



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2025 – 04:28 PM JST

PDB ID : 9J7G / pdb_00009j7g
Title : Crystal structure of Keap1_compound_8
Authors : Xu, K.
Deposited on : 2024-08-18
Resolution : 2.99 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 Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

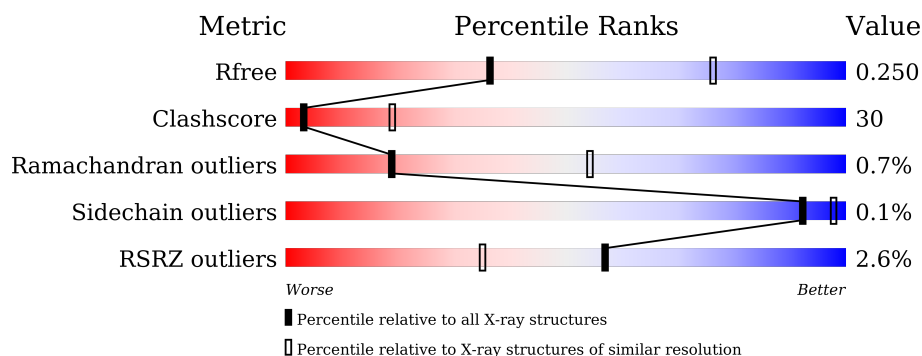
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 59%, green 40%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 60% 39% </div> </div>
1	B	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 59%, green 37%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 59% 39% </div> </div>
1	C	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 43%, green 50%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 43% 53% </div> </div>
1	X	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 61%, green 37%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 61% 37% </div> </div>

2 Entry composition [i](#)

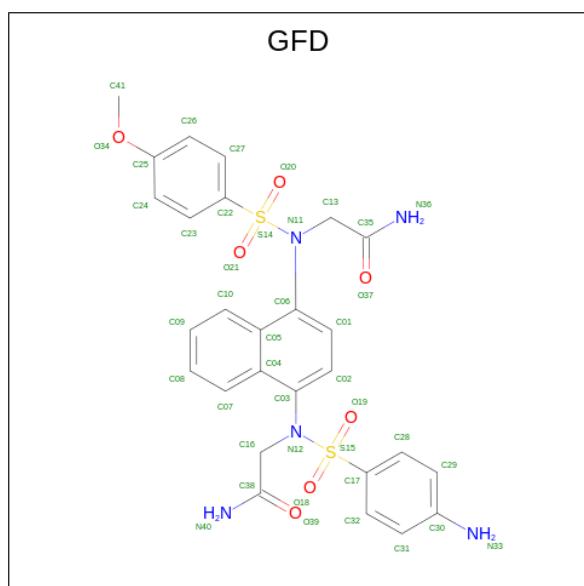
There are 3 unique types of molecules in this entry. The entry contains 9206 atoms, of which 180 are hydrogens and 0 are deuteriums.

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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2201	1368	398	420	15			
1	B	285	Total	C	N	O	S	0	0	0
			2193	1363	397	418	15			
1	C	279	Total	C	N	O	S	0	1	0
			2160	1345	390	410	15			
1	X	287	Total	C	N	O	S	0	0	0
			2208	1372	400	421	15			

- Molecule 2 is 2-[(4-aminophenyl)sulfonyl]-[4-[(2-azanyl-2-oxidanylidene-ethyl)-(4-methoxyphenyl)sulfonyl-amino]naphthalen-1-yl]amino]ethanamide (CCD ID: GFD) (formula: C₂₇H₂₇N₅O₇S₂).



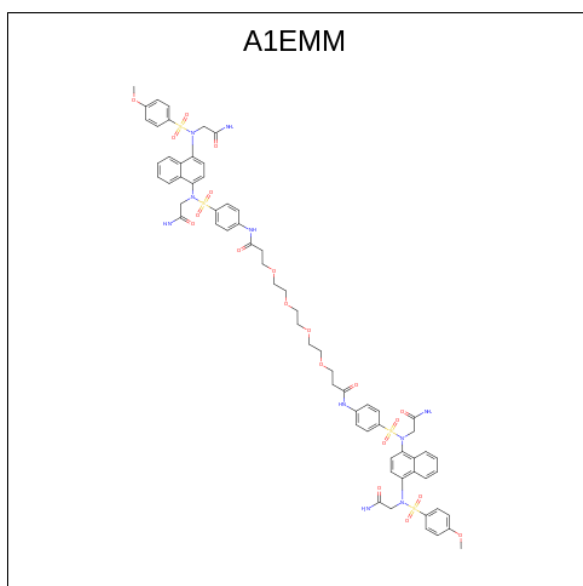
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	
			136	54	54	10	14	4	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	S	
			136	54	54	10	14	4	
								0	1

- Molecule 3 is {N}-[4-[(2-azanyl-2-oxidanylidene-ethyl)-[4-[(2-azanyl-2-oxidanylidene-ethyl)-(4-methoxyphenyl)sulfonyl-amino]naphthalen-1-yl]sulfamoyl]phenyl]-3-[2-[2-[2-[3-[4-[(2-azanyl-2-oxidanylidene-ethyl)-[4-[(2-azanyl-2-oxidanylidene-ethyl)-(4-methoxyphenyl)sulfonyl-amino]naphthalen-1-yl]sulfamoyl]phenyl]amino]-3-oxidanylidene-propoxy]ethoxy]ethoxy]ethoxy]propanamide (CCD ID: A1EMM) (formula: C₆₆H₇₂N₁₀O₂₀S₄) (labeled as "Ligand of Interest" by depositor).

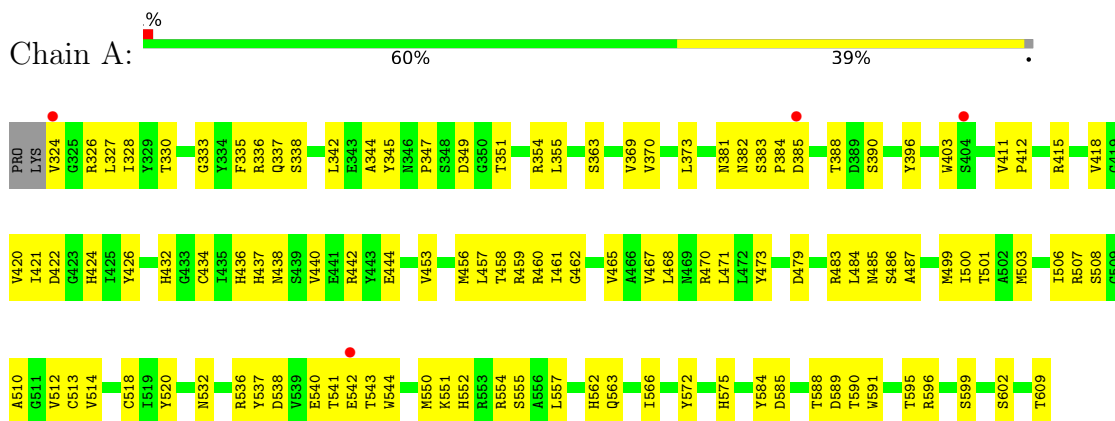


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	X	1	Total	C	H	N	O	S	
			172	66	72	10	20	4	
								0	0

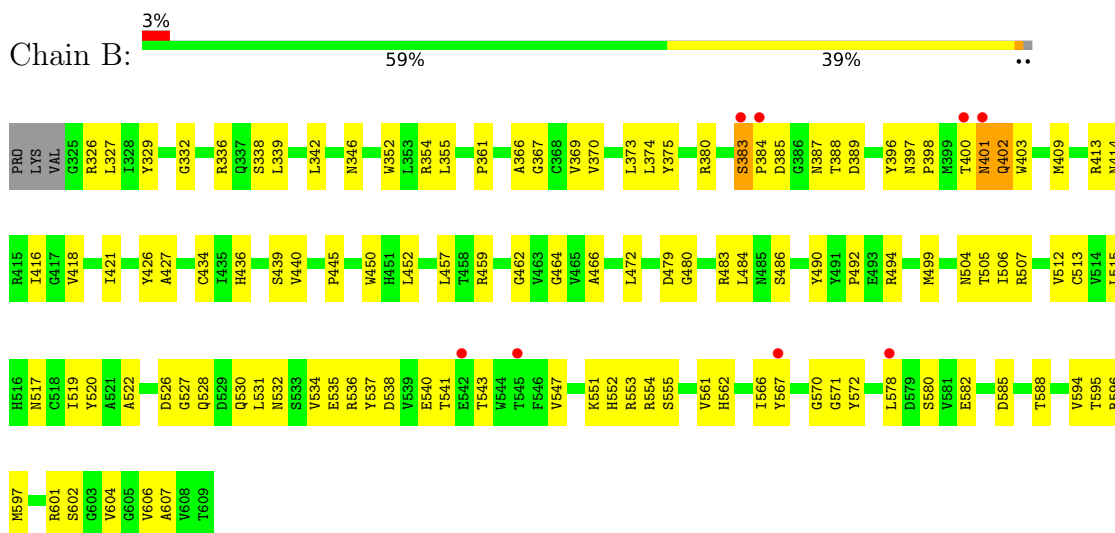
3 Residue-property plots [i](#)

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

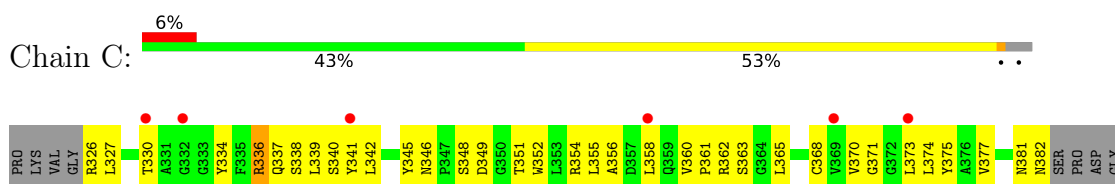
• Molecule 1: Kelch-like ECH-associated protein 1

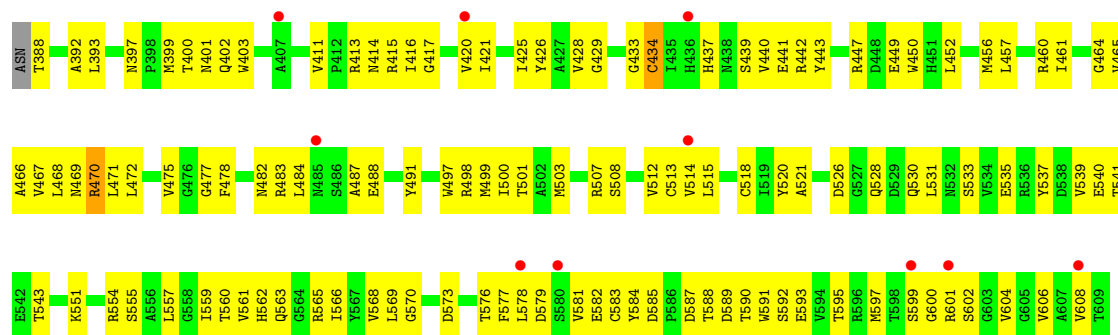


• Molecule 1: Kelch-like ECH-associated protein 1

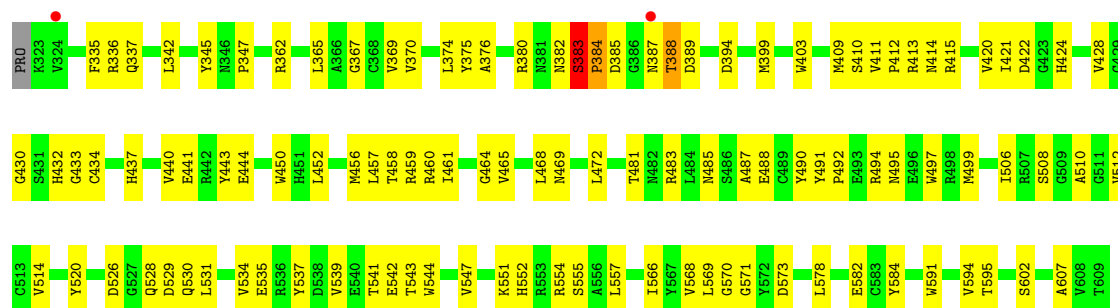


• Molecule 1: Kelch-like ECH-associated protein 1





● Molecule 1: Kelch-like ECH-associated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.47Å 74.15Å 123.11Å 90.00° 100.86° 90.00°	Depositor
Resolution (Å)	44.56 – 2.99 44.56 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.56-2.99) 93.2 (44.56-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.199 , 0.250 0.205 , 0.250	Depositor DCC
R_{free} test set	37370 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	72.3	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9206	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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: GFD, A1EMM

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	0.50	0/2254	0.70	0/3068
1	B	0.50	0/2246	0.74	2/3057 (0.1%)
1	C	0.44	0/2214	0.75	4/3011 (0.1%)
1	X	0.55	1/2261 (0.0%)	0.78	0/3076
All	All	0.50	1/8975 (0.0%)	0.74	6/12212 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	X	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	510	ALA	C-N	6.09	1.36	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	470	ARG	NE-CZ-NH1	-13.24	108.26	121.50
1	C	470	ARG	NE-CZ-NH2	10.62	128.76	119.20
1	C	470	ARG	CG-CD-NE	-8.52	93.25	112.00
1	C	434	CYS	CA-CB-SG	-6.86	98.63	114.40
1	B	401	ASN	N-CA-C	-6.46	97.04	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	ASN	CA-CB-CG	6.19	118.79	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	434	CYS	Peptide
1	C	336	ARG	Peptide
1	X	383	SER	Peptide

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	2201	0	2092	111	0
1	B	2193	0	2081	120	2
1	C	2160	0	2058	197	2
1	X	2208	0	2099	116	0
2	A	82	54	0	3	0
2	C	82	54	0	11	0
3	X	100	72	0	6	0
All	All	9026	180	8330	522	2

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 30.

