



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:38 PM UTC

PDB ID : 7WGD / pdb_00007wgd
Title : X-ray structure of thermostabilized Drosophila dopamine transporter with GABA transporter1-like substitutions in the binding site, in substrate-free form.
Authors : Joseph, D.; Penmatsa, A.
Deposited on : 2021-12-28
Resolution : 3.20 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

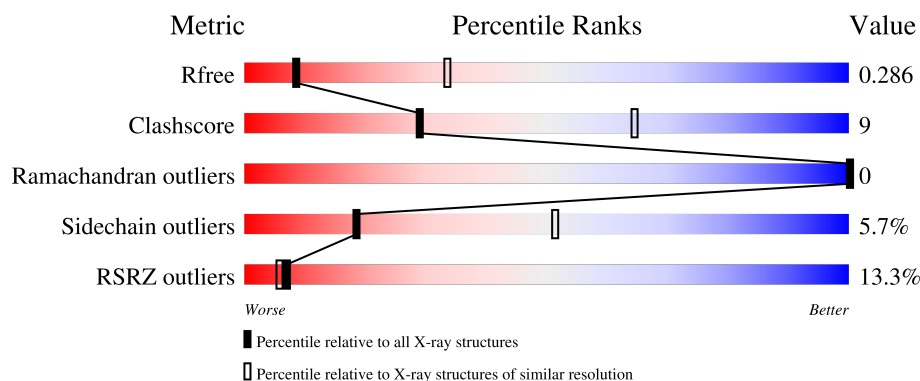
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	536	18% 76% 23% .
2	L	214	7% 76% 24% .
3	H	219	8% 76% 22% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7574 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 Sodium-dependent dopamine transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4228	2833	657	720	18	0	1	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	TYR	PHE	engineered mutation	UNP Q7K4Y6
A	46	GLY	ASP	engineered mutation	UNP Q7K4Y6
A	74	ALA	VAL	engineered mutation	UNP Q7K4Y6
A	117	SER	ALA	engineered mutation	UNP Q7K4Y6
A	120	LEU	VAL	engineered mutation	UNP Q7K4Y6
A	121	ASN	ASP	engineered mutation	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	GLN	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ARG	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	?	-	PRO	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	?	-	ILE	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ASP	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	MET	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLU	deletion	UNP Q7K4Y6
A	?	-	THR	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	MET	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	ASP	deletion	UNP Q7K4Y6
A	?	-	THR	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	275	ALA	VAL	engineered mutation	UNP Q7K4Y6
A	311	ALA	VAL	engineered mutation	UNP Q7K4Y6
A	325	LEU	PHE	engineered mutation	UNP Q7K4Y6
A	327	SER	VAL	engineered mutation	UNP Q7K4Y6
A	384	SER	GLU	engineered mutation	UNP Q7K4Y6
A	415	ALA	LEU	engineered mutation	UNP Q7K4Y6
A	422	GLN	SER	engineered mutation	UNP Q7K4Y6
A	425	THR	GLY	engineered mutation	UNP Q7K4Y6
A	426	VAL	SER	engineered mutation	UNP Q7K4Y6
A	538	LEU	GLY	engineered mutation	UNP Q7K4Y6

- Molecule 2 is a protein called Antibody fragment (9D5) Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1618	1005	266	339	8			

- Molecule 3 is a protein called Antibody fragment (9D5) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1643	1032	278	325	8			

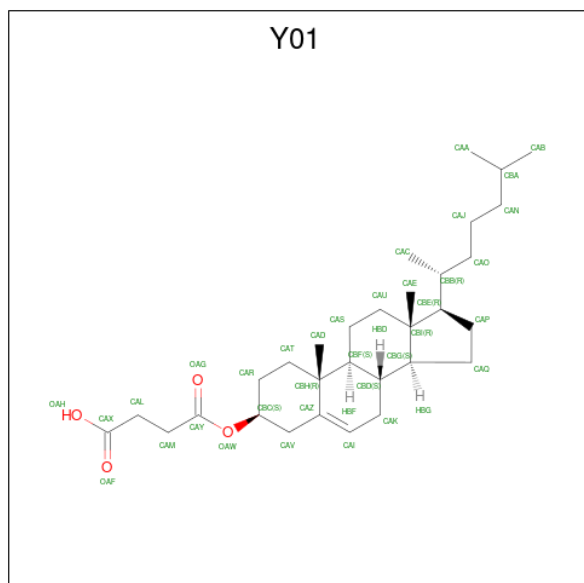
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Na 2 2	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

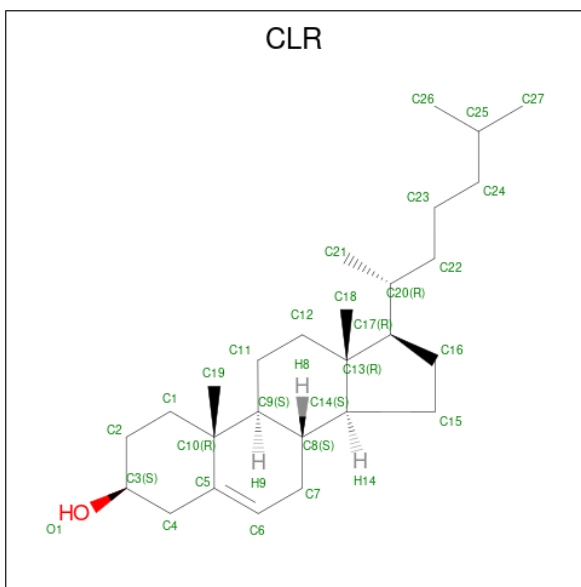
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			35	31	4		

