



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:35 AM UTC

PDB ID : 3QBK / pdb_00003qbk
Title : Bromide-bound form of pharaonis halorhodopsin
Authors : Kouyama, T.; Kanada, S.
Deposited on : 2011-01-13
Resolution : 2.20 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

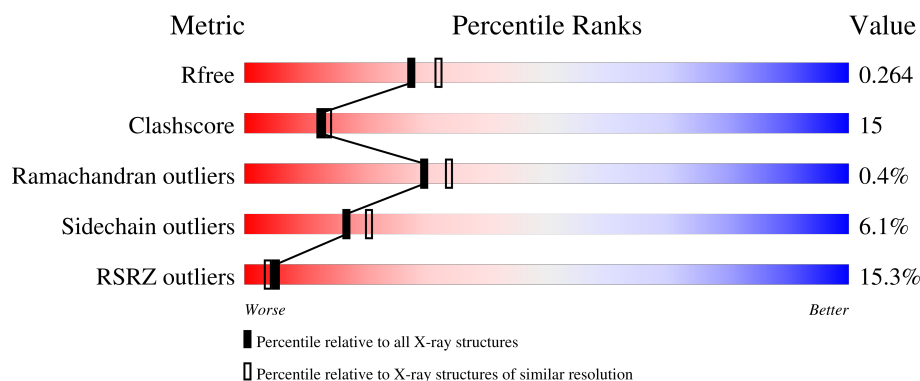
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	291	7% 66% 20% • 10%
1	B	291	7% 67% 19% • 11%
1	D	291	28% 55% 32% • 11%

2 Entry composition [i](#)

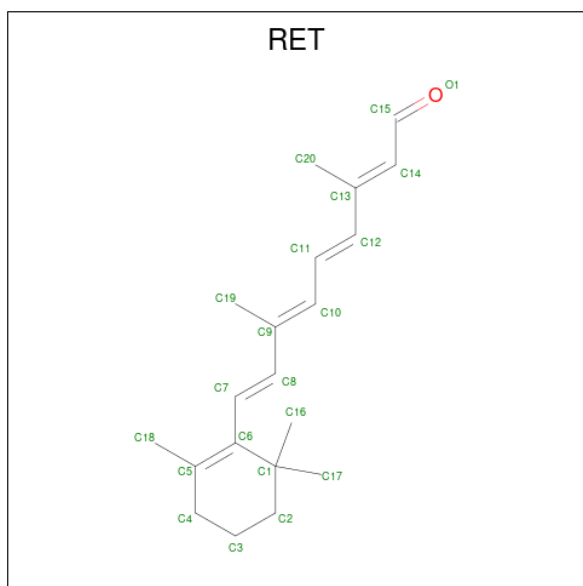
There are 5 unique types of molecules in this entry. The entry contains 6153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Halorhodopsin.

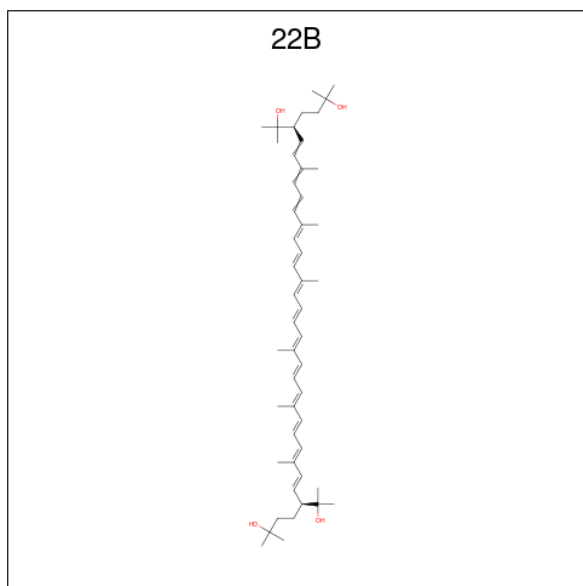
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			1968	1305	300	352	11			
1	B	259	Total	C	N	O	S	0	0	0
			1957	1299	298	349	11			
1	D	259	Total	C	N	O	S	0	0	0
			1957	1299	298	349	11			

- Molecule 2 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		
2	B	1	Total	C	0	0
			20	20		
2	D	1	Total	C	0	0
			20	20		

- Molecule 3 is BACTERIORUBERIN (CCD ID: 22B) (formula: $C_{50}H_{76}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			27	25	2		
3	B	1	Total	C	O	0	0
			27	25	2		

- Molecule 4 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Br	0	0
			3	3		
4	B	1	Total	Br	0	0
			1	1		
4	D	2	Total	Br	0	0
			2	2		

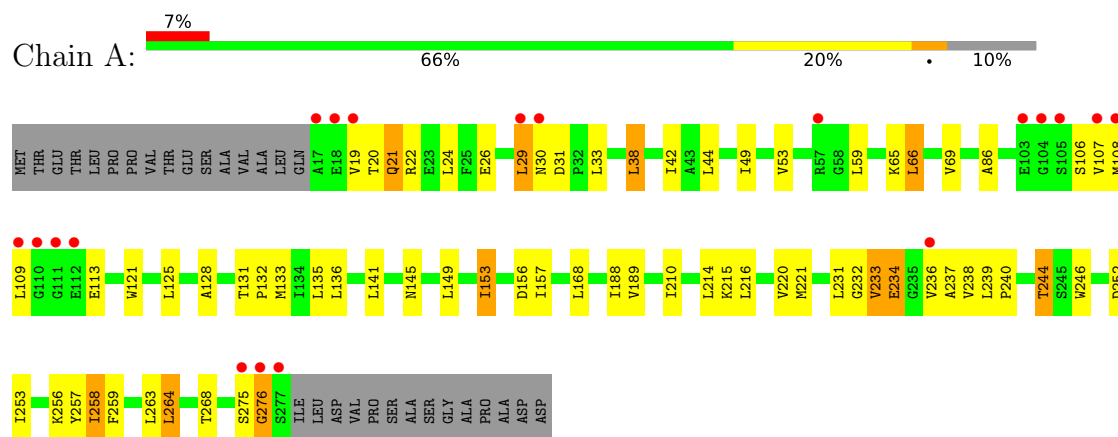
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total	O	0	0
			52	52		
5	B	65	Total	O	0	0
			65	65		
5	D	34	Total	O	0	0
			34	34		

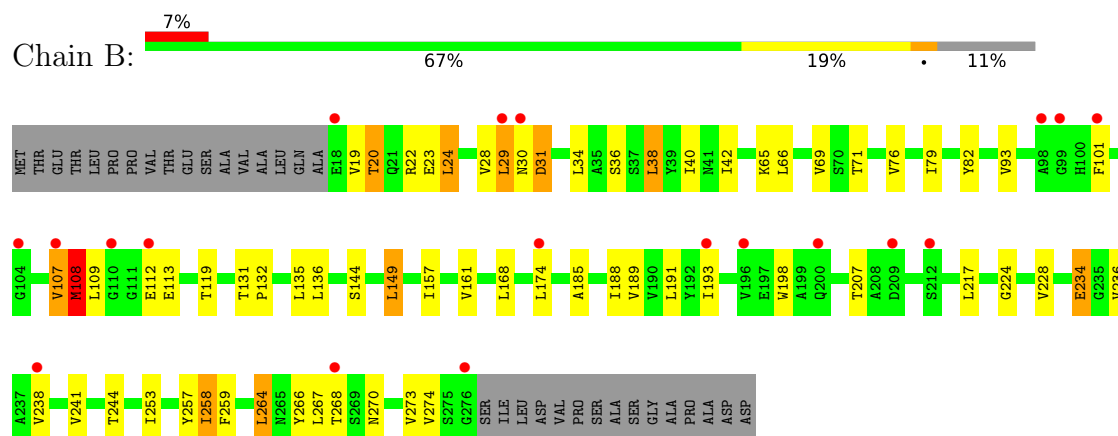
3 Residue-property plots [i](#)

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.

