



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:00 AM UTC

PDB ID : 3QBL / pdb_00003qbl
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 ⓘ 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

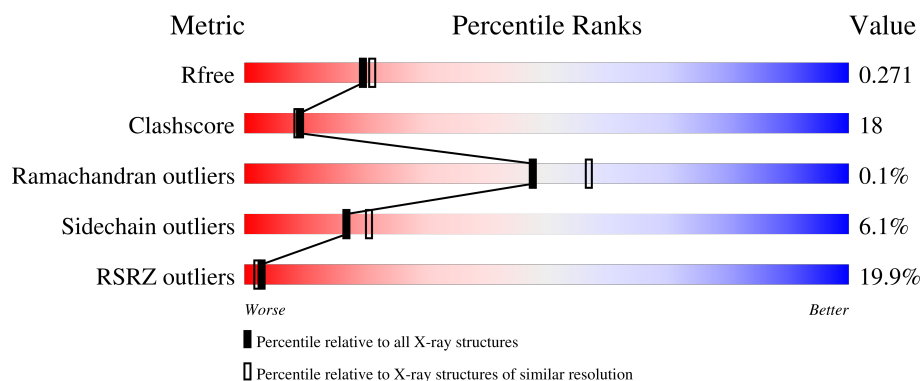
1 Overall quality at a glance

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	9% 60% 26% • 11%
1	B	291	6% 63% 21% 5% 11%
1	D	291	39% 47% 38% • 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	-

2 Entry composition [i](#)

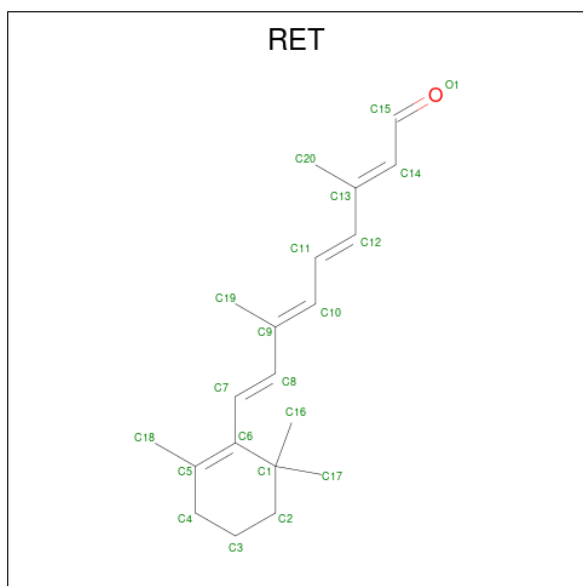
There are 5 unique types of molecules in this entry. The entry contains 6151 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

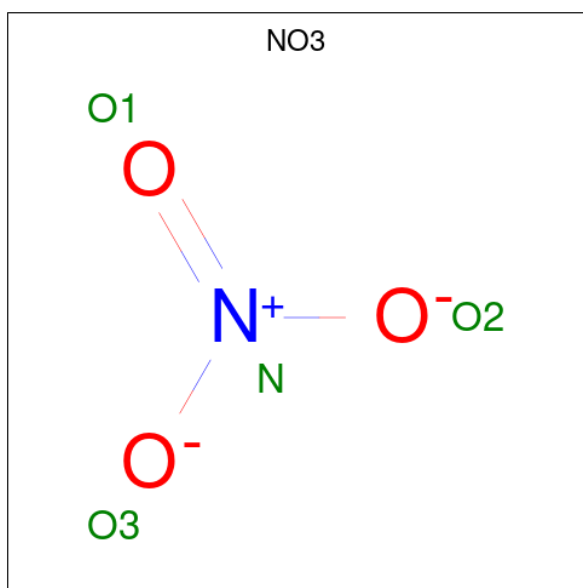
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1963	1302	299	351	11			
1	B	259	Total	C	N	O	S	0	0	0
			1957	1299	298	349	11			
1	D	259	Total	C	N	O	S	0	0	0
			1957	1299	298	349	11			

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



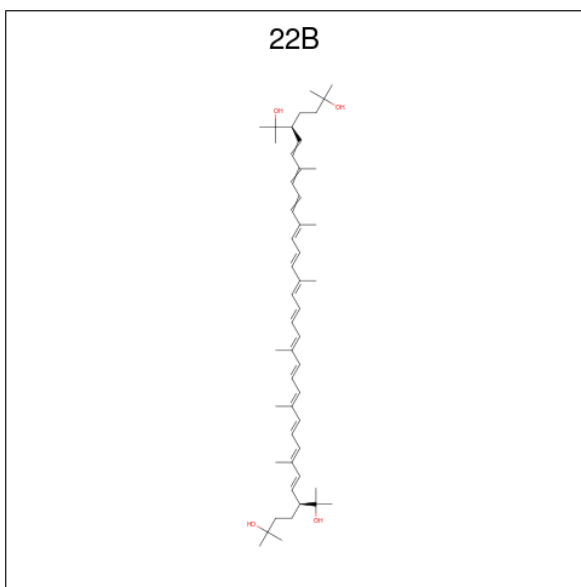
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		
2	B	1	Total	C	0	0
			20	20		
2	D	1	Total	C	0	0
			20	20		

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO_3).



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

- Molecule 4 is BACTERIORUBERIN (CCD ID: 22B) (formula: $\text{C}_{50}\text{H}_{76}\text{O}_4$).



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

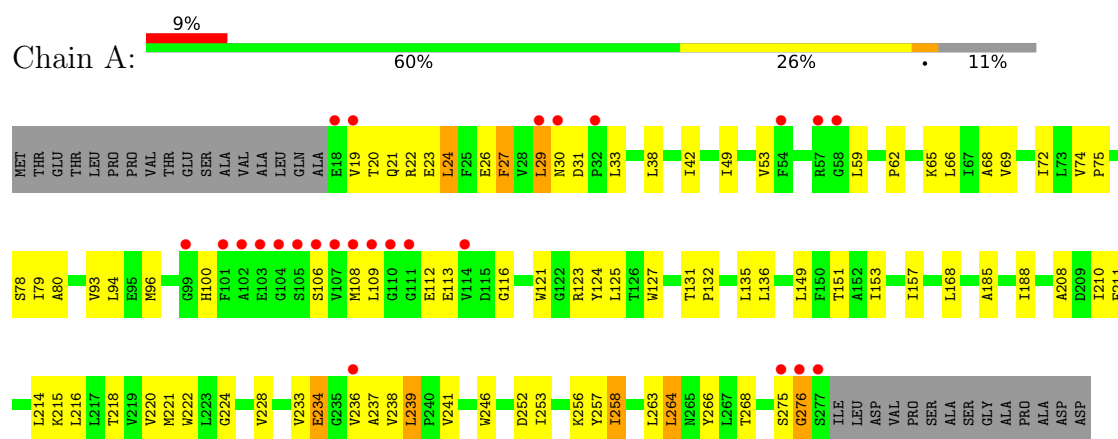
- Molecule 5 is water.