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $\text{C}_{27}\text{H}_{46}\text{O}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			28	27	1		

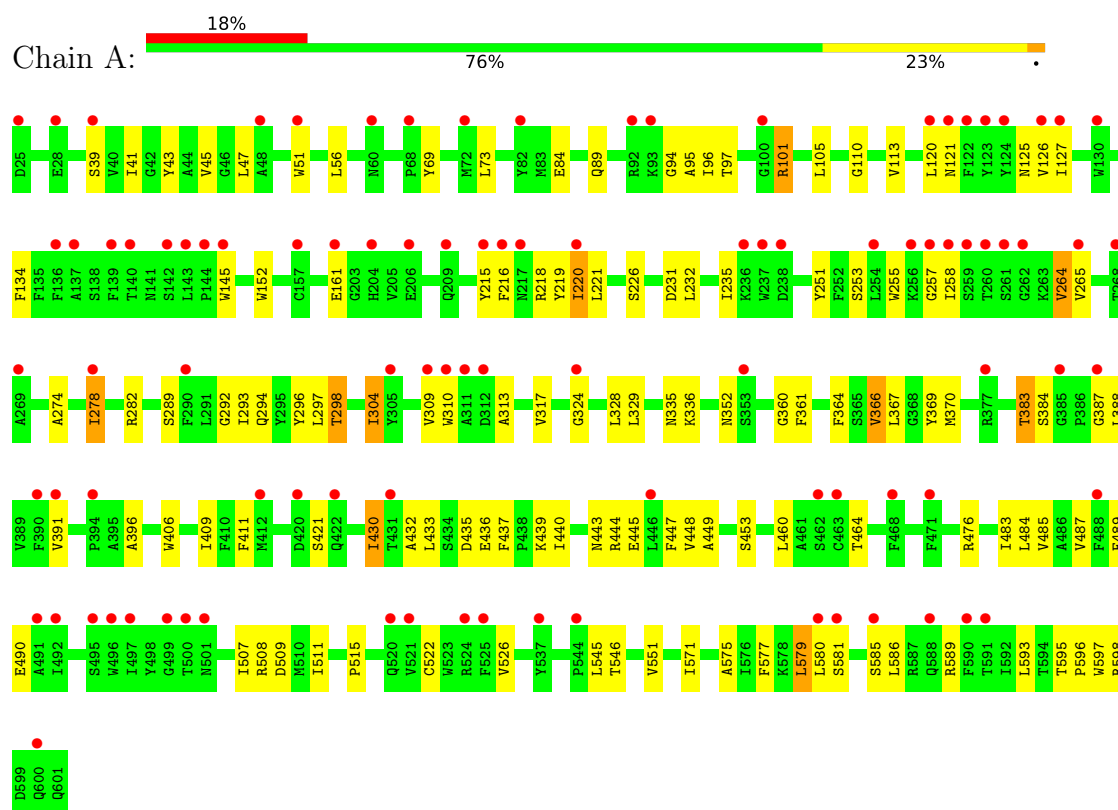
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	16	Total	O	0	0
			16	16		
8	L	3	Total	O	0	0
			3	3		

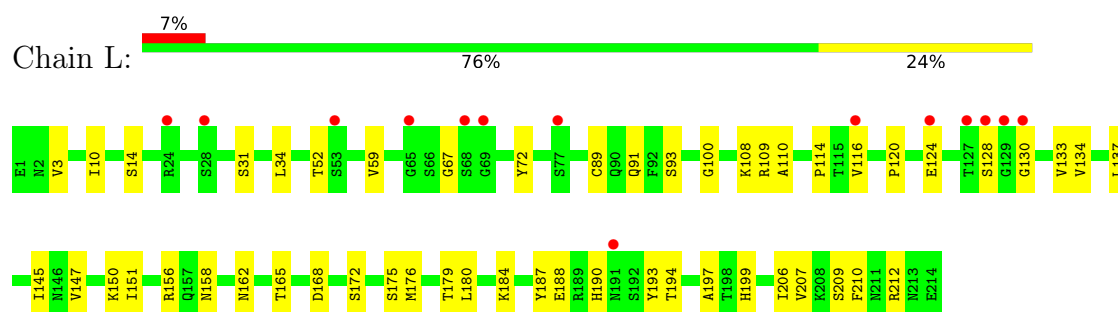
3 Residue-property plots

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.

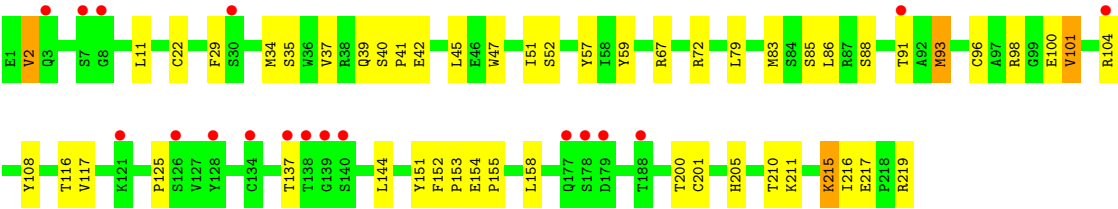
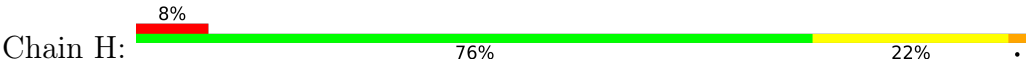
- Molecule 1: Sodium-dependent dopamine transporter



