



# Full wwPDB X-ray Structure Validation Report

Nov 7, 2014 – 07:33 AM EST

PDB ID : 2AD5  
Title : Mechanisms of feedback regulation and drug resistance of CTP synthetases:  
structure of the E. coli CTPS/CTP complex at 2.8-Angstrom resolution.  
Authors : Endrizzi, J.A.; Kim, H.; Anderson, P.M.; Baldwin, E.P.  
Deposited on : 2005-07-19  
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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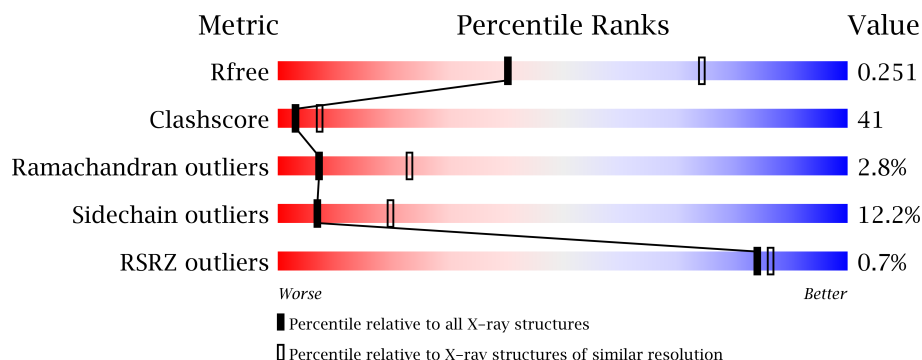
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : trunk24103  
Percentile statistics : 23426  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk24103

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	77520	2045 (2.80-2.80)
Clashscore	88313	2463 (2.80-2.80)
Ramachandran outliers	86584	2419 (2.80-2.80)
C $\alpha$ geometry	86677	2429 (2.80-2.80)
Sidechain outliers	86556	2421 (2.80-2.80)
RSRZ outliers	77580	2048 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	545	
1	B	545	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8694 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

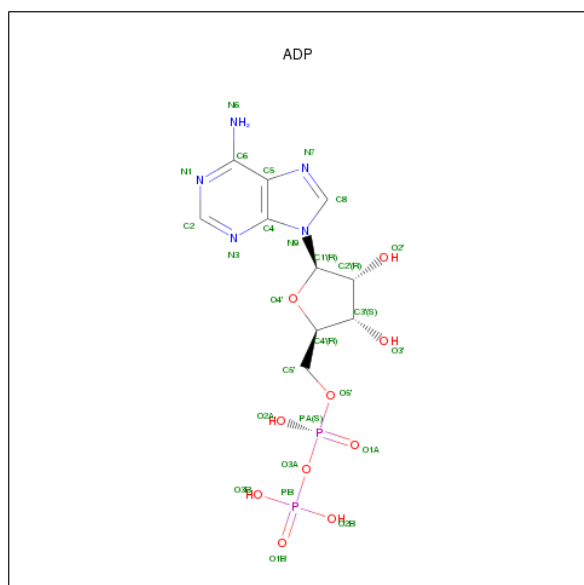
- Molecule 1 is a protein called CTP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	16	0	0
			4156	2625	726	784	21			
1	B	536	Total	C	N	O	S	11	0	0
			4172	2636	729	786	21			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

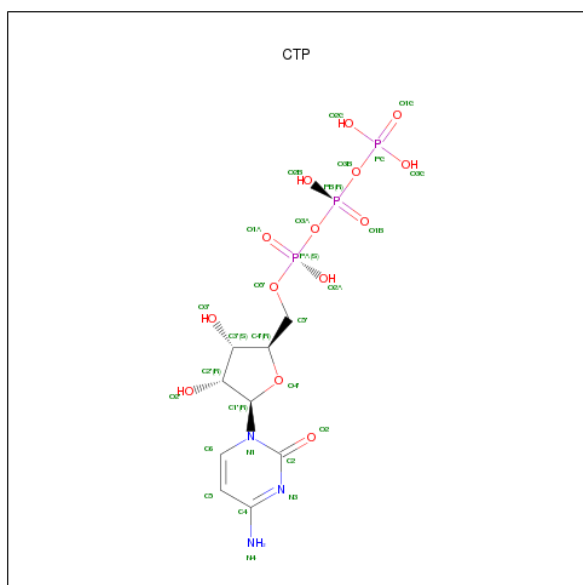
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula:  $C_9H_{16}N_3O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total	O	0	0
			130	130		
5	B	122	Total	O	0	0
			122	122		



