



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 11:49 AM EDT

PDB ID : 1YBG  
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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

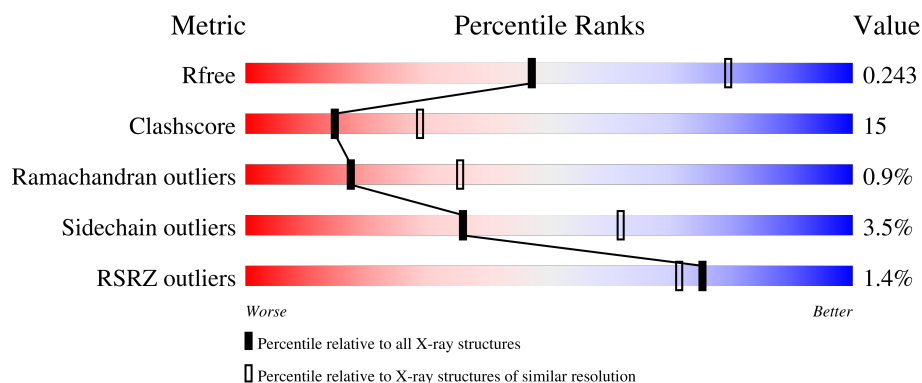
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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  $\geq 3$ , 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	<div> <div>0%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>•</div> </div> </div>
1	B	419	<div> <div>0%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>•</div> </div> </div>
1	C	419	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>•</div> </div> </div>
1	D	419	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>•</div> </div> </div>

## 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.

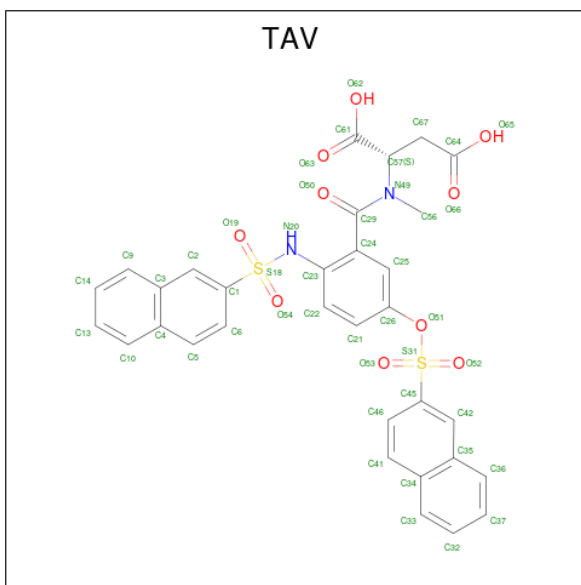
- Molecule 1 is a protein called UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

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 (three-letter code: TAV) (formula: C<sub>32</sub>H<sub>26</sub>N<sub>2</sub>O<sub>10</sub>S<sub>2</sub>).



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

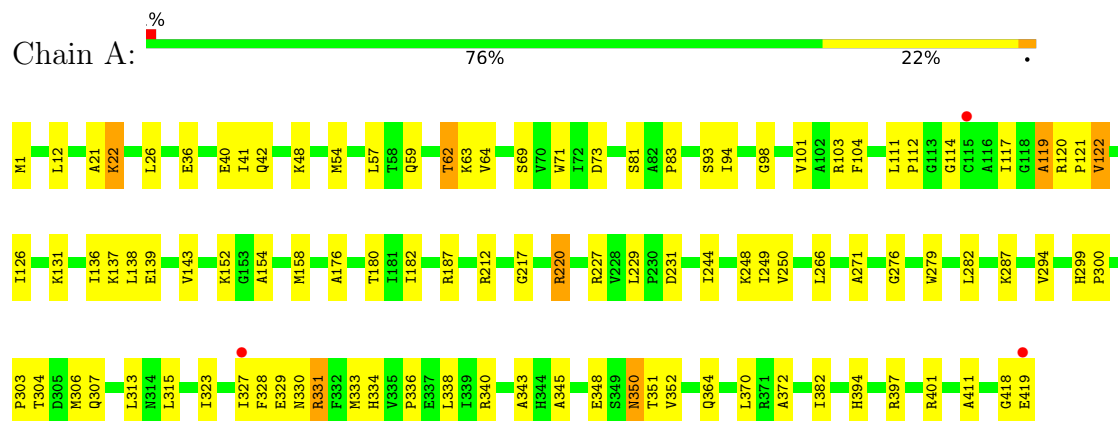
- Molecule 3 is water.

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

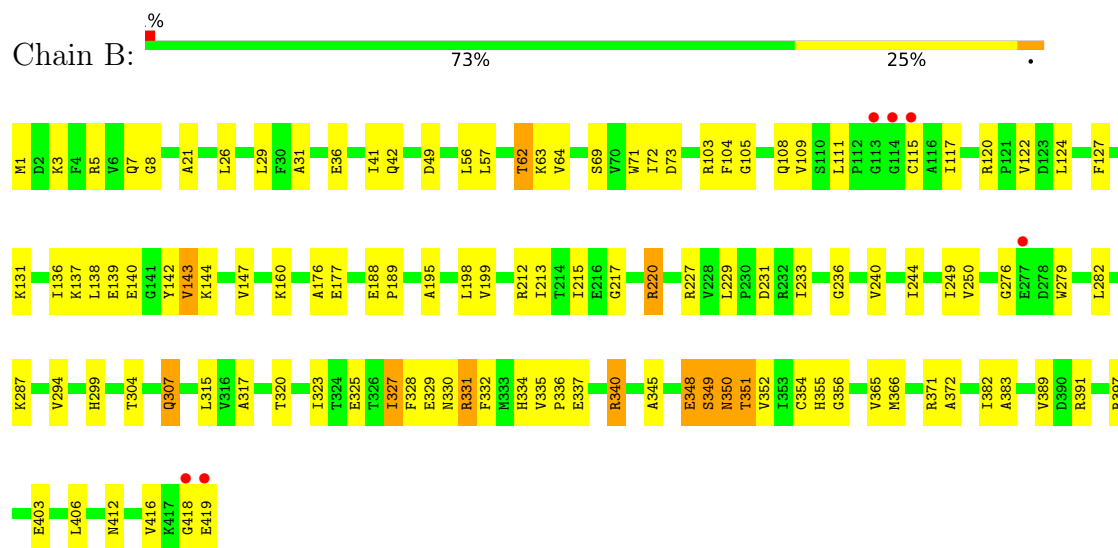
### 3 Residue-property plots [i](#)