- Molecule 2: Antibody fragment (9D5) Light Chain



- Molecule 3: Antibody fragment (9D5) heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.39Å 140.71Å 168.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 3.20 48.43 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.43-3.20) 99.9 (48.43-3.20)	Depositor EDS
R_{merge}	0.72	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.19Å)	Xtriage
Refinement program	PHENIX v1.20rc4-4425	Depositor
R, R_{free}	0.244 , 0.286 0.249 , 0.286	Depositor DCC
R_{free} test set	1921 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	93.8	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7574	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: CL, NA, Y01, CLR

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	0.14	0/4373	0.29	0/5980
2	L	0.10	0/1656	0.33	0/2253
3	H	0.11	0/1682	0.31	0/2292
All	All	0.13	0/7711	0.30	0/10525

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

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	4228	0	4135	75	0
2	L	1618	0	1518	32	0
3	H	1643	0	1589	24	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	35	0	48	0	0
7	A	28	0	46	0	0
8	A	16	0	0	0	0
8	L	3	0	0	0	0
All	All	7574	0	7336	129	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 9.

All (129) 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)
2:L:150:LYS:HB2	2:L:194:THR:HB	1.73	0.70
3:H:158:LEU:HD11	3:H:201:CYS:HB2	1.73	0.70
3:H:29:PHE:O	3:H:72:ARG:NH2	2.28	0.67
2:L:190:HIS:O	2:L:212:ARG:NH1	2.29	0.66
1:A:324:GLY:HA3	1:A:487:VAL:HG22	1.79	0.65
3:H:39:GLN:HB3	3:H:45:LEU:HD23	1.81	0.63
1:A:489:PHE:HD2	1:A:571:ILE:HG21	1.64	0.62
1:A:39:SER:HA	1:A:265:VAL:HG21	1.81	0.62
1:A:219:TYR:HD2	1:A:220:ILE:HD12	1.64	0.62
1:A:433:LEU:HB3	1:A:440:ILE:HD11	1.82	0.61
1:A:487:VAL:HA	1:A:490:GLU:HB2	1.82	0.60
1:A:95:ALA:HA	1:A:329:LEU:HD23	1.82	0.60
3:H:51:ILE:HD13	3:H:72:ARG:HG3	1.83	0.60
2:L:124:GLU:N	2:L:124:GLU:OE1	2.35	0.60
1:A:101:ARG:HG3	1:A:597:TRP:HB3	1.85	0.59
2:L:109:ARG:NH1	2:L:110:ALA:O	2.34	0.57
1:A:43:TYR:HA	1:A:421:SER:HA	1.85	0.57
1:A:94:GLY:N	1:A:435:ASP:OD2	2.37	0.57
3:H:67:ARG:HG2	3:H:85:SER:HB3	1.87	0.56
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.87	0.56
2:L:197:ALA:HB3	2:L:206:ILE:HG23	1.89	0.55
2:L:156:ARG:NH1	2:L:158:ASN:O	2.39	0.55
1:A:522:CYS:HA	1:A:526:VAL:HG12	1.88	0.55
1:A:121:ASN:O	1:A:125:ASN:ND2	2.39	0.55
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.88	0.54
3:H:205:HIS:HB3	3:H:210:THR:HB	1.89	0.54
1:A:255:TRP:HA	1:A:448:VAL:HG11	1.90	0.54
1:A:366:VAL:HA	1:A:369:TYR:HB3	1.90	0.53
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.90	0.53
1:A:489:PHE:CD2	1:A:571:ILE:HG21	2.43	0.53
2:L:91:GLN:HG2	2:L:93:SER:H	1.74	0.53
1:A:507:ILE:HD11	1:A:515:PRO:HG3	1.90	0.52
1:A:253:SER:HB2	1:A:264:VAL:HG11	1.90	0.52
1:A:89:GLN:NE2	1:A:336:LYS:O	2.43	0.51
1:A:145:TRP:HB3	1:A:215:TYR:CD2	2.45	0.51
3:H:52:SER:HB3	3:H:57:TYR:HB2	1.92	0.51
3:H:200:THR:HG22	3:H:215:LYS:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:133:VAL:HG23	2:L:180:LEU:HB3	1.93	0.51
1:A:89:GLN:HG3	1:A:335:ASN:HB2	1.93	0.50
1:A:387:GLY:O	1:A:391:VAL:HG22	2.11	0.50
1:A:51:TRP:HH2	1:A:127:ILE:HD13	1.77	0.50
2:L:187:TYR:O	2:L:193:TYR:OH	2.30	0.50
1:A:579:LEU:HD13	1:A:593:LEU:HD12	1.94	0.49
2:L:120:PRO:HB3	2:L:210:PHE:CE2	2.47	0.49
2:L:184:LYS:NZ	2:L:188:GLU:OE1	2.44	0.49
2:L:114:PRO:HD3	2:L:199:HIS:CD2	2.48	0.49
1:A:69:TYR:HA	1:A:313:ALA:HB1	1.93	0.49
3:H:88:SER:O	3:H:91:THR:HG22	2.13	0.49
1:A:73:LEU:HA	1:A:317:VAL:HG11	1.94	0.49
3:H:35:SER:OG	3:H:47:TRP:NE1	2.42	0.49
1:A:96:ILE:HA	1:A:110:GLY:HA3	1.95	0.48
1:A:585:SER:O	1:A:589:ARG:HB2	2.13	0.48
3:H:154:GLU:HG3	3:H:155:PRO:HA	1.95	0.48
1:A:508:ARG:NE	3:H:100:GLU:O	2.46	0.48
