Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 05:32 PM EDT

PDB ID	:	3QBL
Title	:	Pharaonis halorhodopsin complexed with nitrate
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

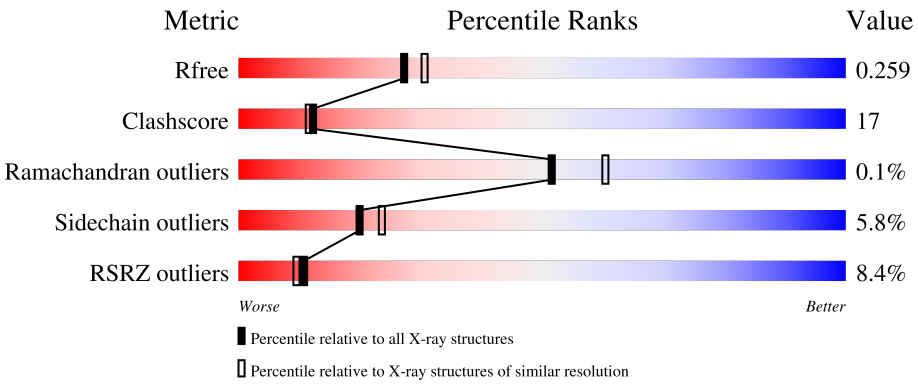
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	4% 63% 24% • 11%
1	B	291	2% 66% 20% • 11%
1	D	291	16% 48% 40% • 11%

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
3	NO3	A	293	-	-	X	-
4	22B	D	300	-	-	-	X

2 Entry composition (i)

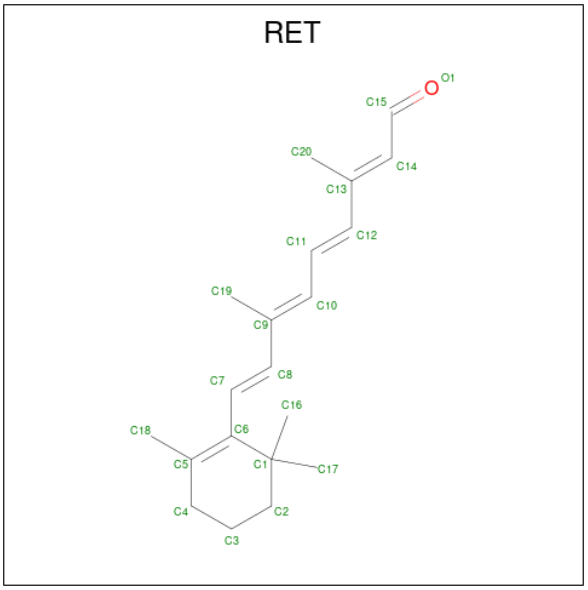
There are 5 unique types of molecules in this entry. The entry contains 6151 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

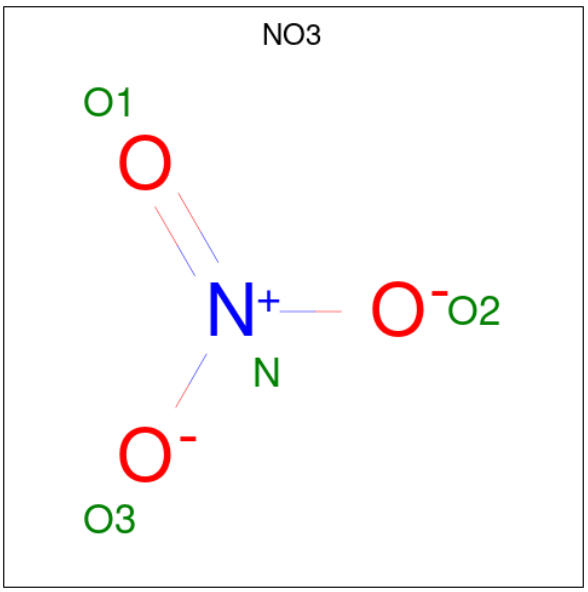
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	1963	1302	299	351	11	0	0	0
1	B	259	1957	1299	298	349	11	0	0	0
1	D	259	1957	1299	298	349	11	0	0	0

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



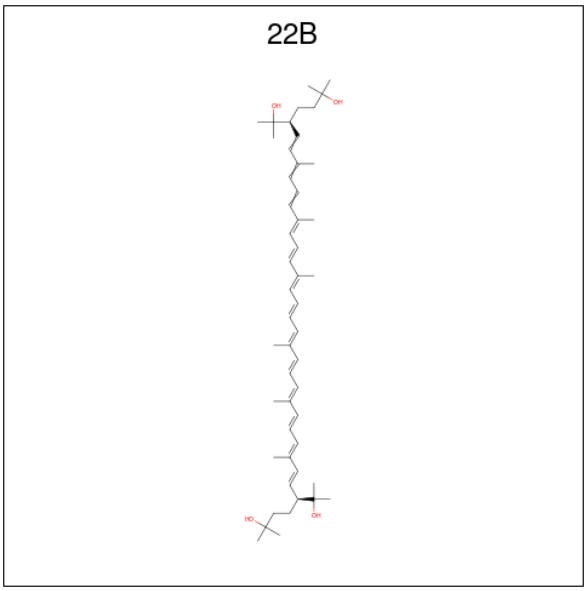
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
2	A	1	20	20	0	0
2	B	1	20	20	0	0
2	D	1	20	20	0	0

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
3	A	1	4	1	3	0	0
			Total	N	O		
3	A	1	4	1	3	0	0
			Total	N	O		
3	A	1	4	1	3	0	0
			Total	N	O		
3	B	1	4	1	3	0	0
			Total	N	O		
3	D	1	4	1	3	0	0
			Total	N	O		
3	D	1	4	1	3	0	0

- Molecule 4 is BACTERIORUBERIN (three-letter code: 22B) (formula: $C_{50}H_{76}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	27	25	2	0	0
			Total	C	O		
4	D	1	27	25	2	0	0

- Molecule 5 is water.

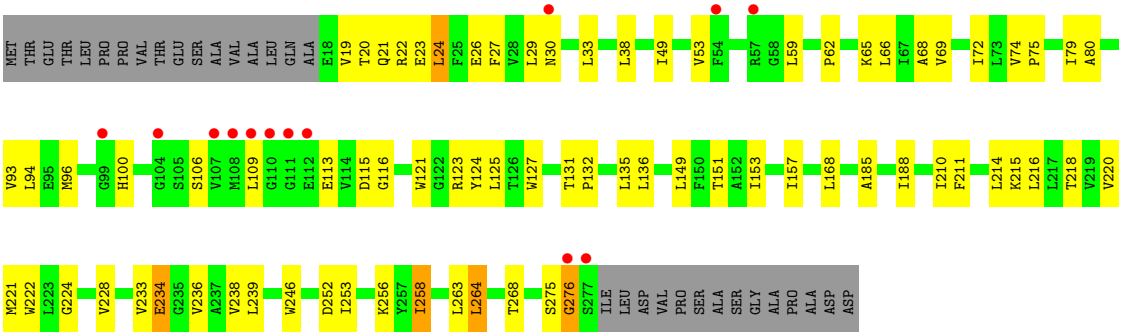
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	49	49	49	0	0
			Total	O		
5	B	59	59	59	0	0
			Total	O		
5	D	28	28	28	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