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.

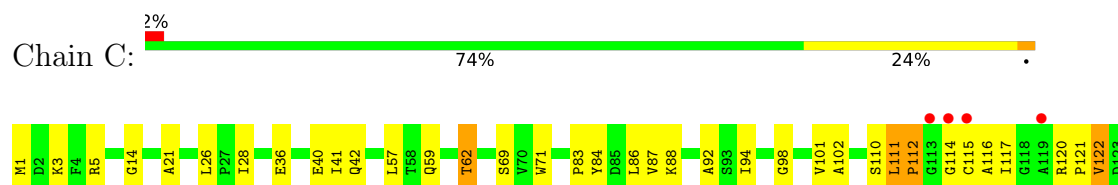
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

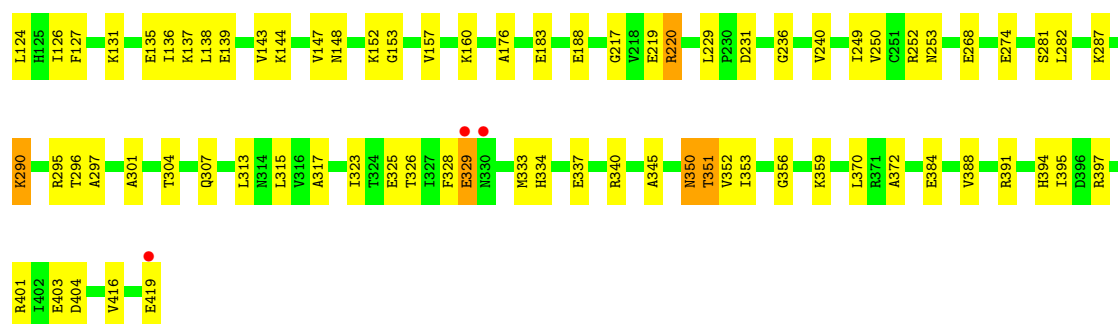


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

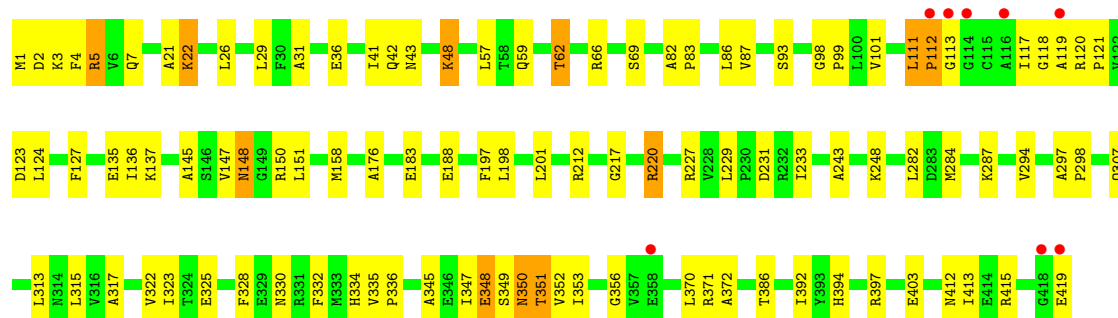
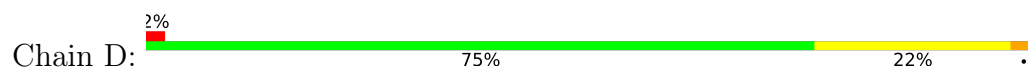


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





- 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, $\alpha$ , $\beta$ , $\gamma$	84.08Å 134.60Å 175.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.00 – 2.60 15.60 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (16.00-2.60) 99.8 (15.60-2.60)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.62Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , 0.253 0.196 , 0.243	Depositor DCC
$R_{free}$ test set	1842 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TAV, IAS

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	0/3204	0.71	0/4339
1	B	0.49	0/3210	0.69	0/4345
1	C	0.51	0/3231	0.72	0/4374
1	D	0.49	0/3199	0.71	0/4330
All	All	0.50	0/12844	0.71	0/17388

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3156	0	3218	105	0
1	B	3162	0	3236	110	0
1	C	3171	0	3238	109	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	397	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 15.