1:A:292:GLY:HA3	1:A:364:PHE:O	2.14	0.48
1:A:304:ILE:O	1:A:310:TRP:NE1	2.44	0.48
1:A:84:GLU:HG2	1:A:328:LEU:HB2	1.95	0.47
2:L:194:THR:HG23	2:L:209:SER:HB2	1.96	0.47
2:L:151:ILE:HD12	2:L:156:ARG:HD2	1.95	0.47
1:A:383:THR:HG22	1:A:384:SER:H	1.80	0.47
1:A:293:ILE:HD12	1:A:361:PHE:HD1	1.78	0.47
1:A:430:ILE:HG22	1:A:447:PHE:CE1	2.49	0.47
2:L:151:ILE:HD11	2:L:180:LEU:HD21	1.96	0.47
1:A:437:PHE:O	1:A:440:ILE:HG12	2.16	0.46
2:L:31:SER:O	2:L:52:THR:HG23	2.15	0.46
3:H:2:VAL:HG11	3:H:108:TYR:CE1	2.51	0.46
1:A:507:ILE:O	1:A:511:ILE:HG12	2.16	0.46
1:A:257:GLY:HA2	1:A:444:ARG:NH2	2.31	0.46
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.98	0.46
3:H:93:MET:HE2	3:H:93:MET:HB2	1.85	0.46
1:A:282:ARG:HD2	1:A:406:TRP:CZ2	2.51	0.45
2:L:165:THR:HG22	2:L:175:SER:H	1.81	0.45
1:A:278:ILE:HG13	1:A:409:ILE:HD12	1.98	0.45
2:L:116:VAL:HG22	2:L:137:LEU:HD22	1.98	0.45
2:L:134:VAL:HG22	2:L:179:THR:HG23	1.97	0.45
3:H:34:MET:HB3	3:H:79:LEU:HD22	1.99	0.45
1:A:51:TRP:HA	1:A:388:LEU:HD23	1.99	0.45
1:A:251:TYR:C	1:A:253:SER:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:52:THR:HG22	2:L:72:TYR:HE2	1.82	0.45
1:A:430:ILE:HG22	1:A:447:PHE:HE1	1.82	0.44
1:A:577:PHE:O	1:A:581:SER:HB2	2.17	0.44
1:A:294:GLN:O	1:A:298:THR:OG1	2.32	0.44
1:A:226:SER:OG	1:A:231:ASP:O	2.28	0.44
2:L:187:TYR:CE2	2:L:212:ARG:HD2	2.53	0.44
1:A:274:ALA:O	1:A:278:ILE:HG12	2.18	0.44
1:A:296:TYR:CZ	1:A:360:GLY:HA3	2.53	0.44
1:A:45:VAL:HG12	1:A:352:ASN:HA	2.00	0.43
2:L:34:LEU:HD13	2:L:72:TYR:CD1	2.53	0.43
3:H:11:LEU:HA	3:H:116:THR:O	2.18	0.43
1:A:152:TRP:O	1:A:218:ARG:HD3	2.19	0.43
1:A:97:THR:OG1	1:A:436:GLU:OE1	2.28	0.43
1:A:134:PHE:HB3	1:A:411:PHE:CE2	2.54	0.43
1:A:483:ILE:O	1:A:487:VAL:HG23	2.19	0.43
1:A:105:LEU:HB2	1:A:593:LEU:HB3	2.01	0.42
2:L:89:CYS:O	2:L:100:GLY:N	2.44	0.42
1:A:509:ASP:OD1	3:H:59:TYR:OH	2.34	0.42
1:A:95:ALA:H	1:A:432:ALA:HB2	1.85	0.42
1:A:235:ILE:HA	1:A:464:THR:HA	2.02	0.42
1:A:449:ALA:O	1:A:453:SER:OG	2.35	0.42
2:L:137:LEU:HD11	2:L:147:VAL:HG12	2.02	0.42
1:A:51:TRP:C	1:A:51:TRP:CD1	2.97	0.42
1:A:235:ILE:HD11	1:A:460:LEU:HD22	2.02	0.42
2:L:114:PRO:HD3	2:L:199:HIS:HD2	1.84	0.42
1:A:439:LYS:O	1:A:443:ASN:ND2	2.53	0.42
1:A:575:ALA:O	1:A:579:LEU:HB2	2.20	0.42
1:A:585:SER:OG	1:A:586:LEU:N	2.52	0.41
1:A:219:TYR:CD2	1:A:220:ILE:HD12	2.49	0.41
2:L:14:SER:N	2:L:108:LYS:HB2	2.35	0.41
2:L:67:GLY:HA3	2:L:72:TYR:HA	2.02	0.41
2:L:162:ASN:HB3	2:L:176:MET:HE3	2.01	0.41
1:A:406:TRP:HE3	1:A:409:ILE:HD11	1.85	0.41
1:A:476:ARG:HA	1:A:476:ARG:HD2	1.70	0.41
1:A:507:ILE:HG13	1:A:515:PRO:HD3	2.02	0.41
3:H:40:SER:HB2	3:H:41:PRO:HD2	2.01	0.41
1:A:41:ILE:O	1:A:45:VAL:HG22	2.20	0.41
3:H:101:VAL:HG13	3:H:104:ARG:HB2	2.03	0.41
1:A:47:LEU:HD13	1:A:127:ILE:HG21	2.02	0.41
1:A:370:MET:SD	1:A:396:ALA:HB2	2.61	0.41
2:L:193:TYR:HB2	2:L:210:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HG22	1:A:110:GLY:C	2.46	0.41
2:L:128:SER:O	2:L:130:GLY:N	2.54	0.41
2:L:168:ASP:O	2:L:172:SER:HA	2.20	0.41
1:A:445:GLU:H	1:A:445:GLU:CD	2.27	0.41
2:L:52:THR:HG22	2:L:72:TYR:CE2	2.56	0.40
1:A:216:PHE:O	1:A:221:LEU:HB2	2.19	0.40
3:H:152:PHE:HA	3:H:153:PRO:HA	1.87	0.40
3:H:144:LEU:HB3	3:H:216:ILE:HG21	2.02	0.40
1:A:296:TYR:HB2	1:A:364:PHE:CG	2.56	0.40
1:A:595:THR:HA	1:A:596:PRO:HD3	1.94	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	535/536 (100%)	510 (95%)	25 (5%)	0	100	100
2	L	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
3	H	217/219 (99%)	203 (94%)	14 (6%)	0	100	100
All	All	964/969 (100%)	914 (95%)	50 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	431/441 (98%)	404 (94%)	27 (6%)	16	48
2	L	183/187 (98%)	178 (97%)	5 (3%)	39	68
3	H	182/187 (97%)	169 (93%)	13 (7%)	13	44
All	All	796/815 (98%)	751 (94%)	45 (6%)	18	51