All (522) 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:C:599:SER:O	1:C:601:ARG:NH1	1.57	1.34
1:C:399:MET:HE3	1:C:399:MET:HA	1.24	1.16
1:B:534:VAL:HG13	1:B:547:VAL:HG23	1.35	1.09
1:C:588:THR:HG23	1:C:590:THR:H	1.20	1.05
1:C:569:LEU:HD23	1:C:581:VAL:HB	1.39	1.03
1:B:494:ARG:HG3	1:B:494:ARG:HH11	1.25	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:554:ARG:HB3	1:C:557:LEU:HD11	1.39	1.01
1:X:410:SER:HB3	1:X:441:GLU:OE2	1.62	1.00
1:C:585:ASP:HB3	1:C:588:THR:HG22	1.44	1.00
1:B:578:LEU:HD12	1:B:580:SER:HB3	1.41	0.99
1:C:456:MET:HE1	1:C:460:ARG:HD2	1.42	0.99
1:B:387:ASN:HB3	1:X:481:THR:HG22	1.42	0.98
1:B:486:SER:HB2	1:B:499:MET:HE1	1.46	0.98
1:C:585:ASP:HB3	1:C:588:THR:CG2	1.94	0.97
1:X:399:MET:HE2	1:X:399:MET:HA	1.51	0.93
1:C:579:ASP:OD2	1:C:600:GLY:HA3	1.70	0.92
1:C:399:MET:HA	1:C:399:MET:CE	2.00	0.91
1:C:360:VAL:HG23	1:C:362:ARG:HD3	1.51	0.90
1:B:387:ASN:HB2	1:X:481:THR:HA	1.56	0.87
1:B:352:TRP:HE1	1:B:595:THR:HG21	1.40	0.87
1:C:526:ASP:HB3	1:C:531:LEU:HD11	1.54	0.87
1:C:588:THR:HG23	1:C:590:THR:N	1.91	0.84
1:C:342:LEU:HD22	1:C:403:TRP:HZ2	1.43	0.84
1:C:415:ARG:HD2	2:C:701[A]:GFD:O39	1.78	0.83
1:C:551:LYS:HB2	1:C:582:GLU:OE2	1.79	0.83
1:C:579:ASP:OD2	1:C:600:GLY:CA	2.28	0.82
1:A:486:SER:HB2	1:A:499:MET:HE1	1.60	0.82
1:A:457:LEU:HD12	1:A:499:MET:HG2	1.62	0.82
1:C:467:VAL:O	1:C:514:VAL:HG11	1.79	0.82
1:B:400:THR:O	1:B:401:ASN:HB3	1.76	0.82
1:X:457:LEU:HD12	1:X:499:MET:HG2	1.63	0.81
1:C:507:ARG:HH22	1:C:533:SER:HB2	1.44	0.81
1:A:575:HIS:HB3	1:C:336:ARG:NH2	1.95	0.81
1:A:385:ASP:O	1:C:482:ASN:ND2	2.15	0.80
1:C:368:CYS:SG	1:C:425:ILE:HD13	2.22	0.80
1:C:561:VAL:HG12	1:C:566:ILE:HA	1.62	0.80
1:B:383:SER:CB	1:B:384:PRO:HD2	2.11	0.80
1:B:483:ARG:HH11	1:B:483:ARG:HG3	1.46	0.80
1:A:424:HIS:NE2	1:A:444:GLU:OE1	2.14	0.79
1:C:346:ASN:HB3	1:C:351:THR:OG1	1.81	0.79
1:X:557:LEU:HD23	1:X:557:LEU:H	1.48	0.78
1:A:487:ALA:HB3	1:A:500:ILE:HD11	1.65	0.78
1:C:327:LEU:CD2	1:C:346:ASN:HB2	2.13	0.78
1:C:487:ALA:O	1:C:499:MET:HG3	1.85	0.77
1:B:551:LYS:HD2	1:B:552:HIS:HB2	1.67	0.76
1:X:541:THR:HG22	1:X:543:THR:HG23	1.66	0.76
1:C:327:LEU:HD23	1:C:346:ASN:HB2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:TYR:CZ	1:C:442:ARG:HD3	2.20	0.76
1:C:559:ILE:H	1:C:606:VAL:HG21	1.50	0.76
1:C:426:TYR:CZ	1:C:442:ARG:CD	2.69	0.76
1:X:494:ARG:HG3	1:X:494:ARG:HH11	1.51	0.76
1:C:568:VAL:O	1:C:581:VAL:HG23	1.86	0.76
1:C:569:LEU:CD2	1:C:581:VAL:HB	2.17	0.75
1:C:569:LEU:HD22	1:C:597:MET:HE2	1.69	0.75
1:C:569:LEU:HD23	1:C:581:VAL:CB	2.17	0.74
1:X:415:ARG:NH1	3:X:701:A1EMM:OA0	2.21	0.74
1:C:573:ASP:HB2	1:C:578:LEU:HD21	1.67	0.74
1:C:362:ARG:NH2	1:C:392:ALA:HB3	2.03	0.74
1:C:602:SER:OG	2:C:701[B]:GFD:S14	2.45	0.73
1:C:426:TYR:CE2	1:C:442:ARG:HD3	2.23	0.73
1:C:585:ASP:CB	1:C:588:THR:HG22	2.17	0.73
1:A:436:HIS:CD2	1:A:461:ILE:HD13	2.24	0.73
1:B:397:ASN:O	1:B:401:ASN:N	2.19	0.73
1:C:393:LEU:HD22	1:C:450:TRP:HZ2	1.54	0.73
1:B:494:ARG:HG3	1:B:494:ARG:NH1	1.99	0.72
1:C:352:TRP:HE1	1:C:595:THR:HG21	1.55	0.72
1:X:526:ASP:HB3	1:X:531:LEU:HD21	1.70	0.72
1:A:518:CYS:SG	1:A:536:ARG:HD2	2.30	0.72
1:B:332:GLY:O	1:B:604:VAL:HG12	1.91	0.71
1:A:575:HIS:HB3	1:C:336:ARG:HH22	1.54	0.71
1:X:541:THR:HG22	1:X:543:THR:CG2	2.20	0.71
1:C:342:LEU:HD22	1:C:403:TRP:CZ2	2.25	0.71
1:C:393:LEU:HD22	1:C:450:TRP:CZ2	2.25	0.71
1:A:585:ASP:HB3	1:A:588:THR:CG2	2.21	0.71
1:A:588:THR:O	1:A:590:THR:HG23	1.91	0.70
1:X:387:ASN:O	1:X:388:THR:HG22	1.91	0.70
1:A:383:SER:HB2	1:A:384:PRO:HD2	1.73	0.70
1:X:412:PRO:HG2	1:X:432:HIS:CE1	2.27	0.70
1:B:457:LEU:HD12	1:B:499:MET:HG2	1.73	0.69
1:C:602:SER:OG	2:C:701[B]:GFD:O20	2.06	0.69
1:B:585:ASP:HB3	1:B:588:THR:OG1	1.92	0.68
1:A:460:ARG:HG2	1:A:460:ARG:HH11	1.58	0.68
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.76	0.68
1:C:551:LYS:HB2	1:C:582:GLU:CD	2.18	0.68
1:B:342:LEU:HD22	1:B:403:TRP:CZ2	2.27	0.68
1:B:396:TYR:OH	1:B:401:ASN:OD1	2.09	0.68
1:X:399:MET:HA	1:X:399:MET:CE	2.22	0.68
1:X:428:VAL:CG2	1:X:465:VAL:HG21	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:VAL:HG13	1:B:607:ALA:HB1	1.76	0.67
1:C:503:MET:HE2	1:C:535:GLU:OE1	1.95	0.67
1:B:515:LEU:CD1	1:B:561:VAL:HG21	2.24	0.67
1:C:334:TYR:HE2	1:C:382:ASN:ND2	1.93	0.67
1:X:369:VAL:HG23	1:X:607:ALA:HB1	1.77	0.67
1:A:462:GLY:HA3	2:A:701[B]:GFD:N40	2.10	0.66
1:C:515:LEU:HB3	1:C:520:TYR:CE1	2.30	0.66
1:X:428:VAL:HG21	1:X:465:VAL:HG21	1.78	0.66
1:C:338:SER:HB2	1:C:361:PRO:HB2	1.77	0.66
1:C:428:VAL:HA	1:C:440:VAL:HG13	1.78	0.66
1:C:561:VAL:HG12	1:C:566:ILE:CA	2.26	0.66
1:B:534:VAL:HG13	1:B:547:VAL:CG2	2.21	0.66
1:B:562:HIS:HB3	1:B:567:TYR:CE1	2.31	0.66
1:X:494:ARG:HG3	1:X:494:ARG:NH1	2.11	0.65
1:X:457:LEU:CD1	1:X:499:MET:HG2	2.26	0.65
1:B:401:ASN:O	1:B:402:GLN:HB2	1.95	0.65
1:C:488:GLU:HB3	1:C:499:MET:HE2	1.79	0.65
1:C:585:ASP:HB3	1:C:588:THR:HG21	1.79	0.64
1:X:594:VAL:HG23	1:X:595:THR:HG22	1.79	0.64
1:C:334:TYR:HB2	1:C:363:SER:HB2	1.80	0.64
1:C:600:GLY:C	1:C:601:ARG:HD3	2.23	0.64
1:A:424:HIS:HE2	1:A:444:GLU:CD	2.06	0.64
1:C:488:GLU:HG3	1:C:497:TRP:CE3	2.33	0.63
1:A:557:LEU:HD23	1:A:557:LEU:H	1.63	0.63
1:C:360:VAL:CG2	1:C:362:ARG:HD3	2.28	0.63
1:X:409:MET:HE1	1:X:413:ARG:HB2	1.79	0.63
1:X:487:ALA:O	1:X:499:MET:HE3	1.99	0.63
1:C:565:ARG:NH2	1:C:585:ASP:HB2	2.14	0.63
1:X:399:MET:HE2	1:X:399:MET:CA	2.26	0.63
1:C:442:ARG:HG2	1:C:442:ARG:HH11	1.64	0.62
1:C:334:TYR:HE2	1:C:382:ASN:HD22	1.47	0.62
1:B:380:ARG:HG3	1:B:389:ASP:OD1	1.99	0.62
1:B:551:LYS:NZ	1:B:552:HIS:HB2	2.15	0.62
1:C:370:VAL:CG2	1:C:420:VAL:HG21	2.30	0.62
1:B:551:LYS:CD	1:B:552:HIS:HB2	2.30	0.61
1:C:352:TRP:HE1	1:C:595:THR:CG2	2.13	0.61
1:B:551:LYS:CE	1:B:552:HIS:HB2	2.29	0.61
1:A:456:MET:SD	1:A:460:ARG:HD2	2.39	0.61
1:C:565:ARG:HE	1:C:585:ASP:HB2	1.66	0.61
1:X:443:TYR:HB2	1:X:450:TRP:CE2	2.36	0.61
1:A:338:SER:HB2	1:A:382:ASN:HB3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ARG:NH1	1:B:527:GLY:HA2	2.16	0.61
1:B:528:GLN:NE2	1:X:383:SER:HA	2.15	0.61
1:C:491:TYR:HE2	1:C:498:ARG:HG3	1.65	0.61
1:C:507:ARG:NH2	1:C:533:SER:HB2	2.15	0.61
1:X:342:LEU:HD22	1:X:403:TRP:CZ2	2.35	0.61
1:B:387:ASN:CB	1:X:481:THR:HA	2.30	0.61
1:C:565:ARG:NE	1:C:585:ASP:HB2	2.16	0.60
1:X:430:GLY:O	1:X:437:HIS:HB2	1.99	0.60
1:B:436:HIS:NE2	1:B:480:GLY:HA2	2.16	0.60
1:C:565:ARG:HH21	1:C:585:ASP:HB2	1.66	0.60
1:C:561:VAL:HG12	1:C:566:ILE:CB	2.31	0.60
1:X:456:MET:HE1	1:X:460:ARG:HB2	1.84	0.60
1:X:485:ASN:HB3	1:X:506:ILE:HG12	1.84	0.60
1:B:483:ARG:HG3	1:B:483:ARG:NH1	2.14	0.60
1:A:370:VAL:HG22	1:A:420:VAL:HG11	1.84	0.60
1:C:456:MET:HE1	1:C:460:ARG:CD	2.24	0.60
1:A:459:ARG:O	1:A:479:ASP:HA	2.02	0.59
1:A:424:HIS:NE2	1:A:444:GLU:CD	2.59	0.59
1:X:456:MET:SD	1:X:460:ARG:HD2	2.42	0.59
1:C:554:ARG:HB3	1:C:557:LEU:CD1	2.23	0.59
1:B:440:VAL:O	1:B:452:LEU:HD23	2.03	0.59
1:X:529:ASP:OD2	1:X:529:ASP:N	2.35	0.59
1:A:487:ALA:O	1:A:500:ILE:HG13	2.03	0.58
1:A:337:GLN:HB3	1:A:382:ASN:ND2	2.18	0.58
1:A:458:THR:HG21	1:A:484:LEU:HD13	1.84	0.58
1:B:387:ASN:HB3	1:X:481:THR:CG2	2.27	0.58
1:C:327:LEU:HD21	1:C:346:ASN:HB2	1.86	0.58
1:X:337:GLN:HB2	1:X:382:ASN:HD21	1.69	0.58
1:C:338:SER:O	1:C:339:LEU:HD23	2.03	0.58
1:X:534:VAL:HG23	1:X:547:VAL:CG2	2.34	0.58
1:B:479:ASP:HB3	1:B:484:LEU:HD11	1.85	0.58
1:A:585:ASP:HB3	1:A:588:THR:HG23	1.85	0.58
1:C:477:GLY:C	1:C:484:LEU:HD23	2.29	0.58
1:X:506:ILE:O	1:X:526:ASP:HA	2.03	0.58
1:B:336:ARG:NH2	1:X:528:GLN:O	2.35	0.57
1:B:352:TRP:NE1	1:B:595:THR:HG21	2.14	0.57
1:B:383:SER:CB	1:B:384:PRO:CD	2.82	0.57
1:C:414:ASN:CG	1:C:415:ARG:HD3	2.29	0.57
1:X:541:THR:O	1:X:543:THR:HG23	2.04	0.57
1:A:602:SER:OG	2:A:701[B]:GFD:O20	2.18	0.57
1:C:585:ASP:O	1:C:588:THR:HG22	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:HIS:HB3	1:B:567:TYR:HE1	1.68	0.57
1:X:542:GLU:O	1:X:542:GLU:HG2	2.03	0.57