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

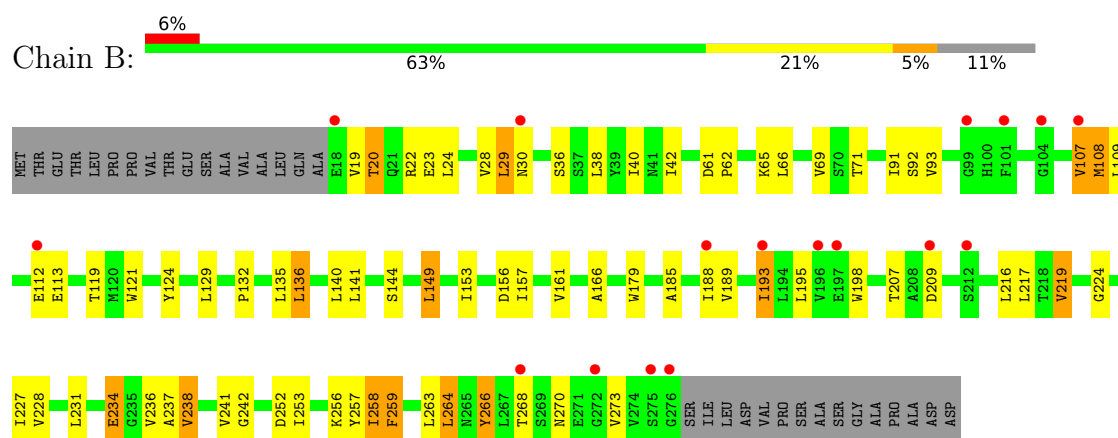
3 Residue-property plots [i](#)

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.

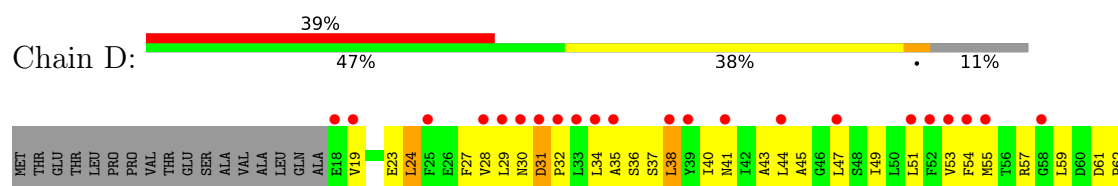
• Molecule 1: Halorhodopsin



• Molecule 1: Halorhodopsin



• Molecule 1: Halorhodopsin



ASP	V220	G143	R63	
VAL	M221	S144	A64	
PRO	W222	M145	K65	
SER	L223	A146	L66	
ALA	G224	T147	I67	
SER	Y225	K148	A68	
GLY	P226	L149	V69	
ALA	I227	F150	S70	
PRO	V228	T151	T71	
ALA	W229	A152	I72	
ASP	A230	I153	L73	
ASP	L231	T154	V74	
	G232	F155	P75	
	V233		I79	
	E234	L164		
	G235	A167	V93	
	V236	L168	L94	
	A237			
	V238		H100	
	L239	S171	F101	
	P240	S172	A102	
	V241	H173	E103	
	G242	L174	G104	
	Y243		S105	
	T244	W177	S106	
	S245		V107	
	W246	Y180	M108	
	A247	A181	L109	
	Y248		G110	
	S249	C184	G111	
	A250	A185	E112	
	L251	C186	E113	
	D252	F187	V114	
	I253	I188	D115	
	V254	V189	G116	
	A255	V190	V117	
	K256	L191	V118	
	Y257	Y192	T119	
	I258	I193	M120	
	F259	L194	W121	
	A260	L195	G122	
	F261	V196	R123	
	L262	E197	Y124	
	L263	W198		
	L264	A199	W127	
	N265	Q200	A128	
	Y266		L129	
	L267		S130	
	T268		T131	
	S269	D209	P132	
	N270	I210	M133	
	E271	F211	I134	
	G272	S212	L135	
	V273	T213	L136	
	V274	L214	A137	
	S275	W215	L138	
	G276	L216	G139	
	SER	L217		
	ILE	T218	A142	
	LEU	V219		

4 Data and refinement statistics

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 15.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (15.00-2.20) 95.8 (15.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.267 0.259 , 0.271	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)	0.41 , 92.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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: NO3, RET, 22B

