



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:28 AM UTC

PDB ID : 1NF7 / pdb_00001nf7
Title : Ternary complex of the human type II Inosine Monophosphate Dehydrogenase with Ribavirin Monophosphate and C2-Mycophenolic Adenine Dinucleotide
Authors : Risal, D.; Strickler, M.D.; Goldstein, B.M.
Deposited on : 2002-12-13
Resolution : 2.65 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

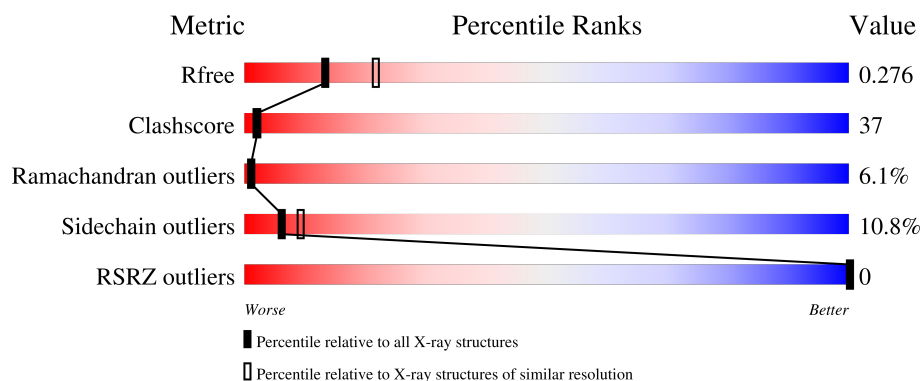
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	514	
1	B	514	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7114 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.

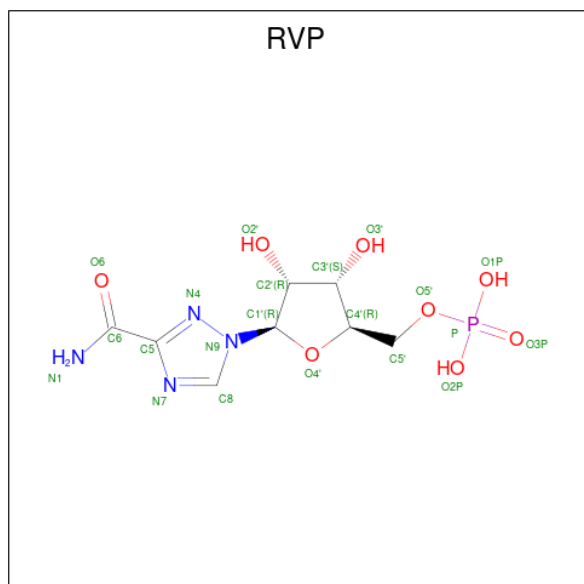
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3440	2176	587	658	19			
1	B	454	Total	C	N	O	S	0	0	0
			3440	2176	587	658	19			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

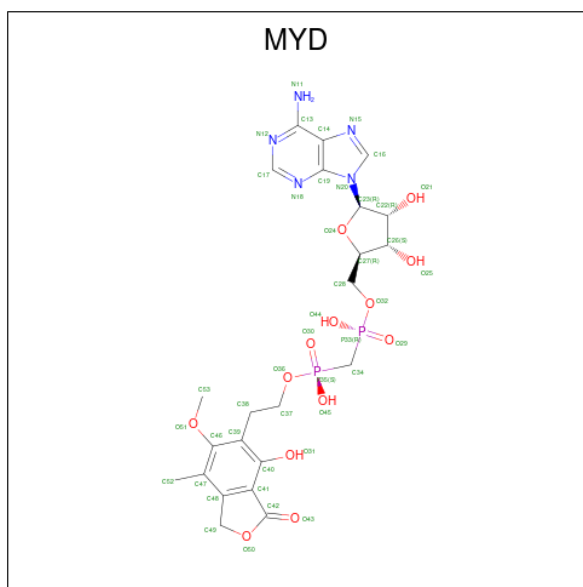
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is RIBAVIRIN MONOPHOSPHATE (CCD ID: RVP) (formula: C₈H₁₃N₄O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	8	4	8	1		
3	B	1	Total	C	N	O	P	0	0
			21	8	4	8	1		

- Molecule 4 is {[5-(6-AMINO-PURIN-7-YL)-3,4-DIHYDROXY-TETRAHYDRO-FURAN-2-YLMETHOXY]-HYDROXY-PHOSPHORYLMETHYL}-PHOSPHONIC ACID MONO-[2-(4-HYDROXY-6-METHOXY-7-METHYL-3-OXO-1,3-DIHYDRO-ISOBENZOFURAN-5-YL)-ETHYL] ESTER (CCD ID: MYD) (formula: $C_{23}H_{29}N_5O_{13}P_2$).



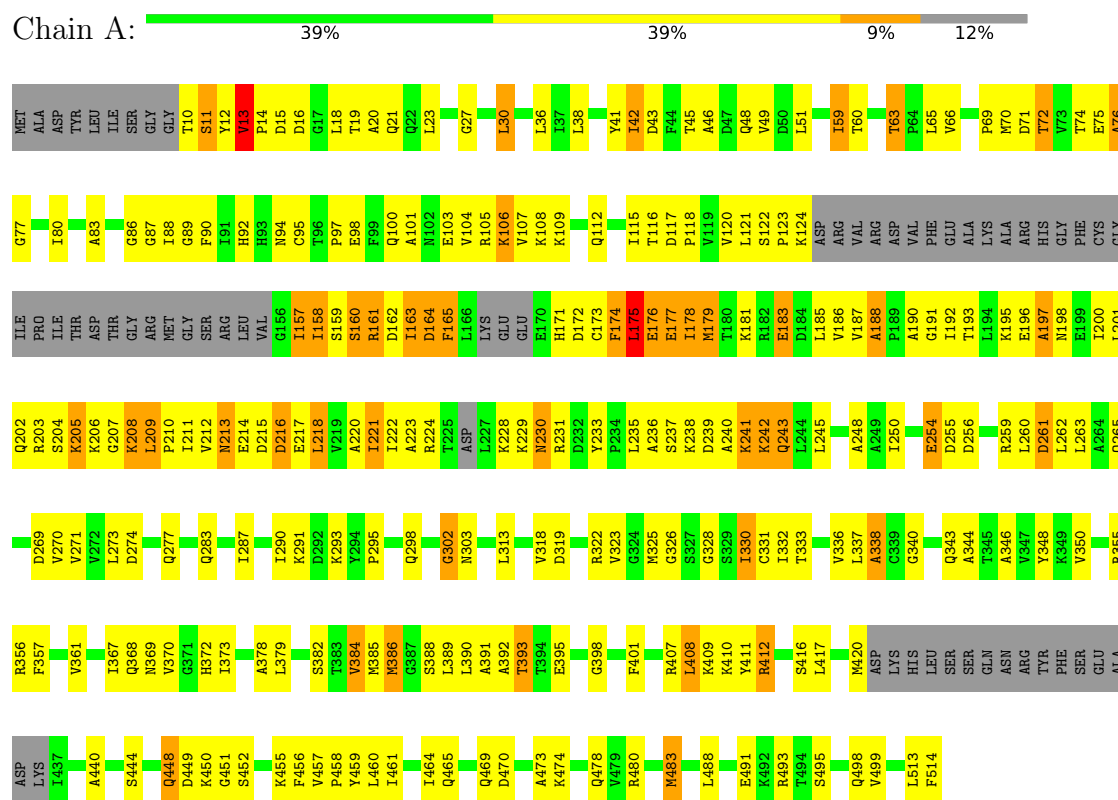
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	47	Total	O	0	0
			47	47		

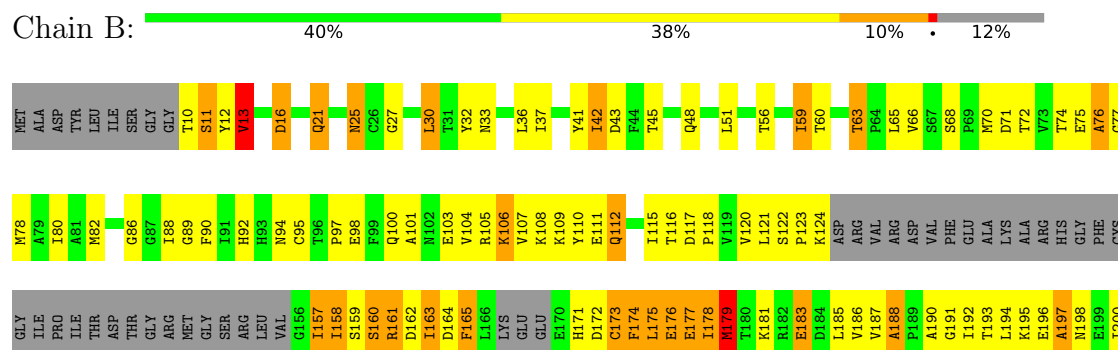
3 Residue-property plots

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: Inosine-5'-monophosphate dehydrogenase 2



• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



L201	Q202	R203	S204	K205	K206	G207	K208	L209	P210	I211	V212	N213	E214	D215	D216	E217	L218	I221	I222	A223	R224	T225	ASP	L227	K228	K229	N230	R231	D232	Y233	P234	L235	A236	S237	K238	D239	A240	K241	K242	Q243	L244	L245	A248	A249	I250	G251	T252	H253	E254	D255	D256	K257	Y258	R259	L260	D261	L262
L263	R356	F357	V361	Q368	N369	V370	G371	H372	I373	A376	L377	A378	L379	V384	M385	M386	G387	S388	L389	L390	A391	A392	T393	T394	E395	G398	E399	Y400	F401	F402	R407	L408	K409	R410	Y411	R412	G413	M414	L417	M420	ASP	LYS	HIS	LEU	SER	SER	GLN	ASN	ARG	TYR	PHE	SER					
GLU	ALA	ASP	LYS	I437	K438	V439	A440	V443	S444	V447	Q448	D449	K450	G451	K455	F456	V457	P458	Y459	L460	I461	I464	Q465	H466	S467	C468	Q469	D470	K474	Q478	V479	R480	M483	Y484	S485	L488	E491	K492	R493	L513	F514																

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	146.58Å 146.58Å 128.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.24 – 2.65 41.24 – 2.65	Depositor EDS
% Data completeness (in resolution range)	64.7 (41.24-2.65) 75.9 (41.24-2.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.277 0.258 , 0.276	Depositor DCC
R_{free} test set	3470 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.429 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7114	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYD, K, UNL, RVP

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	0.70	0/3489	0.92	10/4705 (0.2%)
1	B	0.72	2/3489 (0.1%)	0.94	10/4705 (0.2%)
All	All	0.71	2/6978 (0.0%)	0.93	20/9410 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	437	ILE	CG1-CD1	9.36	1.88	1.51
1	B	179	MET	SD-CE	5.43	1.93	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	437	ILE	CB-CG1-CD1	-11.58	89.47	113.80
1	B	165	PHE	N-CA-C	6.95	119.95	110.35
1	A	165	PHE	N-CA-C	6.41	119.19	110.35
1	B	191	GLY	N-CA-C	-6.06	107.80	115.31
1	A	233	TYR	CA-C-N	5.93	125.55	119.56
1	A	233	TYR	C-N-CA	5.93	125.55	119.56
1	B	513	LEU	N-CA-C	5.87	120.61	112.45
1	B	233	TYR	CA-C-N	5.87	125.49	119.56
1	B	233	TYR	C-N-CA	5.87	125.49	119.56
1	B	228	LYS	N-CA-C	-5.59	105.66	112.88
1	A	228	LYS	N-CA-C	-5.59	105.67	112.88
1	B	59	ILE	N-CA-C	5.46	117.43	108.97
1	A	59	ILE	N-CA-C	5.38	117.30	108.97
1	A	513	LEU	N-CA-C	5.34	119.87	112.45
1	A	191	GLY	N-CA-C	-5.30	108.74	115.31
1	A	188	ALA	CA-C-N	5.27	125.47	120.31
1	A	188	ALA	C-N-CA	5.27	125.47	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	LEU	N-CA-C	5.10	116.53	111.07
1	B	188	ALA	CA-C-N	5.06	125.27	120.31
1	B	188	ALA	C-N-CA	5.06	125.27	120.31

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	3440	0	3498	258	0
1	B	3440	0	3498	262	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	21	0	11	1	0
3	B	21	0	11	1	0
4	A	43	0	25	4	0
4	B	43	0	25	5	0
5	B	11	0	0	1	0
6	A	46	0	0	2	0
6	B	47	0	0	6	0
All	All	7114	0	7068	526	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 37.

