



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:58 AM UTC

PDB ID : 1YBG / pdb_00001ybg
Title : MurA inhibited by a derivative of 5-sulfonyl-anthranilic acid
Authors : Eschenburg, S.; Priestman, M.A.; Abdul-Latif, F.A.; Delachaux, C.; Fassy, F.; Schonbrunn, E.
Deposited on : 2004-12-20
Resolution : 2.60 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

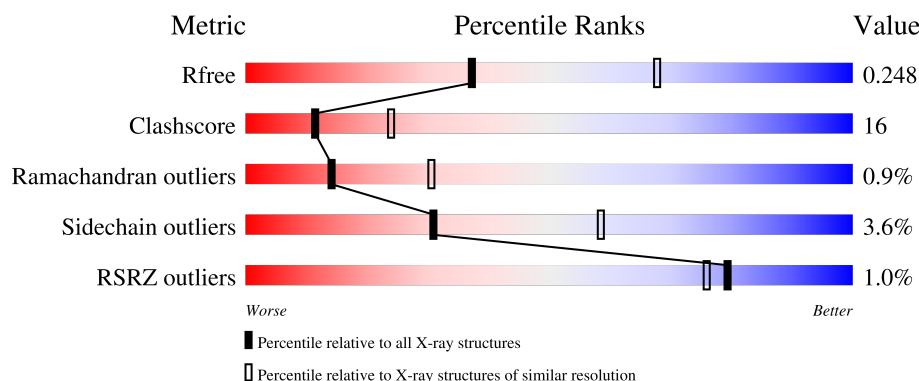
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	419	72% 24% .
1	B	419	67% 30% .
1	C	419	71% 26% .
1	D	419	74% 24% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13267 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.

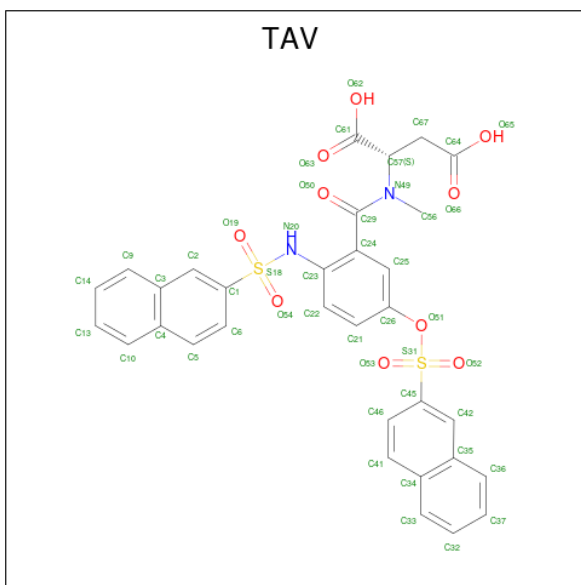
- Molecule 1 is a protein called UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	3	0
			3156	1983	554	605	14			
1	B	419	Total	C	N	O	S	0	3	0
			3162	1987	560	601	14			
1	C	419	Total	C	N	O	S	0	6	0
			3171	1995	555	607	14			
1	D	419	Total	C	N	O	S	0	2	0
			3155	1984	558	599	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	engineered mutation	UNP P33038
B	67	IAS	ASN	engineered mutation	UNP P33038
C	67	IAS	ASN	engineered mutation	UNP P33038
D	67	IAS	ASN	engineered mutation	UNP P33038

- Molecule 2 is N-METHYL-N-{2-[(2-NAPHTHYLSULFONYL)AMINO]-5-[(2-NAPHTHYLSULFONYL)OXY]BENZOYL}-L-ASPARTIC ACID (CCD ID: TAV) (formula: C₃₂H₂₆N₂O₁₀S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 46	C 32	N 2	O 10	S 2	0	0
2	B	1	Total 46	C 32	N 2	O 10	S 2	0	0
2	C	1	Total 46	C 32	N 2	O 10	S 2	0	0
2	D	1	Total 46	C 32	N 2	O 10	S 2	0	0

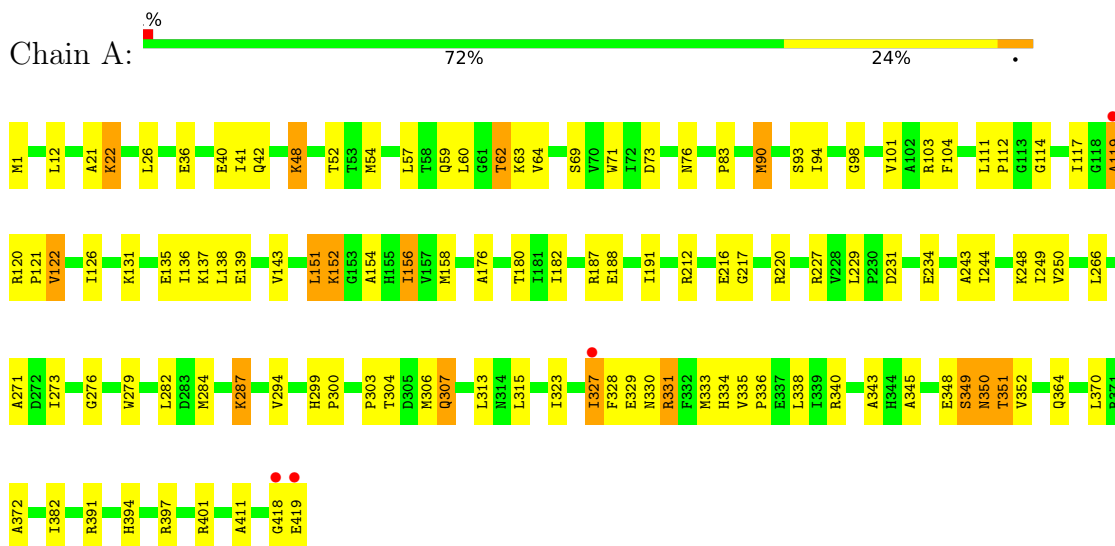
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	115	Total O 115 115	0	0
3	B	102	Total O 102 102	0	0
3	C	135	Total O 135 135	0	0
3	D	87	Total O 87 87	0	0

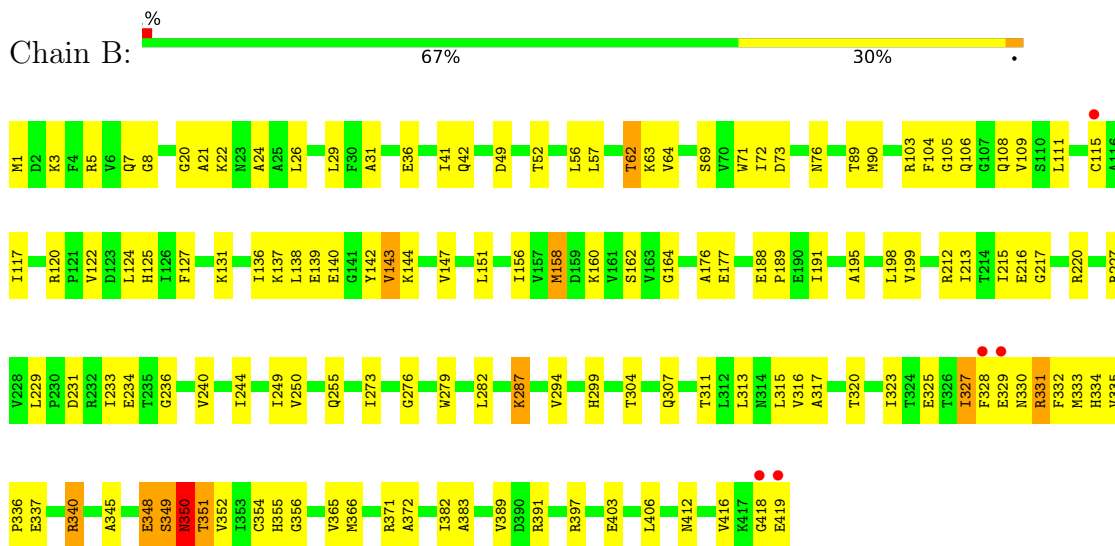
3 Residue-property plots

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: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

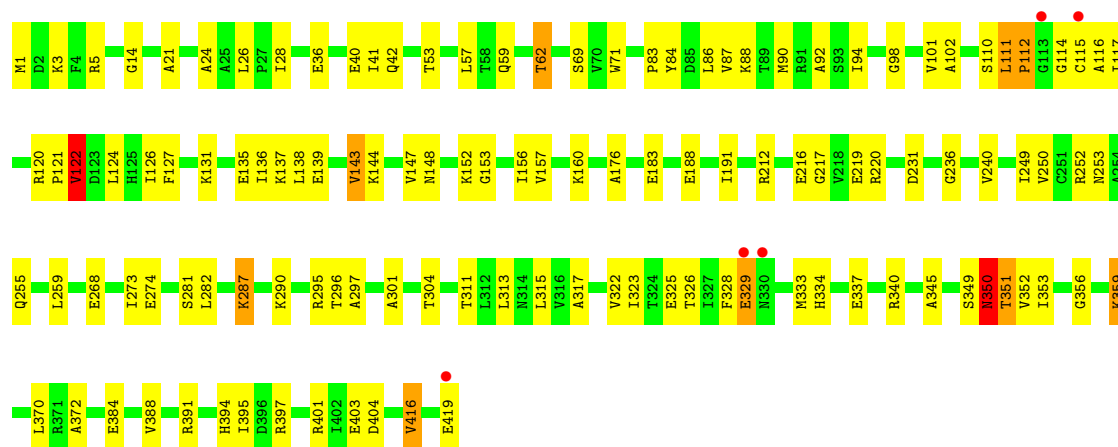


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

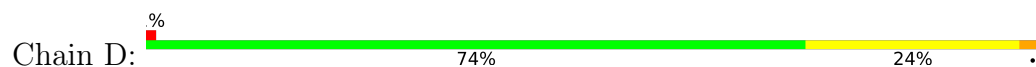


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





● Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.08Å 134.60Å 175.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.00 – 2.60 16.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (16.00-2.60) 99.3 (16.00-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.62Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.253 0.204 , 0.248	Depositor DCC
R_{free} test set	1842 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13267	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IAS, TAV

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	0.63	0/3204	1.03	13/4339 (0.3%)
1	B	0.63	1/3210 (0.0%)	1.01	16/4345 (0.4%)
1	C	0.67	0/3231	1.05	13/4374 (0.3%)
1	D	0.62	0/3199	1.03	8/4330 (0.2%)
All	All	0.64	1/12844 (0.0%)	1.03	50/17388 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	MET	SD-CE	-5.07	1.66	1.79