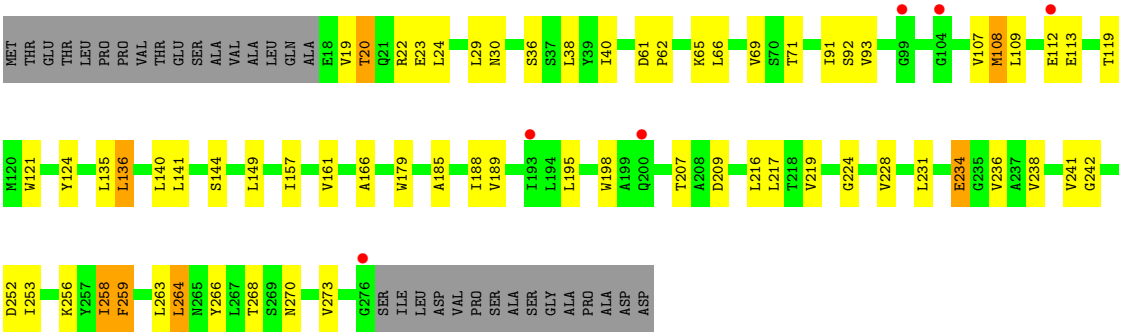
• Molecule 1: Halorhodopsin

Chain A:



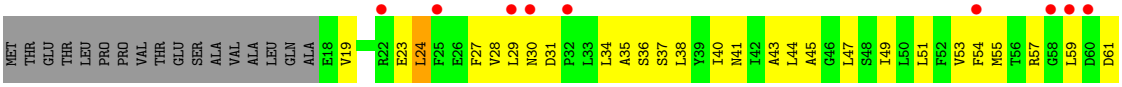
• Molecule 1: Halorhodopsin

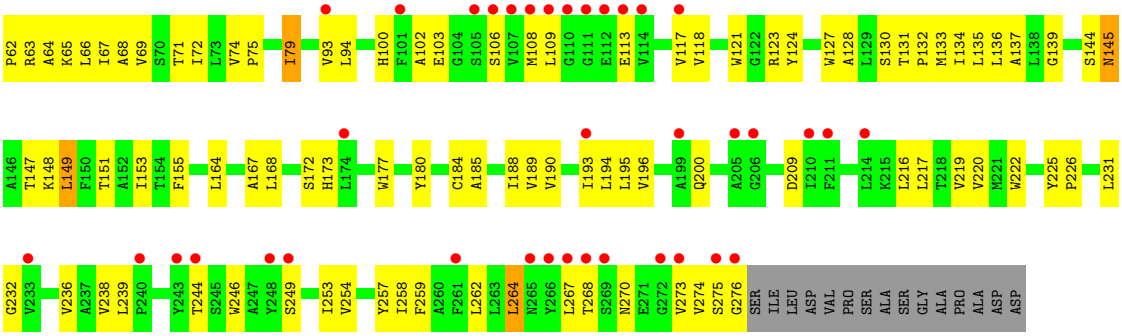
Chain B:



• Molecule 1: Halorhodopsin

Chain D:




P62 R63 A64 K65 L66 I67 A68 V69 S70 T71 I72 L73 V74 P75 I79 V93 L94 H100 F101 A102 E103 G104 S105 S106 V107 M108 L109 G110 G111 E112 E113 V114 V117 V118 W121 G122 R123 Y124 W127 A128 L129 S130 T131 P132 M133 I134 L135 L136 A137 L138 G139 S144 N145
A146 T147 K148 L149 F150 T151 A152 I153 T154 F155 L164 A167 L168 S172 H173 L174 W177 Y180 C184 A185 I188 V189 V190 I193 L194 L195 V196 A199 Q200 A205 G206 D209 I210 F211 L214 K215 L216 L217 T218 V219 V220 M221 W222 Y225 P226 L231
G232 V233 V236 A237 V238 L239 P240 Y243 T244 S245 W246 A247 Y248 S249 I253 V254 Y257 I258 F259 A260 P261 L262 L263 L264 N265 Y266 L267 T268 S269 N270 E271 G272 V273 V274 S275 G276 SER ILE LEU ASP VAL PRO SER ALA SER GLY ALA PRO ALA ASP ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.75Å 100.03Å 99.33Å 90.00° 127.23° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 50.02 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (15.00-2.20) 96.1 (50.02-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.267 0.250 , 0.259	Depositor DCC
R_{free} test set	2885 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 94.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6151	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 22B, NO3, RET

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	0.39	0/2009	0.59	0/2751
1	B	0.38	0/2003	0.59	0/2743
1	D	0.33	0/2003	0.55	0/2743
All	All	0.37	0/6015	0.58	0/8237

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1963	0	2014	53	0
1	B	1957	0	2009	50	0
1	D	1957	0	2009	101	0
2	A	20	0	27	1	0
2	B	20	0	27	1	0
2	D	20	0	27	1	0
3	A	12	0	0	4	0
3	B	4	0	0	1	0
3	D	8	0	0	1	0
4	B	27	0	37	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	27	0	37	2	0
5	A	49	0	0	5	1
5	B	59	0	0	3	0
5	D	28	0	0	3	0
All	All	6151	0	6187	207	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 17.