All (397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:MET:HE3	1:C:391:ARG:HE	1.54	0.73
1:C:83:PRO:CG	1:C:86:LEU:HD12	2.19	0.72
1:C:1:MET:CE	1:C:391:ARG:HE	2.02	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:B:350:ASN:H	1:B:350:ASN:ND2	1.80	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:HE1	1:C:391:ARG:NH2	2.07	0.69
1:A:57:LEU:O	1:A:62:THR:HG23	1.92	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
1:A:350:ASN:H	1:A:350:ASN:ND2	1.86	0.68
1:C:84:TYR:HD1	1:C:110:SER:HG	1.40	0.68
1:C:42:GLN:HA	1:C:69:SER:HB3	1.75	0.68
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:57:LEU:O	1:D:62:THR:CG2	2.43	0.65
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:A:333:MET:HE1	1:D:347:ILE:HG21	1.80	0.63
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:C:1:MET:HE1	1:C:391:ARG:HH21	1.62	0.63
1:C:57:LEU:C	1:C:62:THR:HG23	2.19	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: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:D:57:LEU:C	1:D:62:THR:HG23	2.19	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:22:LYS:HZ1	1:D:397:ARG:HH11	1.48	0.61
1:C:323:ILE:HB	1:C:352:VAL:CG1	2.32	0.60
1:B:57:LEU:C	1:B:62:THR:HG23	2.23	0.60
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:336:PRO:HG2	1:C:333:MET:HE2	1.85	0.58
1:A:57:LEU:C	1:A:62:THR:HG23	2.24	0.58
1:B:124:LEU:HD11	1:B:160:LYS:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1:MET:HE1	1:C:391:ARG:CZ	2.36	0.56
1:C:127:PHE:O	1:C:131:LYS:HG2	2.04	0.56
1:D:22:LYS:HZ1	1:D:397:ARG:NH1	2.03	0.56
1:A:176:ALA:O	1:A:217:GLY:HA3	2.05	0.56
1:C:120:ARG:O	1:C:121:PRO:C	2.44	0.55
1:B:49:ASP:CG	1:B:397[A]:ARG:HH21	2.09	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:D:353:ILE:HD12	1:D:353:ILE:N	2.22	0.55
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:C:1:MET:HE1	1:C:391:ARG:NE	2.22	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:A:352:VAL:HG13	1:A:352:VAL:O	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ALA:HB2	1:C:231:ASP:HA	1.90	0.53
1:B:63:LYS:HB2	1:B:73:ASP:HB3	1.90	0.53
1:C:1:MET:CE	1:C:391:ARG:NE	2.71	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: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: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:C:313:LEU:C	1:C:313:LEU:HD23	2.30	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
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: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: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:A:119:ALA:O	1:A:120:ARG:C	2.50	0.50
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:A:158:MET:HE1	1:C:117:ILE:HB	1.92	0.50
1:B:282:LEU:C	1:B:282:LEU:HD23	2.31	0.50
1:B:366:MET:CG	1:B:391:ARG:HD2	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:313:LEU:C	1:D:313:LEU:HD23	2.32	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:282:LEU:C	1:A:282:LEU:HD23	2.33	0.49
1:A:57:LEU:O	1:A:62:THR:CG2	2.60	0.49
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:282:LEU:HD23	1:D:282:LEU:C	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:370:LEU:CD1	1:C:395:ILE:HA	2.46	0.46
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: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:329:GLU:O	1:A:330:ASN:C	2.53	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: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:337:GLU:CD	1:B:340:ARG:HH21	2.20	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:PRO:HG2	1:D:86:LEU:CB	2.39	0.45
1:A:333:MET:HE1	1:D:347:ILE:CD1	2.47	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: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: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
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: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: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:D:350:ASN:N	1:D:350:ASN:ND2	2.49	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:A:333:MET:CE	1:D:347:ILE:HD12	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:ILE:HD12	1:C:353:ILE:H	1.84	0.42
1:D:330:ASN:C	1:D:332:PHE:H	2.23	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:A:313:LEU:C	1:A:313:LEU:HD23	2.40	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:D:158:MET:HE2	1:D:158:MET:HA	2.00	0.42
1:A:248:LYS:HA	1:A:282:LEU:O	2.20	0.42
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:101:VAL:HG13	1:C:102:ALA:N	2.35	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:A:333:MET:HE1	1:D:347:ILE:HD13	2.02	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:328:PHE:O	1:B:329:GLU:C	2.58	0.41
1:C:14:GLY:O	1:C:249:ILE:HA	2.21	0.41
1:C:152:LYS:O	1:C:153:GLY:C	2.59	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:B:56:LEU:HD23	1:B:56:LEU:C	2.41	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:B:320:THR:OG1	1:B:355:HIS:ND1	2.46	0.40
1:C:282:LEU:C	1:C:282:LEU:HD23	2.41	0.40
1:D:48:LYS:HD3	1:D:48:LYS:C	2.42	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: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: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

### 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	418/419 (100%)	402 (96%)	14 (3%)	2 (0%)	29	52
1	B	418/419 (100%)	402 (96%)	10 (2%)	6 (1%)	11	22
1	C	421/419 (100%)	404 (96%)	12 (3%)	5 (1%)	13	27
1	D	417/419 (100%)	402 (96%)	13 (3%)	2 (0%)	29	52
All	All	1674/1676 (100%)	1610 (96%)	49 (3%)	15 (1%)	17	35

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%)	320 (96%)	12 (4%)	35	61
1	B	332/329 (101%)	321 (97%)	11 (3%)	38	64
1	C	335/329 (102%)	325 (97%)	10 (3%)	41	67
1	D	331/329 (101%)	317 (96%)	14 (4%)	30	55
All	All	1330/1316 (101%)	1283 (96%)	47 (4%)	36	62

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	62	THR
1	A	81	SER
1	A	122	VAL
1	A	152	LYS
1	A	220	ARG
1	A	229	LEU
1	A	307	GLN
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	220	ARG
1	B	229	LEU
1	B	307	GLN
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	220	ARG
1	C	229	LEU
1	C	290	LYS
1	C	307	GLN
1	C	350	ASN

