



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:23 PM UTC

PDB ID : 5OSC / pdb_00005osc
Title : GLIC-GABAAR alpha1 chimera crystallized in complex with pregnenolone sulfate at pH 4.5
Authors : Lavery, D.C.; Gold, M.G.; Smart, T.G.
Deposited on : 2017-08-17
Resolution : 3.10 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

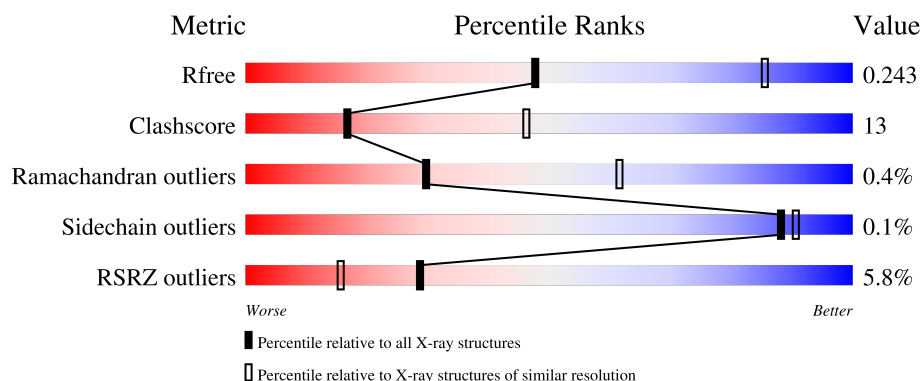
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	336	
1	B	336	
1	C	336	
1	D	336	
1	E	336	

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
2	ACT	A	501	-	-	X	-
2	ACT	B	501	-	-	X	-
2	ACT	D	501	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13188 atoms, of which 405 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 Proton-gated ion channel, Gamma-aminobutyric acid receptor subunit alpha-2, Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2488	1627	400	455	6			
1	B	312	Total	C	N	O	S	0	0	0
			2490	1627	402	455	6			
1	C	312	Total	C	N	O	S	0	0	0
			2490	1627	402	455	6			
1	D	312	Total	C	N	O	S	0	0	0
			2484	1624	399	455	6			
1	E	312	Total	C	N	O	S	0	0	0
			2484	1624	399	455	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	VAL	GLY	conflict	UNP P26048
A	312	SER	-	linker	UNP P26048
A	313	GLN	-	linker	UNP P26048
A	314	PRO	-	linker	UNP P26048
A	315	ALA	-	linker	UNP P26048
A	316	ARG	-	linker	UNP P26048
A	317	ALA	-	linker	UNP P26048
A	318	ALA	-	linker	UNP P26048
A	429	HIS	-	expression tag	UNP P62812
A	430	HIS	-	expression tag	UNP P62812
A	431	HIS	-	expression tag	UNP P62812
A	432	HIS	-	expression tag	UNP P62812
A	433	HIS	-	expression tag	UNP P62812
A	434	HIS	-	expression tag	UNP P62812
A	435	HIS	-	expression tag	UNP P62812
A	436	HIS	-	expression tag	UNP P62812
B	258	VAL	GLY	conflict	UNP P26048
B	312	SER	-	linker	UNP P26048

Continued on next page...

Continued from previous page...

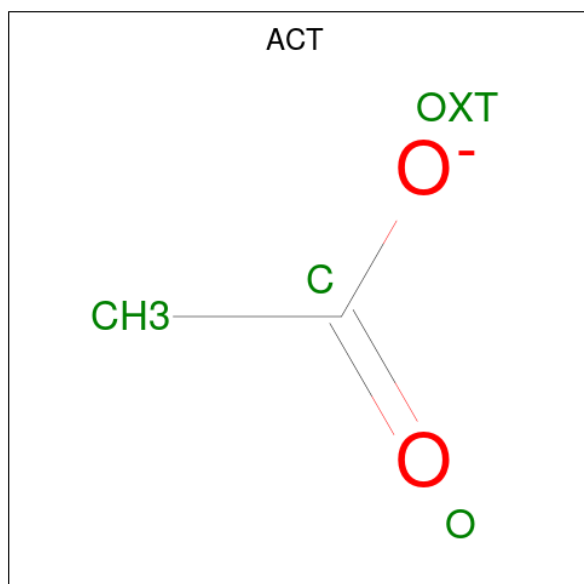
Chain	Residue	Modelled	Actual	Comment	Reference
B	313	GLN	-	linker	UNP P26048
B	314	PRO	-	linker	UNP P26048
B	315	ALA	-	linker	UNP P26048
B	316	ARG	-	linker	UNP P26048
B	317	ALA	-	linker	UNP P26048
B	318	ALA	-	linker	UNP P26048
B	429	HIS	-	expression tag	UNP P62812
B	430	HIS	-	expression tag	UNP P62812
B	431	HIS	-	expression tag	UNP P62812
B	432	HIS	-	expression tag	UNP P62812
B	433	HIS	-	expression tag	UNP P62812
B	434	HIS	-	expression tag	UNP P62812
B	435	HIS	-	expression tag	UNP P62812
B	436	HIS	-	expression tag	UNP P62812
C	258	VAL	GLY	conflict	UNP P26048
C	312	SER	-	linker	UNP P26048
C	313	GLN	-	linker	UNP P26048
C	314	PRO	-	linker	UNP P26048
C	315	ALA	-	linker	UNP P26048
C	316	ARG	-	linker	UNP P26048
C	317	ALA	-	linker	UNP P26048
C	318	ALA	-	linker	UNP P26048
C	429	HIS	-	expression tag	UNP P62812
C	430	HIS	-	expression tag	UNP P62812
C	431	HIS	-	expression tag	UNP P62812
C	432	HIS	-	expression tag	UNP P62812
C	433	HIS	-	expression tag	UNP P62812
C	434	HIS	-	expression tag	UNP P62812
C	435	HIS	-	expression tag	UNP P62812
C	436	HIS	-	expression tag	UNP P62812
D	258	VAL	GLY	conflict	UNP P26048
D	312	SER	-	linker	UNP P26048
D	313	GLN	-	linker	UNP P26048
D	314	PRO	-	linker	UNP P26048
D	315	ALA	-	linker	UNP P26048
D	316	ARG	-	linker	UNP P26048
D	317	ALA	-	linker	UNP P26048
D	318	ALA	-	linker	UNP P26048
D	429	HIS	-	expression tag	UNP P62812
D	430	HIS	-	expression tag	UNP P62812
D	431	HIS	-	expression tag	UNP P62812
D	432	HIS	-	expression tag	UNP P62812

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	433	HIS	-	expression tag	UNP P62812
D	434	HIS	-	expression tag	UNP P62812
D	435	HIS	-	expression tag	UNP P62812
D	436	HIS	-	expression tag	UNP P62812
E	258	VAL	GLY	conflict	UNP P26048
E	312	SER	-	linker	UNP P26048
E	313	GLN	-	linker	UNP P26048
E	314	PRO	-	linker	UNP P26048
E	315	ALA	-	linker	UNP P26048
E	316	ARG	-	linker	UNP P26048
E	317	ALA	-	linker	UNP P26048
E	318	ALA	-	linker	UNP P26048
E	429	HIS	-	expression tag	UNP P62812
E	430	HIS	-	expression tag	UNP P62812
E	431	HIS	-	expression tag	UNP P62812
E	432	HIS	-	expression tag	UNP P62812
E	433	HIS	-	expression tag	UNP P62812
E	434	HIS	-	expression tag	UNP P62812
E	435	HIS	-	expression tag	UNP P62812
E	436	HIS	-	expression tag	UNP P62812

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

Continued on next page...

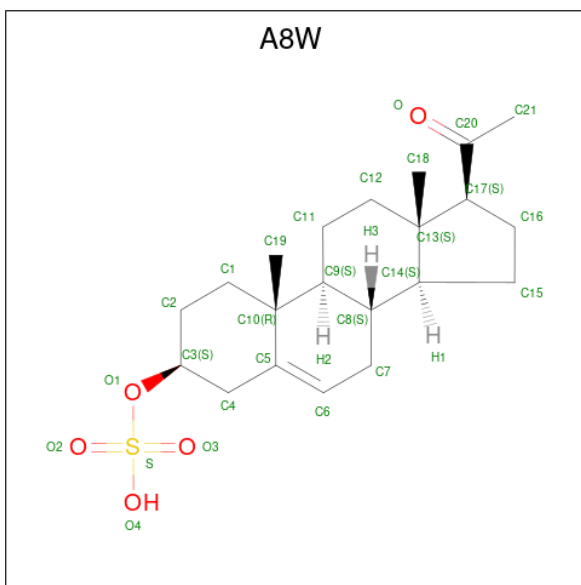
Continued from previous page...

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

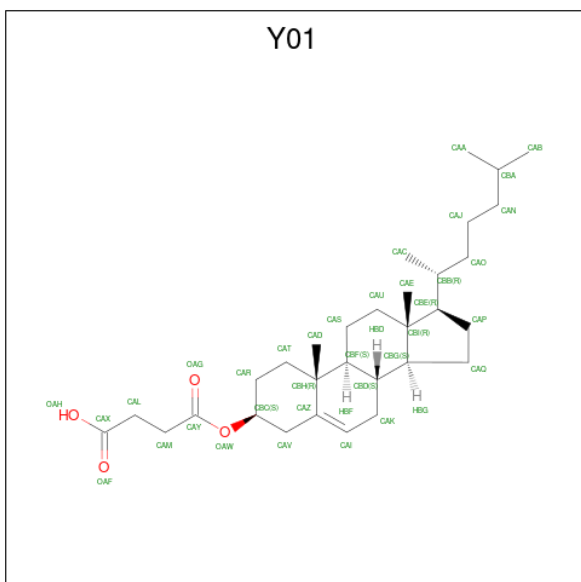
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

- Molecule 4 is Pregnenolone sulfate (CCD ID: A8W) (formula: C₂₁H₃₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 59	C 21	H 32	O 5	S 1	0	0
4	B	1	Total 59	C 21	H 32	O 5	S 1	0	0
4	C	1	Total 59	C 21	H 32	O 5	S 1	0	0
4	D	1	Total 59	C 21	H 32	O 5	S 1	0	0
4	E	1	Total 59	C 21	H 32	O 5	S 1	0	0

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).

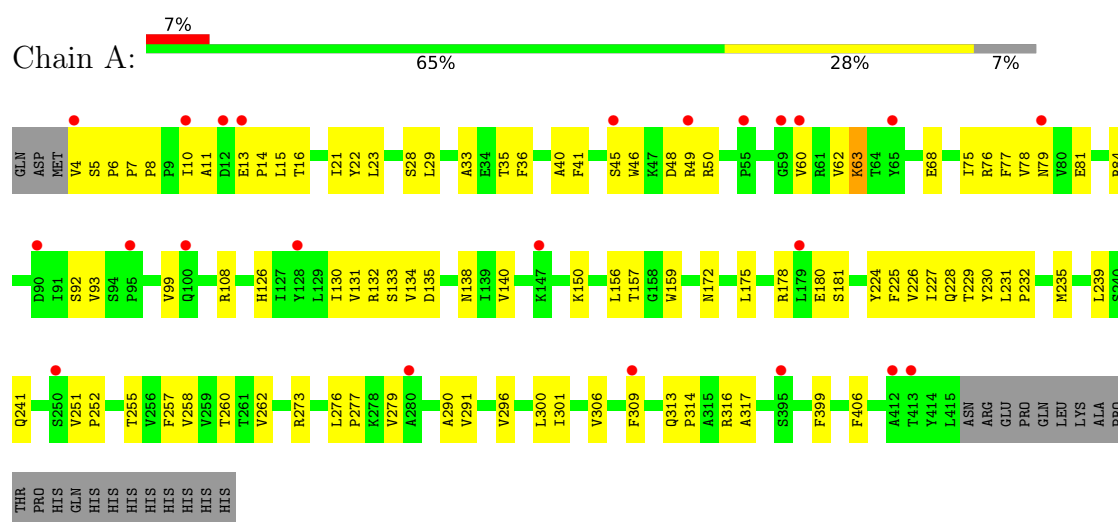


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			84	31	49	4		
5	B	1	Total	C	H	O	0	0
			84	31	49	4		
5	B	1	Total	C	H	O	0	0
			84	31	49	4		
5	D	1	Total	C	H	O	0	0
			84	31	49	4		
5	E	1	Total	C	H	O	0	0
			84	31	49	4		