All (207) 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	1.44	0.97
1:D:231:LEU:HB3	1:D:239:LEU:HD13	1.62	0.82
1:D:28:VAL:HG13	1:D:34:LEU:HD12	1.61	0.82
1:B:270:ASN:HB3	1:B:273:VAL:CG1	2.12	0.80
1:A:236:VAL:HG13	1:A:238:VAL:HG13	1.64	0.78
1:D:254:VAL:HA	1:D:258:ILE:HG22	1.66	0.77
1:D:65:LYS:O	1:D:69:VAL:HG23	1.85	0.76
1:D:108:MET:HA	1:D:113:GLU:HA	1.67	0.76
1:D:145:ASN:HD21	1:D:148:LYS:HG3	1.51	0.75
1:B:270:ASN:HB3	1:B:273:VAL:HG12	1.69	0.74
1:D:45:ALA:HB3	1:D:79:ILE:HG23	1.70	0.73
1:D:193:ILE:HD12	1:D:194:LEU:N	2.04	0.72
1:B:20:THR:HG21	5:B:535:HOH:O	1.89	0.72
1:D:123:ARG:HD2	5:D:506:HOH:O	1.91	0.71
1:D:23:GLU:HB3	1:D:109:LEU:HB3	1.72	0.70
1:D:131:THR:OG1	1:D:132:PRO:HD3	1.91	0.70
1:D:185:ALA:O	1:D:188:ILE:HG12	1.93	0.69
1:A:20:THR:HG21	1:A:22:ARG:NH1	2.08	0.68
1:B:20:THR:HG22	1:B:23:GLU:H	1.57	0.68
1:B:19:VAL:HG21	1:B:93:VAL:HG11	1.76	0.67
1:D:106:SER:HB3	1:D:113:GLU:HG2	1.76	0.67
1:D:54:PHE:HB3	1:D:57:ARG:NH1	2.10	0.67
1:D:145:ASN:C	1:D:145:ASN:HD22	2.00	0.66
1:A:238:VAL:HG23	1:A:239:LEU:CD1	2.24	0.65
1:B:256:LYS:HE2	3:B:359:NO3:O1	1.97	0.64
1:D:164:LEU:O	1:D:168:LEU:HD23	1.97	0.64
1:D:40:ILE:O	1:D:44:LEU:HG	1.98	0.63
1:D:217:LEU:HD11	1:D:254:VAL:HG12	1.79	0.63
1:A:20:THR:HG22	1:A:21:GLN:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:O	1:B:30:ASN:HB2	1.99	0.63
1:B:236:VAL:HG13	1:B:238:VAL:HG13	1.80	0.62
1:D:28:VAL:HG13	1:D:34:LEU:CD1	2.29	0.62
1:D:254:VAL:HA	1:D:258:ILE:CG2	2.29	0.61
1:A:62:PRO:HA	3:A:293:NO3:O1	1.99	0.61
1:A:65:LYS:O	1:A:69:VAL:HG23	1.99	0.61
3:A:360:NO3:O1	1:B:62:PRO:HA	2.02	0.60
1:D:238:VAL:HG23	1:D:239:LEU:CD1	2.32	0.60
1:B:65:LYS:O	1:B:69:VAL:HG23	2.03	0.59
1:D:190:VAL:O	1:D:193:ILE:HG13	2.03	0.58
1:A:22:ARG:HG3	1:A:23:GLU:N	2.19	0.57
1:B:119:THR:HG23	1:B:234:GLU:OE1	2.05	0.57
1:A:29:LEU:O	1:A:30:ASN:HB2	2.05	0.57
1:B:185:ALA:O	1:B:188:ILE:HG12	2.04	0.57
1:D:238:VAL:HG23	1:D:239:LEU:HD12	1.87	0.56
1:D:27:PHE:CZ	1:D:118:VAL:HG21	2.40	0.56
1:D:64:ALA:O	1:D:267:LEU:HD21	2.06	0.56
1:D:71:THR:HG21	1:D:264:LEU:HD13	1.88	0.56
1:D:131:THR:O	1:D:135:LEU:HD13	2.05	0.56
1:D:216:LEU:O	1:D:220:VAL:HG23	2.06	0.56
1:B:108:MET:HA	1:B:112:GLU:O	2.06	0.55
1:A:256:LYS:HE2	3:A:359:NO3:O2	2.06	0.55
1:D:19:VAL:HG21	1:D:93:VAL:HG11	1.88	0.55
1:B:71:THR:HG21	1:B:264:LEU:HD13	1.88	0.55
1:D:145:ASN:ND2	1:D:148:LYS:H	2.04	0.55
1:B:93:VAL:HG13	1:B:93:VAL:O	2.06	0.55
1:A:20:THR:HG21	1:A:22:ARG:HG2	1.88	0.55
1:D:24:LEU:O	1:D:28:VAL:HG23	2.07	0.55
1:B:207:THR:HG22	1:B:266:TYR:OH	2.07	0.55
1:D:29:LEU:C	1:D:31:ASP:H	2.10	0.54
1:D:267:LEU:HD11	1:D:274:VAL:HG21	1.87	0.54
1:A:20:THR:CG2	1:A:22:ARG:HG2	2.37	0.54
1:A:233:VAL:HG23	1:A:234:GLU:OE1	2.08	0.54
1:A:264:LEU:O	1:A:268:THR:HG22	2.07	0.54
1:A:234:GLU:HG3	5:A:511:HOH:O	2.07	0.54
1:B:188:ILE:HG13	1:B:189:VAL:N	2.23	0.54
1:D:124:TYR:HD1	1:D:127:TRP:CZ3	2.27	0.53
1:B:107:VAL:O	1:B:108:MET:HB2	2.07	0.53
1:A:20:THR:HG22	1:A:22:ARG:H	1.74	0.53
1:A:275:SER:O	1:A:276:GLY:O	2.27	0.53
1:D:232:GLY:HA3	1:D:244:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ALA:O	1:D:47:LEU:HD13	2.10	0.52
1:D:167:ALA:HB2	5:D:514:HOH:O	2.09	0.51
1:B:108:MET:HA	1:B:113:GLU:HA	1.92	0.51
1:D:232:GLY:CA	1:D:244:THR:HG21	2.41	0.51
1:D:61:ASP:OD2	1:D:275:SER:HA	2.11	0.50
1:D:254:VAL:CA	1:D:258:ILE:HG22	2.40	0.50
1:D:100:HIS:CD2	1:D:102:ALA:H	2.29	0.50
1:D:108:MET:HB2	1:D:113:GLU:HG3	1.93	0.50
1:B:258:ILE:HG13	1:B:259:PHE:N	2.26	0.50
1:D:217:LEU:HD11	1:D:254:VAL:CG1	2.42	0.50
1:A:116:GLY:HA2	5:A:516:HOH:O	2.09	0.50
1:D:225:TYR:N	1:D:226:PRO:HD2	2.26	0.50
1:D:109:LEU:HD22	1:D:109:LEU:N	2.27	0.50
1:A:20:THR:CG2	1:A:21:GLN:N	2.75	0.49
1:A:234:GLU:HB2	5:A:508:HOH:O	2.11	0.49
1:D:249:SER:O	1:D:253:ILE:HG13	2.12	0.49
1:A:151:THR:HG21	4:B:300:22B:H253	1.95	0.49
1:A:68:ALA:O	1:A:72:ILE:HG13	2.13	0.49
1:A:253:ILE:O	1:A:258:ILE:HG23	2.13	0.49
1:B:136:LEU:HD22	1:B:140:LEU:CD1	2.43	0.49
1:B:144:SER:OG	1:B:149:LEU:HD22	2.12	0.49
1:B:270:ASN:HB3	1:B:273:VAL:HG11	1.92	0.49
1:B:270:ASN:O	1:B:273:VAL:HG12	2.13	0.49
1:D:94:LEU:HD11	1:D:168:LEU:HD13	1.94	0.49
1:D:254:VAL:O	1:D:258:ILE:HG22	2.14	0.48
1:D:267:LEU:CD1	1:D:274:VAL:HG21	2.43	0.48
1:B:217:LEU:C	1:B:217:LEU:HD23	2.32	0.48
1:D:270:ASN:HB3	1:D:273:VAL:CG2	2.43	0.48
1:B:29:LEU:O	1:B:30:ASN:CB	2.62	0.48
1:A:210:ILE:HG23	1:A:211:PHE:N	2.29	0.48
1:B:236:VAL:HG22	1:B:236:VAL:O	2.14	0.48
1:B:259:PHE:C	1:B:259:PHE:CD1	2.87	0.48
1:D:36:SER:O	1:D:40:ILE:HG12	2.15	0.47
1:D:145:ASN:C	1:D:145:ASN:ND2	2.67	0.47