1:A:421:ILE:HG23	1:A:470:ARG:HG3	1.85	0.57
1:B:342:LEU:HD22	1:B:403:TRP:HZ2	1.68	0.57
1:B:352:TRP:HE1	1:B:595:THR:CG2	2.15	0.56
1:C:461:ILE:HG12	1:C:478:PHE:HB3	1.86	0.56
1:B:515:LEU:HD13	1:B:561:VAL:HG21	1.86	0.56
1:B:551:LYS:HD2	1:B:551:LYS:C	2.30	0.56
1:A:468:LEU:HD13	1:A:514:VAL:HG21	1.86	0.56
1:C:413:ARG:HD3	1:C:429:GLY:O	2.04	0.56
1:A:421:ILE:CG2	1:A:470:ARG:HG3	2.35	0.56
1:C:397:ASN:HB3	1:C:400:THR:HB	1.87	0.56
1:A:507:ARG:HG2	1:A:507:ARG:HH11	1.71	0.56
1:A:520:TYR:OH	1:A:536:ARG:NH1	2.39	0.56
1:C:346:ASN:HD21	1:C:348:SER:HB2	1.71	0.56
1:X:335:PHE:O	1:X:336:ARG:HB2	2.06	0.56
1:B:515:LEU:HD12	1:B:561:VAL:HG21	1.87	0.56
1:C:358:LEU:HD22	1:C:360:VAL:H	1.71	0.56
1:C:441:GLU:HA	1:C:452:LEU:HA	1.88	0.56
1:C:579:ASP:OD2	1:C:600:GLY:N	2.39	0.56
1:X:537:TYR:HE2	1:X:539:VAL:HG12	1.71	0.56
1:C:334:TYR:HB2	1:C:363:SER:CB	2.36	0.55
1:C:508:SER:OG	2:C:701[B]:GFD:N40	2.39	0.55
1:X:365:LEU:HD12	1:X:376:ALA:HB1	1.88	0.55
1:B:466:ALA:CB	1:B:519:ILE:HG23	2.36	0.55
1:B:400:THR:O	1:B:401:ASN:O	2.24	0.55
1:C:421:ILE:HG13	1:C:467:VAL:HG21	1.87	0.55
1:C:515:LEU:HB3	1:C:520:TYR:HE1	1.71	0.55
1:B:530:GLN:HG2	1:B:572:TYR:O	2.07	0.55
1:X:443:TYR:HB2	1:X:450:TRP:CD2	2.41	0.55
1:X:512:VAL:HA	1:X:520:TYR:O	2.07	0.55
1:X:424:HIS:CD2	1:X:444:GLU:HG3	2.42	0.55
1:C:507:ARG:HH22	1:C:533:SER:CB	2.15	0.55
1:A:512:VAL:HA	1:A:520:TYR:O	2.07	0.54
1:C:559:ILE:N	1:C:606:VAL:HG21	2.21	0.54
1:X:374:LEU:HD12	1:X:375:TYR:N	2.22	0.54
1:C:370:VAL:HG23	1:C:420:VAL:HG21	1.90	0.54
1:C:468:LEU:HD23	1:C:469:ASN:HB2	1.90	0.54
1:X:345:TYR:CE2	1:X:347:PRO:HA	2.42	0.54
1:C:346:ASN:HB3	1:C:351:THR:HG1	1.70	0.54
1:X:428:VAL:HG21	1:X:465:VAL:CG2	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:THR:HG22	1:C:561:VAL:N	2.22	0.54
1:C:326:ARG:NH1	1:C:562:HIS:HA	2.22	0.54
1:C:465:VAL:HG13	1:C:472:LEU:CD1	2.38	0.54
1:A:330:THR:HG23	1:A:330:THR:O	2.07	0.54
1:A:486:SER:HB2	1:A:499:MET:CE	2.35	0.54
1:A:541:THR:OG1	1:A:543:THR:HG22	2.08	0.54
1:C:352:TRP:NE1	1:C:595:THR:HG21	2.23	0.53
1:C:417:GLY:O	1:C:428:VAL:HG12	2.08	0.53
1:B:504:ASN:ND2	1:B:535:GLU:OE1	2.41	0.53
1:C:456:MET:CE	1:C:460:ARG:HD2	2.26	0.53
1:A:381:ASN:OD1	1:A:390:SER:HB2	2.08	0.53
1:C:370:VAL:CG2	1:C:420:VAL:CG2	2.86	0.53
1:C:345:TYR:OH	1:C:595:THR:OG1	2.26	0.53
1:C:583:CYS:N	1:C:592:SER:O	2.41	0.53
1:A:337:GLN:NE2	1:C:528:GLN:HA	2.24	0.53
1:C:428:VAL:HG23	1:C:440:VAL:CG2	2.37	0.52
1:A:415:ARG:HB3	1:A:462:GLY:H	1.74	0.52
1:X:571:GLY:HA2	1:X:602:SER:HB2	1.90	0.52
1:A:503:MET:SD	1:A:507:ARG:HD2	2.49	0.52
1:C:565:ARG:CZ	1:C:585:ASP:HB2	2.40	0.52
1:B:505:THR:O	1:B:507:ARG:HG3	2.09	0.52
1:B:541:THR:O	1:B:543:THR:HG23	2.09	0.52
1:C:500:ILE:HG13	1:C:501:THR:O	2.10	0.52
1:A:345:TYR:CE1	1:A:595:THR:HG21	2.45	0.52
1:B:374:LEU:CD1	1:B:607:ALA:HB3	2.40	0.52
1:C:466:ALA:HB1	1:C:514:VAL:HG13	1.90	0.52
1:B:385:ASP:OD1	1:B:385:ASP:N	2.43	0.52
1:B:494:ARG:NH1	1:B:494:ARG:CG	2.72	0.52
1:X:569:LEU:N	1:X:569:LEU:HD12	2.25	0.52
1:C:371:GLY:O	1:C:373:LEU:HD12	2.09	0.52
1:X:380:ARG:HG3	1:X:389:ASP:OD1	2.09	0.52
1:A:326:ARG:HG2	1:A:609:THR:OXT	2.10	0.51
1:A:424:HIS:CD2	1:A:444:GLU:CD	2.88	0.51
1:A:460:ARG:HG2	1:A:460:ARG:NH1	2.25	0.51
1:C:411:VAL:HG21	1:C:437:HIS:CE1	2.45	0.51
1:C:415:ARG:HD2	2:C:701[B]:GFD:O37	2.10	0.51
1:X:370:VAL:HG22	1:X:420:VAL:HG11	1.92	0.51
1:B:436:HIS:O	1:B:459:ARG:HD3	2.10	0.51
1:A:555:SER:OG	2:A:701[B]:GFD:O18	2.28	0.51
1:B:515:LEU:HD13	1:B:561:VAL:CG2	2.41	0.51
1:B:571:GLY:C	1:B:602:SER:HB2	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:THR:HG22	1:C:402:GLN:HG2	1.92	0.51
1:X:362:ARG:NH1	1:X:394:ASP:OD2	2.44	0.51
1:B:380:ARG:HD2	1:B:387:ASN:OD1	2.10	0.51
1:B:551:LYS:HD2	1:B:552:HIS:N	2.26	0.51
1:C:577:PHE:C	1:C:578:LEU:HD22	2.35	0.51
1:A:588:THR:O	1:A:590:THR:CG2	2.58	0.51
1:B:327:LEU:HD22	1:B:346:ASN:HB2	1.92	0.51
1:B:336:ARG:HH22	1:X:529:ASP:HA	1.76	0.51
1:B:434:CYS:HA	1:X:434:CYS:SG	2.51	0.51
1:B:530:GLN:OE1	1:B:530:GLN:N	2.43	0.51
1:A:347:PRO:HG2	1:A:562:HIS:CE1	2.46	0.51
1:A:487:ALA:CB	1:A:500:ILE:HD11	2.38	0.51
1:X:534:VAL:HG23	1:X:547:VAL:HG22	1.93	0.51
1:C:400:THR:O	1:C:402:GLN:HG2	2.09	0.51
1:C:554:ARG:HD3	1:C:570:GLY:O	2.10	0.51
1:C:563:GLN:OE1	1:C:563:GLN:HA	2.10	0.51
1:A:585:ASP:CG	1:A:588:THR:HG22	2.36	0.50
1:B:528:GLN:CD	1:X:383:SER:HA	2.36	0.50
1:C:541:THR:O	1:C:543:THR:HG23	2.11	0.50
1:X:460:ARG:HH21	1:X:488:GLU:CG	2.24	0.50
1:B:597:MET:HE1	1:B:601:ARG:CG	2.41	0.50
1:C:349:ASP:OD2	1:C:351:THR:HG23	2.10	0.50
1:X:374:LEU:HD12	1:X:375:TYR:H	1.77	0.50
1:A:487:ALA:HB3	1:A:500:ILE:CD1	2.39	0.50
1:B:421:ILE:HB	1:B:426:TYR:HE1	1.76	0.50
1:C:327:LEU:HD23	1:C:346:ASN:CB	2.39	0.50
1:A:483:ARG:HB3	1:A:506:ILE:CG2	2.42	0.50
1:B:464:GLY:HA3	1:B:512:VAL:CG2	2.41	0.50
1:B:534:VAL:CG1	1:B:547:VAL:HG23	2.24	0.50
1:C:464:GLY:HA3	1:C:512:VAL:CG2	2.42	0.50
1:C:356:ALA:HB2	1:C:401:ASN:ND2	2.26	0.50
1:X:494:ARG:HH11	1:X:494:ARG:CG	2.24	0.50
1:B:434:CYS:HG	1:X:434:CYS:CB	2.24	0.49
1:C:561:VAL:HG12	1:C:566:ILE:HB	1.93	0.49
1:A:336:ARG:HG3	1:A:336:ARG:HH11	1.77	0.49
1:C:442:ARG:HG2	1:C:442:ARG:NH1	2.27	0.49
1:C:464:GLY:HA3	1:C:512:VAL:HG21	1.94	0.49
1:C:530:GLN:H	1:C:530:GLN:NE2	2.10	0.49
1:X:551:LYS:HG3	1:X:552:HIS:CD2	2.47	0.49
1:C:345:TYR:HA	1:C:351:THR:O	2.12	0.49
1:X:566:ILE:HB	1:X:584:TYR:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:530:GLN:OE1	1:X:530:GLN:N	2.45	0.49
1:A:335:PHE:O	1:A:336:ARG:HB2	2.13	0.49
1:A:349:ASP:O	1:A:351:THR:HG23	2.13	0.49
1:B:595:THR:HG22	1:B:596:ARG:N	2.28	0.49
1:A:369:VAL:HG21	1:A:609:THR:HB	1.95	0.49
1:B:472:LEU:HB3	1:B:490:TYR:HB3	1.95	0.49
1:A:440:VAL:HG23	1:A:453:VAL:HG23	1.93	0.48
1:X:345:TYR:CE1	1:X:595:THR:HG21	2.48	0.48
1:X:383:SER:CB	1:X:384:PRO:CD	2.90	0.48
1:X:424:HIS:NE2	1:X:444:GLU:HG3	2.28	0.48
1:C:584:TYR:OH	1:C:589:ASP:OD2	2.25	0.48
1:C:560:THR:HG22	1:C:561:VAL:H	1.79	0.48
1:X:414:ASN:OD1	3:X:701:A1EMM:N95	2.46	0.48
1:C:478:PHE:HD1	1:C:483:ARG:HG2	1.78	0.48
1:X:457:LEU:HD12	1:X:499:MET:CG	2.41	0.48
1:A:485:ASN:HD21	1:X:452:LEU:CD1	2.26	0.48
1:B:513:CYS:SG	1:B:566:ILE:HD13	2.54	0.48
1:C:555:SER:C	1:C:557:LEU:HD12	2.39	0.48
1:C:584:TYR:HB2	1:C:591:TRP:CE2	2.48	0.48
1:X:472:LEU:HB3	1:X:490:TYR:HB3	1.95	0.48
1:A:575:HIS:CB	1:C:336:ARG:NH2	2.73	0.48
1:C:341:TYR:N	1:C:341:TYR:CD1	2.81	0.48
1:X:573:ASP:HB3	1:X:578:LEU:HD11	1.95	0.48
1:C:426:TYR:OH	1:C:442:ARG:NE	2.46	0.48
1:C:597:MET:SD	1:C:601:ARG:CZ	3.02	0.48
1:X:468:LEU:HD13	1:X:514:VAL:HG21	1.96	0.48
1:X:535:GLU:HG3	1:X:544:TRP:CE3	2.48	0.48
1:C:349:ASP:CG	1:C:351:THR:HG23	2.38	0.47
1:A:381:ASN:HB2	1:A:388:THR:HG22	1.96	0.47
1:A:507:ARG:HG2	1:A:507:ARG:NH1	2.28	0.47
1:B:462:GLY:HA3	3:X:701:A1EMM:N59	2.29	0.47
1:B:520:TYR:CE2	1:B:536:ARG:HD3	2.49	0.47
1:C:341:TYR:N	1:C:341:TYR:HD1	2.12	0.47
1:X:412:PRO:HG2	1:X:432:HIS:ND1	2.28	0.47
1:X:530:GLN:HG3	1:X:555:SER:CB	2.43	0.47
1:C:393:LEU:HD21	1:C:443:TYR:CE2	2.49	0.47
1:C:400:THR:HG22	1:C:402:GLN:CG	2.44	0.47
1:X:554:ARG:HD3	1:X:570:GLY:O	2.15	0.47
1:A:442:ARG:HG2	1:A:442:ARG:HH11	1.79	0.47
1:C:401:ASN:ND2	1:C:401:ASN:O	2.47	0.47
1:A:457:LEU:HD12	1:A:499:MET:CG	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ARG:C	1:A:484:LEU:HD23	2.40	0.47
1:C:349:ASP:OD1	1:C:351:THR:N	2.26	0.47
1:A:338:SER:HB2	1:A:382:ASN:CB	2.42	0.47
1:A:411:VAL:HG21	1:A:437:HIS:CE1	2.49	0.47
1:A:342:LEU:HD13	1:A:403:TRP:HZ2	1.79	0.47
1:B:342:LEU:HG	1:B:355:LEU:HB2	1.96	0.47
1:C:354:ARG:O	1:C:355:LEU:HD23	2.14	0.47
1:C:373:LEU:HD12	1:C:373:LEU:N	2.30	0.47
1:C:582:GLU:HA	1:C:593:GLU:HA	1.96	0.47
1:A:328:ILE:O	1:A:344:ALA:HA	2.15	0.47
1:C:365:LEU:HB2	1:C:377:VAL:O	2.15	0.47
1:C:371:GLY:C	1:C:373:LEU:HD12	2.39	0.47
1:C:421:ILE:CG1	1:C:467:VAL:HG21	2.44	0.47
1:C:508:SER:OG	2:C:701[A]:GFD:O37	2.32	0.47