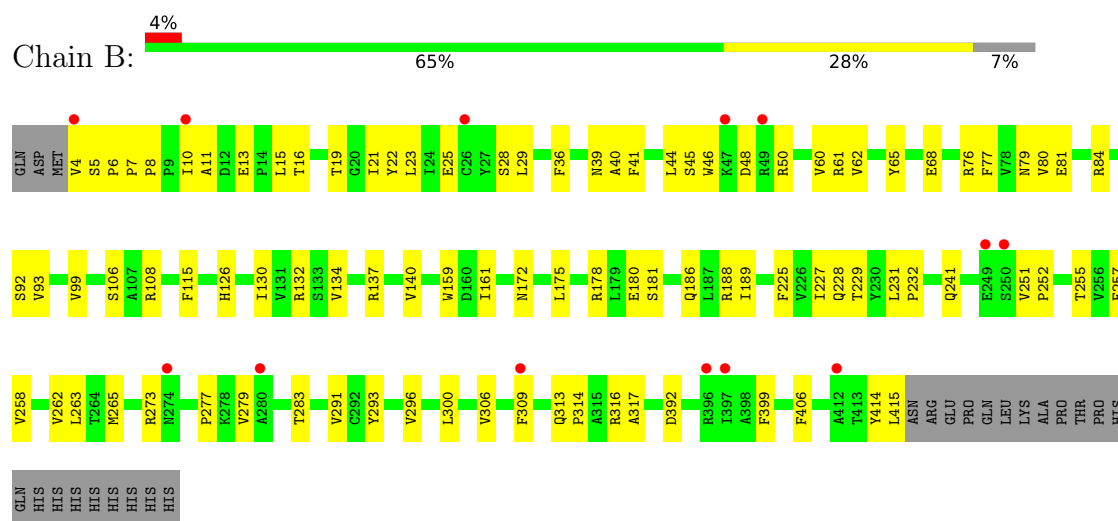
3 Residue-property plots

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

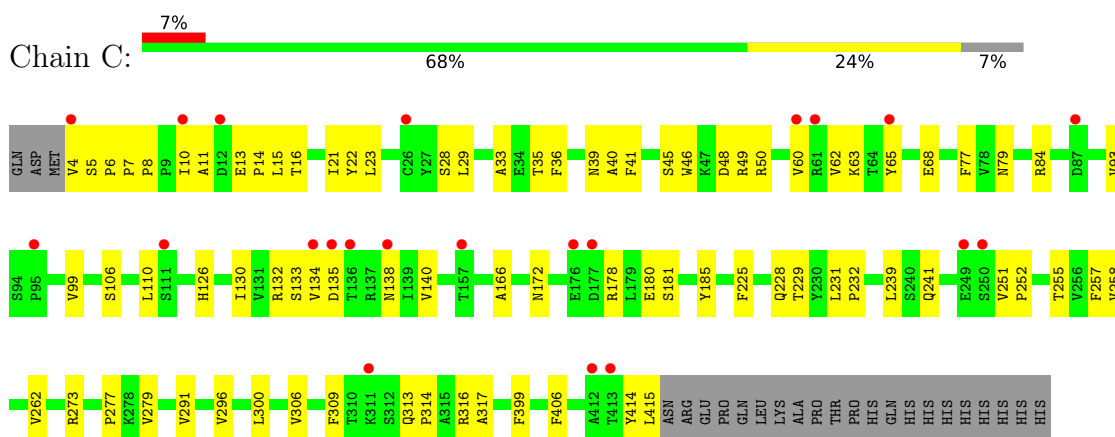
- Molecule 1: Proton-gated ion channel, Gamma-aminobutyric acid receptor subunit alpha-2, Gamma-aminobutyric acid receptor subunit alpha-1



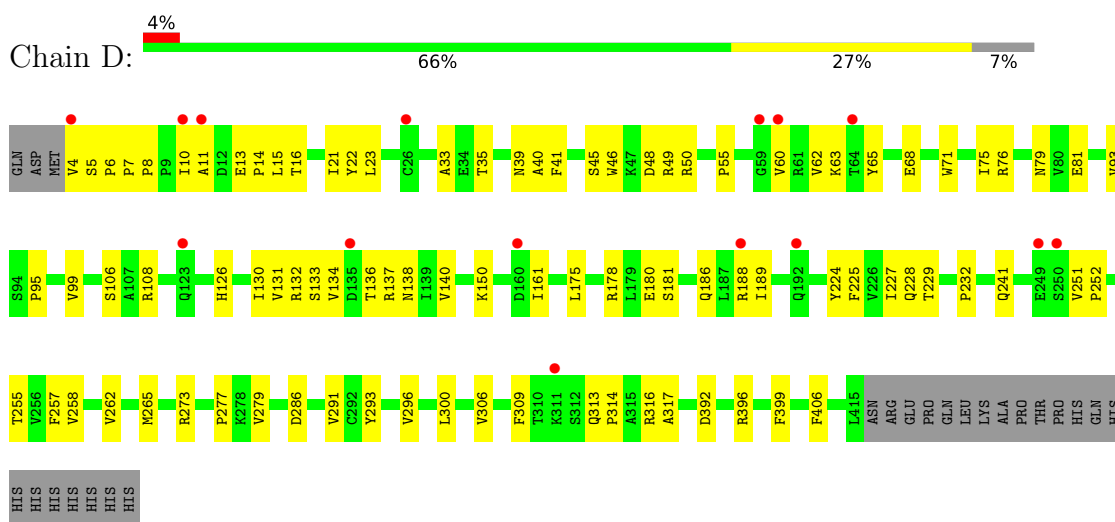
- Molecule 1: Proton-gated ion channel, Gamma-aminobutyric acid receptor subunit alpha-2, Gamma-aminobutyric acid receptor subunit alpha-1



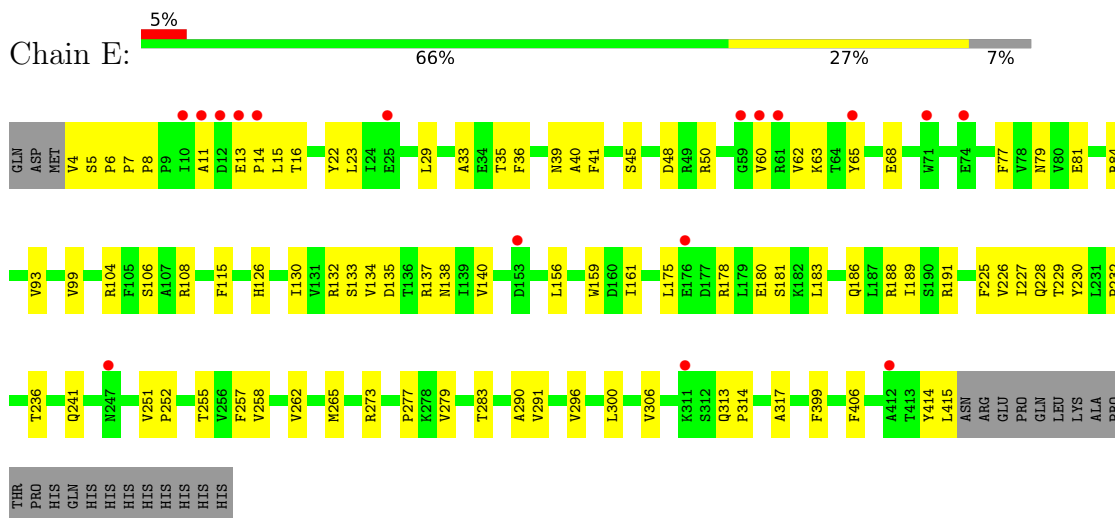
- Molecule 1: Proton-gated ion channel, Gamma-aminobutyric acid receptor subunit alpha-2, Gamma-aminobutyric acid receptor subunit alpha-1



- Molecule 1: Proton-gated ion channel, Gamma-aminobutyric acid receptor subunit alpha-2, Gamma-aminobutyric acid receptor subunit alpha-1



- Molecule 1: Proton-gated ion channel, Gamma-aminobutyric acid receptor subunit alpha-2, Gamma-aminobutyric acid receptor subunit alpha-1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.31Å 133.18Å 161.86Å 90.00° 102.71° 90.00°	Depositor
Resolution (Å)	29.92 – 3.10 29.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.92-3.10) 99.2 (29.92-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.211 , 0.246 0.210 , 0.243	Depositor DCC
R_{free} test set	3864 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13188	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A8W, CL, ACT, Y01

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	0.10	0/2553	0.30	0/3496
1	B	0.10	0/2555	0.29	0/3499
1	C	0.09	0/2555	0.29	0/3499
1	D	0.10	0/2549	0.29	0/3492
1	E	0.09	0/2549	0.29	0/3492
All	All	0.10	0/12761	0.29	0/17478

