



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2023 – 05:25 am GMT

PDB ID : 2VCT
Title : Glutathione transferase A2-2 in complex with delta-4-andostrene-3-17- dione
Authors : Tars, K.; Olin, B.; Mannervik, B.
Deposited on : 2007-09-27
Resolution : 2.10 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

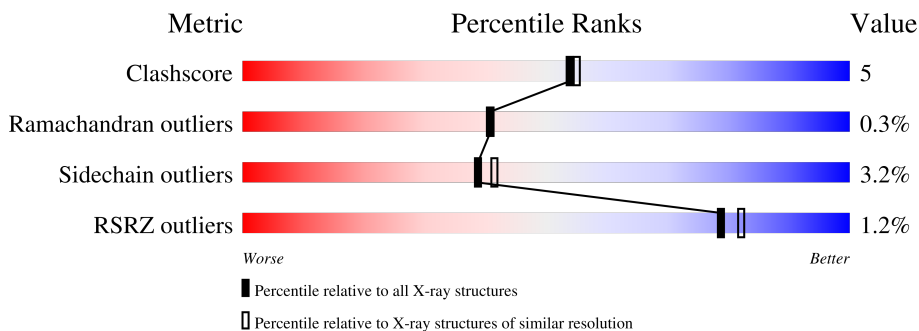
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



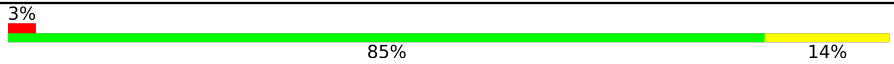

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	222	88% 11%
1	B	222	85% 14%
1	C	222	83% 14% .
1	D	222	90% 8% .
1	E	222	% 86% 13% .
1	F	222	84% 15% .

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Mol	Chain	Length	Quality of chain
1	G	222	 3% 85% 14%
1	H	222	 5% 82% 16%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16109 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.

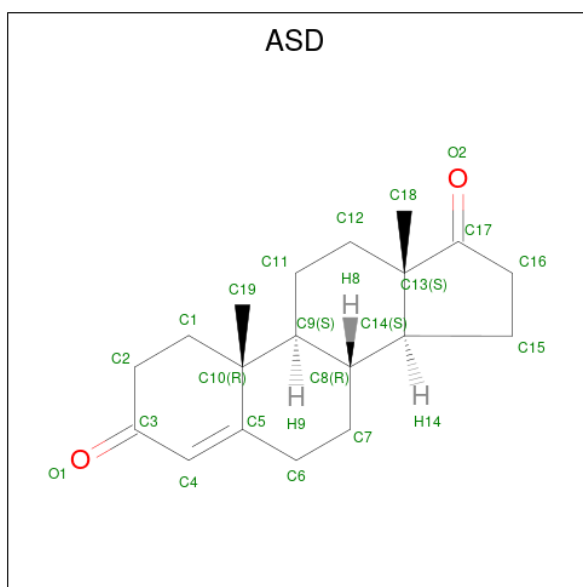
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	1800	1164	299	330	7	0	0	0
1	B	221	1800	1164	299	330	7	0	0	0
1	C	221	1800	1164	299	330	7	0	0	0
1	D	221	1800	1164	299	330	7	0	0	0
1	E	221	1800	1164	299	330	7	0	0	0
1	F	221	1800	1164	299	330	7	0	0	0
1	G	221	1800	1164	299	330	7	0	0	0
1	H	221	1800	1164	299	330	7	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	THR	SER	variant	UNP P09210
B	112	THR	SER	variant	UNP P09210
C	112	THR	SER	variant	UNP P09210
D	112	THR	SER	variant	UNP P09210
E	112	THR	SER	variant	UNP P09210
F	112	THR	SER	variant	UNP P09210
G	112	THR	SER	variant	UNP P09210
H	112	THR	SER	variant	UNP P09210

- Molecule 2 is 4-ANDROSTENE-3-17-DIONE (three-letter code: ASD) (formula: C₁₉H₂₆O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			21	19 2		
2	B	1	Total	C O	0	0
			21	19 2		
2	C	1	Total	C O	0	0
			21	19 2		
2	D	1	Total	C O	0	0
			21	19 2		


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	297	Total	O	0	0
			297	297		
3	B	281	Total	O	0	0
			281	281		
3	C	284	Total	O	0	0
			284	284		
3	D	255	Total	O	0	0
			255	255		
3	E	123	Total	O	0	0
			123	123		
3	F	165	Total	O	0	0
			165	165		
3	G	115	Total	O	0	0
			115	115		
3	H	105	Total	O	0	0
			105	105		

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.

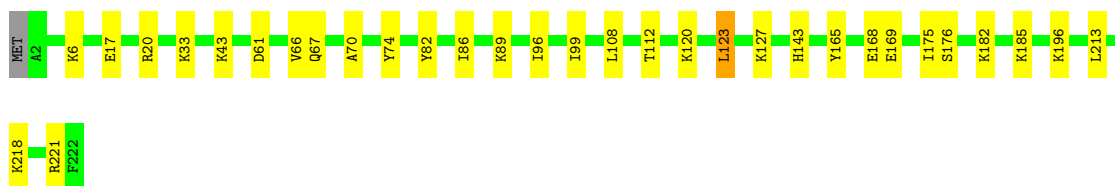
- Molecule 1: GLUTATHIONE S-TRANSFERASE A2

Chain A: 




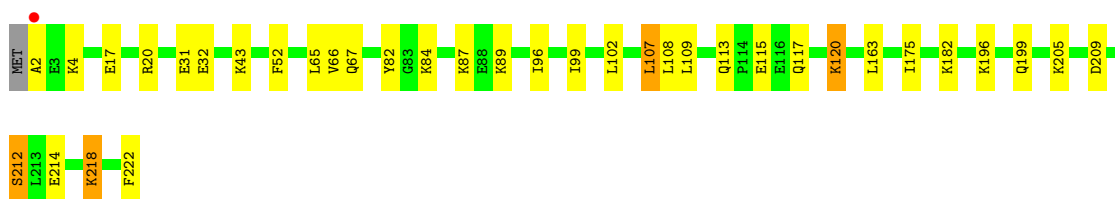
- Molecule 1: GLUTATHIONE S-TRANSFERASE A2