1:B:436:HIS:CD2	1:B:480:GLY:HA2	2.49	0.47
1:C:478:PHE:CD1	1:C:483:ARG:HG2	2.50	0.47
1:B:483:ARG:NH1	1:B:483:ARG:CG	2.77	0.46
1:B:397:ASN:O	1:B:401:ASN:CA	2.63	0.46
1:C:513:CYS:HB3	1:C:566:ILE:CD1	2.45	0.46
1:A:418:VAL:HA	1:A:426:TYR:O	2.15	0.46
1:C:413:ARG:HB2	1:C:416:ILE:HD12	1.97	0.46
1:B:594:VAL:O	1:B:595:THR:OG1	2.30	0.46
1:C:554:ARG:NH1	1:C:554:ARG:HG3	2.30	0.46
1:B:434:CYS:CB	1:X:434:CYS:SG	3.03	0.46
1:B:571:GLY:O	1:B:602:SER:HB2	2.15	0.46
1:A:336:ARG:HG3	1:A:336:ARG:NH1	2.29	0.46
1:B:326:ARG:HH11	1:B:326:ARG:HB3	1.81	0.46
1:X:428:VAL:HG12	1:X:440:VAL:HG13	1.98	0.46
1:B:551:LYS:HG3	1:B:582:GLU:CD	2.40	0.46
1:C:584:TYR:HB2	1:C:591:TRP:CZ2	2.51	0.46
1:X:468:LEU:O	1:X:469:ASN:C	2.59	0.46
1:B:519:ILE:HD12	1:B:537:TYR:HD2	1.80	0.46
1:A:326:ARG:NH2	1:A:563:GLN:HG3	2.31	0.46
1:A:499:MET:HE3	1:A:499:MET:HB3	1.79	0.46
1:A:537:TYR:HB2	1:A:544:TRP:CH2	2.51	0.46
1:C:569:LEU:HD23	1:C:581:VAL:CG2	2.46	0.45
1:C:576:THR:HG22	1:C:577:PHE:O	2.16	0.45
1:X:335:PHE:O	1:X:336:ARG:CB	2.64	0.45
1:X:428:VAL:HG22	1:X:465:VAL:HG21	1.96	0.45
1:X:487:ALA:O	1:X:499:MET:CE	2.64	0.45
1:A:355:LEU:HD13	1:A:396:TYR:OH	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ILE:HD12	1:A:501:THR:O	2.17	0.45
1:B:490:TYR:O	1:B:492:PRO:HD3	2.16	0.45
1:C:466:ALA:HB2	1:C:512:VAL:HG12	1.98	0.45
1:C:561:VAL:HG13	1:C:566:ILE:HD12	1.98	0.45
1:C:362:ARG:HB2	1:C:365:LEU:HD13	1.97	0.45
1:A:483:ARG:HB3	1:A:506:ILE:HG21	1.97	0.45
1:C:413:ARG:NH1	1:C:439:SER:O	2.50	0.45
1:C:428:VAL:CA	1:C:440:VAL:HG13	2.46	0.45
1:X:490:TYR:CE2	1:X:492:PRO:HA	2.52	0.45
1:X:554:ARG:NH2	1:X:582:GLU:HG3	2.31	0.45
1:A:326:ARG:O	1:A:327:LEU:HD23	2.17	0.45
1:A:354:ARG:O	1:A:355:LEU:HD23	2.17	0.45
1:B:595:THR:HG22	1:B:596:ARG:H	1.81	0.45
1:X:409:MET:HB3	1:X:441:GLU:OE1	2.16	0.45
1:C:330:THR:OG1	1:C:604:VAL:HG11	2.17	0.45
1:X:530:GLN:HG3	1:X:555:SER:HB3	1.99	0.45
1:C:518:CYS:HB3	1:C:537:TYR:O	2.16	0.44
1:B:367:GLY:HA2	1:B:375:TYR:O	2.17	0.44
1:C:488:GLU:HG3	1:C:497:TRP:HE3	1.79	0.44
1:A:585:ASP:HB3	1:A:588:THR:HG22	1.94	0.44
1:B:336:ARG:NH2	1:X:529:ASP:HA	2.32	0.44
1:X:384:PRO:O	1:X:385:ASP:HB2	2.18	0.44
1:X:568:VAL:HG23	1:X:568:VAL:O	2.17	0.44
1:B:597:MET:HE1	1:B:601:ARG:HG2	1.98	0.44
1:C:415:ARG:HD2	2:C:701[B]:GFD:N36	2.33	0.44
1:A:537:TYR:HB2	1:A:544:TRP:CZ2	2.53	0.44
1:B:366:ALA:HB1	1:B:418:VAL:HG22	1.99	0.44
1:C:457:LEU:N	1:C:488:GLU:OE1	2.48	0.44
1:B:522:ALA:HB2	1:B:534:VAL:HG23	1.99	0.44
1:B:526:ASP:HB3	1:B:531:LEU:HD21	1.99	0.44
1:B:554:ARG:HD3	1:B:570:GLY:O	2.18	0.44
1:C:467:VAL:HG23	1:C:471:LEU:O	2.18	0.44
1:C:475:VAL:HB	1:C:512:VAL:HG21	1.99	0.44
1:C:561:VAL:CG1	1:C:566:ILE:HD12	2.48	0.44
1:B:398:PRO:O	1:B:401:ASN:HB2	2.18	0.44
1:B:551:LYS:HG3	1:B:582:GLU:OE2	2.18	0.44
1:C:560:THR:HG21	1:C:608:VAL:HG22	1.99	0.44
1:X:490:TYR:HB2	1:X:497:TRP:CZ3	2.53	0.44
1:C:381:ASN:O	1:C:388:THR:N	2.50	0.43
1:X:464:GLY:HA3	1:X:512:VAL:CG2	2.48	0.43
1:C:374:LEU:HD12	1:C:375:TYR:H	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:342:LEU:HD22	1:X:403:TRP:HZ2	1.81	0.43
1:A:333:GLY:O	1:A:363:SER:HB3	2.18	0.43
1:A:420:VAL:HA	1:A:424:HIS:O	2.19	0.43
1:A:542:GLU:HG3	1:B:434:CYS:HB3	2.01	0.43
1:B:597:MET:CE	1:B:601:ARG:CD	2.96	0.43
1:X:383:SER:OG	1:X:384:PRO:HD3	2.19	0.43
1:X:411:VAL:HG21	1:X:437:HIS:CE1	2.53	0.43
1:X:508:SER:OG	3:X:701:A1EMM:O70	2.37	0.43
1:X:537:TYR:OH	1:X:542:GLU:HG3	2.19	0.43
1:A:342:LEU:HD23	1:A:355:LEU:HB2	2.00	0.43
1:A:507:ARG:HB3	1:A:510:ALA:HB2	2.00	0.43
1:A:540:GLU:O	1:B:434:CYS:HB2	2.19	0.43
1:B:373:LEU:N	1:B:373:LEU:HD23	2.33	0.43
1:X:367:GLY:HA2	1:X:375:TYR:O	2.18	0.43
1:B:338:SER:O	1:B:361:PRO:HB3	2.19	0.43
1:X:552:HIS:HB2	1:X:554:ARG:HH21	1.83	0.43
1:B:464:GLY:HA3	1:B:512:VAL:HG21	2.01	0.43
1:C:373:LEU:HD12	1:C:373:LEU:H	1.83	0.43
1:A:440:VAL:HG23	1:A:453:VAL:CG2	2.49	0.43
1:B:370:VAL:HG11	1:B:445:PRO:HG2	2.01	0.43
1:C:340:SER:HB3	1:C:358:LEU:H	1.83	0.43
1:C:468:LEU:HD21	1:C:469:ASN:OD1	2.18	0.43
1:A:369:VAL:HA	1:A:373:LEU:O	2.18	0.42
1:B:409:MET:HG2	1:B:450:TRP:CE2	2.53	0.42
1:C:393:LEU:HD21	1:C:443:TYR:CD2	2.54	0.42
1:C:581:VAL:O	1:C:581:VAL:HG13	2.19	0.42
1:B:532:ASN:HB3	1:B:553:ARG:HA	2.01	0.42
1:C:503:MET:HE1	1:C:507:ARG:HD2	2.02	0.42
1:A:458:THR:HG21	1:A:484:LEU:CD1	2.46	0.42
1:B:551:LYS:HD2	1:B:552:HIS:CB	2.46	0.42
1:C:428:VAL:HG23	1:C:440:VAL:HG22	2.01	0.42
1:C:466:ALA:HB1	1:C:514:VAL:CG1	2.49	0.42
1:X:458:THR:HG22	1:X:459:ARG:O	2.19	0.42
1:A:538:ASP:OD1	1:A:540:GLU:HG3	2.20	0.42
1:A:483:ARG:NH1	1:A:508:SER:OG	2.52	0.42
1:C:452:LEU:HD12	1:C:452:LEU:O	2.19	0.42
1:A:421:ILE:HG12	1:A:467:VAL:HG11	2.01	0.42
1:B:354:ARG:HG3	1:B:354:ARG:HH11	1.85	0.42
1:C:554:ARG:C	1:C:557:LEU:HD11	2.44	0.42
1:X:537:TYR:HB2	1:X:544:TRP:CE2	2.55	0.42
1:A:336:ARG:O	1:A:337:GLN:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:ARG:HG2	1:C:449:GLU:CD	2.44	0.42
1:C:602:SER:CB	2:C:701[B]:GFD:O20	2.67	0.42
1:X:421:ILE:O	1:X:422:ASP:C	2.62	0.42
1:X:557:LEU:HD12	1:X:568:VAL:HB	2.01	0.42
1:A:595:THR:OG1	1:A:596:ARG:N	2.53	0.42
1:A:422:ASP:O	1:A:422:ASP:CG	2.63	0.42
1:X:428:VAL:O	1:X:428:VAL:HG23	2.19	0.42
1:X:483:ARG:HB3	1:X:506:ILE:CG2	2.49	0.42
1:A:513:CYS:SG	1:A:566:ILE:HD13	2.60	0.42
1:B:479:ASP:OD1	1:B:479:ASP:C	2.63	0.42
1:C:415:ARG:HD2	2:C:701[B]:GFD:C35	2.48	0.42
1:B:329:TYR:O	1:B:606:VAL:HA	2.20	0.41
1:A:584:TYR:HB2	1:A:591:TRP:CE2	2.55	0.41
1:A:589:ASP:O	1:A:589:ASP:CG	2.63	0.41
1:B:517:ASN:ND2	1:B:540:GLU:OE1	2.52	0.41
1:A:468:LEU:HD13	1:A:514:VAL:CG2	2.50	0.41
1:X:409:MET:O	1:X:410:SER:C	2.63	0.41
1:A:396:TYR:HB2	1:A:403:TRP:CD2	2.55	0.41
1:A:470:ARG:O	1:A:471:LEU:HD23	2.20	0.41
1:B:597:MET:HE1	1:B:601:ARG:CD	2.50	0.41
1:C:428:VAL:HG23	1:C:440:VAL:CG1	2.50	0.41
1:C:585:ASP:OD2	1:C:587:ASP:HB2	2.19	0.41
1:A:412:PRO:HD2	1:A:432:HIS:ND1	2.35	0.41
1:A:440:VAL:CG2	1:A:453:VAL:HG23	2.50	0.41
1:B:530:GLN:HG3	1:B:555:SER:CB	2.50	0.41
1:B:530:GLN:HG3	1:B:555:SER:HB3	2.01	0.41
1:C:363:SER:OG	2:C:701[A]:GFD:O18	2.36	0.41
1:C:503:MET:HE1	1:C:521:ALA:HB3	2.03	0.41
1:C:338:SER:C	1:C:339:LEU:HD23	2.45	0.41
1:X:430:GLY:C	1:X:461:ILE:HG22	2.45	0.41
1:X:441:GLU:HB2	1:X:450:TRP:CE3	2.56	0.41
1:X:483:ARG:HB3	1:X:506:ILE:HG21	2.02	0.41
1:X:491:TYR:O	1:X:495:ASN:N	2.52	0.41
1:A:381:ASN:N	1:A:388:THR:O	2.52	0.41
1:B:436:HIS:CD2	1:B:480:GLY:CA	3.04	0.41
1:B:512:VAL:HA	1:B:520:TYR:O	2.20	0.41
1:C:468:LEU:HD23	1:C:468:LEU:C	2.46	0.41
1:A:532:ASN:HA	1:A:550:MET:HE3	2.02	0.41
1:A:540:GLU:O	1:B:434:CYS:N	2.48	0.41
1:C:441:GLU:HG3	1:C:450:TRP:CE3	2.55	0.41
1:C:465:VAL:HG13	1:C:472:LEU:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:TYR:CE1	1:C:539:VAL:HA	2.56	0.41
1:X:483:ARG:NH1	1:X:483:ARG:HG3	2.36	0.41
1:X:490:TYR:HB2	1:X:497:TRP:CH2	2.55	0.41
1:X:584:TYR:HB2	1:X:591:TRP:CH2	2.55	0.41
1:X:555:SER:OG	3:X:701:A1EMM:O69	2.39	0.41
1:X:568:VAL:C	1:X:569:LEU:HD12	2.46	0.41
1:A:465:VAL:HA	1:A:473:TYR:O	2.21	0.40
1:B:339:LEU:N	1:B:339:LEU:HD23	2.36	0.40
1:C:354:ARG:C	1:C:355:LEU:HG	2.46	0.40
1:A:324:VAL:O	1:A:324:VAL:HG13	2.21	0.40
1:A:485:ASN:HD21	1:X:452:LEU:HD12	1.86	0.40
1:A:554:ARG:HA	1:A:572:TYR:O	2.20	0.40
1:B:505:THR:OG1	1:B:507:ARG:NH1	2.54	0.40
1:A:551:LYS:HE2	1:A:552:HIS:NE2	2.36	0.40
1:B:538:ASP:OD1	1:B:538:ASP:C	2.63	0.40
1:C:337:GLN:OE1	1:C:382:ASN:HB3	2.22	0.40
1:C:554:ARG:HG3	1:C:554:ARG:HH11	1.87	0.40
1:C:581:VAL:HG12	1:C:595:THR:O	2.21	0.40
1:A:415:ARG:HB3	1:A:462:GLY:N	2.37	0.40
1:A:438:ASN:HB3	1:A:459:ARG:HA	2.04	0.40
1:C:433:GLY:O	1:C:434:CYS:C	2.63	0.40
1:C:602:SER:OG	2:C:701[A]:GFD:S15	2.76	0.40
1:B:413:ARG:NH2	1:B:439:SER:OG	2.51	0.40
1:B:414:ASN:ND2	3:X:701:A1EMM:O56	2.47	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:THR:OG1	1:C:540:GLU:OE2[1_455]	1.79	0.41
1:B:401:ASN:O	1:C:470:ARG:NH1[1_455]	1.93	0.27

