



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:51 AM UTC

PDB ID : 3HND / pdb_00003hnd
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effector TTP and substrate GDP
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.
Deposited on : 2009-05-31
Resolution : 3.21 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

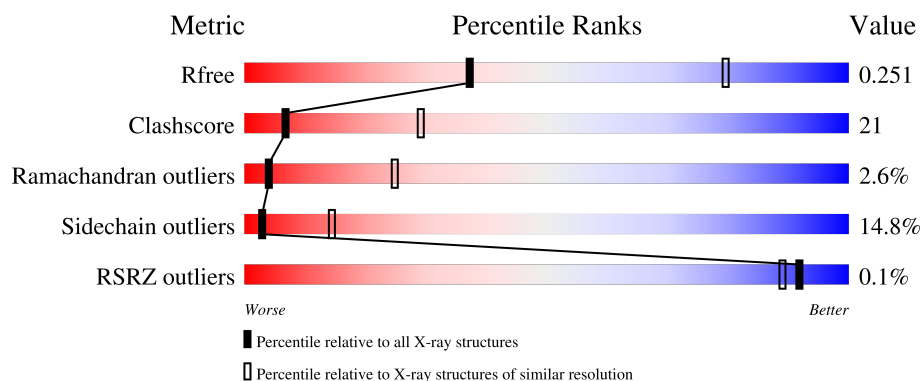
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	792	
1	B	792	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11566 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.

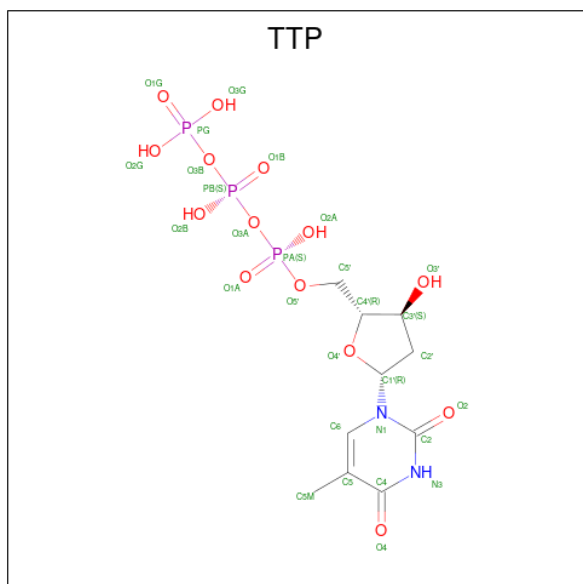
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5720	3640	959	1088	33			
1	B	735	Total	C	N	O	S	0	1	0
			5678	3608	956	1083	31			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

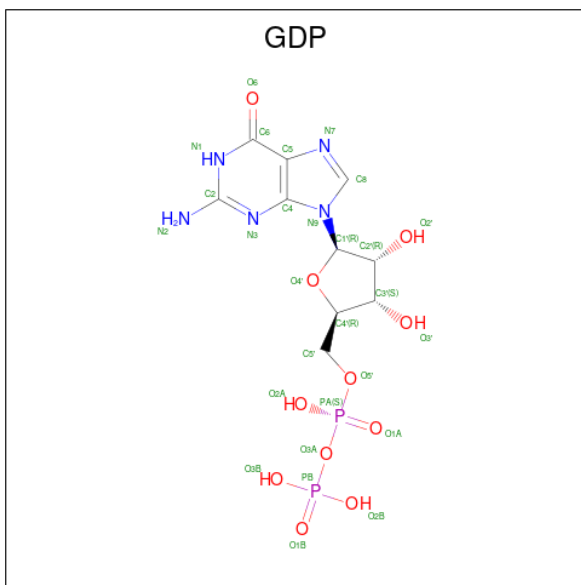
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
3	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

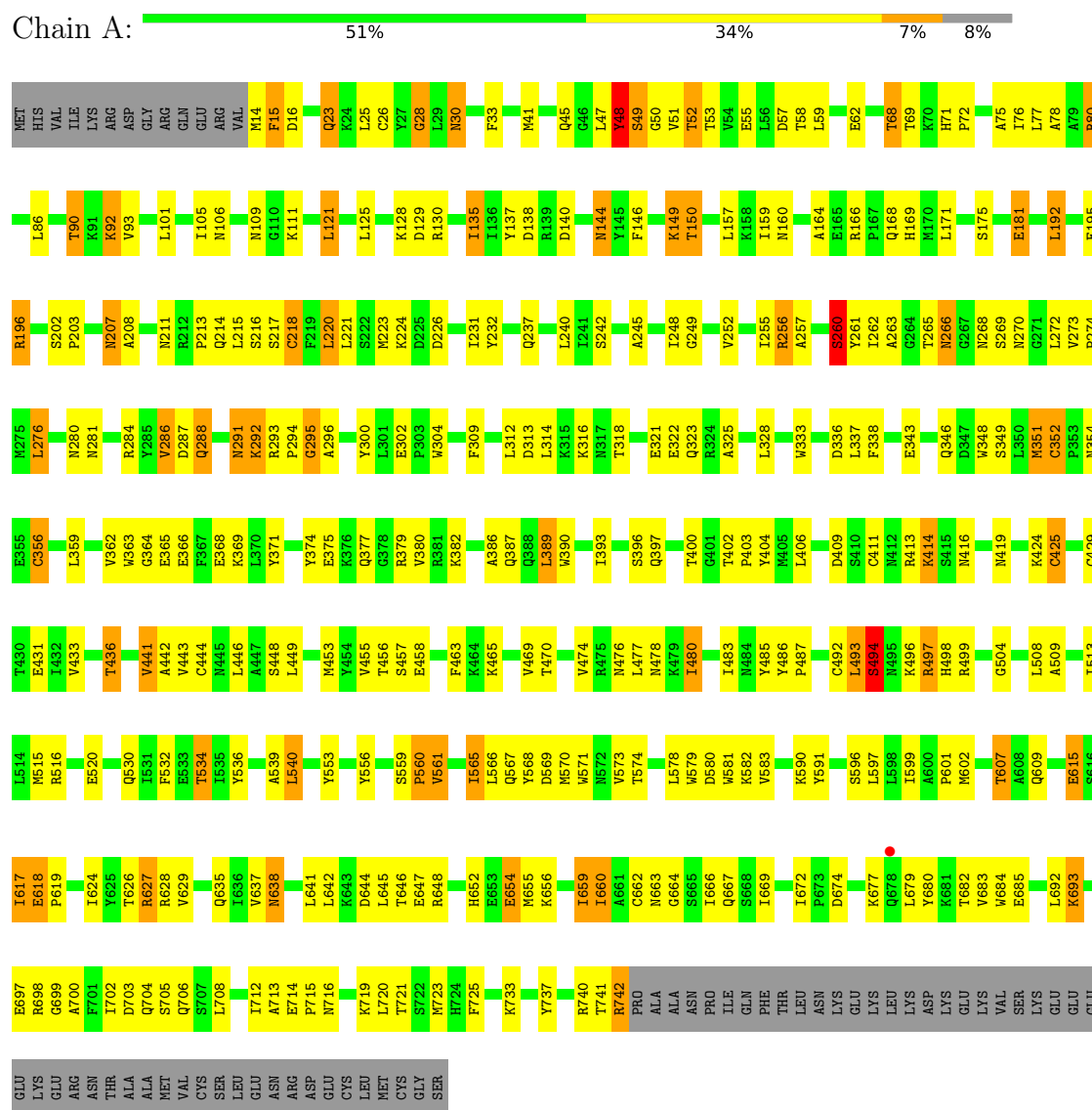
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	B	14	Total	O	0	0
			14	14		

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: Ribonucleoside-diphosphate reductase large subunit



- Molecule 1: Ribonucleoside-diphosphate reductase large subunit



ASN	L642	Y537	C352	A263	Q168	K88	MET
PRO	K643	T456	P353	N270	H169	E89	H2
ILE	E541	S457	L359	G271	V176	T90	V3
GLN	R648	E458	L359	L272	H179	K91	I4
PHE	G649	S543	G364	V273	K180	V93	K5
THR	L650	C544	E365	P274	T187	F94	R6
LEU	G651	Y556	E366	M275	I187	S95	R5
ASN	H652	P560	F367	L276	N191	E99	V13
LYS	R655	V561	E368	N280	N191	E99	D16
LYS	N663	V474	Y371	N281	N191	E99	K17
LYS	I565	L477	Y374	T282	S194	I105	T18
ASP	L566	M478	Y374	A283	E195	I106	I19
LYS	G567	M479	R379	R284	R196	P107	S20
GLU	E671	I480	R379	V286	N109	H108	R21
LYS	I672	L578	V383	D287	F198	G110	I22
VAL	D675	W579	V383	Q288	T199	K111	M31
SER	L676	D580	V384	Q289	S202	H112	M31
LYS	L676	W581	K385	G289	P203	S113	P36
GLU	L679	K582	A386	G290	N211	V116	I39
GLU	Y680	V583	L389	G291	R212	A117	T40
GLU	L584	L584	L389	K292	P213	K118	V43
LYS	I686	V488	I394	R293	Q214	S119	V43
GLU	S687	E490	E395	P294	L215	T120	I44
ARG	Q688	L493	T398	A298	S216	D122	L47
ASN	V691	S494	T398	I299	S217	I123	Y48
THR	L692	G592	T402	Y300	C218	V124	SER
ALA	K693	N595	P403	L301	F219	L125	GLY
MET	E697	S596	Y404	E302	L220	A126	GLY
VAL	R698	T501	M405	L306	L221	N127	T52
CYS	R698	P601	Y407	F309	S222	K128	T53
SER	F701	M602	K408	Y407	M223	D129	V54
LEU	F701	P603	D409	L314	K224	R130	E55
GLU	Q706	T604	D409	K315	D225	L131	E55
ASN	S707	L508	M416	K315	D226	L131	T58
ARG	L708	A509	Q417	K316	S227	N132	L59
ASP	N709	D510	Q418	N317	I228	I135	L59
GLU	I710	E618	Q418	T318	C238	I136	A64
CYS	H711	P619	S426	Q323	S242	Y137	A65
LEU	I712	I624	M427	Q323	K243	D138	T66
MET	I712	I624	M427	Q323	S242	R139	T66
CYS	Y717	I624	M427	Q323	K243	D140	T69
GLY	G718	I624	M427	Q323	S244	A245	K70
SER	H724	R628	VAL	F329	I248	E152	H71
	F725	LEU	SER	F329	G249	R153	P72
	Y726	GLY	GLY	W333	V250	S154	D73
	Y726	GLY	GLY	W333	V250	S154	I76
	Y738	E633	D439	L337	S253	I159	A79
	L739	F634	E440	F338	C254	N160	R80
	R740	Q635	V441	M339	I255	G161	V83
	T741	I636	A442	K340	R256	K162	S84
	R741	V637	V443	R341	A257	V163	S84
	R742	N638	C144	R341	Y261	R166	R85
PRO	P639	T534	M445	W348	I262	P167	R86
ALA	H640	I535	N445	M351	I262	P167	H87
ALA	L641	Y536	L451	M351	I262	P167	H87