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.48	0/2009	0.95	10/2751 (0.4%)
1	B	0.46	0/2003	0.95	10/2743 (0.4%)
1	D	0.37	0/2003	0.90	7/2743 (0.3%)
All	All	0.44	0/6015	0.94	27/8237 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	LEU	N-CA-C	-9.88	98.25	110.41
1	A	42	ILE	N-CA-C	-7.74	102.90	110.72
1	B	107	VAL	N-CA-C	6.96	117.53	111.90
1	B	153	ILE	N-CA-C	6.63	116.78	110.42
1	B	238	VAL	N-CA-C	-6.07	106.32	113.42
1	A	29	LEU	N-CA-C	-5.88	102.73	110.43
1	B	42	ILE	N-CA-C	-5.88	104.78	110.72
1	B	156	ASP	N-CA-C	-5.86	104.97	111.36
1	A	237	ALA	N-CA-C	5.75	119.35	111.54
1	B	257	TYR	N-CA-C	5.61	117.26	111.03
1	B	266	TYR	N-CA-C	-5.58	104.89	110.97
1	D	31	ASP	CA-C-N	5.53	126.75	119.84
1	D	31	ASP	C-N-CA	5.53	126.75	119.84
1	D	131	THR	CA-C-N	-5.49	113.24	119.28
1	D	131	THR	C-N-CA	-5.49	113.24	119.28
1	A	27	PHE	N-CA-C	-5.41	105.29	111.14
1	A	257	TYR	N-CA-C	5.32	116.94	111.03
1	A	241	VAL	N-CA-C	5.29	116.64	110.62
1	D	195	LEU	N-CA-C	5.27	116.71	111.07
1	A	78	SER	N-CA-C	5.27	117.02	111.28
1	A	31	ASP	CA-C-N	5.23	126.37	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ASP	C-N-CA	5.23	126.37	119.84
1	D	219	VAL	N-CA-C	5.12	115.74	110.36
1	B	219	VAL	N-CA-C	5.10	115.82	110.62
1	A	208	ALA	N-CA-C	5.05	117.17	111.11
1	B	227	ILE	N-CA-C	-5.04	105.93	110.82
1	D	79	ILE	CB-CA-C	-5.02	105.36	112.14

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	1963	0	2014	56	0
1	B	1957	0	2009	56	0
1	D	1957	0	2009	107	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
4	D	27	0	37	2	0
5	A	49	0	0	5	1
5	B	59	0	0	4	0
5	D	28	0	0	3	0
All	All	6151	0	6187	222	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 18.

All (222) 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:108:MET:HE3	1:D:113:GLU:HB2	1.67	0.75
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:A:220:VAL:HG12	1:A:221:MET:HE2	1.67	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:145:ASN:C	1:D:145:ASN:HD22	2.00	0.70
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: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: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
1:A:20:THR:HG22	1:A:21:GLN:N	2.14	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:29:LEU:C	1:D:31:ASP:H	2.10	0.58
1:D:190:VAL:O	1:D:193:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LEU:HD21	1:D:120:MET:HE1	1.85	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: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:B:217:LEU:HD23	1:B:217:LEU:C	2.32	0.53
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:B:259:PHE:CD1	1:B:259:PHE:C	2.87	0.52
1:D:232:GLY:HA3	1:D:244:THR:HG21	1.91	0.52
1:D:145:ASN:C	1:D:145:ASN:ND2	2.67	0.52
1:A:275:SER:O	1:A:276:GLY:C	2.53	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:D:109:LEU:HD22	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: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:D:36:SER:O	1:D:40:ILE:HG12	2.15	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:O	1:D:66:LEU:HD23	2.14	0.47
1:D:68:ALA:O	1:D:72:ILE:HG13	2.13	0.47
1:A:19:VAL:HG23	1:A:19:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:108:MET:HE3	1:A:112:GLU:O	2.18	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:29:LEU:C	1:D:31:ASP:N	2.73	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:30:ASN:C	1:D:32:PRO:HD3	2.43	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
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:193:ILE:HD12	1:D:193:ILE:C	2.43	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:A:266:TYR:CD2	1:A:266:TYR:C	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:129:LEU:C	1:B:132:PRO:HD2	2.43	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
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:D:131:THR:HG1	1:D:132:PRO:HD3	1.83	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:B:193:ILE:HD12	1:B:193:ILE:C	2.45	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:B:28:VAL:C	1:B:29:LEU:O	2.58	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:B:65:LYS:NZ	5:B:531:HOH:O	2.53	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:133:MET:HE2	1:D:133:MET:HA	2.02	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:O	1:D:30:ASN:HB2	2.20	0.41
1:A:124:TYR:HD1	1:A:127:TRP:CZ3	2.39	0.41
1:D:63:ARG:O	1:D:67:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:236:VAL:O	1:B:237:ALA:C	2.64	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:108:MET:HE3	1:B:112:GLU:C	2.46	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:220:VAL:CG1	1:A:221:MET:HE2	2.45	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 ⓘ

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	258/291 (89%)	249 (96%)	8 (3%)	1 (0%)	30	34
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%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	GLY

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%)	195 (94%)	13 (6%)	16	19
1	B	207/233 (89%)	192 (93%)	15 (7%)	13	15
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	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	234	GLU
1	A	239	LEU
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

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Mol	Chain	Res	Type
1	B	149	LEU
1	B	193	ILE
1	B	209	ASP
1	B	216	LEU
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 ⓘ