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ILE	N-CA-C	8.46	120.01	108.17
1	A	188	GLU	N-CA-C	7.41	118.12	109.60
1	B	151	LEU	N-CA-C	-7.36	100.81	110.53
1	C	156	ILE	N-CA-C	7.27	118.35	108.17
1	D	273	ILE	N-CA-C	7.27	118.95	108.48
1	C	350	ASN	N-CA-C	-7.17	105.37	112.97
1	C	273	ILE	N-CA-C	7.12	118.86	108.53
1	A	191	ILE	N-CA-C	-7.05	103.91	110.53
1	D	156	ILE	N-CA-C	7.01	117.98	108.17
1	C	311	THR	N-CA-C	-6.99	103.74	111.36
1	D	84	TYR	N-CA-C	6.72	118.26	111.07
1	A	234	GLU	N-CA-C	-6.54	104.23	111.36
1	B	311	THR	N-CA-C	-6.35	104.28	111.14
1	C	255	GLN	CA-C-N	6.28	126.48	119.32
1	C	255	GLN	C-N-CA	6.28	126.48	119.32
1	A	76	ASN	N-CA-C	6.23	120.65	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	ILE	N-CA-C	6.18	117.67	108.46
1	A	307	GLN	N-CA-C	5.99	117.47	111.07
1	C	143	VAL	N-CA-C	-5.96	99.28	107.99
1	A	135	GLU	N-CA-C	-5.87	100.93	110.20
1	A	156	ILE	N-CA-C	5.86	116.38	108.17
1	A	349	SER	CB-CA-C	-5.85	108.15	116.34
1	D	20	GLY	N-CA-C	-5.83	104.62	112.14
1	B	22	LYS	N-CA-C	-5.83	105.27	112.38
1	C	24	ALA	N-CA-C	-5.80	106.75	113.88
1	B	350	ASN	N-CA-C	-5.77	106.86	112.97
1	C	322	VAL	N-CA-C	5.72	116.10	107.75
1	D	307	GLN	N-CA-C	5.71	117.18	111.07
1	B	76	ASN	N-CA-C	5.67	119.87	111.87
1	B	89	THR	N-CA-C	5.65	120.02	113.18
1	D	120	ARG	CA-C-N	5.63	126.88	119.84
1	D	120	ARG	C-N-CA	5.63	126.88	119.84
1	B	255	GLN	CA-C-N	5.62	126.86	119.84
1	B	255	GLN	C-N-CA	5.62	126.86	119.84
1	A	335	VAL	CB-CA-C	-5.54	108.48	114.35
1	B	24	ALA	N-CA-C	-5.54	107.07	113.88
1	A	90	MET	N-CA-C	5.53	117.68	108.99
1	A	60	LEU	N-CA-C	-5.44	106.00	113.30
1	B	162	SER	N-CA-C	5.41	117.20	108.34
1	A	151	LEU	N-CA-C	-5.40	103.56	110.53
1	C	191	ILE	N-CA-C	-5.33	105.52	110.53
1	C	212	ARG	N-CA-C	5.31	117.73	108.76
1	C	259	LEU	N-CA-C	5.27	118.83	111.56
1	B	191	ILE	N-CA-C	-5.22	105.44	110.72
1	B	234	GLU	N-CA-C	-5.22	105.49	111.07
1	C	359	LYS	N-CA-C	5.20	117.16	108.99
1	B	106	GLN	N-CA-C	5.13	116.21	108.46
1	B	20	GLY	N-CA-C	-5.12	105.54	112.14
1	D	311	THR	N-CA-C	-5.12	105.70	111.28
1	B	316	VAL	N-CA-C	-5.03	107.81	112.43

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	3156	0	3218	114	0
1	B	3162	0	3236	118	0
1	C	3171	0	3238	113	0
1	D	3155	0	3234	100	0
2	A	46	0	24	4	0
2	B	46	0	24	3	0
2	C	46	0	24	6	0
2	D	46	0	24	3	0
3	A	115	0	0	9	0
3	B	102	0	0	3	0
3	C	135	0	0	4	0
3	D	87	0	0	6	0
All	All	13267	0	13022	417	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 16.

