



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:08 AM UTC

PDB ID : 1B3O / pdb_00001b3o
Title : TERNARY COMPLEX OF HUMAN TYPE-II INOSINE MONOPHOSPHATE DEHYDROGENASE WITH 6-CL-IMP AND SELENAZOLE ADENINE DINUCLEOTIDE
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Deposited on : 1998-12-14
Resolution : 2.90 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

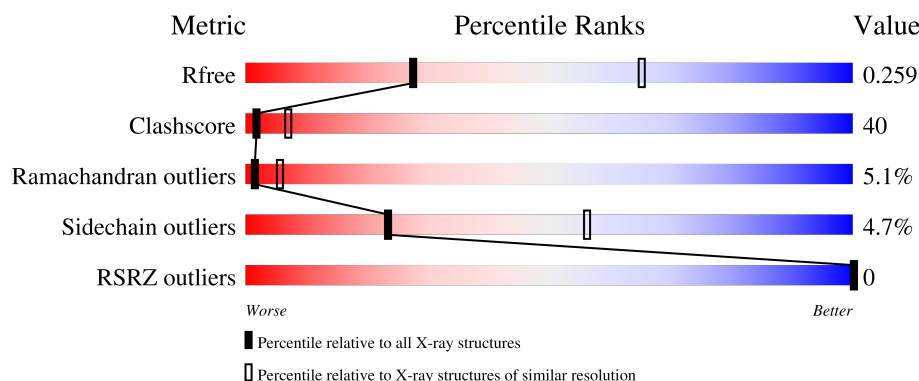
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

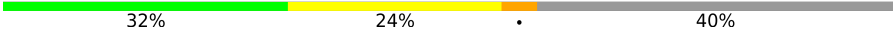
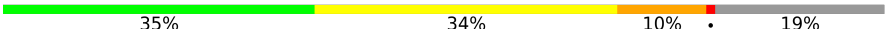
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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](#)

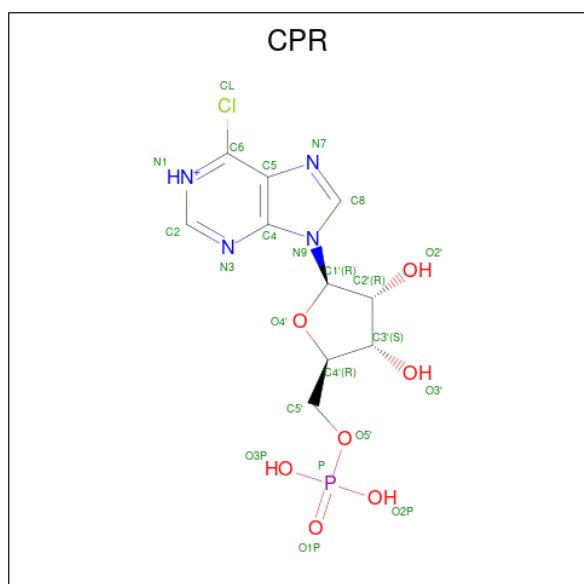
There are 5 unique types of molecules in this entry. The entry contains 5536 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (INOSINE MONOPHOSPHATE DEHYDROGENASE 2).

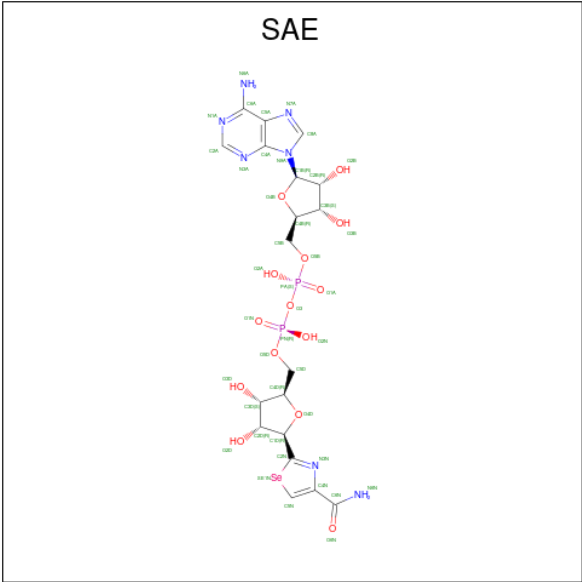
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	3
			2275	1434	389	439	13			
1	B	414	Total	C	N	O	S	0	0	4
			3085	1941	535	591	18			

- Molecule 2 is 6-CHLOROPURINE RIBOSIDE, 5'-MONOPHOSPHATE (CCD ID: CPR) (formula: $C_{10}H_{13}ClN_4O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	4	7	1		

- Molecule 3 is SELENAZOLE-4-CARBOXYAMIDE-ADENINE DINUCLEOTIDE (CCD ID: SAE) (formula: $C_{19}H_{25}N_7O_{14}P_2Se$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	Se	0	0
			43	19	7	14	2	1		
3	B	1	Total	C	N	O	P	Se	0	0
			43	19	7	14	2	1		

- Molecule 4 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	15	Total	X	15	0
			15	15		

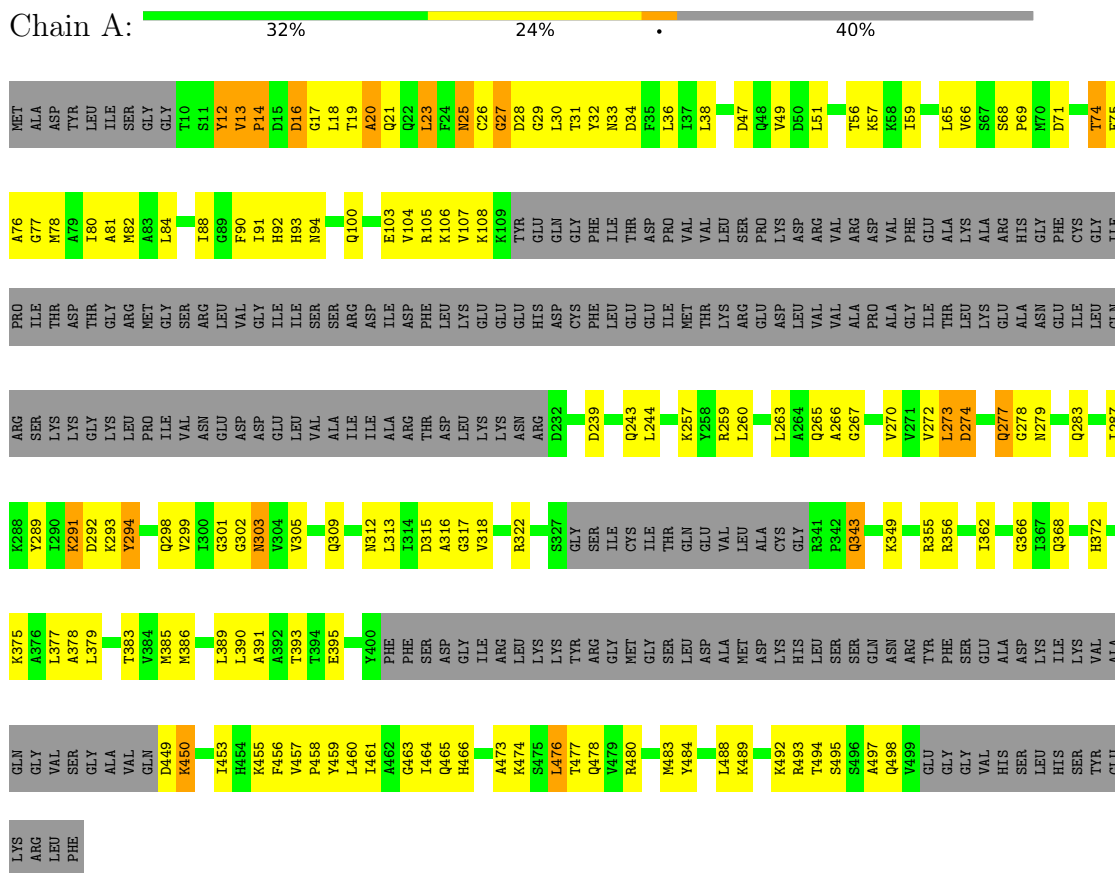
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	20	Total	O	0	0
			20	20		

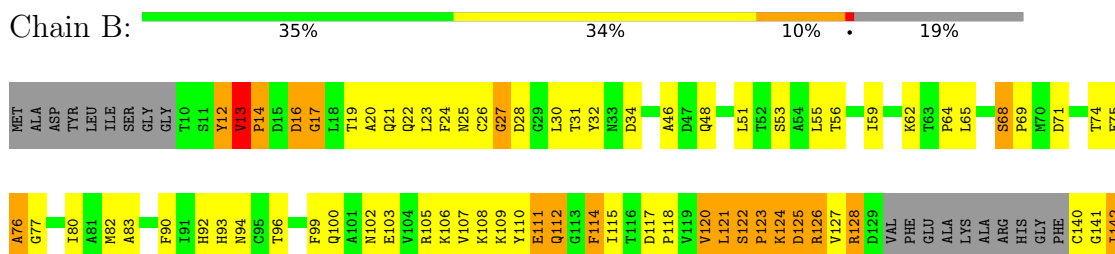
3 Residue-property plots

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: PROTEIN (INOSINE MONOPHOSPHATE DEHYDROGENASE 2)



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A497	ASP	K349	W271	R203	P143
Q498	LYS	V350	V272	S204	I144
V499	HIS	S351	L273	K205	T145
GLU	LEU	E352	D274	K206	D146
GLY	SER			G207	T147
GLY	SER	R355	Q277	K208	G148
VAL	GLN	R356		L209	R149
HIS	ASN		S280	P210	M150
SER	ARG	A363	I281	I211	G151
LEU	TYR	D364	Q282	V212	S152
HIS	PHE		Q283	N213	R153
SER	SER	Q368	I284	E214	L154
GLY	SER		N285	D215	V155
TYR	GLU	H372	K286	D216	G156
GLU	ALA	I373	I287	E217	V157
LYS	ASP	A374		L218	I158
ARG	LYS	K375	K291	V219	S159
LEU	ILE	A376	D292	A220	SER
PHE	VAL	L377	K293	I221	ARG
	VAL	A378	Y294	I222	ASP
	GLN	L379	P295	A223	ILE
	GLY			R224	ASP
	VAL	T383	Q298	T225	PHE
	SER	V384	V299	D226	LEU
	GLY	K385	I300	L227	LYS
	ALA	N386	G301	K228	GLU
	VAL	G387	G302	K229	GLU
	GLN	S388	N303	N230	GLU
		L389	V304	R231	HIS
		L390	V305	D232	ASP
		K450	T306	Y233	CYS
				P234	PHE
		I453	Q309	L235	LEU
		H454	L313	A236	GLU
		K455		S237	
		F456	A316	K238	I178
		V457	G317	D239	R179
		P458	V318		T180
		Y459	D319	K242	K181
		L460	A320	Q243	R182
		I461	L321	G246	E183
			R322	G247	D184
		I464		C246	L185
		Q465		A248	V186
			G328	A249	V187
		I471	S329		A188
		G472	I330	H253	P189
		A473	C331		A190
			I332	D256	G191
		L476	T333		I192
		T477	Q334	R259	T193
		Q478	E335	L260	L194
			V336	D261	K195
		M483	L337	L262	E196
			A338	L263	A197
		L488		A264	N198
				Q265	E199
		R493		D269	I200
		T494			L201
		S495			Q202
		S496		V270	