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	2488	0	2463	74	0
1	B	2490	0	2463	73	0
1	C	2490	0	2463	61	0
1	D	2484	0	2452	62	0
1	E	2484	0	2452	69	0
2	A	4	0	3	2	0
2	B	8	0	6	2	0
2	C	4	0	3	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	8	0	6	2	0
2	E	8	0	6	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	27	32	0	0	0
4	B	27	32	0	0	0
4	C	27	32	0	0	0
4	D	27	32	0	0	0
4	E	27	32	0	0	0
5	A	35	49	49	5	0
5	B	70	98	98	2	0
5	D	35	49	49	1	0
5	E	35	49	49	2	0
All	All	12783	405	12562	325	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (325) 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:D:6:PRO:HG3	1:D:134:VAL:HG21	1.43	0.99
1:A:6:PRO:HG3	1:A:134:VAL:HG21	1.51	0.93
1:E:8:PRO:HD3	1:E:50:ARG:HD2	1.58	0.85
1:A:8:PRO:HD3	1:A:50:ARG:HD2	1.64	0.77
1:C:6:PRO:HG3	1:C:134:VAL:HG21	1.68	0.75
1:B:65:TYR:HE1	1:B:93:VAL:HG21	1.54	0.73
1:D:76:ARG:NH1	2:D:501:ACT:O	2.22	0.72
1:D:48:ASP:OD1	1:D:50:ARG:HD3	1.90	0.72
1:E:6:PRO:HG3	1:E:134:VAL:HG21	1.72	0.70
1:E:306:VAL:HG13	1:E:317:ALA:HB1	1.75	0.69
1:E:39:ASN:HD22	1:E:106:SER:HB3	1.57	0.69
1:A:13:GLU:HG3	1:A:14:PRO:HD2	1.74	0.69
1:B:6:PRO:HG3	1:B:134:VAL:HG21	1.73	0.67
1:C:62:VAL:HG23	1:C:63:LYS:H	1.60	0.67
1:C:8:PRO:HD3	1:C:50:ARG:HD2	1.78	0.66
1:C:48:ASP:OD1	1:C:50:ARG:HD3	1.95	0.65
1:B:8:PRO:HD3	1:B:50:ARG:HD2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:VAL:HG11	1:E:300:LEU:HD13	1.79	0.64
1:E:13:GLU:HG3	1:E:14:PRO:HD2	1.79	0.64
1:B:306:VAL:HG13	1:B:317:ALA:HB1	1.80	0.64
1:A:7:PRO:HA	1:A:50:ARG:HH11	1.63	0.63
1:D:62:VAL:HG23	1:D:63:LYS:H	1.63	0.63
1:E:48:ASP:OD1	1:E:50:ARG:HD3	1.97	0.63
1:C:132:ARG:CZ	1:C:178:ARG:HB2	2.29	0.63
1:D:306:VAL:HG13	1:D:317:ALA:HB1	1.81	0.63
1:E:79:ASN:ND2	1:E:126:HIS:O	2.25	0.63
1:B:10:ILE:HG22	1:B:13:GLU:OE2	1.99	0.62
1:E:65:TYR:HE1	1:E:93:VAL:HG21	1.64	0.62
1:B:48:ASP:OD1	1:B:50:ARG:HD3	1.99	0.61
1:A:132:ARG:CZ	1:A:178:ARG:HB2	2.30	0.61
1:D:55:PRO:HG3	1:D:95:PRO:HB3	1.83	0.60
1:E:7:PRO:HA	1:E:50:ARG:HH11	1.67	0.60
1:A:130:ILE:HA	1:A:181:SER:O	2.02	0.60
1:E:258:VAL:HG11	1:E:300:LEU:CD1	2.32	0.60
1:D:15:LEU:HB2	1:D:137:ARG:CZ	2.32	0.60
1:A:48:ASP:OD1	1:A:50:ARG:HD3	2.02	0.59
1:B:68:GLU:OE1	1:B:68:GLU:N	2.35	0.59
1:E:16:THR:HA	1:E:140:VAL:O	2.02	0.59
1:E:62:VAL:HG23	1:E:63:LYS:H	1.66	0.59
1:D:65:TYR:HE1	1:D:93:VAL:HG21	1.67	0.59
1:C:258:VAL:HG11	1:C:300:LEU:HD13	1.85	0.59
1:E:262:VAL:HG22	1:E:296:VAL:HG12	1.84	0.59
1:C:13:GLU:HG3	1:C:14:PRO:HD2	1.84	0.58
1:B:23:LEU:HA	1:B:40:ALA:HB2	1.85	0.58
1:B:130:ILE:HD13	2:B:501:ACT:H2	1.85	0.58
1:E:186:GLN:OE1	1:E:188:ARG:NH2	2.36	0.58
1:A:301:ILE:HG13	5:A:504:Y01:HAC3	1.85	0.58
1:E:68:GLU:N	1:E:68:GLU:OE1	2.35	0.58
1:D:8:PRO:HD3	1:D:50:ARG:HD2	1.85	0.58
1:D:81:GLU:OE1	1:D:108:ARG:NH1	2.37	0.58
1:A:77:PHE:CE2	1:A:84:ARG:HD3	2.38	0.58
1:B:130:ILE:HA	1:B:181:SER:O	2.03	0.57
1:E:81:GLU:OE1	1:E:108:ARG:NH1	2.37	0.57
1:A:79:ASN:ND2	1:A:126:HIS:O	2.34	0.57
1:E:23:LEU:HA	1:E:40:ALA:HB2	1.86	0.57
1:A:229:THR:C	1:A:232:PRO:HD2	2.29	0.57
1:A:75:ILE:HD13	1:A:131:VAL:HB	1.86	0.56
1:B:241:GLN:NE2	1:B:399:PHE:HB3	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:PRO:CD	1:E:50:ARG:HD2	2.31	0.56
1:C:65:TYR:HE1	1:C:93:VAL:HG21	1.70	0.56
1:D:130:ILE:HD13	2:D:501:ACT:H2	1.88	0.56
1:E:13:GLU:CG	1:E:14:PRO:HD2	2.34	0.56
1:A:132:ARG:NH2	1:A:178:ARG:HB2	2.21	0.56
1:D:68:GLU:OE1	1:D:68:GLU:N	2.38	0.56
1:C:258:VAL:HG11	1:C:300:LEU:CD1	2.35	0.56
1:D:227:ILE:HD11	1:E:273:ARG:CZ	2.35	0.56
1:A:227:ILE:HD11	1:B:273:ARG:CZ	2.36	0.56
1:E:251:VAL:HB	1:E:252:PRO:HD3	1.88	0.56
1:A:62:VAL:HG11	1:A:92:SER:HB3	1.86	0.56
1:D:13:GLU:HG3	1:D:14:PRO:HD2	1.88	0.56
1:A:16:THR:HA	1:A:140:VAL:O	2.06	0.55
1:A:241:GLN:NE2	1:A:399:PHE:HB3	2.21	0.55
1:D:130:ILE:HA	1:D:181:SER:O	2.06	0.55
1:C:10:ILE:HD12	1:C:49:ARG:CZ	2.36	0.55
1:C:28:SER:O	1:C:36:PHE:HA	2.06	0.55
1:C:68:GLU:N	1:C:68:GLU:OE1	2.36	0.55
1:A:8:PRO:CD	1:A:50:ARG:HD2	2.35	0.55
1:A:291:VAL:HG21	1:A:406:PHE:CE1	2.42	0.55
1:A:76:ARG:NH1	2:A:501:ACT:O	2.39	0.55
1:C:258:VAL:CG1	1:C:300:LEU:HD13	2.36	0.55
1:A:21:ILE:HA	1:A:41:PHE:O	2.07	0.55
1:B:28:SER:O	1:B:36:PHE:HA	2.05	0.55
1:C:5:SER:HB2	1:C:6:PRO:HD2	1.88	0.55
1:D:7:PRO:HA	1:D:50:ARG:HH11	1.72	0.55
5:D:505:Y01:HAC1	5:D:505:Y01:HAU2	1.88	0.55
1:B:258:VAL:HG11	1:B:300:LEU:CD1	2.37	0.55
1:A:262:VAL:HG22	1:A:296:VAL:HG12	1.88	0.55
1:D:79:ASN:ND2	1:D:126:HIS:O	2.34	0.55
1:D:186:GLN:OE1	1:D:188:ARG:NH2	2.40	0.55
1:E:15:LEU:HB2	1:E:137:ARG:CZ	2.37	0.54
1:B:77:PHE:CE2	1:B:84:ARG:HD3	2.43	0.54
1:D:23:LEU:HA	1:D:40:ALA:HB2	1.88	0.54
1:B:258:VAL:HG11	1:B:300:LEU:HD13	1.90	0.54
1:C:130:ILE:HA	1:C:181:SER:O	2.08	0.54
1:D:251:VAL:HB	1:D:252:PRO:HD3	1.90	0.54
1:A:4:VAL:HG12	1:A:5:SER:N	2.23	0.54
1:A:4:VAL:HG12	1:A:5:SER:H	1.73	0.53
1:C:291:VAL:HG21	1:C:406:PHE:CE1	2.43	0.53
1:E:258:VAL:CG1	1:E:300:LEU:HD13	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:THR:HA	1:B:140:VAL:O	2.08	0.53
1:D:258:VAL:HG11	1:D:300:LEU:CD1	2.38	0.53
1:B:4:VAL:HG12	1:B:5:SER:N	2.24	0.53
1:B:61:ARG:HG3	1:B:62:VAL:HG23	1.89	0.53
1:B:309:PHE:CD2	1:B:316:ARG:HD2	2.44	0.53
1:C:13:GLU:CG	1:C:14:PRO:HD2	2.38	0.53
1:E:4:VAL:HG12	1:E:5:SER:N	2.24	0.53
1:A:5:SER:HB2	1:A:6:PRO:HD2	1.91	0.53
1:A:60:VAL:HG12	1:A:62:VAL:H	1.73	0.53
1:C:7:PRO:HA	1:C:50:ARG:HH11	1.74	0.53
1:D:75:ILE:CD1	1:D:131:VAL:HB	2.39	0.53
1:D:45:SER:HA	1:D:99:VAL:O	2.09	0.52
1:C:77:PHE:CE2	1:C:84:ARG:HD3	2.45	0.52
1:B:5:SER:HB2	1:B:6:PRO:HD2	1.91	0.52
1:B:79:ASN:ND2	1:B:126:HIS:O	2.38	0.52
1:E:133:SER:HB3	1:E:138:ASN:HA	1.91	0.52
1:D:33:ALA:O	1:D:35:THR:HG23	2.10	0.52
1:B:262:VAL:HG22	1:B:296:VAL:HG12	1.92	0.52
1:A:33:ALA:O	1:A:35:THR:HG23	2.10	0.52
1:B:4:VAL:HG12	1:B:5:SER:H	1.74	0.51
1:C:251:VAL:HB	1:C:252:PRO:HD3	1.91	0.51
1:D:309:PHE:CD2	1:D:316:ARG:HD2	2.44	0.51
1:B:65:TYR:HE1	1:B:93:VAL:CG2	2.22	0.51
5:B:505:Y01:HAC1	5:B:505:Y01:HAE2	1.92	0.51
1:E:4:VAL:HG12	1:E:5:SER:H	1.75	0.51
1:A:251:VAL:HB	1:A:252:PRO:HD3	1.93	0.51
1:A:258:VAL:HG11	1:A:300:LEU:CD1	2.41	0.51
5:B:506:Y01:HAU2	5:B:506:Y01:HAC1	1.92	0.51
1:D:4:VAL:HG12	1:D:5:SER:N	2.25	0.51
1:D:132:ARG:CZ	1:D:178:ARG:HB2	2.41	0.51
1:E:77:PHE:CE2	1:E:84:ARG:HD3	2.45	0.51
1:A:10:ILE:HD12	1:A:49:ARG:CZ	2.41	0.51
1:A:133:SER:HB3	1:A:138:ASN:HA	1.93	0.51
1:C:62:VAL:HG23	1:C:63:LYS:N	2.26	0.51
1:B:25:GLU:HG3	1:C:110:LEU:HD23	1.92	0.50
1:D:258:VAL:HG11	1:D:300:LEU:HD13	1.93	0.50
1:E:130:ILE:HD13	2:E:501:ACT:H2	1.94	0.50
1:C:4:VAL:HG12	1:C:5:SER:N	2.26	0.50
1:D:229:THR:C	1:D:232:PRO:HD2	2.36	0.50
5:E:505:Y01:HAC1	5:E:505:Y01:HAU2	1.93	0.50
1:D:225:PHE:HA	1:D:228:GLN:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:ILE:HA	1:E:181:SER:O	2.11	0.50
1:C:39:ASN:HD22	1:C:106:SER:HB3	1.75	0.50
1:E:45:SER:HA	1:E:99:VAL:O	2.12	0.50
1:B:265:MET:HE3	1:B:265:MET:HA	1.94	0.50
1:A:77:PHE:HE2	1:A:84:ARG:HD3	1.75	0.49
1:A:277:PRO:O	1:A:279:VAL:N	2.43	0.49
1:B:251:VAL:HB	1:B:252:PRO:HD3	1.94	0.49
1:D:75:ILE:HD13	1:D:131:VAL:HB	1.92	0.49
1:E:313:GLN:N	1:E:314:PRO:HD3	2.27	0.49
1:A:78:VAL:HA	1:E:104:ARG:HH22	1.76	0.49
1:A:7:PRO:CA	1:A:50:ARG:HH11	2.25	0.49
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.94	0.49
1:B:39:ASN:HD22	1:B:106:SER:HB3	1.77	0.49
1:B:313:GLN:N	1:B:314:PRO:HD3	2.27	0.49
1:D:161:ILE:HA	1:D:189:ILE:HG22	1.94	0.49
1:E:22:TYR:O	1:E:40:ALA:HB1	2.13	0.49
1:C:79:ASN:ND2	1:C:126:HIS:O	2.37	0.49