All (417) 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:1:MET:HE3	1:C:391:ARG:HE	1.18	1.04
1:D:111:LEU:HD23	1:D:112:PRO:HD2	1.36	1.03
1:B:350:ASN:H	1:B:350:ASN:HD22	1.01	0.98
1:A:111:LEU:HD11	1:A:143:VAL:HG23	1.44	0.98
1:A:111:LEU:HD11	1:A:143:VAL:CG2	1.95	0.97
1:C:350:ASN:HD22	1:C:350:ASN:H	1.07	0.97
1:D:7:GLN:HB2	1:D:412:ASN:HB3	1.45	0.95
1:D:350:ASN:HD22	1:D:350:ASN:H	1.15	0.94
1:A:350:ASN:HD22	1:A:350:ASN:H	1.09	0.93
1:A:59:GLN:NE2	1:A:83:PRO:HG3	1.83	0.92
1:B:327:ILE:HA	3:B:449:HOH:O	1.70	0.90
1:D:150:ARG:HD3	3:D:453:HOH:O	1.73	0.88
1:D:123:ASP:HB2	3:D:482:HOH:O	1.75	0.87
1:B:227:ARG:HD2	3:B:461:HOH:O	1.75	0.86
1:B:111:LEU:HD11	1:B:143:VAL:HG22	1.58	0.86
1:C:359:LYS:HD3	1:C:384:GLU:HB2	1.58	0.86
1:C:121:PRO:O	1:C:122:VAL:HB	1.71	0.85
1:C:36:GLU:OE1	1:C:220:ARG:HD2	1.75	0.85
1:D:111:LEU:HD23	1:D:112:PRO:CD	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LEU:HD12	1:C:143:VAL:HG22	1.59	0.84
1:D:42:GLN:HA	1:D:69:SER:HB3	1.60	0.83
1:C:26:LEU:HD12	2:C:750:TAV:O52	1.78	0.83
1:A:136:ILE:HB	1:C:138[B]:LEU:HD23	1.59	0.83
1:C:1:MET:HE3	1:C:391:ARG:NE	1.94	0.82
1:D:83:PRO:HG2	1:D:86:LEU:HB2	1.60	0.82
1:A:333:MET:O	1:A:336:PRO:HD2	1.80	0.81
1:B:327:ILE:HG22	1:B:328:PHE:HD1	1.44	0.81
1:B:350:ASN:HD22	1:B:350:ASN:N	1.77	0.81
1:C:88:LYS:HA	1:C:112:PRO:HG2	1.62	0.81
1:D:57:LEU:O	1:D:62:THR:HG23	1.81	0.81
1:A:227:ARG:HD2	3:A:517:HOH:O	1.80	0.80
1:C:350:ASN:HD22	1:C:350:ASN:N	1.77	0.80
1:A:117:ILE:HG22	1:C:124:LEU:HD23	1.64	0.80
1:C:40:GLU:HG3	1:C:71:TRP:NE1	1.97	0.80
1:B:366:MET:HG3	1:B:391:ARG:HD2	1.64	0.79
1:D:350:ASN:HD22	1:D:350:ASN:N	1.77	0.78
1:D:5:ARG:NH1	1:D:5:ARG:HB3	1.97	0.78
1:A:350:ASN:HD22	1:A:350:ASN:N	1.76	0.77
1:B:57:LEU:O	1:B:62:THR:HG23	1.84	0.77
1:B:137:LYS:NZ	1:D:137:LYS:HE2	2.00	0.76
1:A:139:GLU:HB3	1:C:135[A]:GLU:HG3	1.67	0.76
1:C:350:ASN:H	1:C:350:ASN:ND2	1.84	0.75
1:A:370:LEU:HB2	1:A:397:ARG:HH22	1.52	0.75
1:D:350:ASN:H	1:D:350:ASN:ND2	1.84	0.74
1:A:111:LEU:CD1	1:A:143:VAL:HG23	2.18	0.74
1:D:83:PRO:HG3	1:D:86:LEU:HD12	1.70	0.74
1:D:248[A]:LYS:HE3	3:D:465:HOH:O	1.89	0.73
1:C:83:PRO:CG	1:C:86:LEU:HD12	2.19	0.72
1:A:21:ALA:HB2	1:A:231:ASP:HA	1.71	0.71
1:B:142:TYR:CE1	1:B:144:LYS:HE3	2.25	0.71
1:B:142:TYR:HE1	1:B:144:LYS:HE3	1.55	0.71
1:A:370:LEU:HB2	1:A:397:ARG:NH2	2.06	0.70
1:C:94:ILE:HG21	2:C:750:TAV:H6	1.73	0.70
1:A:26:LEU:HD12	2:A:550:TAV:O52	1.92	0.70
1:C:1:MET:CE	1:C:391:ARG:HE	2.02	0.69
1:A:57:LEU:O	1:A:62:THR:HG23	1.92	0.69
1:C:1:MET:HE1	1:C:391:ARG:HH21	1.57	0.69
1:C:337:GLU:O	1:C:340:ARG:HG2	1.92	0.69
1:A:117:ILE:HD12	1:C:127:PHE:HB3	1.76	0.68
1:C:295:ARG:HD2	3:C:481:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ASN:H	1:A:350:ASN:ND2	1.86	0.68
1:C:42:GLN:HA	1:C:69:SER:HB3	1.75	0.68
1:C:57:LEU:C	1:C:62:THR:HG23	2.19	0.67
1:C:57:LEU:O	1:C:62:THR:CG2	2.42	0.67
1:B:131:LYS:HG3	1:D:117:ILE:HD11	1.76	0.67
1:C:295:ARG:CZ	1:C:326:THR:HG21	2.25	0.67
1:D:36:GLU:OE1	1:D:220:ARG:HD2	1.95	0.67
1:B:340:ARG:HG2	1:B:340:ARG:HH11	1.59	0.67
1:A:334:HIS:HB3	1:A:372:ALA:HB1	1.76	0.66
1:D:57:LEU:C	1:D:62:THR:HG23	2.19	0.66
1:D:22:LYS:NZ	1:D:397:ARG:HH11	1.93	0.66
1:B:176:ALA:O	1:B:217:GLY:HA3	1.96	0.66
1:C:401:ARG:NH1	1:C:404:ASP:OD1	2.29	0.66
1:B:327:ILE:HG22	1:B:328:PHE:CD1	2.29	0.65
1:A:333:MET:HE1	1:D:347:ILE:HD12	1.77	0.65
1:D:57:LEU:O	1:D:62:THR:CG2	2.43	0.65
1:B:57:LEU:C	1:B:62:THR:HG23	2.23	0.64
1:C:57:LEU:O	1:C:62:THR:HG23	1.98	0.64
1:C:121:PRO:O	1:C:122:VAL:CB	2.46	0.64
1:D:83:PRO:CG	1:D:86:LEU:HD12	2.26	0.64
1:A:187:ARG:HD3	3:A:432:HOH:O	1.98	0.64
1:A:42:GLN:HA	1:A:69:SER:HB3	1.79	0.64
1:B:137:LYS:HB3	1:B:144:LYS:HB2	1.80	0.63
1:B:138:LEU:HB2	1:D:136:ILE:HB	1.79	0.63
1:B:304:THR:HB	1:B:327:ILE:HD12	1.79	0.63
1:A:340:ARG:NH2	1:A:364:GLN:O	2.32	0.62
1:B:57:LEU:O	1:B:62:THR:CG2	2.46	0.62
1:B:136:ILE:HG22	1:B:138:LEU:HD13	1.80	0.62
1:A:36:GLU:OE1	1:A:220:ARG:HD2	1.98	0.62
1:C:83:PRO:HG3	1:C:86:LEU:HD12	1.80	0.62
1:A:40:GLU:HG3	1:A:71:TRP:NE1	2.15	0.62
1:A:57:LEU:C	1:A:62:THR:HG23	2.24	0.62
1:A:158:MET:HE2	1:A:158:MET:HA	1.82	0.62
1:A:327:ILE:HG13	1:A:328:PHE:HD1	1.64	0.62
1:C:40:GLU:HG3	1:C:71:TRP:CD1	2.35	0.62
1:A:59:GLN:HE21	1:A:83:PRO:HG3	1.62	0.61
1:A:333:MET:HE1	1:D:347:ILE:CD1	2.29	0.61
1:A:331:ARG:HG2	1:A:331:ARG:HH11	1.65	0.61
1:A:401:ARG:NH1	1:A:401:ARG:HB2	2.16	0.61
1:D:158:MET:HE2	1:D:158:MET:HA	1.83	0.61
1:B:350:ASN:H	1:B:350:ASN:ND2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ASP:CG	1:B:397[A]:ARG:HH21	2.09	0.60
1:C:323:ILE:HB	1:C:352:VAL:CG1	2.32	0.60
1:C:120:ARG:O	1:C:121:PRO:C	2.44	0.60
1:C:1:MET:HE1	1:C:391:ARG:NH2	2.16	0.59
1:A:1:MET:HB3	1:A:419:GLU:HA	1.83	0.59
1:C:295:ARG:HB3	3:C:522:HOH:O	2.02	0.59
1:A:187:ARG:NH1	3:A:432:HOH:O	2.36	0.59
1:B:1:MET:HB3	1:B:419:GLU:HA	1.84	0.59
1:A:136:ILE:HG22	1:A:138:LEU:CD2	2.33	0.59
1:B:36:GLU:OE1	1:B:220:ARG:HD2	2.03	0.59
1:C:176:ALA:O	1:C:217:GLY:HA3	2.03	0.58
1:A:137:LYS:HD3	1:A:139:GLU:OE2	2.03	0.58
1:B:233:ILE:HG21	1:B:371:ARG:CZ	2.34	0.58
1:B:124:LEU:HD11	1:B:160:LYS:HE3	1.85	0.58
1:D:323:ILE:HB	1:D:352:VAL:CG1	2.33	0.58
1:D:188:GLU:HG2	2:D:850:TAV:H32	1.85	0.58
1:A:59:GLN:HE22	1:A:83:PRO:HG3	1.64	0.57
1:D:1:MET:HE3	1:D:391:ARG:HG2	1.86	0.57
1:B:109:VAL:O	1:B:142:TYR:HB2	2.04	0.57
1:B:137:LYS:HD3	1:B:139:GLU:OE2	2.05	0.57
1:A:48:LYS:HD3	3:A:470:HOH:O	2.05	0.57
1:C:304:THR:HG21	1:C:328:PHE:HE1	1.70	0.57
1:B:26:LEU:HD12	2:B:650:TAV:O52	2.04	0.57
1:C:83:PRO:HG2	1:C:86:LEU:HD12	1.85	0.57
1:C:370:LEU:HB2	1:C:397:ARG:HH22	1.70	0.57
1:C:126:ILE:HG23	1:C:136:ILE:HG21	1.86	0.57
1:D:7:GLN:HB2	1:D:412:ASN:CB	2.29	0.57
1:C:268:GLU:O	1:C:290:LYS:HD2	2.06	0.56
1:C:313:LEU:C	1:C:313:LEU:HD23	2.30	0.56
1:C:127:PHE:O	1:C:131:LYS:HG2	2.04	0.56
1:A:176:ALA:O	1:A:217:GLY:HA3	2.05	0.56
1:A:119:ALA:O	1:A:120:ARG:C	2.50	0.55
1:B:52:THR:HG22	1:B:90:MET:HE2	1.87	0.55
1:A:330:ASN:CG	1:A:333:MET:HE2	2.32	0.55
1:B:282:LEU:C	1:B:282:LEU:HD23	2.31	0.55
1:B:103:ARG:HD3	1:B:104:PHE:CE1	2.41	0.55
1:B:137:LYS:CE	1:D:137:LYS:HE2	2.37	0.55
1:C:334:HIS:HB3	1:C:372:ALA:HB1	1.88	0.55
1:A:1:MET:HE3	1:A:391:ARG:HG2	1.88	0.55
1:D:353:ILE:HD12	1:D:353:ILE:N	2.22	0.55
1:D:313:LEU:C	1:D:313:LEU:HD23	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:MET:HE1	1:D:347:ILE:HG21	1.88	0.54
1:B:334:HIS:HB3	1:B:372:ALA:HB1	1.90	0.54
1:B:304:THR:OG1	1:B:331:ARG:NH1	2.41	0.54
1:A:282:LEU:C	1:A:282:LEU:HD23	2.33	0.54
1:D:5:ARG:HB3	1:D:5:ARG:HH11	1.71	0.54
1:C:323:ILE:HB	1:C:352:VAL:HG12	1.90	0.54
1:B:117:ILE:HG22	1:D:124:LEU:HD22	1.89	0.54
1:B:3:LYS:HG3	1:B:416:VAL:CG2	2.38	0.54
2:C:750:TAV:O19	2:C:750:TAV:H22	2.07	0.54
1:B:137:LYS:HZ1	1:D:137:LYS:HE2	1.73	0.53
1:D:334:HIS:HB3	1:D:372:ALA:HB1	1.91	0.53
1:A:117:ILE:HD11	1:C:131:LYS:HE3	1.91	0.53
1:A:304:THR:OG1	1:A:331:ARG:NH1	2.41	0.53
1:B:117:ILE:HG22	1:D:124:LEU:CD2	2.38	0.53
1:D:22:LYS:NZ	1:D:397:ARG:NH1	2.56	0.53
1:C:3:LYS:HG3	1:C:416:VAL:HG22	1.90	0.53
1:B:325:GLU:HG2	1:B:328:PHE:O	2.09	0.53
1:B:332:PHE:HB3	1:B:335:VAL:HG23	1.90	0.53
1:A:352:VAL:HG13	1:A:352:VAL:O	2.08	0.53
1:C:21:ALA:HB2	1:C:231:ASP:HA	1.90	0.53
1:C:53:THR:OG1	1:C:90:MET:HE1	2.09	0.53
1:B:63:LYS:HB2	1:B:73:ASP:HB3	1.90	0.53
1:A:212:ARG:HG3	1:A:212:ARG:O	2.09	0.52
1:C:84:TYR:HA	1:C:110:SER:CB	2.40	0.52
1:D:282:LEU:HD23	1:D:282:LEU:C	2.33	0.52
1:D:5:ARG:HH11	1:D:5:ARG:CB	2.22	0.52
1:C:87:VAL:HG11	1:C:110:SER:O	2.09	0.52
1:D:22:LYS:HZ1	1:D:397:ARG:HH11	1.57	0.52
1:D:42:GLN:HA	1:D:69:SER:CB	2.36	0.52
1:C:98:GLY:O	1:C:101:VAL:HG12	2.10	0.52
1:B:140:GLU:HB2	1:B:142:TYR:CE2	2.45	0.52
1:B:287:LYS:HB2	1:B:287:LYS:NZ	2.25	0.52
1:B:333:MET:HE2	1:B:333:MET:N	2.24	0.52
1:B:21:ALA:HB2	1:B:231:ASP:HA	1.92	0.52
1:C:287:LYS:HB2	1:C:287:LYS:NZ	2.25	0.52
1:A:131:LYS:CG	1:C:117:ILE:HD11	2.40	0.52
1:B:329:GLU:OE2	1:C:350:ASN:HB3	2.09	0.52
1:A:401:ARG:CB	1:A:401:ARG:HH11	2.22	0.51
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.91	0.51
1:C:252:ARG:O	1:C:253:ASN:HB2	2.11	0.51
1:D:5:ARG:NH1	1:D:5:ARG:CB	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:LYS:HB2	1:D:287:LYS:NZ	2.25	0.51
1:A:26:LEU:CD1	2:A:550:TAV:O52	2.58	0.51
1:A:243:ALA:O	1:A:284:MET:HE2	2.11	0.51
1:D:233:ILE:HG21	1:D:371:ARG:CZ	2.41	0.51
1:A:117:ILE:HD11	1:C:131:LYS:CE	2.40	0.51
1:B:49:ASP:OD1	1:B:397[A]:ARG:NH2	2.44	0.51
1:B:332:PHE:HB3	1:B:335:VAL:CG2	2.40	0.51
1:D:2:ASP:OD1	1:D:415:ARG:HD3	2.11	0.51
1:C:370:LEU:HD13	1:C:394:HIS:O	2.10	0.51
1:B:336:PRO:HG2	1:C:333:MET:HE2	1.92	0.51
1:D:322:VAL:HG22	1:D:353:ILE:HG13	1.93	0.51
1:A:138:LEU:HB2	1:C:136:ILE:HB	1.92	0.51
1:B:330:ASN:O	1:B:331:ARG:HB2	2.10	0.51
1:D:176:ALA:O	1:D:217:GLY:HA3	2.11	0.51
1:A:370:LEU:HD22	1:A:397:ARG:NH1	2.26	0.51
1:B:348:GLU:O	1:B:349:SER:HB2	2.10	0.51
1:D:135:GLU:HB3	3:D:438:HOH:O	2.10	0.51
1:B:177:GLU:HG2	3:B:521:HOH:O	2.10	0.50
1:D:323:ILE:HB	1:D:352:VAL:HG12	1.93	0.50
1:B:366:MET:CG	1:B:391:ARG:HD2	2.35	0.50
1:C:304:THR:HG21	1:C:328:PHE:CE1	2.46	0.50
1:D:87:VAL:HG22	1:D:93:SER:HB3	1.93	0.50
1:A:41:ILE:O	1:A:69:SER:HB2	2.10	0.50
1:D:21:ALA:HB2	1:D:231:ASP:HA	1.93	0.50
1:A:401:ARG:NH1	1:A:401:ARG:CB	2.75	0.50
1:A:329:GLU:O	1:A:330:ASN:C	2.53	0.50
1:B:136:ILE:HG22	1:B:138:LEU:CD1	2.41	0.50
1:C:1:MET:HB3	1:C:419:GLU:HA	1.94	0.50
1:B:105:GLY:HA2	1:B:147:VAL:HG12	1.94	0.50
1:B:307:GLN:NE2	1:B:325:GLU:OE2	2.45	0.50
1:D:31:ALA:HB1	1:D:198:LEU:HD21	1.93	0.50
1:D:325:GLU:HG2	1:D:328:PHE:O	2.11	0.50
1:A:52:THR:HG22	1:A:90:MET:HE2	1.92	0.50
1:B:337:GLU:CD	1:B:340:ARG:HH21	2.20	0.50