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	142.26Å 142.26Å 174.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.90 100.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	86.4 (100.00-2.90) 86.4 (100.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.85Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.244 , 0.270 0.233 , 0.259	Depositor DCC
R_{free} test set	3253 reflections (9.62%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 19.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for -h,k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5536	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: CPR, UNX, SAE

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	0.64	0/2308	1.14	15/3122 (0.5%)
1	B	0.76	4/3125 (0.1%)	1.23	31/4224 (0.7%)
All	All	0.71	4/5433 (0.1%)	1.20	46/7346 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	MET	SD-CE	6.97	1.97	1.79
1	B	336	VAL	CA-CB	5.41	1.59	1.53
1	B	128	ARG	C-N	-5.26	1.25	1.33
1	B	399	GLU	C-N	-5.01	1.26	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	THR	N-CA-C	9.60	124.17	108.52
1	B	301	GLY	N-CA-C	9.06	121.96	111.36
1	B	111	GLU	N-CA-C	-8.90	98.77	110.43
1	B	23	LEU	N-CA-C	8.54	120.67	111.36
1	A	343	GLN	N-CA-C	8.47	121.28	111.11
1	A	303	ASN	N-CA-C	8.44	122.95	110.30
1	B	181	LYS	N-CA-C	8.20	128.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	ALA	N-CA-C	-7.92	102.63	111.82
1	B	152	SER	N-CA-C	7.57	121.59	109.86
1	B	16	ASP	N-CA-C	7.35	122.30	109.80
1	B	343	GLN	N-CA-C	7.32	119.95	111.02
1	A	274	ASP	N-CA-C	7.13	121.35	108.17
1	A	316	ALA	N-CA-C	-6.93	103.93	112.38
1	B	122	SER	CA-C-N	6.65	128.15	119.84
1	B	122	SER	C-N-CA	6.65	128.15	119.84
1	A	74	THR	N-CA-C	6.60	119.70	109.07
1	B	68	SER	N-CA-C	6.47	119.22	110.29
1	B	364	ASP	N-CA-C	6.46	119.42	107.99
1	B	457	VAL	CB-CA-C	-6.46	107.57	113.70
1	A	68	SER	N-CA-C	6.38	119.09	110.29
1	B	156	GLY	N-CA-C	6.31	120.22	110.88
1	B	65	LEU	N-CA-C	6.29	118.95	108.20
1	B	259	ARG	N-CA-C	-6.21	104.42	111.07
1	B	225	THR	N-CA-C	6.16	120.40	113.01
1	A	294	TYR	CA-C-N	6.11	126.00	119.28
1	A	294	TYR	C-N-CA	6.11	126.00	119.28
1	B	142	ILE	CA-C-N	6.09	126.43	119.92
1	B	142	ILE	C-N-CA	6.09	126.43	119.92
1	B	331	CYS	N-CA-C	6.03	121.15	113.55
1	B	303	ASN	N-CA-C	5.96	118.90	109.96
1	B	229	LYS	N-CA-C	5.92	123.41	110.80
1	A	301	GLY	N-CA-C	5.77	119.39	111.54
1	A	476	LEU	N-CA-C	-5.69	105.06	112.23
1	B	208	LYS	N-CA-C	5.40	117.87	107.44
1	B	233	TYR	CA-C-N	5.38	125.05	119.56
1	B	233	TYR	C-N-CA	5.38	125.05	119.56
1	B	228	LYS	N-CA-C	5.38	122.26	110.80
1	A	25	ASN	N-CA-C	-5.34	104.75	113.19
1	A	299	VAL	N-CA-C	5.24	115.51	108.17
1	A	65	LEU	N-CA-C	5.13	117.92	109.76
1	B	349	LYS	N-CA-C	5.13	116.68	111.14
1	B	184	ASP	CA-C-N	5.10	128.59	121.24
1	B	184	ASP	C-N-CA	5.10	128.59	121.24
1	B	12	TYR	N-CA-C	5.06	119.92	113.55
1	A	29	GLY	N-CA-C	-5.05	101.21	113.18
1	A	23	LEU	N-CA-C	5.03	118.57	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Sidechain

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	2275	0	2294	140	0
1	B	3085	0	3161	299	0
2	A	22	0	11	1	0
2	B	22	0	11	2	0
3	A	43	0	23	5	0
3	B	43	0	23	4	0
4	B	15	0	0	0	0
5	A	11	0	0	0	0
5	B	20	0	0	0	0
All	All	5536	0	5523	442	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 40.