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.16Å 115.83Å 221.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.94 – 3.21 49.94 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.94-3.21) 98.3 (49.94-3.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.254 0.187 , 0.251	Depositor DCC
R_{free} test set	1576 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	97.0	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 102.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11566	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, TTP, MG, GDP

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	0.77	1/5847 (0.0%)	1.07	20/7950 (0.3%)
1	B	0.81	5/5806 (0.1%)	1.08	16/7905 (0.2%)
All	All	0.79	6/11653 (0.1%)	1.07	36/15855 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	ASP	CG-OD2	8.90	1.42	1.25
1	B	180[A]	LYS	CG-CD	-8.32	1.27	1.52
1	B	180[B]	LYS	CG-CD	-8.32	1.27	1.52
1	B	129	ASP	CG-OD1	5.24	1.35	1.25
1	B	129	ASP	C-N	5.16	1.41	1.33
1	A	135	ILE	CA-CB	5.06	1.60	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	ILE	CA-C-N	7.00	126.52	119.24
1	A	669	ILE	C-N-CA	7.00	126.52	119.24
1	A	559	SER	CA-C-N	6.93	128.50	119.84
1	A	559	SER	C-N-CA	6.93	128.50	119.84
1	A	291	ASN	N-CA-C	6.83	120.75	109.96
1	A	207	ASN	N-CA-C	6.26	121.98	113.97
1	A	672	ILE	CA-C-N	6.09	127.46	119.84
1	A	672	ILE	C-N-CA	6.09	127.46	119.84
1	B	603	PRO	N-CA-C	-6.06	102.73	111.22
1	A	618	GLU	N-CA-C	5.88	117.06	109.65
1	B	212	ARG	CA-C-N	5.84	127.14	119.84
1	B	212	ARG	C-N-CA	5.84	127.14	119.84
1	B	257	ALA	N-CA-C	5.82	118.05	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	395	GLU	N-CA-C	-5.70	105.15	111.36
1	A	667	GLN	N-CA-C	5.62	117.40	111.28
1	A	181	GLU	N-CA-C	5.58	119.19	112.38
1	B	578	LEU	N-CA-C	5.57	117.79	111.11
1	B	459	HIS	N-CA-C	5.46	118.65	111.28
1	A	684	TRP	N-CA-C	-5.35	106.72	113.20
1	B	655	MET	N-CA-C	5.35	118.91	112.38
1	B	556	TYR	N-CA-C	5.34	116.79	110.97
1	A	268	ASN	N-CA-C	5.31	117.04	108.34
1	A	356	CYS	CA-C-N	5.30	126.47	119.84
1	A	356	CYS	C-N-CA	5.30	126.47	119.84
1	B	366	GLU	N-CA-C	5.25	117.08	111.36
1	B	293	ARG	CA-C-N	5.23	126.38	119.84
1	B	293	ARG	C-N-CA	5.23	126.38	119.84
1	B	451	LEU	N-CA-C	5.23	117.66	111.33
1	B	16	ASP	N-CA-C	-5.21	107.58	114.04
1	A	444	CYS	N-CA-C	5.12	117.70	108.48
1	B	262	ILE	CB-CA-C	-5.12	105.28	111.88
1	A	346	GLN	N-CA-C	5.04	115.95	108.60
1	A	607	THR	N-CA-C	-5.03	105.50	111.69
1	A	638	ASN	CA-C-N	5.01	126.11	119.84
1	A	638	ASN	C-N-CA	5.01	126.11	119.84
1	B	129	ASP	N-CA-C	5.01	117.14	111.02

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	5720	0	5543	247	0
1	B	5678	0	5414	240	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	13	3	0
3	B	29	0	13	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	28	0	12	2	0
4	B	28	0	12	1	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
6	A	18	0	0	4	0
6	B	14	0	0	1	0
All	All	11566	0	11007	483	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 21.