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	101	ARG
1	A	113	VAL
1	A	120	LEU
1	A	126	VAL
1	A	161	GLU
1	A	220	ILE
1	A	232	LEU
1	A	258	ILE
1	A	264	VAL
1	A	278	ILE
1	A	289	SER
1	A	297	LEU
1	A	298	THR
1	A	304	ILE
1	A	309	VAL
1	A	366	VAL
1	A	383	THR
1	A	430	ILE
1	A	484	LEU
1	A	485	VAL
1	A	545	LEU
1	A	546	THR
1	A	551	VAL
1	A	579	LEU
1	A	580	LEU
1	A	598	ARG
2	L	3	VAL
2	L	10	ILE
2	L	59	VAL
2	L	145	ILE
2	L	207	VAL
3	H	2	VAL
3	H	37	VAL

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Mol	Chain	Res	Type
3	H	42	GLU
3	H	93	MET
3	H	96	CYS
3	H	98	ARG
3	H	101	VAL
3	H	117	VAL
3	H	137	THR
3	H	211	LYS
3	H	215	LYS
3	H	217	GLU
3	H	219	ARG

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	91	ASN
1	A	601	GLN
2	L	54	ASN
2	L	139	ASN
2	L	162	ASN
3	H	170	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
7	CLR	A	705	-	31,31,31	3.70	16 (51%)	48,48,48	1.93	16 (33%)
6	Y01	A	704	-	38,38,38	4.53	21 (55%)	57,57,57	2.13	18 (31%)

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
7	CLR	A	705	-	-	2/10/68/68	0/4/4/4
6	Y01	A	704	-	-	8/19/77/77	0/4/4/4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	704	Y01	CAS-CBF	-10.24	1.36	1.53
6	A	704	Y01	CBH-CAZ	-10.06	1.33	1.52
6	A	704	Y01	CAK-CAI	-8.83	1.32	1.50
7	A	705	CLR	C11-C9	8.66	1.68	1.53
7	A	705	CLR	C12-C11	8.56	1.70	1.53
6	A	704	Y01	CAI-CAZ	-8.33	1.15	1.33
6	A	704	Y01	CAV-CAZ	8.18	1.68	1.51
6	A	704	Y01	CBD-CBG	-8.00	1.38	1.53
6	A	704	Y01	CAK-CBD	7.68	1.65	1.53
7	A	705	CLR	C12-C13	-7.29	1.41	1.54
6	A	704	Y01	CAU-CBI	6.36	1.65	1.54
6	A	704	Y01	CBH-CBF	6.05	1.65	1.56
7	A	705	CLR	C6-C5	-5.42	1.21	1.33
7	A	705	CLR	C1-C2	5.32	1.64	1.53
6	A	704	Y01	CAU-CAS	5.29	1.64	1.53
7	A	705	CLR	C7-C6	-5.21	1.39	1.50
7	A	705	CLR	C16-C15	5.15	1.68	1.54
6	A	704	Y01	CAV-CBC	4.73	1.62	1.52
6	A	704	Y01	CBI-CBE	-4.57	1.46	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	705	CLR	C10-C9	-4.52	1.48	1.56
7	A	705	CLR	C8-C14	-4.22	1.45	1.53
6	A	704	Y01	OAW-CBC	-3.77	1.37	1.46
7	A	705	CLR	C13-C14	-3.59	1.48	1.55
6	A	704	Y01	CBD-CBF	3.50	1.60	1.53
7	A	705	CLR	C1-C10	3.29	1.60	1.54
6	A	704	Y01	CAT-CAR	-3.18	1.47	1.53
7	A	705	CLR	C2-C3	3.07	1.58	1.51
6	A	704	Y01	CAP-CBE	2.99	1.60	1.54
6	A	704	Y01	CAQ-CAP	2.87	1.61	1.54
7	A	705	CLR	C8-C9	2.78	1.58	1.53
6	A	704	Y01	OAW-CAY	2.75	1.42	1.34
7	A	705	CLR	C15-C14	2.69	1.59	1.54
6	A	704	Y01	CAL-CAX	2.55	1.56	1.50
7	A	705	CLR	C10-C5	-2.30	1.48	1.52
6	A	704	Y01	OAF-CAX	2.20	1.29	1.22
7	A	705	CLR	C4-C5	-2.15	1.47	1.51
6	A	704	Y01	CAQ-CBG	2.04	1.58	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	704	Y01	CBC-CAV-CAZ	-5.46	103.39	111.45
6	A	704	Y01	CAV-CAZ-CAI	-5.19	113.54	120.57
6	A	704	Y01	CAK-CAI-CAZ	4.40	132.45	125.02
6	A	704	Y01	CBH-CBF-CBD	-4.17	106.63	112.71
6	A	704	Y01	CAK-CBD-CBF	-4.15	104.92	109.72
7	A	705	CLR	C11-C9-C8	-3.92	106.31	111.78
6	A	704	Y01	OAW-CAY-CAM	3.86	119.84	111.48
7	A	705	CLR	C15-C14-C8	-3.80	113.04	119.10
7	A	705	CLR	C12-C13-C17	-3.65	111.22	116.60
7	A	705	CLR	C12-C11-C9	-3.56	107.09	113.14
6	A	704	Y01	CAP-CAQ-CBG	-3.36	98.57	105.14
6	A	704	Y01	CAS-CAU-CBI	-3.33	107.13	112.74
7	A	705	CLR	C16-C15-C14	-3.23	98.83	105.14
6	A	704	Y01	CBI-CBE-CBB	-3.21	114.54	119.50
7	A	705	CLR	C4-C5-C6	-3.13	116.32	120.57
6	A	704	Y01	CBH-CAZ-CAI	3.06	127.39	122.93
6	A	704	Y01	CBI-CBG-CBD	-2.92	110.27	114.41
7	A	705	CLR	C16-C17-C20	-2.83	107.90	112.18
6	A	704	Y01	CBF-CBH-CAZ	2.78	113.72	109.65
7	A	705	CLR	C14-C8-C9	-2.74	105.51	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	705	CLR	C21-C20-C22	-2.66	106.22	110.34
7	A	705	CLR	C12-C13-C14	2.64	111.20	107.25
7	A	705	CLR	C1-C10-C5	2.62	113.26	108.74
7	A	705	CLR	C4-C5-C10	2.61	119.76	116.42
7	A	705	CLR	C17-C13-C14	2.57	103.05	100.10
7	A	705	CLR	C3-C4-C5	-2.57	107.96	112.05
6	A	704	Y01	CAQ-CBG-CBD	-2.45	115.19	119.10
7	A	705	CLR	C1-C2-C3	-2.31	107.42	110.48
6	A	704	Y01	CBF-CBD-CBG	-2.23	106.17	109.09
6	A	704	Y01	CAP-CBE-CBB	-2.18	108.89	112.18
7	A	705	CLR	C23-C22-C20	-2.08	109.26	115.08
6	A	704	Y01	CBG-CBI-CBE	2.08	102.48	100.10
6	A	704	Y01	CAV-CAZ-CBH	2.07	119.07	116.42
6	A	704	Y01	CBC-OAW-CAY	-2.02	112.96	117.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