1:C:88:LYS:HA	1:C:112:PRO:CG	2.38	0.50
1:D:317:ALA:O	1:D:356:GLY:HA3	2.12	0.50
1:A:244:ILE:HD12	1:A:382:ILE:HD13	1.93	0.49
1:C:5:ARG:HG3	1:C:388:VAL:HG22	1.94	0.49
1:D:3:LYS:HA	1:D:392:ILE:HG12	1.93	0.49
1:D:243:ALA:HA	1:D:284:MET:CG	2.43	0.49
1:A:57:LEU:O	1:A:62:THR:CG2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ARG:HG2	1:B:5:ARG:HH11	1.78	0.49
1:B:29:LEU:HD23	1:B:41:ILE:HD12	1.93	0.49
1:A:131:LYS:HG2	1:C:117:ILE:HD11	1.95	0.49
1:B:212:ARG:O	1:B:212:ARG:HG3	2.12	0.49
1:B:340:ARG:HG2	1:B:340:ARG:NH1	2.26	0.49
1:B:111:LEU:HD11	1:B:143:VAL:CG2	2.38	0.48
1:B:124:LEU:HD11	1:B:160:LYS:CE	2.42	0.48
1:D:315:LEU:HD21	1:D:345:ALA:HB2	1.95	0.48
1:C:94:ILE:CG2	2:C:750:TAV:H6	2.41	0.48
1:C:147:VAL:HG22	1:C:148:ASN:N	2.29	0.48
1:C:188:GLU:HG2	2:C:750:TAV:H32	1.95	0.48
1:B:5:ARG:HG2	1:B:5:ARG:NH1	2.27	0.48
1:D:5:ARG:HB3	1:D:5:ARG:CZ	2.44	0.48
1:A:350:ASN:N	1:A:350:ASN:ND2	2.49	0.48
1:D:7:GLN:HG3	1:D:412:ASN:OD1	2.14	0.47
1:C:111:LEU:HD12	1:C:143:VAL:CG2	2.38	0.47
1:C:57:LEU:O	1:C:62:THR:HG22	2.12	0.47
1:B:328:PHE:HD1	1:B:328:PHE:H	1.62	0.47
1:D:330:ASN:C	1:D:332:PHE:H	2.23	0.47
1:A:111:LEU:HD22	1:A:122:VAL:HG11	1.96	0.47
1:A:249:ILE:HG12	1:A:250:VAL:N	2.28	0.47
1:A:287:LYS:HB2	1:A:287:LYS:NZ	2.29	0.47
1:C:249:ILE:HG12	1:C:250:VAL:N	2.30	0.47
1:D:22:LYS:HZ1	1:D:397:ARG:NH1	2.13	0.47
1:D:26:LEU:HD12	2:D:850:TAV:O52	2.14	0.47
2:D:850:TAV:O19	2:D:850:TAV:H22	2.15	0.47
1:A:313:LEU:C	1:A:313:LEU:HD23	2.40	0.47
1:B:158:MET:HE2	1:B:158:MET:HA	1.97	0.46
1:B:336:PRO:CG	1:C:333:MET:HE2	2.44	0.46
1:C:124:LEU:HD11	1:C:160:LYS:HE3	1.97	0.46
1:D:48:LYS:O	1:D:48:LYS:HD3	2.15	0.46
1:D:148:ASN:HD22	1:D:148:ASN:HA	1.48	0.46
1:B:244:ILE:HD12	1:B:382:ILE:HD13	1.97	0.46
1:C:137[B]:LYS:HB3	1:C:144:LYS:HB2	1.98	0.46
1:B:31:ALA:HB1	1:B:198:LEU:HD21	1.98	0.46
1:B:328:PHE:CD1	1:B:328:PHE:N	2.84	0.46
1:D:348:GLU:O	1:D:349:SER:HB2	2.16	0.46
1:D:353:ILE:HD12	1:D:353:ILE:H	1.79	0.46
1:A:114:GLY:HA3	1:A:120:ARG:HH22	1.80	0.46
1:B:328:PHE:O	1:B:329:GLU:C	2.58	0.46
1:C:370:LEU:CD1	1:C:395:ILE:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ASN:HB2	1:D:227[A]:ARG:NH1	2.31	0.46
1:D:147:VAL:HG21	1:D:151:LEU:HD23	1.98	0.45
1:D:335:VAL:HB	1:D:336:PRO:HD3	1.96	0.45
1:C:152:LYS:O	1:C:153:GLY:C	2.59	0.45
1:D:119:ALA:O	1:D:121:PRO:HD3	2.17	0.45
1:D:183:GLU:OE1	1:D:212:ARG:NH2	2.42	0.45
1:A:22:LYS:HB3	3:A:449:HOH:O	2.16	0.45
1:A:276:GLY:HA3	1:A:279:TRP:CE2	2.51	0.45
1:A:303:PRO:HG2	1:A:306:MET:HB2	1.99	0.45
1:A:397:ARG:HD2	1:A:397:ARG:O	2.16	0.45
1:C:353:ILE:HD12	1:C:353:ILE:N	2.31	0.45
1:B:56:LEU:HD23	1:B:56:LEU:C	2.41	0.45
1:B:249:ILE:HG12	1:B:250:VAL:N	2.31	0.45
1:C:350:ASN:N	1:C:350:ASN:ND2	2.50	0.45
1:A:139:GLU:CB	1:C:135[A]:GLU:HG3	2.43	0.45
1:B:328:PHE:HD1	1:B:328:PHE:N	2.14	0.45
1:C:315:LEU:HD21	1:C:345:ALA:HB2	1.98	0.45
1:B:315:LEU:HD21	1:B:345:ALA:HB2	1.98	0.45
1:D:1:MET:HB3	1:D:419:GLU:HA	1.99	0.45
1:D:48:LYS:HD3	1:D:48:LYS:C	2.42	0.45
1:D:294:VAL:HB	1:D:323:ILE:CD1	2.46	0.45
2:A:550:TAV:H22	2:A:550:TAV:O19	2.16	0.45
1:C:3:LYS:HG3	1:C:416:VAL:CG2	2.46	0.45
1:C:282:LEU:C	1:C:282:LEU:HD23	2.41	0.45
1:C:317:ALA:O	1:C:356:GLY:HA3	2.17	0.45
1:A:370:LEU:HD13	1:A:394:HIS:O	2.17	0.45
1:C:157:VAL:HG22	1:C:183:GLU:HG3	1.97	0.45
1:C:296:THR:OG1	1:C:325:GLU:OE1	2.30	0.45
1:D:83:PRO:HG2	1:D:86:LEU:CB	2.39	0.45
1:B:317:ALA:O	1:B:356:GLY:HA3	2.16	0.45
1:B:139:GLU:OE2	1:B:144:LYS:NZ	2.35	0.44
1:C:57:LEU:HB3	1:C:62:THR:HG21	2.00	0.44
1:D:41:ILE:O	1:D:69:SER:HB2	2.17	0.44
1:A:156:ILE:CG2	1:A:158:MET:HE3	2.48	0.44
1:B:327:ILE:HG22	1:B:328:PHE:N	2.33	0.44
1:B:71:TRP:CH2	1:B:73:ASP:HB2	2.53	0.44
1:B:125:HIS:CE1	1:B:164:GLY:C	2.95	0.44
1:C:137[A]:LYS:HB3	1:C:144:LYS:HB2	2.00	0.44
1:D:4:PHE:CD2	1:D:413:ILE:HD11	2.53	0.44
1:D:330:ASN:O	1:D:332:PHE:N	2.47	0.44
1:A:330:ASN:ND2	1:D:347:ILE:HG21	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137[A]:LYS:HE2	1:C:139:GLU:OE2	2.18	0.44
1:A:12:LEU:HD21	1:A:411:ALA:HB2	2.00	0.43
1:A:151:LEU:C	1:A:152:LYS:HD3	2.42	0.43
1:C:57:LEU:C	1:C:62:THR:CG2	2.87	0.43
1:B:57:LEU:HB3	1:B:62:THR:HG21	2.01	0.43
1:C:115:CYS:O	1:C:116:ALA:HB3	2.18	0.43
1:D:22:LYS:HE3	1:D:397:ARG:HD2	2.00	0.43
1:D:98:GLY:O	1:D:101:VAL:HG12	2.17	0.43
1:A:331:ARG:HH11	1:A:331:ARG:CG	2.31	0.43
1:A:397:ARG:HD2	1:A:397:ARG:C	2.43	0.43
1:C:42:GLN:HA	1:C:69:SER:CB	2.45	0.43
1:D:197:PHE:CZ	1:D:201:LEU:HD11	2.53	0.43
1:C:1:MET:CE	1:C:391:ARG:HH21	2.28	0.43
1:D:99:PRO:HD3	3:D:481:HOH:O	2.17	0.43
1:B:328:PHE:CD2	1:B:331:ARG:HD3	2.54	0.43
1:B:236:GLY:O	1:B:240:VAL:HG23	2.18	0.43
1:B:213:ILE:HG22	1:B:215:ILE:HD11	2.00	0.43
1:B:350:ASN:N	1:B:350:ASN:ND2	2.49	0.43
1:B:117:ILE:HD12	1:D:127:PHE:HB3	2.01	0.43
1:C:121:PRO:HB2	2:C:750:TAV:C2	2.49	0.43
1:A:182:ILE:O	1:A:212:ARG:HA	2.19	0.43
1:B:111:LEU:HD22	1:B:122:VAL:HG21	2.01	0.43
1:B:127:PHE:CD2	1:D:120:ARG:NH1	2.87	0.43
1:B:188:GLU:HG2	2:B:650:TAV:H32	2.01	0.43
1:B:320:THR:HA	1:B:354:CYS:O	2.19	0.43
1:D:7:GLN:OE1	1:D:386:THR:HG23	2.19	0.43
1:A:114:GLY:HA3	1:A:120:ARG:NH2	2.34	0.42
1:B:276:GLY:HA3	1:B:279:TRP:CE2	2.54	0.42
1:B:189:PRO:HD3	1:B:299:HIS:CD2	2.54	0.42
1:C:28:ILE:HG22	1:C:41:ILE:HD13	2.01	0.42
1:C:353:ILE:HD12	1:C:353:ILE:H	1.84	0.42
1:B:7:GLN:HB2	1:B:412:ASN:HB3	2.01	0.42
1:B:8:GLY:HA3	1:B:383:ALA:O	2.19	0.42
1:D:322:VAL:HG13	1:D:351:THR:HG23	2.02	0.42
1:D:352:VAL:HG13	1:D:352:VAL:O	2.20	0.42
1:A:137:LYS:CD	1:A:139:GLU:OE2	2.67	0.42
1:B:124:LEU:HD21	1:D:118:GLY:HA3	2.02	0.42
1:B:329:GLU:HG2	1:C:329:GLU:OE1	2.20	0.42
1:C:57:LEU:HB3	1:C:62:THR:CG2	2.48	0.42
1:C:84:TYR:HD1	1:C:110:SER:OG	2.02	0.42
1:A:248:LYS:HA	1:A:282:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ARG:HG2	3:A:443:HOH:O	2.19	0.42
1:B:351:THR:HG23	1:B:352:VAL:N	2.35	0.42
1:C:274:GLU:HB2	1:C:281:SER:OG	2.20	0.42
1:A:131:LYS:HG3	1:C:117:ILE:HD11	2.02	0.42
1:C:1:MET:CE	1:C:391:ARG:NE	2.71	0.42
1:C:101:VAL:HG13	1:C:102:ALA:N	2.35	0.42
1:A:156:ILE:HG22	1:A:158:MET:HE3	2.02	0.42
1:A:138:LEU:CD1	1:A:143:VAL:HG22	2.50	0.41
1:A:138:LEU:HD13	1:A:143:VAL:HG22	2.01	0.41
1:A:315:LEU:HD12	1:A:338:LEU:HD13	2.01	0.41
1:A:370:LEU:HD22	1:A:397:ARG:CZ	2.50	0.41
1:B:406:LEU:HD23	1:B:406:LEU:HA	1.82	0.41
1:D:297:ALA:HB1	1:D:298:PRO:CD	2.49	0.41
1:A:340:ARG:HH11	1:A:340:ARG:HG2	1.85	0.41
1:B:136:ILE:CG2	1:B:138:LEU:CD1	2.98	0.41
1:D:22:LYS:HE3	1:D:397:ARG:CD	2.51	0.41
1:B:233:ILE:HG21	1:B:371:ARG:NE	2.36	0.41
1:C:295:ARG:CD	3:C:481:HOH:O	2.59	0.41
1:A:63:LYS:HB2	1:A:73:ASP:HB3	2.02	0.41
1:B:5:ARG:HH12	1:B:7:GLN:NE2	2.18	0.41
1:B:42:GLN:HA	1:B:69:SER:HB3	2.02	0.41
1:B:131:LYS:CG	1:D:117:ILE:HD11	2.47	0.41
1:B:195:ALA:O	1:B:199:VAL:HG23	2.21	0.41
1:B:313:LEU:HD23	1:B:313:LEU:C	2.46	0.41
1:A:93:SER:HB2	3:A:484:HOH:O	2.20	0.41
1:A:98:GLY:O	1:A:101:VAL:HG12	2.21	0.41
1:A:315:LEU:HD22	1:A:343:ALA:HB1	2.02	0.41
1:B:156:ILE:HG22	1:B:158:MET:HE3	2.02	0.41
1:B:294:VAL:HB	1:B:323:ILE:CD1	2.50	0.41
1:B:340:ARG:NH1	1:B:340:ARG:CG	2.82	0.41
1:C:297:ALA:HB3	1:C:301:ALA:CB	2.50	0.41
1:D:370:LEU:HD13	1:D:394:HIS:O	2.21	0.41
1:A:112:PRO:HB2	1:A:120:ARG:HD2	2.02	0.41
1:A:299:HIS:CG	1:A:300:PRO:HA	2.56	0.41
1:A:401:ARG:HH11	1:A:401:ARG:HB3	1.85	0.41
1:B:29:LEU:HD23	1:B:41:ILE:CD1	2.51	0.41
1:D:135:GLU:O	1:D:145:ALA:HA	2.20	0.41
1:A:103:ARG:HD3	1:A:104:PHE:CE1	2.56	0.41
1:A:154:ALA:O	1:A:180:THR:HA	2.21	0.41
1:C:349:SER:C	1:C:351:THR:H	2.29	0.41
1:C:14:GLY:O	1:C:249:ILE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ASN:C	1:D:332:PHE:N	2.79	0.41
1:A:54:MET:HG2	1:A:64:VAL:HG11	2.03	0.40
1:B:108:GLN:HA	1:B:143:VAL:O	2.21	0.40
1:C:236:GLY:O	1:C:240:VAL:HG23	2.20	0.40
1:A:294:VAL:HB	1:A:323:ILE:HD13	2.03	0.40
1:A:349:SER:C	1:A:351:THR:H	2.28	0.40
1:B:64:VAL:HG13	1:B:72:ILE:HD13	2.03	0.40
1:A:299:HIS:ND1	1:A:300:PRO:HA	2.36	0.40
2:B:650:TAV:O19	2:B:650:TAV:H22	2.22	0.40
1:C:83:PRO:HG2	1:C:86:LEU:HB2	2.02	0.40
1:D:29:LEU:HA	1:D:29:LEU:HD23	1.92	0.40
1:A:227:ARG:NH1	3:A:517:HOH:O	2.55	0.40
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.96	0.40
1:A:315:LEU:HD21	1:A:345:ALA:HB2	2.02	0.40
1:B:57:LEU:HB3	1:B:62:THR:CG2	2.51	0.40
1:D:66:ARG:HG3	3:D:478:HOH:O	2.20	0.40
1:D:82:ALA:HA	1:D:83:PRO:HD2	1.90	0.40
1:A:94:ILE:HG21	2:A:550:TAV:H6	2.03	0.40
1:A:121:PRO:HD2	3:A:503:HOH:O	2.20	0.40
1:A:126:ILE:CG2	1:A:136:ILE:HG21	2.52	0.40
1:A:158:MET:HE2	1:C:117:ILE:HB	2.02	0.40
1:A:271:ALA:HB1	1:A:282:LEU:HG	2.04	0.40
1:A:397:ARG:HE	1:A:397:ARG:HB3	1.69	0.40
1:B:320:THR:OG1	1:B:355:HIS:ND1	2.46	0.40
1:B:336:PRO:HG2	1:C:333:MET:CE	2.50	0.40
1:B:365:VAL:O	1:B:389:VAL:HA	2.22	0.40
1:C:219:GLU:HB2	3:C:552:HOH:O	2.22	0.40
1:C:351:THR:CG2	1:C:352:VAL:N	2.83	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	418/419 (100%)	402 (96%)	14 (3%)	2 (0%)	24	46
1	B	418/419 (100%)	402 (96%)	10 (2%)	6 (1%)	9	19
1	C	421/419 (100%)	404 (96%)	12 (3%)	5 (1%)	10	23
1	D	417/419 (100%)	402 (96%)	13 (3%)	2 (0%)	24	46
All	All	1674/1676 (100%)	1610 (96%)	49 (3%)	15 (1%)	14	30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	327	ILE
1	B	331	ARG
1	C	122	VAL
1	C	329	GLU
1	A	119	ALA
1	B	115	CYS
1	B	349	SER
1	C	92	ALA
1	C	112	PRO
1	D	112	PRO
1	A	418	GLY
1	B	120	ARG
1	C	114	GLY
1	B	418	GLY
1	D	113	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	332/329 (101%)	318 (96%)	14 (4%)	26	52
1	B	332/329 (101%)	321 (97%)	11 (3%)	33	61
1	C	335/329 (102%)	325 (97%)	10 (3%)	36	64
1	D	331/329 (101%)	317 (96%)	14 (4%)	26	52
All	All	1330/1316 (101%)	1281 (96%)	49 (4%)	31	57