1:E:229:THR:C	1:E:232:PRO:HD2	2.37	0.49
1:A:13:GLU:CG	1:A:14:PRO:HD2	2.40	0.49
1:D:22:TYR:O	1:D:40:ALA:HB1	2.12	0.49
1:A:258:VAL:HG11	1:A:300:LEU:HD13	1.94	0.49
1:B:25:GLU:CG	1:C:110:LEU:HD23	2.42	0.49
1:B:258:VAL:CG1	1:B:300:LEU:HD13	2.43	0.49
1:B:265:MET:HE3	1:B:265:MET:CA	2.42	0.49
1:C:8:PRO:CD	1:C:50:ARG:HD2	2.42	0.49
1:C:313:GLN:N	1:C:314:PRO:HD3	2.28	0.49
1:B:227:ILE:HD11	1:C:273:ARG:CZ	2.43	0.49
1:B:414:TYR:O	1:B:415:LEU:HD23	2.13	0.49
1:C:4:VAL:HG12	1:C:5:SER:H	1.76	0.49
1:D:39:ASN:HD22	1:D:106:SER:HB3	1.77	0.49
1:D:262:VAL:HG22	1:D:296:VAL:HG12	1.94	0.49
1:E:60:VAL:HG12	1:E:62:VAL:H	1.77	0.49
1:B:81:GLU:OE1	1:B:108:ARG:NH1	2.46	0.49
1:D:4:VAL:HG12	1:D:5:SER:H	1.77	0.49
1:D:5:SER:HB2	1:D:6:PRO:HD2	1.93	0.49
1:D:13:GLU:CG	1:D:14:PRO:HD2	2.43	0.49
1:A:62:VAL:CG1	1:A:92:SER:HB3	2.42	0.48
1:A:313:GLN:N	1:A:314:PRO:HD3	2.28	0.48
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.93	0.48
1:B:161:ILE:HA	1:B:189:ILE:HG22	1.94	0.48
1:E:5:SER:HB2	1:E:6:PRO:HD2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:THR:C	1:C:232:PRO:HD2	2.38	0.48
1:D:10:ILE:HD12	1:D:49:ARG:CZ	2.43	0.48
1:E:7:PRO:CA	1:E:50:ARG:HH11	2.26	0.48
1:A:23:LEU:HB2	1:A:150:LYS:CB	2.43	0.48
1:A:257:PHE:CE1	1:B:255:THR:HG23	2.49	0.48
5:A:504:Y01:HAC1	5:A:504:Y01:HAE2	1.96	0.48
1:C:23:LEU:HA	1:C:40:ALA:HB2	1.94	0.48
1:A:258:VAL:CG1	1:A:300:LEU:HD13	2.44	0.48
1:C:16:THR:HA	1:C:140:VAL:O	2.14	0.48
1:A:81:GLU:OE1	1:A:108:ARG:NH1	2.47	0.48
1:B:277:PRO:O	1:B:279:VAL:N	2.44	0.48
1:D:21:ILE:HA	1:D:41:PHE:O	2.13	0.48
1:B:7:PRO:HA	1:B:50:ARG:HH11	1.79	0.48
1:D:224:TYR:HD1	1:E:273:ARG:HH21	1.62	0.48
1:B:45:SER:HA	1:B:99:VAL:O	2.13	0.48
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.95	0.48
1:A:23:LEU:HA	1:A:40:ALA:HB2	1.96	0.48
1:A:68:GLU:OE1	1:A:68:GLU:N	2.41	0.48
1:B:76:ARG:NH1	2:B:501:ACT:O	2.47	0.48
1:D:313:GLN:N	1:D:314:PRO:HD3	2.28	0.48
1:D:175:LEU:HB3	1:D:180:GLU:HG3	1.96	0.48
1:C:33:ALA:O	1:C:35:THR:HG23	2.14	0.47
1:B:22:TYR:O	1:B:40:ALA:HB1	2.15	0.47
1:B:172:ASN:HA	1:B:180:GLU:O	2.15	0.47
1:B:186:GLN:OE1	1:B:188:ARG:NH2	2.47	0.47
1:D:291:VAL:HG21	1:D:406:PHE:CE1	2.48	0.47
1:B:60:VAL:HG12	1:B:62:VAL:H	1.79	0.47
1:C:262:VAL:HG22	1:C:296:VAL:HG12	1.95	0.47
1:E:135:ASP:HB2	1:E:178:ARG:NH2	2.29	0.47
1:E:161:ILE:HA	1:E:189:ILE:HG22	1.96	0.47
1:C:306:VAL:HG13	1:C:317:ALA:HB1	1.95	0.47
1:A:277:PRO:HG2	1:A:279:VAL:HG13	1.96	0.47
1:E:290:ALA:HA	5:E:505:Y01:OAH	2.14	0.47
1:A:306:VAL:HG13	1:A:317:ALA:HB1	1.96	0.47
1:D:258:VAL:CG1	1:D:300:LEU:HD13	2.45	0.46
1:A:172:ASN:HA	1:A:180:GLU:O	2.15	0.46
1:B:115:PHE:O	1:B:283:THR:HG22	2.16	0.46
1:E:115:PHE:O	1:E:283:THR:HG22	2.16	0.46
1:B:62:VAL:CG1	1:B:92:SER:HB3	2.46	0.46
1:C:7:PRO:CA	1:C:50:ARG:HH11	2.29	0.46
1:A:175:LEU:HB3	1:A:180:GLU:HG3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:PHE:CE1	1:D:255:THR:HG23	2.51	0.46
1:E:291:VAL:HG21	1:E:406:PHE:CE1	2.51	0.46
1:A:23:LEU:HB2	1:A:150:LYS:HB2	1.97	0.45
1:E:29:LEU:HD23	1:E:159:TRP:NE1	2.31	0.45
1:C:60:VAL:HG12	1:C:62:VAL:H	1.79	0.45
1:D:62:VAL:HG23	1:D:63:LYS:N	2.30	0.45
1:E:226:VAL:HA	1:E:230:TYR:HB2	1.98	0.45
1:A:75:ILE:CD1	1:A:131:VAL:HB	2.44	0.45
1:B:77:PHE:HE2	1:B:84:ARG:HD3	1.78	0.45
1:C:132:ARG:NH2	1:C:178:ARG:HB2	2.31	0.45
1:B:77:PHE:HB3	1:B:80:VAL:CG2	2.47	0.45
1:B:175:LEU:HB3	1:B:180:GLU:HG3	1.98	0.45
1:C:239:LEU:HD13	1:D:300:LEU:HD22	1.99	0.45
1:E:236:THR:HB	1:E:265:MET:HE1	1.98	0.44
1:B:132:ARG:CZ	1:B:178:ARG:HB2	2.47	0.44
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.98	0.44
1:A:28:SER:O	1:A:36:PHE:HA	2.17	0.44
1:C:21:ILE:HA	1:C:41:PHE:O	2.17	0.44
1:D:6:PRO:HG2	1:D:136:THR:HB	1.99	0.44
1:E:156:LEU:HD23	1:E:156:LEU:HA	1.72	0.44
1:C:45:SER:HA	1:C:99:VAL:O	2.18	0.44
1:A:157:THR:HG21	1:B:277:PRO:HB2	2.00	0.44
1:C:29:LEU:HD13	1:C:36:PHE:HB3	1.99	0.44
1:A:93:VAL:HG12	1:A:99:VAL:HG22	1.99	0.44
1:C:172:ASN:HA	1:C:180:GLU:O	2.17	0.44
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.77	0.44
1:B:93:VAL:HG12	1:B:99:VAL:HG22	2.00	0.44
1:D:273:ARG:NH1	1:D:286:ASP:OD2	2.50	0.44
1:E:277:PRO:O	1:E:279:VAL:N	2.47	0.44
1:B:134:VAL:HG23	1:B:137:ARG:H	1.83	0.43
1:D:133:SER:HB3	1:D:138:ASN:HA	2.00	0.43
1:A:309:PHE:CD2	1:A:316:ARG:HD2	2.52	0.43
1:B:21:ILE:HA	1:B:41:PHE:O	2.18	0.43
1:D:392:ASP:O	1:D:396:ARG:HG3	2.18	0.43
1:A:226:VAL:HA	1:A:230:TYR:HB2	1.98	0.43
1:B:62:VAL:HG21	1:C:135:ASP:CG	2.44	0.43
1:B:225:PHE:HA	1:B:228:GLN:HB3	1.99	0.43
1:E:77:PHE:HE2	1:E:84:ARG:HD3	1.83	0.43
1:A:290:ALA:HA	5:A:504:Y01:HAL1	1.99	0.43
1:B:291:VAL:HG21	1:B:406:PHE:CE1	2.53	0.43
1:C:15:LEU:HD11	1:C:46:TRP:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:SER:HB3	1:C:138:ASN:HA	2.00	0.43
1:B:306:VAL:HG21	1:B:392:ASP:OD1	2.19	0.43
1:C:225:PHE:HA	1:C:228:GLN:HB3	2.01	0.43
1:E:29:LEU:HD13	1:E:36:PHE:HB3	2.00	0.43
1:E:132:ARG:CZ	1:E:178:ARG:HB2	2.49	0.43
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.99	0.43
1:C:77:PHE:CD2	1:C:84:ARG:HD3	2.54	0.43
1:D:4:VAL:HG12	1:D:71:TRP:HB2	2.00	0.43
1:D:23:LEU:HB2	1:D:150:LYS:CB	2.48	0.43
1:D:241:GLN:NE2	1:D:399:PHE:HB3	2.34	0.43
1:E:33:ALA:O	1:E:35:THR:HG23	2.19	0.43
1:C:277:PRO:O	1:C:279:VAL:N	2.45	0.42
1:A:260:THR:HB	1:B:263:LEU:HD11	2.00	0.42
1:B:29:LEU:HD23	1:B:159:TRP:NE1	2.35	0.42
1:C:166:ALA:HB2	1:C:185:TYR:CD2	2.54	0.42
1:E:62:VAL:HG23	1:E:63:LYS:N	2.34	0.42
1:E:236:THR:HG21	1:E:265:MET:HE2	2.01	0.42
1:A:239:LEU:HD13	1:B:300:LEU:HD22	2.01	0.42
1:D:16:THR:HA	1:D:140:VAL:O	2.19	0.42
1:A:273:ARG:CZ	1:E:227:ILE:HD11	2.49	0.42
1:B:23:LEU:HA	1:B:40:ALA:CB	2.50	0.42
1:C:277:PRO:HG2	1:C:279:VAL:HG13	2.01	0.42
1:D:277:PRO:O	1:D:279:VAL:N	2.49	0.42
1:A:225:PHE:HA	1:A:228:GLN:HB3	2.02	0.42
1:A:276:LEU:HB3	1:A:277:PRO:HD2	2.02	0.42
1:B:77:PHE:CB	1:B:80:VAL:HG21	2.50	0.42
1:C:241:GLN:NE2	1:C:399:PHE:HB3	2.34	0.42
1:B:229:THR:C	1:B:232:PRO:HD2	2.45	0.42
1:C:309:PHE:CD2	1:C:316:ARG:HD2	2.55	0.42
1:C:414:TYR:O	1:C:415:LEU:HD23	2.20	0.42
1:A:224:TYR:HD1	1:B:273:ARG:HH21	1.67	0.41
2:A:501:ACT:H3	1:E:41:PHE:CE2	2.55	0.41
1:E:23:LEU:HA	1:E:40:ALA:CB	2.49	0.41
1:A:235:MET:HE2	1:B:293:TYR:HE1	1.84	0.41
1:B:22:TYR:HB3	1:B:41:PHE:HB2	2.02	0.41
1:C:22:TYR:O	1:C:40:ALA:HB1	2.21	0.41
1:A:29:LEU:HD13	1:A:36:PHE:HB3	2.03	0.41
5:A:504:Y01:HAJ2	5:A:504:Y01:HAC2	1.81	0.41
1:A:45:SER:HA	1:A:99:VAL:O	2.20	0.41
1:A:255:THR:HG23	1:E:257:PHE:CE1	2.55	0.41
1:E:175:LEU:HB3	1:E:180:GLU:HG3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:HA	1:A:231:LEU:HD23	1.81	0.41
1:B:19:THR:HG22	1:B:44:LEU:HD22	2.02	0.41
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.84	0.41
1:E:63:LYS:O	1:E:93:VAL:HG22	2.20	0.41
1:C:10:ILE:HD12	1:C:49:ARG:NE	2.36	0.41
1:A:135:ASP:HB3	1:E:62:VAL:HG21	2.02	0.41
1:A:262:VAL:CG2	1:A:296:VAL:HG12	2.50	0.41
1:E:183:LEU:HD23	1:E:183:LEU:HA	1.94	0.41
5:A:504:Y01:HAC1	5:A:504:Y01:HAU2	2.02	0.41
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.90	0.41
1:D:257:PHE:CE1	1:E:255:THR:HG23	2.55	0.41
1:A:29:LEU:HD23	1:A:159:TRP:NE1	2.36	0.41
1:D:60:VAL:HG12	1:D:62:VAL:H	1.86	0.41
1:E:225:PHE:HA	1:E:228:GLN:HB3	2.02	0.41
1:E:262:VAL:CG2	1:E:296:VAL:HG12	2.50	0.41
1:E:241:GLN:NE2	1:E:399:PHE:HB3	2.36	0.40
1:E:414:TYR:O	1:E:415:LEU:HD23	2.21	0.40
1:D:265:MET:HB3	1:D:293:TYR:HD2	1.86	0.40
1:B:257:PHE:CE1	1:C:255:THR:HG23	2.56	0.40
1:C:130:ILE:HD13	2:C:501:ACT:H2	2.02	0.40
1:E:159:TRP:CZ3	1:E:191:ARG:HB2	2.57	0.40