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

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	360	-	1,3,3	3.15	1 (100%)	0,3,3	-	-
4	22B	B	300	-	26,26,53	3.33	12 (46%)	31,35,72	2.03	8 (25%)
3	NO3	D	360	-	1,3,3	3.29	1 (100%)	0,3,3	-	-
4	22B	D	300	-	26,26,53	3.37	12 (46%)	31,35,72	2.03	9 (29%)
3	NO3	A	359	-	1,3,3	2.91	1 (100%)	0,3,3	-	-
2	RET	A	292	1	20,20,21	2.24	6 (30%)	27,27,28	1.72	7 (25%)
3	NO3	B	359	-	1,3,3	2.93	1 (100%)	0,3,3	-	-
3	NO3	D	359	-	1,3,3	3.28	1 (100%)	0,3,3	-	-
3	NO3	A	293	-	1,3,3	3.34	1 (100%)	0,3,3	-	-
2	RET	D	292	1	20,20,21	2.34	5 (25%)	27,27,28	1.81	8 (29%)
2	RET	B	292	1	20,20,21	2.22	5 (25%)	27,27,28	1.80	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
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	D	292	1	-	0/13/30/31	0/1/1/1
2	RET	B	292	1	-	0/13/30/31	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	300	22B	C2-C3	9.70	1.64	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	300	22B	C2-C3	9.51	1.64	1.49
4	D	300	22B	C1-C2	6.77	1.62	1.55
4	B	300	22B	C1-C2	6.35	1.62	1.55
2	D	292	RET	C1-C6	6.28	1.61	1.53
4	D	300	22B	C21-C2	6.03	1.61	1.53
2	B	292	RET	C1-C6	6.03	1.61	1.53
2	A	292	RET	C1-C6	5.94	1.61	1.53
4	B	300	22B	C21-C2	5.86	1.61	1.53
2	D	292	RET	C5-C6	4.65	1.42	1.34
2	A	292	RET	C5-C6	4.63	1.42	1.34
2	D	292	RET	C14-C13	4.49	1.36	1.33
4	D	300	22B	C16-C1	4.26	1.59	1.52
2	B	292	RET	C14-C13	4.26	1.36	1.33
4	D	300	22B	C19-C9	4.15	1.59	1.50
4	B	300	22B	C16-C1	4.09	1.59	1.52
4	B	300	22B	C19-C9	3.97	1.58	1.50
4	B	300	22B	O27-C23	3.94	1.54	1.44
4	D	300	22B	O27-C23	3.94	1.54	1.44
2	B	292	RET	C5-C6	3.80	1.40	1.34
4	D	300	22B	C22-C21	3.52	1.62	1.53
4	B	300	22B	C22-C21	3.49	1.62	1.53
4	D	300	22B	C17-C1	3.39	1.58	1.52
3	A	293	NO3	O1-N	3.34	1.40	1.24
4	D	300	22B	C20-C13	3.32	1.57	1.50
4	B	300	22B	C17-C1	3.30	1.58	1.52
3	D	360	NO3	O1-N	3.29	1.40	1.24
3	D	359	NO3	O1-N	3.28	1.40	1.24
2	A	292	RET	C14-C13	3.19	1.35	1.33
3	A	360	NO3	O1-N	3.15	1.39	1.24
2	A	292	RET	C7-C6	3.14	1.55	1.45
2	B	292	RET	C7-C6	3.11	1.55	1.45
4	B	300	22B	C20-C13	3.09	1.57	1.50
2	D	292	RET	C7-C6	3.06	1.55	1.45
3	B	359	NO3	O1-N	2.93	1.38	1.24
2	A	292	RET	C2-C3	-2.93	1.45	1.52
3	A	359	NO3	O1-N	2.91	1.38	1.24
4	B	300	22B	C18-C5	2.71	1.56	1.50
2	B	292	RET	C2-C3	-2.71	1.46	1.52
4	D	300	22B	C18-C5	2.69	1.56	1.50
2	D	292	RET	C2-C3	-2.65	1.46	1.52
4	D	300	22B	C4-C3	2.54	1.38	1.32
4	B	300	22B	C4-C3	2.52	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	300	22B	C22-C23	2.13	1.60	1.53
4	B	300	22B	C8-C9	2.13	1.50	1.46
2	A	292	RET	C18-C5	2.01	1.54	1.50

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	300	22B	C20-C13-C12	4.64	125.17	118.09
4	B	300	22B	C21-C22-C23	4.50	124.63	116.24
4	B	300	22B	C20-C13-C12	4.19	124.48	118.09
4	D	300	22B	C21-C22-C23	4.11	123.90	116.24
4	B	300	22B	C16-C1-C2	3.99	117.06	111.71
4	D	300	22B	C16-C1-C2	3.72	116.70	111.71
4	B	300	22B	C17-C1-C16	-3.64	105.20	110.52
2	B	292	RET	C1-C6-C7	3.59	125.39	115.65
4	D	300	22B	C17-C1-C16	-3.58	105.29	110.52
4	D	300	22B	C4-C5-C6	-3.57	113.40	119.01
2	D	292	RET	C1-C6-C7	3.52	125.19	115.65
4	B	300	22B	C4-C5-C6	-3.48	113.53	119.01
2	B	292	RET	C1-C6-C5	-3.33	118.08	122.64
2	D	292	RET	C1-C6-C5	-3.20	118.27	122.64
2	A	292	RET	C20-C13-C12	3.13	122.86	118.09
2	B	292	RET	C19-C9-C8	3.12	122.86	118.09
4	D	300	22B	C12-C13-C14	-3.02	110.52	118.55
2	A	292	RET	C1-C6-C5	-3.02	118.51	122.64
4	D	300	22B	C18-C5-C4	3.00	122.68	118.09
2	B	292	RET	C2-C1-C6	2.99	114.78	110.44
4	B	300	22B	C18-C5-C4	2.99	122.65	118.09
2	A	292	RET	C7-C8-C9	2.98	130.64	126.23
2	A	292	RET	C1-C6-C7	2.89	123.48	115.65
2	A	292	RET	C2-C1-C6	2.77	114.46	110.44
2	D	292	RET	C20-C13-C12	2.76	122.30	118.09
4	B	300	22B	C12-C13-C14	-2.75	111.23	118.55
2	B	292	RET	C8-C9-C10	-2.72	114.72	119.01
2	D	292	RET	C2-C1-C6	2.68	114.33	110.44
2	D	292	RET	C19-C9-C8	2.54	121.96	118.09
4	B	300	22B	C24-C23-C22	2.33	118.41	111.51
2	B	292	RET	C17-C1-C6	2.32	113.89	110.24
2	A	292	RET	C17-C1-C6	2.31	113.86	110.24
4	D	300	22B	C24-C23-C22	2.29	118.31	111.51
2	B	292	RET	C20-C13-C12	2.26	121.53	118.09
2	B	292	RET	C7-C6-C5	-2.18	116.53	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	292	RET	C7-C6-C5	-2.18	116.54	121.56
2	D	292	RET	C2-C3-C4	2.12	115.93	111.28
2	D	292	RET	C17-C1-C6	2.09	113.53	110.24
2	A	292	RET	C19-C9-C8	2.08	121.27	118.09
4	D	300	22B	C8-C9-C10	-2.02	115.83	119.01

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	B	300	22B	C21-C2-C3-C4
4	D	300	22B	C21-C2-C3-C4
4	D	300	22B	C2-C21-C22-C23

There are no ring outliers.