All (483) 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:A:713:ALA:O	1:A:715:PRO:HD3	1.52	1.09
1:A:256:ARG:HG3	1:A:256:ARG:HH11	1.18	1.08
1:A:742:ARG:HA	1:A:742:ARG:NE	1.65	1.04
1:A:196:ARG:HG2	1:A:196:ARG:HH11	1.18	1.04
1:B:108:HIS:C	1:B:110:GLY:H	1.60	1.03
1:A:90:THR:HG21	1:A:166:ARG:HE	1.27	0.99
1:B:106:ASN:HD21	1:B:108:HIS:N	1.61	0.99
1:A:742:ARG:HA	1:A:742:ARG:HE	0.83	0.98
1:B:106:ASN:HD21	1:B:107:PRO:C	1.72	0.98
1:A:240:LEU:HD23	1:B:228:ILE:HD11	1.47	0.97
1:A:742:ARG:HE	1:A:742:ARG:CA	1.77	0.95
1:A:211:ASN:O	1:A:213:PRO:HD3	1.67	0.94
1:B:478:ASN:ND2	1:B:499:ARG:HH12	1.68	0.91
1:A:288:GLN:HE21	1:A:288:GLN:HA	1.36	0.90
1:B:106:ASN:ND2	1:B:107:PRO:C	2.30	0.90
1:B:130:ARG:HG2	1:B:130:ARG:HH11	1.37	0.88
1:A:90:THR:CG2	1:A:166:ARG:HE	1.86	0.88
1:B:106:ASN:CG	1:B:107:PRO:N	2.30	0.88
1:B:52:THR:HB	1:B:55:GLU:HB3	1.56	0.87
1:A:446:LEU:HB3	1:A:602:MET:HE2	1.57	0.86
1:B:478:ASN:HD21	1:B:499:ARG:NH1	1.72	0.86
1:B:478:ASN:HD21	1:B:499:ARG:HH12	0.88	0.86
1:B:394:ILE:HD11	1:B:717:TYR:HD2	1.40	0.85
1:B:108:HIS:C	1:B:110:GLY:N	2.30	0.84
1:B:688:GLN:HA	1:B:691:VAL:HG13	1.60	0.84
1:A:265:THR:O	1:A:266:ASN:HB2	1.78	0.82
1:A:693:LYS:O	1:A:697:GLU:HG3	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HD23	1:B:228:ILE:CD1	2.09	0.81
1:B:527:LEU:O	1:B:531:ILE:HG23	1.81	0.81
1:B:106:ASN:ND2	1:B:108:HIS:N	2.30	0.80
1:B:106:ASN:ND2	1:B:107:PRO:N	2.30	0.79
1:A:713:ALA:O	1:A:715:PRO:CD	2.30	0.79
1:B:429:CYS:SG	4:B:803:GDP:H3'	2.22	0.79
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.65	0.78
1:A:30:ASN:HD21	1:A:33:PHE:HD1	1.32	0.78
1:B:221:LEU:HA	1:B:436:THR:HG21	1.65	0.78
1:A:92:LYS:HE2	1:A:92:LYS:H	1.48	0.77
1:A:218:CYS:HB3	4:A:803:GDP:O2'	1.85	0.76
1:A:223:MET:CE	1:A:231:ILE:HA	2.14	0.76
1:A:256:ARG:HG3	1:A:256:ARG:NH1	1.96	0.74
1:A:349:SER:HB2	1:A:380:VAL:CG2	2.17	0.74
1:B:518:PRO:HG2	1:B:521:SER:HB3	1.70	0.74
1:A:90:THR:HG21	1:A:166:ARG:NE	2.02	0.74
1:B:127:ASN:O	1:B:129:ASP:N	2.20	0.74
1:B:394:ILE:CD1	1:B:717:TYR:HD2	2.00	0.74
1:A:223:MET:HE2	1:A:231:ILE:HG12	1.70	0.73
1:B:504:GLY:HA3	1:B:602:MET:HE1	1.71	0.73
1:B:127:ASN:O	1:B:128:LYS:C	2.30	0.73
1:B:530:GLN:O	1:B:534:THR:HG22	1.88	0.73
1:A:662:CYS:C	1:A:664:GLY:H	1.97	0.72
1:B:109:ASN:O	1:B:110:GLY:C	2.32	0.71
1:A:256:ARG:HH11	1:A:256:ARG:CG	1.99	0.71
1:A:414:LYS:HB3	1:A:570:MET:HB3	1.73	0.71
1:B:374:TYR:HE2	1:B:379:ARG:NH1	1.89	0.71
1:A:135:ILE:HG21	1:A:137:TYR:CE2	2.25	0.71
1:A:534:THR:HB	1:A:579:TRP:HE1	1.56	0.70
1:A:273:VAL:HG22	1:A:314:LEU:HD21	1.72	0.69
1:B:510:ASP:OD1	1:B:640:HIS:HE1	1.75	0.69
1:B:71:HIS:HD2	1:B:73:ASP:H	1.40	0.69
1:A:476:ASN:O	1:A:480:ILE:HD12	1.93	0.69
1:B:394:ILE:HD11	1:B:717:TYR:CD2	2.25	0.69
1:A:465:LYS:O	1:A:469:VAL:HG23	1.93	0.68
1:A:374:TYR:HE2	1:A:379:ARG:HH21	1.40	0.68
1:A:456:THR:C	1:A:458:GLU:H	1.99	0.68
1:A:221:LEU:HA	1:A:436:THR:HG21	1.76	0.68
1:B:129:ASP:CG	1:B:130:ARG:N	2.52	0.67
1:B:451:LEU:HD22	1:B:531:ILE:HD12	1.75	0.67
1:A:214:GLN:HE22	1:A:216:SER:HB2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:THR:HB	1:B:403:PRO:HA	1.77	0.67
1:B:709:ASN:OD1	1:B:738:TYR:HB2	1.95	0.67
1:A:261:TYR:CE1	1:A:263:ALA:HA	2.30	0.66
1:A:429:CYS:SG	4:A:803:GDP:H3'	2.35	0.66
1:A:692:LEU:HD23	1:A:708:LEU:HD21	1.78	0.66
1:B:213:PRO:HB2	1:B:215:LEU:HG	1.77	0.66
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.59	0.66
1:A:196:ARG:HG2	1:A:196:ARG:NH1	1.95	0.66
1:A:349:SER:HB2	1:A:380:VAL:HG23	1.77	0.66
1:B:712:ILE:O	1:B:741:THR:HA	1.96	0.66
1:B:256:ARG:HA	1:B:353:PRO:HD2	1.76	0.66
1:B:618:GLU:HB2	1:B:619:PRO:CD	2.26	0.66
1:A:196:ARG:HH11	1:A:196:ARG:CG	2.03	0.65
1:B:83:VAL:HG21	1:B:140:ASP:HB3	1.76	0.65
1:B:693:LYS:O	1:B:697:GLU:HG3	1.96	0.65
1:B:126:ALA:O	1:B:127:ASN:ND2	2.30	0.65
1:A:638:ASN:HD22	1:A:641:LEU:HB2	1.59	0.65
1:A:47:LEU:O	1:A:49:SER:N	2.29	0.65
1:A:402:THR:HB	1:A:403:PRO:HA	1.79	0.65
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.31	0.65
1:B:79:ALA:O	1:B:83:VAL:HG12	1.97	0.65
1:B:109:ASN:O	1:B:111:LYS:N	2.30	0.64
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.78	0.64
1:B:126:ALA:C	1:B:127:ASN:ND2	2.54	0.64
1:A:195:GLU:C	1:A:196:ARG:HG3	2.22	0.64
1:B:19:THR:HG23	1:B:36:PRO:HB2	1.80	0.64
1:B:125:LEU:C	1:B:127:ASN:H	2.06	0.64
1:A:719:LYS:O	1:A:723:MET:HG2	1.98	0.63
1:A:90:THR:CG2	1:A:166:ARG:NE	2.58	0.63
1:B:309:PHE:HB2	6:B:931:HOH:O	1.98	0.63
1:A:220:LEU:N	1:A:220:LEU:CD2	2.61	0.63
1:A:478:ASN:OD1	1:A:499:ARG:NH1	2.31	0.63
1:B:351:MET:HE3	1:B:371:TYR:CE1	2.34	0.63
1:A:226:ASP:OD2	1:A:256:ARG:NH1	2.31	0.62
1:A:101:LEU:HD13	1:A:157:LEU:HD13	1.81	0.62
1:A:159:ILE:HG22	1:A:160:ASN:HD22	1.64	0.62
1:B:317:ASN:HA	1:B:326:ARG:HE	1.65	0.62
1:A:662:CYS:O	1:A:664:GLY:N	2.33	0.62
1:A:638:ASN:HD22	1:A:641:LEU:CB	2.13	0.62
1:B:635:GLN:O	1:B:636:ILE:HG13	2.00	0.61
1:A:463:PHE:HD2	1:A:534:THR:HG21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:PRO:HG2	1:A:706:GLN:HB3	1.82	0.60
1:B:84:SER:HA	1:B:87:HIS:HB2	1.82	0.60
1:B:284:ARG:HD2	1:B:327:ASP:OD2	2.02	0.60
1:A:609:GLN:NE2	1:A:627:ARG:HD3	2.17	0.60
1:B:228:ILE:C	1:B:228:ILE:HD12	2.27	0.60
1:B:471:LYS:NZ	1:B:541:GLU:OE1	2.34	0.60
1:B:688:GLN:HA	1:B:691:VAL:CG1	2.31	0.60
1:A:121:LEU:HD22	1:A:125:LEU:HG	1.83	0.59
1:B:222:SER:OG	1:B:436:THR:HB	2.02	0.59
1:B:339:MET:HE3	1:B:725:PHE:CZ	2.38	0.59
1:B:374:TYR:CE2	1:B:379:ARG:NH1	2.69	0.59
1:A:348:TRP:HB2	1:A:386:ALA:HB2	1.83	0.58
1:B:652:HIS:CE1	1:B:655:MET:HB2	2.38	0.58
1:B:710:ILE:HG22	1:B:739:LEU:HD23	1.84	0.58
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.03	0.58
1:B:618:GLU:HB2	1:B:619:PRO:HD2	1.85	0.58
1:B:80:ARG:HA	1:B:83:VAL:HG12	1.84	0.58
1:A:456:THR:C	1:A:458:GLU:N	2.58	0.58
1:B:221:LEU:HD21	1:B:248:ILE:HG21	1.85	0.58
1:B:534:THR:HB	1:B:579:TRP:HE1	1.67	0.58
1:A:286:VAL:O	1:A:286:VAL:CG2	2.52	0.58
1:A:624:ILE:HD12	1:A:624:ILE:O	2.03	0.58
1:A:702:ILE:HG22	1:A:704:GLN:O	2.03	0.58
1:B:120:THR:O	1:B:124:VAL:HG23	2.02	0.58
1:B:220:LEU:HD22	1:B:427:ASN:HB3	1.85	0.58
1:B:337:LEU:HG	1:B:368:GLU:HG2	1.84	0.58
1:A:292:LYS:O	1:A:293:ARG:HB2	2.03	0.58
1:A:159:ILE:HG12	1:A:164:ALA:HB2	1.85	0.57
1:A:288:GLN:HA	1:A:288:GLN:NE2	2.13	0.57
1:A:530:GLN:O	1:A:534:THR:HG22	2.04	0.57
1:B:159:ILE:HG23	1:B:159:ILE:O	2.05	0.57
1:A:286:VAL:O	1:A:286:VAL:HG22	2.04	0.57
1:B:637:VAL:HG13	1:B:642:LEU:HD22	1.87	0.57
1:A:14:MET:HG3	1:A:15:PHE:H	1.69	0.57
1:A:638:ASN:ND2	1:A:641:LEU:HB2	2.19	0.57
3:A:802:TTP:C5M	1:B:243:LYS:HG3	2.33	0.57
1:B:6:ARG:H	1:B:6:ARG:HD3	1.69	0.57
1:A:256:ARG:HD3	1:A:260:SER:HB3	1.86	0.56
1:A:390:TRP:NE1	1:A:721:THR:HG23	2.20	0.56
1:A:356:CYS:HB3	1:A:374:TYR:CD1	2.39	0.56
1:B:108:HIS:O	1:B:110:GLY:N	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:HIS:CE1	1:A:654:GLU:HB3	2.40	0.56
1:B:71:HIS:CD2	1:B:73:ASP:H	2.23	0.56
1:B:602:MET:HG2	1:B:603:PRO:O	2.04	0.56
1:A:15:PHE:CD2	1:A:15:PHE:C	2.83	0.56
1:A:221:LEU:HB3	1:A:441:VAL:HB	1.87	0.56
1:A:260:SER:OG	1:A:352:CYS:SG	2.63	0.56
1:B:86:LEU:HD11	1:B:163:VAL:HG22	1.87	0.56
1:B:191:ASN:O	1:B:195:GLU:HB2	2.06	0.56
1:B:298:ALA:HA	1:B:329:PHE:HB2	1.88	0.55