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	284/288 (99%)	277 (98%)	7 (2%)	0	100	100
1	B	283/288 (98%)	266 (94%)	13 (5%)	4 (1%)	9	37
1	C	276/288 (96%)	264 (96%)	12 (4%)	0	100	100
1	X	285/288 (99%)	268 (94%)	13 (5%)	4 (1%)	9	37
All	All	1128/1152 (98%)	1075 (95%)	45 (4%)	8 (1%)	19	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	383	SER
1	X	383	SER
1	B	402	GLN
1	B	506	ILE
1	X	388	THR
1	X	433	GLY
1	B	388	THR
1	X	384	PRO

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	232/234 (99%)	231 (100%)	1 (0%)	89	95
1	B	230/234 (98%)	230 (100%)	0	100	100
1	C	228/234 (97%)	228 (100%)	0	100	100
1	X	232/234 (99%)	232 (100%)	0	100	100
All	All	922/936 (98%)	921 (100%)	1 (0%)	92	98

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

Mol	Chain	Res	Type
1	A	599	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	GLN
1	A	359	GLN
1	A	432	HIS
1	A	436	HIS
1	B	528	GLN
1	B	563	GLN
1	C	381	ASN
1	C	424	HIS
1	C	451	HIS
1	C	504	ASN
1	C	530	GLN
1	X	469	ASN
1	X	575	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](#)

5 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	GFD	A	701[A]	-	44,44,44	2.85	16 (36%)	59,65,65	2.83	16 (36%)
2	GFD	A	701[B]	-	44,44,44	3.08	16 (36%)	59,65,65	2.90	17 (36%)
3	A1EMM	X	701	-	107,107,107	3.60	36 (33%)	138,152,152	3.08	46 (33%)
2	GFD	C	701[B]	-	44,44,44	2.93	14 (31%)	59,65,65	2.65	13 (31%)
2	GFD	C	701[A]	-	44,44,44	2.89	14 (31%)	59,65,65	2.83	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
2	GFD	A	701[A]	-	-	10/42/42/42	0/4/4/4
2	GFD	A	701[B]	-	-	8/42/42/42	0/4/4/4
3	A1EMM	X	701	-	-	38/109/109/109	0/8/8/8
2	GFD	C	701[B]	-	-	14/42/42/42	0/4/4/4
2	GFD	C	701[A]	-	-	12/42/42/42	0/4/4/4

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	701	A1EMM	S14-N11	11.76	1.81	1.65
3	X	701	A1EMM	C07-N12	11.60	1.55	1.44
3	X	701	A1EMM	S13-N12	11.20	1.80	1.65
3	X	701	A1EMM	S67-N68	10.93	1.80	1.65
3	X	701	A1EMM	C74-N81	10.02	1.53	1.44
3	X	701	A1EMM	S82-N81	9.27	1.78	1.65
3	X	701	A1EMM	C16-S13	8.24	1.87	1.76
3	X	701	A1EMM	C71-N68	8.21	1.52	1.44
2	A	701[B]	GFD	S15-N12	8.10	1.76	1.65
2	A	701[B]	GFD	C17-S15	7.18	1.86	1.76
2	C	701[A]	GFD	C17-S15	7.16	1.86	1.76
2	C	701[B]	GFD	C22-S14	7.10	1.86	1.76
3	X	701	A1EMM	C34-N33	7.04	1.51	1.35
2	A	701[A]	GFD	S14-N11	7.00	1.75	1.65
2	C	701[B]	GFD	C03-N12	6.88	1.50	1.44
3	X	701	A1EMM	C64-S67	6.82	1.85	1.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701[A]	GFD	C17-S15	6.78	1.85	1.76
2	A	701[B]	GFD	C22-S14	6.77	1.85	1.76
2	C	701[B]	GFD	C06-N11	6.59	1.50	1.44
2	C	701[A]	GFD	C03-N12	6.58	1.50	1.44
3	X	701	A1EMM	C10-N11	6.57	1.50	1.44
2	C	701[A]	GFD	S14-N11	6.50	1.74	1.65
2	A	701[A]	GFD	C22-S14	6.48	1.85	1.76
2	A	701[B]	GFD	C03-N12	6.42	1.50	1.44
2	A	701[B]	GFD	S14-N11	6.34	1.74	1.65
2	C	701[B]	GFD	S15-N12	6.33	1.74	1.65
2	C	701[B]	GFD	C17-S15	6.33	1.85	1.76
2	A	701[B]	GFD	C06-N11	6.23	1.50	1.44
2	C	701[A]	GFD	C06-N11	6.05	1.49	1.44
2	C	701[A]	GFD	C22-S14	6.01	1.84	1.76
3	X	701	A1EMM	C15-S14	5.90	1.84	1.76
2	C	701[B]	GFD	S14-N11	5.89	1.73	1.65
2	A	701[A]	GFD	C06-N11	5.73	1.49	1.44
2	A	701[A]	GFD	C03-N12	5.69	1.49	1.44
2	C	701[A]	GFD	S15-N12	5.60	1.73	1.65
3	X	701	A1EMM	O85-S82	5.28	1.49	1.43
2	A	701[A]	GFD	S15-N12	5.17	1.72	1.65
3	X	701	A1EMM	C98-N99	4.94	1.48	1.32
3	X	701	A1EMM	C54-N55	4.59	1.47	1.32
2	A	701[B]	GFD	C38-N40	4.41	1.47	1.32
3	X	701	A1EMM	C83-S82	4.35	1.82	1.76
2	A	701[A]	GFD	C38-N40	4.33	1.46	1.32
2	C	701[B]	GFD	C38-N40	4.26	1.46	1.32
2	A	701[A]	GFD	C35-N36	4.25	1.46	1.32
2	C	701[A]	GFD	C38-N40	4.25	1.46	1.32
3	X	701	A1EMM	C94-N95	4.21	1.46	1.32
2	C	701[A]	GFD	C35-N36	4.18	1.46	1.32
3	X	701	A1EMM	C58-N59	4.17	1.46	1.32
3	X	701	A1EMM	O70-S67	4.00	1.48	1.43
3	X	701	A1EMM	O17-S13	3.95	1.47	1.43
3	X	701	A1EMM	C28-N33	3.93	1.49	1.41
2	A	701[B]	GFD	O19-S15	3.93	1.47	1.43
2	C	701[B]	GFD	C35-N36	3.91	1.45	1.32
2	C	701[A]	GFD	O21-S14	3.89	1.47	1.43
3	X	701	A1EMM	C50-N51	3.88	1.44	1.35
2	C	701[B]	GFD	O21-S14	3.83	1.47	1.43
2	A	701[B]	GFD	C35-N36	3.82	1.45	1.32
2	A	701[B]	GFD	O20-S14	3.82	1.47	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701[A]	GFD	O19-S15	3.69	1.47	1.43
3	X	701	A1EMM	C76-C75	3.66	1.45	1.38
2	C	701[B]	GFD	O19-S15	3.66	1.47	1.43
2	C	701[A]	GFD	O19-S15	3.64	1.47	1.43
2	A	701[A]	GFD	O21-S14	3.58	1.47	1.43
3	X	701	A1EMM	C73-C72	-3.57	1.36	1.43
2	A	701[B]	GFD	O21-S14	3.55	1.47	1.43
2	C	701[A]	GFD	O20-S14	3.55	1.47	1.43
2	A	701[A]	GFD	O20-S14	3.54	1.47	1.43
3	X	701	A1EMM	O91-C88	3.38	1.44	1.37
3	X	701	A1EMM	C35-C34	3.31	1.57	1.51
2	C	701[B]	GFD	O20-S14	3.23	1.47	1.43
2	C	701[B]	GFD	O18-S15	2.96	1.46	1.43
2	C	701[A]	GFD	O18-S15	2.95	1.46	1.43
3	X	701	A1EMM	O20-S14	2.91	1.46	1.43
2	A	701[B]	GFD	C07-C04	-2.84	1.36	1.42
2	A	701[B]	GFD	C30-N33	2.78	1.48	1.38
2	A	701[B]	GFD	O34-C25	2.68	1.43	1.37
3	X	701	A1EMM	C97-C98	2.63	1.55	1.52
2	A	701[A]	GFD	C30-N33	2.62	1.47	1.38
2	A	701[A]	GFD	O18-S15	2.61	1.46	1.43
3	X	701	A1EMM	O84-S82	2.53	1.46	1.43
2	A	701[B]	GFD	O18-S15	2.46	1.46	1.43
3	X	701	A1EMM	C08-C09	2.44	1.43	1.38
2	C	701[B]	GFD	C30-N33	2.41	1.46	1.38
2	C	701[A]	GFD	C30-N33	2.38	1.46	1.38
2	A	701[B]	GFD	C05-C04	-2.38	1.39	1.43
3	X	701	A1EMM	O69-S67	2.31	1.46	1.43
2	A	701[A]	GFD	C05-C04	-2.26	1.39	1.43
2	A	701[A]	GFD	C07-C04	-2.26	1.37	1.42
3	X	701	A1EMM	C29-C30	2.22	1.42	1.38
3	X	701	A1EMM	O36-C34	-2.20	1.18	1.23
2	C	701[B]	GFD	C07-C04	-2.17	1.37	1.42
3	X	701	A1EMM	C05-C04	-2.16	1.39	1.43
3	X	701	A1EMM	C49-C50	2.15	1.55	1.51
2	C	701[A]	GFD	C07-C04	-2.14	1.37	1.42
2	A	701[A]	GFD	O34-C25	2.08	1.41	1.37
3	X	701	A1EMM	C52-N51	2.07	1.45	1.41