10 monomers are involved in 12 short contacts:

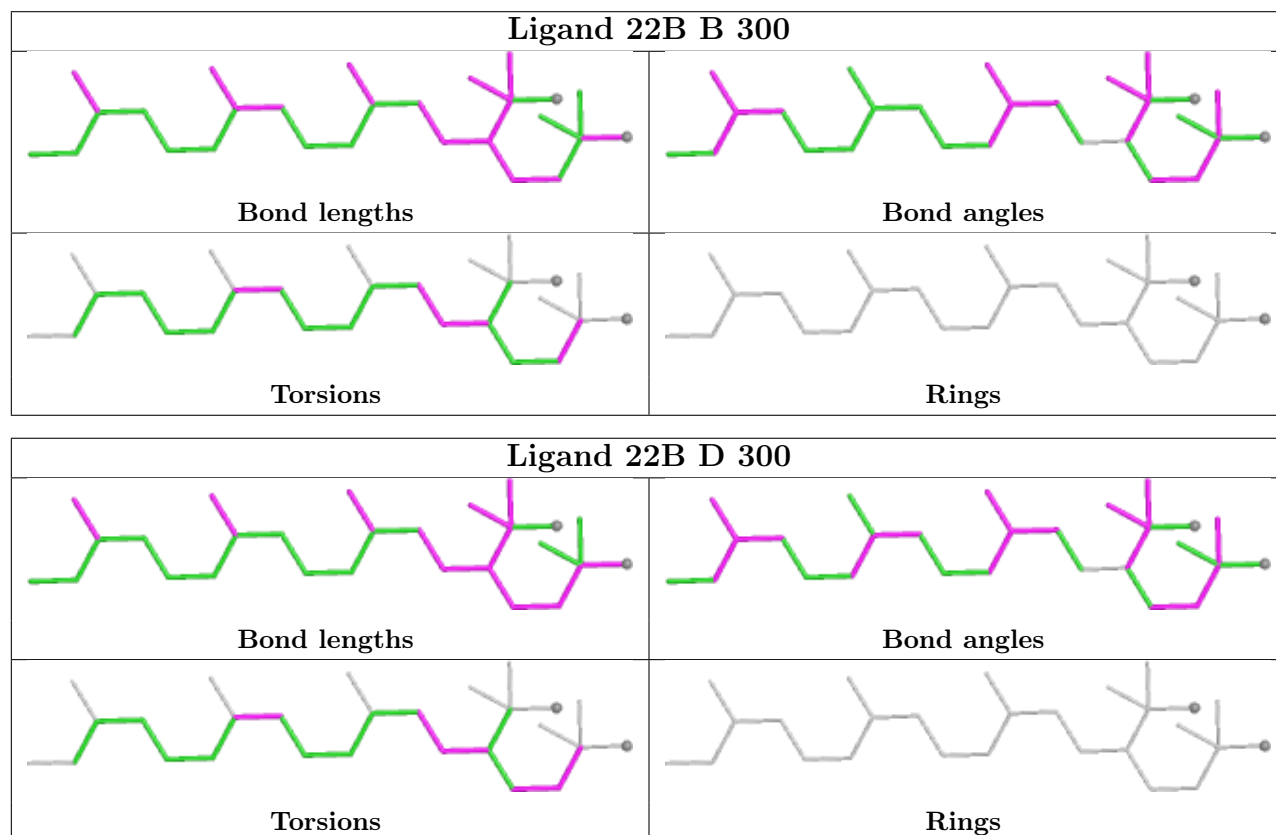
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	360	NO3	1	0
4	B	300	22B	1	0
3	D	360	NO3	1	0
4	D	300	22B	2	0
3	A	359	NO3	1	0
2	A	292	RET	1	0
3	B	359	NO3	1	0
3	A	293	NO3	2	0
2	D	292	RET	1	0