1:B:451:LEU:HD13	1:B:531:ILE:HD11	1.88	0.55
1:B:481:ILE:HD11	1:B:501:ILE:CD1	2.36	0.55
1:B:518:PRO:HD3	1:B:679:LEU:CD2	2.36	0.55
1:A:232:TYR:OH	1:B:282:THR:HG23	2.06	0.55
1:A:288:GLN:HE21	1:A:288:GLN:CA	2.16	0.55
1:A:390:TRP:HE1	1:A:721:THR:HG23	1.70	0.55
1:A:135:ILE:HG21	1:A:137:TYR:CZ	2.41	0.55
1:B:4:ILE:H	1:B:51:VAL:HG13	1.72	0.55
1:B:125:LEU:C	1:B:127:ASN:N	2.61	0.55
1:B:126:ALA:C	1:B:127:ASN:HD22	2.14	0.55
1:A:349:SER:HB2	1:A:380:VAL:HG21	1.86	0.55
1:B:130:ARG:HH11	1:B:130:ARG:CG	2.14	0.55
1:B:286:VAL:HG22	1:B:286:VAL:O	2.07	0.55
1:B:179:HIS:HD2	1:B:479:LYS:NZ	2.05	0.55
1:A:402:THR:HG22	1:A:404:TYR:CE1	2.42	0.55
1:A:516:ARG:NH2	1:A:644:ASP:OD2	2.30	0.55
1:A:580:ASP:CG	1:A:583:VAL:HG23	2.31	0.55
1:A:705:SER:OG	1:A:706:GLN:N	2.38	0.55
1:A:302:GLU:HG2	1:A:333:TRP:HB3	1.88	0.54
1:A:534:THR:HB	1:A:579:TRP:NE1	2.21	0.54
1:A:416:ASN:HA	1:A:560:PRO:HG2	1.89	0.54
1:A:646:THR:C	1:A:648:ARG:H	2.16	0.54
1:A:662:CYS:C	1:A:664:GLY:N	2.66	0.54
1:B:227:SER:HA	3:B:802:TTP:C5'	2.38	0.54
1:A:90:THR:HG21	1:A:166:ARG:HG2	1.89	0.54
1:B:275:MET:HE3	1:B:276:LEU:HD13	1.90	0.54
1:A:196:ARG:NH1	1:A:196:ARG:CG	2.67	0.53
1:B:518:PRO:HD3	1:B:679:LEU:HD23	1.89	0.53
1:B:117:ALA:HB3	1:B:120:THR:HB	1.90	0.53
1:A:68:THR:OG1	1:A:75:ALA:HB2	2.07	0.53
1:B:504:GLY:HA3	1:B:602:MET:CE	2.37	0.53
1:A:362:VAL:HG22	1:A:366:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:PRO:HD2	1:A:485:TYR:HB2	1.91	0.53
1:A:699:GLY:HA2	1:A:702:ILE:HD12	1.91	0.53
1:B:478:ASN:C	1:B:478:ASN:HD22	2.16	0.53
1:A:474:VAL:HG21	1:A:539:ALA:HA	1.91	0.52
1:B:242:SER:HB3	1:B:286:VAL:HG22	1.92	0.52
1:A:448:SER:HA	1:A:504:GLY:O	2.08	0.52
1:A:498:HIS:O	1:A:596:SER:HB3	2.09	0.52
1:B:160:ASN:O	1:B:162:LYS:N	2.41	0.52
1:A:240:LEU:CD2	1:B:228:ILE:HD11	2.31	0.52
1:B:292:LYS:HE3	1:B:293:ARG:HH11	1.73	0.52
1:B:351:MET:HE3	1:B:371:TYR:HE1	1.73	0.52
1:B:273:VAL:HG22	1:B:314:LEU:HD21	1.92	0.52
1:B:280:ASN:HA	1:B:328:LEU:HD21	1.90	0.52
1:B:315:LYS:NZ	1:B:328:LEU:O	2.36	0.52
1:B:333:TRP:NE1	1:B:408:LYS:HG3	2.24	0.52
1:A:304:TRP:CZ2	1:A:359:LEU:HB3	2.45	0.52
1:A:431:GLU:N	1:A:431:GLU:OE2	2.43	0.51
1:A:414:LYS:HA	1:A:570:MET:SD	2.50	0.51
1:A:703:ASP:HB3	6:A:942:HOH:O	2.11	0.51
1:A:30:ASN:ND2	1:A:33:PHE:HD1	2.05	0.51
1:B:80:ARG:HA	1:B:83:VAL:CG1	2.40	0.51
1:A:223:MET:HE3	1:A:231:ILE:HA	1.93	0.51
1:A:666:ILE:HG23	1:A:677:LYS:HG2	1.92	0.51
1:A:77:LEU:O	1:A:78:ALA:C	2.53	0.51
1:A:364:GLY:N	1:A:409:ASP:OD1	2.38	0.51
1:A:411:CYS:HB3	1:A:433:VAL:HG11	1.92	0.51
1:A:566:LEU:O	1:A:569:ASP:HB2	2.11	0.51
1:A:166:ARG:HG3	1:A:169:HIS:CE1	2.46	0.51
1:A:265:THR:O	1:A:266:ASN:CB	2.53	0.51
1:A:601:PRO:HG2	1:A:706:GLN:CB	2.41	0.51
1:B:223:MET:CG	1:B:255:ILE:HD11	2.40	0.51
1:A:242:SER:HB3	1:A:286:VAL:HG22	1.92	0.51
1:A:565:ILE:HG22	1:A:569:ASP:HB2	1.93	0.51
1:B:93:VAL:HG22	1:B:132:ASN:OD1	2.10	0.51
1:B:478:ASN:OD1	1:B:595:ASN:ND2	2.39	0.51
1:A:213:PRO:O	1:A:215:LEU:HG	2.10	0.50
1:B:365:GLU:CD	1:B:365:GLU:H	2.19	0.50
1:A:72:PRO:HD3	1:A:642:LEU:HD23	1.92	0.50
1:A:270:ASN:HB3	1:A:274:PRO:HG2	1.93	0.50
1:B:36:PRO:O	1:B:39:ILE:HG22	2.11	0.50
1:B:676:LEU:HD23	1:B:679:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:O	1:A:276:LEU:HB2	2.12	0.50
1:A:300:TYR:HE2	1:A:406:LEU:HD13	1.77	0.50
1:B:40:THR:HG22	1:B:44:ILE:HD12	1.93	0.50
1:B:195:GLU:HB3	1:B:197:TRP:CD1	2.46	0.50
1:A:226:ASP:OD2	1:A:256:ARG:HG3	2.12	0.50
1:A:638:ASN:ND2	1:A:641:LEU:CB	2.75	0.50
1:B:118:LYS:HG3	1:B:211:ASN:OD1	2.11	0.50
1:B:106:ASN:CG	1:B:108:HIS:N	2.70	0.50
1:A:69:THR:HG22	1:A:635:GLN:O	2.12	0.50
1:B:39:ILE:O	1:B:43:VAL:HG23	2.12	0.49
1:B:105:ILE:O	1:B:106:ASN:O	2.30	0.49
1:B:219:PHE:O	1:B:248:ILE:HA	2.11	0.49
1:B:292:LYS:HE3	1:B:293:ARG:NH1	2.26	0.49
1:A:71:HIS:CG	1:A:72:PRO:HD2	2.46	0.49
1:B:109:ASN:C	1:B:111:LYS:N	2.70	0.49
1:B:139:ARG:HD3	1:B:194:SER:OG	2.11	0.49
1:B:484:ASN:OD1	1:B:485:TYR:N	2.45	0.49
1:B:533:GLU:HG2	1:B:701:PHE:CZ	2.48	0.49
1:A:76:ILE:O	1:A:80:ARG:HG2	2.11	0.49
1:B:136:ILE:HB	1:B:139:ARG:HD2	1.94	0.49
1:B:287:ASP:C	1:B:289:GLY:H	2.21	0.49
1:B:500:PRO:O	1:B:501:ILE:HD13	2.12	0.49
1:B:261:TYR:CE1	1:B:263:ALA:HA	2.48	0.49
1:A:343:GLU:HB3	1:A:725:PHE:CE2	2.48	0.49
1:A:414:LYS:HB3	1:A:570:MET:CB	2.43	0.49
1:B:262:ILE:HD12	3:B:802:TTP:O4'	2.12	0.49
1:B:105:ILE:C	1:B:106:ASN:O	2.56	0.48
1:B:214:GLN:OE1	1:B:244:SER:HB3	2.12	0.48
1:B:339:MET:HE3	1:B:725:PHE:CE2	2.49	0.48
1:A:477:LEU:HA	1:A:480:ILE:HD13	1.94	0.48
1:B:106:ASN:OD1	1:B:108:HIS:N	2.46	0.48
1:A:90:THR:HG21	1:A:166:ARG:CG	2.44	0.48
1:B:427:ASN:ND2	1:B:429:CYS:H	2.11	0.48
1:A:48:TYR:HA	1:A:51:VAL:HG22	1.95	0.48
1:B:480:ILE:O	1:B:481:ILE:C	2.55	0.48
1:A:365:GLU:H	1:A:365:GLU:CD	2.21	0.48
1:B:225:ASP:OD2	1:B:225:ASP:C	2.56	0.48
1:B:227:SER:HA	3:B:802:TTP:H5'2	1.95	0.48
1:A:220:LEU:N	1:A:220:LEU:HD23	2.29	0.48
1:A:712:ILE:O	1:A:741:THR:HG22	2.13	0.48
1:A:86:LEU:O	1:A:90:THR:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ASN:CG	1:B:292:LYS:H	2.22	0.48
1:B:3:VAL:HG13	1:B:51:VAL:HA	1.95	0.48
1:A:48:TYR:C	1:A:50:GLY:H	2.22	0.47
1:A:146:PHE:O	1:A:150:THR:OG1	2.32	0.47
1:A:683:VAL:C	1:A:685:GLU:H	2.20	0.47
1:A:325:ALA:HB1	1:A:328:LEU:HD12	1.96	0.47
1:B:129:ASP:CG	1:B:130:ARG:H	2.22	0.47
1:A:23:GLN:C	1:A:25:LEU:H	2.22	0.47
1:A:242:SER:O	1:A:245:ALA:N	2.48	0.47
1:A:352:CYS:C	1:A:354:ASN:H	2.23	0.47
1:A:416:ASN:OD1	1:A:561:VAL:HG13	2.14	0.47
1:B:299:ILE:HD13	1:B:328:LEU:HD13	1.97	0.47
1:B:111:LYS:O	1:B:113:SER:OG	2.31	0.47
1:B:44:ILE:O	1:B:44:ILE:CG2	2.62	0.47
1:A:202:SER:O	1:A:203:PRO:C	2.57	0.46
1:A:284:ARG:HA	1:A:294:PRO:HB3	1.96	0.46
1:B:6:ARG:HB3	1:B:53:THR:HB	1.97	0.46
1:B:481:ILE:HD11	1:B:501:ILE:HD13	1.97	0.46
1:A:349:SER:OG	1:A:375:GLU:OE1	2.22	0.46
1:A:336:ASP:O	1:A:337:LEU:C	2.57	0.46
1:A:513:ILE:HG21	1:A:680:TYR:HE2	1.79	0.46
1:A:617:ILE:H	1:A:617:ILE:HG13	1.59	0.46
1:A:281:ASN:N	1:A:281:ASN:HD22	2.11	0.46
1:A:396:SER:O	1:A:400:THR:N	2.35	0.46
1:B:179:HIS:HD2	1:B:479:LYS:HZ3	1.62	0.46
1:B:441:VAL:HG12	1:B:490:GLU:HB2	1.97	0.46
1:B:6:ARG:HD2	1:B:53:THR:HG21	1.97	0.46
1:B:602:MET:HE3	1:B:604:THR:HG23	1.97	0.46
1:B:742:ARG:HA	1:B:742:ARG:NH1	2.30	0.46
1:A:144:ASN:H	1:A:144:ASN:HD22	1.64	0.46
1:B:18:ILE:O	1:B:22:ILE:HG12	2.16	0.46
1:A:220:LEU:HB2	1:A:442:ALA:HB3	1.97	0.46
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.82	0.46
1:B:532:PHE:CD2	1:B:698:ARG:HG3	2.51	0.46
1:B:121:LEU:C	1:B:123:ILE:N	2.71	0.46
1:B:291:ASN:CG	1:B:292:LYS:N	2.73	0.46
1:B:666:ILE:HD11	1:B:680:TYR:HB2	1.98	0.46
1:A:149:LYS:HG2	1:A:629:VAL:HG11	1.98	0.46
1:A:641:LEU:HD21	1:A:666:ILE:HD13	1.97	0.45
1:A:652:HIS:ND1	1:A:654:GLU:HB3	2.31	0.45
1:B:86:LEU:HD11	1:B:163:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:SER:O	1:A:49:SER:OG	2.30	0.45
1:A:553:TYR:CZ	1:A:556:TYR:HA	2.51	0.45
1:B:39:ILE:HD11	1:B:64:ALA:HB2	1.98	0.45
1:B:106:ASN:HD21	1:B:108:HIS:CA	2.27	0.45
1:A:211:ASN:O	1:A:213:PRO:CD	2.52	0.45
1:A:532:PHE:CE2	1:A:698:ARG:HD3	2.52	0.45
1:B:149:LYS:HA	1:B:152:GLU:HG2	1.98	0.45
1:A:14:MET:HG3	1:A:15:PHE:N	2.30	0.45
1:A:419:ASN:OD1	1:A:419:ASN:N	2.50	0.45
1:B:106:ASN:HD21	1:B:108:HIS:CB	2.30	0.45