All (526) 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:B:437:ILE:CG1	1:B:437:ILE:CD1	1.88	1.52
1:B:179:MET:HE1	1:B:181:LYS:HE2	1.32	1.08
1:A:157:ILE:HD12	1:A:157:ILE:H	1.27	0.99
1:B:437:ILE:CD1	1:B:437:ILE:CB	2.41	0.98
1:B:270:VAL:HG12	1:B:298:GLN:HB2	1.45	0.97
1:B:157:ILE:H	1:B:157:ILE:HD12	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ALA:HB1	1:A:449:ASP:HA	1.46	0.94
1:A:473:ALA:HA	1:A:478:GLN:HE21	1.32	0.94
1:B:392:ALA:HB1	1:B:449:ASP:HA	1.50	0.92
1:B:72:THR:HG21	1:B:411:TYR:HA	1.51	0.92
1:A:270:VAL:HG12	1:A:298:GLN:HB2	1.51	0.91
1:B:333:THR:HG23	1:B:337:LEU:HD12	1.53	0.91
1:A:201:LEU:HD11	1:A:209:LEU:H	1.39	0.88
1:A:373:ILE:HG23	1:A:384:VAL:HG11	1.52	0.88
1:A:412:ARG:HB3	1:A:444:SER:HA	1.53	0.88
1:B:201:LEU:HD11	1:B:209:LEU:H	1.39	0.87
1:B:172:ASP:HB2	1:B:178:ILE:HG23	1.56	0.86
1:A:172:ASP:HB2	1:A:178:ILE:HG23	1.56	0.85
1:A:36:LEU:HG	1:A:493:ARG:HD2	1.59	0.83
1:A:72:THR:HG21	1:A:411:TYR:HA	1.60	0.83
1:B:211:ILE:HD11	1:B:222:ILE:HG12	1.60	0.83
1:A:211:ILE:HD11	1:A:222:ILE:HG12	1.59	0.82
1:B:379:LEU:HA	1:B:483:MET:HE3	1.61	0.81
1:A:157:ILE:H	1:A:157:ILE:CD1	1.94	0.81
1:B:204:SER:HB2	6:B:928:HOH:O	1.80	0.81
1:B:192:ILE:HD11	1:B:222:ILE:HG13	1.61	0.81
1:B:45:THR:H	1:B:48:GLN:NE2	1.79	0.81
1:A:493:ARG:HH21	1:A:498:GLN:HA	1.45	0.80
1:A:157:ILE:HD12	1:A:157:ILE:N	1.94	0.80
1:A:201:LEU:HD21	1:A:209:LEU:HD22	1.64	0.79
1:A:18:LEU:HD23	1:A:23:LEU:HD13	1.64	0.79
1:B:118:PRO:HG3	1:B:221:ILE:HD11	1.63	0.79
1:B:157:ILE:HD12	1:B:157:ILE:N	1.97	0.79
1:A:179:MET:HE1	1:A:181:LYS:HE2	1.65	0.78
1:B:158:ILE:HG23	1:B:179:MET:SD	2.25	0.77
1:A:172:ASP:HB2	1:A:178:ILE:CG2	2.15	0.76
1:A:237:SER:HB3	1:A:245:LEU:HD12	1.65	0.76
1:A:45:THR:H	1:A:48:GLN:NE2	1.84	0.75
1:B:412:ARG:HB3	1:B:444:SER:HA	1.68	0.75
1:B:437:ILE:CD1	1:B:437:ILE:HB	2.15	0.75
1:B:172:ASP:HB2	1:B:178:ILE:CG2	2.16	0.74
1:A:118:PRO:HG3	1:A:221:ILE:HD11	1.70	0.74
1:B:157:ILE:H	1:B:157:ILE:CD1	1.99	0.74
1:A:178:ILE:O	1:A:179:MET:HG2	1.87	0.74
1:A:160:SER:HA	1:A:163:ILE:CD1	2.18	0.73
1:A:157:ILE:O	1:A:158:ILE:HD13	1.89	0.73
1:A:30:LEU:H	1:A:30:LEU:HD12	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ILE:HG12	1:B:469:GLN:HG2	1.72	0.72
1:B:213:ASN:ND2	1:B:214:GLU:H	1.88	0.72
1:B:183:GLU:CD	1:B:183:GLU:H	1.96	0.71
1:A:333:THR:HG23	1:A:337:LEU:HD12	1.72	0.71
1:B:250:ILE:HD13	1:B:260:LEU:HD13	1.70	0.71
1:B:100:GLN:NE2	1:B:259:ARG:HH11	1.87	0.71
1:A:174:PHE:O	1:A:178:ILE:HG12	1.91	0.71
1:A:261:ASP:O	1:A:265:GLN:HG2	1.90	0.71
1:B:178:ILE:O	1:B:179:MET:HG2	1.91	0.70
1:A:183:GLU:CD	1:A:183:GLU:H	1.98	0.70
1:A:160:SER:HA	1:A:163:ILE:HD12	1.72	0.70
1:A:197:ALA:HB1	1:A:222:ILE:HG21	1.73	0.69
1:B:179:MET:HE1	1:B:181:LYS:CE	2.16	0.69
1:A:105:ARG:NH1	1:A:109:LYS:HD2	2.07	0.69
1:A:386:MET:HE3	1:A:389:LEU:HD23	1.72	0.69
1:A:108:LYS:HG3	1:A:243:GLN:NE2	2.08	0.69
1:A:303:ASN:HA	1:A:322:ARG:O	1.93	0.69
1:B:197:ALA:HB1	1:B:222:ILE:HG21	1.75	0.69
1:A:206:LYS:HG3	1:A:207:GLY:H	1.57	0.69
1:B:261:ASP:O	1:B:265:GLN:HG2	1.93	0.69
1:A:283:GLN:NE2	1:A:302:GLY:H	1.92	0.68
1:B:386:MET:HE3	1:B:389:LEU:HD23	1.76	0.68
1:A:250:ILE:HD13	1:A:260:LEU:HD13	1.75	0.68
1:B:188:ALA:HB2	1:B:209:LEU:HD11	1.76	0.68
1:B:30:LEU:HD12	1:B:30:LEU:H	1.58	0.68
1:A:187:VAL:HG13	1:A:210:PRO:HG2	1.74	0.68
1:B:157:ILE:O	1:B:158:ILE:HD13	1.94	0.68
1:A:42:ILE:HD11	1:A:470:ASP:HA	1.75	0.67
1:A:201:LEU:HD11	1:A:209:LEU:N	2.10	0.67
1:A:210:PRO:HA	1:A:221:ILE:HG23	1.76	0.67
1:B:303:ASN:HA	1:B:322:ARG:O	1.94	0.67
1:A:157:ILE:O	1:A:181:LYS:HG3	1.93	0.67
1:A:106:LYS:HB2	1:A:106:LYS:NZ	2.09	0.67
1:B:36:LEU:HG	1:B:493:ARG:HD3	1.76	0.67
1:B:174:PHE:O	1:B:178:ILE:HG12	1.95	0.67
1:A:51:LEU:HD12	1:A:461:ILE:HG23	1.77	0.67
1:B:157:ILE:O	1:B:181:LYS:HG3	1.95	0.67
4:B:702:MYD:H26	6:B:942:HOH:O	1.95	0.67
1:A:221:ILE:HD12	1:A:221:ILE:H	1.61	0.66
1:A:106:LYS:HG3	1:A:117:ASP:OD1	1.95	0.66
1:B:106:LYS:HG3	1:B:117:ASP:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:CYS:O	1:B:177:GLU:HB2	1.96	0.66
1:A:42:ILE:HG12	1:A:469:GLN:HG2	1.76	0.66
1:B:459:TYR:CD1	1:B:514:PHE:HB3	2.31	0.66
1:A:192:ILE:HG12	1:A:211:ILE:HG12	1.76	0.66
1:B:330:ILE:HD12	1:B:331:CYS:N	2.11	0.66
1:B:101:ALA:HA	1:B:263:LEU:HD23	1.77	0.65
1:B:206:LYS:HG3	1:B:207:GLY:H	1.60	0.65
1:A:185:LEU:HD23	1:A:186:VAL:N	2.11	0.65
1:A:177:GLU:C	1:A:179:MET:H	2.05	0.65
1:B:207:GLY:C	1:B:208:LYS:HD2	2.22	0.65
1:A:493:ARG:NH2	1:A:498:GLN:HA	2.11	0.65
1:B:368:GLN:HG2	1:B:372:HIS:CD2	2.32	0.65
1:B:157:ILE:HG22	1:B:158:ILE:N	2.12	0.64
1:B:51:LEU:HD12	1:B:461:ILE:HG23	1.79	0.64
1:B:197:ALA:O	1:B:201:LEU:HD23	1.96	0.64
1:B:198:ASN:O	1:B:201:LEU:HB2	1.98	0.64
1:B:273:LEU:HD13	1:B:283:GLN:HG3	1.77	0.64
1:B:37:ILE:HG23	1:B:488:LEU:HD21	1.79	0.64
1:B:12:TYR:O	1:B:13:VAL:HG22	1.98	0.64
1:B:213:ASN:CG	1:B:214:GLU:H	2.06	0.64
1:B:193:THR:CG2	1:B:195:LYS:HG3	2.28	0.63
1:B:201:LEU:HD21	1:B:209:LEU:HD22	1.78	0.63
1:B:160:SER:HA	1:B:163:ILE:CD1	2.28	0.63
1:B:210:PRO:HA	1:B:221:ILE:HG23	1.80	0.63
1:B:192:ILE:HG12	1:B:211:ILE:HG12	1.81	0.63
1:A:192:ILE:HD11	1:A:222:ILE:HG13	1.81	0.63
1:B:211:ILE:N	1:B:211:ILE:HD12	2.14	0.63
1:A:69:PRO:HG3	1:A:90:PHE:CB	2.29	0.63
1:A:100:GLN:NE2	1:A:263:LEU:HD11	2.13	0.63
1:B:283:GLN:O	1:B:287:ILE:HG12	1.98	0.63
1:A:157:ILE:HG22	1:A:158:ILE:N	2.13	0.62
1:A:158:ILE:HG23	1:A:179:MET:SD	2.39	0.62
1:A:450:LYS:HD3	1:A:456:PHE:CE1	2.33	0.62
1:B:283:GLN:NE2	1:B:302:GLY:H	1.97	0.62
1:B:455:LYS:C	1:B:458:PRO:HD2	2.24	0.62
1:B:187:VAL:HG13	1:B:210:PRO:HG2	1.80	0.62
1:B:177:GLU:C	1:B:179:MET:H	2.05	0.62
1:B:106:LYS:HB2	1:B:106:LYS:NZ	2.15	0.62
1:B:45:THR:H	1:B:48:GLN:HE21	1.47	0.62
1:A:459:TYR:CD1	1:A:514:PHE:HB3	2.35	0.62
1:B:11:SER:OG	1:B:11:SER:O	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HD23	1:B:186:VAL:N	2.16	0.61
1:B:221:ILE:HD12	1:B:221:ILE:H	1.65	0.61
1:A:69:PRO:HG3	1:A:90:PHE:HB2	1.80	0.61
1:A:173:CYS:O	1:A:177:GLU:HB2	2.00	0.61
1:B:42:ILE:HD11	1:B:470:ASP:HA	1.81	0.61
1:B:368:GLN:HG2	1:B:372:HIS:HD2	1.64	0.61
1:A:457:VAL:HB	1:A:458:PRO:HD3	1.81	0.61
1:B:63:THR:HG23	1:B:86:GLY:C	2.25	0.61
1:B:65:LEU:HD12	1:B:457:VAL:HG13	1.82	0.61
1:B:252:THR:HA	1:B:286:MET:HG3	1.83	0.61
1:A:157:ILE:HG22	1:A:158:ILE:H	1.66	0.61
1:B:474:LYS:H	1:B:478:GLN:NE2	1.99	0.61
1:A:106:LYS:HB2	1:A:106:LYS:HZ2	1.63	0.60
1:A:179:MET:CE	1:A:179:MET:HA	2.31	0.60
1:B:105:ARG:NH1	1:B:109:LYS:HD2	2.16	0.60
1:B:241:LYS:HE2	1:B:241:LYS:N	2.15	0.60
1:B:257:LYS:HD2	1:B:289:TYR:CZ	2.36	0.60
1:B:160:SER:HA	1:B:163:ILE:HD12	1.84	0.60
1:B:211:ILE:CD1	1:B:222:ILE:HG12	2.30	0.60
1:A:337:LEU:O	1:A:338:ALA:HB2	2.00	0.60
1:A:283:GLN:O	1:A:287:ILE:HG12	2.01	0.60
1:B:108:LYS:HG3	1:B:243:GLN:NE2	2.17	0.60
1:B:201:LEU:HD11	1:B:209:LEU:N	2.13	0.60
1:A:63:THR:HG23	1:A:86:GLY:C	2.27	0.59
1:A:213:ASN:ND2	1:A:214:GLU:H	2.00	0.59
1:A:211:ILE:CD1	1:A:222:ILE:HG12	2.30	0.59
1:A:273:LEU:HD13	1:A:283:GLN:HG3	1.83	0.59
4:A:701:MYD:H26	6:A:948:HOH:O	2.02	0.59
1:B:157:ILE:HG22	1:B:158:ILE:H	1.65	0.59
1:B:212:VAL:HG12	1:B:218:LEU:HA	1.83	0.59
1:A:158:ILE:HD12	1:A:179:MET:HB3	1.84	0.59
1:A:197:ALA:O	1:A:201:LEU:HD23	2.01	0.59
4:B:702:MYD:O36	4:B:702:MYD:H532	2.02	0.59
1:B:88:ILE:HG12	1:B:89:GLY:N	2.16	0.59
1:A:213:ASN:CG	1:A:214:GLU:H	2.09	0.59
1:A:287:ILE:HD12	1:A:318:VAL:HG12	1.85	0.59
1:A:332:ILE:O	1:A:336:VAL:HG22	2.02	0.59
1:A:211:ILE:O	1:A:218:LEU:HD22	2.03	0.59
1:B:25:ASN:HD21	1:B:349:LYS:NZ	2.01	0.58
1:B:337:LEU:O	1:B:338:ALA:HB2	2.02	0.58
1:B:457:VAL:HB	1:B:458:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:HB	1:A:221:ILE:HD13	1.85	0.58
1:A:203:ARG:HG2	1:A:203:ARG:HH11	1.67	0.58
1:B:450:LYS:HD3	1:B:456:PHE:CE1	2.38	0.58