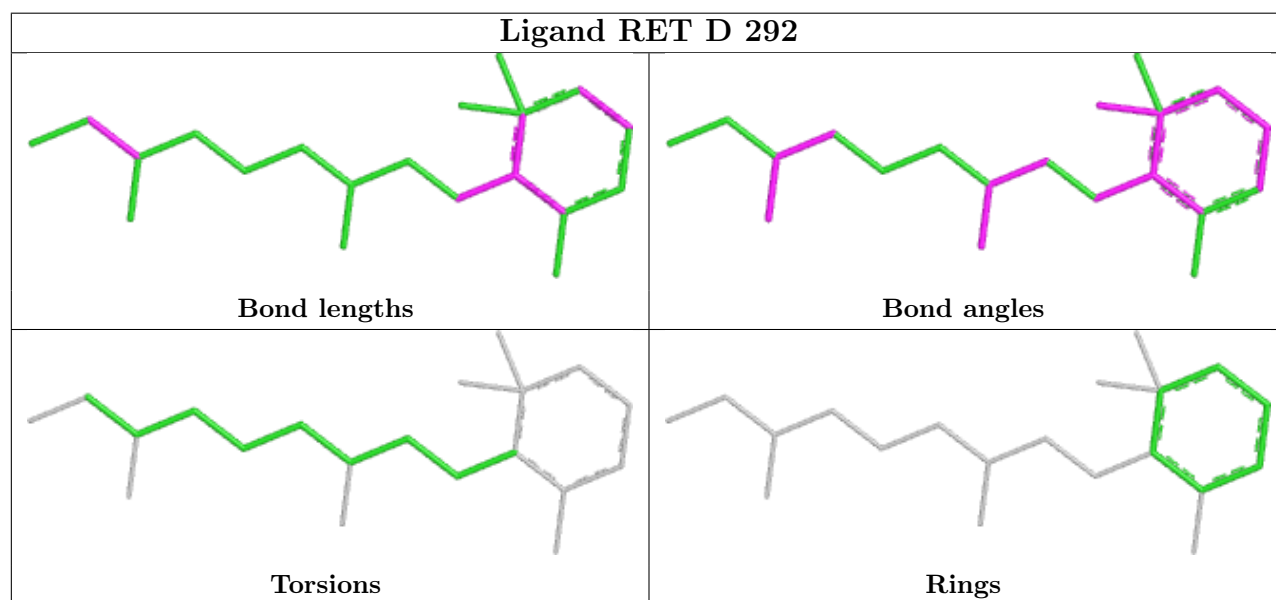
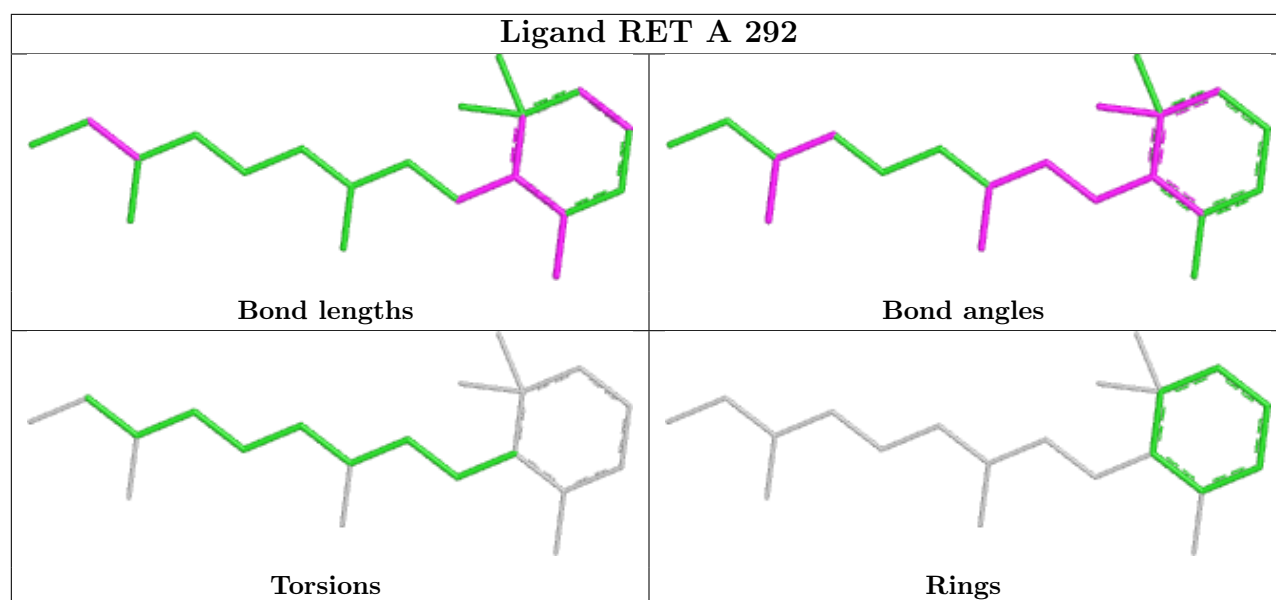
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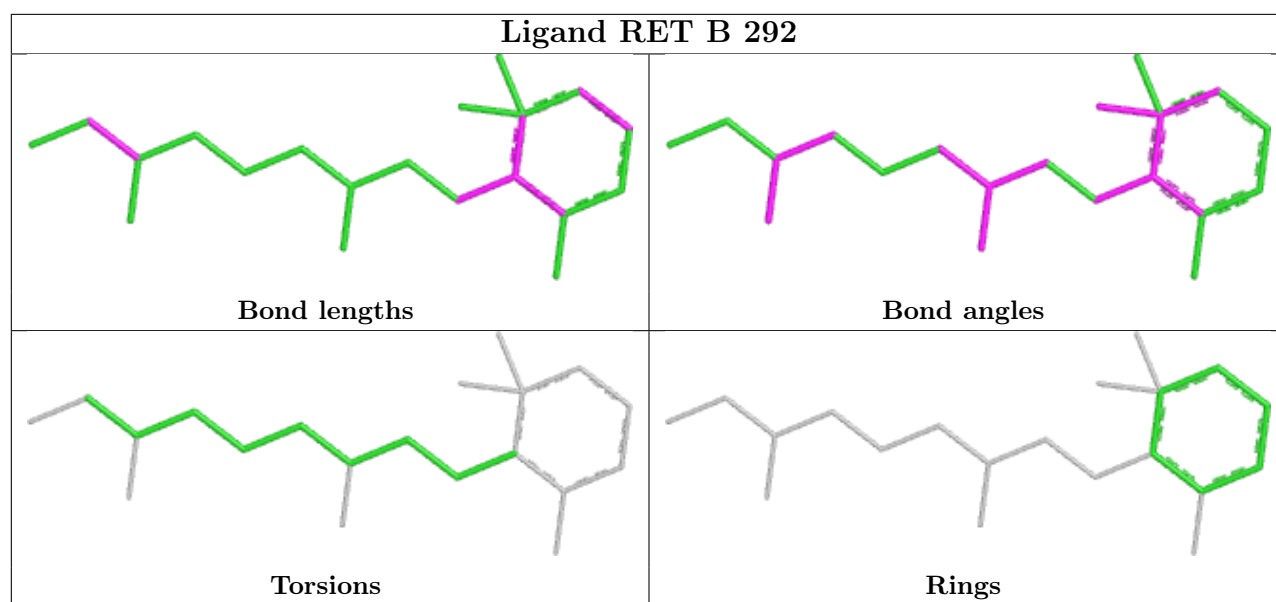
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	292	RET	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	260/291 (89%)	0.63	25 (9%) 13 11	24, 37, 67, 82	0
1	B	259/291 (89%)	0.57	17 (6%) 24 21	24, 39, 53, 69	0
1	D	259/291 (89%)	2.01	113 (43%) 0 0	36, 56, 77, 98	0
All	All	778/873 (89%)	1.07	155 (19%) 3 2	24, 43, 72, 98	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	112	GLU	8.6
1	A	111	GLY	7.1
1	D	109	LEU	6.0
1	B	276	GLY	6.0
1	A	110	GLY	5.7
1	D	114	VAL	5.6
1	D	249	SER	5.5
1	A	107	VAL	5.4
1	D	193	ILE	5.4
1	D	231	LEU	5.2
1	D	227	ILE	5.1
1	D	260	ALA	4.8
1	D	275	SER	4.8
1	D	111	GLY	4.8
1	A	276	GLY	4.7
1	A	30	ASN	4.6
1	D	245	SER	4.5
1	D	110	GLY	4.5
1	A	104	GLY	4.4
1	A	277	SER	4.3
1	A	109	LEU	4.2
1	D	30	ASN	4.2
1	D	240	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	242	GLY	3.9
1	D	210	ILE	3.8
1	B	104	GLY	3.8
1	D	34	LEU	3.8
1	D	113	GLU	3.8
1	D	267	LEU	3.6
1	D	199	ALA	3.6
1	A	106	SER	3.5
1	D	266	TYR	3.5
1	D	54	PHE	3.5
1	D	216	LEU	3.5
1	D	105	SER	3.5
1	D	211	PHE	3.5
1	D	235	GLY	3.5
1	D	239	LEU	3.5
1	D	255	ALA	3.4
1	B	268	THR	3.4
1	A	105	SER	3.4
1	D	243	TYR	3.3
1	D	212	SER	3.3
1	D	51	LEU	3.3
1	D	247	ALA	3.3
1	B	193	ILE	3.3
1	A	108	MET	3.2
1	D	224	GLY	3.2
1	D	29	LEU	3.2
1	D	230	ALA	3.2
1	D	116	GLY	3.2
1	A	29	LEU	3.2
1	A	275	SER	3.2
1	B	99	GLY	3.2
1	D	107	VAL	3.2
1	D	258	ILE	3.2
1	A	54	PHE	3.1
1	D	117	VAL	3.1
1	A	57	ARG	3.1
1	D	58	GLY	3.1
1	A	102	ALA	3.1
1	D	250	ALA	3.1
1	D	276	GLY	3.0
1	D	28	VAL	3.0
1	D	268	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	270	ASN	3.0
1	B	196	VAL	3.0
1	D	232	GLY	3.0
1	B	112	GLU	3.0
1	A	236	VAL	3.0
1	D	269	SER	3.0
1	D	220	VAL	2.9
1	D	100	HIS	2.9
1	D	229	TRP	2.9
1	B	212	SER	2.9
1	D	181	ALA	2.9
1	D	214	LEU	2.9
1	D	217	LEU	2.9
1	A	19	VAL	2.9
1	B	209	ASP	2.9
1	D	248	TYR	2.8
1	D	173	HIS	2.8
1	D	118	VAL	2.8
1	D	238	VAL	2.8
1	D	188	ILE	2.8
1	B	30	ASN	2.8
1	D	205	ALA	2.8
1	D	236	VAL	2.7
1	D	119	THR	2.7
1	D	272	GLY	2.7
1	D	55	MET	2.7
1	A	18	GLU	2.7
1	D	108	MET	2.7
1	A	114	VAL	2.7
1	D	274	VAL	2.6
1	D	195	LEU	2.6
1	D	131	THR	2.6
1	B	188	ILE	2.6
1	D	196	VAL	2.6
1	D	106	SER	2.6
1	B	18	GLU	2.6
1	D	233	VAL	2.6
1	D	252	ASP	2.5
1	D	187	PHE	2.5
1	A	99	GLY	2.5
1	D	222	TRP	2.5
1	D	19	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	237	ALA	2.5
1	B	107	VAL	2.4
1	D	53	VAL	2.4
1	D	273	VAL	2.4
1	D	33	LEU	2.4
1	D	47	LEU	2.4
1	D	142	ALA	2.4
1	B	272	GLY	2.4
1	D	32	PRO	2.4
1	D	191	LEU	2.4
1	D	31	ASP	2.4
1	D	35	ALA	2.4
1	D	261	PHE	2.4
1	D	192	TYR	2.3
1	D	120	MET	2.3
1	B	197	GLU	2.3
1	A	103	GLU	2.3
1	D	171	SER	2.3
1	D	52	PHE	2.3
1	D	259	PHE	2.3
1	D	262	LEU	2.3
1	D	102	ALA	2.3
1	D	69	VAL	2.3
1	D	39	TYR	2.2
1	D	228	VAL	2.2
1	B	275	SER	2.2
1	D	44	LEU	2.2
1	D	25	PHE	2.2
1	D	101	PHE	2.2
1	A	32	PRO	2.2
1	D	226	PRO	2.2
1	D	174	LEU	2.1
1	B	101	PHE	2.1
1	D	41	ASN	2.1
1	A	101	PHE	2.1
1	D	177	TRP	2.1
1	D	18	GLU	2.1
1	D	265	ASN	2.1
1	D	93	VAL	2.1
1	D	254	VAL	2.1
1	D	139	GLY	2.1
1	D	221	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	38	LEU	2.0
1	D	241	VAL	2.0
1	A	58	GLY	2.0
1	D	197	GLU	2.0
1	D	209	ASP	2.0
1	D	263	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