Chain B: 




- Molecule 1: GLUTATHIONE S-TRANSFERASE A2

Chain C: 




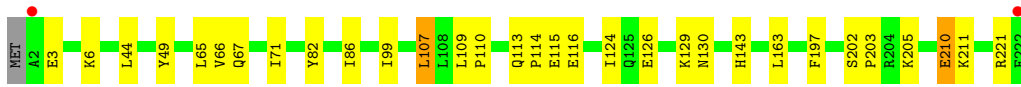
- Molecule 1: GLUTATHIONE S-TRANSFERASE A2

Chain D: 

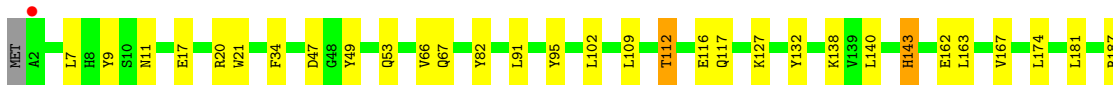
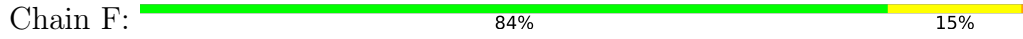


- Molecule 1: GLUTATHIONE S-TRANSFERASE A2

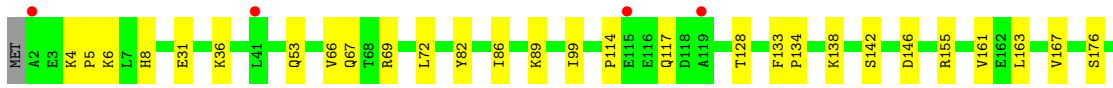
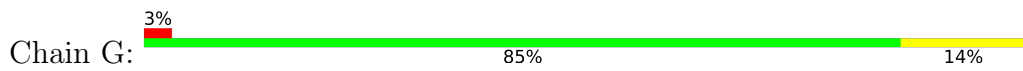
Chain E: 



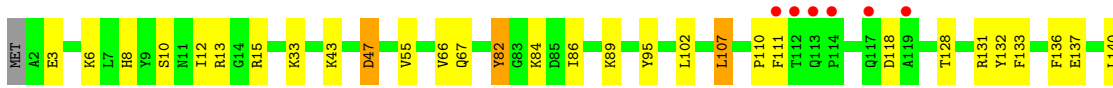
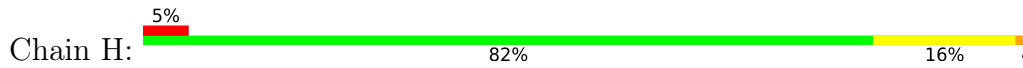
● Molecule 1: GLUTATHIONE S-TRANSFERASE A2



● Molecule 1: GLUTATHIONE S-TRANSFERASE A2



● Molecule 1: GLUTATHIONE S-TRANSFERASE A2



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.55Å 97.34Å 110.30Å 90.00° 115.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 36.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.10) 62.5 (36.64-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.288 0.227 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtrriage
Anisotropy	0.463	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.130 for l,-k,h	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16109	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.65% 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: ASD

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	0.72	0/1835	0.75	0/2465
1	B	0.64	0/1835	0.73	0/2465
1	C	0.71	0/1835	0.77	1/2465 (0.0%)
1	D	0.65	0/1835	0.72	2/2465 (0.1%)
1	E	0.51	0/1835	0.62	1/2465 (0.0%)
1	F	0.52	0/1835	0.68	1/2465 (0.0%)
1	G	0.48	0/1835	0.60	0/2465
1	H	0.47	0/1835	0.58	1/2465 (0.0%)
All	All	0.60	0/14680	0.68	6/19720 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	LEU	CA-CB-CG	6.15	129.45	115.30
1	E	107	LEU	CA-CB-CG	5.55	128.07	115.30
1	F	7	LEU	CA-CB-CG	5.51	127.97	115.30
1	H	107	LEU	CA-CB-CG	5.45	127.82	115.30
1	D	123	LEU	CA-CB-CG	5.22	127.30	115.30
1	D	208	MET	CA-CB-CG	-5.20	104.45	113.30

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	1800	0	1858	21	0
1	B	1800	0	1858	22	0
1	C	1800	0	1858	27	0
1	D	1800	0	1858	17	0
1	E	1800	0	1858	14	0
1	F	1800	0	1858	20	0
1	G	1800	0	1858	19	0
1	H	1800	0	1858	22	0
2	A	21	0	26	0	0
2	B	21	0	26	0	0
2	C	21	0	26	5	0
2	D	21	0	26	0	0
3	A	297	0	0	8	0
3	B	281	0	0	10	0
3	C	284	0	0	9	0
3	D	255	0	0	8	0
3	E	123	0	0	5	0
3	F	165	0	0	1	0
3	G	115	0	0	7	0
3	H	105	0	0	3	0
All	All	16109	0	14968	157	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 5.