All (442) 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:105:ARG:HH12	1:B:109:LYS:HG2	1.18	1.06
1:B:386:MET:HE3	1:B:389:LEU:HD23	1.39	1.02
1:B:181:LYS:HE2	1:B:181:LYS:H	1.20	1.01
1:B:224:ARG:HB3	1:B:227:LEU:HD11	1.46	0.97
1:B:227:LEU:HD13	1:B:228:LYS:N	1.80	0.96
1:B:198:ASN:HA	1:B:201:LEU:HD12	1.44	0.95
1:B:122:SER:N	1:B:148:GLY:HA2	1.81	0.94
1:B:270:VAL:HG12	1:B:298:GLN:HB2	1.49	0.94
1:A:277:GLN:C	1:A:277:GLN:HE21	1.75	0.94
1:B:201:LEU:HD22	1:B:206:LYS:HA	1.52	0.92
1:B:207:GLY:O	1:B:223:ALA:HA	1.70	0.90
1:A:270:VAL:HG12	1:A:298:GLN:HB2	1.54	0.90
1:B:203:ARG:HH21	1:B:205:LYS:HB2	1.39	0.88
1:B:212:VAL:HG11	1:B:216:ASP:HA	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:GLN:HE21	1:B:343:GLN:HA	1.40	0.87
1:B:277:GLN:HE21	1:B:277:GLN:C	1.82	0.86
1:B:204:SER:C	1:B:206:LYS:H	1.83	0.86
1:B:239:ASP:OD2	1:B:243:GLN:HB2	1.75	0.86
1:B:198:ASN:O	1:B:201:LEU:HB2	1.76	0.85
1:B:203:ARG:NE	1:B:205:LYS:H	1.74	0.85
1:B:224:ARG:HB3	1:B:227:LEU:CD1	2.07	0.84
1:B:291:LYS:HE2	1:B:291:LYS:HA	1.60	0.83
1:B:368:GLN:H	1:B:372:HIS:HD2	1.26	0.81
1:B:75:GLU:OE2	1:B:92:HIS:HE1	1.63	0.81
1:A:368:GLN:H	1:A:372:HIS:HD2	1.26	0.81
1:B:330:ILE:HG23	1:B:335:GLU:HB2	1.62	0.81
1:B:198:ASN:HB3	1:B:224:ARG:HH12	1.46	0.80
1:A:283:GLN:HE22	1:A:302:GLY:HA3	1.46	0.80
1:A:473:ALA:HA	1:A:478:GLN:NE2	1.97	0.79
1:A:239:ASP:OD2	1:A:243:GLN:HB2	1.83	0.79
1:B:92:HIS:HD2	1:B:94:ASN:HB3	1.45	0.79
1:B:203:ARG:HD2	1:B:204:SER:N	1.97	0.79
1:B:114:PHE:O	1:B:115:ILE:HD13	1.83	0.78
1:B:330:ILE:HG12	1:B:335:GLU:HG2	1.65	0.78
1:B:483:MET:HB3	1:B:488:LEU:HD23	1.63	0.78
1:A:16:ASP:HB2	1:A:489:LYS:HG3	1.65	0.78
1:B:153:ARG:HA	1:B:216:ASP:O	1.83	0.78
1:A:493:ARG:HE	1:A:498:GLN:HG2	1.48	0.78
1:B:204:SER:O	1:B:206:LYS:N	2.16	0.78
1:B:207:GLY:O	1:B:208:LYS:HD2	1.84	0.77
1:B:111:GLU:O	1:B:112:GLN:HG2	1.84	0.77
1:B:181:LYS:H	1:B:181:LYS:CE	1.98	0.77
1:B:203:ARG:HD2	1:B:203:ARG:C	2.09	0.76
1:B:213:ASN:OD1	1:B:217:GLU:HB2	1.85	0.76
1:B:144:ILE:HG12	1:B:156:GLY:CA	2.16	0.76
1:B:181:LYS:HE2	1:B:181:LYS:N	2.00	0.76
1:A:31:THR:HG22	1:A:32:TYR:N	2.01	0.75
1:B:12:TYR:CE2	1:B:14:PRO:HA	2.22	0.75
1:A:291:LYS:HA	1:A:291:LYS:HE2	1.69	0.74
1:B:227:LEU:HD13	1:B:227:LEU:C	2.12	0.74
1:B:144:ILE:HD11	1:B:179:MET:SD	2.28	0.74
1:B:203:ARG:NH1	1:B:204:SER:HB3	2.04	0.73
1:B:204:SER:O	1:B:206:LYS:HG3	1.88	0.73
1:B:261:ASP:O	1:B:265:GLN:HG3	1.87	0.73
1:A:473:ALA:HA	1:A:478:GLN:HE21	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:HH12	1:B:109:LYS:CG	2.00	0.73
1:B:115:ILE:HG22	1:B:118:PRO:HD3	1.70	0.72
1:B:31:THR:HG22	1:B:32:TYR:N	2.03	0.72
1:B:207:GLY:HA2	1:B:224:ARG:H	1.54	0.72
1:B:283:GLN:HE22	1:B:302:GLY:HA3	1.54	0.72
1:A:92:HIS:HD2	1:A:94:ASN:HB3	1.54	0.72
1:A:16:ASP:CB	1:A:489:LYS:HG3	2.20	0.72
1:B:82:MET:HE1	1:B:453:ILE:HD12	1.72	0.72
1:B:471:ILE:HD12	1:B:488:LEU:HD13	1.71	0.71
1:A:26:CYS:HB3	1:A:28:ASP:OD2	1.89	0.71
1:B:206:LYS:C	1:B:206:LYS:HD2	2.16	0.71
1:B:337:LEU:O	1:B:338:ALA:HB2	1.89	0.70
1:B:150:MET:CE	1:B:220:ALA:HA	2.21	0.70
1:A:277:GLN:HE22	1:A:279:ASN:N	1.89	0.70
1:B:155:VAL:HG12	1:B:155:VAL:O	1.92	0.70
1:A:277:GLN:HE22	1:A:279:ASN:H	1.39	0.69
1:B:157:ILE:O	1:B:158:ILE:HG23	1.91	0.69
1:B:197:ALA:O	1:B:201:LEU:HG	1.92	0.69
1:B:105:ARG:NH1	1:B:109:LYS:HG2	2.02	0.69
1:B:120:VAL:HG11	1:B:150:MET:HB2	1.74	0.69
1:A:31:THR:HG22	1:A:33:ASN:H	1.56	0.69
1:A:270:VAL:CG1	1:A:298:GLN:HB2	2.22	0.69
1:A:283:GLN:O	1:A:287:ILE:HG12	1.93	0.69
1:A:386:MET:CE	1:A:389:LEU:HD23	2.23	0.69
1:B:198:ASN:CB	1:B:224:ARG:HH12	2.05	0.69
1:B:193:THR:HG23	1:B:196:GLU:H	1.58	0.69
1:B:157:ILE:HG22	1:B:158:ILE:N	2.08	0.68
1:B:203:ARG:HG3	1:B:204:SER:H	1.57	0.68
1:B:305:VAL:H	1:B:309:GLN:NE2	1.92	0.68
1:B:283:GLN:O	1:B:287:ILE:HG12	1.94	0.68
1:B:331:CYS:O	1:B:332:ILE:HB	1.92	0.68
1:B:494:THR:O	1:B:497:ALA:HB3	1.93	0.67
1:A:75:GLU:O	1:A:77:GLY:N	2.27	0.67
1:A:456:PHE:O	1:A:459:TYR:HB3	1.95	0.67
1:A:483:MET:HB3	1:A:488:LEU:HD23	1.78	0.66
1:B:120:VAL:HG21	1:B:150:MET:N	2.11	0.66
1:B:333:THR:O	1:B:334:GLN:HB3	1.95	0.66
1:B:211:ILE:O	1:B:218:LEU:HD12	1.95	0.66
1:B:203:ARG:NH2	1:B:205:LYS:HB2	2.09	0.66
1:B:473:ALA:HA	1:B:478:GLN:NE2	2.11	0.66
1:B:204:SER:C	1:B:206:LYS:N	2.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ALA:O	1:B:483:MET:HG2	1.95	0.66
1:A:31:THR:CG2	1:A:32:TYR:N	2.60	0.65
1:A:51:LEU:HD12	1:A:461:ILE:HG23	1.77	0.65
1:B:227:LEU:O	1:B:227:LEU:HD22	1.97	0.65
1:B:225:THR:HG22	1:B:225:THR:O	1.97	0.65
1:B:16:ASP:O	1:B:17:GLY:O	2.13	0.65
1:B:121:LEU:C	1:B:148:GLY:HA2	2.21	0.65
1:B:144:ILE:HG13	1:B:144:ILE:O	1.97	0.65
1:B:112:GLN:OE1	1:B:243:GLN:HG2	1.96	0.65
1:B:333:THR:O	1:B:333:THR:HG22	1.97	0.65
1:A:305:VAL:H	1:A:309:GLN:NE2	1.95	0.64
1:B:121:LEU:HA	1:B:148:GLY:O	1.97	0.64
1:A:104:VAL:O	1:A:108:LYS:HG2	1.98	0.64
1:A:494:THR:N	1:A:497:ALA:HB3	2.12	0.63
1:A:305:VAL:H	1:A:309:GLN:HE22	1.46	0.63
1:A:449:ASP:O	1:A:450:LYS:O	2.15	0.63
1:B:12:TYR:HE2	1:B:14:PRO:HA	1.62	0.63
1:B:303:ASN:OD1	1:B:322:ARG:HD3	1.99	0.63
1:B:203:ARG:CD	1:B:204:SER:N	2.62	0.63
1:A:303:ASN:CG	3:A:600:SAE:H62N	2.08	0.62
1:B:75:GLU:O	1:B:77:GLY:N	2.32	0.62
1:B:69:PRO:HG3	1:B:90:PHE:HB2	1.82	0.62
1:B:150:MET:HE1	1:B:220:ALA:HA	1.80	0.62
1:B:239:ASP:CG	1:B:243:GLN:HB2	2.25	0.62
1:B:471:ILE:HD12	1:B:488:LEU:CD1	2.29	0.62
1:B:203:ARG:CG	1:B:204:SER:N	2.62	0.61
1:B:12:TYR:C	1:B:13:VAL:HG13	2.25	0.61
1:B:51:LEU:HD12	1:B:461:ILE:HG23	1.80	0.61
1:B:238:LYS:HA	1:B:243:GLN:O	2.00	0.61
1:B:64:PRO:HA	1:B:383:THR:HG22	1.82	0.61
1:B:277:GLN:C	1:B:277:GLN:NE2	2.57	0.61
1:B:457:VAL:O	1:B:461:ILE:HG13	2.00	0.61
1:B:142:ILE:N	1:B:142:ILE:HD12	2.16	0.60
1:A:69:PRO:HG3	1:A:90:PHE:HB2	1.82	0.60
1:B:201:LEU:CD2	1:B:206:LYS:HA	2.29	0.60
1:A:395:GLU:CD	1:A:395:GLU:H	2.08	0.60
1:B:100:GLN:HG2	1:B:263:LEU:HD21	1.82	0.60
1:B:203:ARG:HD2	1:B:204:SER:HB3	1.83	0.60
1:B:212:VAL:CG1	1:B:216:ASP:HA	2.31	0.60
1:B:144:ILE:HG12	1:B:156:GLY:HA3	1.82	0.60
1:B:12:TYR:O	1:B:13:VAL:O	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:THR:HG22	1:B:32:TYR:H	1.66	0.60
1:B:337:LEU:O	1:B:338:ALA:CB	2.48	0.60
1:B:75:GLU:OE2	1:B:92:HIS:CE1	2.52	0.59
1:B:395:GLU:N	1:B:395:GLU:OE1	2.35	0.59
1:A:25:ASN:OD1	1:A:349:LYS:HE2	2.03	0.59
1:B:22:GLN:O	1:B:26:CYS:SG	2.60	0.59
1:A:277:GLN:C	1:A:277:GLN:NE2	2.56	0.58
1:B:55:LEU:HG	1:B:56:THR:HG23	1.83	0.58
1:A:74:THR:O	1:A:75:GLU:HG3	2.04	0.58
1:B:270:VAL:CG1	1:B:298:GLN:HB2	2.29	0.58
1:A:368:GLN:H	1:A:372:HIS:CD2	2.15	0.58
1:A:378:ALA:O	1:A:483:MET:HG2	2.04	0.58
1:B:460:LEU:O	1:B:464:ILE:HG13	2.04	0.57
1:A:377:LEU:HD13	1:A:476:LEU:HD13	1.86	0.57
1:B:292:ASP:O	1:B:295:PRO:HD3	2.03	0.57
1:B:118:PRO:HD2	1:B:150:MET:SD	2.44	0.57
1:B:368:GLN:H	1:B:372:HIS:CD2	2.15	0.57
1:A:31:THR:CG2	1:A:32:TYR:H	2.18	0.56
1:B:26:CYS:O	1:B:27:GLY:C	2.47	0.56
1:A:19:THR:O	1:A:20:ALA:C	2.47	0.56
1:A:75:GLU:HA	1:A:91:ILE:HD12	1.87	0.56
1:A:366:GLY:O	1:A:368:GLN:HG3	2.05	0.56
1:B:31:THR:CG2	1:B:32:TYR:N	2.69	0.56
1:A:493:ARG:NE	1:A:498:GLN:HG2	2.19	0.56
1:B:182:ARG:O	1:B:182:ARG:HD3	2.05	0.56
1:A:100:GLN:HG2	1:A:263:LEU:HD21	1.88	0.56
1:B:198:ASN:CA	1:B:224:ARG:HH12	2.18	0.56
1:B:157:ILE:CG2	1:B:158:ILE:N	2.68	0.56
1:A:477:THR:HA	1:A:480:ARG:NH1	2.21	0.56
1:B:62:LYS:HB3	1:B:235:LEU:HD22	1.88	0.56
1:B:193:THR:HG22	1:B:196:GLU:CD	2.31	0.56
1:A:33:ASN:OD1	1:A:372:HIS:HE1	1.89	0.56
1:A:277:GLN:NE2	1:A:279:ASN:H	2.02	0.55
1:B:103:GLU:OE1	1:B:106:LYS:HE3	2.07	0.55
1:A:303:ASN:ND2	3:A:600:SAE:H62N	2.03	0.55
1:B:144:ILE:O	1:B:144:ILE:CG1	2.54	0.55
1:A:273:LEU:HD11	1:A:287:ILE:HD13	1.88	0.55
1:B:82:MET:HE1	1:B:453:ILE:CD1	2.35	0.55
1:A:270:VAL:HG12	1:A:298:GLN:CB	2.32	0.55
1:B:291:LYS:HA	1:B:291:LYS:CE	2.34	0.55
1:B:333:THR:O	1:B:334:GLN:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:VAL:HG13	1:A:272:VAL:O	2.07	0.55
1:B:291:LYS:HE2	1:B:291:LYS:CA	2.35	0.55
1:B:125:ASP:O	1:B:126:ARG:HD2	2.06	0.54
1:A:12:TYR:O	1:A:13:VAL:O	2.26	0.54
1:A:26:CYS:O	1:A:28:ASP:N	2.40	0.54
1:B:144:ILE:CD1	1:B:156:GLY:HA3	2.36	0.54
1:B:199:GLU:O	1:B:202:GLN:N	2.32	0.54
1:B:212:VAL:CG1	1:B:215:ASP:O	2.55	0.54
1:A:395:GLU:CD	1:A:395:GLU:N	2.64	0.54
1:B:92:HIS:CD2	1:B:94:ASN:HB3	2.35	0.54
1:B:108:LYS:HB3	1:B:243:GLN:NE2	2.23	0.54
1:B:13:VAL:O	1:B:13:VAL:HG22	2.06	0.54
1:A:390:LEU:O	1:A:393:THR:HG23	2.08	0.54
1:B:25:ASN:OD1	1:B:349:LYS:HE2	2.08	0.54
1:B:227:LEU:C	1:B:227:LEU:HD22	2.33	0.54
1:B:456:PHE:O	1:B:459:TYR:HB3	2.08	0.53
1:A:257:LYS:O	1:A:260:LEU:HB3	2.07	0.53
1:B:154:LEU:HD12	1:B:218:LEU:HD13	1.91	0.53
1:B:26:CYS:O	1:B:28:ASP:N	2.41	0.53
1:B:190:ALA:HB2	1:B:219:VAL:HG11	1.90	0.53
1:A:313:LEU:O	1:A:318:VAL:HG13	2.09	0.53
1:A:80:ILE:HG13	1:A:107:VAL:HG22	1.91	0.53
1:B:122:SER:OG	1:B:148:GLY:N	2.41	0.53
1:B:203:ARG:HG3	1:B:204:SER:N	2.20	0.53
1:A:74:THR:HG22	1:A:91:ILE:HD13	1.90	0.53
1:B:330:ILE:HG12	1:B:335:GLU:CG	2.36	0.53
1:A:36:LEU:HG	1:A:493:ARG:HD3	1.91	0.52
1:A:265:GLN:C	1:A:267:GLY:H	2.16	0.52
1:A:493:ARG:HH21	1:A:498:GLN:HG2	1.74	0.52
1:A:455:LYS:C	1:A:458:PRO:HD2	2.33	0.52
1:B:203:ARG:HD2	1:B:204:SER:CB	2.40	0.52
1:B:207:GLY:H	1:B:224:ARG:HB2	1.75	0.52
1:B:343:GLN:HA	1:B:343:GLN:NE2	2.19	0.52
1:A:277:GLN:HE21	1:A:278:GLY:N	2.08	0.52
1:B:145:THR:OG1	1:B:146:ASP:N	2.43	0.52
1:B:328:GLY:HA2	2:B:631:CPR:O1P	2.09	0.52
1:A:93:HIS:HB3	1:A:100:GLN:HE22	1.75	0.52
1:A:343:GLN:NE2	1:A:343:GLN:HA	2.24	0.52
1:A:26:CYS:O	1:A:27:GLY:C	2.54	0.51
1:B:334:GLN:O	1:B:335:GLU:HB2	2.08	0.51
1:B:56:THR:OG1	1:B:59:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:C	1:B:121:LEU:HD22	2.35	0.51
1:B:343:GLN:HE21	1:B:343:GLN:CA	2.10	0.51