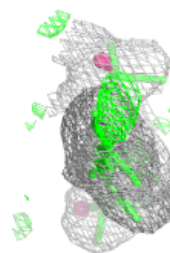
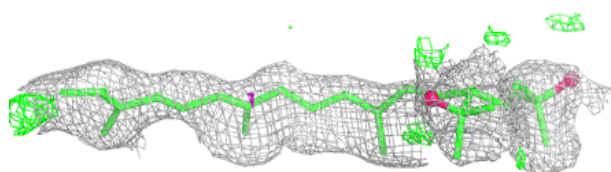
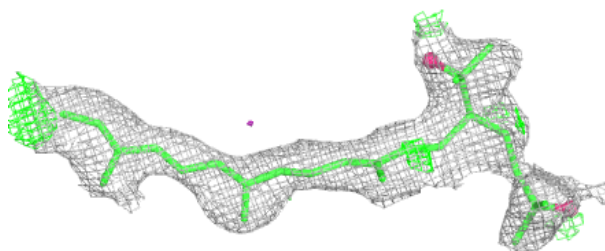
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	22B	B	300	27/54	0.67	0.21	60,64,70,71	0
4	22B	D	300	27/54	0.67	0.22	84,86,92,92	0
3	NO3	A	293	4/4	0.71	0.24	76,77,77,78	0
2	RET	D	292	20/21	0.83	0.15	44,48,50,51	0
3	NO3	A	360	4/4	0.87	0.20	69,70,70,72	0
3	NO3	D	360	4/4	0.89	0.20	56,56,56,58	0
3	NO3	D	359	4/4	0.93	0.11	44,45,47,49	0
2	RET	A	292	20/21	0.94	0.08	25,28,32,32	0
3	NO3	A	359	4/4	0.94	0.12	34,39,40,44	0
2	RET	B	292	20/21	0.95	0.07	29,31,32,33	0
3	NO3	B	359	4/4	0.97	0.07	33,36,37,38	0