All (157) 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)
3:A:2141:HOH:O	1:B:86:ILE:HG22	1.58	1.03
1:B:33:LYS:HB2	3:B:2064:HOH:O	1.65	0.96
3:G:2011:HOH:O	1:H:89:LYS:HD3	1.72	0.90
1:H:89:LYS:HG3	3:H:2040:HOH:O	1.74	0.86
1:A:64:LYS:HG3	3:A:2036:HOH:O	1.79	0.82
1:B:6:LYS:HG2	3:B:2064:HOH:O	1.79	0.81
1:E:210:GLU:HB2	3:E:2123:HOH:O	1.82	0.80
1:D:107:LEU:CD1	3:D:2014:HOH:O	2.30	0.79
1:C:113:GLN:HG2	3:C:2178:HOH:O	1.87	0.74
1:A:59:GLU:HG2	1:A:64:LYS:CD	2.20	0.72
1:H:140:LEU:HB3	1:H:180:LEU:HD22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:ILE:HG23	1:E:163:LEU:HD22	1.72	0.71
1:A:31:GLU:HG2	3:A:2004:HOH:O	1.93	0.68
1:D:213:LEU:HD23	3:D:2247:HOH:O	1.93	0.68
1:G:134:PRO:O	1:G:138:LYS:HB2	1.95	0.67
1:D:215:GLU:HB2	3:D:2249:HOH:O	1.95	0.66
1:A:82:TYR:O	1:A:89:LYS:HG2	1.95	0.66
1:G:176:SER:HA	3:G:2089:HOH:O	1.96	0.65
1:B:112:THR:HG21	1:B:120:LYS:HD2	1.79	0.64
1:C:222:PHE:CD1	2:C:1223:ASD:H61	2.33	0.63
1:H:6:LYS:HD3	1:H:33:LYS:HD2	1.79	0.63
1:B:127:LYS:HG2	3:B:2185:HOH:O	1.98	0.63
1:A:89:LYS:CE	3:A:2159:HOH:O	2.47	0.62
1:C:222:PHE:CG	2:C:1223:ASD:H62	2.35	0.62
1:H:102:LEU:HD23	1:H:163:LEU:HD21	1.81	0.61
1:C:65:LEU:HD22	3:C:2121:HOH:O	2.01	0.61
1:D:208:MET:HG3	3:D:2241:HOH:O	2.01	0.60
1:G:53:GLN:HB2	1:H:131:ARG:HH21	1.66	0.60
1:C:66:VAL:O	1:C:67:GLN:HB2	2.00	0.60
1:A:59:GLU:HG2	1:A:64:LYS:HD2	1.83	0.60
1:B:176:SER:HA	1:B:182:LYS:HE3	1.83	0.59
1:H:43:LYS:O	1:H:47:ASP:HB2	2.01	0.59
1:D:208:MET:HG2	1:D:212:SER:OG	2.03	0.59
1:A:64:LYS:HE3	3:A:2110:HOH:O	2.02	0.59
1:B:165:TYR:O	1:B:169:GLU:HG3	2.03	0.58
1:G:99:ILE:HG23	1:G:163:LEU:HD22	1.85	0.58
1:A:183:ALA:O	1:A:187:ARG:HG3	2.04	0.58
1:D:215:GLU:HG2	1:D:219:ILE:HD12	1.85	0.57
1:C:4:LYS:HD2	1:C:31:GLU:HG3	1.87	0.57
1:C:109:LEU:HD13	1:C:120:LYS:HB3	1.87	0.56
1:B:89:LYS:HE3	3:B:2153:HOH:O	2.05	0.56
1:C:222:PHE:CG	2:C:1223:ASD:C6	2.89	0.56
1:B:185:LYS:HE2	3:B:2115:HOH:O	2.04	0.56
1:B:168:GLU:HG3	3:B:2223:HOH:O	2.06	0.55
1:A:89:LYS:HE2	3:A:2159:HOH:O	2.05	0.55
1:A:3:GLU:HG3	1:A:4:LYS:N	2.22	0.55
1:B:17:GLU:OE1	1:B:20:ARG:HD2	2.08	0.54
1:A:59:GLU:HG2	1:A:64:LYS:HD3	1.90	0.54
1:E:65:LEU:HB3	1:E:71:ILE:HG12	1.90	0.54
1:F:187:ARG:HD3	1:G:146:ASP:OD2	2.08	0.53
1:G:67:GLN:NE2	3:G:2034:HOH:O	2.42	0.53
1:F:21:TRP:NE1	1:F:162:GLU:HG3	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LYS:HD2	1:D:31:GLU:HG3	1.89	0.53
1:F:209:ASP:O	1:F:213:LEU:HB2	2.09	0.53
1:C:175:ILE:HG12	1:C:182:LYS:HG3	1.91	0.52
1:C:214:GLU:O	1:C:218:LYS:HG2	2.09	0.52
1:D:107:LEU:HD12	3:D:2014:HOH:O	2.04	0.52
1:F:112:THR:HG22	1:F:117:GLN:HG3	1.91	0.52
1:G:89:LYS:HE3	3:G:2048:HOH:O	2.09	0.52
1:C:96:ILE:HA	1:C:99:ILE:HD12	1.91	0.52
1:E:109:LEU:HD22	1:E:124:ILE:HD12	1.91	0.52
1:A:190:ASN:ND2	3:A:2260:HOH:O	2.37	0.52
1:B:123:LEU:HD12	3:B:2185:HOH:O	2.09	0.52
1:C:66:VAL:HG22	1:D:94:MET:SD	2.51	0.51
1:C:52:PHE:CZ	1:D:98:GLY:HA3	2.46	0.51
1:H:82:TYR:CD1	1:H:89:LYS:HG2	2.45	0.51
1:C:17:GLU:OE1	1:C:20:ARG:HD2	2.11	0.51
1:F:140:LEU:HA	1:F:143:HIS:CE1	2.46	0.51
1:F:11:ASN:OD1	1:F:205:LYS:HE3	2.11	0.51
1:F:112:THR:HG23	1:F:116:GLU:HB2	1.92	0.51
1:G:114:PRO:HA	1:G:117:GLN:HG3	1.92	0.50
1:G:161:VAL:HG21	1:G:188:ILE:HG13	1.94	0.50
1:B:6:LYS:CG	3:B:2064:HOH:O	2.46	0.50
1:B:168:GLU:CG	3:B:2223:HOH:O	2.60	0.50
1:E:110:PRO:HD3	3:E:2067:HOH:O	2.09	0.50
3:C:2121:HOH:O	1:D:94:MET:HB2	2.12	0.50
1:E:203:PRO:O	1:E:205:LYS:NZ	2.42	0.50
1:F:17:GLU:OE1	1:F:20:ARG:HD2	2.11	0.49
1:D:102:LEU:HD23	1:D:163:LEU:HD21	1.93	0.49
1:F:167:VAL:HG13	1:F:174:LEU:HD12	1.95	0.49
1:C:222:PHE:HB3	3:C:2282:HOH:O	2.11	0.49
1:F:127:LYS:HE3	3:F:2108:HOH:O	2.13	0.48
1:G:69:ARG:NH2	3:G:2036:HOH:O	2.45	0.48
1:A:112:THR:HG21	1:A:120:LYS:HE3	1.96	0.48
1:A:217:ARG:O	1:A:221:ARG:HA	2.12	0.48
1:F:66:VAL:O	1:F:67:GLN:HB2	2.13	0.48
1:H:136:PHE:HE2	3:H:2047:HOH:O	1.95	0.48
1:H:128:THR:O	1:H:133:PHE:HB2	2.13	0.48
1:D:118:ASP:O	3:D:2153:HOH:O	2.20	0.48
1:H:8:HIS:CE1	1:H:33:LYS:HD3	2.48	0.48