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	48	LYS
1	A	62	THR
1	A	122	VAL
1	A	152	LYS
1	A	216	GLU
1	A	229	LEU
1	A	287	LYS
1	A	307	GLN
1	A	327	ILE
1	A	331	ARG
1	A	348	GLU
1	A	350	ASN
1	A	351	THR
1	B	62	THR
1	B	143	VAL
1	B	216	GLU
1	B	229	LEU
1	B	287	LYS
1	B	340	ARG
1	B	348	GLU
1	B	350	ASN
1	B	351	THR
1	B	403[A]	GLU
1	B	403[B]	GLU
1	C	59	GLN
1	C	62	THR
1	C	111	LEU
1	C	122	VAL
1	C	216	GLU
1	C	287	LYS
1	C	350	ASN
1	C	351	THR
1	C	403	GLU
1	C	416	VAL
1	D	5	ARG
1	D	22	LYS
1	D	48	LYS
1	D	59	GLN
1	D	62	THR
1	D	111	LEU
1	D	148	ASN

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Mol	Chain	Res	Type
1	D	216	GLU
1	D	229	LEU
1	D	287	LYS
1	D	348	GLU
1	D	350	ASN
1	D	351	THR
1	D	403	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	148	ASN
1	A	307	GLN
1	A	330	ASN
1	A	350	ASN
1	B	42	GLN
1	B	148	ASN
1	B	350	ASN
1	B	394	HIS
1	C	108	GLN
1	C	148	ASN
1	C	350	ASN
1	C	394	HIS
1	D	13	GLN
1	D	148	ASN
1	D	184	ASN
1	D	299	HIS
1	D	344	HIS
1	D	350	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	IAS	B	67	1	6,7,8	1.15	0	3,8,10	0.91	0
1	IAS	A	67	1	6,7,8	0.96	0	3,8,10	1.06	0
1	IAS	C	67	1	6,7,8	1.03	0	3,8,10	1.15	0
1	IAS	D	67	1	6,7,8	0.92	0	3,8,10	0.99	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IAS	B	67	1	-	0/7/7/8	-
1	IAS	A	67	1	-	0/7/7/8	-
1	IAS	C	67	1	-	0/7/7/8	-
1	IAS	D	67	1	-	0/7/7/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TAV	B	650	-	50,50,50	2.72	18 (36%)	71,74,74	2.81	10 (14%)
2	TAV	C	750	-	50,50,50	2.77	15 (30%)	71,74,74	2.95	11 (15%)
2	TAV	A	550	-	50,50,50	2.84	18 (36%)	71,74,74	2.78	11 (15%)
2	TAV	D	850	-	50,50,50	2.90	19 (38%)	71,74,74	2.89	10 (14%)