1:A:207:GLY:HA2	1:A:224:ARG:HD2	1.85	0.58
1:A:330:ILE:HD12	1:A:331:CYS:N	2.19	0.58
1:B:106:LYS:HB2	1:B:106:LYS:HZ2	1.69	0.58
1:B:123:PRO:HB3	1:B:176:GLU:HB2	1.87	0.57
1:B:332:ILE:O	1:B:336:VAL:HG22	2.03	0.57
1:A:455:LYS:C	1:A:458:PRO:HD2	2.29	0.57
1:A:115:ILE:HD12	1:A:221:ILE:HB	1.86	0.57
1:B:326:GLY:HA2	1:B:331:CYS:SG	2.44	0.57
1:A:101:ALA:HA	1:A:263:LEU:HD23	1.85	0.57
1:B:193:THR:HG22	1:B:195:LYS:HG3	1.87	0.57
1:A:211:ILE:HD12	1:A:211:ILE:N	2.20	0.56
1:A:283:GLN:HE22	1:A:302:GLY:N	2.03	0.56
4:A:701:MYD:O36	4:A:701:MYD:H532	2.05	0.56
1:A:75:GLU:O	1:A:77:GLY:N	2.38	0.56
1:B:202:GLN:HA	1:B:224:ARG:HH12	1.69	0.56
1:B:408:LEU:HD23	1:B:408:LEU:C	2.30	0.56
1:A:41:TYR:CE2	1:A:43:ASP:HB3	2.41	0.56
1:A:221:ILE:HD12	1:A:221:ILE:N	2.20	0.56
1:B:160:SER:O	1:B:161:ARG:C	2.49	0.56
1:A:198:ASN:O	1:A:201:LEU:HB2	2.05	0.56
1:A:66:VAL:HG22	1:A:88:ILE:HG22	1.88	0.56
1:A:92:HIS:HD2	1:A:94:ASN:H	1.53	0.56
1:A:197:ALA:CB	1:A:222:ILE:HG21	2.36	0.56
1:B:159:SER:HB2	1:B:161:ARG:NE	2.21	0.56
1:B:92:HIS:CD2	1:B:94:ASN:H	2.24	0.55
1:B:41:TYR:CE2	1:B:43:ASP:HB3	2.40	0.55
1:A:12:TYR:O	1:A:13:VAL:HG22	2.06	0.55
1:B:239:ASP:OD1	1:B:243:GLN:HG3	2.07	0.55
1:A:368:GLN:H	1:A:372:HIS:HD2	1.55	0.55
1:B:25:ASN:HD21	1:B:349:LYS:HZ2	1.53	0.55
1:A:12:TYR:C	1:A:13:VAL:HG13	2.31	0.54
1:B:75:GLU:O	1:B:77:GLY:N	2.40	0.54
1:B:248:ALA:O	1:B:271:VAL:HA	2.07	0.54
1:A:248:ALA:O	1:A:271:VAL:HA	2.07	0.54
1:A:273:LEU:CD1	1:A:283:GLN:HG3	2.36	0.54
1:A:283:GLN:HE22	1:A:302:GLY:H	1.55	0.54
1:A:115:ILE:HG22	1:A:118:PRO:HD3	1.90	0.54
1:A:211:ILE:HD11	1:A:222:ILE:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:C	1:A:408:LEU:HD23	2.33	0.54
1:A:92:HIS:CD2	1:A:94:ASN:H	2.24	0.54
1:B:122:SER:OG	1:B:124:LYS:HG2	2.08	0.54
1:A:160:SER:O	1:A:161:ARG:C	2.51	0.54
1:A:203:ARG:HG2	1:A:203:ARG:NH1	2.21	0.54
1:B:158:ILE:HD12	1:B:179:MET:HB3	1.89	0.54
1:B:221:ILE:HD12	1:B:221:ILE:N	2.23	0.54
1:A:179:MET:HE1	1:A:181:LYS:CE	2.35	0.54
1:A:245:LEU:HD23	1:A:269:ASP:OD1	2.09	0.53
1:B:74:THR:HG21	1:B:90:PHE:N	2.22	0.53
1:B:159:SER:O	1:B:161:ARG:HG2	2.08	0.53
1:B:378:ALA:O	1:B:483:MET:HG2	2.08	0.53
1:A:175:LEU:HA	1:A:178:ILE:CG1	2.38	0.53
1:B:211:ILE:HD11	1:B:222:ILE:H	1.73	0.53
1:A:196:GLU:O	1:A:200:ILE:HG13	2.08	0.53
1:A:63:THR:HG23	1:A:86:GLY:O	2.09	0.53
1:B:274:ASP:OD1	1:B:322:ARG:NH1	2.42	0.53
1:B:197:ALA:CB	1:B:222:ILE:HG21	2.38	0.53
1:A:207:GLY:C	1:A:208:LYS:HD2	2.34	0.53
1:A:328:GLY:HA2	3:A:600:RVP:O3P	2.09	0.53
1:B:37:ILE:HG23	1:B:488:LEU:CD2	2.39	0.53
1:B:37:ILE:CG2	1:B:488:LEU:HD21	2.38	0.53
1:B:213:ASN:ND2	1:B:215:ASP:H	2.07	0.53
1:B:192:ILE:HD12	1:B:193:THR:H	1.74	0.52
1:B:407:ARG:CD	1:B:449:ASP:HB3	2.40	0.52
1:A:51:LEU:CD1	1:A:461:ILE:HG23	2.37	0.52
1:A:75:GLU:O	1:A:76:ALA:C	2.52	0.52
1:B:10:THR:HG22	1:B:12:TYR:HB2	1.92	0.52
1:B:78:MET:O	1:B:82:MET:HB2	2.09	0.52
1:A:106:LYS:HE3	1:A:117:ASP:CG	2.34	0.52
1:B:66:VAL:HG22	1:B:88:ILE:HG22	1.91	0.52
1:B:97:PRO:HB2	1:B:262:LEU:HD12	1.91	0.52
1:B:293:LYS:O	1:B:295:PRO:HD3	2.09	0.52
1:B:388:SER:C	1:B:390:LEU:H	2.17	0.52
1:B:224:ARG:HA	6:B:929:HOH:O	2.10	0.52
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.74	0.52
1:B:458:PRO:HA	1:B:461:ILE:HD12	1.92	0.52
1:A:188:ALA:HB2	1:A:209:LEU:HD11	1.92	0.52
1:A:461:ILE:O	1:A:465:GLN:HG3	2.10	0.52
1:B:75:GLU:O	1:B:76:ALA:C	2.52	0.52
1:A:104:VAL:HG21	1:A:263:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HH11	1:A:109:LYS:HD2	1.73	0.51
1:A:192:ILE:HG21	1:A:211:ILE:HG21	1.92	0.51
1:A:193:THR:CG2	1:A:195:LYS:HG3	2.40	0.51
1:B:215:ASP:O	1:B:217:GLU:N	2.43	0.51
1:A:100:GLN:HE21	1:A:263:LEU:HD21	1.74	0.51
1:A:388:SER:C	1:A:390:LEU:H	2.18	0.51
1:B:211:ILE:O	1:B:218:LEU:HD22	2.10	0.51
1:B:287:ILE:HD12	1:B:318:VAL:HG12	1.91	0.51
1:B:313:LEU:O	1:B:318:VAL:HG22	2.11	0.51
1:A:386:MET:HE1	1:A:460:LEU:HD13	1.93	0.51
1:B:97:PRO:HB3	1:B:259:ARG:HA	1.91	0.51
1:B:386:MET:HE1	1:B:460:LEU:CD1	2.40	0.51
1:A:97:PRO:HB2	1:A:262:LEU:HD12	1.92	0.51
1:A:313:LEU:O	1:A:318:VAL:HG22	2.10	0.51
1:B:13:VAL:O	1:B:13:VAL:CG2	2.58	0.51
1:B:215:ASP:O	1:B:217:GLU:HG2	2.11	0.51
1:A:97:PRO:HB3	1:A:259:ARG:HA	1.91	0.51
1:A:106:LYS:HZ2	1:A:106:LYS:CB	2.24	0.51
1:A:215:ASP:O	1:A:217:GLU:N	2.43	0.51
1:A:162:ASP:O	1:A:163:ILE:C	2.54	0.51
1:A:398:GLY:C	1:A:409:LYS:HE3	2.36	0.51
1:B:63:THR:HG23	1:B:86:GLY:O	2.11	0.51
1:B:398:GLY:C	1:B:409:LYS:HE3	2.36	0.51
1:B:460:LEU:O	1:B:464:ILE:HG13	2.11	0.51
1:A:123:PRO:HB3	1:A:176:GLU:HB2	1.94	0.50
1:A:11:SER:O	1:A:11:SER:OG	2.22	0.50
1:A:208:LYS:HA	1:A:222:ILE:O	2.11	0.50
1:B:177:GLU:C	1:B:179:MET:N	2.70	0.50
1:A:326:GLY:HA2	1:A:331:CYS:SG	2.51	0.50
1:B:203:ARG:HH11	1:B:203:ARG:HG2	1.76	0.50
1:A:293:LYS:O	1:A:295:PRO:HD3	2.11	0.50
1:B:175:LEU:HA	1:B:178:ILE:CG1	2.41	0.50
1:A:115:ILE:HG13	1:A:223:ALA:HB2	1.92	0.50
1:B:283:GLN:OE1	1:B:302:GLY:HA3	2.12	0.50
1:A:65:LEU:HD12	1:A:457:VAL:HG13	1.93	0.50
1:A:179:MET:HA	1:A:179:MET:HE2	1.94	0.50
1:A:212:VAL:HG12	1:A:218:LEU:HA	1.94	0.50
1:B:187:VAL:HG12	1:B:188:ALA:H	1.76	0.50
1:A:382:SER:HA	1:A:480:ARG:HH21	1.77	0.49
1:A:159:SER:O	1:A:161:ARG:HG2	2.12	0.49
1:B:94:ASN:HB2	1:B:414:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLU:N	1:B:395:GLU:OE1	2.45	0.49
1:A:206:LYS:HG3	1:A:207:GLY:N	2.25	0.49
1:B:208:LYS:HD2	1:B:208:LYS:N	2.26	0.49
1:A:46:ALA:O	1:A:49:VAL:HG23	2.13	0.49
1:A:105:ARG:O	1:A:109:LYS:HG2	2.12	0.49
1:B:208:LYS:HA	1:B:222:ILE:O	2.12	0.49
1:A:105:ARG:HH11	1:A:105:ARG:HG2	1.78	0.49
1:A:159:SER:HB2	1:A:161:ARG:NE	2.28	0.49
1:A:202:GLN:HA	1:A:224:ARG:HH12	1.78	0.49
1:A:241:LYS:N	1:A:241:LYS:HE2	2.28	0.49
1:B:104:VAL:HG21	1:B:263:LEU:HD22	1.93	0.49
1:B:254:GLU:C	1:B:256:ASP:H	2.21	0.49
1:A:74:THR:HG21	1:A:90:PHE:N	2.28	0.48
1:B:209:LEU:HD23	1:B:209:LEU:O	2.12	0.48
1:A:177:GLU:C	1:A:179:MET:N	2.70	0.48
1:A:348:TYR:CE1	1:A:483:MET:HE1	2.48	0.48
1:A:186:VAL:HG11	1:A:204:SER:HB3	1.95	0.48
1:B:98:GLU:H	1:B:98:GLU:CD	2.21	0.48
1:B:161:ARG:H	1:B:161:ARG:HD3	1.78	0.48
1:B:202:GLN:O	1:B:205:LYS:HD2	2.13	0.48
1:A:122:SER:OG	1:A:123:PRO:HD2	2.13	0.48
1:B:88:ILE:HG12	1:B:89:GLY:H	1.77	0.48
1:A:254:GLU:C	1:A:256:ASP:H	2.21	0.48
1:B:437:ILE:N	5:B:811:UNL:CA	2.77	0.48
1:B:257:LYS:HD2	1:B:289:TYR:CE1	2.47	0.48
1:B:51:LEU:CD1	1:B:461:ILE:HG23	2.44	0.48
1:B:398:GLY:O	1:B:409:LYS:HE3	2.14	0.48
1:B:115:ILE:HG22	1:B:118:PRO:HD3	1.96	0.48
1:B:162:ASP:O	1:B:163:ILE:C	2.57	0.48
1:A:386:MET:HE1	1:A:460:LEU:CD1	2.44	0.47
1:B:158:ILE:CD1	1:B:179:MET:HB3	2.43	0.47
1:B:201:LEU:HD21	1:B:209:LEU:HB3	1.96	0.47
1:B:417:LEU:HG	1:B:440:ALA:HB2	1.96	0.47
1:A:88:ILE:HG12	1:A:89:GLY:N	2.30	0.47
1:A:333:THR:CG2	1:A:337:LEU:HD12	2.41	0.47
1:B:203:ARG:HG2	1:B:203:ARG:NH1	2.29	0.47
1:B:206:LYS:HG3	1:B:207:GLY:N	2.28	0.47
1:A:120:VAL:HG22	1:A:121:LEU:N	2.29	0.47
1:A:417:LEU:HG	1:A:440:ALA:HB2	1.96	0.47
1:B:215:ASP:O	1:B:216:ASP:C	2.57	0.47
1:B:298:GLN:HA	1:B:319:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ILE:O	1:B:465:GLN:HG3	2.13	0.47
1:A:236:ALA:HB3	1:A:238:LYS:HE2	1.97	0.47
1:A:298:GLN:HA	1:A:319:ASP:OD2	2.13	0.47
1:B:237:SER:HB3	1:B:245:LEU:HD12	1.96	0.47
1:A:108:LYS:HD2	1:A:108:LYS:HA	1.74	0.47
1:B:108:LYS:O	1:B:243:GLN:NE2	2.43	0.47
1:B:120:VAL:HG22	1:B:121:LEU:N	2.28	0.47
1:A:100:GLN:HG2	1:A:263:LEU:HD21	1.97	0.47
1:A:343:GLN:OE1	1:A:343:GLN:HA	2.15	0.47
1:A:159:SER:O	1:A:161:ARG:N	2.47	0.47
1:A:323:VAL:HG23	1:A:361:VAL:HG13	1.96	0.47
1:A:215:ASP:O	1:A:216:ASP:C	2.57	0.47
1:A:355:ARG:C	1:A:357:PHE:H	2.23	0.47
1:B:352:GLU:CD	1:B:352:GLU:O	2.58	0.46
1:B:394:THR:HA	1:B:400:TYR:OH	2.15	0.46
1:A:13:VAL:O	1:A:13:VAL:CG2	2.63	0.46
1:A:157:ILE:HD13	1:A:185:LEU:HD13	1.96	0.46
1:A:218:LEU:C	1:A:218:LEU:HD13	2.41	0.46