There are no symmetry-related clashes.

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	310/336 (92%)	297 (96%)	11 (4%)	2 (1%)	21	52
1	B	310/336 (92%)	299 (96%)	10 (3%)	1 (0%)	36	67
1	C	310/336 (92%)	298 (96%)	11 (4%)	1 (0%)	36	67
1	D	310/336 (92%)	299 (96%)	10 (3%)	1 (0%)	36	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	310/336 (92%)	298 (96%)	11 (4%)	1 (0%)	36	67
All	All	1550/1680 (92%)	1491 (96%)	53 (3%)	6 (0%)	30	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	B	11	ALA
1	C	11	ALA
1	D	11	ALA
1	E	11	ALA
1	A	63	LYS

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	272/302 (90%)	271 (100%)	1 (0%)	84	86
1	B	272/302 (90%)	272 (100%)	0	100	100
1	C	272/302 (90%)	272 (100%)	0	100	100
1	D	271/302 (90%)	271 (100%)	0	100	100
1	E	271/302 (90%)	271 (100%)	0	100	100
All	All	1358/1510 (90%)	1357 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	A8W	A	503	-	30,30,30	0.19	0	45,49,49	0.71	2 (4%)
2	ACT	D	502	-	3,3,3	0.82	0	3,3,3	1.35	0
2	ACT	A	501	-	3,3,3	0.83	0	3,3,3	1.34	0
4	A8W	E	504	-	30,30,30	0.16	0	45,49,49	0.71	2 (4%)
5	Y01	B	505	-	38,38,38	0.73	0	57,57,57	1.78	15 (26%)
5	Y01	E	505	-	38,38,38	0.66	0	57,57,57	1.42	9 (15%)
2	ACT	E	501	-	3,3,3	0.81	0	3,3,3	1.38	0
5	Y01	D	505	-	38,38,38	0.64	0	57,57,57	1.32	7 (12%)
5	Y01	B	506	-	38,38,38	0.63	0	57,57,57	1.36	8 (14%)
2	ACT	B	501	-	3,3,3	0.82	0	3,3,3	1.35	0
2	ACT	E	502	-	3,3,3	0.82	0	3,3,3	1.32	0
4	A8W	C	503	-	30,30,30	0.21	0	45,49,49	0.72	2 (4%)
4	A8W	D	504	-	30,30,30	0.20	0	45,49,49	0.83	2 (4%)
5	Y01	A	504	-	38,38,38	0.64	0	57,57,57	1.41	10 (17%)
4	A8W	B	504	-	30,30,30	0.17	0	45,49,49	0.73	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	B	502	-	3,3,3	0.82	0	3,3,3	1.33	0
2	ACT	C	501	-	3,3,3	0.82	0	3,3,3	1.35	0
2	ACT	D	501	-	3,3,3	0.82	0	3,3,3	1.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A8W	A	503	-	-	7/9/67/67	0/4/4/4
4	A8W	E	504	-	-	6/9/67/67	0/4/4/4
5	Y01	B	505	-	-	4/19/77/77	0/4/4/4
5	Y01	E	505	-	-	6/19/77/77	0/4/4/4
5	Y01	D	505	-	-	5/19/77/77	0/4/4/4
5	Y01	B	506	-	-	0/19/77/77	0/4/4/4
4	A8W	C	503	-	-	5/9/67/67	0/4/4/4
4	A8W	D	504	-	-	9/9/67/67	0/4/4/4
5	Y01	A	504	-	-	4/19/77/77	0/4/4/4
4	A8W	B	504	-	-	7/9/67/67	0/4/4/4

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	505	Y01	OAW-CAY-CAM	4.19	120.54	111.48
5	B	505	Y01	CAK-CBD-CBF	-3.99	105.11	109.72
5	D	505	Y01	OAW-CAY-CAM	3.80	119.69	111.48
5	B	505	Y01	CAR-CBC-CAV	3.76	116.20	110.97
5	B	506	Y01	OAW-CAY-CAM	3.62	119.31	111.48
5	E	505	Y01	OAW-CAY-CAM	3.58	119.22	111.48
5	B	505	Y01	CBI-CBE-CBB	-3.47	114.14	119.50
5	B	506	Y01	CBI-CBE-CBB	-3.30	114.40	119.50
5	A	504	Y01	CBC-OAW-CAY	3.21	125.47	117.80
4	E	504	A8W	O3-S-O2	3.18	124.50	112.24
5	B	505	Y01	CBI-CBG-CBD	-3.18	109.90	114.41
4	A	503	A8W	O3-S-O2	3.17	124.45	112.24
4	D	504	A8W	O3-S-O2	3.16	124.43	112.24
4	B	504	A8W	O3-S-O2	3.15	124.39	112.24
5	E	505	Y01	CAK-CBD-CBF	-3.14	106.09	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	Y01	CBI-CBG-CBD	-3.12	109.99	114.41
4	C	503	A8W	O3-S-O2	3.10	124.17	112.24
5	E	505	Y01	CBI-CBE-CBB	-3.08	114.74	119.50
5	A	504	Y01	CBI-CBE-CBB	-3.08	114.74	119.50
5	A	504	Y01	OAW-CAY-CAM	2.97	117.90	111.48
5	E	505	Y01	CBI-CBG-CBD	-2.94	110.24	114.41
5	D	505	Y01	CBI-CBE-CBB	-2.89	115.04	119.50
4	C	503	A8W	O4-S-O1	-2.81	99.91	106.37
5	B	505	Y01	CBG-CBI-CBE	2.80	103.31	100.10
5	B	505	Y01	CAE-CBI-CAU	2.68	114.56	110.61
4	A	503	A8W	O4-S-O1	-2.67	100.25	106.37
5	B	505	Y01	CAS-CBF-CBD	2.64	115.46	111.78
4	D	504	A8W	O4-S-O1	-2.62	100.35	106.37
5	A	504	Y01	OAW-CBC-CAR	2.61	114.53	108.37
5	B	505	Y01	CAS-CAU-CBI	-2.60	108.36	112.74
4	B	504	A8W	O4-S-O1	-2.59	100.42	106.37
5	B	506	Y01	CBI-CBG-CBD	-2.53	110.82	114.41
5	B	505	Y01	CAU-CBI-CBG	-2.53	103.46	107.25
4	E	504	A8W	O4-S-O1	-2.51	100.59	106.37
5	B	505	Y01	CBD-CAK-CAI	-2.51	109.29	112.76
5	D	505	Y01	CAQ-CBG-CBD	-2.49	115.13	119.10
5	A	504	Y01	CAQ-CBG-CBI	-2.47	100.94	103.84
5	A	504	Y01	CAT-CBH-CBF	2.44	111.97	108.74
5	B	506	Y01	CAQ-CBG-CBD	-2.43	115.22	119.10
5	E	505	Y01	CAS-CAU-CBI	-2.40	108.68	112.74
5	B	506	Y01	CAC-CBB-CBE	-2.40	109.28	112.88
5	B	505	Y01	CAQ-CBG-CBI	-2.40	101.01	103.84
5	E	505	Y01	CAQ-CBG-CBD	-2.38	115.31	119.10
5	B	505	Y01	CAJ-CAO-CBB	-2.31	108.61	115.08
5	B	505	Y01	CBH-CBF-CBD	-2.30	109.36	112.71
5	D	505	Y01	CAQ-CBG-CBI	-2.27	101.17	103.84
5	E	505	Y01	CAQ-CBG-CBI	-2.25	101.19	103.84
5	B	506	Y01	CAJ-CAO-CBB	-2.24	108.82	115.08
5	E	505	Y01	CAS-CBF-CBD	2.23	114.89	111.78
5	D	505	Y01	CBI-CBG-CBD	-2.22	111.26	114.41
5	B	505	Y01	CAT-CAR-CBC	2.22	113.95	110.33
5	A	504	Y01	CAQ-CBG-CBD	-2.19	115.61	119.10
5	D	505	Y01	CAK-CBD-CBF	-2.16	107.23	109.72
5	B	506	Y01	CAQ-CBG-CBI	-2.14	101.32	103.84
5	E	505	Y01	CBH-CBF-CBD	-2.13	109.60	112.71
5	D	505	Y01	CAS-CAU-CBI	-2.10	109.20	112.74
5	B	506	Y01	CAV-CAZ-CAI	-2.04	117.80	120.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	Y01	CBG-CBI-CBE	2.01	102.41	100.10
5	A	504	Y01	CAV-CAZ-CAI	-2.01	117.85	120.57

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	A8W	C3-O1-S-O2
4	A	503	A8W	C3-O1-S-O3
4	A	503	A8W	C3-O1-S-O4
4	B	504	A8W	C3-O1-S-O3
4	B	504	A8W	C3-O1-S-O4
4	C	503	A8W	C2-C3-O1-S
4	D	504	A8W	C3-O1-S-O3
4	D	504	A8W	C3-O1-S-O4
5	A	504	Y01	CAR-CBC-OAW-CAY
5	B	505	Y01	CAM-CAY-OAW-CBC
5	D	505	Y01	CAV-CBC-OAW-CAY
5	E	505	Y01	CAV-CBC-OAW-CAY
5	B	505	Y01	OAG-CAY-OAW-CBC
4	C	503	A8W	C13-C17-C20-C21
4	D	504	A8W	C13-C17-C20-C21
4	E	504	A8W	C13-C17-C20-O
5	D	505	Y01	CAO-CAJ-CAN-CBA
4	B	504	A8W	C3-O1-S-O2
4	D	504	A8W	C3-O1-S-O2
4	E	504	A8W	C3-O1-S-O2
4	D	504	A8W	C2-C3-O1-S
4	D	504	A8W	C4-C3-O1-S
5	A	504	Y01	CAM-CAY-OAW-CBC
5	E	505	Y01	CAM-CAY-OAW-CBC
4	A	503	A8W	C13-C17-C20-C21
4	D	504	A8W	C13-C17-C20-O
4	E	504	A8W	C13-C17-C20-C21
5	D	505	Y01	CAX-CAL-CAM-CAY
5	E	505	Y01	CAX-CAL-CAM-CAY
5	A	504	Y01	OAG-CAY-OAW-CBC
4	E	504	A8W	C3-O1-S-O4
5	E	505	Y01	OAG-CAY-OAW-CBC
4	A	503	A8W	C16-C17-C20-O
4	B	504	A8W	C16-C17-C20-C21
4	C	503	A8W	C16-C17-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	503	A8W	C13-C17-C20-O
4	A	503	A8W	C16-C17-C20-C21
4	B	504	A8W	C16-C17-C20-O
4	C	503	A8W	C16-C17-C20-O
4	D	504	A8W	C16-C17-C20-C21
4	A	503	A8W	C13-C17-C20-O
4	D	504	A8W	C16-C17-C20-O
4	E	504	A8W	C16-C17-C20-C21
4	B	504	A8W	C13-C17-C20-C21
4	E	504	A8W	C16-C17-C20-O
5	E	505	Y01	CAO-CAJ-CAN-CBA
4	B	504	A8W	C13-C17-C20-O
5	B	505	Y01	CAJ-CAN-CBA-CAA
5	A	504	Y01	CAN-CAJ-CAO-CBB
5	B	505	Y01	CAJ-CAO-CBB-CAC
5	D	505	Y01	CAL-CAM-CAY-OAW
5	D	505	Y01	CAL-CAM-CAY-OAG
5	E	505	Y01	CAM-CAL-CAX-OAH