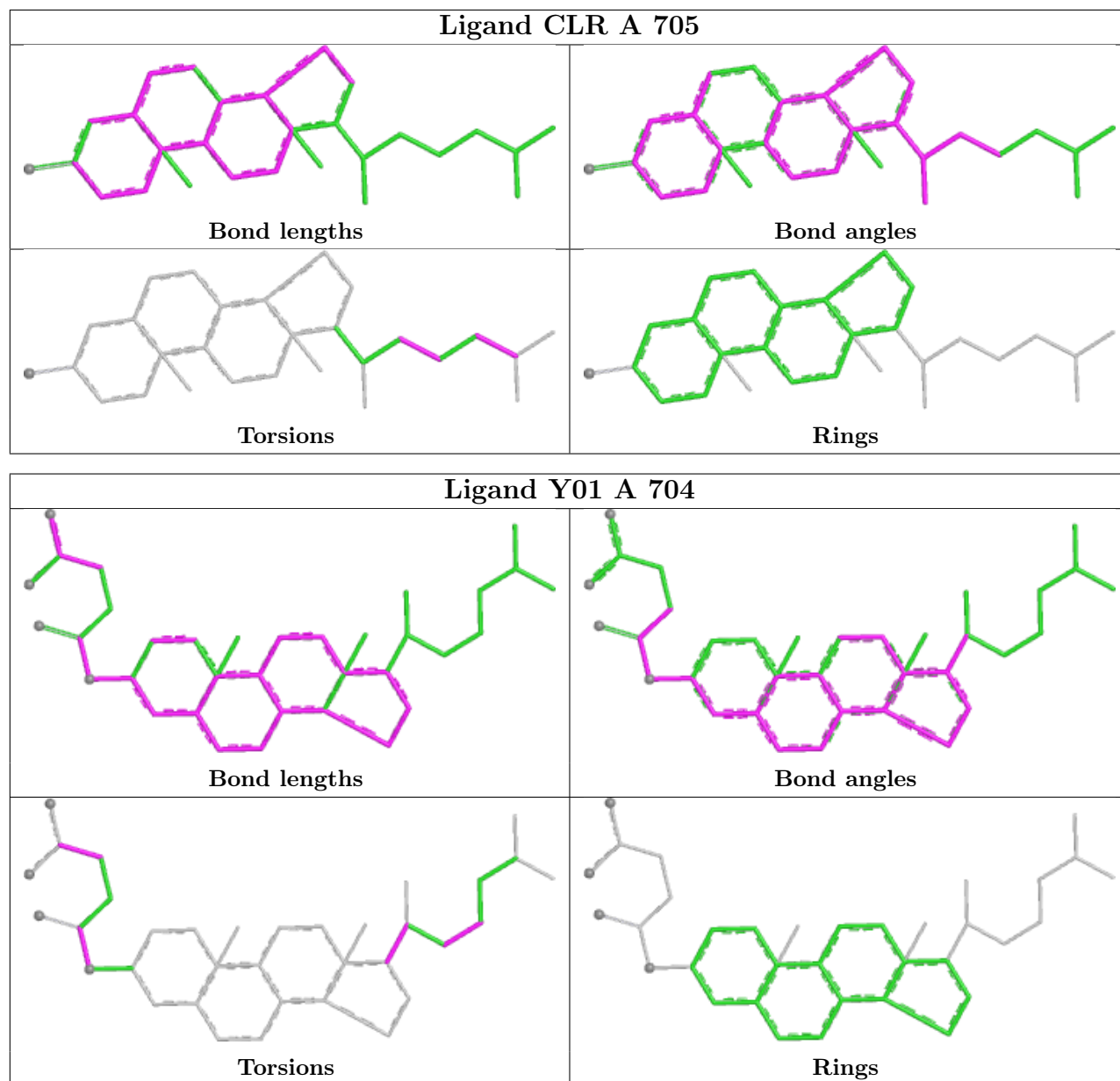
Mol	Chain	Res	Type	Atoms
6	A	704	Y01	CAN-CAJ-CAO-CBB
6	A	704	Y01	CAM-CAY-OAW-CBC
6	A	704	Y01	OAG-CAY-OAW-CBC
7	A	705	CLR	C20-C22-C23-C24
6	A	704	Y01	CAC-CBB-CBE-CBI
6	A	704	Y01	CAM-CAL-CAX-OAH
6	A	704	Y01	CAM-CAL-CAX-OAF
7	A	705	CLR	C23-C24-C25-C26
6	A	704	Y01	CAO-CBB-CBE-CBI
6	A	704	Y01	CAC-CBB-CBE-CAP