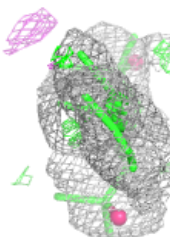
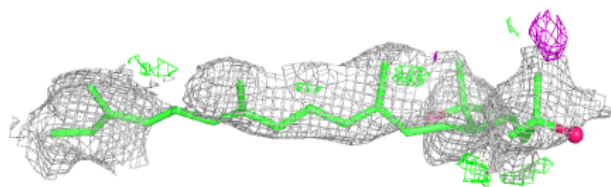
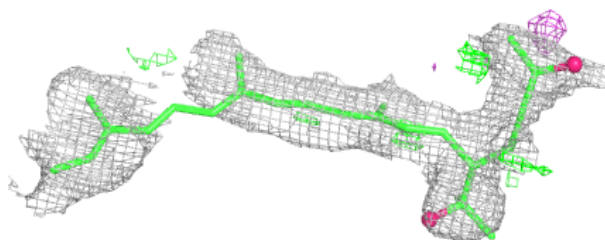
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 22B 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)

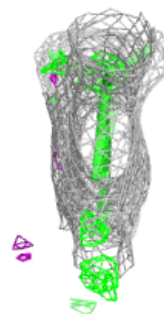
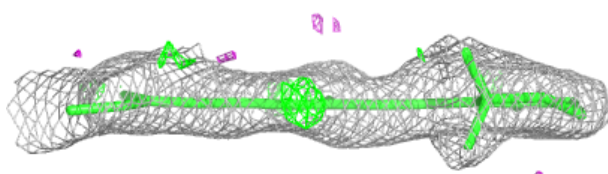
**Electron density around 22B D 300:**

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

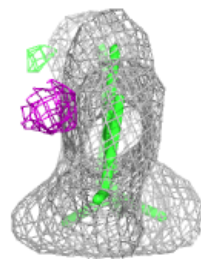
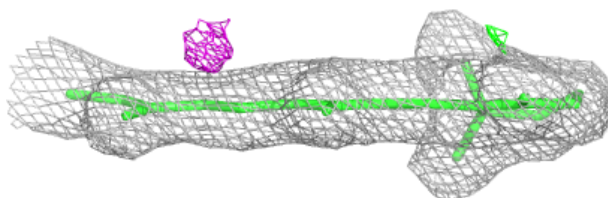
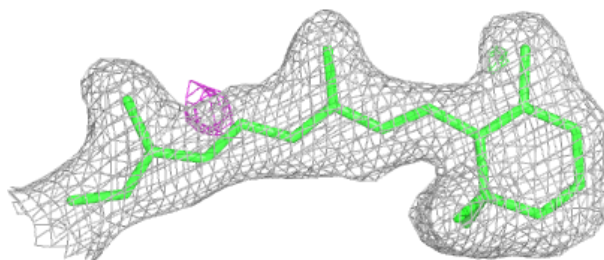


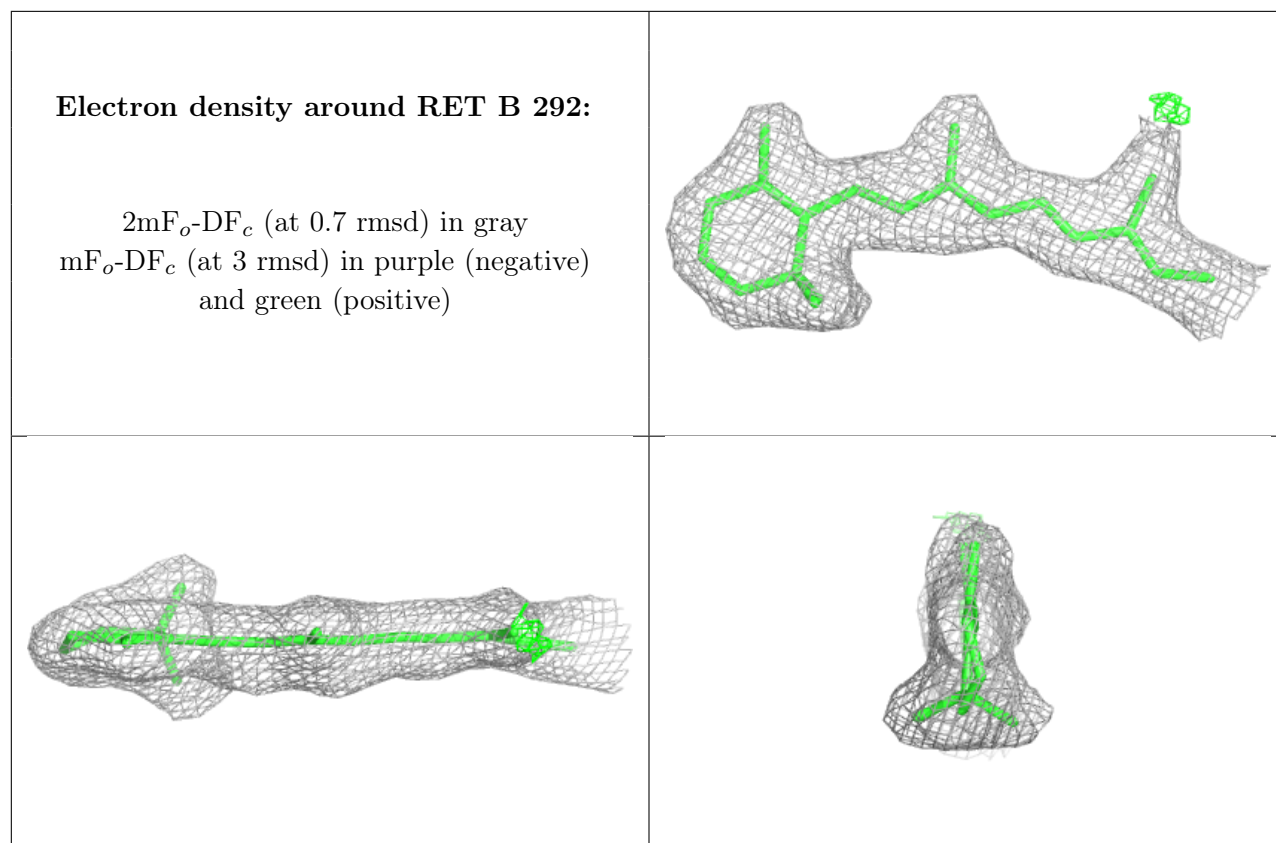
Electron density around RET D 292:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.