1:B:212:VAL:HG13	1:B:217:GLU:O	2.10	0.51
1:B:196:GLU:O	1:B:199:GLU:HB2	2.10	0.51
1:B:270:VAL:HG12	1:B:298:GLN:CB	2.33	0.51
1:B:127:VAL:HG22	1:B:128:ARG:H	1.75	0.51
1:B:455:LYS:C	1:B:458:PRO:HD2	2.36	0.51
1:B:355:ARG:HG3	1:B:356:ARG:N	2.25	0.51
1:A:494:THR:H	1:A:497:ALA:HB3	1.75	0.50
1:B:140:CYS:SG	1:B:141:GLY:N	2.83	0.50
1:B:198:ASN:HB3	1:B:224:ARG:NH1	2.20	0.50
1:A:283:GLN:HE22	1:A:302:GLY:CA	2.22	0.50
1:B:346:ALA:O	1:B:350:VAL:HG23	2.11	0.50
1:B:181:LYS:HG2	1:B:183:GLU:HG2	1.93	0.50
1:B:493:ARG:NH2	1:B:498:GLN:HG2	2.25	0.50
1:B:12:TYR:O	1:B:13:VAL:HG13	2.11	0.50
1:B:375:LYS:O	1:B:379:LEU:HG	2.11	0.50
1:B:76:ALA:O	1:B:80:ILE:HG13	2.11	0.50
1:B:218:LEU:HD11	1:B:220:ALA:O	2.12	0.50
1:B:71:ASP:HB3	1:B:92:HIS:CD2	2.46	0.50
1:B:120:VAL:O	1:B:121:LEU:HB3	2.12	0.50
1:B:303:ASN:CG	3:B:601:SAE:H62N	2.20	0.50
1:B:398:GLY:O	1:B:399:GLU:C	2.54	0.50
1:A:84:LEU:HD23	1:A:244:LEU:HD21	1.92	0.49
1:B:190:ALA:HA	1:B:211:ILE:CG2	2.42	0.49
1:B:227:LEU:CD1	1:B:227:LEU:C	2.82	0.49
1:B:313:LEU:O	1:B:318:VAL:HG22	2.12	0.49
1:B:115:ILE:C	1:B:117:ASP:H	2.20	0.49
1:B:157:ILE:CG2	1:B:158:ILE:H	2.26	0.49
1:B:212:VAL:HG12	1:B:215:ASP:O	2.12	0.49
1:B:228:LYS:HB2	1:B:228:LYS:NZ	2.27	0.49
1:B:352:GLU:CD	1:B:352:GLU:C	2.81	0.49
1:B:461:ILE:O	1:B:465:GLN:HG3	2.12	0.49
1:B:186:VAL:HG13	1:B:205:LYS:NZ	2.28	0.49
1:B:203:ARG:HH11	1:B:204:SER:HB3	1.77	0.49
1:B:206:LYS:HD2	1:B:207:GLY:N	2.28	0.49
1:A:277:GLN:NE2	1:A:278:GLY:N	2.60	0.49
1:B:31:THR:CG2	1:B:32:TYR:H	2.24	0.49
1:B:150:MET:HE2	1:B:220:ALA:HA	1.93	0.49
1:B:306:THR:OG1	1:B:309:GLN:HG3	2.13	0.49
1:B:336:VAL:HG23	1:B:336:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:GLN:CD	3:B:601:SAE:SE1N	3.06	0.48
1:B:377:LEU:HD13	1:B:476:LEU:HD13	1.95	0.48
1:B:147:THR:C	1:B:149:ARG:H	2.22	0.48
1:B:115:ILE:O	1:B:117:ASP:N	2.47	0.48
1:B:199:GLU:O	1:B:200:ILE:C	2.56	0.48
1:B:203:ARG:HE	1:B:205:LYS:CB	2.26	0.48
1:B:203:ARG:O	1:B:204:SER:HB2	2.13	0.48
1:B:227:LEU:CD1	1:B:227:LEU:N	2.76	0.48
1:B:368:GLN:N	1:B:372:HIS:HD2	2.05	0.48
1:A:477:THR:HA	1:A:480:ARG:HH11	1.78	0.48
1:B:19:THR:HG22	1:B:21:GLN:H	1.79	0.48
1:B:213:ASN:C	1:B:215:ASP:H	2.22	0.48
1:A:26:CYS:C	1:A:28:ASP:N	2.70	0.48
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.78	0.48
1:B:224:ARG:NE	1:B:225:THR:H	2.11	0.48
1:B:212:VAL:HG12	1:B:213:ASN:N	2.29	0.48
1:B:115:ILE:HG22	1:B:118:PRO:CD	2.42	0.48
1:B:127:VAL:HG22	1:B:128:ARG:N	2.28	0.48
1:B:283:GLN:HE22	1:B:302:GLY:CA	2.24	0.48
1:B:193:THR:HG22	1:B:196:GLU:OE2	2.13	0.47
1:A:103:GLU:HA	1:A:103:GLU:OE1	2.14	0.47
1:B:93:HIS:H	1:B:93:HIS:CD2	2.31	0.47
3:B:601:SAE:H51A	3:B:601:SAE:PN	2.54	0.47
1:A:343:GLN:HA	1:A:343:GLN:HE21	1.79	0.47
1:B:28:ASP:HB3	1:B:30:LEU:HG	1.95	0.47
1:B:150:MET:O	1:B:150:MET:HG2	2.14	0.47
1:B:80:ILE:HG13	1:B:107:VAL:HG22	1.97	0.47
1:A:31:THR:HG22	1:A:32:TYR:H	1.74	0.47
1:A:100:GLN:OE1	1:A:259:ARG:HD3	2.15	0.47
1:B:144:ILE:CG1	1:B:156:GLY:HA3	2.44	0.47
1:B:198:ASN:CB	1:B:224:ARG:NH1	2.75	0.47
1:A:56:THR:OG1	1:A:59:ILE:HG12	2.14	0.47
1:A:291:LYS:HA	1:A:291:LYS:CE	2.41	0.47
1:B:105:ARG:NH1	1:B:105:ARG:HG2	2.30	0.47
1:B:144:ILE:HG12	1:B:156:GLY:C	2.40	0.47
1:B:494:THR:H	1:B:497:ALA:CB	2.27	0.47
1:A:18:LEU:HD22	1:A:18:LEU:N	2.29	0.47
1:A:66:VAL:O	1:A:385:MET:HA	2.15	0.47
1:B:363:ALA:HB3	1:B:384:VAL:HG22	1.96	0.47
1:B:125:ASP:O	1:B:126:ARG:CD	2.63	0.46
1:A:19:THR:O	1:A:21:GLN:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LYS:O	1:B:206:LYS:O	2.33	0.46
1:B:213:ASN:ND2	1:B:215:ASP:OD2	2.48	0.46
1:B:494:THR:H	1:B:497:ALA:HB2	1.81	0.46
1:B:51:LEU:CD1	1:B:461:ILE:HG23	2.45	0.46
1:B:124:LYS:H	1:B:124:LYS:HD2	1.80	0.46
1:A:80:ILE:HG23	1:A:244:LEU:CD1	2.46	0.46
1:B:303:ASN:HA	1:B:322:ARG:O	2.16	0.46
1:B:471:ILE:O	1:B:471:ILE:HG13	2.15	0.46
3:A:600:SAE:H51A	3:A:600:SAE:PN	2.55	0.46
1:B:203:ARG:CZ	1:B:204:SER:HB3	2.45	0.46
1:B:13:VAL:O	1:B:13:VAL:CG2	2.63	0.46
1:B:453:ILE:HG23	1:B:457:VAL:HG23	1.97	0.46
1:B:96:THR:OG1	1:B:99:PHE:HB2	2.15	0.46
1:B:388:SER:N	2:B:631:CPR:O3P	2.38	0.46
1:B:390:LEU:O	1:B:392:ALA:N	2.49	0.46
1:A:23:LEU:HD11	1:A:492:LYS:CG	2.46	0.46
1:A:303:ASN:OD1	1:A:322:ARG:HD3	2.16	0.46
1:A:483:MET:CB	1:A:488:LEU:HD23	2.45	0.46
1:A:274:ASP:OD2	3:A:600:SAE:O2D	2.33	0.46
1:A:460:LEU:O	1:A:464:ILE:HG13	2.16	0.46
1:A:303:ASN:HA	1:A:322:ARG:O	2.16	0.45
1:B:188:ALA:HB1	1:B:192:ILE:HD13	1.98	0.45
1:A:75:GLU:OE2	1:A:92:HIS:HE1	1.98	0.45
1:B:300:ILE:HG12	1:B:320:ALA:HB3	1.97	0.45
1:B:90:PHE:HA	1:B:247:GLY:O	2.17	0.45
1:A:483:MET:HB3	1:A:488:LEU:CD2	2.44	0.45
1:B:154:LEU:N	1:B:216:ASP:O	2.48	0.45
1:A:343:GLN:HE21	1:A:343:GLN:CA	2.29	0.45
1:A:12:TYR:HE2	1:A:14:PRO:HA	1.82	0.45
1:B:20:ALA:O	1:B:24:PHE:HD2	1.99	0.45
1:B:181:LYS:O	1:B:182:ARG:CB	2.62	0.45
1:B:496:SER:O	1:B:497:ALA:C	2.60	0.45
1:A:293:LYS:O	1:A:294:TYR:CG	2.70	0.45
1:B:157:ILE:HG22	1:B:158:ILE:H	1.80	0.45
1:A:395:GLU:OE1	1:A:453:ILE:HG12	2.17	0.44
1:A:13:VAL:HA	1:A:14:PRO:HD3	1.85	0.44
1:A:23:LEU:O	1:A:28:ASP:OD2	2.35	0.44
1:B:246:CYS:N	1:B:269:ASP:OD2	2.37	0.44
1:A:28:ASP:HB3	1:A:30:LEU:HD21	1.98	0.44
1:A:49:VAL:HA	1:A:474:LYS:O	2.17	0.44
1:B:198:ASN:CA	1:B:224:ARG:NH1	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:HD12	1:A:287:ILE:HD11	1.99	0.44
1:B:199:GLU:C	1:B:201:LEU:N	2.73	0.44
1:B:125:ASP:HB3	1:B:126:ARG:H	1.40	0.44
1:B:281:ILE:HG13	1:B:285:ASN:ND2	2.33	0.44
1:B:225:THR:O	1:B:225:THR:CG2	2.64	0.44
1:A:71:ASP:HB3	1:A:92:HIS:CD2	2.53	0.44
1:A:355:ARG:HG3	1:A:356:ARG:N	2.32	0.44
1:B:249:ALA:HB1	1:B:274:ASP:HB2	2.00	0.44
1:B:280:SER:O	1:B:284:ILE:HG13	2.18	0.44
1:A:265:GLN:C	1:A:267:GLY:N	2.74	0.43
1:A:277:GLN:NE2	1:A:279:ASN:N	2.61	0.43
1:A:375:LYS:O	1:A:379:LEU:HG	2.18	0.43
1:B:112:GLN:OE1	1:B:243:GLN:CG	2.64	0.43
1:B:235:LEU:O	1:B:236:ALA:C	2.61	0.43
1:B:494:THR:N	1:B:497:ALA:HB3	2.34	0.43
1:A:93:HIS:H	1:A:93:HIS:CD2	2.36	0.43
1:A:343:GLN:NE2	1:A:343:GLN:CA	2.82	0.43
1:A:69:PRO:HG3	1:A:90:PHE:CB	2.48	0.43
1:B:144:ILE:CD1	1:B:179:MET:SD	3.04	0.43
1:B:26:CYS:C	1:B:28:ASP:N	2.76	0.43
1:A:78:MET:HE1	1:A:393:THR:OG1	2.18	0.43
1:A:315:ASP:C	1:A:317:GLY:N	2.74	0.43
1:A:483:MET:HE1	1:A:484:TYR:CE1	2.53	0.43
1:B:272:VAL:HG13	1:B:272:VAL:O	2.19	0.43
1:B:122:SER:CB	1:B:123:PRO:HD2	2.49	0.43
1:A:108:LYS:HG3	1:A:266:ALA:O	2.19	0.43
1:A:362:ILE:HG12	1:A:383:THR:OG1	2.19	0.43
1:B:19:THR:O	1:B:20:ALA:C	2.60	0.43
1:B:46:ALA:C	1:B:48:GLN:H	2.27	0.43
1:B:153:ARG:HB2	1:B:153:ARG:HH11	1.84	0.43
1:B:219:VAL:O	1:B:220:ALA:HB2	2.19	0.43
1:A:13:VAL:O	1:A:13:VAL:HG23	2.18	0.42
1:A:395:GLU:OE1	1:A:453:ILE:N	2.49	0.42
1:B:12:TYR:C	1:B:13:VAL:CG1	2.89	0.42
1:B:62:LYS:CB	1:B:235:LEU:HD22	2.49	0.42
1:B:213:ASN:C	1:B:215:ASP:N	2.76	0.42
1:A:47:ASP:OD1	1:A:47:ASP:C	2.62	0.42
1:B:30:LEU:HD22	1:B:34:ASP:HB3	1.99	0.42
1:B:16:ASP:CG	1:B:17:GLY:H	2.26	0.42
1:B:303:ASN:ND2	3:B:601:SAE:H62N	2.16	0.42
1:B:21:GLN:O	1:B:22:GLN:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:SER:OG	1:B:64:PRO:HB3	2.20	0.42
1:B:75:GLU:O	1:B:76:ALA:C	2.62	0.42
1:B:102:ASN:O	1:B:106:LYS:HG3	2.19	0.42
1:A:28:ASP:HB3	1:A:30:LEU:CD2	2.49	0.42
1:A:461:ILE:O	1:A:465:GLN:HG3	2.19	0.42
1:B:111:GLU:HG3	1:B:242:LYS:O	2.20	0.42
1:B:202:GLN:CG	1:B:203:ARG:N	2.82	0.42
1:B:373:ILE:HG21	1:B:464:ILE:HD11	2.02	0.42
1:B:394:THR:C	1:B:396:ALA:H	2.26	0.42
1:A:90:PHE:N	1:A:90:PHE:CD1	2.87	0.42
1:A:108:LYS:O	1:A:243:GLN:NE2	2.53	0.42
1:B:120:VAL:HG21	1:B:149:ARG:C	2.44	0.42
1:B:203:ARG:HE	1:B:205:LYS:HB3	1.83	0.42
1:B:203:ARG:CZ	1:B:205:LYS:H	2.31	0.41
1:A:80:ILE:O	1:A:81:ALA:C	2.63	0.41
1:A:312:ASN:N	1:A:312:ASN:HD22	2.18	0.41
1:B:68:SER:HA	1:B:69:PRO:HD3	1.81	0.41
1:A:80:ILE:HG12	1:A:107:VAL:HG13	2.01	0.41
1:A:463:GLY:O	1:A:466:HIS:HB3	2.21	0.41
1:B:120:VAL:HG23	1:B:121:LEU:N	2.34	0.41
1:B:155:VAL:O	1:B:155:VAL:CG1	2.63	0.41
1:B:193:THR:CG2	1:B:196:GLU:HG3	2.50	0.41
1:B:293:LYS:O	1:B:293:LYS:HG2	2.20	0.41
1:A:19:THR:HG22	1:A:21:GLN:H	1.85	0.41
1:B:194:LEU:HD23	1:B:222:ILE:HD13	2.02	0.41
1:B:198:ASN:HA	1:B:224:ARG:NH1	2.36	0.41
1:B:110:TYR:HE2	1:B:117:ASP:OD1	2.03	0.41
1:B:115:ILE:CG2	1:B:118:PRO:HD3	2.45	0.41
1:B:181:LYS:H	1:B:181:LYS:CD	2.34	0.41
1:B:142:ILE:N	1:B:142:ILE:CD1	2.82	0.41
1:A:105:ARG:O	1:A:106:LYS:C	2.64	0.41
1:A:386:MET:HE3	1:A:389:LEU:HD23	2.00	0.41
1:A:56:THR:O	1:A:57:LYS:C	2.64	0.41
1:A:293:LYS:O	1:A:293:LYS:HG2	2.21	0.41
1:B:188:ALA:HA	1:B:189:PRO:HD3	1.87	0.41
1:B:199:GLU:O	1:B:202:GLN:HB3	2.21	0.41
1:B:199:GLU:O	1:B:202:GLN:CB	2.68	0.41
1:B:218:LEU:CD1	1:B:220:ALA:O	2.69	0.41
1:B:253:HIS:O	1:B:256:ASP:HB2	2.20	0.41
1:A:16:ASP:HB3	1:A:489:LYS:HG3	2.02	0.41
1:A:31:THR:N	1:A:34:ASP:OD2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:HD11	1:A:287:ILE:CD1	2.50	0.41
1:A:455:LYS:HD3	1:A:455:LYS:HA	1.91	0.41
1:A:457:VAL:O	1:A:461:ILE:HG13	2.21	0.41
1:A:494:THR:O	1:A:495:SER:C	2.64	0.41
1:B:225:THR:O	1:B:228:LYS:HD3	2.22	0.40
1:A:492:LYS:HE2	1:A:492:LYS:HB3	1.84	0.40
1:B:207:GLY:C	1:B:208:LYS:HD2	2.45	0.40
1:B:390:LEU:O	1:B:391:ALA:C	2.63	0.40
1:A:292:ASP:OD1	1:A:292:ASP:C	2.64	0.40
1:B:141:GLY:O	1:B:208:LYS:HG2	2.21	0.40
1:B:146:ASP:HB3	1:B:152:SER:OG	2.21	0.40
1:B:352:GLU:O	1:B:355:ARG:HG2	2.21	0.40
1:B:494:THR:N	1:B:497:ALA:CB	2.84	0.40
1:A:82:MET:HG3	1:A:88:ILE:H	1.87	0.40
1:A:272:VAL:O	1:A:274:ASP:N	2.55	0.40
1:B:83:ALA:O	1:B:236:ALA:HA	2.21	0.40
1:B:231:ARG:H	1:B:231:ARG:HG3	1.36	0.40
2:A:631:CPR:O2'	3:A:600:SAE:N6N	2.55	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	299/514 (58%)	249 (83%)	39 (13%)	11 (4%)	2	11
1	B	406/514 (79%)	304 (75%)	77 (19%)	25 (6%)	1	3
All	All	705/1028 (69%)	553 (78%)	116 (16%)	36 (5%)	1	6