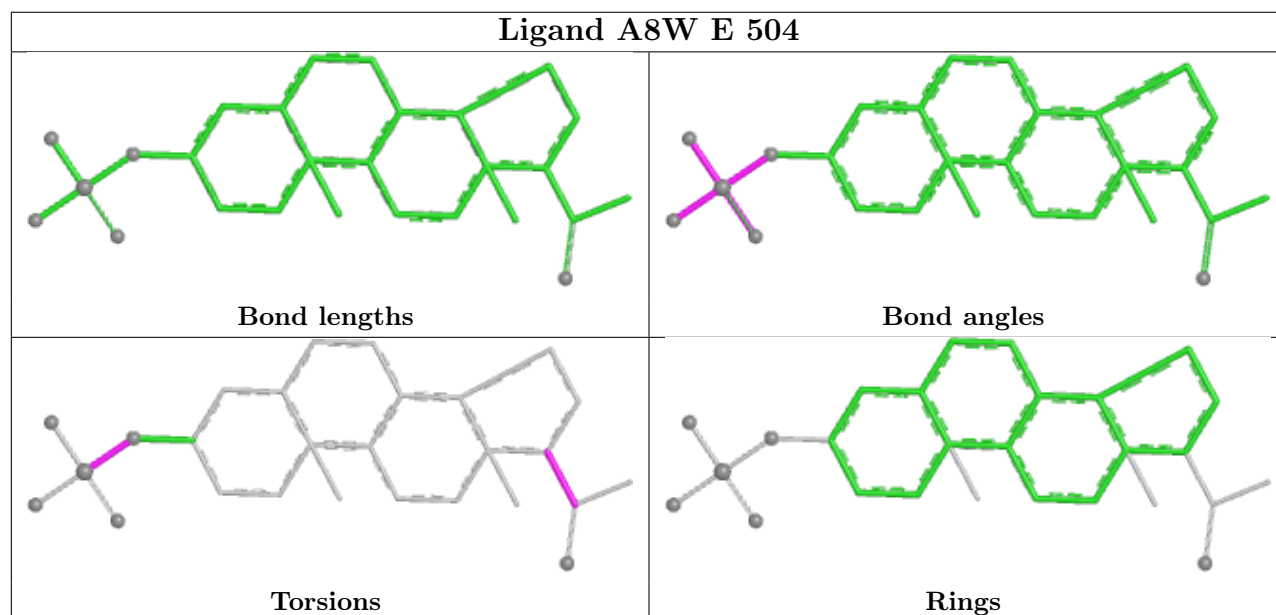
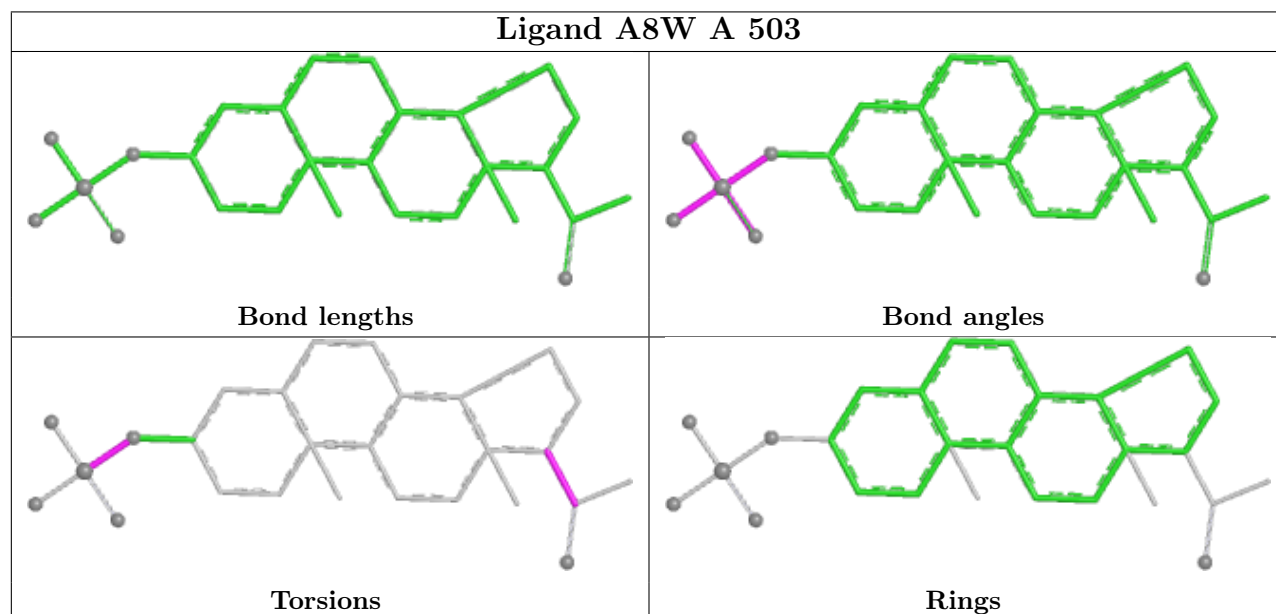
There are no ring outliers.

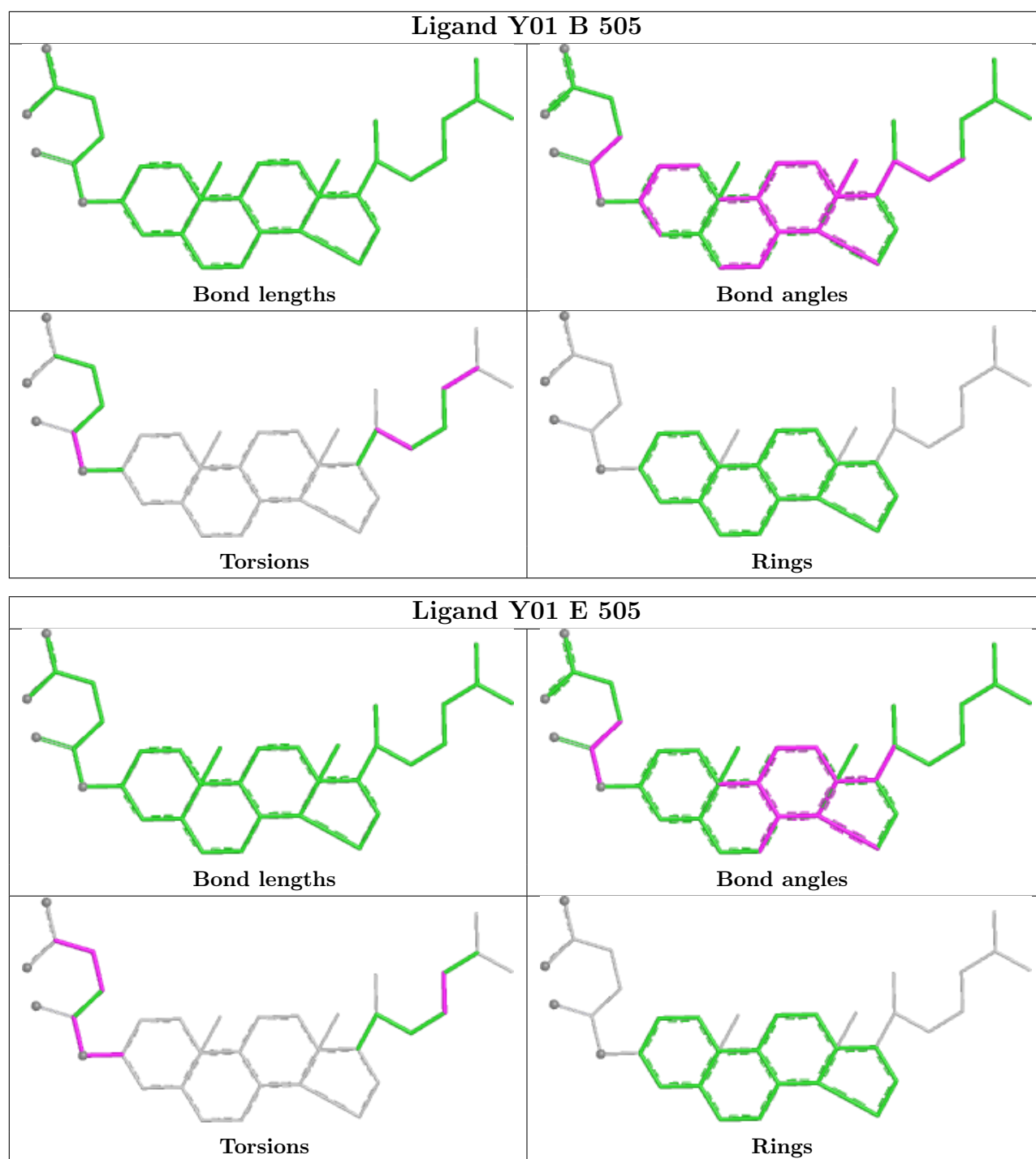
10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ACT	2	0
5	B	505	Y01	1	0
5	E	505	Y01	2	0
2	E	501	ACT	1	0
5	D	505	Y01	1	0
5	B	506	Y01	1	0
2	B	501	ACT	2	0
5	A	504	Y01	5	0
2	C	501	ACT	1	0
2	D	501	ACT	2	0

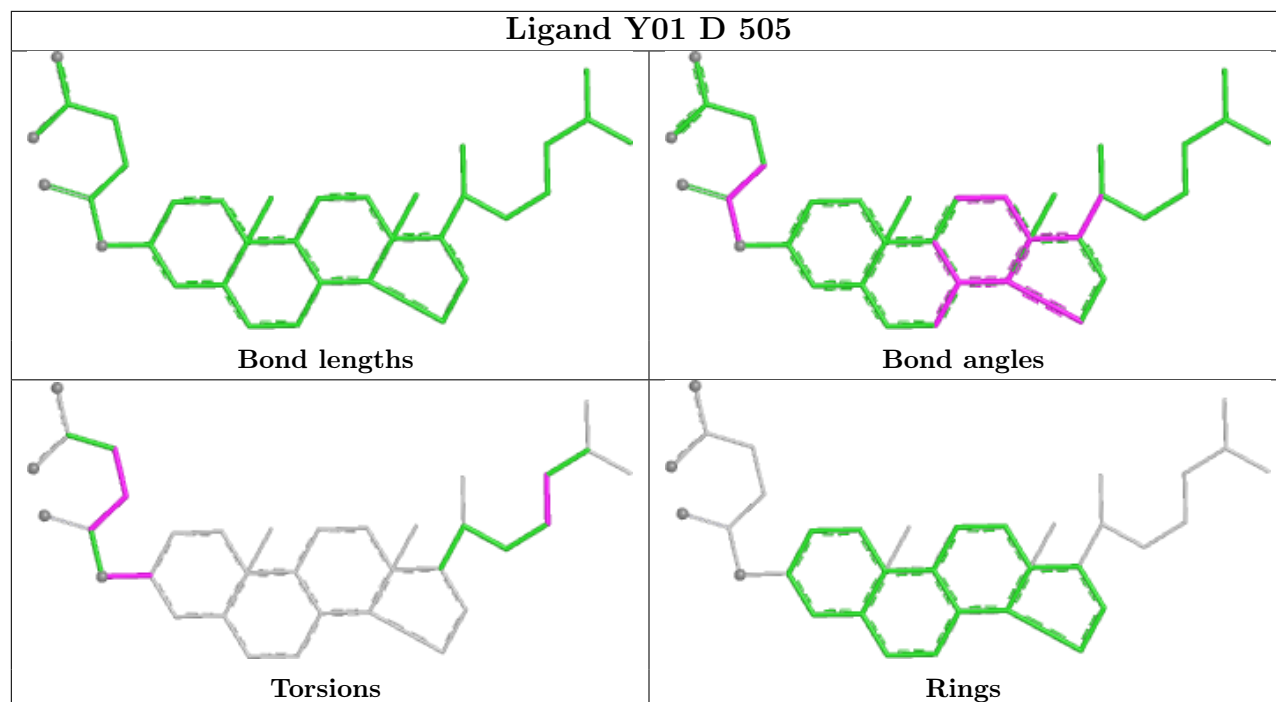
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