All (110) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701[B]	GFD	O21-S14-O20	-11.78	100.44	119.52
2	C	701[A]	GFD	O19-S15-O18	-11.53	100.83	119.52
2	C	701[B]	GFD	O21-S14-O20	-11.30	101.21	119.52
2	A	701[A]	GFD	O19-S15-O18	-11.10	101.53	119.52
3	X	701	A1EMM	O85-S82-O84	-11.05	101.61	119.52
3	X	701	A1EMM	C64-S67-N68	10.77	121.60	106.92
3	X	701	A1EMM	O19-S14-O20	-10.67	102.24	119.52
2	A	701[A]	GFD	O21-S14-O20	-10.62	102.31	119.52
3	X	701	A1EMM	O17-S13-O18	-10.31	102.81	119.52
3	X	701	A1EMM	O85-S82-N81	10.15	118.72	106.71
3	X	701	A1EMM	O70-S67-O69	-10.12	103.12	119.52
2	C	701[A]	GFD	O21-S14-O20	-9.98	103.35	119.52
2	C	701[B]	GFD	O19-S15-O18	-9.85	103.55	119.52
2	A	701[B]	GFD	O19-S15-O18	-9.85	103.55	119.52
3	X	701	A1EMM	O17-S13-N12	8.69	116.99	106.71
3	X	701	A1EMM	O20-S14-N11	8.21	116.42	106.71
2	A	701[B]	GFD	O20-S14-N11	6.36	114.24	106.71
2	A	701[B]	GFD	O18-S15-N12	5.85	113.63	106.71
3	X	701	A1EMM	O20-S14-C15	-5.84	100.66	108.05
2	A	701[A]	GFD	O19-S15-N12	5.45	113.16	106.71
3	X	701	A1EMM	C49-C50-N51	5.18	123.72	114.59
3	X	701	A1EMM	C35-C34-N33	5.15	123.66	114.59
2	C	701[A]	GFD	O18-S15-N12	5.14	112.79	106.71
2	A	701[A]	GFD	O18-S15-N12	5.12	112.77	106.71
2	C	701[A]	GFD	O19-S15-N12	5.11	112.76	106.71
2	C	701[A]	GFD	O18-S15-C17	5.11	114.51	108.05
2	C	701[B]	GFD	O21-S14-C22	5.02	114.39	108.05
3	X	701	A1EMM	O69-S67-N68	4.97	112.58	106.71
2	A	701[A]	GFD	O21-S14-N11	4.88	112.48	106.71
2	C	701[B]	GFD	O21-S14-N11	4.87	112.47	106.71
2	A	701[A]	GFD	O20-S14-N11	4.86	112.46	106.71
2	A	701[B]	GFD	O19-S15-N12	4.68	112.25	106.71
2	C	701[B]	GFD	O18-S15-N12	4.63	112.18	106.71
2	C	701[A]	GFD	O20-S14-N11	4.59	112.14	106.71
3	X	701	A1EMM	C15-S14-N11	4.58	113.16	106.92
2	C	701[B]	GFD	O19-S15-N12	4.55	112.09	106.71
2	C	701[A]	GFD	O21-S14-N11	4.45	111.98	106.71
2	A	701[A]	GFD	O18-S15-C17	4.42	113.64	108.05
3	X	701	A1EMM	C76-C71-N68	4.36	124.82	119.75
2	A	701[B]	GFD	O19-S15-C17	4.12	113.26	108.05
2	A	701[A]	GFD	C13-N11-S14	4.11	124.24	117.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	701	A1EMM	C97-N68-S67	3.94	123.94	117.23
2	A	701[B]	GFD	C07-C04-C03	-3.87	116.06	122.74
2	C	701[A]	GFD	C13-N11-S14	3.86	123.81	117.23
3	X	701	A1EMM	O69-S67-C64	-3.84	103.19	108.05
2	C	701[A]	GFD	O19-S15-C17	3.84	112.91	108.05
3	X	701	A1EMM	C77-C72-C71	-3.83	116.13	122.74
2	A	701[B]	GFD	C01-C06-N11	-3.70	115.43	119.75
2	C	701[A]	GFD	C02-C03-N12	-3.69	115.45	119.75
3	X	701	A1EMM	O19-S14-N11	3.67	111.05	106.71
2	A	701[B]	GFD	C16-N12-S15	3.54	123.26	117.23
3	X	701	A1EMM	O19-S14-C15	3.53	112.51	108.05
3	X	701	A1EMM	C97-C98-N99	3.52	121.41	115.86
3	X	701	A1EMM	C57-N12-S13	3.48	123.16	117.23
2	A	701[B]	GFD	C02-C03-N12	-3.47	115.70	119.75
2	A	701[B]	GFD	C07-C04-C05	3.45	122.73	118.45
3	X	701	A1EMM	C30-C16-S13	3.45	123.39	119.76
3	X	701	A1EMM	O61-C50-N51	-3.44	117.35	123.63
2	C	701[B]	GFD	C07-C04-C03	-3.43	116.81	122.74
2	A	701[A]	GFD	O19-S15-C17	3.31	112.24	108.05
2	A	701[B]	GFD	C13-C35-N36	3.30	121.06	115.86
2	C	701[B]	GFD	C16-C38-N40	3.29	121.05	115.86
2	A	701[B]	GFD	O21-S14-C22	3.27	112.18	108.05
2	A	701[A]	GFD	O20-S14-C22	3.22	112.12	108.05
2	A	701[A]	GFD	C02-C03-N12	-3.15	116.08	119.75
3	X	701	A1EMM	C80-C73-C74	-3.14	117.32	122.74
2	C	701[A]	GFD	C07-C04-C03	-3.14	117.33	122.74
2	A	701[B]	GFD	O21-S14-N11	3.09	110.37	106.71
2	A	701[A]	GFD	C07-C04-C03	-3.09	117.41	122.74
3	X	701	A1EMM	C71-C72-C73	3.04	122.61	119.33
2	C	701[B]	GFD	O20-S14-C22	3.01	111.85	108.05
2	C	701[B]	GFD	C07-C04-C05	2.92	122.08	118.45
2	C	701[A]	GFD	O21-S14-C22	2.91	111.73	108.05
3	X	701	A1EMM	C75-C74-N81	2.87	123.09	119.75
2	C	701[B]	GFD	O18-S15-C17	2.83	111.63	108.05
3	X	701	A1EMM	O85-S82-C83	2.80	111.59	108.05
2	C	701[A]	GFD	C01-C06-N11	-2.77	116.52	119.75
3	X	701	A1EMM	O84-S82-C83	2.72	111.49	108.05
3	X	701	A1EMM	C65-C64-S67	2.68	122.58	119.76
2	A	701[B]	GFD	C06-N11-S14	-2.65	113.50	117.24
2	C	701[B]	GFD	C02-C03-N12	-2.62	116.69	119.75
3	X	701	A1EMM	O36-C34-N33	-2.62	118.84	123.63
3	X	701	A1EMM	C71-N68-S67	-2.62	113.54	117.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	701	A1EMM	O84-S82-N81	2.54	109.72	106.71
2	C	701[A]	GFD	C17-S15-N12	-2.53	103.47	106.92
3	X	701	A1EMM	O17-S13-C16	2.51	111.23	108.05
3	X	701	A1EMM	C53-N11-S14	2.50	121.49	117.23
3	X	701	A1EMM	O36-C34-C35	-2.47	117.50	122.02
2	A	701[A]	GFD	C07-C04-C05	2.46	121.51	118.45
2	C	701[A]	GFD	C07-C04-C05	2.46	121.51	118.45
2	A	701[B]	GFD	C22-S14-N11	2.46	110.27	106.92
2	A	701[A]	GFD	C01-C06-N11	-2.43	116.91	119.75
3	X	701	A1EMM	C79-C80-C73	-2.35	117.63	120.89
3	X	701	A1EMM	C74-C73-C72	2.33	121.84	119.33
3	X	701	A1EMM	C03-C04-C07	-2.29	118.79	122.74
3	X	701	A1EMM	C77-C72-C73	2.26	121.25	118.45
3	X	701	A1EMM	C83-S82-N81	-2.23	103.87	106.92
2	A	701[A]	GFD	C17-S15-N12	-2.23	103.88	106.92
3	X	701	A1EMM	C78-C77-C72	-2.20	117.84	120.89
2	C	701[A]	GFD	C41-O34-C25	-2.20	112.74	117.51
3	X	701	A1EMM	C75-C74-C73	-2.16	116.08	119.94
2	A	701[B]	GFD	C16-C38-N40	2.12	119.21	115.86
3	X	701	A1EMM	C90-C83-S82	-2.12	117.53	119.76
3	X	701	A1EMM	O18-S13-N12	2.10	109.19	106.71
3	X	701	A1EMM	C06-C05-C10	-2.08	119.16	122.74
2	C	701[A]	GFD	C13-C35-N36	2.06	119.12	115.86
2	A	701[A]	GFD	O21-S14-C22	2.06	110.65	108.05
2	C	701[A]	GFD	C06-N11-S14	2.06	120.15	117.24
3	X	701	A1EMM	C57-C58-N59	2.03	119.07	115.86
2	C	701[B]	GFD	C16-N12-S15	2.01	120.66	117.23

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701[A]	GFD	C35-C13-N11-S14
2	A	701[A]	GFD	N12-C16-C38-O39
2	A	701[B]	GFD	N11-C13-C35-N36
2	A	701[B]	GFD	N11-C13-C35-O37
2	A	701[B]	GFD	C35-C13-N11-C06
2	C	701[A]	GFD	C35-C13-N11-S14
2	C	701[A]	GFD	N12-C16-C38-O39
2	C	701[B]	GFD	N11-C13-C35-N36
2	C	701[B]	GFD	N11-C13-C35-O37
2	C	701[B]	GFD	C35-C13-N11-C06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	701[B]	GFD	C35-C13-N11-S14
3	X	701	A1EMM	C34-C35-C37-O38
3	X	701	A1EMM	O47-C48-C49-C50
3	X	701	A1EMM	N12-C57-C58-N59
3	X	701	A1EMM	N12-C57-C58-O60
3	X	701	A1EMM	C94-C93-N81-C74
3	X	701	A1EMM	N68-C97-C98-N99
3	X	701	A1EMM	N68-C97-C98-OA0
3	X	701	A1EMM	O61-C50-N51-C52
2	C	701[B]	GFD	C24-C25-O34-C41
2	C	701[B]	GFD	C26-C25-O34-C41
3	X	701	A1EMM	C49-C50-N51-C52
2	A	701[B]	GFD	C26-C25-O34-C41
2	A	701[B]	GFD	C24-C25-O34-C41
3	X	701	A1EMM	O38-C39-C40-O41
3	X	701	A1EMM	C93-N81-S82-O85
3	X	701	A1EMM	O44-C45-C46-O47
2	A	701[A]	GFD	C24-C25-O34-C41
2	C	701[A]	GFD	C24-C25-O34-C41
2	A	701[A]	GFD	C26-C25-O34-C41
2	A	701[A]	GFD	N12-C16-C38-N40
2	C	701[A]	GFD	N12-C16-C38-N40
3	X	701	A1EMM	N11-C53-C54-O56
2	C	701[A]	GFD	C26-C25-O34-C41
2	C	701[A]	GFD	C16-N12-S15-O19
2	C	701[B]	GFD	C13-N11-S14-C22
3	X	701	A1EMM	C53-N11-S14-O20
3	X	701	A1EMM	C97-N68-S67-C64
3	X	701	A1EMM	C97-N68-S67-O69
2	A	701[A]	GFD	C16-N12-S15-O19
2	A	701[B]	GFD	C13-N11-S14-O20
2	C	701[B]	GFD	C13-N11-S14-O20
2	C	701[A]	GFD	C38-C16-N12-C03
3	X	701	A1EMM	N11-C53-C54-N55
3	X	701	A1EMM	C54-C53-N11-C10
2	A	701[A]	GFD	C13-N11-S14-O21
2	C	701[A]	GFD	C13-N11-S14-O21
2	C	701[B]	GFD	C16-N12-S15-O18
3	X	701	A1EMM	C49-C48-O47-C46
2	C	701[B]	GFD	C13-N11-S14-O21
3	X	701	A1EMM	C53-N11-S14-O19
3	X	701	A1EMM	C93-N81-S82-O84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	X	701	A1EMM	N33-C34-C35-C37
3	X	701	A1EMM	O36-C34-C35-C37
3	X	701	A1EMM	C46-C45-O44-C43
3	X	701	A1EMM	C53-N11-S14-C15
3	X	701	A1EMM	C97-N68-S67-O70
3	X	701	A1EMM	C42-C43-O44-C45
2	A	701[B]	GFD	C35-C13-N11-S14
3	X	701	A1EMM	C58-C57-N12-S13
3	X	701	A1EMM	C94-C93-N81-S82
3	X	701	A1EMM	C57-N12-S13-O18
3	X	701	A1EMM	C43-C42-O41-C40
2	C	701[A]	GFD	C16-N12-S15-C17
3	X	701	A1EMM	C93-N81-S82-C83
3	X	701	A1EMM	N81-C93-C94-N95
2	A	701[A]	GFD	C35-C13-N11-C06
3	X	701	A1EMM	N81-C93-C94-O96
2	A	701[A]	GFD	C16-N12-S15-C17
2	A	701[B]	GFD	C13-N11-S14-C22
2	C	701[A]	GFD	C01-C06-N11-C13
2	C	701[B]	GFD	C02-C03-N12-C16
3	X	701	A1EMM	C22-C23-O31-C32
3	X	701	A1EMM	C24-C23-O31-C32
3	X	701	A1EMM	O41-C42-C43-O44
3	X	701	A1EMM	C58-C57-N12-C07
2	C	701[A]	GFD	C16-N12-S15-O18
2	C	701[B]	GFD	C04-C03-N12-C16
2	C	701[B]	GFD	C05-C06-N11-C13
2	A	701[A]	GFD	C13-N11-S14-C22
2	C	701[A]	GFD	C13-N11-S14-C22
2	C	701[B]	GFD	C16-N12-S15-C17