1:A:256:ARG:HG2	1:A:354:ASN:HB2	1.99	0.45
1:B:263:ALA:HB3	3:B:802:TTP:O1G	2.17	0.45
1:A:571:TRP:CD1	1:A:700:ALA:HA	2.52	0.45
1:A:682:THR:N	1:A:685:GLU:OE1	2.46	0.45
1:B:238:CYS:O	1:B:242:SER:HB2	2.17	0.45
1:B:498:HIS:O	1:B:596:SER:OG	2.28	0.45
1:A:536:TYR:CZ	1:A:540:LEU:HD11	2.51	0.45
1:A:641:LEU:O	1:A:645:LEU:HG	2.16	0.45
1:A:23:GLN:C	1:A:25:LEU:N	2.75	0.45
1:B:130:ARG:NH2	1:B:187:ILE:HD12	2.32	0.45
1:A:703:ASP:HB2	6:A:941:HOH:O	2.15	0.45
1:B:225:ASP:OD2	1:B:227:SER:OG	2.23	0.45
1:B:286:VAL:O	1:B:286:VAL:CG2	2.64	0.45
1:B:517:TYR:CE1	1:B:523:GLU:HB3	2.52	0.45
1:A:424:LYS:O	1:A:425:CYS:HB3	2.17	0.44
1:A:374:TYR:HE2	1:A:379:ARG:NH2	2.11	0.44
1:A:470:THR:O	1:A:474:VAL:HG23	2.17	0.44
1:B:501:ILE:HD12	1:B:501:ILE:HA	1.66	0.44
1:A:565:ILE:HG23	1:A:569:ASP:HB3	1.99	0.44
1:A:641:LEU:HD13	1:A:680:TYR:CD1	2.53	0.44
1:B:202:SER:HB2	1:B:203:PRO:HD3	1.99	0.44
1:B:253:SER:OG	1:B:302:GLU:HG3	2.17	0.44
1:A:456:THR:O	1:A:458:GLU:N	2.50	0.44
1:B:39:ILE:CG2	1:B:40:THR:N	2.80	0.44
1:B:108:HIS:N	1:B:110:GLY:H	2.14	0.44
1:B:121:LEU:HD12	1:B:122:ASP:N	2.33	0.44
1:B:166:ARG:O	1:B:169:HIS:HB2	2.18	0.44
1:B:518:PRO:CD	1:B:679:LEU:HD23	2.47	0.44
1:B:584:LEU:O	1:B:587:LYS:HG2	2.16	0.44
1:B:221:LEU:CD2	1:B:248:ILE:CG2	2.96	0.44
1:B:650:LEU:HD12	1:B:671:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASN:HD21	1:A:111:LYS:CB	2.30	0.44
1:A:287:ASP:O	1:A:288:GLN:HB2	2.17	0.44
1:A:567:GLN:HA	1:A:570:MET:HE3	1.99	0.44
1:A:742:ARG:NE	1:A:742:ARG:CA	2.51	0.44
1:B:108:HIS:H	1:B:110:GLY:H	1.66	0.44
1:B:123:ILE:O	1:B:126:ALA:HB3	2.17	0.44
1:B:532:PHE:CG	1:B:698:ARG:HG3	2.53	0.44
1:A:52:THR:HG23	1:A:55:GLU:OE1	2.18	0.44
1:B:527:LEU:O	1:B:527:LEU:HG	2.18	0.44
1:A:337:LEU:HD21	1:A:371:TYR:HD2	1.82	0.44
1:B:560:PRO:O	1:B:565:ILE:HB	2.18	0.44
1:A:270:ASN:HD22	1:A:270:ASN:HA	1.66	0.43
1:A:624:ILE:HG12	1:A:660:ILE:HG13	2.00	0.43
1:B:481:ILE:HD11	1:B:501:ILE:HD11	1.98	0.43
1:B:566:LEU:HD12	1:B:568:TYR:OH	2.18	0.43
1:A:389:LEU:O	1:A:390:TRP:C	2.61	0.43
1:A:567:GLN:HA	1:A:567:GLN:NE2	2.33	0.43
1:B:197:TRP:CZ3	1:B:465:LYS:HD3	2.52	0.43
1:B:242:SER:HB3	1:B:286:VAL:CG2	2.48	0.43
1:B:359:LEU:HD12	1:B:359:LEU:HA	1.82	0.43
1:B:587:LYS:HG2	1:B:587:LYS:H	1.66	0.43
1:B:95:SER:HB3	1:B:132:ASN:HD21	1.81	0.43
1:B:675:ASP:O	1:B:679:LEU:HG	2.18	0.43
1:A:486:TYR:HA	1:A:487:PRO:HD3	1.82	0.43
1:A:106:ASN:OD1	1:A:106:ASN:C	2.62	0.43
1:A:214:GLN:NE2	1:A:216:SER:HB2	2.30	0.43
1:A:363:TRP:CH2	1:A:413:ARG:HA	2.54	0.43
1:B:220:LEU:N	1:B:220:LEU:HD23	2.34	0.43
1:A:261:TYR:HE1	1:A:263:ALA:HA	1.80	0.43
1:A:411:CYS:SG	1:A:733:LYS:HB3	2.58	0.43
1:A:463:PHE:CE2	1:A:530:GLN:HB3	2.54	0.43
1:A:638:ASN:ND2	1:A:641:LEU:H	2.16	0.43
1:B:275:MET:CE	1:B:276:LEU:HD13	2.49	0.43
1:B:402:THR:HG22	1:B:404:TYR:CE1	2.54	0.43
1:B:451:LEU:HD11	1:B:505:VAL:HG21	2.01	0.43
1:B:94:PHE:HB2	1:B:135:ILE:CD1	2.49	0.43
1:B:257:ALA:CB	1:B:306:LEU:HB3	2.49	0.43
1:A:92:LYS:HE2	1:A:92:LYS:N	2.23	0.42
1:A:655:MET:HG2	1:A:659:ILE:HD12	2.01	0.42
1:B:140:ASP:OD2	1:B:168:GLN:HG2	2.18	0.42
1:B:416:ASN:OD1	1:B:561:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ASN:HA	1:B:481:ILE:HD12	2.01	0.42
1:B:105:ILE:O	1:B:106:ASN:C	2.62	0.42
1:B:429:CYS:HB2	1:B:431:GLU:OE1	2.19	0.42
1:A:248:ILE:HG22	1:A:249:GLY:N	2.34	0.42
1:A:402:THR:HG22	1:A:404:TYR:CD1	2.54	0.42
1:A:509:ALA:O	1:A:513:ILE:HG12	2.19	0.42
1:B:580:ASP:O	1:B:581:TRP:HB2	2.19	0.42
1:A:338:PHE:HB2	1:A:348:TRP:CH2	2.55	0.42
1:B:248:ILE:HG22	1:B:249:GLY:N	2.34	0.42
1:A:337:LEU:CD2	1:A:371:TYR:HD2	2.32	0.42
1:B:544:CYS:HA	1:B:592:GLY:O	2.19	0.42
1:B:726:TYR:CD2	1:B:726:TYR:C	2.98	0.42
1:B:3:VAL:HG22	1:B:51:VAL:HA	2.01	0.42
1:B:638:ASN:HA	1:B:639:PRO:HD3	1.88	0.42
1:A:287:ASP:O	1:A:287:ASP:CG	2.63	0.42
1:B:93:VAL:HG22	1:B:132:ASN:CG	2.44	0.42
1:B:227:SER:HA	3:B:802:TTP:H5'1	2.02	0.42
1:B:520:GLU:CD	1:B:686:ILE:HG23	2.45	0.42
1:B:2:HIS:N	1:B:13:VAL:HG23	2.34	0.42
1:B:337:LEU:HD22	1:B:341:ARG:HG2	2.02	0.42
1:B:534:THR:HB	1:B:579:TRP:NE1	2.33	0.42
1:A:351:MET:H	1:A:351:MET:HG2	1.72	0.42
1:B:58:THR:O	1:B:59:LEU:C	2.61	0.42
1:A:207:ASN:O	1:A:208:ALA:C	2.62	0.41
1:A:214:GLN:NE2	1:A:216:SER:H	2.17	0.41
1:A:493:LEU:O	1:A:494:SER:C	2.62	0.41
1:A:637:VAL:HB	1:A:642:LEU:HD22	2.01	0.41
1:A:130:ARG:HH11	1:A:130:ARG:HG3	1.85	0.41
1:A:256:ARG:NH2	3:A:802:TTP:O3G	2.44	0.41
1:B:348:TRP:HB2	1:B:386:ALA:HB2	2.01	0.41
1:B:451:LEU:HD13	1:B:531:ILE:CD1	2.49	0.41
1:A:280:ASN:HD22	1:A:281:ASN:ND2	2.19	0.41
1:A:369:LYS:HE2	1:A:369:LYS:HB3	1.80	0.41
1:B:72:PRO:HD3	1:B:642:LEU:HD23	2.02	0.41
1:A:26:CYS:O	1:A:28:GLY:N	2.54	0.41
1:A:321:GLU:C	1:A:323:GLN:H	2.29	0.41
1:B:129:ASP:OD2	1:B:130:ARG:HG3	2.20	0.41
1:B:292:LYS:HB3	1:B:293:ARG:H	1.73	0.41
1:A:359:LEU:HD12	1:A:359:LEU:HA	1.81	0.41
1:A:618:GLU:HA	1:A:619:PRO:HD2	1.84	0.41
1:A:242:SER:HB3	1:A:286:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ILE:HD11	1:A:269:SER:HA	2.01	0.41
1:A:352:CYS:SG	1:A:354:ASN:HB3	2.61	0.41
1:A:478:ASN:CG	1:A:499:ARG:HH12	2.28	0.41
1:A:568:TYR:HD2	1:A:573:VAL:O	2.03	0.41
1:A:590:LYS:HD3	1:A:591:TYR:CZ	2.56	0.41
1:A:615:GLU:CD	1:A:615:GLU:H	2.27	0.41
1:A:192:LEU:HD12	1:A:192:LEU:HA	2.00	0.41
1:A:257:ALA:O	1:A:260:SER:HB2	2.20	0.41
1:A:352:CYS:C	1:A:354:ASN:N	2.78	0.41
1:A:713:ALA:HB1	1:A:742:ARG:HG2	2.02	0.41
1:B:130:ARG:HG2	1:B:130:ARG:NH1	2.16	0.41
1:B:244:SER:O	1:B:245:ALA:HB3	2.19	0.41
1:B:364:GLY:N	1:B:409:ASP:OD2	2.51	0.41
1:B:510:ASP:OD1	1:B:640:HIS:CE1	2.64	0.41
1:A:280:ASN:HD22	1:A:281:ASN:HD22	1.69	0.41
1:B:44:ILE:O	1:B:44:ILE:HG22	2.20	0.41
1:B:69:THR:HG22	1:B:637:VAL:HG12	2.02	0.41
1:A:309:PHE:O	1:A:313:ASP:OD1	2.38	0.41
1:A:380:VAL:HG22	1:A:382:LYS:H	1.86	0.41
1:A:493:LEU:HD22	1:A:497:ARG:HG3	2.03	0.41
1:A:515:MET:O	1:A:516:ARG:HB2	2.21	0.41
1:A:570:MET:HE1	6:A:943:HOH:O	2.19	0.41
1:B:106:ASN:ND2	1:B:107:PRO:CA	2.81	0.41
1:B:203:PRO:HG2	1:B:217:SER:HB3	2.03	0.41
1:B:471:LYS:HG2	1:B:542:ALA:HB2	2.03	0.41
1:B:477:LEU:HA	1:B:480:ILE:HD12	2.01	0.41
1:A:256:ARG:CD	1:A:260:SER:HB3	2.51	0.41
1:B:73:ASP:HA	1:B:76:ILE:HG13	2.03	0.41
1:B:456:THR:HG22	1:B:458:GLU:H	1.86	0.41
1:A:220:LEU:N	1:A:220:LEU:HD22	2.35	0.40
1:A:581:TRP:O	1:A:582:LYS:C	2.63	0.40
1:B:124:VAL:O	1:B:127:ASN:N	2.53	0.40
1:B:406:LEU:HD22	1:B:426:SER:HB2	2.03	0.40
1:A:397:GLN:HG2	1:A:403:PRO:HD2	2.02	0.40
1:B:293:ARG:HA	1:B:294:PRO:HD2	1.65	0.40
1:A:90:THR:HG22	1:A:166:ARG:HE	1.78	0.40
1:A:195:GLU:O	1:A:453:MET:HE2	2.22	0.40
1:A:288:GLN:NE2	1:A:288:GLN:CA	2.79	0.40
1:A:337:LEU:CD2	1:A:371:TYR:CD2	3.04	0.40
1:A:492:CYS:O	1:A:496:LYS:HG2	2.21	0.40
1:A:567:GLN:HA	6:A:943:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PHE:CD2	1:B:199:THR:N	2.90	0.40
1:A:226:ASP:O	3:A:802:TTP:H5'2	2.20	0.40
1:B:536:TYR:O	1:B:537:TYR:C	2.64	0.40
1:B:650:LEU:HD13	1:B:650:LEU:HA	1.92	0.40
1:A:295:GLY:O	1:A:296:ALA:HB3	2.21	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	727/792 (92%)	625 (86%)	84 (12%)	18 (2%)	4	25
1	B	730/792 (92%)	629 (86%)	81 (11%)	20 (3%)	4	24
All	All	1457/1584 (92%)	1254 (86%)	165 (11%)	38 (3%)	4	25