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	TAV	B	650	-	-	13/42/42/42	0/5/5/5
2	TAV	C	750	-	-	9/42/42/42	0/5/5/5
2	TAV	A	550	-	-	9/42/42/42	0/5/5/5
2	TAV	D	850	-	-	12/42/42/42	0/5/5/5

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	550	TAV	O51-C26	9.34	1.57	1.42
2	C	750	TAV	O51-C26	8.78	1.56	1.42
2	D	850	TAV	O51-C26	8.30	1.56	1.42
2	B	650	TAV	O51-C26	7.88	1.55	1.42
2	D	850	TAV	O63-C61	7.34	1.43	1.22
2	C	750	TAV	O63-C61	7.02	1.42	1.22
2	B	650	TAV	O63-C61	6.95	1.42	1.22
2	C	750	TAV	C29-N49	6.92	1.48	1.34
2	A	550	TAV	O63-C61	6.76	1.42	1.22
2	D	850	TAV	C29-N49	6.34	1.47	1.34
2	B	650	TAV	C29-N49	6.24	1.47	1.34
2	A	550	TAV	C29-N49	5.91	1.46	1.34
2	A	550	TAV	O66-C64	5.85	1.41	1.22
2	D	850	TAV	O66-C64	5.47	1.40	1.22
2	C	750	TAV	O66-C64	5.47	1.40	1.22
2	B	650	TAV	O66-C64	5.41	1.39	1.22
2	D	850	TAV	C57-C61	5.37	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	850	TAV	C46-C45	5.09	1.46	1.38
2	A	550	TAV	C46-C45	4.78	1.46	1.38
2	D	850	TAV	C6-C1	4.78	1.46	1.38
2	C	750	TAV	C46-C45	4.60	1.46	1.38
2	C	750	TAV	C6-C1	4.59	1.46	1.38
2	B	650	TAV	C6-C1	4.54	1.46	1.38
2	B	650	TAV	C46-C45	4.41	1.45	1.38
2	A	550	TAV	C6-C1	4.29	1.45	1.38
2	D	850	TAV	C1-S18	4.28	1.83	1.76
2	A	550	TAV	C1-S18	4.17	1.82	1.76
2	D	850	TAV	C14-C13	3.85	1.46	1.38
2	B	650	TAV	O19-S18	3.83	1.48	1.43
2	A	550	TAV	C14-C13	3.76	1.46	1.38
2	B	650	TAV	C14-C13	3.73	1.46	1.38
2	C	750	TAV	C37-C32	3.69	1.46	1.38
2	B	650	TAV	C1-S18	3.50	1.81	1.76
2	A	550	TAV	C57-C61	3.50	1.59	1.52
2	A	550	TAV	C37-C32	3.47	1.45	1.38
2	C	750	TAV	C14-C13	3.46	1.45	1.38
2	C	750	TAV	C1-S18	3.40	1.81	1.76
2	B	650	TAV	C37-C32	3.39	1.45	1.38
2	A	550	TAV	C45-S31	3.38	1.82	1.76
2	D	850	TAV	C37-C32	3.35	1.45	1.38
2	A	550	TAV	C67-C57	3.28	1.62	1.53
2	A	550	TAV	C67-C64	3.15	1.59	1.51
2	C	750	TAV	C45-S31	3.08	1.81	1.76
2	D	850	TAV	C45-S31	3.05	1.81	1.76
2	C	750	TAV	C57-C61	2.95	1.58	1.52
2	B	650	TAV	C57-C61	2.93	1.58	1.52
2	C	750	TAV	O62-C61	-2.86	1.21	1.30
2	B	650	TAV	C67-C57	2.81	1.60	1.53
2	D	850	TAV	C2-C3	2.78	1.48	1.42
2	C	750	TAV	C67-C57	2.73	1.60	1.53
2	D	850	TAV	O62-C61	-2.72	1.22	1.30
2	A	550	TAV	S18-N20	2.67	1.67	1.63
2	B	650	TAV	C45-S31	2.61	1.81	1.76
2	B	650	TAV	C67-C64	2.60	1.57	1.51
2	B	650	TAV	C2-C3	2.50	1.47	1.42
2	D	850	TAV	O65-C64	-2.46	1.22	1.30
2	D	850	TAV	C22-C23	2.45	1.43	1.39
2	B	650	TAV	C4-C3	2.36	1.47	1.42
2	B	650	TAV	O62-C61	-2.35	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	850	TAV	C57-N49	2.35	1.51	1.47
2	A	550	TAV	C57-N49	2.22	1.50	1.47
2	A	550	TAV	O54-S18	2.20	1.46	1.43
2	A	550	TAV	O62-C61	-2.20	1.23	1.30
2	D	850	TAV	C4-C3	2.19	1.47	1.42
2	D	850	TAV	O53-S31	2.19	1.48	1.43
2	A	550	TAV	O65-C64	-2.10	1.23	1.30
2	C	750	TAV	C22-C23	2.03	1.43	1.39
2	D	850	TAV	C9-C3	2.02	1.46	1.42
2	B	650	TAV	O54-S18	2.01	1.45	1.43
2	C	750	TAV	C2-C3	2.00	1.46	1.42

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	750	TAV	C26-O51-S31	21.75	155.94	119.05
2	D	850	TAV	C26-O51-S31	21.32	155.22	119.05
2	A	550	TAV	C26-O51-S31	20.82	154.37	119.05
2	B	650	TAV	C26-O51-S31	20.78	154.30	119.05
2	D	850	TAV	O51-C26-C21	5.05	128.60	118.70
2	B	650	TAV	O51-C26-C21	4.83	128.16	118.70
2	C	750	TAV	O51-C26-C21	4.61	127.73	118.70
2	D	850	TAV	O51-C26-C25	-4.53	108.95	118.46
2	B	650	TAV	O51-C26-C25	-4.40	109.22	118.46
2	A	550	TAV	C1-S18-N20	-4.21	101.65	106.88
2	C	750	TAV	O51-C26-C25	-3.97	110.13	118.46
2	D	850	TAV	C1-S18-N20	-3.93	102.01	106.88
2	C	750	TAV	C1-S18-N20	-3.92	102.02	106.88
2	A	550	TAV	O51-C26-C21	3.78	126.10	118.70
2	C	750	TAV	C61-C57-N49	3.64	114.53	110.26
2	D	850	TAV	O62-C61-C57	3.19	123.73	113.34
2	A	550	TAV	O51-C26-C25	-3.15	111.85	118.46
2	C	750	TAV	O54-S18-C1	-3.14	104.02	107.98
2	C	750	TAV	O62-C61-C57	3.12	123.51	113.34
2	B	650	TAV	O62-C61-C57	3.09	123.43	113.34
2	A	550	TAV	O62-C61-C57	3.05	123.30	113.34
2	A	550	TAV	O51-S31-C45	-2.91	95.62	102.56
2	D	850	TAV	C56-N49-C57	-2.76	112.92	117.70
2	D	850	TAV	O62-C61-O63	-2.67	118.02	124.08
2	C	750	TAV	O65-C64-C67	2.65	122.24	114.00
2	B	650	TAV	C1-S18-N20	-2.62	103.63	106.88
2	D	850	TAV	O65-C64-C67	2.58	122.01	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	550	TAV	C56-N49-C57	-2.38	113.58	117.70
2	A	550	TAV	O65-C64-C67	2.36	121.33	114.00
2	B	650	TAV	C2-C1-S18	2.33	122.01	120.07
2	B	650	TAV	C56-N49-C57	-2.31	113.69	117.70
2	B	650	TAV	O51-S31-C45	-2.26	97.16	102.56
2	B	650	TAV	O65-C64-C67	2.24	120.95	114.00
2	C	750	TAV	C57-C67-C64	2.24	117.19	112.58
2	A	550	TAV	C57-C67-C64	2.20	117.11	112.58
2	B	650	TAV	C6-C1-S18	-2.15	117.39	119.76
2	A	550	TAV	O62-C61-O63	-2.10	119.31	124.08
2	D	850	TAV	O66-C64-C67	-2.08	116.45	122.84
2	D	850	TAV	C2-C1-S18	2.05	121.78	120.07
2	A	550	TAV	C23-C24-C29	-2.03	117.90	120.72
2	C	750	TAV	O66-C64-C67	-2.01	116.67	122.84
2	C	750	TAV	O62-C61-O63	-2.01	119.53	124.08

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	550	TAV	C24-C29-N49-C56
2	A	550	TAV	O50-C29-N49-C56
2	A	550	TAV	C61-C57-N49-C29
2	B	650	TAV	C24-C29-N49-C56
2	B	650	TAV	O50-C29-N49-C56
2	B	650	TAV	C61-C57-N49-C29
2	C	750	TAV	C24-C29-N49-C56
2	C	750	TAV	O50-C29-N49-C56
2	C	750	TAV	C61-C57-N49-C29
2	C	750	TAV	C67-C57-C61-O63
2	D	850	TAV	C24-C29-N49-C56
2	D	850	TAV	O50-C29-N49-C56
2	D	850	TAV	C61-C57-N49-C29
2	A	550	TAV	C26-O51-S31-C45
2	B	650	TAV	C26-O51-S31-C45
2	C	750	TAV	C26-O51-S31-C45
2	D	850	TAV	C26-O51-S31-C45
2	D	850	TAV	C25-C26-O51-S31
2	C	750	TAV	C67-C57-C61-O62
2	C	750	TAV	C25-C26-O51-S31
2	A	550	TAV	C25-C26-O51-S31
2	D	850	TAV	C26-O51-S31-O52