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Mol	Chain	Res	Type
1	C	351	THR
1	C	403	GLU
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
1	D	220	ARG
1	D	229	LEU
1	D	307	GLN
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	148	ASN
1	A	330	ASN
1	A	350	ASN
1	B	148	ASN
1	B	350	ASN
1	C	108	GLN
1	C	350	ASN
1	D	13	GLN
1	D	148	ASN
1	D	184	ASN
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	C	67	1	4,7,8	0.60	0	2,8,10	1.41	0
1	IAS	A	67	1	4,7,8	0.52	0	2,8,10	1.29	0
1	IAS	B	67	1	4,7,8	0.85	0	2,8,10	1.12	0
1	IAS	D	67	1	4,7,8	0.53	0	2,8,10	1.21	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	C	67	1	-	0/3/7/8	-
1	IAS	A	67	1	-	0/3/7/8	-
1	IAS	B	67	1	-	0/3/7/8	-
1	IAS	D	67	1	-	0/3/7/8	-

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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TAV	B	650	-	44,50,50	2.43	13 (29%)	64,74,74	2.98	8 (12%)
2	TAV	C	750	-	44,50,50	2.48	10 (22%)	64,74,74	3.09	5 (7%)
2	TAV	D	850	-	44,50,50	2.51	13 (29%)	64,74,74	3.08	7 (10%)
2	TAV	A	550	-	44,50,50	2.55	12 (27%)	64,74,74	2.95	6 (9%)

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	-	-	8/36/42/42	0/5/5/5
2	TAV	C	750	-	-	6/36/42/42	0/5/5/5
2	TAV	D	850	-	-	9/36/42/42	0/5/5/5
2	TAV	A	550	-	-	6/36/42/42	0/5/5/5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	550	TAV	O51-C26	9.20	1.57	1.42
2	C	750	TAV	O51-C26	8.66	1.56	1.42
2	D	850	TAV	O51-C26	8.18	1.56	1.42
2	B	650	TAV	O51-C26	7.77	1.55	1.42
2	C	750	TAV	C29-N49	6.65	1.48	1.34
2	D	850	TAV	C29-N49	6.09	1.47	1.34
2	B	650	TAV	C29-N49	5.99	1.47	1.34
2	A	550	TAV	C29-N49	5.68	1.46	1.34
2	D	850	TAV	C46-C45	5.07	1.46	1.38
2	A	550	TAV	C46-C45	4.77	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	850	TAV	C6-C1	4.76	1.46	1.38
2	C	750	TAV	C46-C45	4.58	1.46	1.38
2	C	750	TAV	C6-C1	4.57	1.46	1.38
2	B	650	TAV	C6-C1	4.53	1.46	1.38
2	B	650	TAV	C46-C45	4.40	1.45	1.38
2	A	550	TAV	C67-C57	4.36	1.62	1.54
2	A	550	TAV	C6-C1	4.28	1.45	1.38
2	D	850	TAV	C1-S18	4.27	1.83	1.76
2	A	550	TAV	C1-S18	4.16	1.82	1.76
2	B	650	TAV	O19-S18	3.92	1.48	1.43
2	B	650	TAV	C67-C57	3.64	1.60	1.54
2	C	750	TAV	C67-C57	3.52	1.60	1.54
2	B	650	TAV	C1-S18	3.49	1.81	1.76
2	A	550	TAV	C45-S31	3.42	1.82	1.76
2	C	750	TAV	C1-S18	3.39	1.81	1.76
2	D	850	TAV	C14-C13	3.28	1.46	1.38
2	A	550	TAV	C14-C13	3.20	1.46	1.38
2	B	650	TAV	C14-C13	3.18	1.46	1.38
2	C	750	TAV	C37-C32	3.15	1.46	1.38
2	C	750	TAV	C45-S31	3.12	1.81	1.76
2	D	850	TAV	C45-S31	3.09	1.81	1.76
2	A	550	TAV	C37-C32	2.97	1.45	1.38
2	C	750	TAV	C14-C13	2.96	1.45	1.38
2	B	650	TAV	C37-C32	2.90	1.45	1.38
2	D	850	TAV	C37-C32	2.86	1.45	1.38
2	D	850	TAV	C2-C3	2.71	1.48	1.42
2	B	650	TAV	C45-S31	2.64	1.81	1.76
2	D	850	TAV	C57-N49	2.62	1.51	1.47
2	A	550	TAV	S18-N20	2.52	1.67	1.63
2	A	550	TAV	C57-N49	2.46	1.50	1.47
2	B	650	TAV	C2-C3	2.44	1.47	1.42
2	D	850	TAV	C22-C23	2.36	1.43	1.39
2	B	650	TAV	C4-C3	2.33	1.47	1.42
2	A	550	TAV	O54-S18	2.26	1.46	1.43
2	D	850	TAV	C4-C3	2.17	1.47	1.42
2	D	850	TAV	O53-S31	2.15	1.48	1.43
2	B	650	TAV	O54-S18	2.07	1.45	1.43
2	C	750	TAV	O19-S18	2.05	1.45	1.43