1:B:192:ILE:HG21	1:B:211:ILE:HG21	1.98	0.46
1:A:389:LEU:O	1:A:390:LEU:HD23	2.16	0.46
1:B:211:ILE:CD1	1:B:222:ILE:H	2.28	0.46
1:B:369:ASN:O	1:B:370:VAL:C	2.59	0.46
1:B:386:MET:HE1	1:B:460:LEU:HD13	1.97	0.46
1:A:30:LEU:O	1:A:344:ALA:HB3	2.16	0.46
1:A:76:ALA:O	1:A:80:ILE:HG13	2.15	0.46
1:A:158:ILE:HD12	1:A:179:MET:CB	2.44	0.46
1:B:192:ILE:HD12	1:B:193:THR:N	2.30	0.46
1:A:19:THR:HG22	1:A:20:ALA:N	2.29	0.46
1:A:214:GLU:HA	1:A:214:GLU:OE1	2.16	0.46
1:A:235:LEU:O	1:A:236:ALA:C	2.57	0.46
1:A:386:MET:CE	1:A:389:LEU:HD23	2.44	0.46
1:B:103:GLU:O	1:B:107:VAL:HG23	2.15	0.46
1:B:115:ILE:HD12	1:B:221:ILE:HB	1.98	0.46
1:B:158:ILE:HD12	1:B:179:MET:CB	2.45	0.46
1:B:218:LEU:HD13	1:B:218:LEU:C	2.40	0.46
1:B:333:THR:CG2	1:B:337:LEU:HD12	2.34	0.46
1:A:158:ILE:CD1	1:A:179:MET:HB3	2.45	0.46
1:A:495:SER:O	1:A:499:VAL:HG23	2.16	0.46
1:B:70:MET:HE3	1:B:413:GLY:HA2	1.97	0.46
1:A:239:ASP:C	1:A:239:ASP:OD1	2.58	0.46
1:A:10:THR:HG21	1:B:485:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:CD2	1:B:209:LEU:HB3	2.46	0.46
1:A:236:ALA:CB	1:A:238:LYS:HE2	2.45	0.45
1:A:322:ARG:HH11	1:A:385:MET:HE1	1.80	0.45
1:A:192:ILE:HD12	1:A:193:THR:H	1.81	0.45
1:B:328:GLY:HA2	3:B:601:RVP:O3P	2.16	0.45
1:A:59:ILE:HD12	1:A:270:VAL:CG1	2.47	0.45
1:A:108:LYS:HG3	1:A:243:GLN:HE22	1.77	0.45
1:A:378:ALA:O	1:A:483:MET:HG2	2.15	0.45
1:B:16:ASP:OD1	1:B:16:ASP:C	2.59	0.45
1:B:63:THR:CG2	1:B:86:GLY:HA3	2.45	0.45
1:B:118:PRO:CG	1:B:221:ILE:HD11	2.41	0.45
1:B:179:MET:CE	1:B:181:LYS:HE2	2.24	0.45
1:B:235:LEU:O	1:B:236:ALA:C	2.57	0.45
1:A:106:LYS:HG3	1:A:117:ASP:CG	2.40	0.45
1:A:395:GLU:OE1	1:A:395:GLU:N	2.49	0.45
1:A:193:THR:HG22	1:A:195:LYS:HG3	1.99	0.45
1:A:197:ALA:O	1:A:198:ASN:C	2.60	0.45
1:A:211:ILE:CD1	1:A:222:ILE:H	2.30	0.45
1:A:230:ASN:O	1:A:230:ASN:ND2	2.49	0.45
1:B:190:ALA:C	1:B:192:ILE:H	2.23	0.45
1:B:305:VAL:HG23	1:B:306:THR:HG23	1.98	0.45
1:B:197:ALA:O	1:B:198:ASN:C	2.59	0.45
1:A:215:ASP:O	1:A:217:GLU:HG2	2.16	0.45
1:B:72:THR:HG21	1:B:411:TYR:CA	2.33	0.45
1:A:187:VAL:HG12	1:A:188:ALA:H	1.81	0.45
1:A:346:ALA:O	1:A:350:VAL:HG23	2.16	0.45
1:A:379:LEU:C	1:A:483:MET:HE2	2.41	0.45
1:B:351:SER:O	1:B:355:ARG:HG2	2.17	0.45
1:B:355:ARG:C	1:B:357:PHE:H	2.25	0.45
1:A:10:THR:O	1:A:11:SER:HB3	2.17	0.45
1:A:473:ALA:CB	1:A:478:GLN:HG2	2.47	0.45
1:B:159:SER:O	1:B:161:ARG:N	2.49	0.45
1:B:391:ALA:HB3	1:B:447:VAL:HG21	1.99	0.45
1:A:239:ASP:OD1	1:A:243:GLN:HG3	2.17	0.44
1:A:416:SER:O	1:A:420:MET:HG3	2.17	0.44
1:B:240:ALA:C	1:B:242:LYS:H	2.25	0.44
1:B:157:ILE:CG2	1:B:158:ILE:N	2.79	0.44
1:B:193:THR:HG21	1:B:195:LYS:HG3	2.00	0.44
1:B:373:ILE:HG23	1:B:384:VAL:HG21	1.99	0.44
1:B:391:ALA:O	1:B:392:ALA:C	2.60	0.44
1:A:157:ILE:HD13	1:A:185:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ARG:HG3	1:A:356:ARG:N	2.31	0.44
1:A:483:MET:HB3	1:A:488:LEU:HD23	1.98	0.44
1:B:56:THR:HB	1:B:298:GLN:HE21	1.83	0.44
1:A:98:GLU:CD	1:A:98:GLU:H	2.25	0.44
1:A:162:ASP:O	1:A:164:ASP:N	2.50	0.44
1:A:192:ILE:CG2	1:A:211:ILE:HG21	2.47	0.44
1:B:106:LYS:HG3	1:B:117:ASP:CG	2.41	0.44
1:B:106:LYS:HZ2	1:B:106:LYS:CB	2.30	0.44
1:A:337:LEU:O	1:A:338:ALA:CB	2.66	0.44
1:A:408:LEU:HG	1:A:409:LYS:N	2.33	0.44
1:B:179:MET:CE	1:B:179:MET:HA	2.48	0.44
1:B:283:GLN:HE22	1:B:302:GLY:N	2.16	0.44
1:A:190:ALA:C	1:A:192:ILE:H	2.24	0.44
1:B:407:ARG:HD3	1:B:449:ASP:HB3	2.00	0.44
1:A:240:ALA:C	1:A:242:LYS:H	2.26	0.43
1:A:325:MET:SD	1:A:340:GLY:HA2	2.58	0.43
1:B:355:ARG:HG3	1:B:356:ARG:N	2.33	0.43
1:A:185:LEU:O	1:A:187:VAL:HG23	2.17	0.43
1:B:196:GLU:HB3	1:B:200:ILE:CD1	2.48	0.43
1:A:412:ARG:HB3	1:A:444:SER:CA	2.37	0.43
1:A:473:ALA:HA	1:A:478:GLN:NE2	2.15	0.43
1:B:185:LEU:HD23	1:B:185:LEU:C	2.43	0.43
1:A:122:SER:OG	1:A:124:LYS:HG2	2.19	0.43
1:A:369:ASN:O	1:A:370:VAL:C	2.62	0.43
1:A:407:ARG:CD	1:A:449:ASP:HB3	2.48	0.43
1:A:185:LEU:HD23	1:A:185:LEU:C	2.44	0.43
1:A:395:GLU:OE2	1:A:452:SER:OG	2.35	0.43
1:B:70:MET:HG2	1:B:414:MET:HG2	2.00	0.43
1:B:388:SER:C	1:B:390:LEU:N	2.77	0.43
1:B:480:ARG:NH1	6:B:907:HOH:O	2.52	0.43
1:A:157:ILE:CG2	1:A:158:ILE:N	2.81	0.43
1:A:367:ILE:HG13	1:A:384:VAL:HG21	2.00	0.43
1:A:452:SER:N	6:A:929:HOH:O	2.51	0.43
1:B:76:ALA:O	1:B:80:ILE:HG13	2.19	0.43
1:A:10:THR:HG21	1:B:485:SER:CB	2.49	0.43
1:A:66:VAL:O	1:A:385:MET:HA	2.19	0.43
1:B:282:PHE:CD1	4:B:702:MYD:N11	2.87	0.43
1:B:448:GLN:HB3	1:B:449:ASP:H	1.50	0.43
1:A:118:PRO:CG	1:A:221:ILE:HD11	2.45	0.43
1:B:74:THR:HG21	1:B:90:PHE:H	1.84	0.43
1:B:196:GLU:O	1:B:200:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ALA:O	1:B:393:THR:C	2.61	0.43
1:A:209:LEU:O	1:A:209:LEU:HD23	2.19	0.43
1:A:448:GLN:HB3	1:A:449:ASP:H	1.48	0.43
1:B:32:TYR:OH	1:B:376:ALA:HB2	2.18	0.43
1:B:231:ARG:HD2	1:B:233:TYR:OH	2.19	0.43
1:A:103:GLU:O	1:A:107:VAL:HG23	2.18	0.42
1:A:213:ASN:ND2	1:A:215:ASP:H	2.17	0.42
1:B:70:MET:C	1:B:72:THR:H	2.27	0.42
1:A:391:ALA:O	1:A:392:ALA:C	2.62	0.42
1:B:110:TYR:CD2	1:B:110:TYR:C	2.97	0.42
1:B:254:GLU:HA	1:B:254:GLU:OE2	2.19	0.42
1:A:202:GLN:O	1:A:205:LYS:HD2	2.20	0.42
1:B:122:SER:OG	1:B:123:PRO:HD2	2.19	0.42
1:B:187:VAL:HG12	1:B:188:ALA:N	2.34	0.42
1:A:100:GLN:NE2	1:A:263:LEU:HD21	2.34	0.42
1:A:179:MET:HE2	1:A:179:MET:CA	2.49	0.42
1:B:100:GLN:HE21	1:B:100:GLN:HB3	1.64	0.42
1:B:202:GLN:HA	1:B:224:ARG:NH1	2.33	0.42
1:B:258:TYR:O	1:B:261:ASP:HB2	2.20	0.42
1:B:297:LEU:N	6:B:931:HOH:O	2.53	0.42
1:B:108:LYS:HA	1:B:108:LYS:HD2	1.81	0.42
1:B:193:THR:HG22	1:B:194:LEU:N	2.34	0.42
1:B:407:ARG:HD2	1:B:449:ASP:HB3	2.01	0.42
1:B:437:ILE:HG22	1:B:438:LYS:N	2.34	0.42
1:B:111:GLU:O	1:B:112:GLN:C	2.62	0.42
1:B:213:ASN:CG	1:B:214:GLU:N	2.74	0.42
1:A:63:THR:CG2	1:A:86:GLY:HA3	2.49	0.42
1:B:59:ILE:HG22	1:B:60:THR:N	2.34	0.42
1:B:115:ILE:HB	1:B:221:ILE:HD13	2.02	0.42
1:B:239:ASP:CG	1:B:243:GLN:HG3	2.45	0.42
1:A:108:LYS:O	1:A:243:GLN:NE2	2.44	0.42
1:A:460:LEU:O	1:A:464:ILE:HG13	2.19	0.42
1:B:210:PRO:C	1:B:211:ILE:HD12	2.45	0.42
1:A:83:ALA:HA	1:A:87:GLY:O	2.20	0.42
1:A:158:ILE:HG23	1:A:179:MET:HG3	2.02	0.42
1:A:201:LEU:CD2	1:A:209:LEU:HB3	2.50	0.41
1:B:66:VAL:O	1:B:385:MET:HA	2.20	0.41
1:B:100:GLN:NE2	1:B:259:ARG:NH1	2.63	0.41
1:B:437:ILE:CG2	1:B:438:LYS:N	2.83	0.41
1:A:174:PHE:CZ	1:A:177:GLU:HG3	2.55	0.41
1:A:388:SER:C	1:A:390:LEU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASP:OD1	1:B:239:ASP:C	2.62	0.41
1:B:337:LEU:O	1:B:338:ALA:CB	2.68	0.41
1:A:260:LEU:CD2	1:A:290:ILE:HG12	2.51	0.41
1:B:183:GLU:CD	1:B:183:GLU:N	2.71	0.41
1:A:59:ILE:HD12	1:A:270:VAL:HG11	2.03	0.41
1:A:105:ARG:HH11	1:A:109:LYS:CD	2.34	0.41
1:A:197:ALA:C	1:A:201:LEU:HD23	2.45	0.41
1:B:323:VAL:HG23	1:B:361:VAL:HG13	2.02	0.41
1:B:330:ILE:O	1:B:443:VAL:HG22	2.21	0.41
1:A:157:ILE:CG2	1:A:158:ILE:H	2.31	0.41
1:B:63:THR:HG23	1:B:86:GLY:HA3	2.01	0.41
1:B:185:LEU:O	1:B:187:VAL:HG23	2.20	0.41
1:A:218:LEU:HD13	1:A:220:ALA:N	2.36	0.41
4:A:701:MYD:H532	4:A:701:MYD:H381	2.02	0.41
1:A:183:GLU:CD	1:A:183:GLU:N	2.74	0.41
1:A:410:LYS:HB3	1:A:410:LYS:HE2	1.90	0.41
4:B:702:MYD:H532	4:B:702:MYD:H381	2.02	0.41
4:B:702:MYD:H532	4:B:702:MYD:C38	2.51	0.41
1:A:70:MET:C	1:A:72:THR:H	2.29	0.41
1:B:105:ARG:O	1:B:109:LYS:HG2	2.20	0.41
1:A:59:ILE:HG22	1:A:60:THR:N	2.36	0.40
1:A:283:GLN:OE1	1:A:302:GLY:HA3	2.21	0.40
1:B:401:PHE:O	1:B:402:PHE:C	2.65	0.40
1:A:213:ASN:CG	1:A:214:GLU:N	2.77	0.40
4:A:701:MYD:H532	4:A:701:MYD:C38	2.51	0.40
1:B:33:ASN:ND2	6:B:915:HOH:O	2.53	0.40
1:B:157:ILE:CG2	1:B:158:ILE:H	2.29	0.40
1:A:322:ARG:NH1	1:A:385:MET:SD	2.95	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	444/514 (86%)	348 (78%)	69 (16%)	27 (6%)	1	1
1	B	444/514 (86%)	349 (79%)	68 (15%)	27 (6%)	1	1
All	All	888/1028 (86%)	697 (78%)	137 (15%)	54 (6%)	1	1