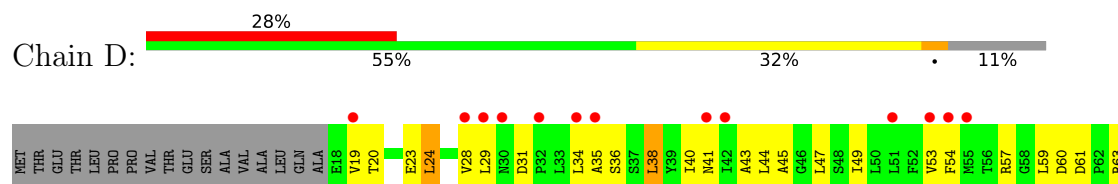
• Molecule 1: Halorhodopsin

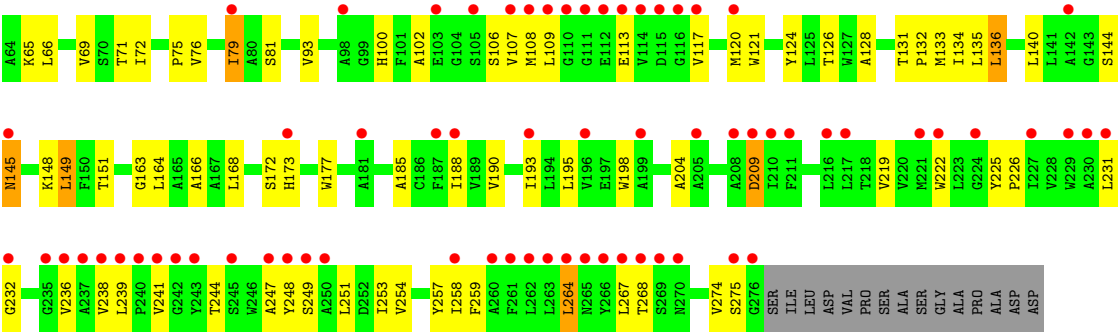


• Molecule 1: Halorhodopsin



• Molecule 1: Halorhodopsin





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.15Å 99.72Å 99.97Å 90.00° 127.80° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 15.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.00-2.20) 97.0 (15.00-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.267 0.245 , 0.264	Depositor DCC
R_{free} test set	2936 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6153	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: 22B, RET, BR

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	0.47	0/2014	0.93	10/2758 (0.4%)
1	B	0.43	0/2003	0.90	6/2743 (0.2%)
1	D	0.37	0/2003	0.86	0/2743
All	All	0.43	0/6020	0.90	16/8244 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	LEU	N-CA-C	-9.14	98.85	110.19
1	A	153	ILE	N-CA-C	6.68	117.46	110.72
1	A	42	ILE	N-CA-C	-6.65	104.01	110.72
1	A	237	ALA	N-CA-C	6.09	120.04	112.24
1	B	107	VAL	N-CA-C	6.03	117.18	112.12
1	B	42	ILE	N-CA-C	-5.95	104.93	110.53
1	A	156	ASP	N-CA-C	-5.56	105.13	111.14
1	A	257	TYR	N-CA-C	5.42	116.88	110.97
1	A	66	LEU	N-CA-C	-5.26	105.46	111.14
1	A	244	THR	N-CA-C	-5.18	105.81	111.82
1	A	31	ASP	CA-C-N	5.15	126.27	119.84
1	A	31	ASP	C-N-CA	5.15	126.27	119.84
1	B	257	TYR	N-CA-C	5.12	116.67	111.14
1	A	29	LEU	N-CA-C	-5.10	103.75	110.43
1	B	31	ASP	CA-C-N	5.03	124.47	119.24
1	B	31	ASP	C-N-CA	5.03	124.47	119.24

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	1968	0	2019	48	0
1	B	1957	0	2009	50	0
1	D	1957	0	2009	85	0
2	A	20	0	27	1	0
2	B	20	0	27	1	0
2	D	20	0	27	2	0
3	A	27	0	37	2	0
3	B	27	0	37	1	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	D	2	0	0	1	0
5	A	52	0	0	2	1
5	B	65	0	0	2	0
5	D	34	0	0	2	0
All	All	6153	0	6192	186	1