R487	G490	S492	G493	D494	D495	Q496	L497	I500	I501	E502	V503	P504	N505	H506	P507	V508	F509	V510	A511	C512	Q513	F514	H515	P516	E517	F518	T519	S520	T521	P522	R523	D524	G525	H526	F527	L528	F529	A530	G531	F532	V533	K534	A535	A536	S537	E538	F539	Q540	R541	R542	Q543	A544	K545	
N419	R420	D421	E422	N423	G424	N425	V426	E427	V428	ARG	SER	GLU	LYS	SER	ASP	LEU	GLY	GLY	T438	P439	R440	L441	G442	A443	Q444	L448	V449	D450	D451	S452	L453	Y458	N459	A460	P461	E465	R466	H467	B468	H469	R470	Y471	E472	V473	N474	L477	L478	K479	Q480	L481	E482	D483	A484	L486
G354	Y355	R356	G357	V358	E359	G360	M361	I362	T363	T364	A365	R366	F367	E370	N371	N372	I373	P374	Y375	C379	L380	G381	M382	Q383	V384	A385	L386	I387	D388	Y389	H392	V393	A394	N395	M396	E397	N400	S401	T402	E403	F404	V405	P406	D407	C408	R409	Y410	P411	V412	V413	A414	L415	E418	
I280	F281	E282	E283	A284	N285	P286	V287	S288	E289	G293	N294	V295	G296	K297	Y298	I299	E300	L301	P302	D303	A304	Y305	K306	E310	K313	N319	R320	V321	S322	K326	L327	I328	D329	S330	Q331	D332	V333	E334	T335	R336	G337	V338	E339	I340	L341	G342	Y343	L344	D345	A346	T347	L348	V349	P350
P216	A218	N219	E220	R221	A222	K223	I224	A225	L226	F227	C228	N229	V230	P231	E232	K233	A234	V235	I236	S237	L238	K239	D240	V241	D242	S243	K246	I247	P248	G249	L250	S253	L256	D257	Y258	I259	I260	R263	F264	S265	L266	N267	C268	P269	E270	A271	N272	L273	S274	E275	W276	E277	Q278	V279
D135	V136	V137	E140	D147	I148	E149	S150	L151	P152	M160	E163	I164	G165	R166	E167	H168	T169	L174	T175	L176	V177	P178	Y179	M180	A181	E185	V186	K187	T188	K189	P190	T191	Q192	H193	S194	E197	L198	I201	D206	I207	L208	L209	C210	R211	S212	D213	R214	A215						

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.27Å 106.38Å 130.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 45.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 98.7 (45.42-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.81Å)	Xtriage
Refinement program	TNT V. 5-F	Depositor
R, $R_{free}$	0.202 , 0.277 0.194 , 0.251	Depositor DCC
$R_{free}$ test set	1865 reflections (3.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 91.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55879 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8694	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, CTP, ADP

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	0.89	37/4232 (0.9%)	1.24	47/5734 (0.8%)
1	B	0.87	35/4248 (0.8%)	1.24	46/5755 (0.8%)
All	All	0.88	72/8480 (0.8%)	1.24	93/11489 (0.8%)