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ALA
1	A	116	THR
1	A	160	SER
1	A	197	ALA
1	A	216	ASP
1	A	338	ALA
1	A	448	GLN
1	B	76	ALA
1	B	116	THR
1	B	160	SER
1	B	197	ALA
1	B	216	ASP
1	B	338	ALA
1	B	448	GLN
1	A	163	ILE
1	A	164	ASP
1	A	174	PHE
1	A	229	LYS
1	A	255	ASP
1	A	393	THR
1	B	164	ASP
1	B	174	PHE
1	B	229	LYS
1	B	255	ASP
1	B	393	THR
1	A	302	GLY
1	B	13	VAL
1	B	163	ILE
1	B	302	GLY
1	A	13	VAL
1	A	21	GLN
1	A	27	GLY
1	A	71	ASP
1	A	171	HIS
1	A	218	LEU

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Mol	Chain	Res	Type
1	B	27	GLY
1	B	71	ASP
1	B	173	CYS
1	B	218	LEU
1	A	95	CYS
1	A	161	ARG
1	A	178	ILE
1	B	95	CYS
1	B	161	ARG
1	B	171	HIS
1	B	178	ILE
1	B	213	ASN
1	A	14	PRO
1	A	213	ASN
1	B	21	GLN
1	B	451	GLY
1	A	158	ILE
1	A	451	GLY
1	B	158	ILE