All (26) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	750	TAV	C26-O51-S31	22.70	155.94	118.95
2	D	850	TAV	C26-O51-S31	22.26	155.22	118.95
2	A	550	TAV	C26-O51-S31	21.73	154.37	118.95
2	B	650	TAV	C26-O51-S31	21.69	154.30	118.95
2	D	850	TAV	O51-C26-C21	5.07	128.60	118.64
2	B	650	TAV	O51-C26-C21	4.84	128.16	118.64
2	C	750	TAV	O51-C26-C21	4.62	127.73	118.64
2	D	850	TAV	O51-C26-C25	-4.42	108.95	118.56
2	B	650	TAV	O51-C26-C25	-4.30	109.22	118.56
2	A	550	TAV	C1-S18-N20	-4.12	101.65	106.83
2	C	750	TAV	O51-C26-C25	-3.88	110.13	118.56
2	D	850	TAV	C1-S18-N20	-3.84	102.01	106.83
2	C	750	TAV	C1-S18-N20	-3.83	102.02	106.83
2	A	550	TAV	O51-C26-C21	3.79	126.10	118.64
2	C	750	TAV	O54-S18-C1	-3.21	104.02	107.97
2	A	550	TAV	O51-C26-C25	-3.09	111.85	118.56
2	D	850	TAV	C24-C29-N49	-2.85	115.15	118.80
2	A	550	TAV	O51-S31-C45	-2.80	95.62	102.45
2	D	850	TAV	C56-N49-C57	-2.72	112.92	117.73
2	B	650	TAV	C1-S18-N20	-2.55	103.63	106.83
2	B	650	TAV	C2-C1-S18	2.35	122.01	120.03
2	A	550	TAV	C56-N49-C57	-2.34	113.58	117.73
2	B	650	TAV	C56-N49-C57	-2.28	113.69	117.73
2	B	650	TAV	C6-C1-S18	-2.19	117.39	119.77
2	B	650	TAV	O51-S31-C45	-2.17	97.16	102.45
2	D	850	TAV	C2-C1-S18	2.07	121.78	120.03

There are no chirality outliers.

All (29) 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	B	650	TAV	C24-C29-N49-C56
2	B	650	TAV	O50-C29-N49-C56
2	C	750	TAV	C24-C29-N49-C56
2	C	750	TAV	O50-C29-N49-C56
2	D	850	TAV	C24-C29-N49-C56
2	D	850	TAV	O50-C29-N49-C56
2	A	550	TAV	C26-O51-S31-C45

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Mol	Chain	Res	Type	Atoms
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	C25-C26-O51-S31
2	A	550	TAV	C25-C26-O51-S31
2	B	650	TAV	C25-C26-O51-S31
2	D	850	TAV	C26-O51-S31-O52
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	D	850	TAV	C21-C26-O51-S31
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	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

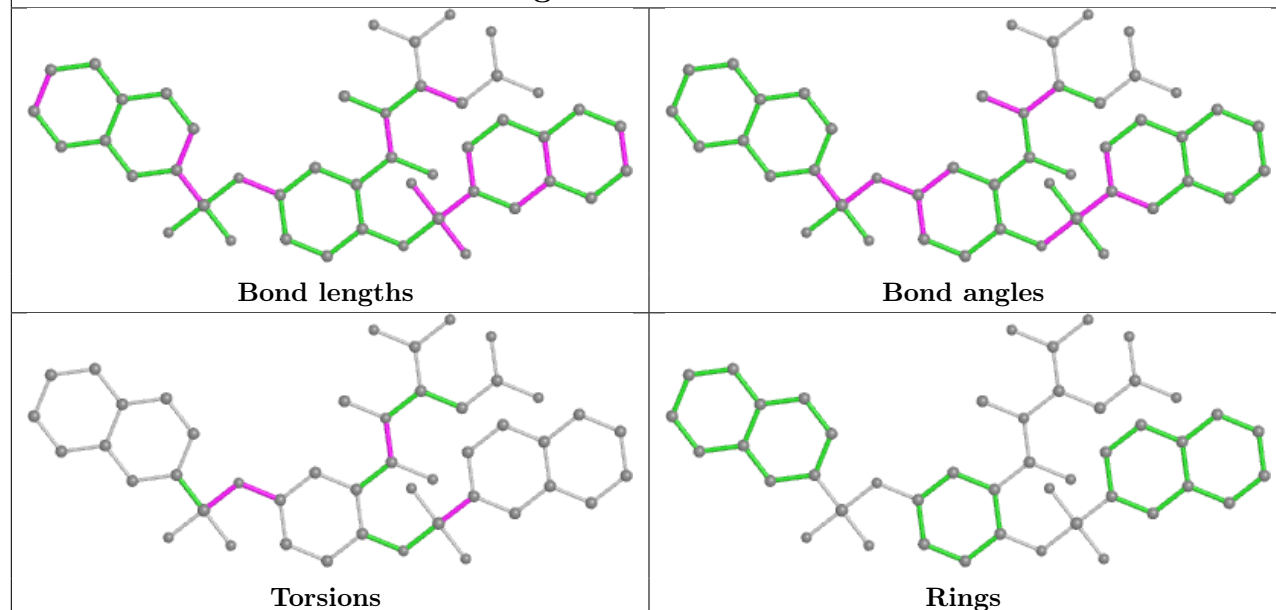
There are no ring outliers.