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 (186) 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:238:VAL:HG23	1:A:239:LEU:HD13	1.47	0.96
1:B:236:VAL:HG13	1:B:238:VAL:HG13	1.56	0.88
1:D:145:ASN:HD21	1:D:148:LYS:HG3	1.49	0.78
1:D:254:VAL:HA	1:D:258:ILE:HG22	1.63	0.77
1:D:195:LEU:HD21	1:D:219:VAL:HG21	1.67	0.77
1:D:65:LYS:O	1:D:69:VAL:HG23	1.85	0.76
1:D:131:THR:OG1	1:D:132:PRO:HD3	1.87	0.74
1:A:220:VAL:HG12	1:A:221:MET:HE2	1.69	0.73
1:B:20:THR:HG22	1:B:23:GLU:H	1.53	0.73
1:D:19:VAL:HG21	1:D:93:VAL:HG11	1.71	0.72
1:A:238:VAL:HG23	1:A:239:LEU:CD1	2.20	0.71
1:D:145:ASN:C	1:D:145:ASN:HD22	2.00	0.70
1:D:100:HIS:CD2	1:D:102:ALA:H	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:THR:HG22	1:A:22:ARG:H	1.59	0.68
1:D:185:ALA:O	1:D:188:ILE:HG12	1.94	0.68
1:D:45:ALA:HB3	1:D:79:ILE:HG23	1.77	0.67
1:D:108:MET:HB2	1:D:113:GLU:HG3	1.77	0.66
1:D:164:LEU:O	1:D:168:LEU:HD23	1.96	0.66
1:A:236:VAL:HG13	1:A:238:VAL:HG13	1.77	0.66
1:B:270:ASN:HB3	1:B:273:VAL:HG12	1.78	0.64
1:D:254:VAL:HA	1:D:258:ILE:CG2	2.27	0.64
1:A:107:VAL:CG2	1:A:109:LEU:HD13	2.29	0.63
1:D:28:VAL:HG13	1:D:34:LEU:HD12	1.79	0.63
1:D:36:SER:O	1:D:40:ILE:HG12	1.99	0.62
1:B:108:MET:HA	1:B:113:GLU:HA	1.81	0.62
1:D:108:MET:HA	1:D:113:GLU:HA	1.80	0.62
1:D:43:ALA:O	1:D:47:LEU:HD13	2.00	0.62
1:A:108:MET:HA	1:A:113:GLU:HA	1.81	0.61
1:D:238:VAL:HG23	1:D:239:LEU:CD1	2.31	0.60
1:D:238:VAL:HG23	1:D:239:LEU:HD13	1.83	0.60
1:D:71:THR:HG21	1:D:264:LEU:HD13	1.85	0.59
1:B:65:LYS:HE2	3:B:300:22B:H243	1.85	0.59
1:B:217:LEU:C	1:B:217:LEU:HD23	2.28	0.59
1:B:270:ASN:O	1:B:273:VAL:HG12	2.03	0.57
1:B:270:ASN:HB3	1:B:273:VAL:CG1	2.35	0.57
1:B:19:VAL:CG2	1:B:93:VAL:HG11	2.36	0.56
3:A:300:22B:H253	1:D:151:THR:HG21	1.86	0.56
1:D:135:LEU:HD11	1:D:222:TRP:CH2	2.40	0.56
1:D:54:PHE:HB3	1:D:57:ARG:NH1	2.20	0.56
1:A:234:GLU:HG3	5:A:511:HOH:O	2.04	0.56
1:A:253:ILE:O	1:A:258:ILE:HG23	2.06	0.56
1:B:93:VAL:HG13	1:B:93:VAL:O	2.05	0.56
1:B:193:ILE:HD12	1:B:193:ILE:C	2.31	0.55
1:D:29:LEU:C	1:D:31:ASP:H	2.14	0.55
1:D:93:VAL:HA	1:D:117:VAL:O	2.06	0.55
1:A:121:TRP:HZ3	1:A:125:LEU:HD22	1.70	0.55
1:B:19:VAL:HG21	1:B:93:VAL:HG11	1.89	0.55
1:B:29:LEU:O	1:B:30:ASN:HB2	2.05	0.55
1:D:254:VAL:CA	1:D:258:ILE:HG22	2.36	0.55
1:A:29:LEU:O	1:A:30:ASN:HB2	2.07	0.55
1:D:24:LEU:O	1:D:28:VAL:HG23	2.07	0.55
1:B:34:LEU:O	1:B:38:LEU:HD22	2.06	0.55
1:B:224:GLY:O	1:B:228:VAL:HG23	2.07	0.54
1:A:107:VAL:HG23	1:A:109:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:VAL:HG23	1:A:234:GLU:OE1	2.08	0.54
1:D:190:VAL:O	1:D:193:ILE:HG13	2.08	0.53
1:B:253:ILE:O	1:B:258:ILE:HG23	2.08	0.53
1:D:108:MET:HE3	1:D:113:GLU:HB2	1.90	0.53
1:A:214:LEU:CD1	1:A:263:LEU:HD13	2.39	0.53
1:D:121:TRP:HA	1:D:124:TYR:CD2	2.44	0.53
1:D:145:ASN:ND2	1:D:148:LYS:H	2.07	0.53
1:D:76:VAL:HA	1:D:79:ILE:HD11	1.91	0.52
1:B:36:SER:O	1:B:40:ILE:HG12	2.09	0.52
1:B:185:ALA:O	1:B:188:ILE:HG12	2.09	0.52
1:D:28:VAL:HG13	1:D:34:LEU:CD1	2.39	0.52
1:A:26:GLU:O	1:A:29:LEU:O	2.27	0.52
1:A:275:SER:O	1:A:276:GLY:C	2.53	0.52
1:B:20:THR:HG23	1:B:22:ARG:H	1.73	0.52
1:D:28:VAL:O	1:D:35:ALA:HB2	2.10	0.52
1:D:49:ILE:O	1:D:53:VAL:HG23	2.10	0.51
1:A:153:ILE:O	1:A:157:ILE:HG13	2.09	0.51
1:D:254:VAL:O	1:D:258:ILE:HG22	2.10	0.51
1:A:20:THR:HG22	1:A:21:GLN:N	2.26	0.51
1:D:38:LEU:HD11	1:D:120:MET:HE1	1.93	0.51
1:A:264:LEU:O	1:A:268:THR:HG22	2.10	0.51
1:A:128:ALA:O	1:A:132:PRO:HG2	2.11	0.51
1:D:20:THR:O	1:D:24:LEU:HD22	2.11	0.51
1:D:29:LEU:C	1:D:31:ASP:N	2.69	0.51
1:B:71:THR:HG21	1:B:264:LEU:HD13	1.92	0.50
1:B:65:LYS:O	1:B:69:VAL:HG23	2.11	0.50
1:D:136:LEU:HD22	1:D:140:LEU:HD11	1.93	0.50
1:D:145:ASN:C	1:D:145:ASN:ND2	2.67	0.50
1:D:61:ASP:OD2	1:D:275:SER:HA	2.12	0.50
1:B:109:LEU:O	1:B:112:GLU:HG2	2.11	0.50
1:A:188:ILE:HG13	1:A:189:VAL:N	2.28	0.49
1:B:207:THR:HG22	1:B:266:TYR:OH	2.13	0.49
1:D:131:THR:O	1:D:135:LEU:HD13	2.13	0.49
1:A:232:GLY:HA2	1:A:239:LEU:HB2	1.95	0.49
1:B:29:LEU:C	1:B:31:ASP:H	2.20	0.49
1:D:100:HIS:CD2	1:D:102:ALA:HB3	2.48	0.49
1:B:38:LEU:HD12	1:B:82:TYR:CD1	2.48	0.49
1:D:81:SER:HB2	1:D:126:THR:HG21	1.95	0.49