1:D:196:VAL:O	1:D:200:GLN:HG2	2.15	0.47
1:B:253:ILE:O	1:B:258:ILE:HG23	2.13	0.47
1:D:128:ALA:O	1:D:132:PRO:HG2	2.14	0.47
1:A:185:ALA:O	1:A:188:ILE:HG13	2.15	0.47
1:D:66:LEU:HD23	1:D:66:LEU:O	2.14	0.47
1:A:275:SER:O	1:A:276:GLY:C	2.53	0.47
1:D:68:ALA:O	1:D:72:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:O	1:A:19:VAL:HG23	2.15	0.47
1:A:24:LEU:HD13	1:A:109:LEU:HD21	1.97	0.47
1:B:36:SER:O	1:B:40:ILE:HG12	2.15	0.47
1:B:121:TRP:HA	1:B:124:TYR:CD2	2.50	0.47
1:B:224:GLY:O	1:B:228:VAL:HG23	2.15	0.47
1:A:123:ARG:HD2	5:A:506:HOH:O	2.15	0.47
1:D:134:ILE:HG23	1:D:259:PHE:CZ	2.50	0.47
1:A:49:ILE:O	1:A:53:VAL:HG23	2.15	0.46
1:B:195:LEU:HD21	1:B:219:VAL:HG21	1.97	0.46
1:D:93:VAL:O	1:D:93:VAL:HG13	2.15	0.46
1:D:144:SER:OG	1:D:148:LYS:HB2	2.16	0.46
1:D:108:MET:HB2	1:D:113:GLU:CG	2.45	0.46
1:B:20:THR:HG22	1:B:22:ARG:N	2.31	0.46
1:D:135:LEU:HD11	1:D:222:TRP:CH2	2.50	0.46
1:D:145:ASN:ND2	1:D:148:LYS:HG3	2.26	0.46
1:A:224:GLY:O	1:A:228:VAL:HG23	2.17	0.45
1:B:109:LEU:HD22	1:B:109:LEU:N	2.31	0.45
1:D:134:ILE:O	1:D:137:ALA:HB3	2.16	0.45
1:D:130:SER:O	1:D:133:MET:HB2	2.15	0.45
1:A:238:VAL:CG2	1:A:239:LEU:HD13	2.32	0.45
1:A:214:LEU:CD1	1:A:263:LEU:HD13	2.47	0.45
1:D:72:ILE:O	1:D:75:PRO:HD2	2.17	0.45
1:A:215:LYS:HE2	1:A:215:LYS:HB3	1.81	0.45
1:A:218:THR:HG23	1:A:222:TRP:NE1	2.31	0.45
1:A:252:ASP:O	1:A:256:LYS:HB2	2.16	0.45
1:D:51:LEU:O	1:D:55:MET:HG3	2.17	0.45
1:D:100:HIS:O	1:D:103:GLU:HB3	2.16	0.45
1:D:63:ARG:HG2	1:D:63:ARG:HH11	1.82	0.45
1:A:153:ILE:O	1:A:157:ILE:HG13	2.16	0.45
1:D:49:ILE:O	1:D:53:VAL:HG23	2.17	0.45
1:B:268:THR:HG23	5:B:516:HOH:O	2.16	0.44
2:B:292:RET:H7	2:B:292:RET:H181	1.81	0.44
1:D:59:LEU:HD21	1:D:268:THR:HG22	1.99	0.44
1:B:91:ILE:HG22	1:B:92:SER:N	2.32	0.44
1:D:28:VAL:O	1:D:35:ALA:HB2	2.17	0.44
1:A:33:LEU:HD22	1:A:246:TRP:HD1	1.81	0.44
1:D:100:HIS:CD2	1:D:102:ALA:HB3	2.53	0.44
1:B:136:LEU:HD22	1:B:140:LEU:HD11	1.99	0.44
1:D:151:THR:HG21	4:D:300:22B:H242	1.99	0.44
1:D:65:LYS:HE3	3:D:360:NO3:O3	2.18	0.44
1:D:254:VAL:HG13	1:D:258:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:SER:HB3	1:A:113:GLU:CG	2.47	0.44
1:B:20:THR:CG2	1:B:22:ARG:H	2.31	0.44
1:D:173:HIS:CD2	1:D:177:TRP:HE1	2.36	0.43
1:A:27:PHE:HB2	1:A:109:LEU:HD12	2.00	0.43
1:A:79:ILE:HG23	1:A:80:ALA:N	2.33	0.43
1:D:231:LEU:HA	1:D:236:VAL:HG12	2.01	0.43
1:D:100:HIS:CE1	5:D:512:HOH:O	2.71	0.43
1:B:263:LEU:HD12	1:B:263:LEU:O	2.19	0.43
1:D:121:TRP:HA	1:D:124:TYR:CD2	2.53	0.43
1:A:22:ARG:HG3	1:A:23:GLU:H	1.82	0.43
1:B:234:GLU:HB2	5:B:509:HOH:O	2.19	0.43
1:D:253:ILE:HA	1:D:257:TYR:CD2	2.54	0.42
1:B:141:LEU:HD22	1:B:263:LEU:HD13	2.01	0.42
1:D:195:LEU:HD21	1:D:219:VAL:HG21	2.01	0.42
1:D:37:SER:HB3	1:D:246:TRP:CD1	2.54	0.42
1:D:108:MET:N	1:D:113:GLU:HG3	2.34	0.42
2:D:292:RET:H7	2:D:292:RET:H181	1.83	0.42
1:D:238:VAL:HG23	1:D:239:LEU:HD13	2.01	0.42
1:A:220:VAL:HG12	1:A:221:MET:CE	2.49	0.42
3:A:293:NO3:O1	1:D:147:THR:HG21	2.19	0.42
1:D:188:ILE:HG13	1:D:189:VAL:N	2.35	0.42
1:D:139:GLY:HA3	1:D:149:LEU:HD11	2.02	0.42
1:B:252:ASP:O	1:B:256:LYS:HB2	2.20	0.42
1:D:132:PRO:HB3	1:D:153:ILE:HG23	2.01	0.42
1:B:241:VAL:HG13	1:B:242:GLY:N	2.35	0.41
1:A:20:THR:N	1:A:23:GLU:OE1	2.45	0.41
2:A:292:RET:H7	2:A:292:RET:H181	1.92	0.41
1:D:93:VAL:HA	1:D:117:VAL:O	2.20	0.41
1:B:166:ALA:HB2	1:B:179:TRP:HB3	2.03	0.41
1:D:145:ASN:HD21	1:D:148:LYS:H	1.67	0.41
1:A:26:GLU:O	1:A:29:LEU:O	2.38	0.41
1:D:61:ASP:HA	1:D:62:PRO:HD2	1.93	0.41
1:D:74:VAL:N	1:D:75:PRO:HD2	2.35	0.41
1:D:63:ARG:HD2	1:D:276:GLY:O	2.19	0.41
1:A:20:THR:HG21	1:A:22:ARG:HH11	1.81	0.41
1:B:231:LEU:O	1:B:238:VAL:HG22	2.21	0.41
1:D:258:ILE:O	1:D:262:LEU:HG	2.20	0.41
1:B:144:SER:HB2	1:B:198:TRP:NE1	2.35	0.41
1:D:29:LEU:C	1:D:31:ASP:N	2.73	0.41
1:D:29:LEU:O	1:D:30:ASN:HB2	2.20	0.41
1:A:124:TYR:HD1	1:A:127:TRP:CZ3	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ARG:O	1:D:67:ILE:HG13	2.21	0.41
1:D:180:TYR:CE1	1:D:184:CYS:SG	3.14	0.41
1:A:131:THR:N	1:A:132:PRO:CD	2.84	0.41
1:B:61:ASP:HA	1:B:62:PRO:HD2	1.94	0.41
1:D:155:PHE:CE1	4:D:300:22B:H192	2.56	0.41
1:D:184:CYS:O	1:D:188:ILE:HG23	2.21	0.41
1:A:96:MET:HB3	1:A:100:HIS:HB3	2.03	0.40
1:A:268:THR:HG23	5:A:543:HOH:O	2.22	0.40
1:B:108:MET:HG2	1:B:113:GLU:HA	2.03	0.40
1:B:157:ILE:O	1:B:161:VAL:HG23	2.22	0.40
1:A:74:VAL:HB	1:A:75:PRO:CD	2.51	0.40
1:A:93:VAL:O	1:A:94:LEU:HD23	2.21	0.40
1:A:121:TRP:HZ3	1:A:125:LEU:HD22	1.86	0.40
1:D:236:VAL:HG13	1:D:238:VAL:HG22	2.03	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]	1.79	0.41