4 monomers are involved in 16 short contacts:

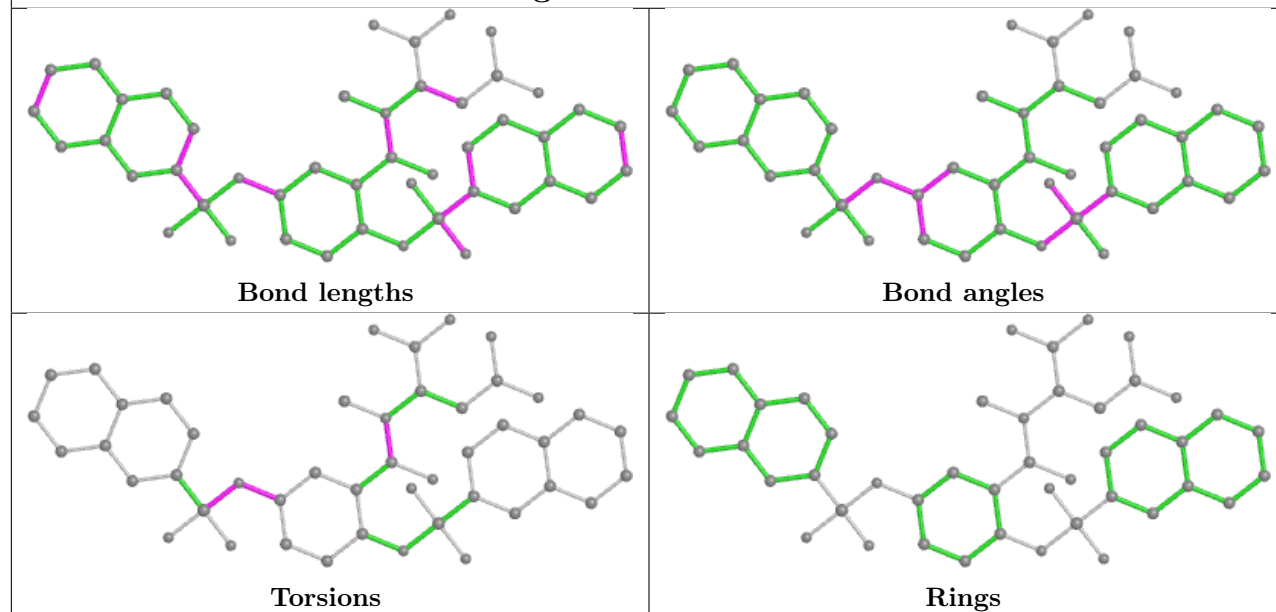
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	650	TAV	3	0
2	C	750	TAV	6	0
2	D	850	TAV	3	0
2	A	550	TAV	4	0

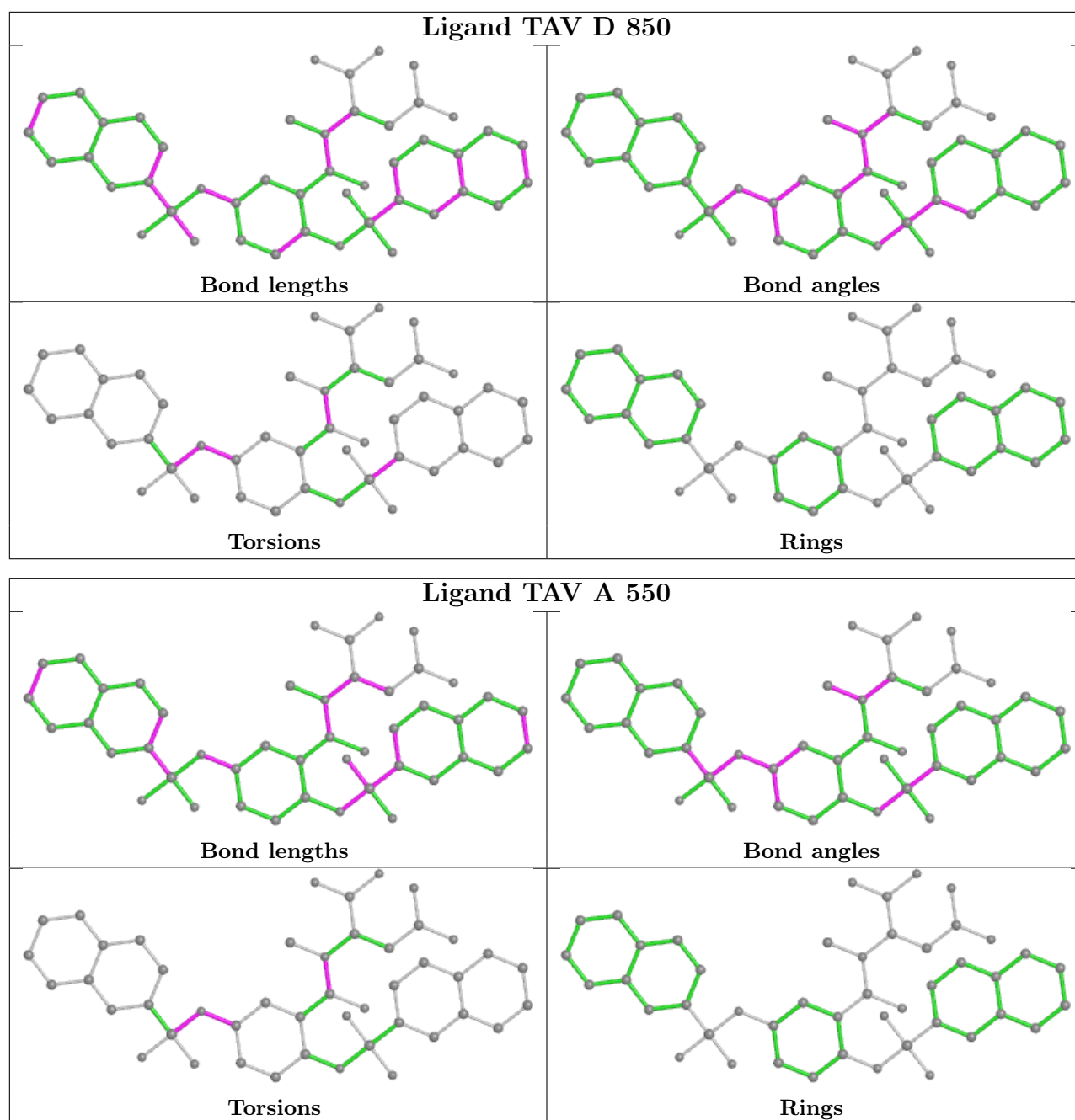
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 TAV B 650