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	TYR
1	A	128	LYS
1	A	224	LYS
1	A	266	ASN
1	A	663	ASN
1	A	714	GLU
1	B	31	MET
1	B	107	PRO
1	B	128	LYS
1	B	161	GLY
1	B	648	ARG
1	A	295	GLY
1	A	457	SER

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Mol	Chain	Res	Type
1	B	109	ASN
1	B	110	GLY
1	B	224	LYS
1	B	718	GLY
1	A	28	GLY
1	A	260	SER
1	A	292	LYS
1	A	377	GLN
1	A	737	TYR
1	B	106	ASN
1	B	292	LYS
1	B	663	ASN
1	A	647	GLU
1	B	160	ASN
1	B	418	GLN
1	A	425	CYS
1	B	91	LYS
1	B	154	SER
1	A	494	SER
1	B	560	PRO
1	B	638	ASN
1	A	393	ILE
1	A	560	PRO
1	B	601	PRO
1	B	636	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	609/693 (88%)	520 (85%)	89 (15%)	3	15
1	B	590/693 (85%)	501 (85%)	89 (15%)	3	13
All	All	1199/1386 (86%)	1021 (85%)	178 (15%)	3	14

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	16	ASP
1	A	23	GLN
1	A	30	ASN
1	A	41	MET
1	A	45	GLN
1	A	48	TYR
1	A	49	SER
1	A	52	THR
1	A	53	THR
1	A	57	ASP
1	A	58	THR
1	A	59	LEU
1	A	62	GLU
1	A	68	THR
1	A	80	ARG
1	A	90	THR
1	A	92	LYS
1	A	93	VAL
1	A	105	ILE
1	A	121	LEU
1	A	129	ASP
1	A	138	ASP
1	A	144	ASN
1	A	149	LYS
1	A	150	THR
1	A	171	LEU
1	A	175	SER
1	A	181	GLU
1	A	192	LEU
1	A	196	ARG
1	A	217	SER
1	A	218	CYS
1	A	220	LEU
1	A	237	GLN
1	A	252	VAL
1	A	256	ARG
1	A	260	SER
1	A	276	LEU
1	A	286	VAL
1	A	288	GLN
1	A	291	ASN
1	A	312	LEU

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Mol	Chain	Res	Type
1	A	316	LYS
1	A	318	THR
1	A	322	GLU
1	A	351	MET
1	A	352	CYS
1	A	368	GLU
1	A	387	GLN
1	A	389	LEU
1	A	414	LYS
1	A	436	THR
1	A	441	VAL
1	A	443	VAL
1	A	449	LEU
1	A	455	VAL
1	A	480	ILE
1	A	483	ILE
1	A	493	LEU
1	A	494	SER
1	A	497	ARG
1	A	508	LEU
1	A	520	GLU
1	A	534	THR
1	A	540	LEU
1	A	561	VAL
1	A	565	ILE
1	A	574	THR
1	A	578	LEU
1	A	597	LEU
1	A	599	ILE
1	A	607	THR
1	A	615	GLU
1	A	617	ILE
1	A	626	THR
1	A	627	ARG
1	A	628	ARG
1	A	654	GLU
1	A	656	LYS
1	A	659	ILE
1	A	660	ILE
1	A	674	ASP
1	A	679	LEU
1	A	693	LYS

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Mol	Chain	Res	Type
1	A	716	ASN
1	A	720	LEU
1	A	740	ARG
1	A	742	ARG
1	B	6	ARG
1	B	16	ASP
1	B	20	SER
1	B	22	ILE
1	B	31	MET
1	B	39	ILE
1	B	47	LEU
1	B	59	LEU
1	B	66	THR
1	B	76	ILE
1	B	89	GLU
1	B	91	LYS
1	B	93	VAL
1	B	99	GLU
1	B	106	ASN
1	B	113	SER
1	B	116	VAL
1	B	118	LYS
1	B	121	LEU
1	B	130	ARG
1	B	138	ASP
1	B	159	ILE
1	B	163	VAL
1	B	176	VAL
1	B	195	GLU
1	B	217	SER
1	B	220	LEU
1	B	222	SER
1	B	228	ILE
1	B	250	VAL
1	B	255	ILE
1	B	270	ASN
1	B	275	MET
1	B	276	LEU
1	B	286	VAL
1	B	288	GLN
1	B	293	ARG
1	B	299	ILE

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Mol	Chain	Res	Type
1	B	301	LEU
1	B	316	LYS
1	B	318	THR
1	B	323	GLN
1	B	337	LEU
1	B	359	LEU
1	B	365	GLU
1	B	379	ARG
1	B	383	VAL
1	B	385	LYS
1	B	389	LEU
1	B	395	GLU
1	B	398	THR
1	B	436	THR
1	B	439	ASP
1	B	441	VAL
1	B	443	VAL
1	B	445	ASN
1	B	460	THR
1	B	474	VAL
1	B	478	ASN
1	B	483	ILE
1	B	488	VAL
1	B	493	LEU
1	B	494	SER
1	B	501	ILE
1	B	505	VAL
1	B	508	LEU
1	B	529	LYS
1	B	531	ILE
1	B	534	THR
1	B	583	VAL
1	B	587	LYS
1	B	590	LYS
1	B	602	MET
1	B	604	THR
1	B	609	GLN
1	B	624	ILE
1	B	637	VAL
1	B	643	LYS
1	B	648	ARG
1	B	650	LEU

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Mol	Chain	Res	Type
1	B	655	MET
1	B	672	ILE
1	B	691	VAL
1	B	692	LEU
1	B	706	GLN
1	B	707	SER
1	B	708	LEU
1	B	710	ILE
1	B	739	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	127	ASN
1	A	144	ASN
1	A	160	ASN
1	A	214	GLN
1	A	237	GLN
1	A	270	ASN
1	A	281	ASN
1	A	288	GLN
1	A	323	GLN
1	A	377	GLN
1	A	495	ASN
1	A	613	ASN
1	A	638	ASN
1	A	652	HIS
1	A	657	ASN
1	A	667	GLN
1	A	688	GLN
1	A	724	HIS
1	B	30	ASN
1	B	85	ASN
1	B	106	ASN
1	B	127	ASN
1	B	144	ASN
1	B	179	HIS
1	B	200	HIS
1	B	237	GLN
1	B	346	GLN
1	B	459	HIS

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Mol	Chain	Res	Type
1	B	478	ASN
1	B	595	ASN
1	B	640	HIS
1	B	678	GLN
1	B	730	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
5	SO4	A	805	-	4,4,4	0.26	0	6,6,6	0.37	0
3	TTP	B	802	2	29,30,30	1.35	4 (13%)	43,47,47	2.21	9 (20%)
5	SO4	A	806	-	4,4,4	0.28	0	6,6,6	0.14	0
4	GDP	B	803	-	29,30,30	1.34	3 (10%)	45,47,47	1.77	7 (15%)
5	SO4	B	804	-	4,4,4	0.19	0	6,6,6	0.29	0
3	TTP	A	802	2	29,30,30	1.18	4 (13%)	43,47,47	2.12	10 (23%)
5	SO4	A	807	-	4,4,4	0.27	0	6,6,6	0.16	0
4	GDP	A	803	-	29,30,30	1.34	3 (10%)	45,47,47	1.93	9 (20%)

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
4	GDP	B	803	-	-	5/16/32/32	0/3/3/3
4	GDP	A	803	-	-	6/16/32/32	0/3/3/3
3	TTP	B	802	2	-	6/22/34/34	0/2/2/2
3	TTP	A	802	2	-	8/22/34/34	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	GDP	PA-O3A	3.71	1.63	1.59
3	B	802	TTP	C6-C5	3.69	1.40	1.34
4	A	803	GDP	PA-O3A	3.66	1.63	1.59
4	A	803	GDP	C5-C4	3.54	1.48	1.38
4	B	803	GDP	C5-C4	3.42	1.48	1.38
3	B	802	TTP	C4-N3	-3.19	1.32	1.38
3	A	802	TTP	C6-N1	-2.78	1.33	1.38
3	A	802	TTP	C6-C5	2.61	1.38	1.34
3	A	802	TTP	C4-N3	-2.42	1.34	1.38
3	B	802	TTP	C6-N1	-2.23	1.34	1.38
3	A	802	TTP	C4-C5	2.22	1.48	1.44
4	B	803	GDP	C5-N7	-2.20	1.34	1.39
4	A	803	GDP	C6-N1	-2.13	1.34	1.38
3	B	802	TTP	C2-N3	-2.07	1.34	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	GDP	C5-C4-N3	-6.85	117.49	128.39
3	B	802	TTP	N3-C2-N1	6.61	123.50	114.89
4	B	803	GDP	C5-C4-N3	-6.28	118.39	128.39
3	B	802	TTP	C4-N3-C2	-6.25	119.15	127.34
3	A	802	TTP	N3-C2-N1	6.15	122.90	114.89
3	A	802	TTP	C4-N3-C2	-6.04	119.42	127.34
4	A	803	GDP	N9-C4-N3	5.45	136.84	125.95
4	A	803	GDP	C2-N3-C4	5.39	121.58	112.30
4	B	803	GDP	C2-N3-C4	5.11	121.09	112.30
4	B	803	GDP	N9-C4-N3	4.92	135.79	125.95
3	B	802	TTP	C5-C6-N1	-4.91	117.98	123.31
3	B	802	TTP	C5-C4-N3	4.74	119.45	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	TTP	O2-C2-N1	-4.61	116.80	122.80
3	A	802	TTP	C5-C6-N1	-4.33	118.61	123.31
3	B	802	TTP	O4-C4-C5	-4.20	120.12	124.92
3	A	802	TTP	O4-C4-C5	-3.85	120.51	124.92
3	B	802	TTP	O2-C2-N1	-3.68	118.01	122.80
3	A	802	TTP	O2G-PG-O3B	3.62	116.76	104.64
3	A	802	TTP	C5-C4-N3	3.50	118.37	115.32
3	B	802	TTP	O2G-PG-O3B	2.91	114.40	104.64
4	B	803	GDP	O6-C6-C5	-2.78	119.20	126.53
3	A	802	TTP	O2B-PB-O3A	2.76	114.73	107.27
4	A	803	GDP	C6-C5-N7	2.68	135.17	130.29
4	A	803	GDP	O6-C6-C5	-2.58	119.72	126.53
4	B	803	GDP	C6-C5-N7	2.54	134.92	130.29
3	B	802	TTP	O4'-C1'-N1	2.54	112.37	107.86
3	A	802	TTP	O2A-PA-O3A	2.46	113.91	107.27
3	B	802	TTP	O2A-PA-O3A	2.35	113.62	107.27
3	A	802	TTP	C6-C5-C4	2.33	119.94	118.02
4	A	803	GDP	C3'-C2'-C1'	2.21	105.64	101.46
4	A	803	GDP	C5-C6-N1	2.19	118.83	113.25
4	A	803	GDP	O2A-PA-O3A	2.17	113.14	107.27
4	A	803	GDP	C4-C5-N7	-2.12	107.30	110.67
4	B	803	GDP	C2'-C3'-C4'	2.08	106.64	102.61
4	B	803	GDP	C5-C6-N1	2.05	118.47	113.25