1:H:10:SER:OG	1:H:12:ILE:HG12	2.14	0.48
1:E:129:LYS:HE3	3:E:2075:HOH:O	2.14	0.48
1:C:102:LEU:HD23	1:C:163:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:VAL:O	1:H:67:GLN:HB2	2.13	0.47
1:A:60:ILE:O	1:A:60:ILE:HG23	2.14	0.47
1:G:66:VAL:O	1:G:67:GLN:HB2	2.14	0.47
1:H:89:LYS:CE	3:H:2043:HOH:O	2.64	0.46
1:B:66:VAL:O	1:B:67:GLN:HB2	2.16	0.46
1:H:137:GLU:OE2	1:H:179:PRO:HD2	2.14	0.46
1:B:61:ASP:OD2	1:B:74:TYR:OH	2.31	0.46
1:B:175:ILE:HG23	1:B:182:LYS:HE2	1.98	0.46
1:H:143:HIS:C	1:H:145:GLN:H	2.19	0.46
1:B:218:LYS:HD2	1:B:218:LYS:HA	1.70	0.45
1:C:32:GLU:OE2	1:C:205:LYS:NZ	2.46	0.45
1:H:15:ARG:HG2	1:H:107:LEU:HD21	1.97	0.45
1:A:36:LYS:HE2	3:A:2058:HOH:O	2.15	0.45
1:B:108:LEU:O	1:B:112:THR:HG23	2.16	0.45
1:F:102:LEU:HD22	1:F:132:TYR:CD2	2.52	0.45
1:C:43:LYS:HE3	3:C:2031:HOH:O	2.17	0.45
1:C:209:ASP:H	1:C:212:SER:HB2	1.81	0.45
1:G:6:LYS:HD3	3:G:2030:HOH:O	2.16	0.45
1:C:87:LYS:HB2	3:C:2155:HOH:O	2.17	0.44
1:C:196:LYS:O	1:C:199:GLN:HB2	2.18	0.44
1:G:184:LEU:O	1:G:188:ILE:HG12	2.18	0.44
1:D:64:LYS:NZ	3:D:2099:HOH:O	2.48	0.44
1:D:99:ILE:HG23	1:D:163:LEU:HD22	1.99	0.44
1:B:196:LYS:NZ	3:B:2254:HOH:O	2.45	0.44
1:F:21:TRP:CE2	1:F:162:GLU:HG3	2.52	0.44
1:F:91:LEU:O	1:F:95:TYR:CD1	2.71	0.44
3:E:2076:HOH:O	1:F:53:GLN:HG3	2.18	0.43
1:C:115:GLU:HB2	3:C:2082:HOH:O	2.18	0.43
1:D:107:LEU:HD13	3:D:2014:HOH:O	2.06	0.43
1:C:222:PHE:CB	2:C:1223:ASD:H62	2.49	0.43
1:A:199:GLN:HB3	1:A:200:PRO:HD2	2.01	0.43
1:F:9:TYR:O	1:F:34:PHE:HA	2.19	0.43
1:B:96:ILE:HA	1:B:99:ILE:HD12	1.99	0.42
1:C:2:ALA:HB3	3:C:2115:HOH:O	2.19	0.42
1:E:44:LEU:O	1:E:49:TYR:HB2	2.19	0.42
1:G:128:THR:O	1:G:133:PHE:HB2	2.18	0.42
1:D:82:TYR:CE1	1:D:89:LYS:HG3	2.54	0.42
1:G:163:LEU:O	1:G:167:VAL:HG23	2.20	0.42
1:H:102:LEU:HD22	1:H:132:TYR:CD2	2.54	0.42
1:E:129:LYS:HB3	3:E:2075:HOH:O	2.18	0.42
1:C:209:ASP:OD1	1:C:212:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:LEU:HD11	1:H:158:ILE:HD11	2.00	0.42
1:G:6:LYS:HE2	1:G:8:HIS:CE1	2.54	0.42
1:E:126:GLU:HG2	1:E:130:ASN:HD22	1.84	0.42
1:G:4:LYS:HA	1:G:5:PRO:HD2	1.82	0.42
1:H:8:HIS:HE1	1:H:33:LYS:HD3	1.84	0.42
1:H:95:TYR:HB3	1:H:136:PHE:HE1	1.85	0.42
1:A:35:ILE:HG23	1:A:40:ASP:HB2	2.01	0.41
1:A:91:LEU:O	1:A:95:TYR:CD1	2.74	0.41
1:G:182:LYS:HE2	3:G:2089:HOH:O	2.20	0.41
1:E:66:VAL:O	1:E:67:GLN:HB2	2.19	0.41
1:A:93:ASP:HB3	1:B:70:ALA:HA	2.03	0.41
1:F:47:ASP:HB3	1:F:49:TYR:CD1	2.56	0.41
1:E:197:PHE:O	1:E:202:SER:OG	2.21	0.41
1:A:188:ILE:O	1:A:191:LEU:HB2	2.21	0.40
1:C:218:LYS:HD2	3:C:2279:HOH:O	2.21	0.40
1:F:109:LEU:O	1:F:112:THR:HB	2.20	0.40
1:F:163:LEU:O	1:F:167:VAL:HG23	2.21	0.40
1:C:108:LEU:CD2	2:C:1223:ASD:H111	2.51	0.40
1:E:210:GLU:HG3	1:E:211:LYS:N	2.36	0.40
1:H:110:PRO:HG2	1:H:111:PHE:CD1	2.56	0.40
1:E:113:GLN:O	1:E:115:GLU:N	2.54	0.40
1:F:181:LEU:HD23	1:F:181:LEU:HA	1.94	0.40
1:G:72:LEU:HB3	1:G:155:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	219/222 (99%)	211 (96%)	8 (4%)	0	100 100
1	B	219/222 (99%)	211 (96%)	8 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	219/222 (99%)	210 (96%)	9 (4%)	0	100	100
1	D	219/222 (99%)	211 (96%)	8 (4%)	0	100	100
1	E	219/222 (99%)	210 (96%)	7 (3%)	2 (1%)	17	12
1	F	219/222 (99%)	212 (97%)	7 (3%)	0	100	100
1	G	219/222 (99%)	205 (94%)	12 (6%)	2 (1%)	17	12
1	H	219/222 (99%)	208 (95%)	9 (4%)	2 (1%)	17	12
All	All	1752/1776 (99%)	1678 (96%)	68 (4%)	6 (0%)	41	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	221	ARG
1	H	13	ARG
1	G	142	SER
1	H	3	GLU
1	E	114	PRO
1	G	86	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/198 (100%)	195 (99%)	2 (1%)	76	82
1	B	197/198 (100%)	191 (97%)	6 (3%)	41	44
1	C	197/198 (100%)	189 (96%)	8 (4%)	30	31
1	D	197/198 (100%)	190 (96%)	7 (4%)	35	36
1	E	197/198 (100%)	189 (96%)	8 (4%)	30	31
1	F	197/198 (100%)	192 (98%)	5 (2%)	47	52
1	G	197/198 (100%)	193 (98%)	4 (2%)	55	60
1	H	197/198 (100%)	187 (95%)	10 (5%)	24	22
All	All	1576/1584 (100%)	1526 (97%)	50 (3%)	39	41