## Ligand TAV C 750





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	418/419 (99%)	-0.60	3 (0%) 87 86	13, 24, 41, 73	0
1	B	418/419 (99%)	-0.59	6 (1%) 75 71	12, 24, 43, 76	0
1	C	418/419 (99%)	-0.56	7 (1%) 70 66	11, 22, 39, 74	0
1	D	418/419 (99%)	-0.48	8 (1%) 66 62	10, 24, 45, 73	0
All	All	1672/1676 (99%)	-0.56	24 (1%) 75 71	10, 23, 43, 76	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	419	GLU	5.1
1	C	419	GLU	5.1
1	A	419	GLU	4.2
1	C	113	GLY	3.9
1	C	115	CYS	3.6
1	D	419	GLU	3.4
1	D	113	GLY	3.4
1	C	114	GLY	3.2
1	C	329	GLU	3.0
1	D	114	GLY	2.8
1	B	115	CYS	2.7
1	D	112	PRO	2.5
1	D	418	GLY	2.4
1	D	116	ALA	2.4
1	A	115	CYS	2.4
1	D	358	GLU	2.4
1	B	113	GLY	2.3
1	A	327	ILE	2.3
1	C	330	ASN	2.3
1	B	418	GLY	2.2
1	C	119	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	119	ALA	2.1
1	B	114	GLY	2.1
1	B	277	GLU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	IAS	B	67	8/9	0.94	0.12	29,30,30,31	0
1	IAS	C	67	8/9	0.94	0.17	24,25,28,29	0
1	IAS	A	67	8/9	0.96	0.21	30,31,32,32	0
1	IAS	D	67	8/9	0.96	0.10	25,26,27,27	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

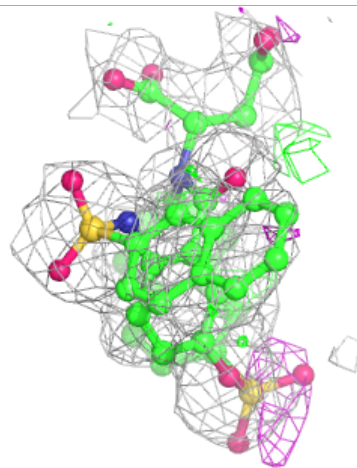
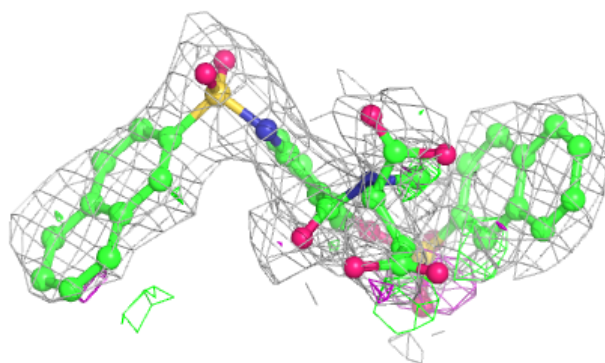
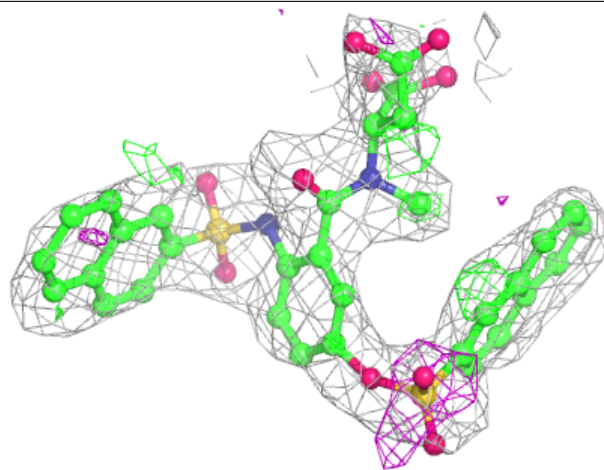
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	TAV	D	850	46/46	0.85	0.24	36,47,60,62	0
2	TAV	B	650	46/46	0.88	0.23	30,39,54,55	0
2	TAV	C	750	46/46	0.88	0.22	30,47,57,63	0
2	TAV	A	550	46/46	0.88	0.20	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.