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	370/420 (88%)	328 (89%)	42 (11%)	5	8
1	B	370/420 (88%)	332 (90%)	38 (10%)	7	10
All	All	740/840 (88%)	660 (89%)	80 (11%)	6	9

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	13	VAL
1	A	15	ASP
1	A	16	ASP

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Mol	Chain	Res	Type
1	A	30	LEU
1	A	38	LEU
1	A	42	ILE
1	A	63	THR
1	A	72	THR
1	A	106	LYS
1	A	112	GLN
1	A	157	ILE
1	A	165	PHE
1	A	175	LEU
1	A	176	GLU
1	A	177	GLU
1	A	179	MET
1	A	183	GLU
1	A	205	LYS
1	A	208	LYS
1	A	209	LEU
1	A	221	ILE
1	A	230	ASN
1	A	231	ARG
1	A	241	LYS
1	A	242	LYS
1	A	243	GLN
1	A	254	GLU
1	A	261	ASP
1	A	274	ASP
1	A	277	GLN
1	A	291	LYS
1	A	330	ILE
1	A	384	VAL
1	A	386	MET
1	A	393	THR
1	A	401	PHE
1	A	408	LEU
1	A	412	ARG
1	A	474	LYS
1	A	483	MET
1	A	491	GLU
1	B	11	SER
1	B	13	VAL
1	B	16	ASP
1	B	21	GLN

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Mol	Chain	Res	Type
1	B	25	ASN
1	B	30	LEU
1	B	42	ILE
1	B	63	THR
1	B	68	SER
1	B	106	LYS
1	B	112	GLN
1	B	157	ILE
1	B	165	PHE
1	B	175	LEU
1	B	176	GLU
1	B	177	GLU
1	B	179	MET
1	B	183	GLU
1	B	205	LYS
1	B	208	LYS
1	B	209	LEU
1	B	211	ILE
1	B	221	ILE
1	B	231	ARG
1	B	242	LYS
1	B	243	GLN
1	B	261	ASP
1	B	277	GLN
1	B	286	MET
1	B	322	ARG
1	B	330	ILE
1	B	393	THR
1	B	401	PHE
1	B	408	LEU
1	B	412	ARG
1	B	467	SER
1	B	488	LEU
1	B	491	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	25	ASN
1	A	48	GLN
1	A	92	HIS

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Mol	Chain	Res	Type
1	A	94	ASN
1	A	102	ASN
1	A	112	GLN
1	A	230	ASN
1	A	283	GLN
1	A	298	GLN
1	A	312	ASN
1	A	334	GLN
1	A	369	ASN
1	A	372	HIS
1	A	441	GLN
1	A	465	GLN
1	A	466	HIS
1	A	478	GLN
1	B	22	GLN
1	B	25	ASN
1	B	33	ASN
1	B	48	GLN
1	B	92	HIS
1	B	100	GLN
1	B	102	ASN
1	B	198	ASN
1	B	230	ASN
1	B	253	HIS
1	B	283	GLN
1	B	298	GLN
1	B	312	ASN
1	B	334	GLN
1	B	368	GLN
1	B	441	GLN
1	B	465	GLN
1	B	466	HIS
1	B	478	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic and 11 are unknown - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	RVP	B	601	-	22,22,22	3.21	5 (22%)	31,33,33	2.27	4 (12%)
4	MYD	A	701	-	43,47,47	2.12	12 (27%)	63,72,72	2.34	26 (41%)
4	MYD	B	702	-	43,47,47	2.06	12 (27%)	63,72,72	2.33	26 (41%)
3	RVP	A	600	-	22,22,22	3.17	5 (22%)	31,33,33	2.20	4 (12%)

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
3	RVP	B	601	-	-	1/14/30/30	0/2/2/2
4	MYD	A	701	-	-	2/25/50/50	0/5/5/5
4	MYD	B	702	-	-	2/25/50/50	0/5/5/5
3	RVP	A	600	-	-	2/14/30/30	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	RVP	N9-N4	-11.03	1.22	1.36
3	B	601	RVP	N9-N4	-10.99	1.22	1.36
3	B	601	RVP	C6-C5	7.44	1.54	1.49
3	A	600	RVP	C6-C5	6.80	1.54	1.49
4	A	701	MYD	O50-C42	5.76	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	MYD	C49-C48	5.60	1.56	1.50
4	B	702	MYD	P33-O44	5.00	1.68	1.56
4	B	702	MYD	O50-C42	4.95	1.42	1.36
4	B	702	MYD	C49-C48	4.91	1.55	1.50
3	A	600	RVP	P-O3P	4.65	1.64	1.50
4	A	701	MYD	P33-O44	4.25	1.66	1.56
3	B	601	RVP	P-O3P	4.12	1.63	1.50
4	B	702	MYD	C41-C42	-3.80	1.41	1.47
4	A	701	MYD	C41-C42	-3.75	1.41	1.47
4	B	702	MYD	C16-N20	-3.69	1.31	1.37
4	A	701	MYD	C16-N20	-3.63	1.31	1.37
4	A	701	MYD	P35-O45	3.60	1.65	1.56
4	A	701	MYD	C26-C27	3.56	1.62	1.53
4	B	702	MYD	P35-O45	3.46	1.64	1.56
3	B	601	RVP	O4'-C1'	3.32	1.49	1.42
4	B	702	MYD	C26-C27	3.30	1.61	1.53
3	A	600	RVP	O4'-C1'	3.00	1.48	1.42
4	A	701	MYD	O51-C46	2.73	1.43	1.38
4	B	702	MYD	C16-N15	2.60	1.36	1.31
4	A	701	MYD	O24-C23	2.55	1.47	1.42
4	A	701	MYD	C40-C39	2.54	1.43	1.40
4	B	702	MYD	O24-C23	2.40	1.47	1.42
3	A	600	RVP	C1'-N9	2.40	1.50	1.46
3	B	601	RVP	C1'-N9	2.38	1.50	1.46
4	B	702	MYD	O51-C46	2.38	1.42	1.38
4	A	701	MYD	O21-C22	2.34	1.48	1.43
4	B	702	MYD	C40-C39	2.32	1.43	1.40
4	B	702	MYD	O21-C22	2.31	1.48	1.43
4	A	701	MYD	C16-N15	2.17	1.35	1.31