1:D:133:MET:HA	1:D:133:MET:HE2	1.95	0.49
1:D:267:LEU:HD11	1:D:274:VAL:HG21	1.94	0.49
1:B:157:ILE:O	1:B:161:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:PHE:C	1:B:259:PHE:CD1	2.91	0.48
1:B:101:PHE:CD2	1:B:236:VAL:HG23	2.48	0.48
1:A:38:LEU:HD23	1:A:86:ALA:HA	1.95	0.48
1:B:188:ILE:HG13	1:B:189:VAL:N	2.28	0.48
1:D:59:LEU:HD21	1:D:268:THR:HG22	1.96	0.48
1:B:108:MET:HA	1:B:112:GLU:O	2.14	0.48
1:B:234:GLU:HB2	5:B:509:HOH:O	2.14	0.47
1:B:241:VAL:HA	1:B:244:THR:HG22	1.96	0.47
1:D:106:SER:HB3	1:D:113:GLU:HG2	1.96	0.47
1:B:76:VAL:O	1:B:79:ILE:HG22	2.14	0.47
1:A:33:LEU:HD22	1:A:246:TRP:HD1	1.80	0.47
1:D:23:GLU:HB3	1:D:109:LEU:HB3	1.96	0.47
1:D:63:ARG:HG2	1:D:63:ARG:HH11	1.80	0.47
1:D:248:TYR:HA	1:D:251:LEU:HD12	1.96	0.47
1:B:144:SER:OG	1:B:149:LEU:HD22	2.15	0.47
1:D:226:PRO:HA	2:D:292:RET:H172	1.97	0.47
1:D:231:LEU:HB3	1:D:239:LEU:HD13	1.96	0.46
1:A:20:THR:CG2	1:A:21:GLN:N	2.78	0.46
2:D:292:RET:H7	2:D:292:RET:H181	1.78	0.46
1:D:126:THR:OG1	4:D:401:BR:BR	2.86	0.46
1:B:38:LEU:HD12	1:B:82:TYR:HD1	1.81	0.46
1:D:131:THR:HB	1:D:222:TRP:CH2	2.50	0.46
1:A:33:LEU:HD22	1:A:246:TRP:CD1	2.51	0.46
1:D:204:ALA:HB2	5:D:518:HOH:O	2.16	0.46
1:B:131:THR:OG1	1:B:132:PRO:HD3	2.16	0.46
1:D:247:ALA:O	1:D:251:LEU:HG	2.15	0.46
1:D:145:ASN:ND2	1:D:148:LYS:HG3	2.26	0.46
1:D:163:GLY:O	1:D:166:ALA:HB3	2.15	0.46
1:B:109:LEU:HD22	1:B:109:LEU:N	2.30	0.45
1:D:93:VAL:O	1:D:93:VAL:HG13	2.16	0.45
1:D:241:VAL:HA	1:D:244:THR:OG1	2.15	0.45
1:D:128:ALA:O	1:D:132:PRO:HG2	2.17	0.45
1:A:19:VAL:O	1:A:19:VAL:HG23	2.16	0.45
1:A:29:LEU:O	1:A:30:ASN:CB	2.65	0.45
1:D:267:LEU:CD1	1:D:274:VAL:HG21	2.46	0.45
1:A:49:ILE:O	1:A:53:VAL:HG23	2.16	0.45
1:D:253:ILE:HA	1:D:257:TYR:CD2	2.52	0.45
1:D:109:LEU:HD22	1:D:109:LEU:N	2.32	0.44
1:B:28:VAL:C	1:B:29:LEU:O	2.56	0.44
1:D:107:VAL:O	1:D:108:MET:HB3	2.17	0.44
1:A:131:THR:N	1:A:132:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ILE:HA	1:B:191:LEU:HD12	1.99	0.44
1:A:65:LYS:HE2	3:A:300:22B:H243	2.00	0.44
1:D:136:LEU:HD22	1:D:140:LEU:CD1	2.48	0.44
1:D:249:SER:O	1:D:253:ILE:HG13	2.18	0.44
1:A:238:VAL:CG2	1:A:239:LEU:HD13	2.33	0.44
1:B:119:THR:HG23	1:B:234:GLU:OE1	2.17	0.44
2:B:292:RET:H7	2:B:292:RET:H181	1.84	0.43
1:A:133:MET:HA	1:A:133:MET:HE2	1.99	0.43
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.84	0.43
1:A:268:THR:HG23	5:A:543:HOH:O	2.19	0.43
1:A:252:ASP:O	1:A:256:LYS:HB2	2.18	0.43
1:A:258:ILE:HG13	1:A:259:PHE:N	2.33	0.43
2:A:292:RET:H181	2:A:292:RET:H7	1.84	0.43
1:D:72:ILE:O	1:D:75:PRO:HD2	2.18	0.43
1:B:241:VAL:HA	1:B:244:THR:CG2	2.49	0.43
1:A:106:SER:HB3	1:A:113:GLU:HG3	2.02	0.42
1:D:100:HIS:CE1	5:D:512:HOH:O	2.72	0.42
1:D:225:TYR:N	1:D:226:PRO:HD2	2.34	0.42
1:A:141:LEU:HD22	1:A:263:LEU:CD1	2.50	0.42
1:D:134:ILE:HG23	1:D:259:PHE:CZ	2.55	0.42
1:B:236:VAL:HG22	1:B:236:VAL:O	2.19	0.42
1:A:20:THR:HG22	1:A:22:ARG:N	2.30	0.42
1:D:131:THR:HG1	1:D:132:PRO:HD3	1.82	0.42
1:D:144:SER:OG	1:D:198:TRP:NE1	2.52	0.42
1:A:215:LYS:HE2	1:A:215:LYS:HB3	1.89	0.42
1:B:19:VAL:HG12	1:B:24:LEU:HD22	2.02	0.42
1:D:60:ASP:C	1:D:65:LYS:HE2	2.44	0.42
1:A:65:LYS:O	1:A:69:VAL:HG23	2.21	0.41
1:B:144:SER:HG	1:B:149:LEU:HD22	1.83	0.41
1:A:239:LEU:HB3	1:A:244:THR:HG22	2.02	0.41
1:B:268:THR:HG23	5:B:516:HOH:O	2.19	0.41
1:A:131:THR:OG1	1:A:132:PRO:HD3	2.20	0.41
1:B:29:LEU:O	1:B:30:ASN:CB	2.69	0.41
1:A:145:ASN:OD1	1:A:145:ASN:C	2.63	0.41
1:B:267:LEU:CD1	1:B:274:VAL:HG21	2.51	0.41
1:D:149:LEU:HD13	1:D:149:LEU:HA	1.94	0.41
1:D:173:HIS:CD2	1:D:177:TRP:HE1	2.39	0.41
1:A:231:LEU:O	1:A:238:VAL:HG22	2.20	0.41
1:D:81:SER:CB	1:D:126:THR:HG21	2.50	0.41
1:D:145:ASN:HD21	1:D:148:LYS:H	1.68	0.41
1:D:193:ILE:C	1:D:193:ILE:HD12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:GLY:CA	1:D:244:THR:HG21	2.50	0.41
1:D:41:ASN:HD22	1:D:41:ASN:HA	1.61	0.41
1:A:240:PRO:O	1:A:244:THR:HG23	2.21	0.40
1:D:231:LEU:HA	1:D:236:VAL:HG12	2.04	0.40
1:A:210:ILE:O	1:A:214:LEU:HG	2.21	0.40
1:B:20:THR:HG22	1:B:23:GLU:N	2.29	0.40
1:B:193:ILE:HD13	1:B:198:TRP:CE2	2.55	0.40
1:D:40:ILE:O	1:D:44:LEU:HG	2.22	0.40
1:B:101:PHE:CE2	1:B:236:VAL:HG23	2.56	0.40