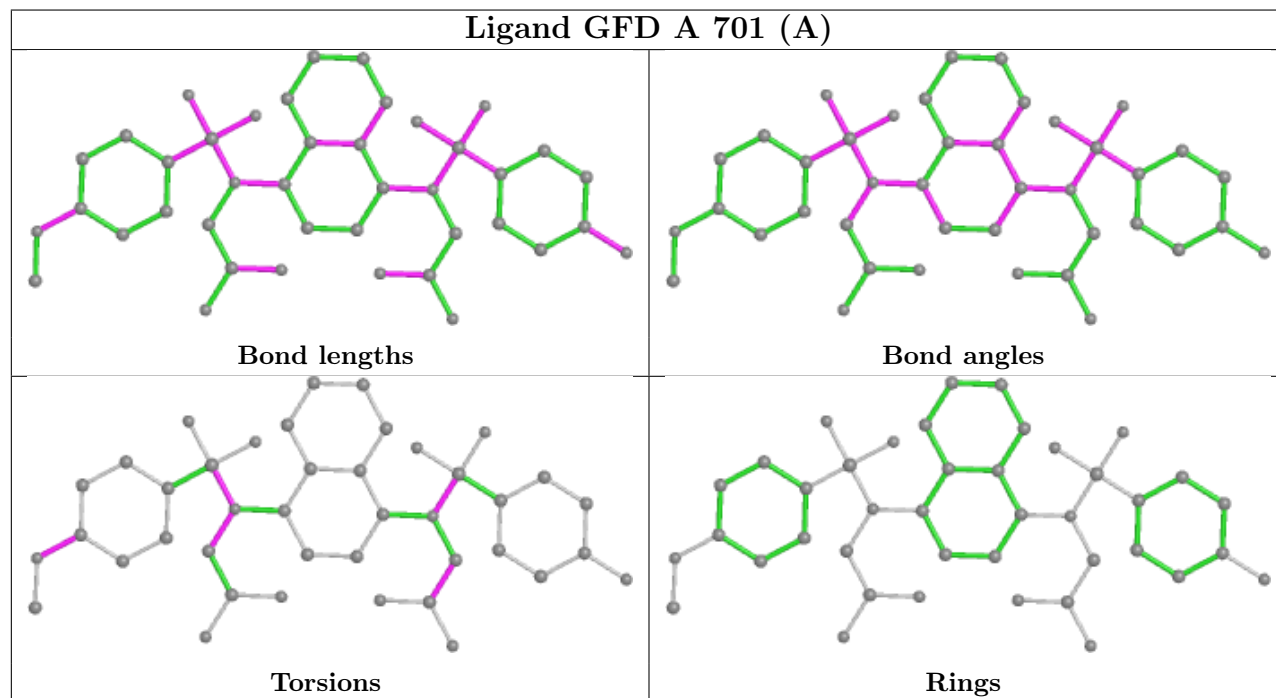
There are no ring outliers.

4 monomers are involved in 20 short contacts:

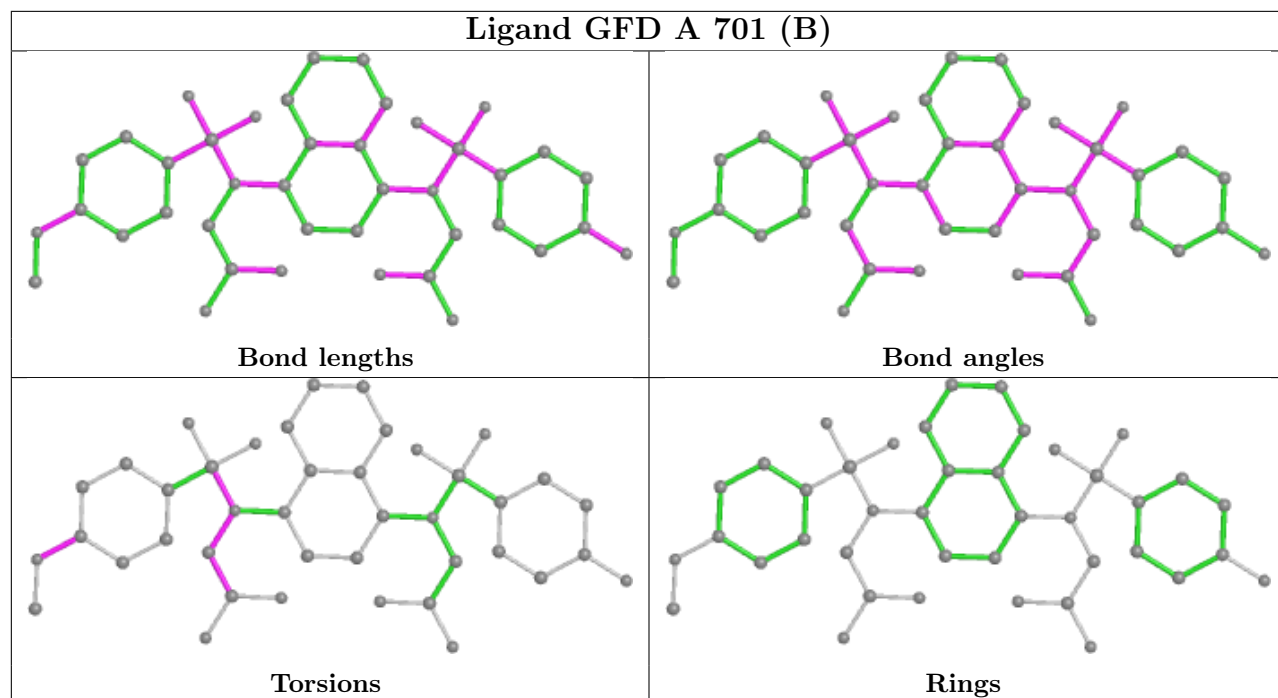
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701[B]	GFD	3	0
3	X	701	A1EMM	6	0
2	C	701[B]	GFD	7	0
2	C	701[A]	GFD	4	0

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

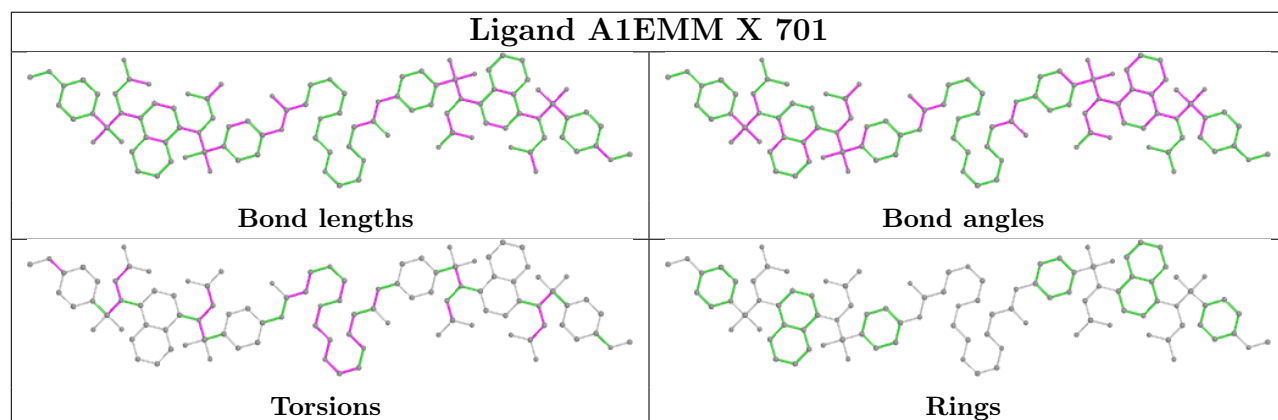
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

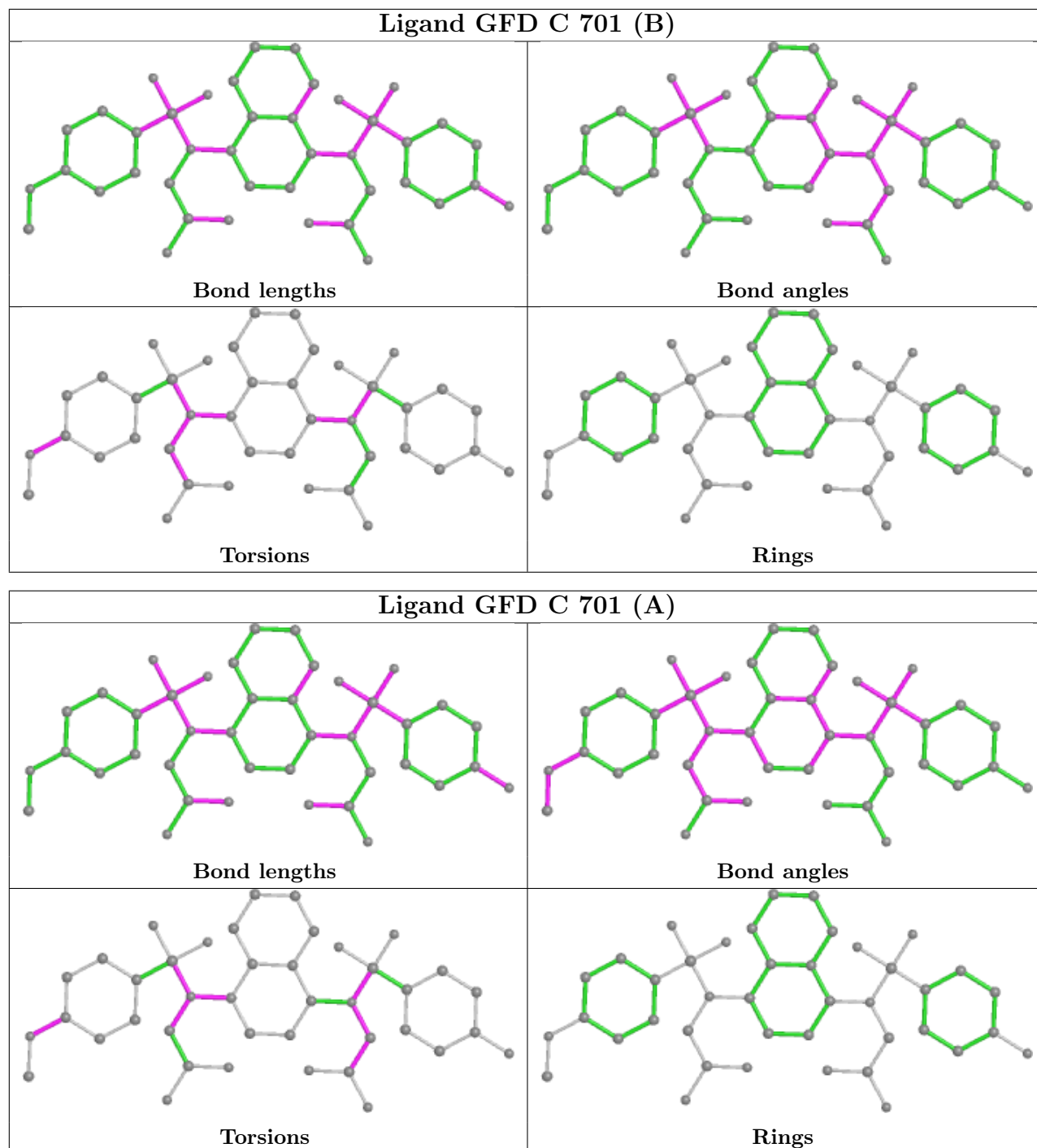


Ligand GFD A 701 (B)



Ligand A1EMM X 701





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	286/288 (99%)	-0.15	4 (1%) 73 52	52, 72, 96, 224	0
1	B	285/288 (98%)	0.23	8 (2%) 55 33	60, 85, 108, 120	0
1	C	279/288 (96%)	0.76	16 (5%) 30 17	85, 126, 152, 169	1 (0%)
1	X	287/288 (99%)	-0.32	2 (0%) 84 68	41, 61, 87, 132	0
All	All	1137/1152 (98%)	0.12	30 (2%) 57 35	41, 79, 144, 224	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	332	GLY	4.5
1	C	580[A]	SER	3.9
1	C	578	LEU	3.8
1	B	384	PRO	3.5
1	B	401	ASN	3.4
1	B	383	SER	3.3
1	C	341	TYR	3.2
1	X	324	VAL	3.2
1	B	400	THR	2.9
1	B	578	LEU	2.9
1	C	358	LEU	2.8
1	C	514	VAL	2.7
1	X	387	ASN	2.6
1	C	608	VAL	2.6
1	A	542	GLU	2.6
1	C	599	SER	2.6
1	B	542	GLU	2.5
1	A	324	VAL	2.4
1	B	545	THR	2.3
1	B	567	TYR	2.2
1	C	436	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	369	VAL	2.1
1	C	420	VAL	2.1
1	C	601	ARG	2.1
1	C	330	THR	2.1
1	C	407	ALA	2.1
1	C	373	LEU	2.0
1	A	385	ASP	2.0
1	A	404	SER	2.0
1	C	485	ASN	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](#)