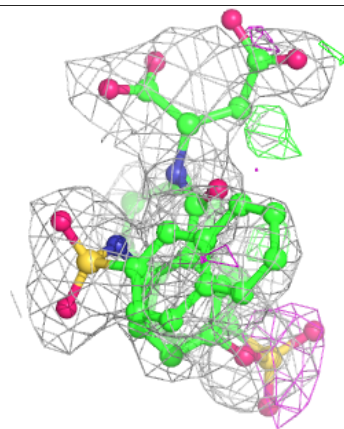
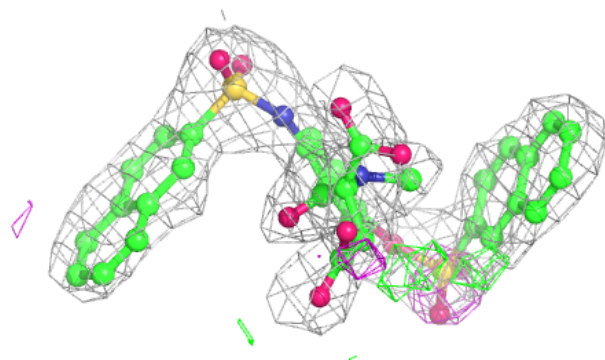
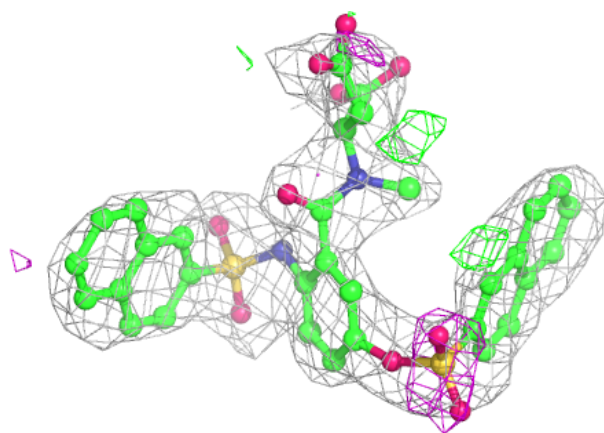
**Electron density around TAV D 850:**

$2mF_o-DF_c$  (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:**

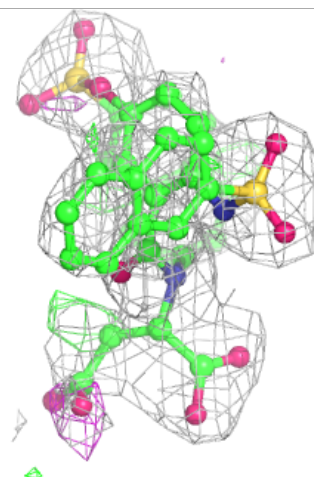
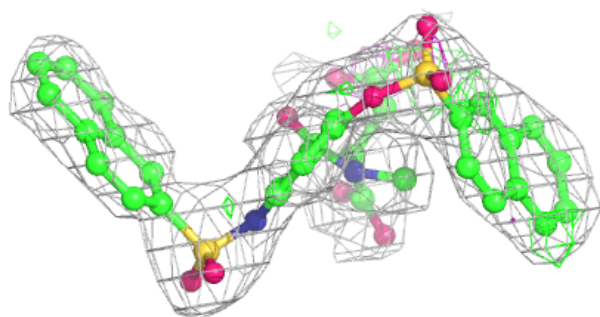
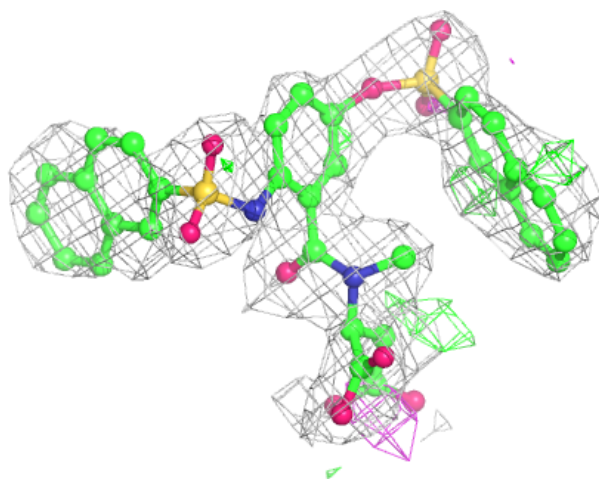
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





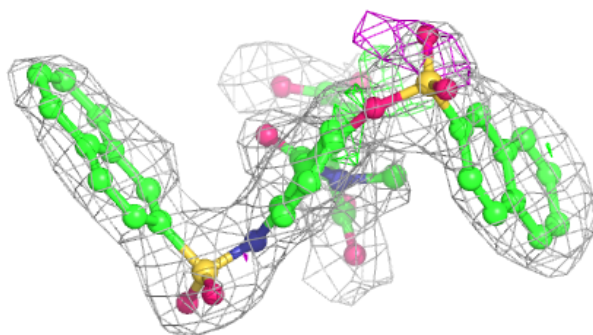
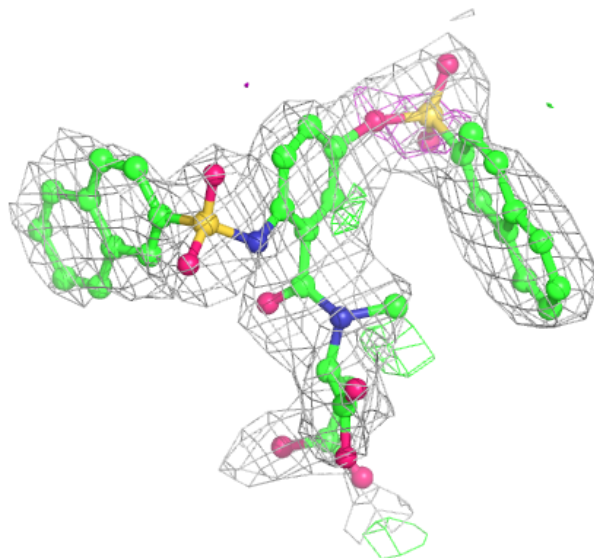
**Electron density around TAV C 750:**

$2mF_o-DF_c$  (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 [i](#)

There are no such residues in this entry.