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	14	PRO
1	A	17	GLY
1	A	76	ALA
1	A	450	LYS
1	B	14	PRO
1	B	17	GLY
1	B	76	ALA
1	B	114	PHE
1	B	205	LYS
1	B	206	LYS
1	B	228	LYS
1	B	229	LYS
1	B	332	ILE
1	B	334	GLN
1	B	335	GLU
1	B	450	LYS
1	A	16	ASP
1	A	27	GLY
1	B	13	VAL
1	B	27	GLY
1	B	123	PRO
1	B	126	ARG
1	B	150	MET
1	B	204	SER
1	B	302	GLY
1	B	338	ALA
1	B	391	ALA
1	A	20	ALA
1	A	273	LEU
1	A	391	ALA
1	B	125	ASP
1	B	236	ALA
1	B	293	LYS
1	B	181	LYS
1	A	289	TYR

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	242/420 (58%)	239 (99%)	3 (1%)	63	86
1	B	333/420 (79%)	309 (93%)	24 (7%)	13	39
All	All	575/840 (68%)	548 (95%)	27 (5%)	23	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	277	GLN
1	A	291	LYS
1	B	13	VAL
1	B	112	GLN
1	B	120	VAL
1	B	121	LEU
1	B	124	LYS
1	B	153	ARG
1	B	158	ILE
1	B	179	MET
1	B	181	LYS
1	B	183	GLU
1	B	186	VAL
1	B	203	ARG
1	B	206	LYS
1	B	209	LEU
1	B	227	LEU
1	B	228	LYS
1	B	229	LYS
1	B	231	ARG
1	B	277	GLN
1	B	291	LYS
1	B	329	SER
1	B	343	GLN
1	B	450	LYS
1	B	471	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN

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Mol	Chain	Res	Type
1	A	92	HIS
1	A	94	ASN
1	A	243	GLN
1	A	265	GLN
1	A	277	GLN
1	A	283	GLN
1	A	285	ASN
1	A	309	GLN
1	A	312	ASN
1	A	343	GLN
1	A	372	HIS
1	A	478	GLN
1	B	22	GLN
1	B	92	HIS
1	B	93	HIS
1	B	94	ASN
1	B	243	GLN
1	B	265	GLN
1	B	277	GLN
1	B	283	GLN
1	B	285	ASN
1	B	309	GLN
1	B	312	ASN
1	B	343	GLN
1	B	368	GLN
1	B	372	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 15 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	SAE	A	600	-	46,47,47	1.77	8 (17%)	65,72,72	2.19	17 (26%)
3	SAE	B	601	-	46,47,47	1.78	8 (17%)	65,72,72	2.19	17 (26%)
2	CPR	B	631	-	24,24,25	1.67	4 (16%)	33,36,38	3.15	13 (39%)
2	CPR	A	631	-	24,24,25	1.39	2 (8%)	33,36,38	3.19	10 (30%)

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	SAE	A	600	-	-	6/28/62/62	0/5/5/5
3	SAE	B	601	-	-	6/28/62/62	0/5/5/5
2	CPR	B	631	-	-	0/10/26/26	0/3/3/3
2	CPR	A	631	-	-	5/10/26/26	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	SAE	SE1N-C2N	-7.38	1.73	1.88
3	A	600	SAE	SE1N-C2N	-7.35	1.73	1.88
2	B	631	CPR	C6-N1	5.77	1.37	1.31
3	B	601	SAE	SE1N-C5N	-5.31	1.71	1.86
3	A	600	SAE	SE1N-C5N	-5.30	1.71	1.86
2	A	631	CPR	C6-N1	4.74	1.36	1.31
3	A	600	SAE	C4N-C6N	3.52	1.53	1.48
3	B	601	SAE	C4N-C6N	3.51	1.53	1.48
2	B	631	CPR	C5-N7	-3.08	1.31	1.39
2	A	631	CPR	C5-N7	-2.67	1.32	1.39
3	B	601	SAE	C4N-N3N	-2.56	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	SAE	C4N-N3N	-2.54	1.33	1.38
2	B	631	CPR	P-O3P	-2.30	1.46	1.54
3	B	601	SAE	O4B-C1B	2.30	1.47	1.42
3	A	600	SAE	O4B-C1B	2.28	1.47	1.42
3	A	600	SAE	C5A-N7A	-2.25	1.35	1.39
3	B	601	SAE	C5A-N7A	-2.24	1.35	1.39
2	B	631	CPR	C4-N9	-2.08	1.32	1.38
3	A	600	SAE	C1B-N9A	2.02	1.51	1.46
3	B	601	SAE	C8A-N7A	2.01	1.35	1.31
3	B	601	SAE	C1B-N9A	2.01	1.51	1.46
3	A	600	SAE	C8A-N7A	2.01	1.35	1.31

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	631	CPR	C6-N1-C2	9.79	128.25	115.77
2	B	631	CPR	C6-N1-C2	9.34	127.68	115.77
2	A	631	CPR	C5-C4-N3	-7.55	115.92	127.24
2	B	631	CPR	C5-C4-N3	-6.66	117.26	127.24
2	B	631	CPR	N1-C2-N3	-6.40	116.87	128.84
2	B	631	CPR	C2-N3-C4	6.36	122.09	111.14
3	B	601	SAE	C5A-C4A-N3A	-6.33	118.00	126.72
3	A	600	SAE	C5A-C4A-N3A	-6.32	118.01	126.72
2	A	631	CPR	N1-C2-N3	-6.24	117.18	128.84
2	A	631	CPR	C2-N3-C4	6.20	121.81	111.14
3	B	601	SAE	N3A-C4A-N9A	6.11	137.56	127.17
3	A	600	SAE	N3A-C4A-N9A	6.11	137.55	127.17
3	B	601	SAE	N3A-C2A-N1A	-5.96	119.56	128.58
3	A	600	SAE	N3A-C2A-N1A	-5.94	119.59	128.58
2	A	631	CPR	N9-C4-N3	5.33	139.04	126.90
3	A	600	SAE	O4B-C4B-C5B	-4.82	93.91	109.33
3	B	601	SAE	O4B-C4B-C5B	-4.81	93.92	109.33
3	A	600	SAE	C4N-N3N-C2N	-4.80	108.73	113.49
3	B	601	SAE	C4N-N3N-C2N	-4.80	108.74	113.49
2	A	631	CPR	C6-C5-N7	-4.52	122.28	132.21
2	B	631	CPR	C6-C5-N7	-4.40	122.53	132.21
2	B	631	CPR	N9-C4-N3	4.36	136.83	126.90
3	B	601	SAE	C2A-N3A-C4A	4.10	121.83	111.83
3	A	600	SAE	C2A-N3A-C4A	4.09	121.83	111.83
3	B	601	SAE	O3B-C3B-C2B	3.96	124.52	111.82
3	A	600	SAE	O3B-C3B-C2B	3.96	124.50	111.82
2	A	631	CPR	O2P-P-O5'	-3.73	96.96	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	SAE	O4B-C1B-N9A	3.71	115.21	108.09
3	B	601	SAE	O4B-C1B-N9A	3.70	115.20	108.09
2	B	631	CPR	O4'-C1'-N9	3.45	116.18	108.36
2	B	631	CPR	C8-N7-C5	-3.36	101.46	104.92
3	B	601	SAE	O4B-C4B-C3B	3.21	111.52	105.15
3	A	600	SAE	O4B-C4B-C3B	3.21	111.52	105.15
2	A	631	CPR	O3'-C3'-C4'	3.18	120.22	111.08
2	B	631	CPR	O3'-C3'-C4'	3.10	119.98	111.08
3	A	600	SAE	O5D-C5D-C4D	2.88	118.81	108.99
3	B	601	SAE	O5D-C5D-C4D	2.88	118.80	108.99
3	B	601	SAE	C2A-N1A-C6A	2.83	123.37	118.73
2	B	631	CPR	C5'-C4'-C3'	-2.82	105.06	115.21
3	A	600	SAE	C2A-N1A-C6A	2.79	123.31	118.73
3	A	600	SAE	C5B-C4B-C3B	-2.77	105.24	115.21
3	B	601	SAE	C5B-C4B-C3B	-2.76	105.28	115.21
3	B	601	SAE	C6A-C5A-C4A	2.68	120.84	117.18
3	A	600	SAE	C6A-C5A-C4A	2.68	120.83	117.18
2	A	631	CPR	C2'-C3'-C4'	-2.65	97.49	102.61
3	A	600	SAE	O5D-PN-O1N	2.55	119.06	108.94
3	B	601	SAE	O5D-PN-O1N	2.54	119.00	108.94
3	B	601	SAE	C6A-C5A-N7A	-2.53	127.21	132.09
3	A	600	SAE	C6A-C5A-N7A	-2.53	127.22	132.09
3	B	601	SAE	C4B-O4B-C1B	-2.44	104.08	109.47
3	A	600	SAE	C4B-O4B-C1B	-2.43	104.09	109.47
2	B	631	CPR	C3'-C2'-C1'	2.36	105.93	101.46
2	A	631	CPR	C2'-C1'-N9	2.12	119.16	113.25
2	B	631	CPR	O4'-C1'-C2'	-2.10	102.12	106.62
2	B	631	CPR	C2'-C3'-C4'	-2.06	98.63	102.61
3	A	600	SAE	O2B-C2B-C3B	2.02	118.30	111.82
3	B	601	SAE	O2B-C2B-C3B	2.01	118.26	111.82

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	631	CPR	C5'-O5'-P-O2P
2	A	631	CPR	C5'-O5'-P-O3P
2	A	631	CPR	C3'-C4'-C5'-O5'
2	A	631	CPR	C5'-O5'-P-O1P
3	A	600	SAE	N3N-C4N-C6N-O6N
3	A	600	SAE	N3N-C4N-C6N-N6N
3	B	601	SAE	N3N-C4N-C6N-O6N

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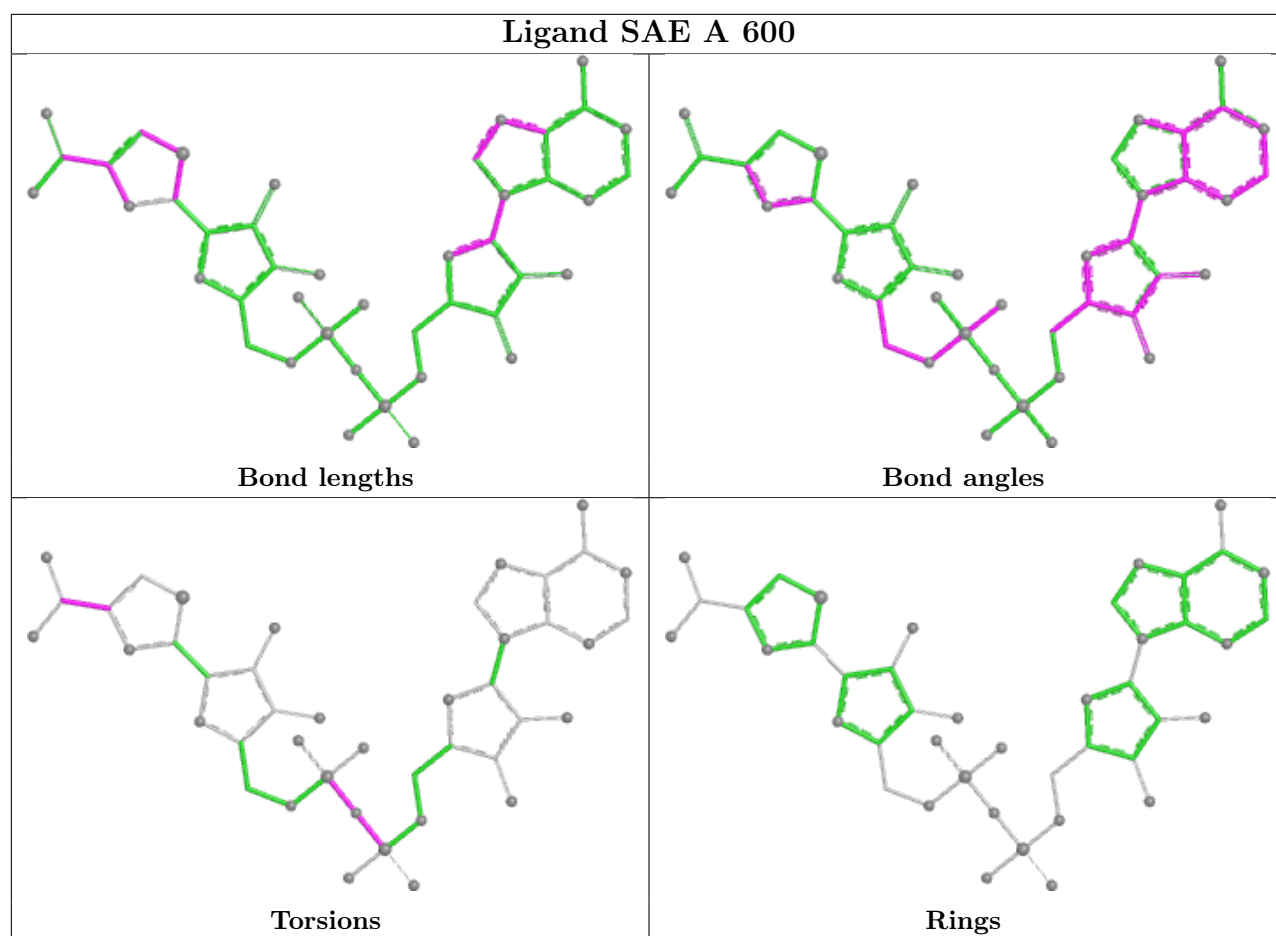
Mol	Chain	Res	Type	Atoms
3	B	601	SAE	N3N-C4N-C6N-N6N
3	A	600	SAE	PN-O3-PA-O5B
3	B	601	SAE	PN-O3-PA-O5B
2	A	631	CPR	O4'-C4'-C5'-O5'
3	A	600	SAE	PA-O3-PN-O1N
3	A	600	SAE	PA-O3-PN-O2N
3	B	601	SAE	PA-O3-PN-O1N
3	B	601	SAE	PA-O3-PN-O2N
3	A	600	SAE	PN-O3-PA-O2A
3	B	601	SAE	PN-O3-PA-O2A