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	GLU	CD-OE2	6.69	1.33	1.25
1	A	499	GLU	CD-OE2	6.64	1.32	1.25
1	A	397	GLU	CD-OE2	6.59	1.32	1.25
1	A	300	GLU	CD-OE2	6.42	1.32	1.25
1	B	185	GLU	CD-OE2	6.14	1.32	1.25
1	B	300	GLU	CD-OE2	6.12	1.32	1.25
1	B	125	GLU	CD-OE1	6.07	1.32	1.25
1	A	132	GLU	CD-OE2	6.05	1.32	1.25
1	A	370	GLU	CD-OE2	6.01	1.32	1.25
1	A	275	GLU	CD-OE1	5.99	1.32	1.25
1	A	310	GLU	CD-OE2	5.97	1.32	1.25
1	B	370	GLU	CD-OE2	5.97	1.32	1.25
1	B	517	GLU	CD-OE1	5.94	1.32	1.25
1	B	167	GLU	CD-OE2	5.92	1.32	1.25
1	A	185	GLU	CD-OE2	5.91	1.32	1.25
1	A	339	GLU	CD-OE2	5.90	1.32	1.25
1	B	270	GLU	CD-OE2	5.90	1.32	1.25
1	B	129	GLU	CD-OE2	5.90	1.32	1.25
1	A	163	GLU	CD-OE2	5.88	1.32	1.25
1	B	427	GLU	CD-OE2	5.88	1.32	1.25
1	A	482	GLU	CD-OE2	5.83	1.32	1.25
1	B	397	GLU	CD-OE2	5.83	1.32	1.25
1	A	334	GLU	CD-OE2	5.81	1.32	1.25
1	A	167	GLU	CD-OE2	5.80	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	GLU	CD-OE2	5.78	1.32	1.25
1	A	125	GLU	CD-OE2	5.74	1.31	1.25
1	B	422	GLU	CD-OE2	5.74	1.31	1.25
1	A	427	GLU	CD-OE2	5.73	1.31	1.25
1	A	517	GLU	CD-OE2	5.73	1.31	1.25
1	B	359	GLU	CD-OE2	5.71	1.31	1.25
1	A	283	GLU	CD-OE2	5.70	1.31	1.25
1	B	339	GLU	CD-OE2	5.70	1.31	1.25
1	B	64	GLU	CD-OE2	5.68	1.31	1.25
1	A	403	GLU	CD-OE2	5.67	1.31	1.25
1	B	334	GLU	CD-OE2	5.66	1.31	1.25
1	B	68	GLU	CD-OE2	5.60	1.31	1.25
1	A	270	GLU	CD-OE2	5.60	1.31	1.25
1	B	163	GLU	CD-OE2	5.59	1.31	1.25
1	A	30	GLU	CD-OE2	5.57	1.31	1.25
1	B	220	GLU	CD-OE2	5.57	1.31	1.25
1	A	64	GLU	CD-OE2	5.57	1.31	1.25
1	B	418	GLU	CD-OE2	5.57	1.31	1.25
1	B	403	GLU	CD-OE1	5.53	1.31	1.25
1	A	359	GLU	CD-OE1	5.53	1.31	1.25
1	B	289	GLU	CD-OE1	5.46	1.31	1.25
1	B	30	GLU	CD-OE2	5.45	1.31	1.25
1	A	277	GLU	CD-OE2	5.43	1.31	1.25
1	B	197	GLU	CD-OE2	5.43	1.31	1.25
1	A	232	GLU	CD-OE2	5.42	1.31	1.25
1	A	418	GLU	CD-OE2	5.42	1.31	1.25
1	B	232	GLU	CD-OE2	5.41	1.31	1.25
1	B	472	GLU	CD-OE2	5.40	1.31	1.25
1	A	103	GLU	CD-OE2	5.38	1.31	1.25
1	A	538	GLU	CD-OE2	5.38	1.31	1.25
1	A	422	GLU	CD-OE1	5.30	1.31	1.25
1	A	68	GLU	CD-OE2	5.30	1.31	1.25
1	B	482	GLU	CD-OE1	5.30	1.31	1.25
1	A	155	GLU	CD-OE2	5.26	1.31	1.25
1	A	220	GLU	CD-OE1	5.22	1.31	1.25
1	B	277	GLU	CD-OE2	5.21	1.31	1.25
1	A	140	GLU	CD-OE2	5.20	1.31	1.25
1	A	59	GLU	CD-OE1	5.17	1.31	1.25
1	A	289	GLU	CD-OE2	5.16	1.31	1.25
1	B	283	GLU	CD-OE2	5.16	1.31	1.25
1	B	140	GLU	CD-OE2	5.16	1.31	1.25
1	A	472	GLU	CD-OE2	5.11	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	GLU	CD-OE2	5.11	1.31	1.25
1	B	538	GLU	CD-OE2	5.07	1.31	1.25
1	B	310	GLU	CD-OE2	5.06	1.31	1.25
1	B	275	GLU	CD-OE2	5.03	1.31	1.25
1	A	465	GLU	CD-OE2	5.01	1.31	1.25
1	B	103	GLU	CD-OE2	5.01	1.31	1.25