All (1) 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)
5:A:600:HOH:O	5:A:600:HOH:O[2_656]	1.55	0.65

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	259/291 (89%)	249 (96%)	9 (4%)	1 (0%)	30	34
1	B	257/291 (88%)	248 (96%)	8 (3%)	1 (0%)	30	34
1	D	257/291 (88%)	247 (96%)	9 (4%)	1 (0%)	30	34
All	All	773/873 (88%)	744 (96%)	26 (3%)	3 (0%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	GLY
1	D	209	ASP
1	B	108	MET

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	208/233 (89%)	194 (93%)	14 (7%)	15	17
1	B	207/233 (89%)	193 (93%)	14 (7%)	14	17
1	D	207/233 (89%)	197 (95%)	10 (5%)	23	30
All	All	622/699 (89%)	584 (94%)	38 (6%)	17	20

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	24	LEU
1	A	38	LEU
1	A	59	LEU
1	A	66	LEU
1	A	135	LEU
1	A	136	LEU
1	A	149	LEU
1	A	168	LEU
1	A	216	LEU
1	A	233	VAL
1	A	234	GLU
1	A	258	ILE
1	A	264	LEU
1	B	20	THR
1	B	24	LEU
1	B	38	LEU
1	B	66	LEU
1	B	107	VAL
1	B	108	MET
1	B	135	LEU
1	B	136	LEU
1	B	149	LEU
1	B	168	LEU
1	B	174	LEU
1	B	234	GLU

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Mol	Chain	Res	Type
1	B	258	ILE
1	B	264	LEU
1	D	24	LEU
1	D	38	LEU
1	D	66	LEU
1	D	79	ILE
1	D	136	LEU
1	D	145	ASN
1	D	149	LEU
1	D	172	SER
1	D	209	ASP
1	D	264	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	265	ASN
1	B	41	ASN
1	B	265	ASN
1	D	41	ASN
1	D	100	HIS
1	D	145	ASN
1	D	270	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	RET	A	292	1	20,20,21	2.38	6 (30%)	27,27,28	1.73	8 (29%)
2	RET	B	292	1	20,20,21	2.42	5 (25%)	27,27,28	1.62	7 (25%)
3	22B	A	300	-	26,26,53	3.31	12 (46%)	31,35,72	2.06	9 (29%)
3	22B	B	300	-	26,26,53	3.38	13 (50%)	31,35,72	2.07	9 (29%)
2	RET	D	292	1	20,20,21	2.18	5 (25%)	27,27,28	1.79	8 (29%)

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	RET	A	292	1	-	0/13/30/31	0/1/1/1
2	RET	B	292	1	-	0/13/30/31	0/1/1/1
3	22B	A	300	-	-	8/31/31/65	-
3	22B	B	300	-	-	8/31/31/65	-
2	RET	D	292	1	-	0/13/30/31	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	300	22B	C2-C3	9.56	1.64	1.49
3	A	300	22B	C2-C3	9.33	1.64	1.49
3	B	300	22B	C1-C2	6.71	1.62	1.55
2	B	292	RET	C1-C6	6.69	1.62	1.53
3	A	300	22B	C1-C2	6.62	1.62	1.55
2	A	292	RET	C1-C6	6.51	1.62	1.53
2	D	292	RET	C1-C6	6.04	1.61	1.53
3	B	300	22B	C21-C2	5.96	1.61	1.53
3	A	300	22B	C21-C2	5.83	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	292	RET	C14-C13	5.13	1.37	1.33
2	A	292	RET	C5-C6	4.34	1.41	1.34
3	B	300	22B	O27-C23	4.22	1.54	1.44
3	B	300	22B	C19-C9	4.18	1.59	1.50
3	A	300	22B	C19-C9	4.17	1.59	1.50
2	A	292	RET	C14-C13	4.17	1.36	1.33
3	A	300	22B	C16-C1	4.14	1.59	1.52
3	B	300	22B	C16-C1	4.06	1.59	1.52
2	D	292	RET	C14-C13	4.02	1.36	1.33
2	B	292	RET	C5-C6	4.02	1.41	1.34
3	A	300	22B	O27-C23	3.93	1.54	1.44
3	B	300	22B	C22-C21	3.89	1.63	1.53
2	D	292	RET	C5-C6	3.80	1.40	1.34
3	A	300	22B	C22-C21	3.57	1.62	1.53
3	A	300	22B	C17-C1	3.57	1.58	1.52
3	A	300	22B	C20-C13	3.30	1.57	1.50
3	B	300	22B	C20-C13	3.28	1.57	1.50
3	B	300	22B	C17-C1	3.17	1.57	1.52
2	D	292	RET	C7-C6	3.07	1.55	1.45
2	A	292	RET	C7-C6	2.91	1.55	1.45
2	B	292	RET	C7-C6	2.89	1.55	1.45
3	B	300	22B	C18-C5	2.78	1.56	1.50
2	A	292	RET	C2-C3	-2.78	1.46	1.52
2	B	292	RET	C2-C3	-2.70	1.46	1.52
2	D	292	RET	C2-C3	-2.63	1.46	1.52
2	A	292	RET	C18-C5	2.60	1.55	1.50
3	A	300	22B	C18-C5	2.56	1.56	1.50
3	B	300	22B	C4-C3	2.44	1.37	1.32
3	A	300	22B	C4-C3	2.43	1.37	1.32
3	B	300	22B	C22-C23	2.06	1.59	1.53
3	B	300	22B	C8-C9	2.01	1.50	1.46
3	A	300	22B	C22-C23	2.00	1.59	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	300	22B	C21-C22-C23	4.74	125.09	116.24
3	A	300	22B	C20-C13-C12	4.62	125.14	118.09
3	B	300	22B	C16-C1-C2	4.61	117.89	111.71
3	A	300	22B	C21-C22-C23	4.60	124.83	116.24
3	B	300	22B	C20-C13-C12	4.18	124.47	118.09
3	A	300	22B	C16-C1-C2	3.86	116.88	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	300	22B	C17-C1-C16	-3.73	105.07	110.52
2	D	292	RET	C1-C6-C7	3.61	125.44	115.65
3	A	300	22B	C17-C1-C16	-3.55	105.34	110.52
3	B	300	22B	C4-C5-C6	-3.47	113.55	119.01
3	A	300	22B	C4-C5-C6	-3.44	113.60	119.01
2	B	292	RET	C1-C6-C7	3.23	124.41	115.65
2	A	292	RET	C1-C6-C7	3.19	124.31	115.65
2	A	292	RET	C7-C8-C9	3.06	130.76	126.23
3	A	300	22B	C12-C13-C14	-3.06	110.42	118.55
2	D	292	RET	C1-C6-C5	-3.04	118.48	122.64
3	A	300	22B	C18-C5-C4	2.96	122.61	118.09
2	A	292	RET	C1-C6-C5	-2.93	118.64	122.64
2	A	292	RET	C19-C9-C8	2.92	122.54	118.09
3	B	300	22B	C18-C5-C4	2.90	122.51	118.09
2	A	292	RET	C8-C9-C10	-2.84	114.54	119.01
2	D	292	RET	C16-C1-C6	2.80	114.64	110.24
2	B	292	RET	C1-C6-C5	-2.78	118.84	122.64
2	D	292	RET	C20-C13-C12	2.74	122.28	118.09
3	B	300	22B	C12-C13-C14	-2.72	111.34	118.55
2	A	292	RET	C2-C1-C6	2.51	114.09	110.44
3	A	300	22B	C24-C23-C22	2.44	118.75	111.51
2	A	292	RET	C17-C1-C6	2.40	114.01	110.24
2	B	292	RET	C2-C1-C6	2.40	113.93	110.44
2	B	292	RET	C8-C9-C10	-2.39	115.26	119.01
2	D	292	RET	C7-C6-C5	-2.37	116.09	121.56
3	B	300	22B	C24-C23-C22	2.33	118.42	111.51
2	D	292	RET	C19-C9-C8	2.28	121.57	118.09
2	D	292	RET	C2-C1-C6	2.25	113.71	110.44
3	A	300	22B	C8-C9-C10	-2.15	115.63	119.01
2	A	292	RET	C20-C13-C12	2.13	121.34	118.09
2	B	292	RET	C19-C9-C8	2.12	121.33	118.09
2	D	292	RET	C8-C9-C10	-2.09	115.72	119.01
2	B	292	RET	C7-C6-C5	-2.08	116.76	121.56
3	B	300	22B	C8-C9-C10	-2.06	115.77	119.01
2	B	292	RET	C20-C13-C12	2.04	121.21	118.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	22B	C1-C2-C3-C4
3	A	300	22B	C7-C8-C9-C10