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	TYR
1	A	123	LEU
1	B	43	LYS
1	B	82	TYR
1	B	123	LEU
1	B	143	HIS
1	B	213	LEU
1	B	221	ARG
1	C	82	TYR
1	C	84	LYS
1	C	89	LYS
1	C	107	LEU
1	C	117	GLN
1	C	120	LYS
1	C	212	SER
1	C	218	LYS
1	D	18	SER
1	D	82	TYR
1	D	123	LEU
1	D	143	HIS
1	D	168	GLU
1	D	169	GLU
1	D	213	LEU
1	E	3	GLU
1	E	6	LYS
1	E	82	TYR
1	E	86	ILE
1	E	107	LEU
1	E	116	GLU
1	E	143	HIS
1	E	210	GLU
1	F	82	TYR
1	F	112	THR
1	F	138	LYS
1	F	143	HIS
1	F	221	ARG
1	G	31	GLU
1	G	36	LYS
1	G	82	TYR
1	G	190	ASN
1	H	47	ASP
1	H	55	VAL

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Mol	Chain	Res	Type
1	H	82	TYR
1	H	84	LYS
1	H	86	ILE
1	H	118	ASP
1	H	142	SER
1	H	177	SER
1	H	180	LEU
1	H	213	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	B	54	GLN
1	C	199	GLN
1	D	53	GLN
1	D	54	GLN
1	E	53	GLN
1	E	54	GLN
1	E	130	ASN
1	F	53	GLN
1	G	11	ASN
1	G	54	GLN
1	G	113	GLN
1	G	190	ASN
1	G	199	GLN
1	H	130	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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
2	ASD	D	1223	-	24,24,24	0.76	0	39,39,39	1.84	10 (25%)
2	ASD	A	1223	-	24,24,24	0.56	0	39,39,39	1.54	9 (23%)
2	ASD	B	1223	-	24,24,24	0.61	0	39,39,39	1.58	6 (15%)
2	ASD	C	1223	-	24,24,24	0.52	0	39,39,39	1.81	9 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ASD	D	1223	-	-	-	0/4/4/4
2	ASD	A	1223	-	-	-	0/4/4/4
2	ASD	B	1223	-	-	-	0/4/4/4
2	ASD	C	1223	-	-	-	0/4/4/4

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1223	ASD	C16-C17-C13	4.73	113.26	108.59
2	B	1223	ASD	C15-C14-C13	4.42	108.04	104.08
2	D	1223	ASD	C15-C14-C13	4.18	107.82	104.08
2	C	1223	ASD	C7-C8-C9	-4.11	105.40	110.49
2	C	1223	ASD	C16-C17-C13	3.79	112.34	108.59
2	A	1223	ASD	C16-C17-C13	3.66	112.20	108.59
2	D	1223	ASD	C9-C10-C5	-3.52	104.14	109.65
2	B	1223	ASD	C16-C17-C13	3.43	111.98	108.59
2	C	1223	ASD	C6-C5-C4	-3.36	115.25	120.87
2	B	1223	ASD	C14-C13-C17	-3.18	96.94	100.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1223	ASD	C14-C13-C17	-3.14	96.99	100.59
2	A	1223	ASD	C1-C2-C3	-3.13	104.92	111.62
2	C	1223	ASD	C5-C4-C3	-2.76	119.21	123.67
2	C	1223	ASD	C15-C16-C17	-2.75	102.94	105.70
2	A	1223	ASD	C15-C14-C13	2.74	106.53	104.08
2	D	1223	ASD	C15-C16-C17	-2.71	102.98	105.70
2	D	1223	ASD	C1-C10-C5	2.70	113.70	108.75
2	C	1223	ASD	C15-C14-C13	2.63	106.43	104.08
2	A	1223	ASD	C6-C7-C8	2.60	116.40	111.69
2	B	1223	ASD	C15-C16-C17	-2.57	103.11	105.70
2	D	1223	ASD	O2-C17-C13	-2.55	122.57	125.96
2	A	1223	ASD	C14-C13-C17	-2.53	97.69	100.59
2	D	1223	ASD	C18-C13-C17	2.49	109.76	105.18
2	C	1223	ASD	C7-C8-C14	-2.46	107.88	112.08
2	A	1223	ASD	C6-C5-C4	-2.39	116.87	120.87
2	B	1223	ASD	C6-C5-C4	-2.31	117.00	120.87
2	D	1223	ASD	C2-C3-C4	2.27	120.24	116.74
2	D	1223	ASD	C7-C8-C9	2.25	113.28	110.49
2	D	1223	ASD	C14-C13-C17	-2.24	98.02	100.59
2	B	1223	ASD	C9-C10-C5	-2.20	106.20	109.65
2	A	1223	ASD	C5-C4-C3	-2.11	120.27	123.67
2	A	1223	ASD	O2-C17-C13	-2.09	123.18	125.96
2	A	1223	ASD	C18-C13-C14	2.05	116.00	112.98
2	C	1223	ASD	C6-C5-C10	2.01	120.47	116.77

There are no chirality outliers.