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	258/291 (89%)	249 (96%)	8 (3%)	1 (0%)	34 37
1	B	257/291 (88%)	244 (95%)	13 (5%)	0	100 100
1	D	257/291 (88%)	239 (93%)	18 (7%)	0	100 100
All	All	772/873 (88%)	732 (95%)	39 (5%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	GLY

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	208/233 (89%)	195 (94%)	13 (6%)	18	20
1	B	207/233 (89%)	194 (94%)	13 (6%)	18	20
1	D	207/233 (89%)	197 (95%)	10 (5%)	25	32
All	All	622/699 (89%)	586 (94%)	36 (6%)	20	23

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	38	LEU
1	A	59	LEU
1	A	66	LEU
1	A	115	ASP
1	A	135	LEU
1	A	136	LEU
1	A	149	LEU
1	A	168	LEU
1	A	216	LEU
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	108	MET
1	B	135	LEU
1	B	136	LEU
1	B	209	ASP
1	B	216	LEU

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Mol	Chain	Res	Type
1	B	234	GLU
1	B	258	ILE
1	B	259	PHE
1	B	264	LEU
1	D	24	LEU
1	D	38	LEU
1	D	41	ASN
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 (6) such sidechains are listed below:

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	NO3	A	359	-	1,3,3	3.16	1 (100%)	0,3,3	-	-
3	NO3	B	359	-	1,3,3	3.19	1 (100%)	0,3,3	-	-
3	NO3	D	360	-	1,3,3	3.57	1 (100%)	0,3,3	-	-
4	22B	B	300	-	25,26,53	3.64	11 (44%)	30,35,72	2.27	9 (30%)
4	22B	D	300	-	25,26,53	3.64	10 (40%)	30,35,72	2.30	10 (33%)
2	RET	A	292	1	20,20,21	2.16	5 (25%)	27,27,28	1.65	7 (25%)
2	RET	B	292	1	20,20,21	2.09	5 (25%)	27,27,28	1.73	8 (29%)
3	NO3	A	293	-	1,3,3	3.63	1 (100%)	0,3,3	-	-
2	RET	D	292	1	20,20,21	2.21	5 (25%)	27,27,28	1.74	7 (25%)
3	NO3	A	360	-	1,3,3	3.42	1 (100%)	0,3,3	-	-
3	NO3	D	359	-	1,3,3	3.56	1 (100%)	0,3,3	-	-

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	22B	B	300	-	-	8/31/31/65	-
4	22B	D	300	-	-	9/31/31/65	-
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
2	RET	D	292	1	-	0/13/30/31	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	300	22B	C2-C3	13.56	1.64	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	300	22B	C2-C3	13.29	1.64	1.49
4	D	300	22B	C21-C2	5.98	1.61	1.53
2	D	292	RET	C1-C6	5.87	1.61	1.53
4	B	300	22B	C21-C2	5.80	1.61	1.53
2	B	292	RET	C1-C6	5.64	1.61	1.53
2	A	292	RET	C1-C6	5.55	1.61	1.53
2	D	292	RET	C5-C6	4.55	1.42	1.34
2	A	292	RET	C5-C6	4.53	1.42	1.34
4	D	300	22B	C16-C1	4.21	1.59	1.52
4	B	300	22B	C16-C1	4.04	1.59	1.52
4	D	300	22B	C19-C9	4.04	1.59	1.50
2	D	292	RET	C14-C13	3.97	1.36	1.33
4	B	300	22B	C19-C9	3.86	1.58	1.50
4	B	300	22B	O27-C23	3.81	1.54	1.44
4	D	300	22B	O27-C23	3.81	1.54	1.44
2	B	292	RET	C14-C13	3.76	1.36	1.33
2	B	292	RET	C5-C6	3.73	1.40	1.34
3	A	293	NO3	O1-N	3.63	1.40	1.24
3	D	360	NO3	O1-N	3.57	1.40	1.24
3	D	359	NO3	O1-N	3.56	1.40	1.24
3	A	360	NO3	O1-N	3.42	1.39	1.24
4	D	300	22B	C17-C1	3.35	1.58	1.52
4	D	300	22B	C22-C21	3.28	1.62	1.53
4	B	300	22B	C17-C1	3.26	1.58	1.52
4	B	300	22B	C22-C21	3.26	1.62	1.53
4	D	300	22B	C20-C13	3.23	1.57	1.50
3	B	359	NO3	O1-N	3.19	1.38	1.24
3	A	359	NO3	O1-N	3.16	1.38	1.24
2	A	292	RET	C7-C6	3.02	1.55	1.45
4	B	300	22B	C20-C13	3.00	1.57	1.50
2	B	292	RET	C7-C6	2.99	1.55	1.45
2	D	292	RET	C7-C6	2.94	1.55	1.45
2	A	292	RET	C14-C13	2.81	1.35	1.33
2	A	292	RET	C2-C3	-2.80	1.45	1.52
4	B	300	22B	C18-C5	2.64	1.56	1.50
4	D	300	22B	C18-C5	2.62	1.56	1.50
2	B	292	RET	C2-C3	-2.59	1.46	1.52
2	D	292	RET	C2-C3	-2.53	1.46	1.52
4	D	300	22B	C4-C3	2.46	1.38	1.32
4	B	300	22B	C4-C3	2.44	1.38	1.32
4	B	300	22B	C8-C9	2.12	1.50	1.45

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	300	22B	C2-C3-C4	6.75	136.12	125.15
4	B	300	22B	C2-C3-C4	6.45	135.64	125.15
4	D	300	22B	C20-C13-C12	4.50	125.17	118.08
4	B	300	22B	C21-C22-C23	4.28	124.63	116.39
4	B	300	22B	C20-C13-C12	4.07	124.48	118.08
4	D	300	22B	C21-C22-C23	3.90	123.90	116.39
4	B	300	22B	C17-C1-C16	-3.75	105.20	110.56
4	B	300	22B	C16-C1-C2	3.70	117.06	111.72
4	D	300	22B	C17-C1-C16	-3.68	105.29	110.56
4	D	300	22B	C4-C5-C6	-3.61	113.40	118.94
4	B	300	22B	C4-C5-C6	-3.53	113.53	118.94
4	D	300	22B	C16-C1-C2	3.45	116.70	111.72
2	B	292	RET	C1-C6-C7	3.40	125.39	115.78
2	D	292	RET	C1-C6-C7	3.33	125.19	115.78
2	B	292	RET	C1-C6-C5	-3.22	118.08	122.61
2	D	292	RET	C1-C6-C5	-3.09	118.27	122.61
2	A	292	RET	C20-C13-C12	3.04	122.86	118.08
2	B	292	RET	C19-C9-C8	3.03	122.86	118.08
4	D	300	22B	C18-C5-C4	2.92	122.68	118.08
2	A	292	RET	C7-C8-C9	2.92	130.64	126.23
2	A	292	RET	C1-C6-C5	-2.91	118.51	122.61
4	B	300	22B	C18-C5-C4	2.90	122.65	118.08
2	B	292	RET	C2-C1-C6	2.79	114.78	110.48
2	B	292	RET	C8-C9-C10	-2.75	114.72	118.94
2	A	292	RET	C1-C6-C7	2.72	123.48	115.78
2	D	292	RET	C20-C13-C12	2.68	122.30	118.08
4	D	300	22B	C12-C13-C14	-2.61	110.52	118.80
2	A	292	RET	C2-C1-C6	2.58	114.46	110.48
2	D	292	RET	C2-C1-C6	2.50	114.33	110.48
2	D	292	RET	C19-C9-C8	2.47	121.96	118.08
4	B	300	22B	C12-C13-C14	-2.38	111.23	118.80
4	B	300	22B	C24-C23-C22	2.27	118.41	111.42
4	D	300	22B	C24-C23-C22	2.23	118.31	111.42
2	B	292	RET	C17-C1-C6	2.21	113.89	110.30
2	A	292	RET	C17-C1-C6	2.20	113.86	110.30
2	B	292	RET	C20-C13-C12	2.19	121.53	118.08
2	B	292	RET	C7-C6-C5	-2.04	116.53	121.46
2	D	292	RET	C2-C3-C4	2.04	115.93	111.38
2	D	292	RET	C7-C6-C5	-2.03	116.54	121.46
2	A	292	RET	C19-C9-C8	2.03	121.27	118.08
4	D	300	22B	C8-C9-C10	-2.02	115.83	118.94

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

There are no ring outliers.