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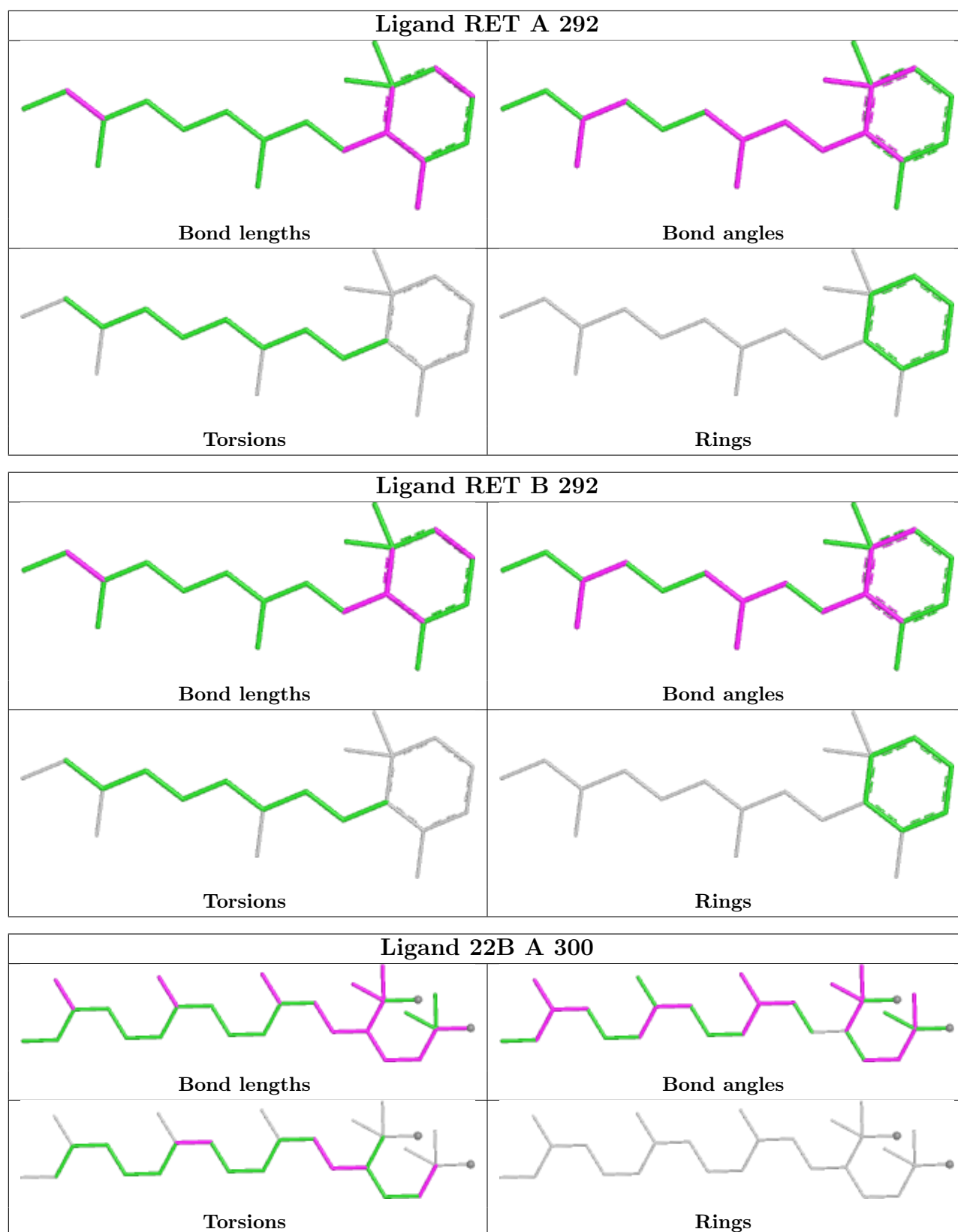
Mol	Chain	Res	Type	Atoms
3	A	300	22B	C21-C22-C23-C24
3	A	300	22B	C21-C22-C23-O27
3	B	300	22B	C1-C2-C3-C4
3	B	300	22B	C2-C3-C4-C5
3	B	300	22B	C7-C8-C9-C10
3	B	300	22B	C21-C22-C23-C24
3	B	300	22B	C21-C22-C23-O27
3	A	300	22B	C7-C8-C9-C19
3	B	300	22B	C7-C8-C9-C19
3	A	300	22B	C21-C22-C23-C25
3	B	300	22B	C21-C22-C23-C25
3	A	300	22B	C21-C2-C3-C4
3	B	300	22B	C21-C2-C3-C4
3	A	300	22B	C2-C3-C4-C5