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	LEU	C-N-CD	-11.39	95.53	120.60
1	B	107	ASP	CB-CG-OD1	-7.74	111.33	118.30
1	A	450	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	B	303	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	B	494	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	B	98	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	B	494	ASP	CB-CG-OD1	7.05	124.64	118.30
1	B	257	ASP	CB-CG-OD2	-7.03	111.98	118.30
1	B	407	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	B	240	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	B	388	ASP	CB-CG-OD1	-6.76	112.21	118.30
1	B	48	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	407	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	B	65	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	A	98	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	B	135	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	B	495	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	B	70	ASP	CB-CG-OD2	-6.57	112.38	118.30
1	B	524	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	A	213	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	B	98	ASP	CB-CG-OD1	6.47	124.12	118.30
1	B	213	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	B	303	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	495	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	451	ASP	CB-CG-OD2	-6.37	112.56	118.30
1	B	345	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	495	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	242	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	A	329	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	451	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	258	ASP	CB-CG-OD1	6.19	123.87	118.30
1	B	450	ASP	CB-CG-OD2	-6.18	112.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	72	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	407	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	65	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	A	70	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	B	388	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	494	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	451	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	A	206	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	332	ASP	CB-CG-OD2	-5.89	112.99	118.30
1	B	240	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	504	PRO	N-CA-CB	5.79	110.25	103.30
1	B	48	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	421	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	A	524	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	B	329	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	388	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	258	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	332	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	345	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	303	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	345	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	257	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	211	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	107	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	257	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	329	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	98	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	107	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	A	303	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	494	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	213	ASP	CB-CA-C	-5.42	99.55	110.40
1	A	44	TYR	CB-CG-CD1	-5.41	117.76	121.00
1	A	240	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	B	483	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	450	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	505	ASN	CB-CA-C	5.35	121.10	110.40
1	B	379	CYS	CB-CA-C	5.35	121.10	110.40
1	B	379	CYS	N-CA-CB	5.34	120.22	110.60
1	A	44	TYR	CA-CB-CG	-5.33	103.28	113.40
1	A	388	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	B	242	ASP	CB-CG-OD2	-5.28	113.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ASP	CB-CG-OD1	5.27	123.05	118.30
1	B	211	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	495	ASP	CB-CG-OD1	5.26	123.04	118.30
1	B	118	HIS	CA-CB-CG	-5.25	104.68	113.60
1	A	407	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	468	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	70	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	166	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	206	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	70	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	421	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	332	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	421	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	B	329	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	504	PRO	N-CA-C	5.12	125.41	112.10
1	B	450	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	483	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	118	HIS	CA-CB-CG	-5.05	105.01	113.60
1	A	94	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4156	0	4162	362	0
1	B	4172	0	4184	327	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	5	0
3	B	27	0	12	4	0
4	A	29	0	12	5	0
4	B	29	0	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	130	0	0	11	0
5	B	122	0	0	12	1
All	All	8694	0	8394	690	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