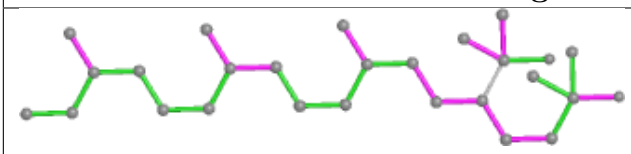
10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	359	NO3	1	0
3	B	359	NO3	1	0
3	D	360	NO3	1	0
4	B	300	22B	1	0
4	D	300	22B	2	0
2	A	292	RET	1	0
2	B	292	RET	1	0
3	A	293	NO3	2	0
2	D	292	RET	1	0
3	A	360	NO3	1	0

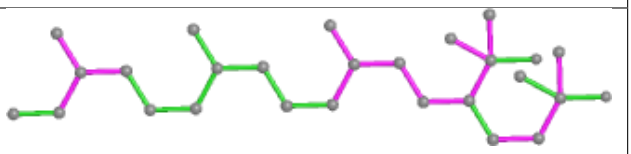
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

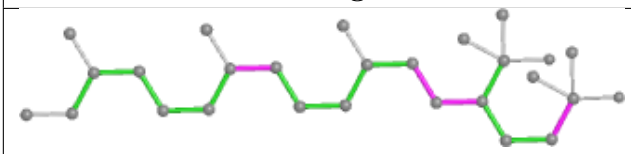
Ligand 22B B 300



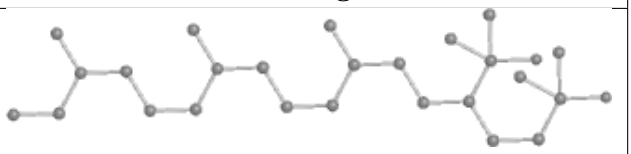
Bond lengths



Bond angles

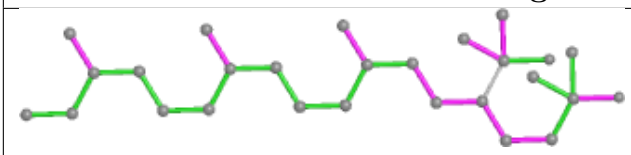


Torsions

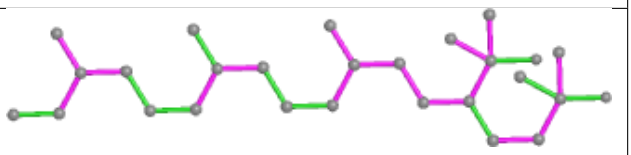


Rings

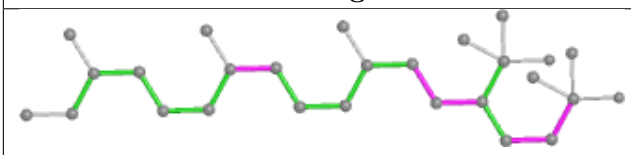
Ligand 22B D 300



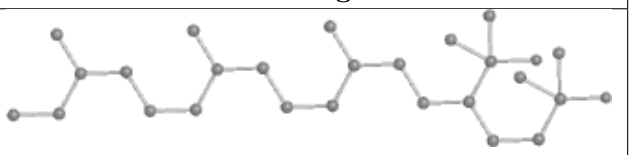
Bond lengths



Bond angles

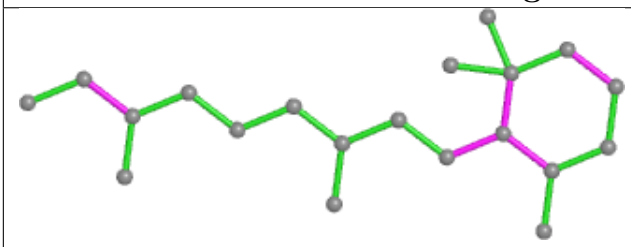


Torsions

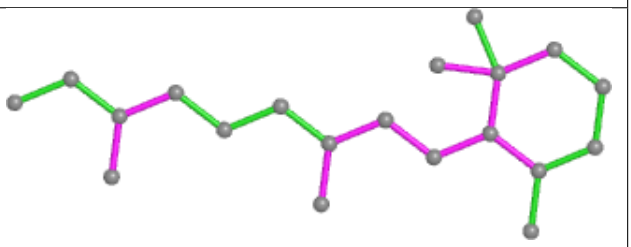


Rings

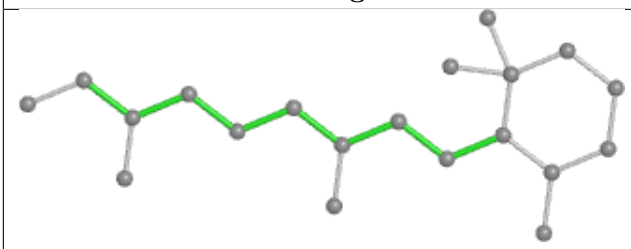
Ligand RET A 292



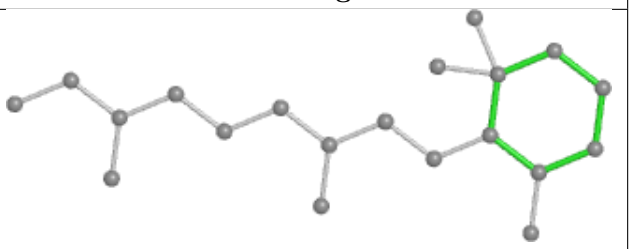
Bond lengths



Bond angles

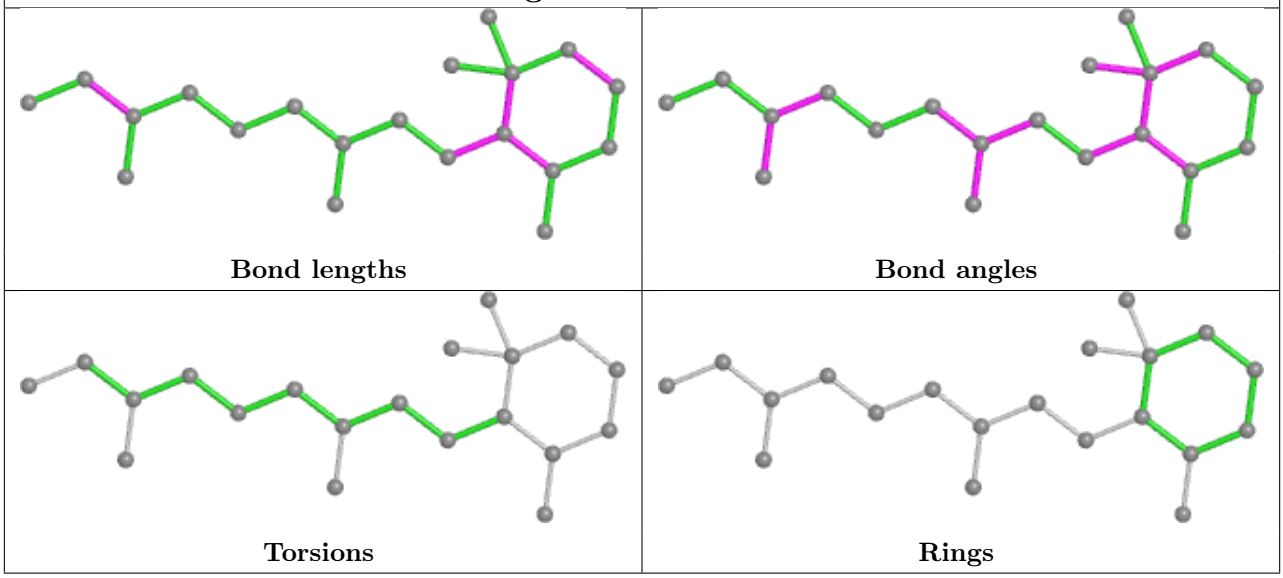


Torsions

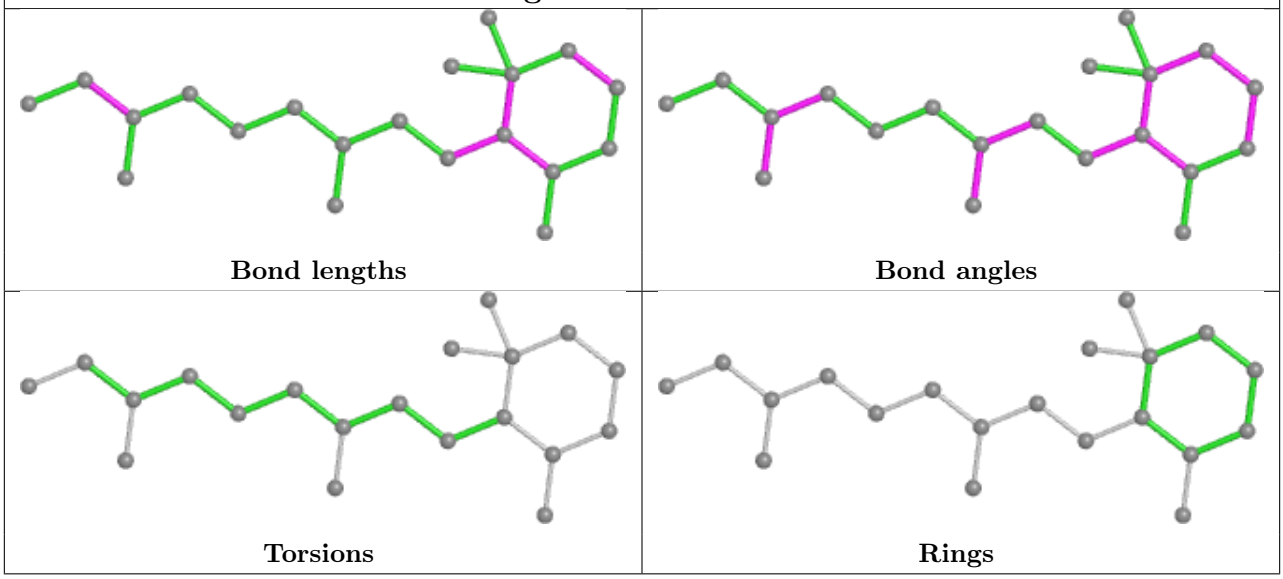


Rings

Ligand RET B 292



Ligand RET D 292



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	260/291 (89%)	0.19	13 (5%)	28	27	24, 37, 67, 82	0
1	B	259/291 (89%)	0.04	6 (2%)	60	58	24, 39, 53, 69	0
1	D	259/291 (89%)	0.93	46 (17%)	1	1	36, 56, 77, 98	0
All	All	778/873 (89%)	0.39	65 (8%)	11	9	24, 43, 72, 98	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	111	GLY	8.5
1	D	109	LEU	6.3
1	B	276	GLY	5.7
1	D	110	GLY	5.5
1	A	107	VAL	5.5
1	D	276	GLY	5.2
1	D	112	GLU	4.8
1	D	268	THR	4.6
1	D	243	TYR	4.5