There are no torsion outliers.

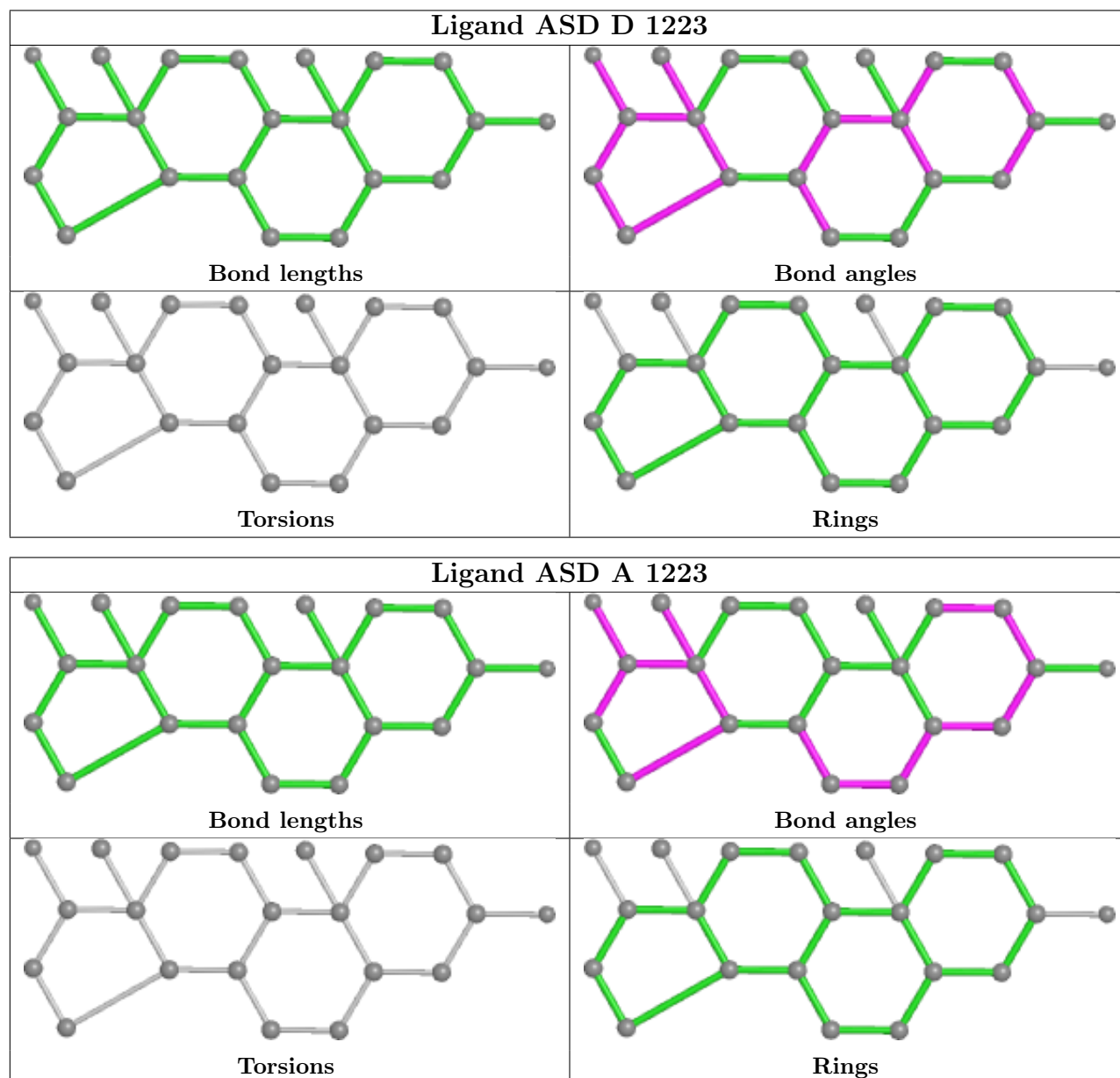
There are no ring outliers.