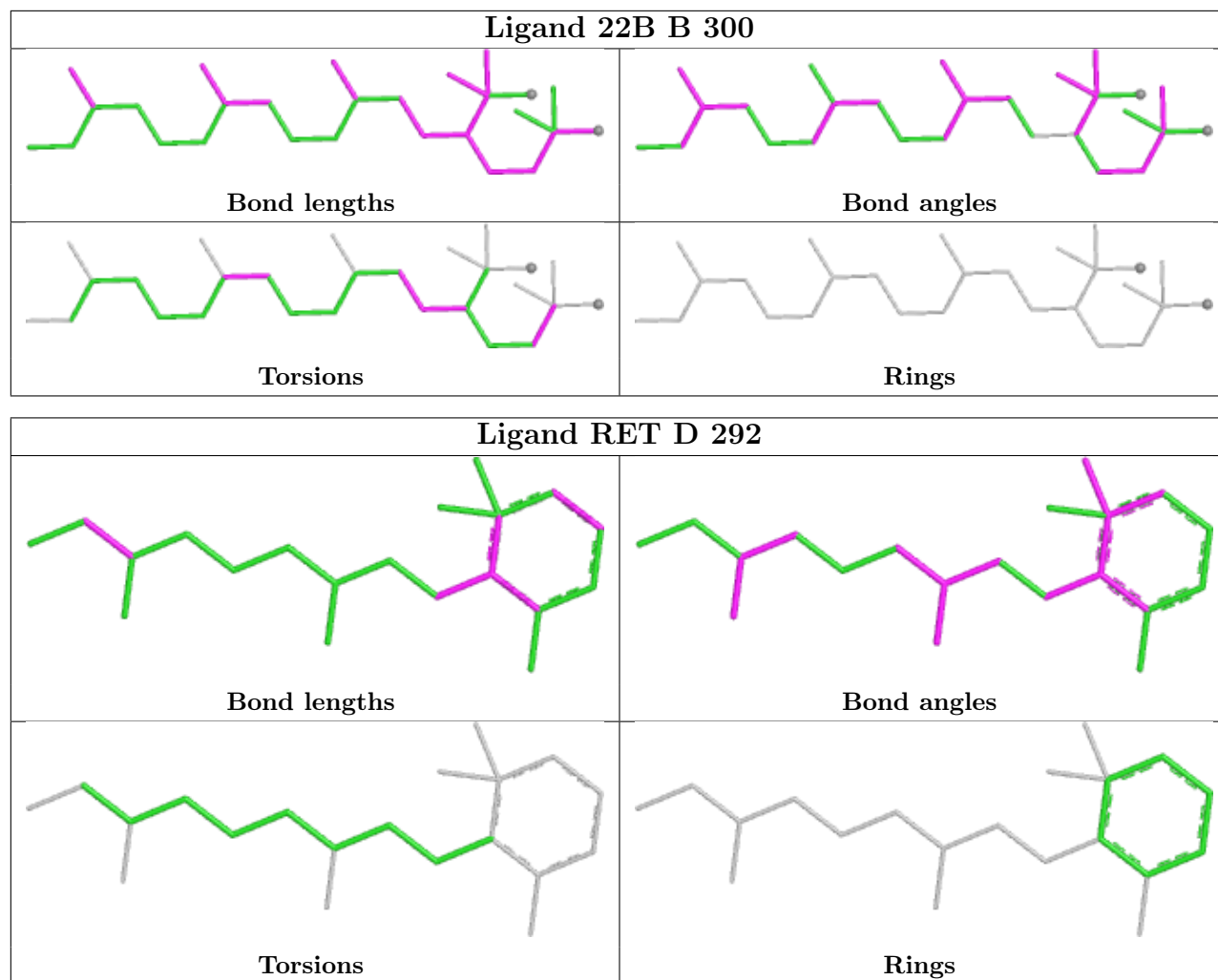
There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	292	RET	1	0
2	B	292	RET	1	0
3	A	300	22B	2	0
3	B	300	22B	1	0
2	D	292	RET	2	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	261/291 (89%)	0.42	19 (7%) 21 18	20, 33, 59, 79	0
1	B	259/291 (89%)	0.56	19 (7%) 21 18	25, 38, 52, 66	0
1	D	259/291 (89%)	1.58	81 (31%) 1 1	32, 50, 71, 92	0
All	All	779/873 (89%)	0.85	119 (15%) 5 4	20, 40, 65, 92	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	GLY	9.1
1	A	110	GLY	5.8
1	B	276	GLY	5.6
1	A	276	GLY	5.6
1	A	17	ALA	5.5
1	D	193	ILE	4.9
1	A	30	ASN	4.7
1	B	99	GLY	4.6
1	D	109	LEU	4.2
1	D	260	ALA	4.1
1	B	104	GLY	4.1
1	D	28	VAL	4.1
1	D	112	GLU	4.0
1	D	32	PRO	3.8
1	A	277	SER	3.7
1	D	110	GLY	3.5
1	D	229	TRP	3.5
1	B	212	SER	3.5
1	D	29	LEU	3.5
1	D	238	VAL	3.5
1	A	107	VAL	3.4
1	A	104	GLY	3.4
1	D	34	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	241	VAL	3.4
1	D	276	GLY	3.4
1	B	112	GLU	3.3
1	D	199	ALA	3.3
1	D	235	GLY	3.3
1	D	108	MET	3.3
1	D	227	ILE	3.3
1	D	240	PRO	3.2
1	A	109	LEU	3.2
1	B	268	THR	3.1
1	B	193	ILE	3.1
1	D	30	ASN	3.1
1	A	236	VAL	3.1
1	D	187	PHE	3.0
1	D	114	VAL	3.0
1	D	239	LEU	3.0
1	A	57	ARG	3.0
1	A	275	SER	3.0
1	D	249	SER	3.0
1	D	261	PHE	3.0
1	D	113	GLU	3.0
1	A	18	GLU	2.9
1	D	111	GLY	2.9
1	D	209	ASP	2.9
1	B	101	PHE	2.9
1	A	108	MET	2.9
1	D	55	MET	2.9
1	D	221	MET	2.9
1	D	258	ILE	2.9
1	D	181	ALA	2.9
1	D	237	ALA	2.8
1	D	188	ILE	2.8
1	D	243	TYR	2.8
1	D	51	LEU	2.8
1	B	30	ASN	2.8
1	D	35	ALA	2.8
1	D	211	PHE	2.7
1	B	200	GLN	2.7
1	B	209	ASP	2.7
1	D	205	ALA	2.7
1	D	236	VAL	2.7
1	D	230	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	42	ILE	2.6
1	D	267	LEU	2.6
1	D	210	ILE	2.6
1	B	196	VAL	2.6
1	A	105	SER	2.5
1	D	107	VAL	2.5
1	D	266	TYR	2.5
1	D	270	ASN	2.5
1	D	19	VAL	2.5
1	D	231	LEU	2.5
1	D	208	ALA	2.5
1	D	245	SER	2.5
1	D	222	TRP	2.4
1	D	248	TYR	2.4
1	D	264	LEU	2.4
1	D	224	GLY	2.4
1	D	232	GLY	2.4
1	A	19	VAL	2.4
1	D	269	SER	2.4
1	A	29	LEU	2.4
1	B	174	LEU	2.4
1	D	268	THR	2.3
1	B	29	LEU	2.3
1	D	275	SER	2.3
1	D	53	VAL	2.3
1	D	262	LEU	2.3
1	D	145	ASN	2.3
1	D	216	LEU	2.3
1	D	98	ALA	2.2
1	D	217	LEU	2.2
1	D	115	ASP	2.2
1	B	110	GLY	2.2
1	D	142	ALA	2.2
1	B	107	VAL	2.2
1	D	242	GLY	2.2
1	B	238	VAL	2.2
1	D	116	GLY	2.2
1	D	117	VAL	2.1
1	D	196	VAL	2.1
1	A	103	GLU	2.1
1	B	18	GLU	2.1
1	D	103	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	98	ALA	2.1
1	D	263	LEU	2.1
1	D	120	MET	2.1
1	D	173	HIS	2.1
1	D	105	SER	2.0
1	A	112	GLU	2.0
1	D	247	ALA	2.0
1	D	265	ASN	2.0
1	D	79	ILE	2.0
1	D	54	PHE	2.0
1	D	250	ALA	2.0
1	D	41	ASN	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](#)