There are no ring outliers.

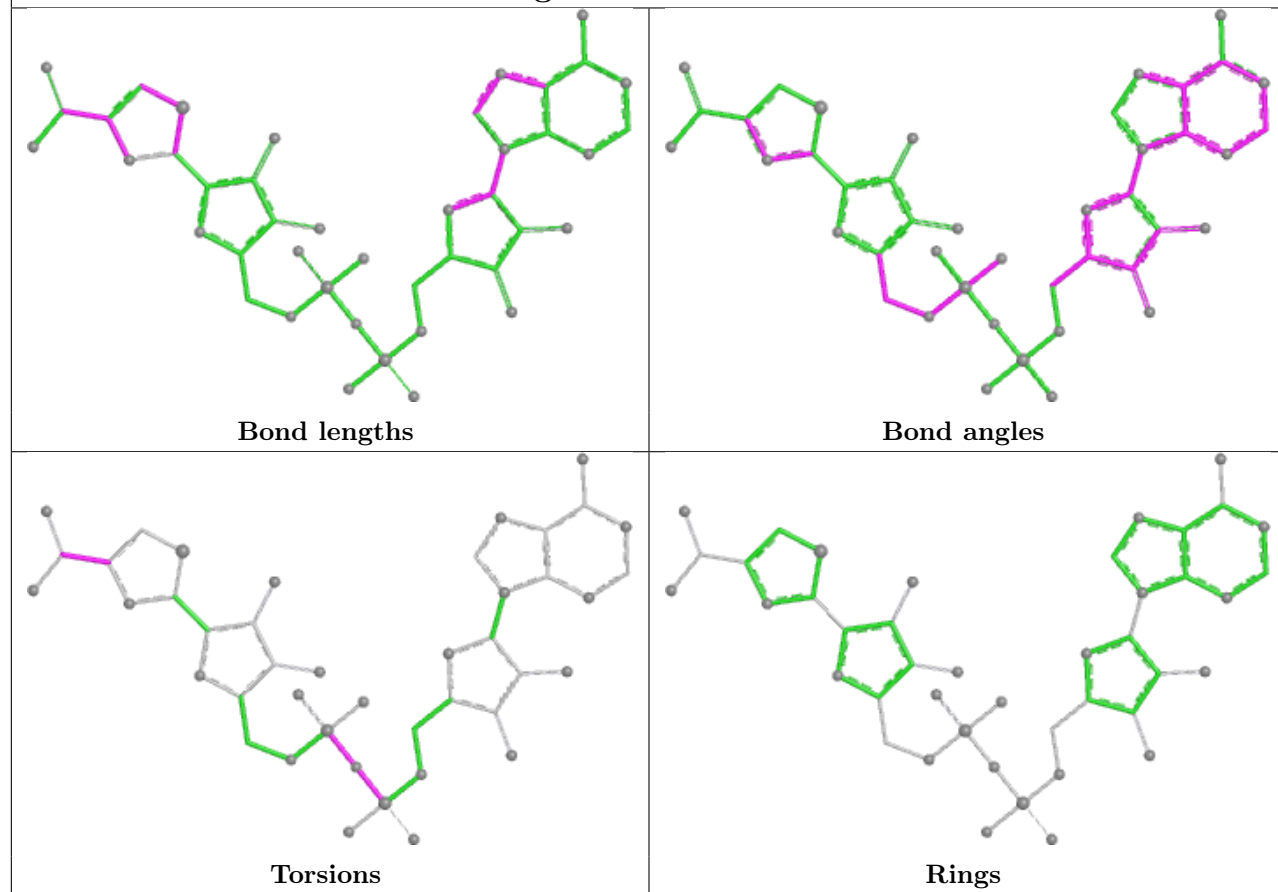
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	SAE	5	0
3	B	601	SAE	4	0
2	B	631	CPR	2	0
2	A	631	CPR	1	0

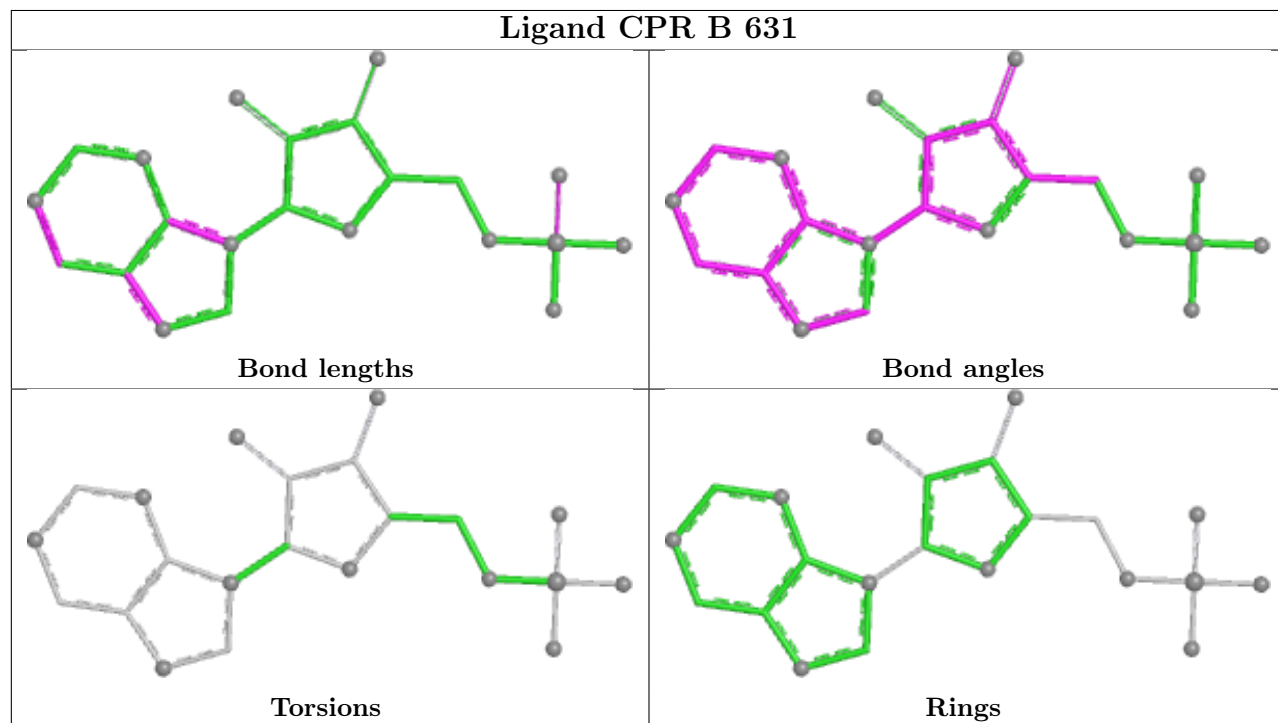
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

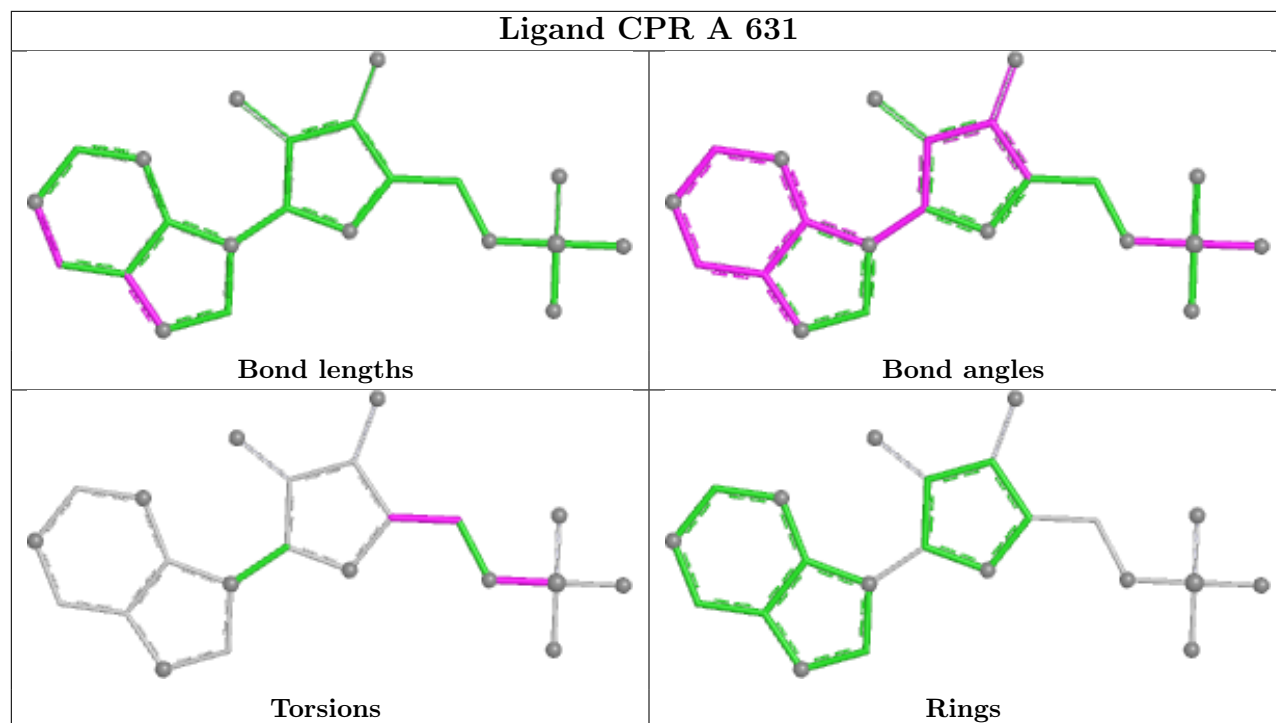


Ligand SAE B 601



Ligand CPR B 631





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 [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	307/514 (59%)	-1.74	0 100 100	12, 32, 55, 88	0
1	B	414/514 (80%)	-1.64	0 100 100	14, 35, 81, 95	0
All	All	721/1028 (70%)	-1.69	0 100 100	12, 34, 78, 95	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
3	SAE	A	600	43/43	0.99	0.05	55,71,91,96	43
3	SAE	B	601	43/43	0.99	0.04	54,76,87,89	43
2	CPR	A	631	22/23	1.00	0.02	30,36,55,57	0
2	CPR	B	631	22/23	1.00	0.02	26,31,53,54	0
4	UNX	B	632	1/1	-	-	20,20,20,20	1
4	UNX	B	633	1/1	-	-	20,20,20,20	1
4	UNX	B	634	1/1	-	-	20,20,20,20	1