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	RVP	N9-C8-N7	-10.23	105.39	110.53
3	A	600	RVP	N9-C8-N7	-9.98	105.52	110.53
4	B	702	MYD	N12-C17-N18	-5.90	119.66	128.58
4	A	701	MYD	N12-C17-N18	-5.72	119.92	128.58
4	B	702	MYD	C14-C19-N18	-5.47	119.19	126.72
4	A	701	MYD	C14-C19-N18	-5.30	119.41	126.72
4	A	701	MYD	C22-C26-C27	-4.84	93.26	102.61
4	A	701	MYD	O50-C49-C48	-4.74	100.81	104.57
4	B	702	MYD	C22-C26-C27	-4.62	93.68	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	702	MYD	O50-C49-C48	-4.54	100.97	104.57
3	B	601	RVP	C8-N9-N4	4.47	112.11	109.87
3	A	600	RVP	C8-N9-N4	4.30	112.02	109.87
4	B	702	MYD	C41-C48-C47	-4.27	118.96	122.68
4	A	701	MYD	C41-C48-C47	-4.25	118.99	122.68
4	A	701	MYD	C17-N18-C19	3.95	121.49	111.83
4	B	702	MYD	C17-N18-C19	3.90	121.35	111.83
4	A	701	MYD	N18-C19-N20	3.87	133.74	127.17
4	A	701	MYD	O32-C28-C27	3.80	121.94	108.99
4	B	702	MYD	O32-C28-C27	3.78	121.88	108.99
4	B	702	MYD	N18-C19-N20	3.71	133.48	127.17
4	B	702	MYD	C19-C14-N15	-3.59	106.48	110.58
4	A	701	MYD	O50-C42-C41	3.39	110.93	108.28
4	A	701	MYD	C19-C14-N15	-3.37	106.72	110.58
4	B	702	MYD	O50-C42-C41	3.31	110.87	108.28
4	A	701	MYD	C53-O51-C46	3.24	123.54	114.74
4	B	702	MYD	C53-O51-C46	3.13	123.25	114.74
4	B	702	MYD	O29-P33-C34	3.07	117.13	109.05
3	B	601	RVP	O2P-P-O1P	3.06	119.29	107.80
4	A	701	MYD	O29-P33-C34	3.03	117.03	109.05
3	A	600	RVP	O2P-P-O1P	2.96	118.90	107.80
4	A	701	MYD	C19-N20-C23	-2.96	119.72	126.63
4	A	701	MYD	C14-N15-C16	2.94	108.06	103.45
4	A	701	MYD	N20-C16-N15	-2.92	109.79	113.94
4	A	701	MYD	O43-C42-C41	-2.89	125.83	130.99
4	B	702	MYD	C19-N20-C23	-2.88	119.89	126.63
4	B	702	MYD	O43-C42-C41	-2.88	125.87	130.99
4	B	702	MYD	C14-N15-C16	2.87	107.96	103.45
4	B	702	MYD	N20-C16-N15	-2.83	109.92	113.94
4	B	702	MYD	C40-C41-C42	2.78	133.09	129.35
4	A	701	MYD	C40-C41-C42	2.72	133.02	129.35
4	B	702	MYD	O25-C26-C27	-2.69	103.36	111.08
4	A	701	MYD	C19-N20-C16	2.66	108.53	105.74
4	A	701	MYD	O25-C26-C27	-2.62	103.54	111.08
4	A	701	MYD	O45-P35-C34	2.60	117.51	106.73
4	B	702	MYD	O45-P35-C34	2.46	116.93	106.73
4	B	702	MYD	C19-N20-C16	2.42	108.28	105.74
4	A	701	MYD	P35-O36-C37	-2.40	114.81	122.28
4	B	702	MYD	P35-O36-C37	-2.37	114.91	122.28
3	A	600	RVP	C6-C5-N4	2.34	124.01	121.98
4	A	701	MYD	O44-P33-C34	2.26	116.10	106.73
3	B	601	RVP	C6-C5-N4	2.21	123.89	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	MYD	C49-C48-C41	2.20	110.72	107.90
4	A	701	MYD	O24-C27-C26	2.16	109.44	105.15
4	B	702	MYD	O44-P33-O29	-2.11	103.09	109.95
4	B	702	MYD	C49-C48-C41	2.09	110.59	107.90
4	B	702	MYD	O50-C42-O43	2.06	123.27	121.09
4	B	702	MYD	O44-P33-C34	2.06	115.24	106.73
4	A	701	MYD	O44-P33-O29	-2.04	103.32	109.95
4	A	701	MYD	O50-C42-O43	2.03	123.23	121.09
4	B	702	MYD	O24-C27-C26	2.02	109.16	105.15

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	RVP	C2'-C1'-N9-N4
3	B	601	RVP	C2'-C1'-N9-N4
4	A	701	MYD	C39-C46-O51-C53
4	B	702	MYD	C39-C46-O51-C53
4	A	701	MYD	P33-C34-P35-O30
4	B	702	MYD	P33-C34-P35-O30
3	A	600	RVP	C2'-C1'-N9-C8

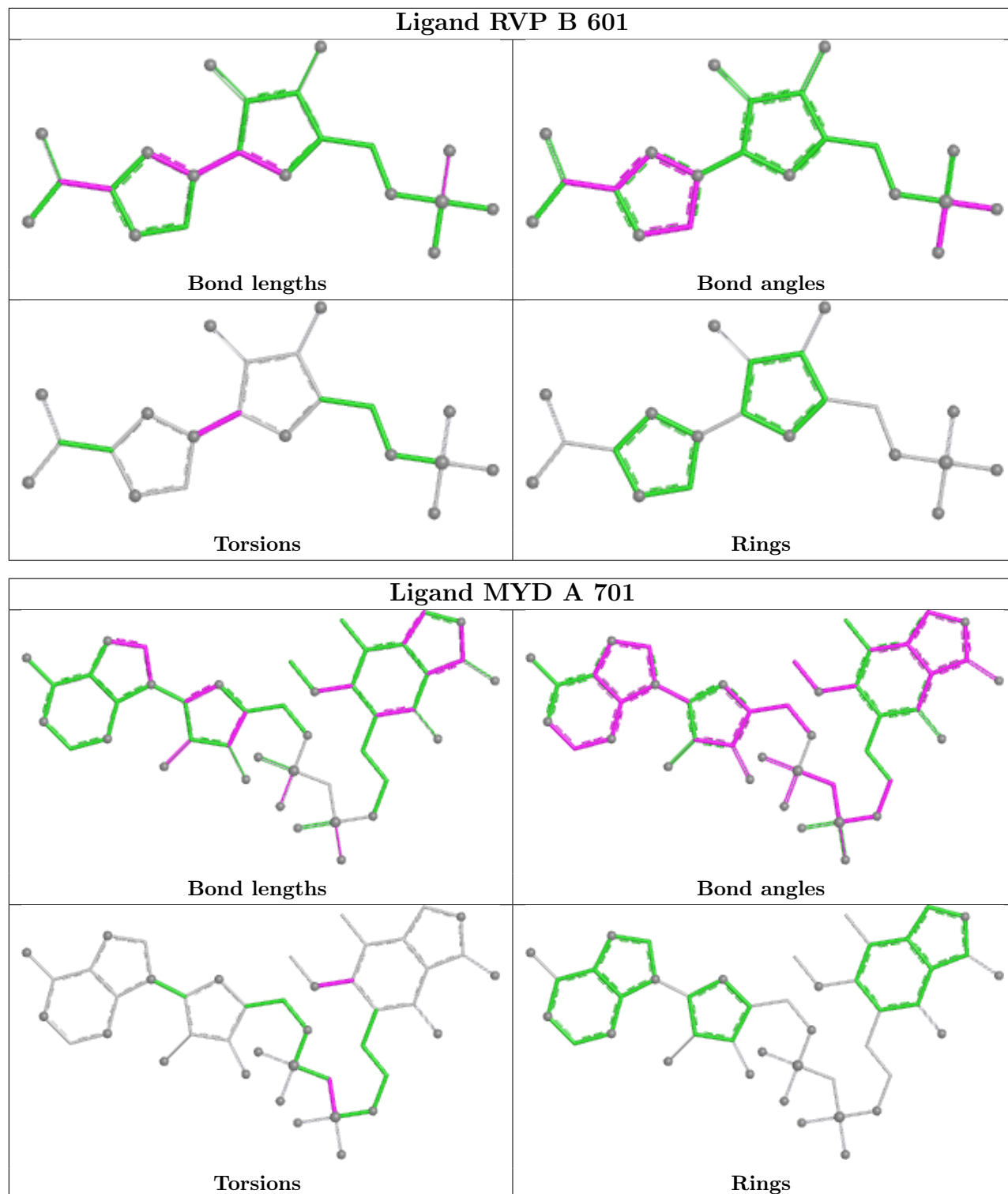
There are no ring outliers.

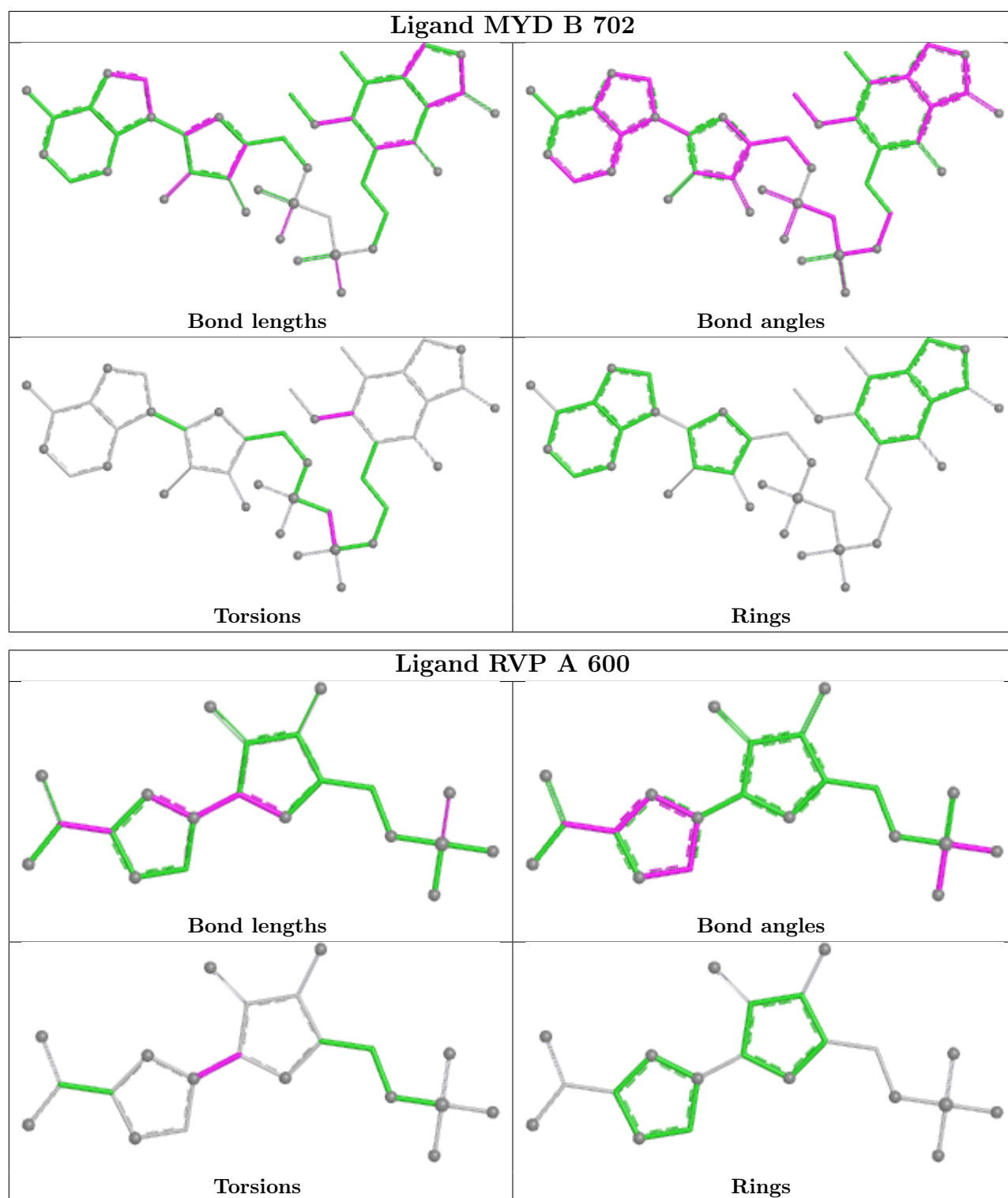
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	RVP	1	0
4	A	701	MYD	4	0
4	B	702	MYD	5	0
3	A	600	RVP	1	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	454/514 (88%)	-1.17	0 100 100	12, 41, 116, 140	0
1	B	454/514 (88%)	-1.20	0 100 100	10, 41, 110, 143	0
All	All	908/1028 (88%)	-1.18	0 100 100	10, 41, 114, 143	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