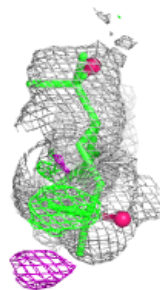
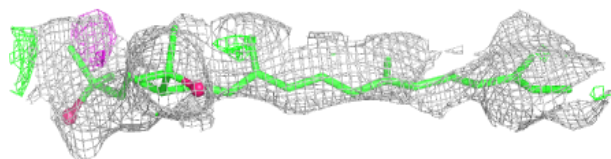
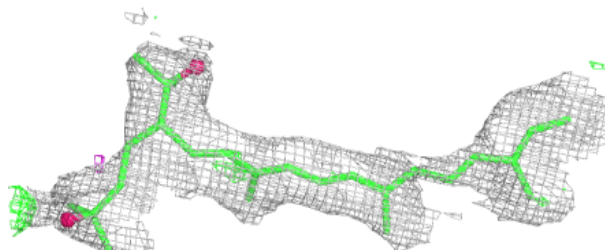
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	22B	A	300	27/54	0.68	0.21	72,77,85,86	0
3	22B	B	300	27/54	0.76	0.16	43,52,60,61	0
2	RET	D	292	20/21	0.81	0.15	40,42,44,46	0
4	BR	A	293	1/1	0.92	0.09	58,58,58,58	0
2	RET	A	292	20/21	0.94	0.07	19,23,27,28	0
2	RET	B	292	20/21	0.94	0.07	25,28,30,30	0
4	BR	D	401	1/1	0.97	0.08	50,50,50,50	0
4	BR	D	402	1/1	0.98	0.04	58,58,58,58	0
4	BR	A	402	1/1	0.99	0.03	43,43,43,43	0
4	BR	A	401	1/1	1.00	0.05	28,28,28,28	0
4	BR	B	401	1/1	1.00	0.07	32,32,32,32	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.

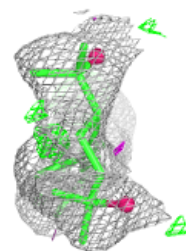
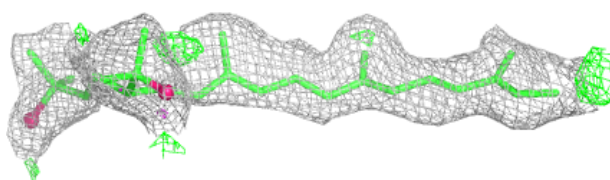
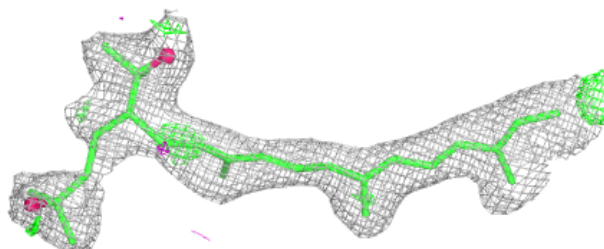
Electron density around 22B A 300:

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

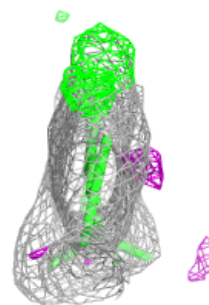
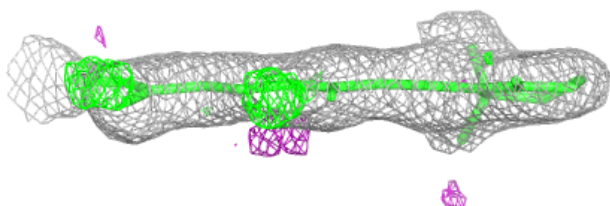
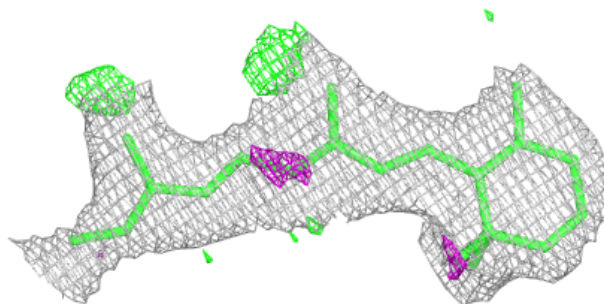


Electron density around 22B B 300:

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

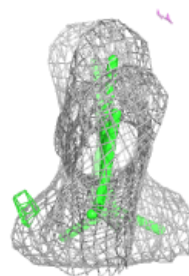
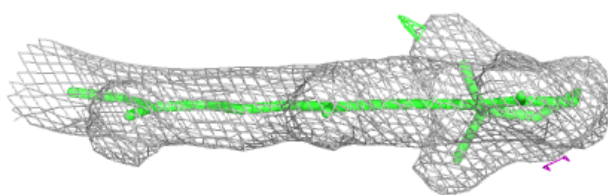
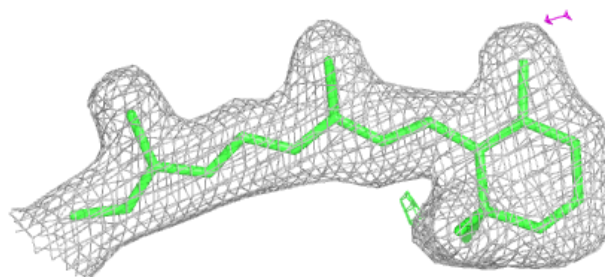
**Electron density around RET D 292:**

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

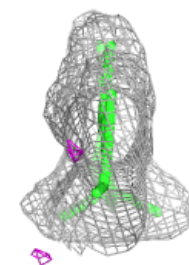
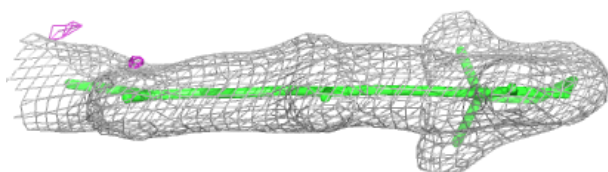
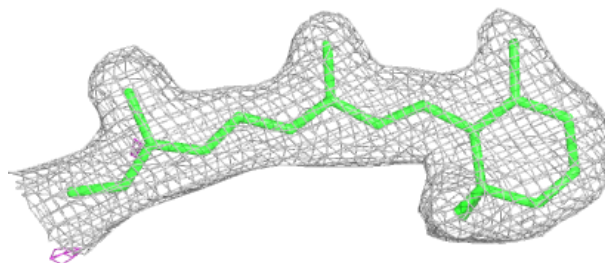


Electron density around RET A 292:

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

**Electron density around RET B 292:**

$2mF_o-DF_c$ (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.