1	A	110	GLY	4.3
1	A	104	GLY	4.2
1	A	111	GLY	4.1
1	D	113	GLU	4.0
1	D	273	VAL	3.9
1	A	277	SER	3.8
1	A	109	LEU	3.8
1	D	240	PRO	3.6
1	D	29	LEU	3.5
1	D	30	ASN	3.5
1	B	112	GLU	3.2
1	A	276	GLY	3.2
1	A	54	PHE	3.1
1	D	58	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	265	ASN	3.0
1	D	269	SER	3.0
1	A	57	ARG	3.0
1	D	275	SER	3.0
1	D	105	SER	2.9
1	D	59	LEU	2.9
1	A	30	ASN	2.9
1	D	114	VAL	2.8
1	A	99	GLY	2.8
1	D	193	ILE	2.8
1	D	108	MET	2.7
1	D	211	PHE	2.7
1	D	60	ASP	2.7
1	D	272	GLY	2.6
1	D	93	VAL	2.6
1	A	112	GLU	2.6
1	D	106	SER	2.6
1	D	249	SER	2.5
1	D	22	ARG	2.5
1	D	267	LEU	2.5
1	D	206	GLY	2.5
1	B	200	GLN	2.5
1	D	107	VAL	2.4
1	B	99	GLY	2.4
1	B	193	ILE	2.4
1	D	174	LEU	2.3
1	D	205	ALA	2.3
1	D	32	PRO	2.3
1	D	54	PHE	2.3
1	D	210	ILE	2.3
1	D	261	PHE	2.3
1	A	108	MET	2.2
1	D	233	VAL	2.1
1	B	104	GLY	2.1
1	D	266	TYR	2.1
1	D	248	TYR	2.1
1	D	25	PHE	2.1
1	D	214	LEU	2.1
1	D	101	PHE	2.1
1	D	199	ALA	2.0
1	D	117	VAL	2.0
1	D	244	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

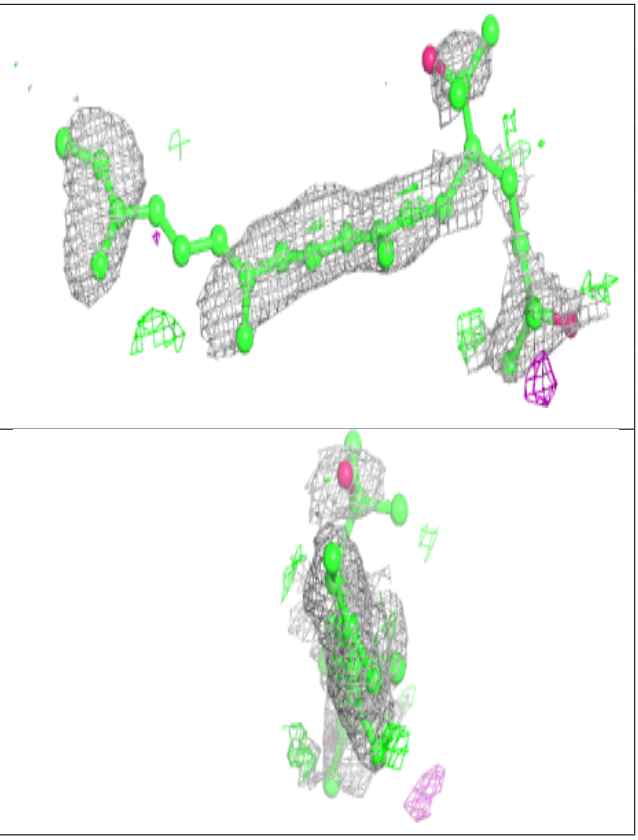
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	22B	D	300	27/54	0.63	0.41	84,86,92,92	0
3	NO3	A	293	4/4	0.64	0.27	76,77,77,78	0
4	22B	B	300	27/54	0.76	0.29	60,64,70,71	0
3	NO3	D	360	4/4	0.83	0.33	56,56,56,58	0
2	RET	D	292	20/21	0.86	0.20	44,48,50,51	0
3	NO3	A	360	4/4	0.92	0.38	69,70,70,72	0
3	NO3	D	359	4/4	0.96	0.18	44,45,47,49	0
2	RET	A	292	20/21	0.96	0.13	25,28,32,32	0
2	RET	B	292	20/21	0.96	0.14	29,31,32,33	0
3	NO3	A	359	4/4	0.97	0.19	34,39,40,44	0
3	NO3	B	359	4/4	0.99	0.14	33,36,37,38	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.