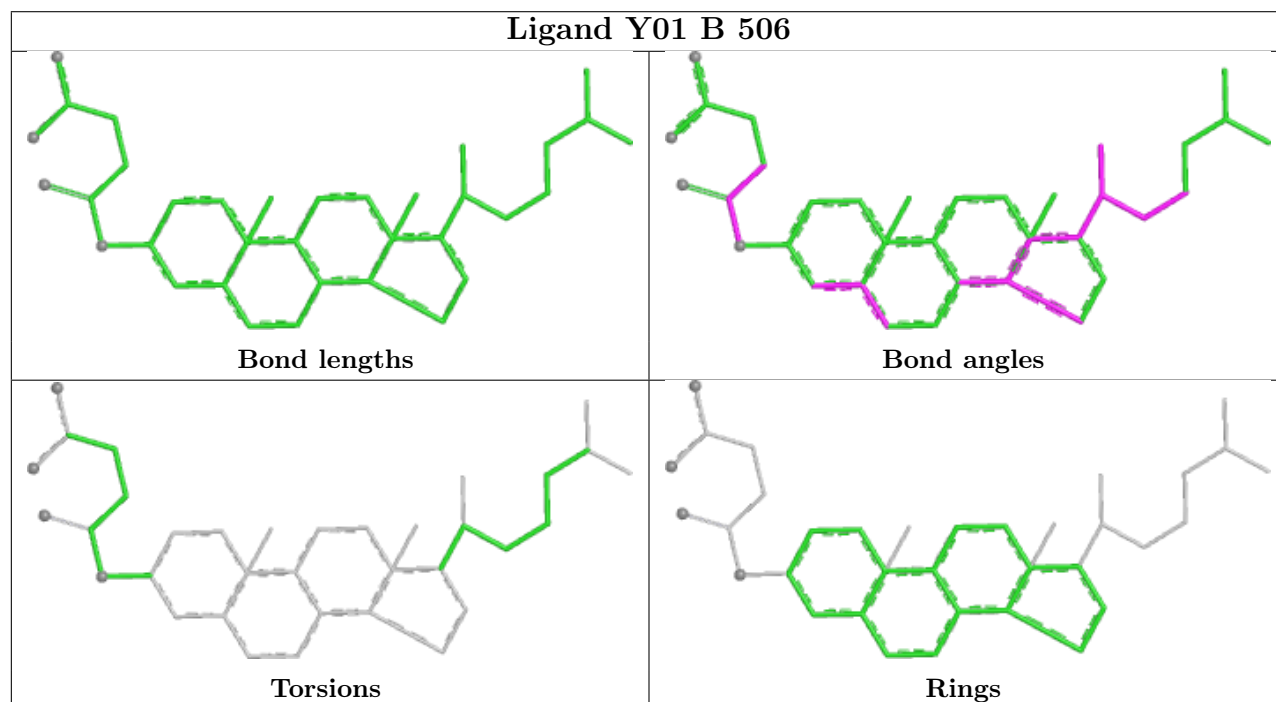


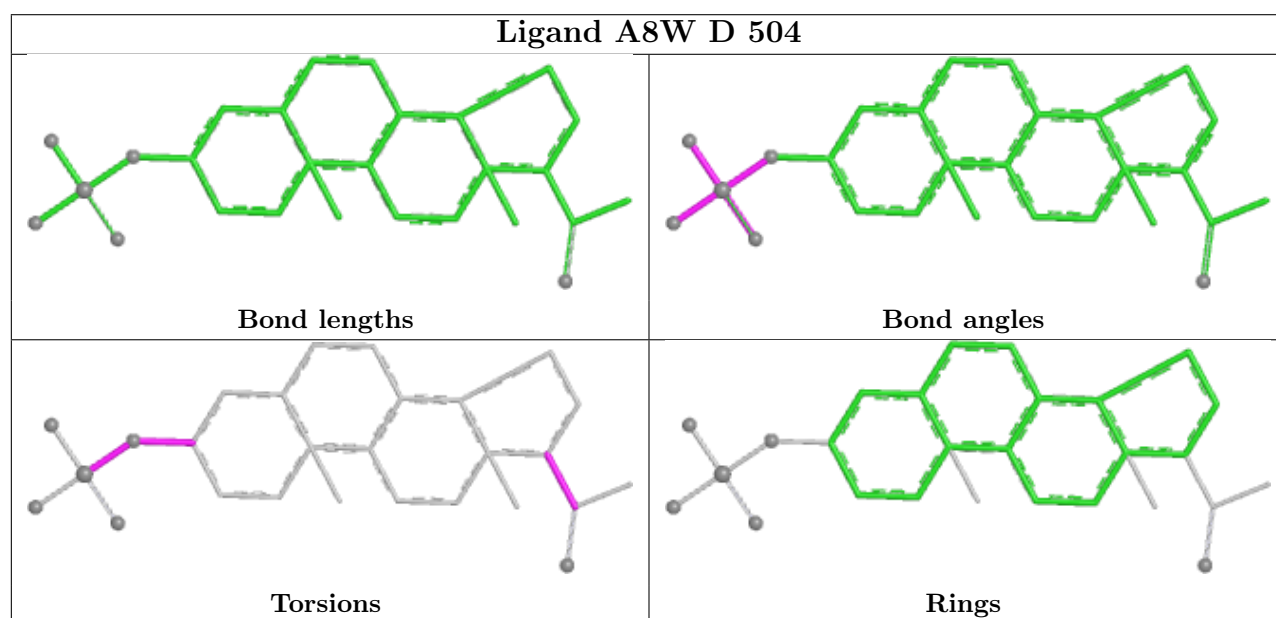
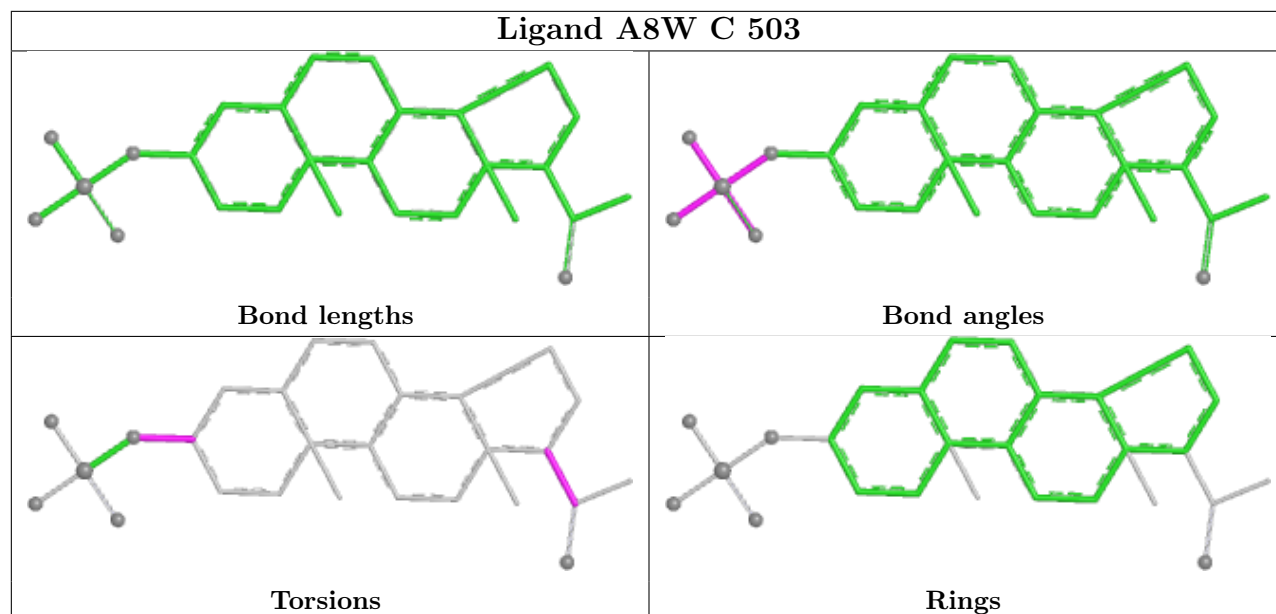


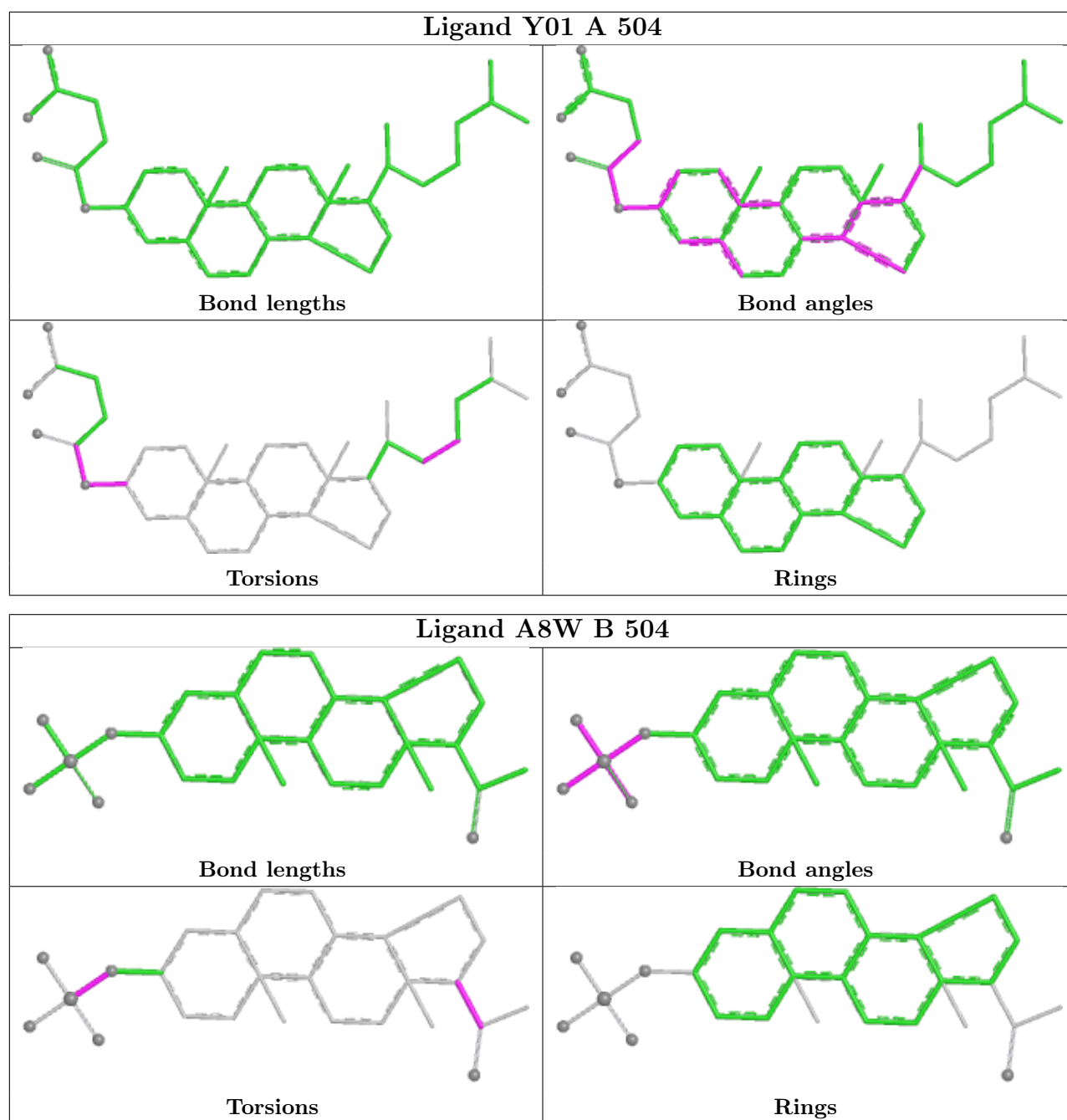
Ligand Y01 D 505



Ligand Y01 B 506







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	312/336 (92%)	0.53	23 (7%) 20 11	74, 104, 142, 178	0
1	B	312/336 (92%)	0.35	13 (4%) 40 22	73, 102, 142, 182	0
1	C	312/336 (92%)	0.45	22 (7%) 22 12	72, 108, 150, 186	0
1	D	312/336 (92%)	0.41	15 (4%) 35 19	73, 104, 145, 184	0
1	E	312/336 (92%)	0.44	17 (5%) 31 17	79, 108, 155, 224	0
All	All	1560/1680 (92%)	0.44	90 (5%) 29 16	72, 105, 149, 224	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	VAL	5.2
1	A	59	GLY	5.1
1	D	60	VAL	4.5
1	C	412	ALA	4.2
1	B	412	ALA	3.9
1	A	90	ASP	3.9
1	A	65	TYR	3.8
1	C	60	VAL	3.8
1	E	12	ASP	3.4
1	C	250	SER	3.4
1	D	135	ASP	3.4
1	A	412	ALA	3.4
1	E	10	ILE	3.3
1	A	395	SER	3.3
1	B	4	VAL	3.3
1	B	397	ILE	3.2
1	E	11	ALA	3.2
1	C	138	ASN	3.2
1	D	11	ALA	3.1
1	A	55	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	311	LYS	3.1
1	D	192	GLN	3.0
1	C	135	ASP	3.0
1	E	71	TRP	3.0
1	D	4	VAL	3.0
1	C	176	GLU	3.0
1	C	95	PRO	2.9
1	E	13	GLU	2.9
1	A	4	VAL	2.9
1	E	59	GLY	2.9
1	A	79	ASN	2.8
1	A	250	SER	2.8
1	A	179	LEU	2.8
1	E	176	GLU	2.8
1	C	26	CYS	2.7
1	C	157	THR	2.7
1	D	123	GLN	2.7
1	A	10	ILE	2.7
1	E	25	GLU	2.7
1	A	100	GLN	2.6
1	D	59	GLY	2.6
1	D	250	SER	2.6
1	C	10	ILE	2.6
1	D	160	ASP	2.6
1	E	61	ARG	2.6
1	D	10	ILE	2.6
1	E	153	ASP	2.5
1	C	134	VAL	2.5
1	E	412	ALA	2.5
1	E	74	GLU	2.5
1	B	280	ALA	2.5
1	A	45	SER	2.4
1	D	249	GLU	2.4
1	C	61	ARG	2.4
1	E	311	LYS	2.4
1	A	309	PHE	2.4
1	E	14	PRO	2.4
1	A	13	GLU	2.4
1	D	26	CYS	2.4
1	C	249	GLU	2.3
1	C	136	THR	2.3
1	B	274	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	12	ASP	2.3
1	E	65	TYR	2.3
1	A	147	LYS	2.3
1	A	95	PRO	2.2
1	B	26	CYS	2.2
1	C	12	ASP	2.2
1	A	280	ALA	2.2
1	C	413	THR	2.2
1	C	65	TYR	2.2
1	C	87	ASP	2.2
1	C	177	ASP	2.1
1	C	4	VAL	2.1
1	E	60	VAL	2.1
1	D	64	THR	2.1
1	A	128	TYR	2.1
1	B	49	ARG	2.1
1	A	413	THR	2.1
1	B	47	LYS	2.1
1	B	396	ARG	2.1
1	B	309	PHE	2.1
1	B	250	SER	2.0
1	C	111	SER	2.0
1	B	10	ILE	2.0
1	E	247	ASN	2.0
1	B	249	GLU	2.0
1	C	311	LYS	2.0
1	A	49	ARG	2.0
1	D	188	ARG	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,