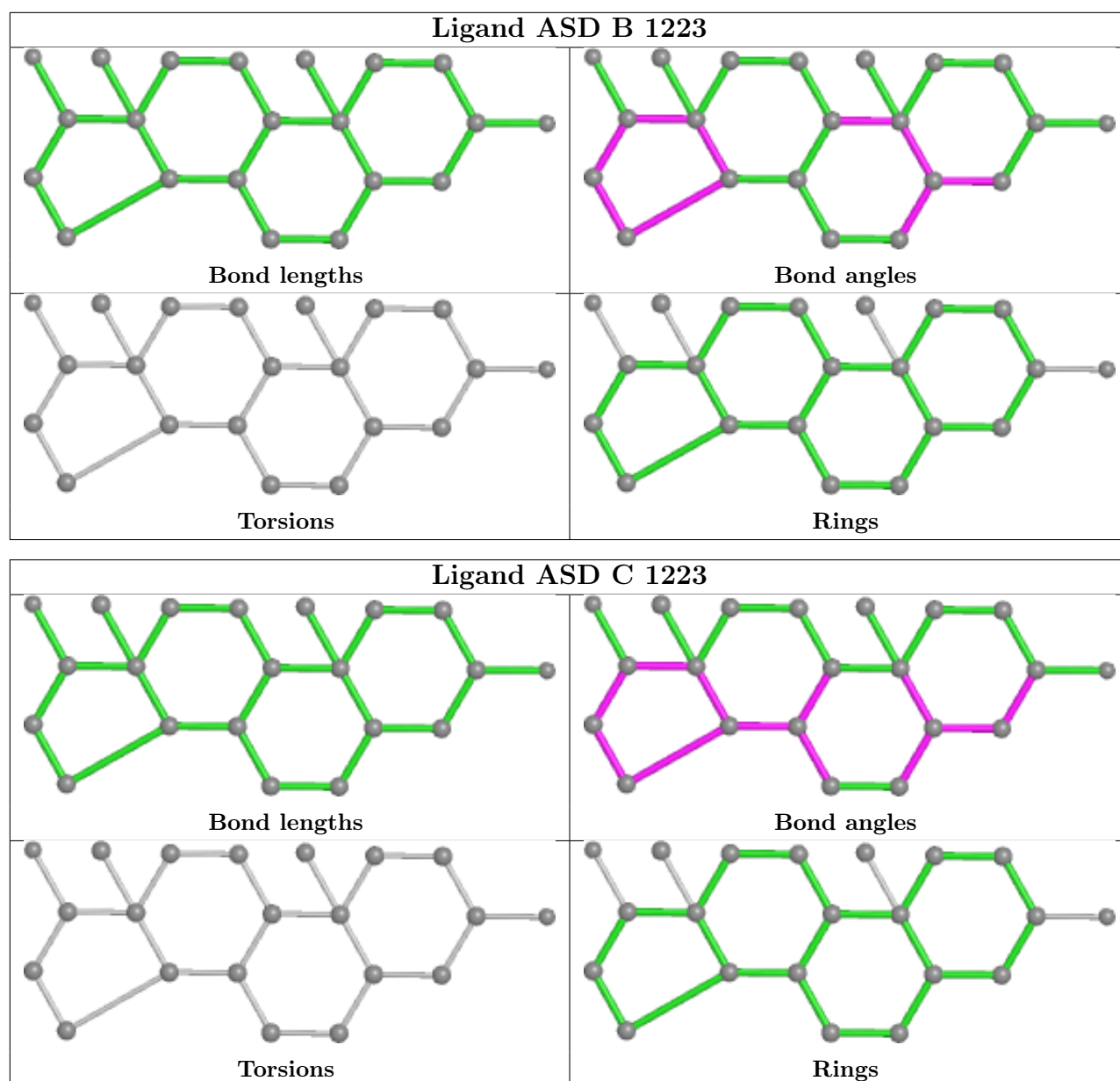
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1223	ASD	5	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	221/222 (99%)	-0.64	1 (0%) 91 92	6, 15, 25, 41	1 (0%)
1	B	221/222 (99%)	-0.55	0 100 100	7, 19, 32, 41	0
1	C	221/222 (99%)	-0.65	1 (0%) 91 92	6, 15, 27, 40	1 (0%)
1	D	221/222 (99%)	-0.62	0 100 100	9, 18, 28, 36	0
1	E	221/222 (99%)	-0.25	2 (0%) 84 86	21, 32, 50, 63	1 (0%)
1	F	221/222 (99%)	-0.42	1 (0%) 91 92	17, 28, 40, 49	0
1	G	221/222 (99%)	0.03	6 (2%) 54 60	21, 37, 56, 65	1 (0%)
1	H	221/222 (99%)	0.08	10 (4%) 33 38	19, 36, 58, 74	0
All	All	1768/1776 (99%)	-0.38	21 (1%) 79 82	6, 24, 49, 74	4 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	ALA	8.1
1	H	222	PHE	4.8
1	E	222	PHE	4.7
1	C	2	ALA	3.5
1	G	2	ALA	3.1
1	H	113	GLN	3.0
1	H	114	PRO	2.9
1	A	2	ALA	2.8
1	G	115	GLU	2.8
1	H	219	ILE	2.8
1	H	213	LEU	2.8
1	G	41	LEU	2.6
1	H	112	THR	2.5
1	E	2	ALA	2.4
1	G	222	PHE	2.4
1	G	220	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	111	PHE	2.3
1	G	119	ALA	2.3
1	H	217	ARG	2.2
1	H	117	GLN	2.1
1	H	119	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