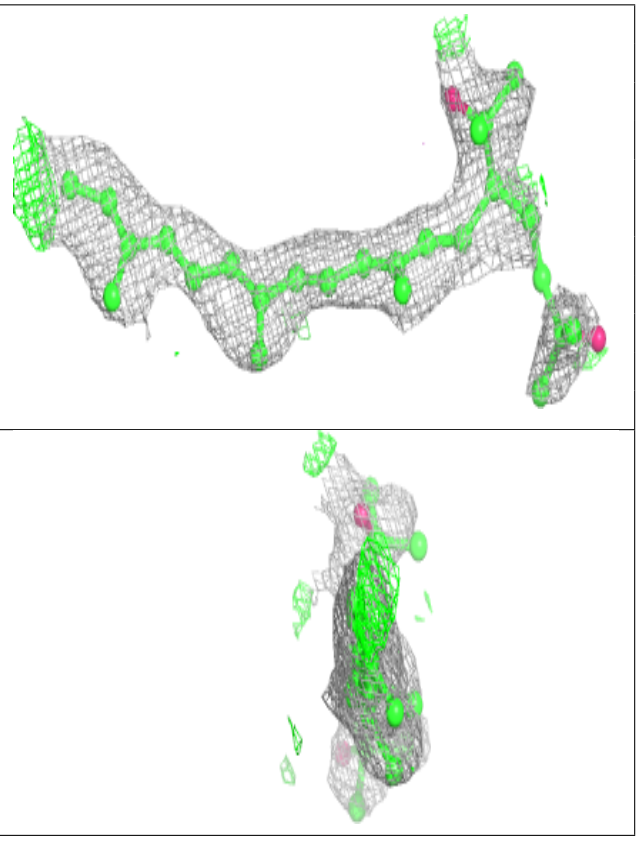
Electron density around 22B D 300:

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



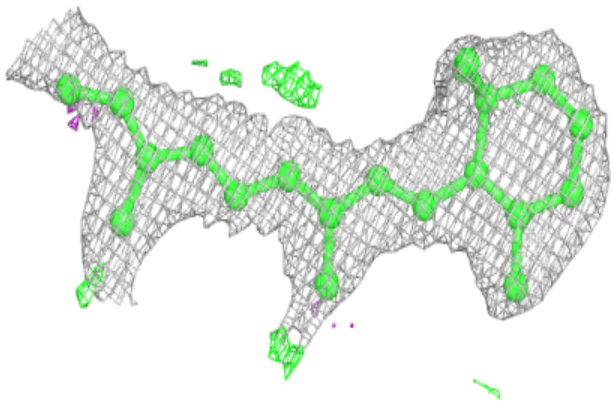
Electron density around 22B B 300:

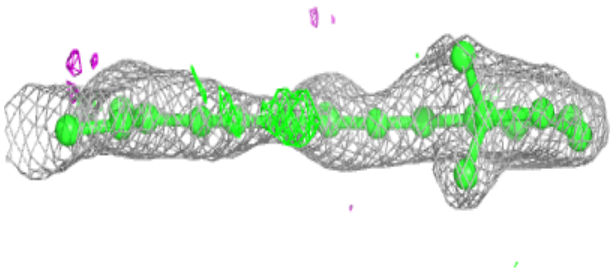
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

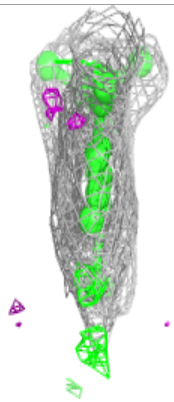


Electron density around RET D 292:

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

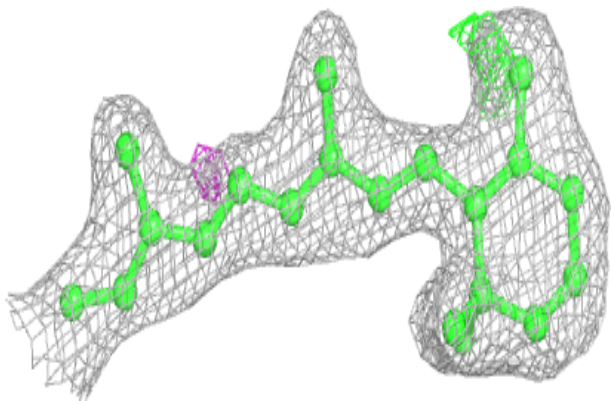


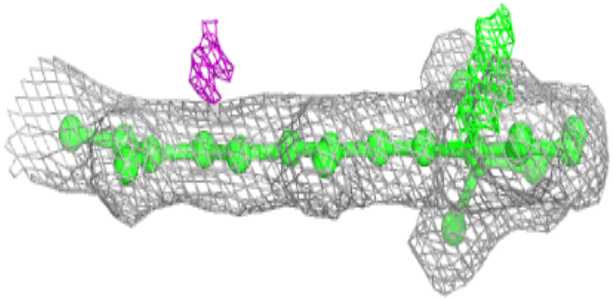


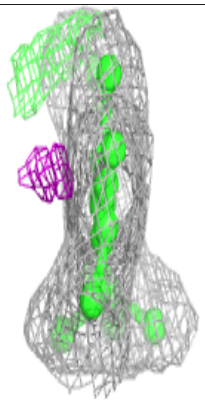


Electron density around RET A 292:

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

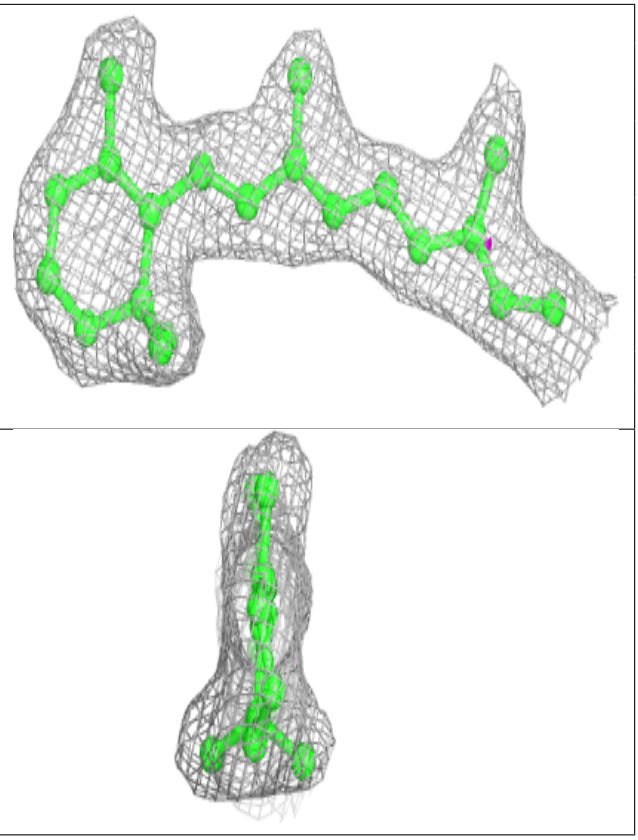






Electron density around RET B 292:

$2mF_o$-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.