All (690) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:MET:HE1	1:A:130:GLY:HA3	1.35	1.09
1:A:301:LEU:HD12	1:A:302:PRO:HD2	1.36	1.06
1:A:396:MET:HE1	1:A:480:GLN:HB3	1.39	1.05
1:A:521:THR:HG22	1:A:524:ASP:H	1.27	0.99
1:A:521:THR:HG23	1:A:522:PRO:HD2	1.41	0.99
1:A:486:LEU:HD12	1:A:487:ARG:H	1.28	0.98
1:B:299:ILE:H	1:B:299:ILE:HD12	1.30	0.95
1:B:349:VAL:HG12	1:B:381:GLY:HA2	1.48	0.94
1:B:400:ASN:HD22	1:B:401:SER:H	1.07	0.93
1:B:382:MET:HE3	1:B:512:CYS:HA	1.50	0.93
1:B:295:VAL:HG13	1:B:328:ILE:HB	1.49	0.92
1:B:426:VAL:HG12	1:B:427:GLU:H	1.34	0.92
1:B:495:ASP:O	1:B:496:GLN:C	2.06	0.92
1:A:426:VAL:HG12	1:A:427:GLU:H	1.34	0.91
1:B:127:VAL:HG11	1:B:160:MET:HE1	1.53	0.91
1:B:519:THR:HG22	1:B:526:HIS:HD2	1.34	0.91
1:B:224:ILE:HA	1:B:227:PHE:CE1	2.06	0.91
1:B:46:ASN:H	1:B:46:ASN:ND2	1.70	0.90
1:B:362:ILE:HA	1:B:384:VAL:HG13	1.53	0.89
1:B:147:ASP:HB3	4:B:1602:CTP:C2	2.08	0.88
1:A:39:MET:CE	1:A:130:GLY:HA3	2.04	0.87
1:B:506:HIS:CG	1:B:507:PRO:HD2	2.09	0.87
1:B:55:ILE:HD11	1:B:298:TYR:HB3	1.57	0.87
1:A:223:LYS:HG3	1:A:227:PHE:CE1	2.10	0.86
1:B:401:SER:HB2	1:B:413:VAL:HB	1.56	0.86
1:B:46:ASN:HD22	1:B:46:ASN:H	1.21	0.85
1:B:297:LYS:HZ1	1:B:354:GLY:HA3	1.41	0.85
1:A:486:LEU:HD12	1:A:487:ARG:N	1.91	0.84
1:B:299:ILE:CG2	1:B:327:LEU:HD13	2.07	0.84
1:B:542:ARG:HA	1:B:545:LYS:HB3	1.60	0.83
1:B:519:THR:HG22	1:B:526:HIS:CD2	2.15	0.80
1:A:362:ILE:HA	1:A:384:VAL:HG13	1.63	0.80
1:B:506:HIS:ND1	1:B:509:PHE:HB2	1.98	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:495:ASP:O	1:A:496:GLN:C	2.17	0.79
4:A:602:CTP:O3G	1:B:188:THR:N	2.15	0.79
1:B:297:LYS:NZ	1:B:354:GLY:HA3	1.98	0.78
1:B:349:VAL:HG12	1:B:381:GLY:CA	2.13	0.78
1:A:127:VAL:HB	1:A:160:MET:CE	2.13	0.78
1:B:506:HIS:CD2	1:B:507:PRO:HD2	2.19	0.77
1:A:278:GLN:O	1:A:282:GLU:HG3	1.84	0.77
1:B:207:ILE:O	1:B:208:LEU:HD23	1.85	0.76
1:B:299:ILE:HG22	1:B:327:LEU:HD13	1.65	0.76
1:A:46:ASN:H	1:A:46:ASN:HD22	1.31	0.76
1:B:296:GLY:C	1:B:299:ILE:HD11	2.05	0.76
1:A:125:GLU:O	1:A:129:GLU:HG3	1.84	0.76
1:A:124:LYS:HA	1:A:160:MET:CE	2.16	0.75
1:A:409:LYS:O	1:A:422:GLU:HA	1.86	0.75
1:B:276:TRP:O	1:B:280:ILE:HG13	1.88	0.74
1:A:124:LYS:HA	1:A:160:MET:HE2	1.70	0.74
1:A:396:MET:CE	1:A:480:GLN:HB3	2.18	0.73
1:B:349:VAL:CG1	1:B:381:GLY:HA2	2.18	0.73
1:B:86:ARG:HD3	1:B:86:ARG:O	1.88	0.73
1:A:409:LYS:HE2	1:A:410:TYR:CE2	2.24	0.73
1:A:17:GLY:HA2	3:A:601:ADP:O1A	1.89	0.72
1:B:54:PRO:HA	1:B:58:GLY:O	1.88	0.72
1:B:345:ASP:OD1	1:B:540:GLN:HB2	1.88	0.72
1:A:421:ASP:HB2	1:A:422:GLU:OE1	1.89	0.72
1:A:403:GLU:HG3	1:A:471:TYR:CE1	2.24	0.72
1:B:289:GLU:HB2	1:B:322:SER:HB3	1.71	0.71
1:A:196:LYS:HD3	5:B:1815:HOH:O	1.89	0.71
1:A:161:ALA:HA	1:A:169:THR:HG21	1.71	0.71
1:A:347:ILE:CD1	1:A:373:ILE:HG21	2.21	0.71
1:A:439:MET:HB2	1:A:470:ARG:HG3	1.73	0.70