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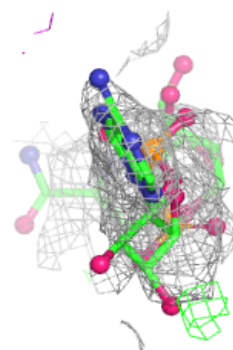
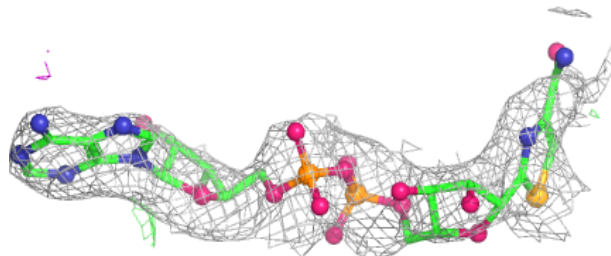
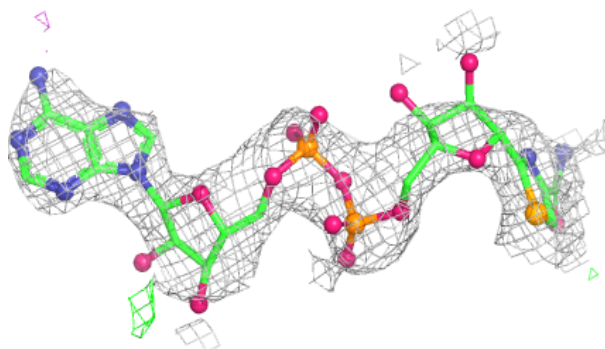
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	UNX	B	635	1/1	-	-	20,20,20,20	1
4	UNX	B	636	1/1	-	-	20,20,20,20	1
4	UNX	B	637	1/1	-	-	20,20,20,20	1
4	UNX	B	638	1/1	-	-	20,20,20,20	1
4	UNX	B	639	1/1	-	-	20,20,20,20	1
4	UNX	B	640	1/1	-	-	20,20,20,20	1
4	UNX	B	641	1/1	-	-	20,20,20,20	1
4	UNX	B	642	1/1	-	-	20,20,20,20	1
4	UNX	B	643	1/1	-	-	20,20,20,20	1
4	UNX	B	644	1/1	-	-	20,20,20,20	1
4	UNX	B	645	1/1	-	-	20,20,20,20	1
4	UNX	B	646	1/1	-	-	20,20,20,20	1

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.

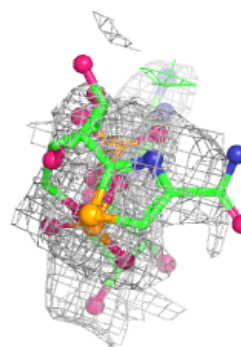
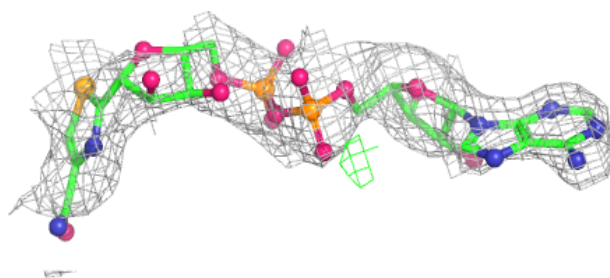
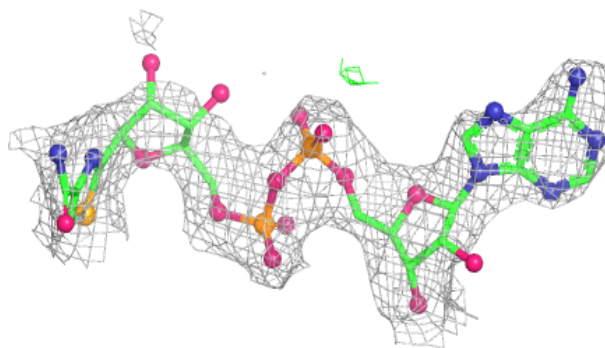
Electron density around SAE A 600:

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

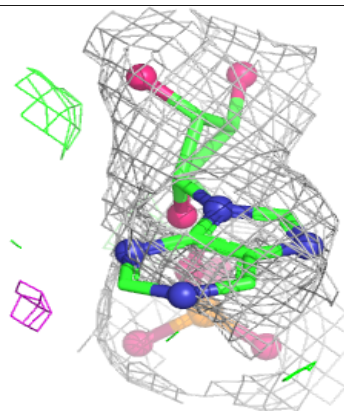
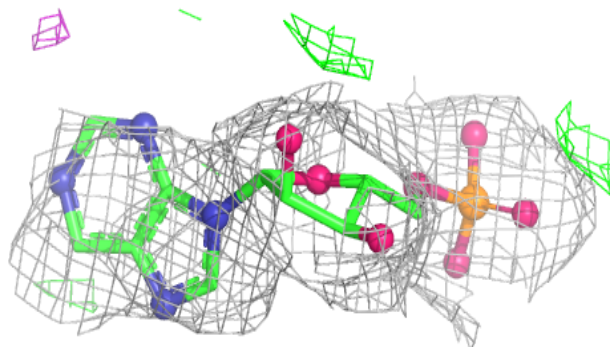
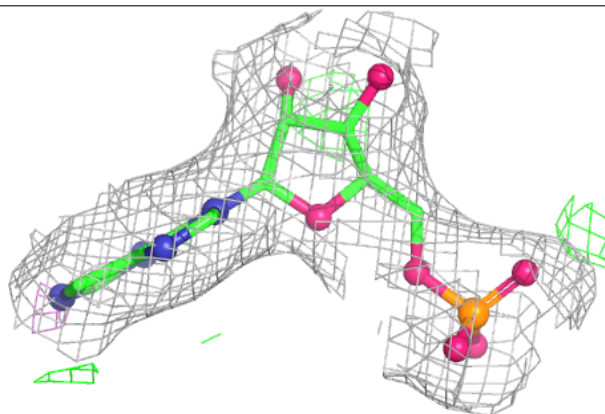


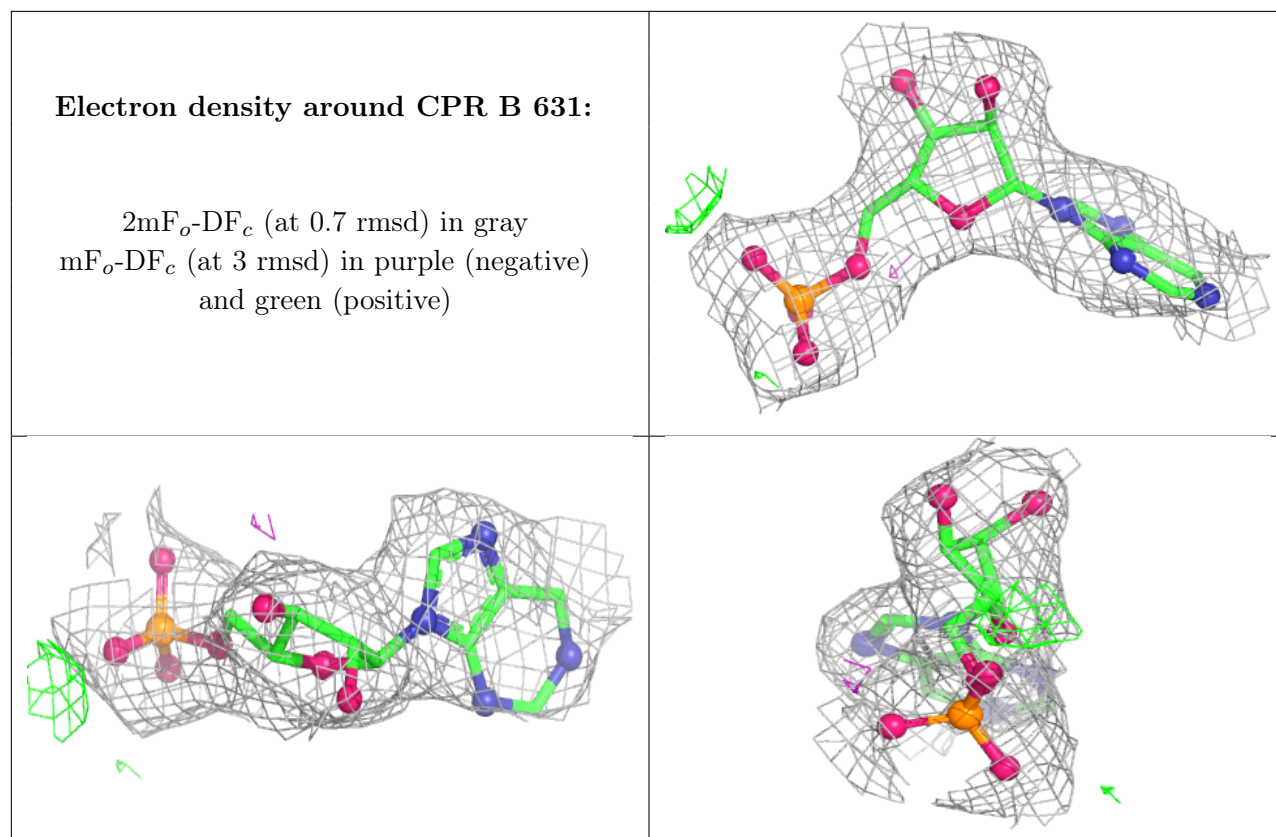
Electron density around SAE B 601:

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

**Electron density around CPR A 631:**

$2mF_o-DF_c$ (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.