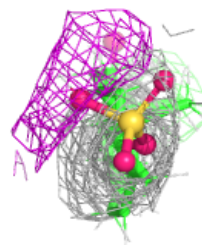
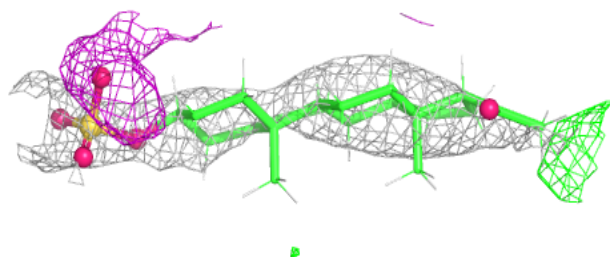
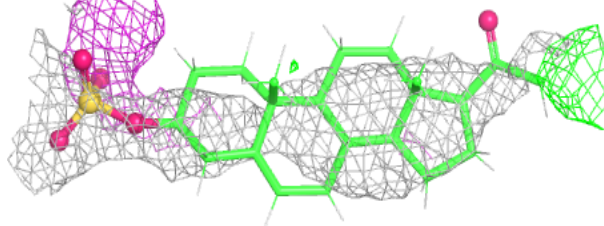
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	A8W	D	504	27/27	0.64	0.24	199,252,286,328	0
5	Y01	A	504	35/35	0.72	0.27	155,203,233,239	0
5	Y01	B	506	35/35	0.74	0.31	153,208,241,250	0
5	Y01	E	505	35/35	0.76	0.25	130,204,228,236	0
4	A8W	A	503	27/27	0.77	0.24	200,240,257,261	0
4	A8W	C	503	27/27	0.78	0.22	190,250,276,315	0
4	A8W	E	504	27/27	0.79	0.20	177,220,243,280	0
5	Y01	B	505	35/35	0.82	0.27	150,213,239,243	0
2	ACT	E	502	4/4	0.83	0.38	119,125,127,129	0
4	A8W	B	504	27/27	0.84	0.17	162,211,243,282	0
5	Y01	D	505	35/35	0.85	0.26	127,213,240,253	0
2	ACT	B	502	4/4	0.87	0.36	109,124,125,127	0
2	ACT	D	502	4/4	0.88	0.35	128,137,139,144	0
3	CL	A	502	1/1	0.92	0.13	89,89,89,89	0
3	CL	B	503	1/1	0.92	0.12	85,85,85,85	0
3	CL	C	502	1/1	0.94	0.16	97,97,97,97	0
2	ACT	D	501	4/4	0.95	0.17	114,115,122,125	0
2	ACT	A	501	4/4	0.95	0.21	117,119,120,123	0
2	ACT	E	501	4/4	0.96	0.12	85,90,96,102	0
3	CL	D	503	1/1	0.96	0.08	85,85,85,85	0
2	ACT	B	501	4/4	0.96	0.15	105,112,118,120	0
2	ACT	C	501	4/4	0.97	0.13	99,105,105,108	0
3	CL	E	503	1/1	0.98	0.07	97,97,97,97	0

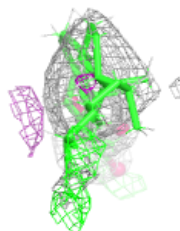
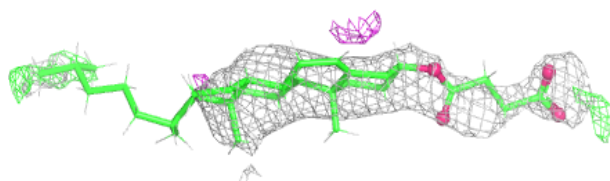
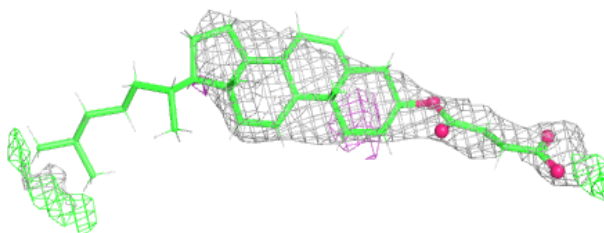
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A8W D 504:

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

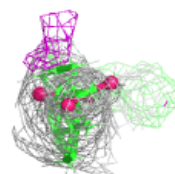
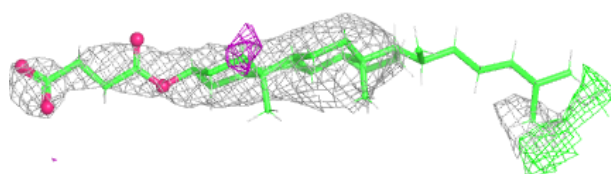
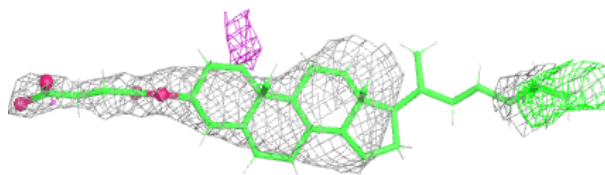
**Electron density around Y01 A 504:**

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

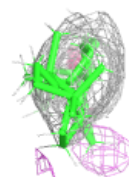
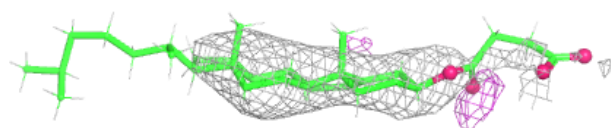
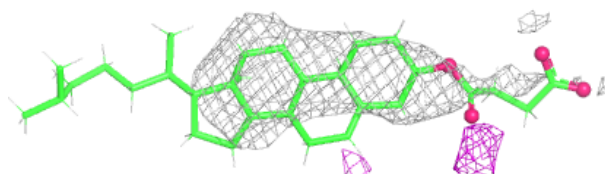


Electron density around Y01 B 506:

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

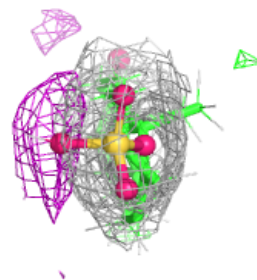
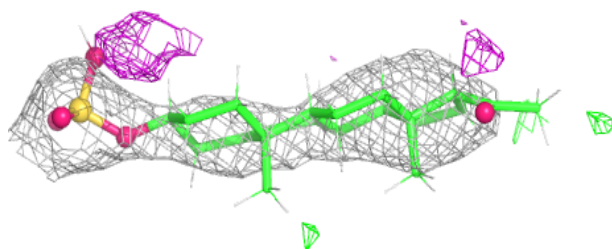
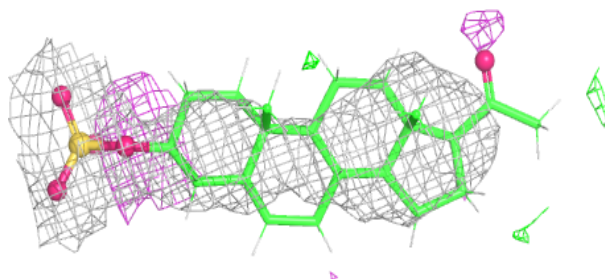
**Electron density around Y01 E 505:**

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

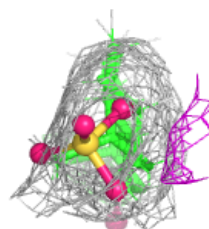
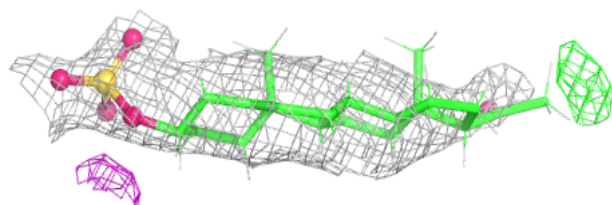
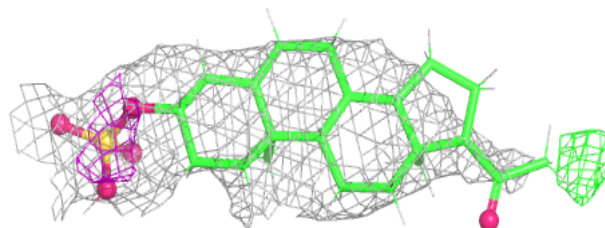


Electron density around A8W A 503:

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

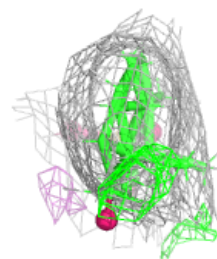
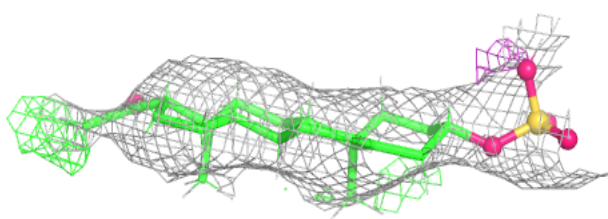
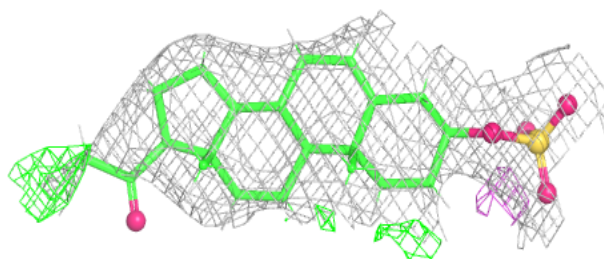
**Electron density around A8W C 503:**

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

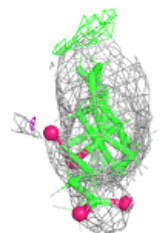
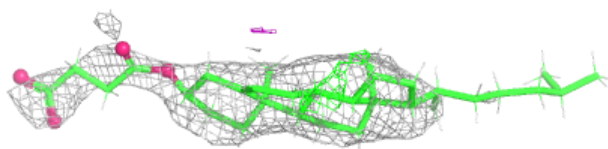
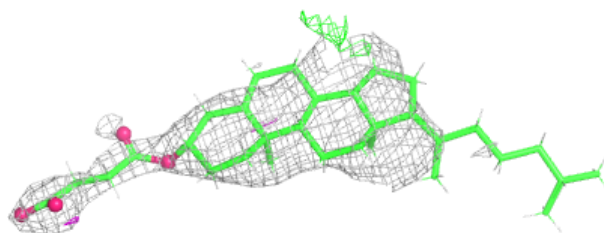


Electron density around A8W E 504:

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

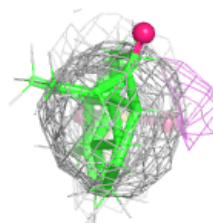
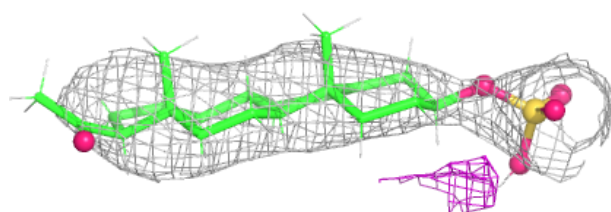
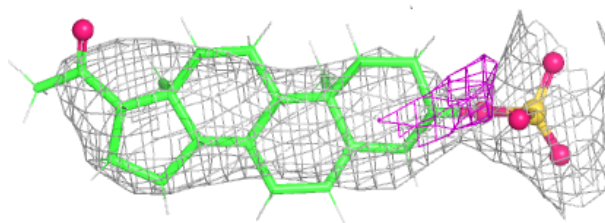
**Electron density around Y01 B 505:**

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

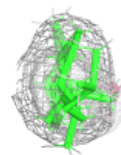
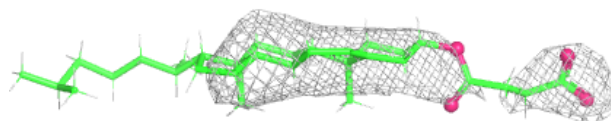
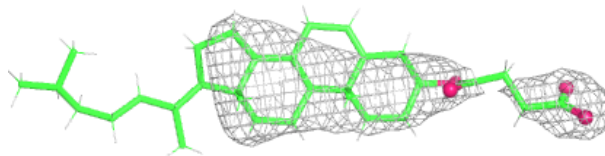


Electron density around A8W B 504:

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

**Electron density around Y01 D 505:**

$2mF_o-DF_c$ (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.