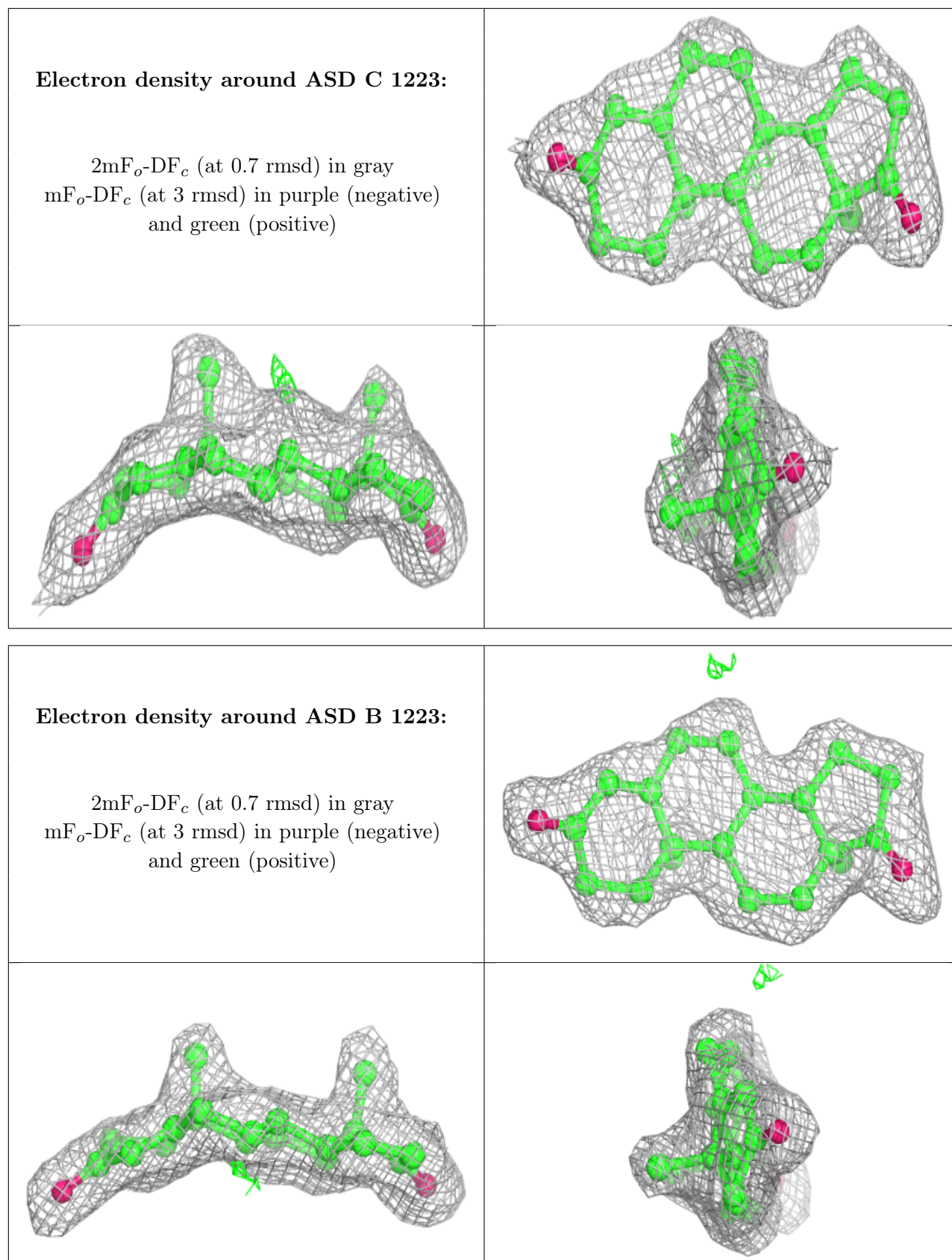
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

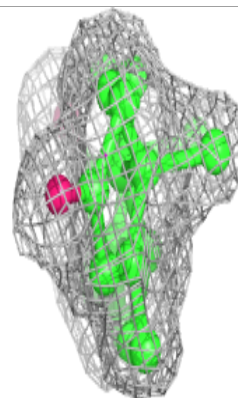
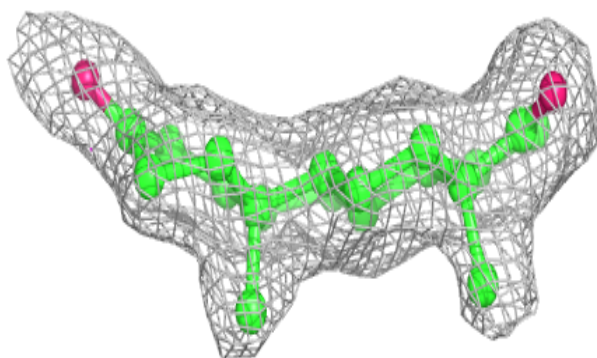
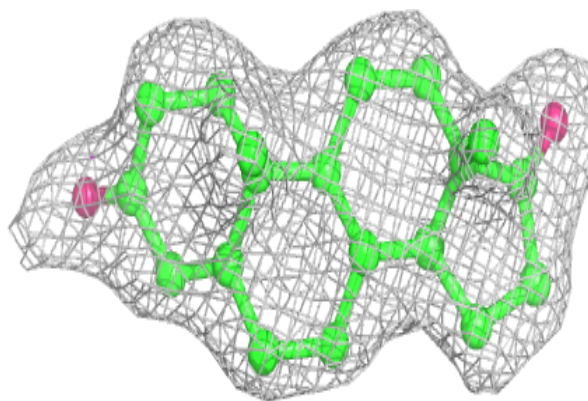
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ASD	C	1223	21/21	0.88	0.13	31,34,40,41	0
2	ASD	B	1223	21/21	0.89	0.13	26,30,34,38	0
2	ASD	A	1223	21/21	0.90	0.12	25,27,30,34	0
2	ASD	D	1223	21/21	0.93	0.14	21,27,34,36	0

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.

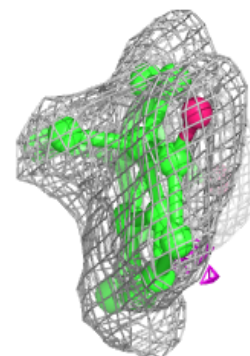
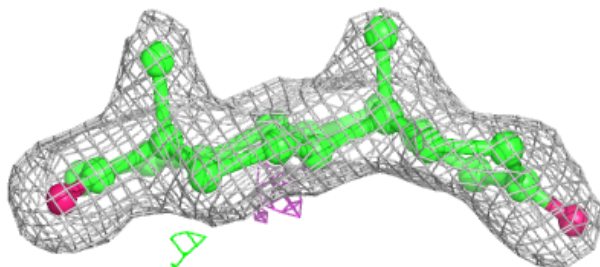
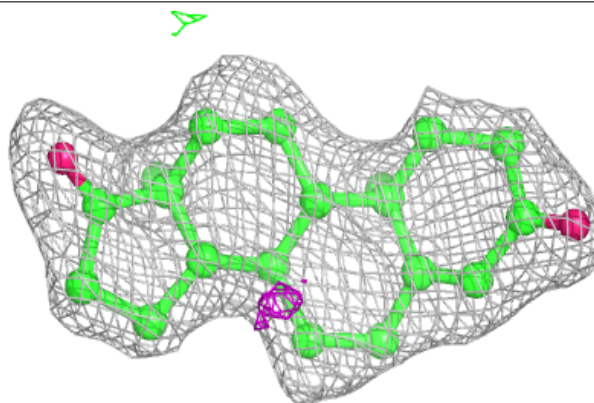


Electron density around ASD A 1223:

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

**Electron density around ASD D 1223:**

$2mF_o-DF_c$ (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.