There are no ring outliers.

No monomer is involved in short contacts.

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	536/536 (100%)	1.07	97 (18%) 3 3	47, 85, 106, 133	1 (0%)
2	L	214/214 (100%)	0.59	14 (6%) 25 16	60, 80, 104, 128	0
3	H	219/219 (100%)	0.51	18 (8%) 17 11	60, 82, 111, 158	0
All	All	969/969 (100%)	0.84	129 (13%) 7 6	47, 84, 107, 158	1 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	TYR	6.9
1	A	524	ARG	6.5
1	A	496	TRP	6.4
3	H	126	SER	6.4
1	A	124	TYR	6.0
1	A	261	SER	5.8
1	A	130	TRP	5.4
1	A	581	SER	5.3
1	A	501	ASN	4.6
1	A	145	TRP	4.5
1	A	422	GLN	4.1
1	A	258	ILE	4.0
2	L	127	THR	4.0
1	A	588	GLN	3.8
1	A	525	PHE	3.8
1	A	391	VAL	3.6
1	A	260	THR	3.6
1	A	269	ALA	3.6
1	A	238	ASP	3.5
1	A	120	LEU	3.5
1	A	324	GLY	3.4
1	A	390	PHE	3.4
1	A	82	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	521	VAL	3.3
2	L	53	SER	3.3
1	A	591	THR	3.3
1	A	122	PHE	3.2
3	H	128	TYR	3.2
1	A	217	ASN	3.2
3	H	139	GLY	3.2
3	H	177	GLN	3.1
1	A	254	LEU	3.1
3	H	178	SER	3.1
1	A	25	ASP	3.1
2	L	65	GLY	3.1
2	L	68	SER	3.1
1	A	499	GLY	3.0
1	A	268	THR	3.0
2	L	77	SER	3.0
3	H	140	SER	3.0
1	A	121	ASN	3.0
1	A	51	TRP	2.9
1	A	144	PRO	2.9
1	A	136	PHE	2.9
1	A	265	VAL	2.9
1	A	290	PHE	2.9
1	A	310	TRP	2.9
2	L	69	GLY	2.9
1	A	257	GLY	2.9
1	A	600	GLN	2.8
2	L	28	SER	2.8
1	A	72	MET	2.8
2	L	191	ASN	2.8
1	A	127	ILE	2.8
1	A	590	PHE	2.7
1	A	520	GLN	2.7
1	A	157	CYS	2.7
1	A	209	GLN	2.7
1	A	140	THR	2.7
1	A	495	SER	2.7
1	A	488	PHE	2.6
3	H	121	LYS	2.6
1	A	353	SER	2.6
1	A	462	SER	2.6
1	A	256	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	129	GLY	2.6
3	H	138	THR	2.6
1	A	48	ALA	2.6
1	A	143	LEU	2.6
1	A	139	PHE	2.5
1	A	431	THR	2.5
1	A	580	LEU	2.5
1	A	262	GLY	2.5
1	A	220	ILE	2.4
1	A	500	THR	2.4
1	A	385	GLY	2.4
3	H	30	SER	2.4
1	A	93	LYS	2.4
1	A	491	ALA	2.4
3	H	3	GLN	2.4
1	A	92	ARG	2.4
1	A	259	SER	2.4
1	A	215	TYR	2.4
1	A	305	TYR	2.4
1	A	387	GLY	2.4
1	A	126	VAL	2.4
1	A	394	PRO	2.4
1	A	236	LYS	2.4
1	A	537	TYR	2.3
1	A	137	ALA	2.3
1	A	311	ALA	2.3
1	A	216	PHE	2.3
1	A	463	CYS	2.3
1	A	204	HIS	2.3
3	H	188	THR	2.3
2	L	124	GLU	2.2
1	A	492	ILE	2.2
1	A	412	MET	2.2
1	A	446	LEU	2.2
1	A	468	PHE	2.2
2	L	128	SER	2.2
1	A	161	GLU	2.2
1	A	68	PRO	2.2
1	A	585	SER	2.2
1	A	237	TRP	2.2
2	L	116	VAL	2.2
1	A	39	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	377	ARG	2.2
1	A	206	GLU	2.2
2	L	130	GLY	2.2
3	H	137	THR	2.1
3	H	104	ARG	2.1
3	H	7	SER	2.1
1	A	60	ASN	2.1
1	A	278	ILE	2.1
1	A	100	GLY	2.1
1	A	544	PRO	2.1
3	H	91	THR	2.1
3	H	8	GLY	2.1
1	A	28	GLU	2.1
1	A	309	VAL	2.0
1	A	312	ASP	2.0
3	H	179	ASP	2.0
1	A	471	PHE	2.0
2	L	24	ARG	2.0
1	A	142	SER	2.0
1	A	420	ASP	2.0
3	H	134	CYS	2.0
1	A	497	ILE	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
6	Y01	A	704	35/35	0.86	0.20	83,99,113,115	0