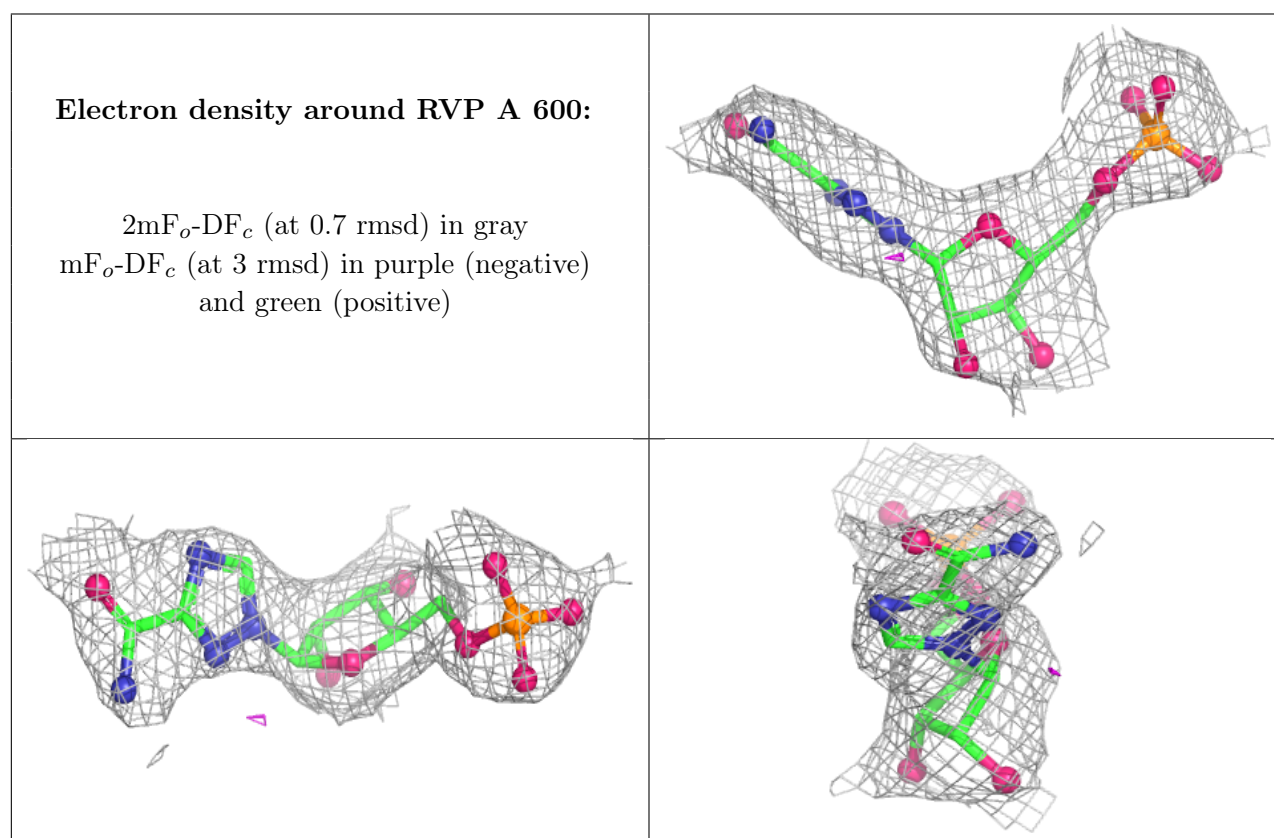
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	UNL	B	806	1/-	0.93	0.10	20,20,20,20	0
5	UNL	B	803	1/-	0.97	0.05	20,20,20,20	0
5	UNL	B	801	1/-	0.98	0.06	20,20,20,20	0
5	UNL	B	804	1/-	0.98	0.05	20,20,20,20	0
5	UNL	B	802	1/-	0.98	0.06	20,20,20,20	0
5	UNL	B	807	1/-	0.98	0.12	20,20,20,20	0
5	UNL	B	809	1/-	0.98	0.04	20,20,20,20	0

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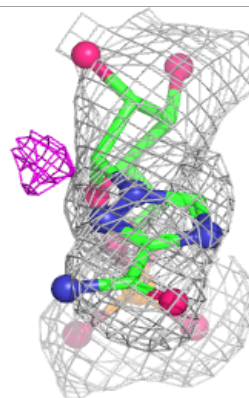
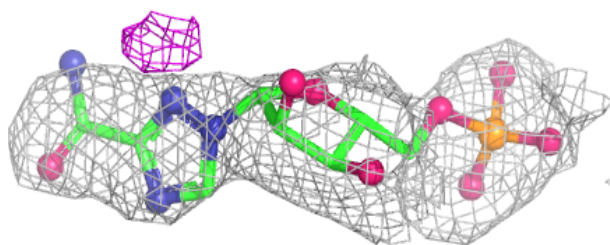
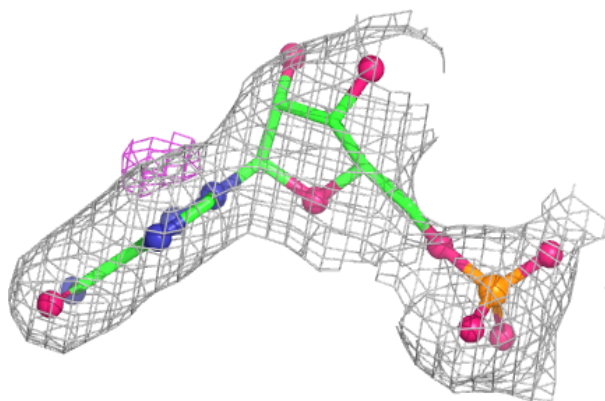
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	K	B	901	1/1	0.99	0.16	106,106,106,106	0
3	RVP	A	600	21/21	0.99	0.03	53,53,53,53	0
3	RVP	B	601	21/21	0.99	0.05	56,56,56,56	0
5	UNL	B	805	1/-	0.99	0.09	20,20,20,20	0
4	MYD	A	701	43/43	0.99	0.04	58,58,58,58	0
4	MYD	B	702	43/43	0.99	0.05	60,60,60,60	0
5	UNL	B	808	1/-	0.99	0.05	20,20,20,20	0
2	K	A	902	1/1	0.99	0.12	100,100,100,100	0
5	UNL	B	810	1/-	0.99	0.11	20,20,20,20	0
5	UNL	B	811	1/-	1.00	0.10	20,20,20,20	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.

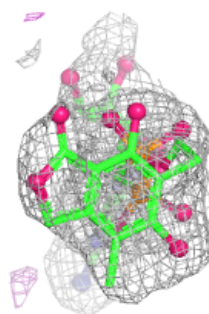
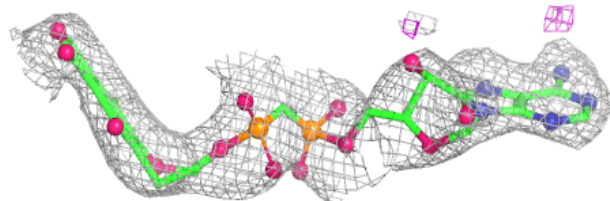
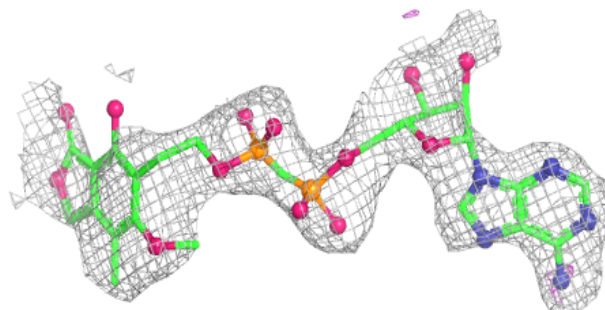


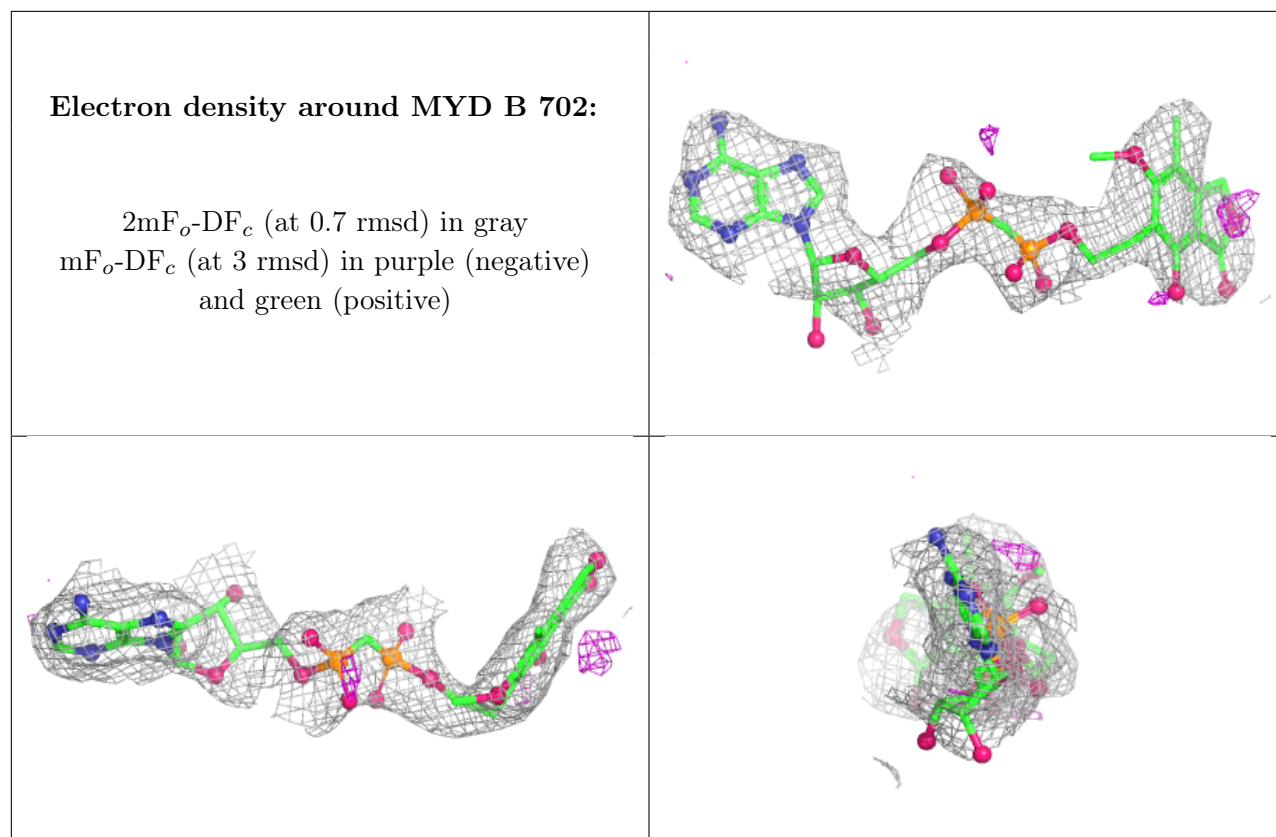
Electron density around RVP B 601:

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

**Electron density around MYD A 701:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.