,15,15,15	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 0Y3 B 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.