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	TTP	C5'-O5'-PA-O1A
3	A	802	TTP	C5'-O5'-PA-O2A
3	A	802	TTP	C5'-O5'-PA-O3A
3	A	802	TTP	PB-O3B-PG-O2G
3	A	802	TTP	PB-O3B-PG-O3G
3	A	802	TTP	O4'-C4'-C5'-O5'
3	B	802	TTP	O4'-C4'-C5'-O5'
4	A	803	GDP	PA-O3A-PB-O2B
4	A	803	GDP	C5'-O5'-PA-O3A
4	A	803	GDP	C5'-O5'-PA-O2A
4	B	803	GDP	C5'-O5'-PA-O3A
4	B	803	GDP	C5'-O5'-PA-O1A
4	B	803	GDP	C5'-O5'-PA-O2A
3	B	802	TTP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	A	802	TTP	C3'-C4'-C5'-O5'
4	B	803	GDP	PA-O3A-PB-O2B
3	B	802	TTP	C5'-O5'-PA-O1A
3	B	802	TTP	PB-O3A-PA-O2A
4	A	803	GDP	C3'-C4'-C5'-O5'
3	A	802	TTP	PB-O3B-PG-O1G
4	A	803	GDP	C4'-C5'-O5'-PA
4	A	803	GDP	O4'-C4'-C5'-O5'
3	B	802	TTP	PB-O3A-PA-O1A
3	B	802	TTP	PG-O3B-PB-O2B
4	B	803	GDP	PB-O3A-PA-O2A

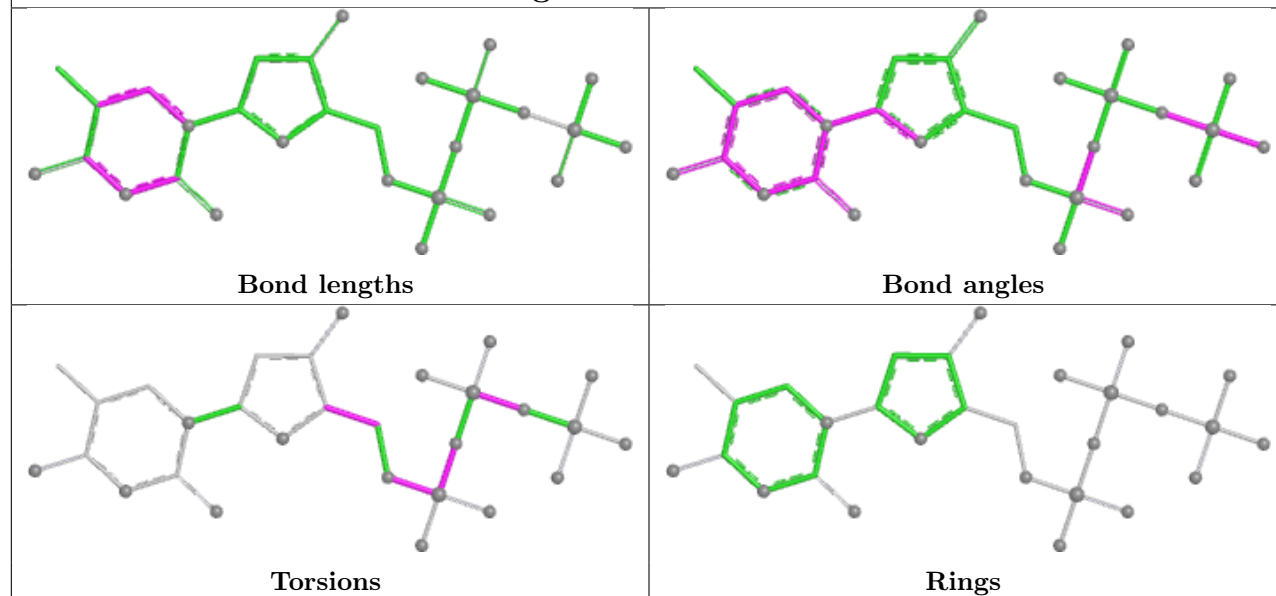
There are no ring outliers.

4 monomers are involved in 11 short contacts:

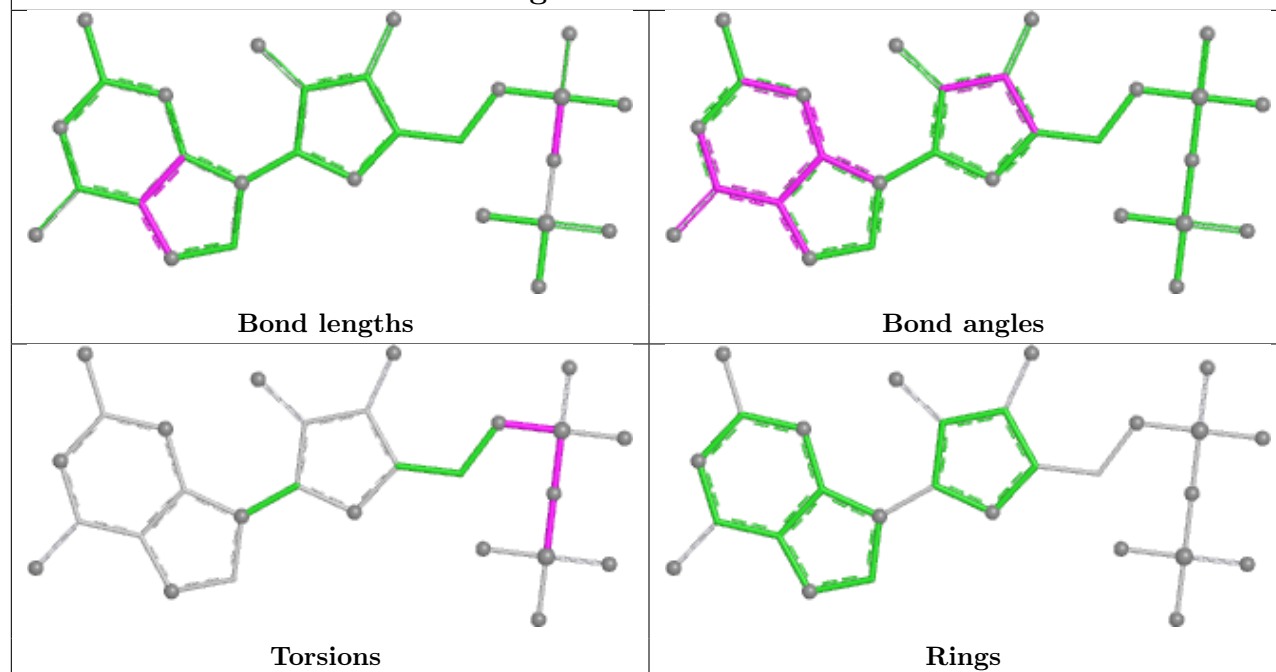
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	TTP	5	0
4	B	803	GDP	1	0
3	A	802	TTP	3	0
4	A	803	GDP	2	0

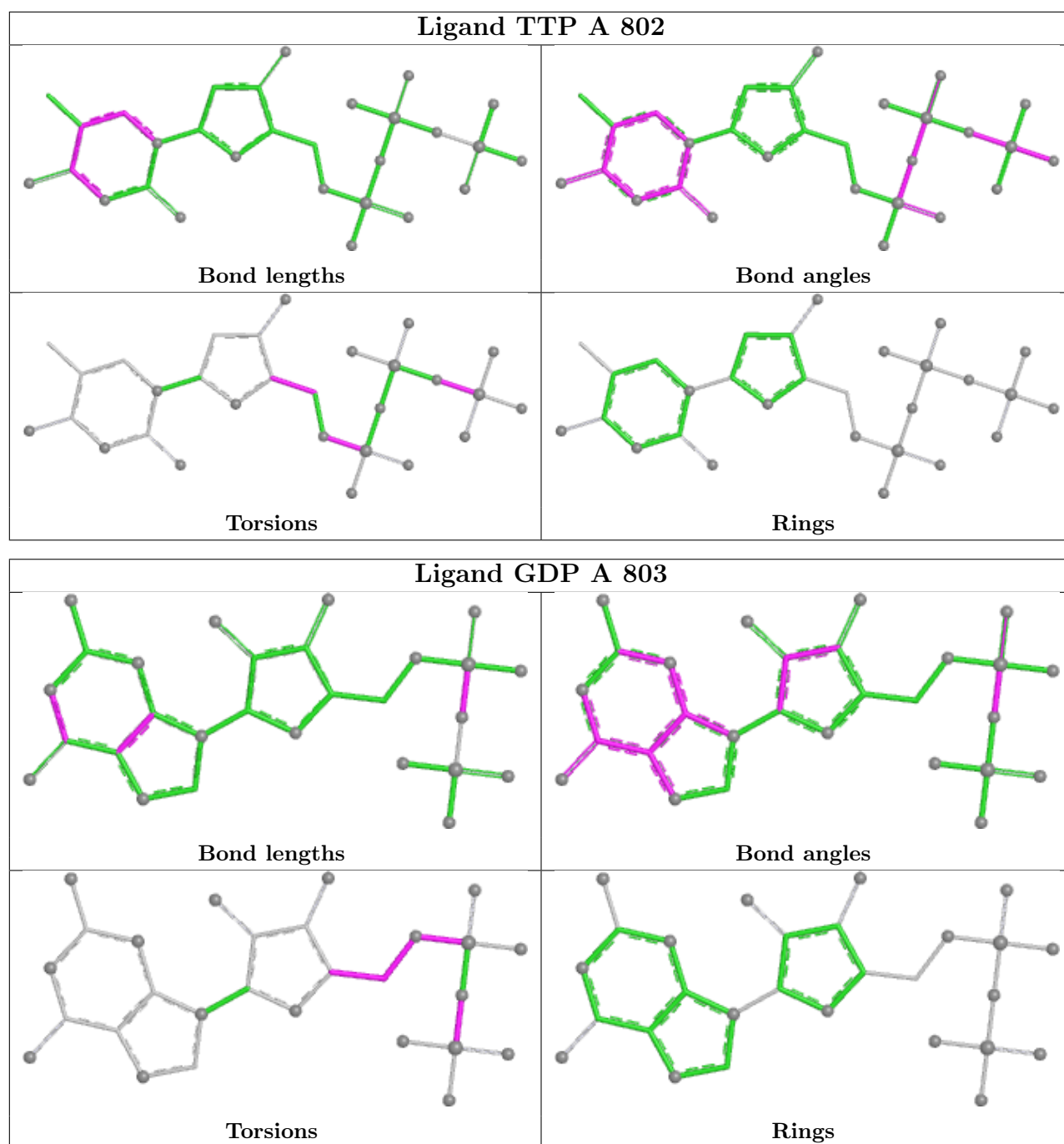
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 TTP B 802



Ligand GDP B 803





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	729/792 (92%)	-0.71	1 (0%) 92 89	73, 97, 126, 149	0
1	B	735/792 (92%)	-0.61	1 (0%) 92 89	70, 107, 150, 198	1 (0%)
All	All	1464/1584 (92%)	-0.66	2 (0%) 92 89	70, 101, 145, 198	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	678	GLN	3.2
1	B	679	LEU	2.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