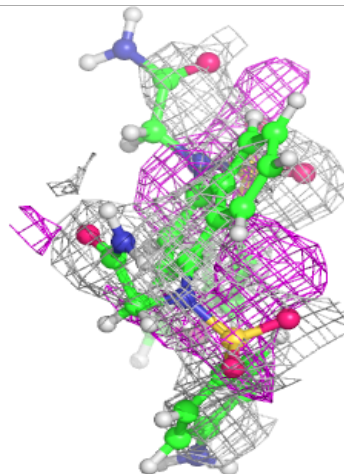
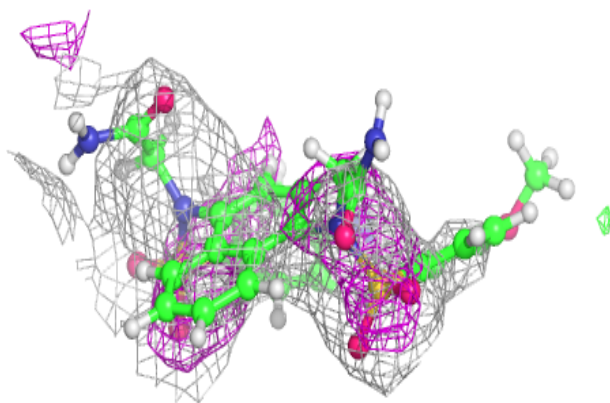
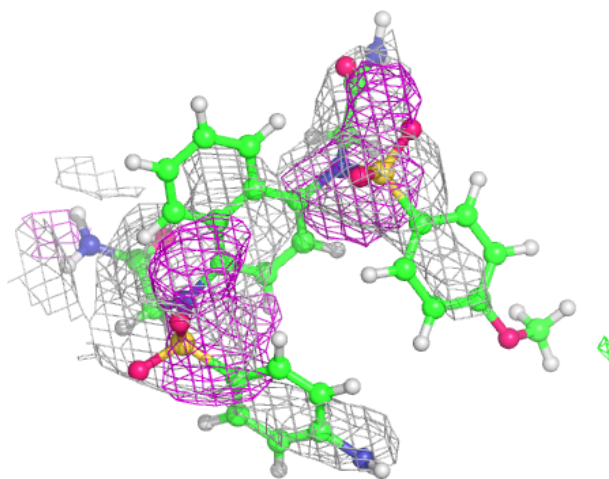
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GFD	C	701[A]	41/41	0.77	0.20	128,141,168,171	68
2	GFD	C	701[B]	41/41	0.77	0.20	127,141,168,170	68
2	GFD	A	701[A]	41/41	0.94	0.14	78,87,105,106	68
2	GFD	A	701[B]	41/41	0.94	0.14	77,88,106,107	68
3	A1EMM	X	701	100/100	0.94	0.12	63,99,131,140	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.

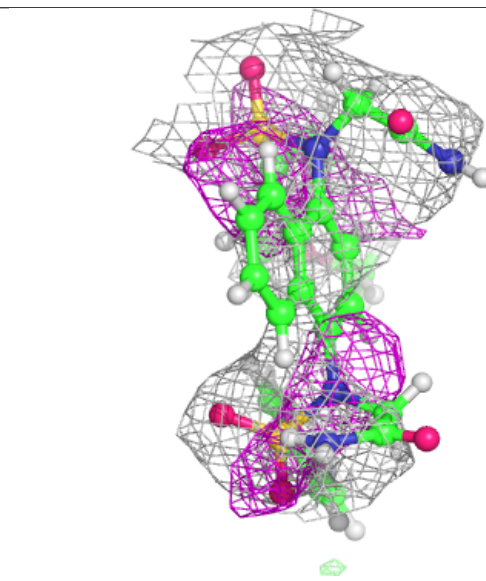
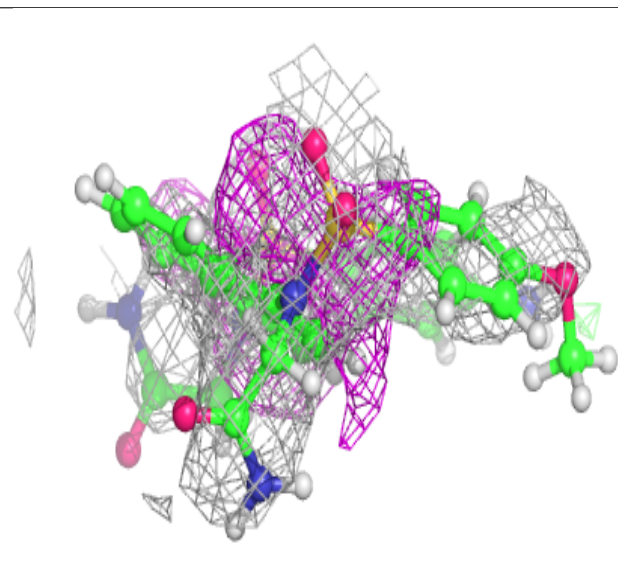
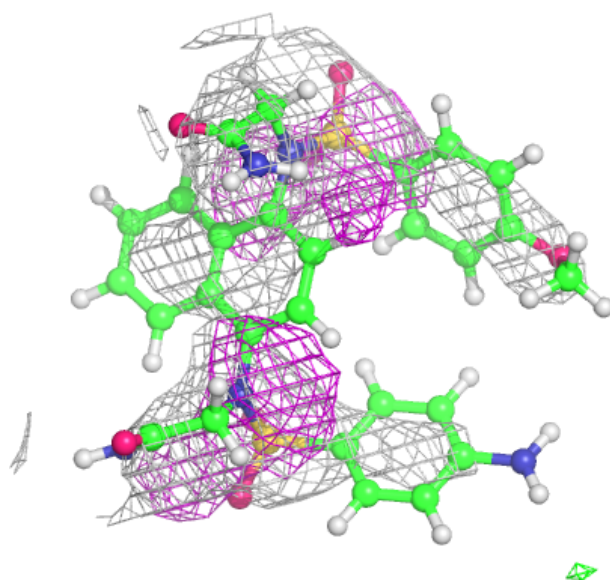
Electron density around GFD C 701 (A):

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



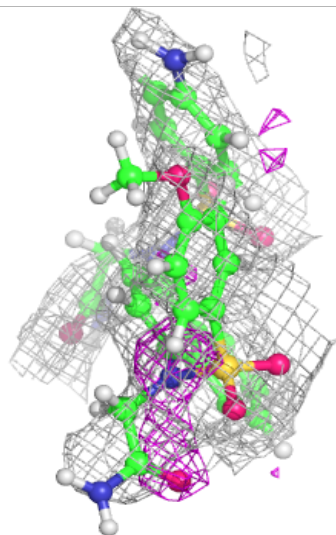
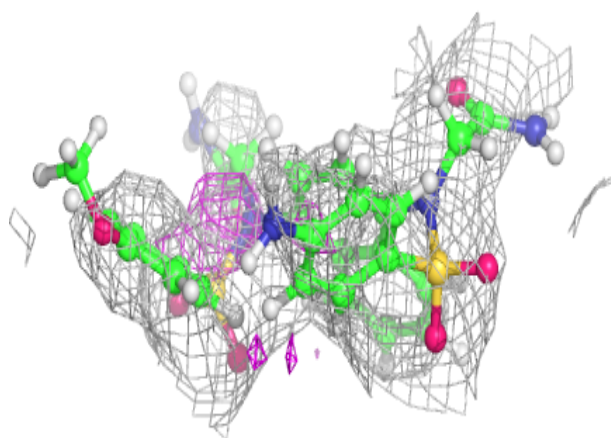
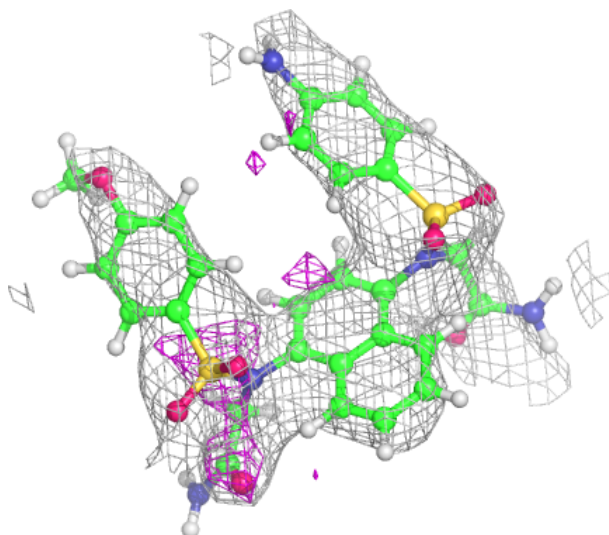
Electron density around GFD C 701 (B):

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



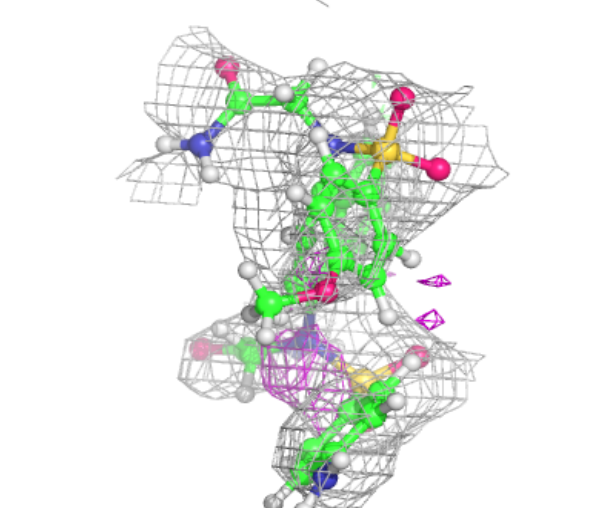
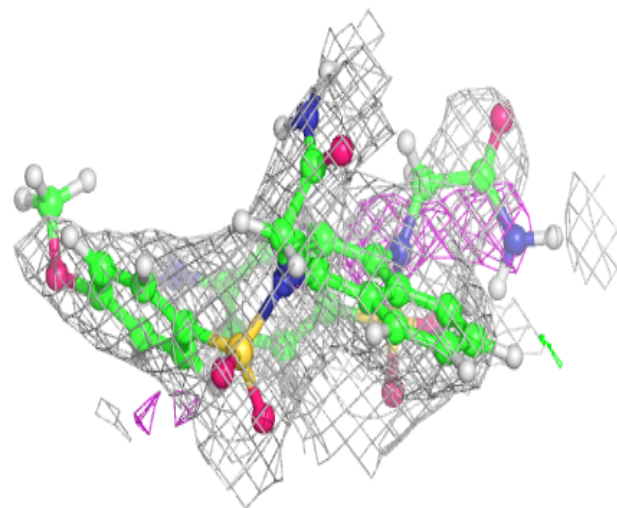
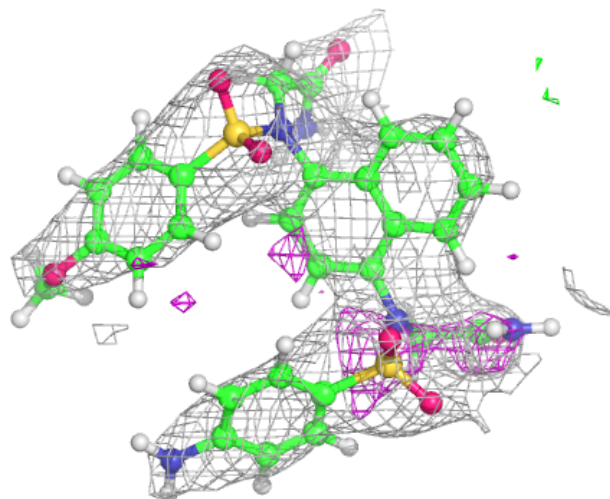
Electron density around GFD A 701 (A):

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



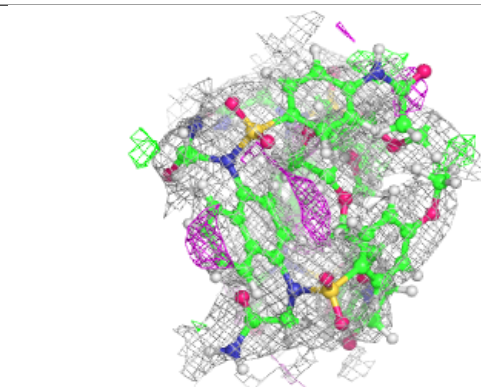
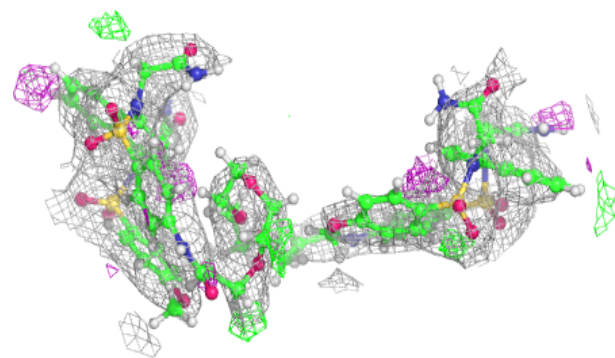
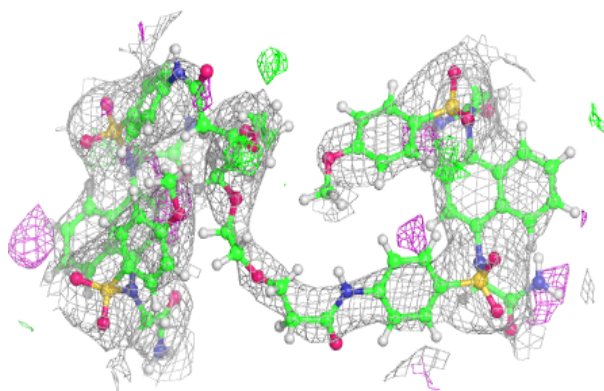
Electron density around GFD A 701 (B):

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



Electron density around A1EMM X 701:

$2mF_o - DF_c$ (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.