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Mol	Chain	Res	Type	Atoms
2	B	650	TAV	C26-O51-S31-O52
2	C	750	TAV	C26-O51-S31-O52
2	A	550	TAV	C26-O51-S31-O52
2	B	650	TAV	N49-C57-C61-O62
2	B	650	TAV	N49-C57-C61-O63
2	D	850	TAV	N49-C57-C61-O62
2	D	850	TAV	N49-C57-C61-O63
2	B	650	TAV	C25-C26-O51-S31
2	B	650	TAV	O66-C64-C67-C57
2	A	550	TAV	O66-C64-C67-C57
2	B	650	TAV	O65-C64-C67-C57
2	B	650	TAV	C26-O51-S31-O53
2	C	750	TAV	C26-O51-S31-O53
2	D	850	TAV	C26-O51-S31-O53
2	A	550	TAV	C26-O51-S31-O53
2	D	850	TAV	C21-C26-O51-S31
2	B	650	TAV	C6-C1-S18-O54
2	B	650	TAV	C2-C1-S18-O54
2	D	850	TAV	C6-C1-S18-O54
2	D	850	TAV	C2-C1-S18-O54
2	A	550	TAV	O65-C64-C67-C57

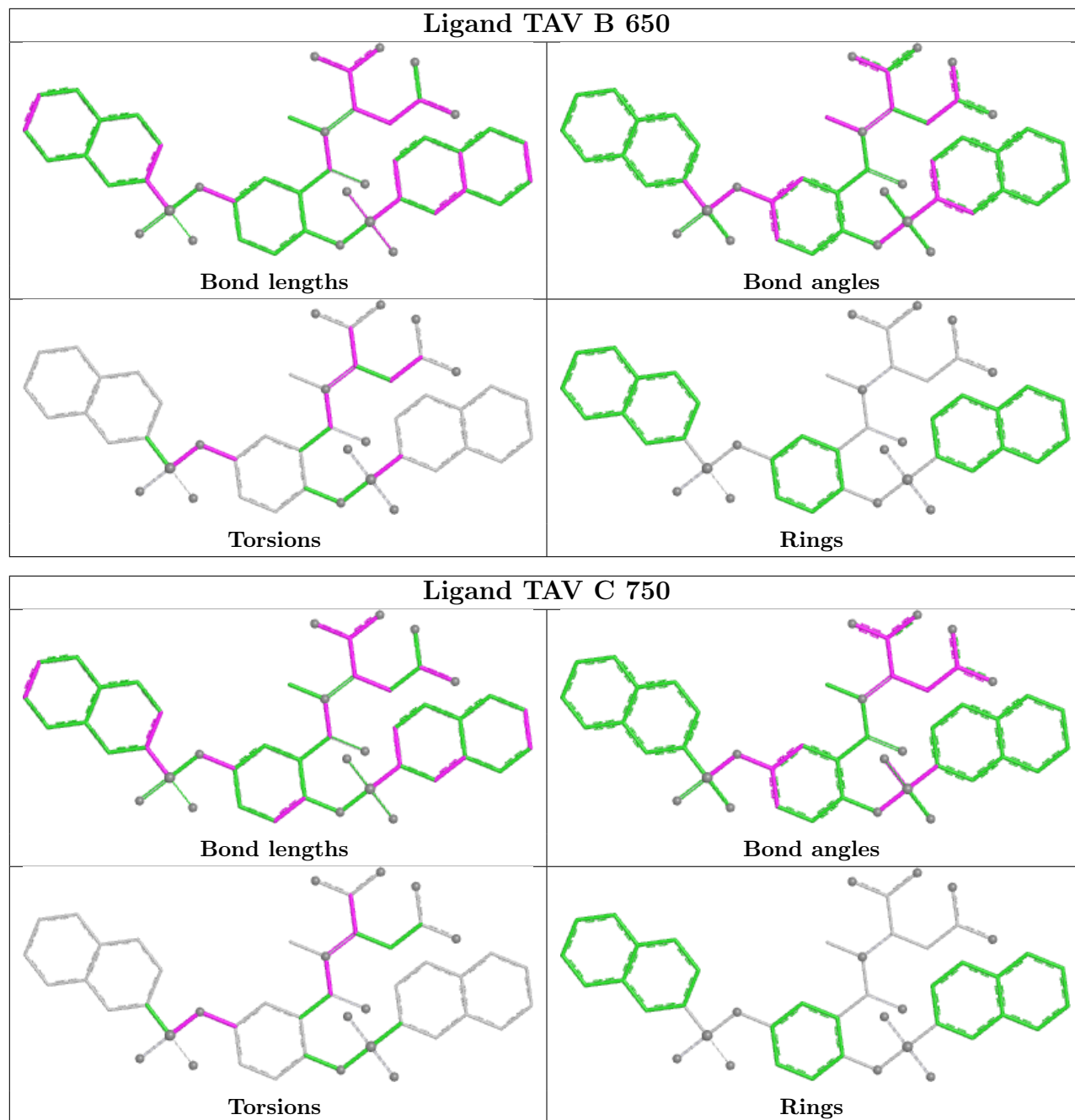
There are no ring outliers.

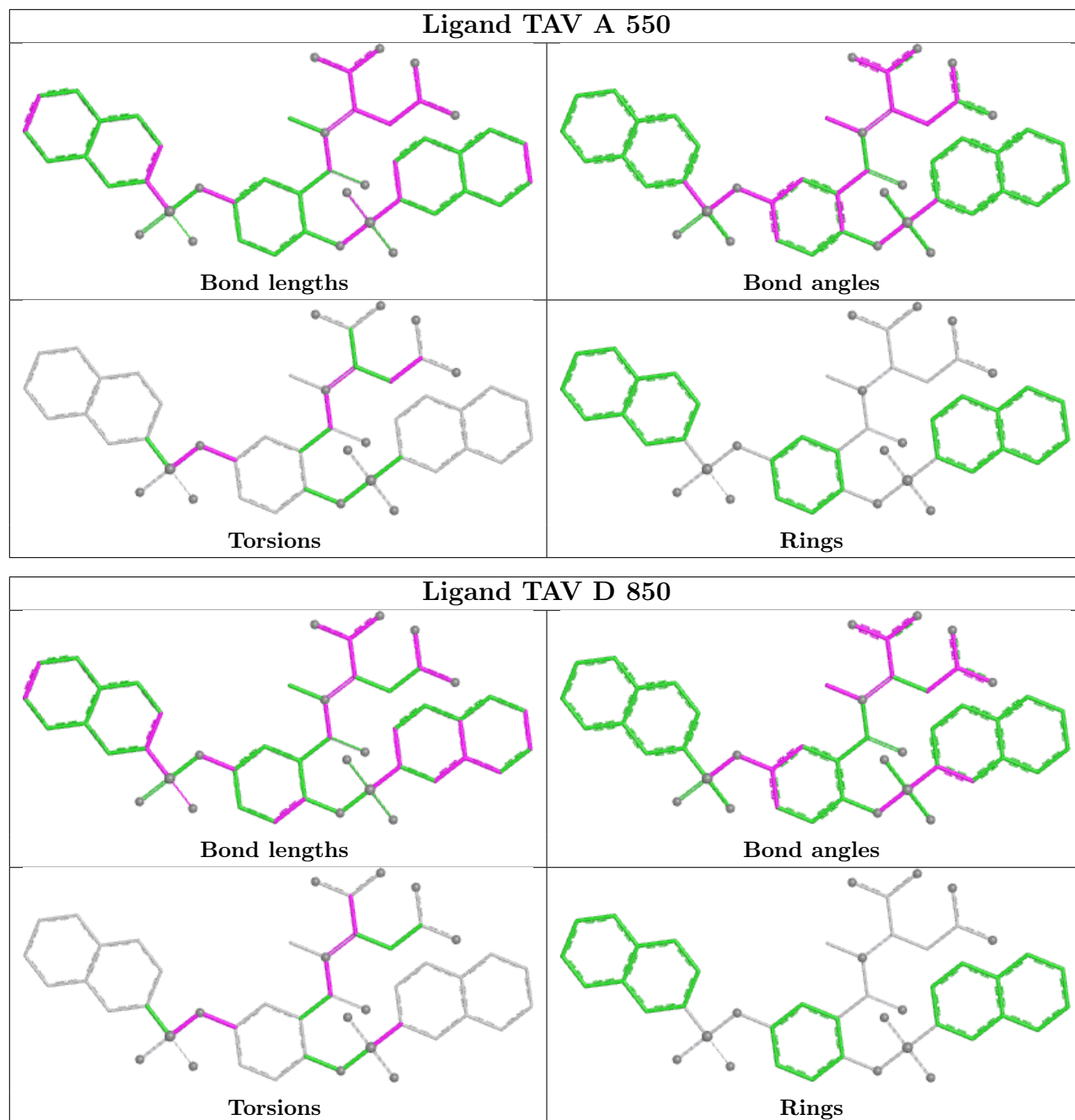
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	650	TAV	3	0
2	C	750	TAV	6	0
2	A	550	TAV	4	0
2	D	850	TAV	3	0

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

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	418/419 (99%)	-0.51	4 (0%) 79 76	13, 24, 41, 73	3 (0%)
1	B	418/419 (99%)	-0.48	5 (1%) 76 73	10, 24, 43, 76	3 (0%)
1	C	418/419 (99%)	-0.46	5 (1%) 76 73	11, 22, 39, 74	6 (1%)
1	D	418/419 (99%)	-0.37	3 (0%) 84 82	10, 24, 45, 73	2 (0%)
All	All	1672/1676 (99%)	-0.46	17 (1%) 79 76	10, 23, 43, 76	14 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	419	GLU	3.9
1	C	330	ASN	3.6
1	C	329	GLU	3.2
1	A	327	ILE	3.1
1	D	116	ALA	3.0
1	A	418	GLY	2.9
1	D	418	GLY	2.6
1	B	115	CYS	2.6
1	B	329	GLU	2.6
1	B	418	GLY	2.5
1	A	419	GLU	2.5
1	C	115	CYS	2.4
1	B	419	GLU	2.3
1	C	113	GLY	2.2
1	B	328	PHE	2.2
1	D	114	GLY	2.0
1	A	119	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	IAS	C	67	8/9	0.87	0.10	24,25,28,29	0
1	IAS	B	67	8/9	0.90	0.08	29,30,30,31	0
1	IAS	A	67	8/9	0.94	0.07	30,31,32,32	0
1	IAS	D	67	8/9	0.95	0.07	25,26,27,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