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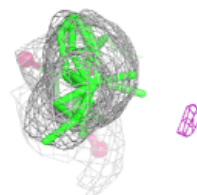
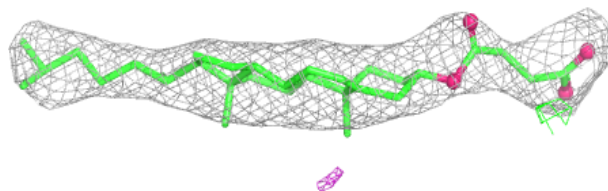
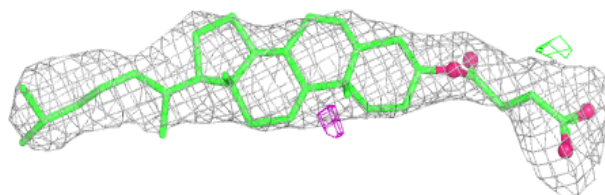
Continued from previous page...

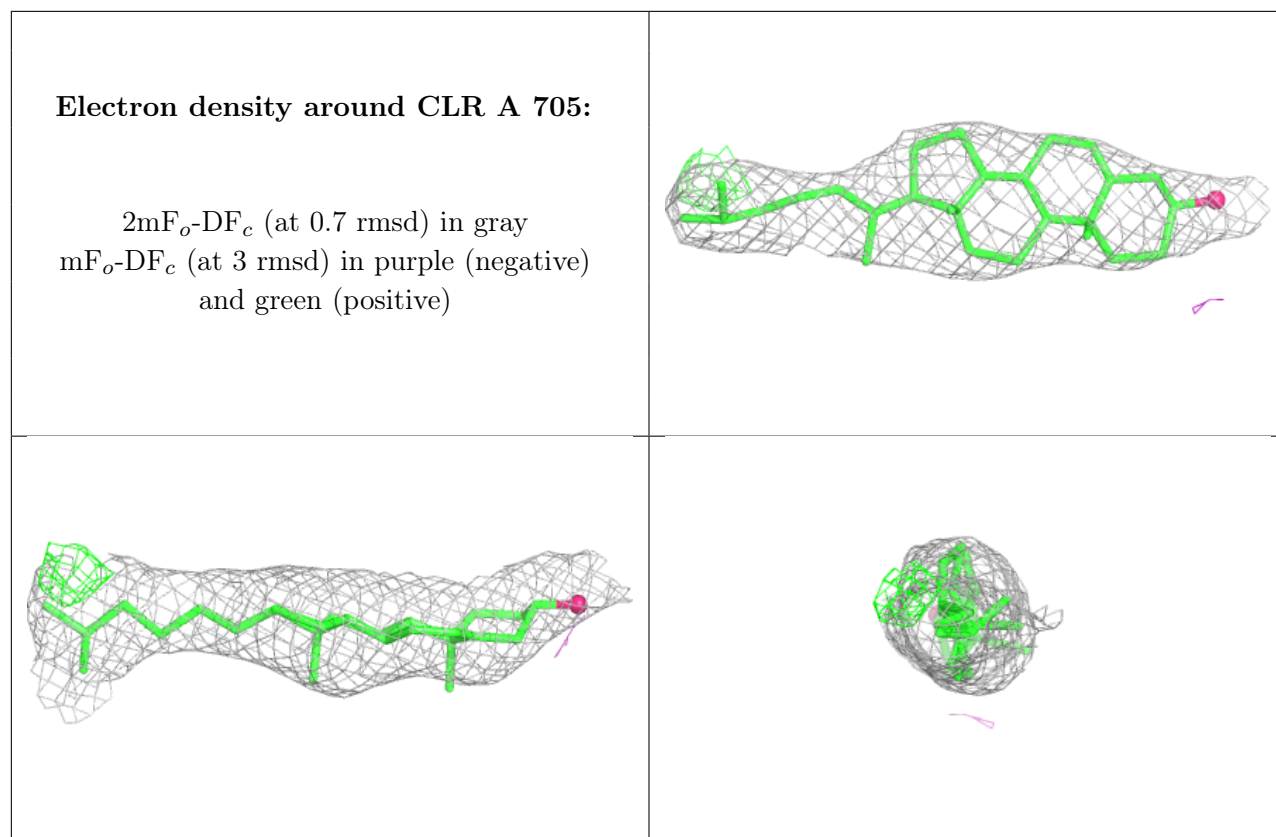
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	A	702	1/1	0.88	0.13	94,94,94,94	0
7	CLR	A	705	28/28	0.90	0.20	67,83,92,94	0
5	CL	A	703	1/1	0.92	0.14	82,82,82,82	0
4	NA	A	701	1/1	0.96	0.10	86,86,86,86	0

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 Y01 A 704:

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.