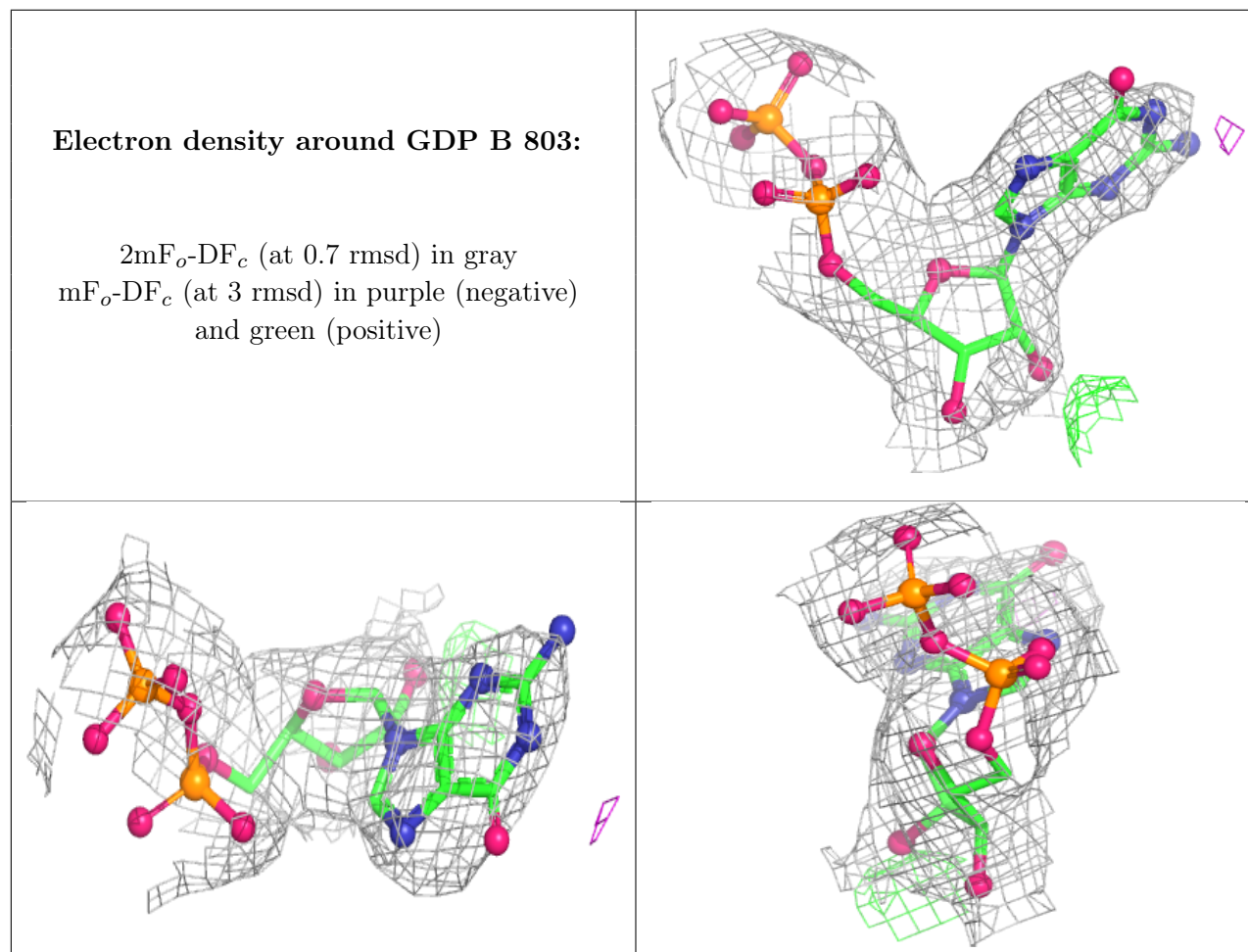
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	801	1/1	0.81	0.16	73,73,73,73	0
2	MG	A	801	1/1	0.82	0.15	92,92,92,92	0
5	SO4	A	807	5/5	0.85	0.06	153,153,153,154	0

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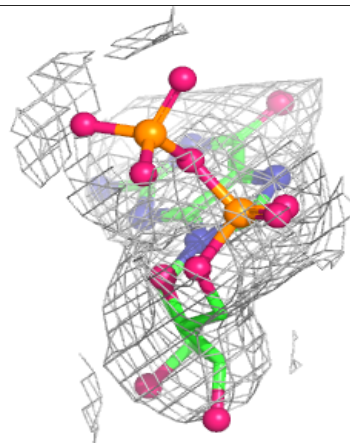
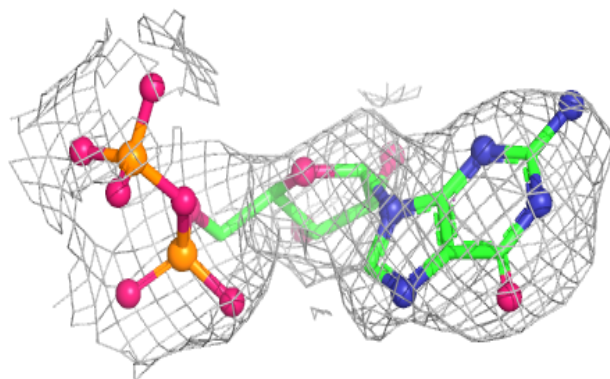
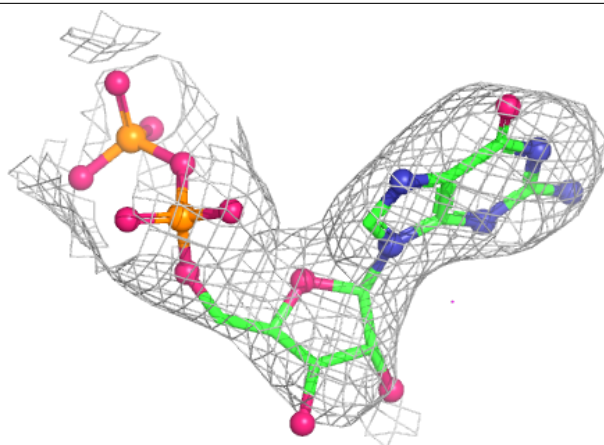
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	A	806	5/5	0.87	0.09	162,163,163,163	0
4	GDP	B	803	28/28	0.90	0.07	113,115,119,119	0
4	GDP	A	803	28/28	0.93	0.08	106,109,109,109	0
5	SO4	B	804	5/5	0.93	0.05	153,153,153,153	0
3	TTP	A	802	29/29	0.97	0.05	75,82,92,94	0
3	TTP	B	802	29/29	0.97	0.05	65,76,83,85	0
5	SO4	A	805	5/5	0.97	0.05	99,99,100,100	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.



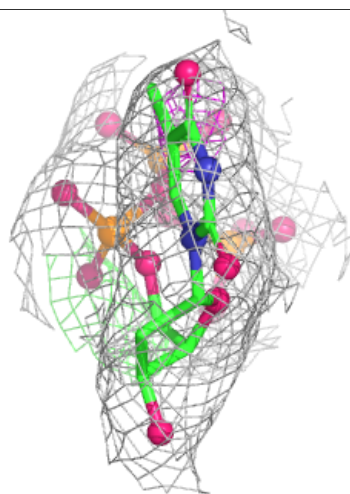
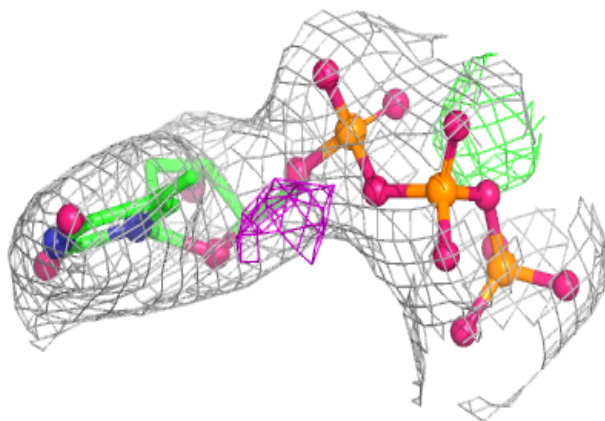
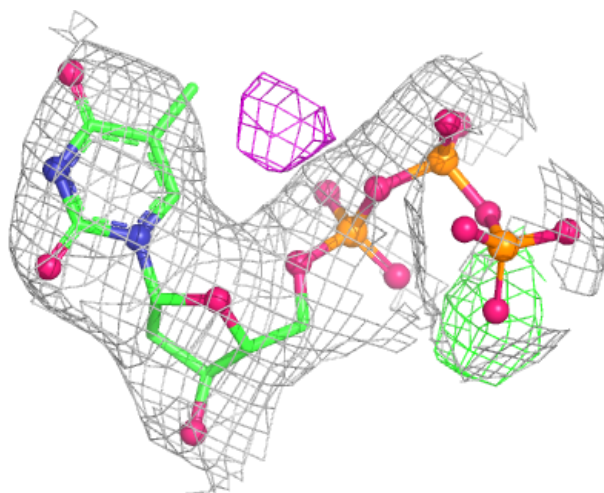
Electron density around GDP A 803:

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



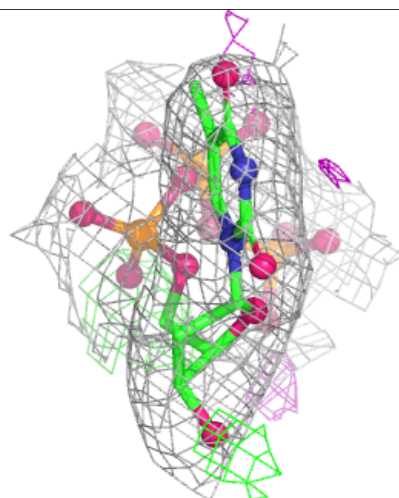
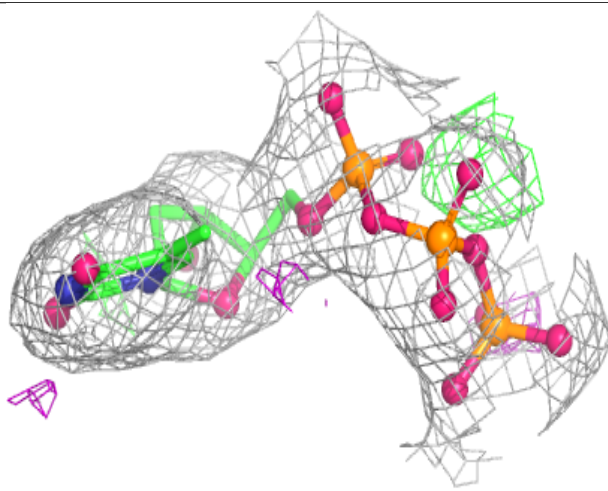
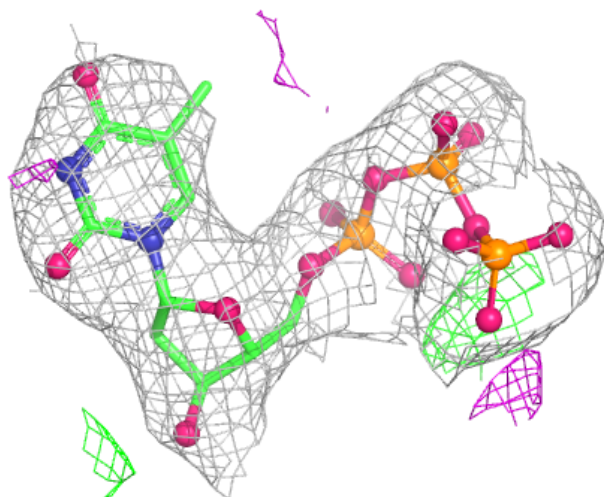
Electron density around TTP A 802:

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



Electron density around TTP B 802:

$2mF_o-DF_c$ (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.