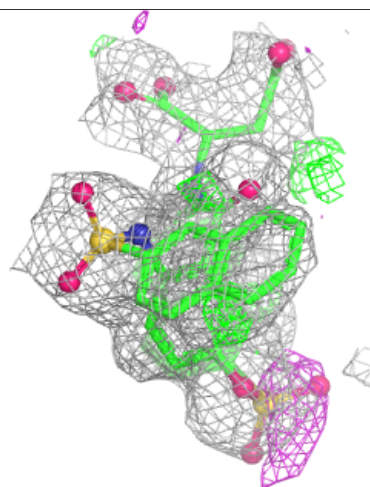
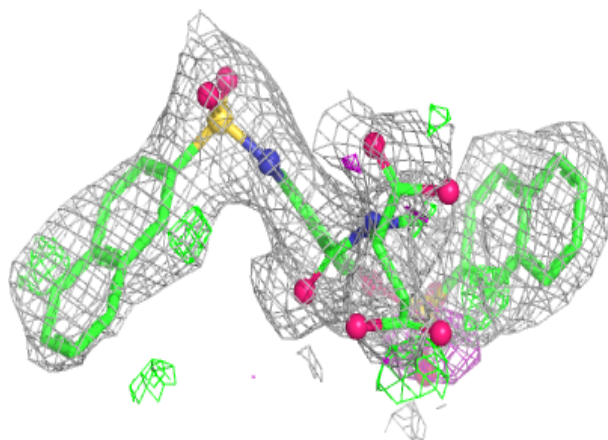
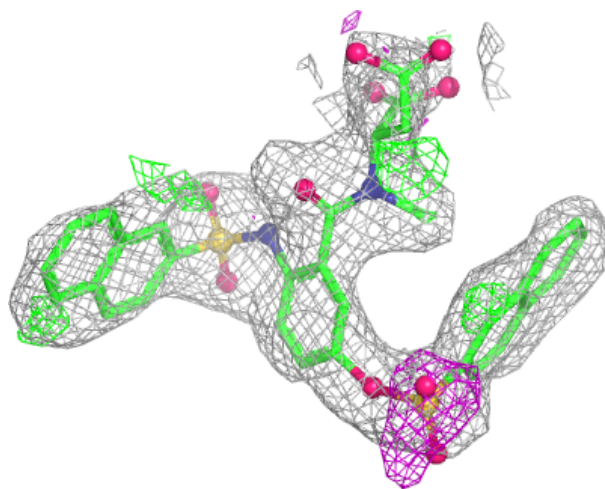
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TAV	D	850	46/46	0.87	0.14	36,47,60,62	0
2	TAV	B	650	46/46	0.88	0.13	30,39,54,55	0
2	TAV	C	750	46/46	0.89	0.13	30,47,57,63	0
2	TAV	A	550	46/46	0.89	0.13	32,36,47,52	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.

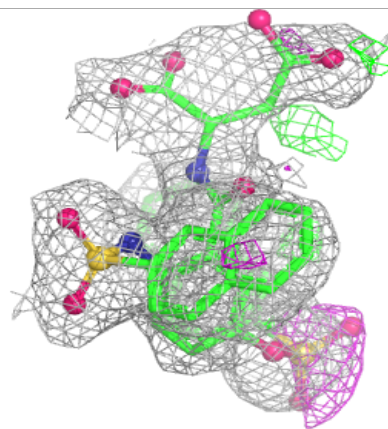
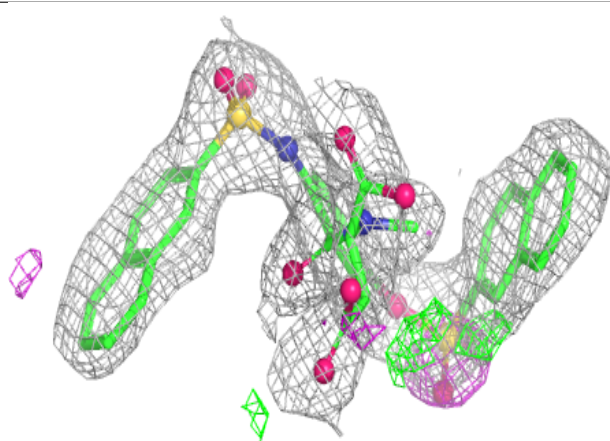
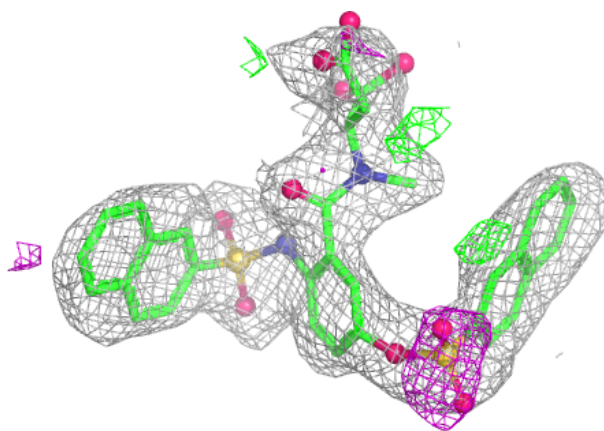
Electron density around TAV D 850:

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



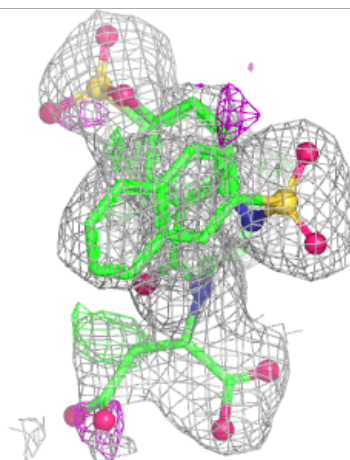
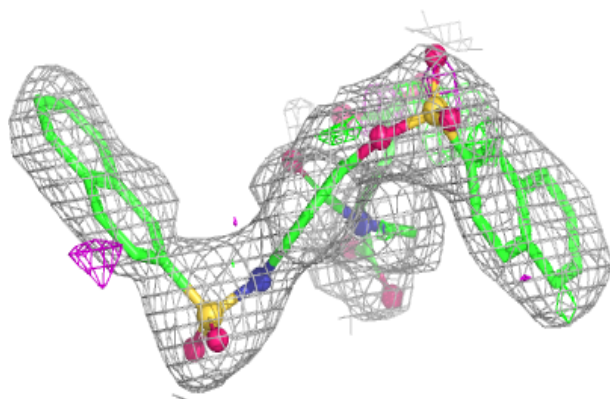
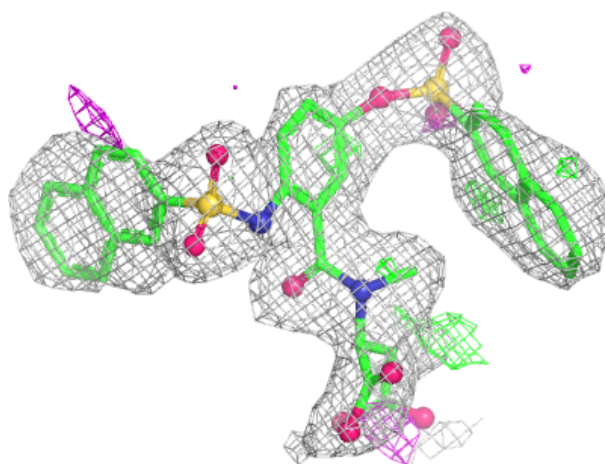
Electron density around TAV B 650:

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



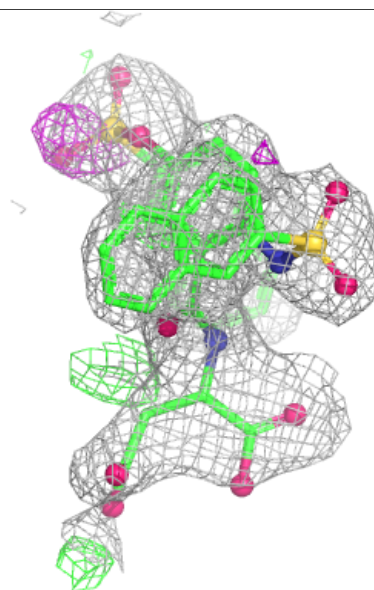
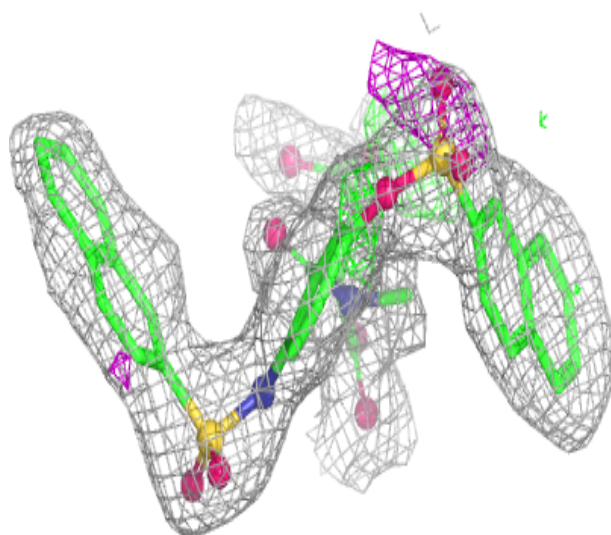
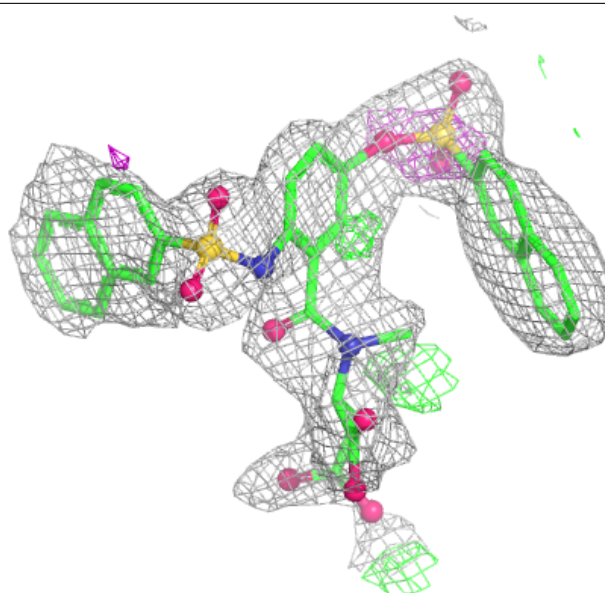
Electron density around TAV C 750:

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



Electron density around TAV A 550:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.