1:A:506:HIS:CG	1:A:507:PRO:HD2	2.27	0.70
1:A:32:ARG:HD3	1:A:269:PRO:O	1.90	0.70
1:A:521:THR:HG22	1:A:524:ASP:N	2.05	0.70
1:B:386:LEU:HD22	1:B:473:VAL:HG22	1.72	0.70
1:B:493:GLY:HA2	1:B:496:GLN:HE21	1.56	0.69
1:A:402:THR:HG23	1:A:414:ALA:HB2	1.74	0.69
1:B:480:GLN:HB2	5:B:1807:HOH:O	1.92	0.69
1:A:65:ASP:OD2	1:A:86:ARG:HD2	1.92	0.69
1:B:147:ASP:HB3	4:B:1602:CTP:O2	1.92	0.69
1:A:400:ASN:HB3	1:A:408:CYS:SG	2.32	0.69
1:A:127:VAL:HB	1:A:160:MET:HE1	1.74	0.68
1:A:453:LEU:O	1:A:456:GLN:HB3	1.94	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:403:GLU:HG3	1:B:471:TYR:CE2	2.29	0.68
1:B:516:PRO:HD2	1:B:517:GLU:OE1	1.94	0.68
1:B:12:VAL:HG12	1:B:13:VAL:HG13	1.74	0.68
1:B:86:ARG:NH1	1:B:89:ASN:HB3	2.09	0.68
1:B:278:GLN:O	1:B:282:GLU:HG3	1.93	0.67
1:A:355:TYR:CD1	1:A:404:PHE:HB3	2.30	0.67
1:A:506:HIS:HD2	1:A:508:TRP:H	1.40	0.67
1:A:473:VAL:HG21	1:A:498:VAL:HB	1.76	0.67
1:A:492:SER:OG	1:A:493:GLY:N	2.28	0.67
1:A:521:THR:CG2	1:A:524:ASP:H	2.06	0.67
1:B:387:ILE:HG22	1:B:388:ASP:N	2.09	0.67
1:B:400:ASN:ND2	1:B:401:SER:H	1.89	0.67
1:B:85:SER:OG	1:B:87:ARG:NH1	2.29	0.66
1:B:86:ARG:HH12	1:B:89:ASN:HB3	1.60	0.66
1:B:192:GLN:HG2	1:B:227:PHE:CZ	2.30	0.66
1:A:289:GLU:HB2	1:A:322:SER:HB3	1.78	0.66
1:B:408:CYS:O	1:B:420:ARG:NH2	2.29	0.66
1:B:415:LEU:HD12	1:B:418:GLU:CD	2.17	0.66
1:B:238:LEU:HD11	1:B:247:ILE:HG23	1.76	0.66
1:A:223:LYS:HA	1:A:227:PHE:HE1	1.60	0.65
1:B:32:ARG:HG2	1:B:269:PRO:O	1.97	0.65
1:B:216:VAL:O	1:B:221:ARG:NH1	2.29	0.65
1:A:301:LEU:O	1:A:303:ASP:N	2.29	0.65
1:A:506:HIS:CD2	1:A:508:TRP:H	2.14	0.65
1:A:105:ARG:HG3	1:A:107:ASP:OD1	1.97	0.65
1:A:275:GLU:O	1:A:279:VAL:HG23	1.97	0.65
1:A:272:ASN:ND2	1:A:274:SER:OG	2.29	0.65
1:A:278:GLN:NE2	1:A:282:GLU:OE2	2.29	0.65
1:B:356:ARG:HD2	5:B:1778:HOH:O	1.97	0.65
1:A:180:MET:O	1:A:184:GLY:N	2.30	0.65
1:B:149:GLU:HG2	4:B:1602:CTP:O2	1.96	0.65
1:A:412:VAL:CG2	1:A:481:ILE:HD11	2.27	0.65
1:A:90:PHE:CE1	1:A:95:ILE:HD11	2.30	0.65
1:B:250:LEU:HD23	1:B:250:LEU:N	2.12	0.65
1:B:48:ASP:OD1	1:B:50:GLY:N	2.29	0.65
1:A:46:ASN:H	1:A:46:ASN:ND2	1.95	0.64
1:A:448:LEU:HD22	1:A:454:VAL:CG1	2.26	0.64
1:B:458:TYR:CE2	1:B:528:LEU:HD12	2.32	0.64
1:A:127:VAL:HB	1:A:160:MET:HE3	1.79	0.64
1:A:543:GLN:N	1:A:543:GLN:OE1	2.30	0.64
1:B:493:GLY:HA2	1:B:496:GLN:NE2	2.12	0.64
1:A:449:VAL:HG21	1:A:488:VAL:O	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:409:LYS:HE3	1:A:422:GLU:HB2	1.79	0.64
1:A:358:VAL:O	1:A:362:ILE:HD12	1.98	0.63
1:A:426:VAL:HG12	1:A:427:GLU:N	2.09	0.63
4:A:602:CTP:O2B	1:B:223:LYS:HE3	1.98	0.63
1:B:362:ILE:CA	1:B:384:VAL:HG13	2.27	0.63
1:B:86:ARG:HD2	5:B:1765:HOH:O	1.99	0.63
1:B:293:GLY:HA3	1:B:344:LEU:HD13	1.79	0.62
1:B:335:THR:HG22	1:B:336:ARG:HG2	1.81	0.62
1:B:107:ASP:N	1:B:107:ASP:OD1	2.29	0.62
1:B:125:GLU:O	1:B:129:GLU:HG3	1.99	0.62
1:B:189:LYS:HB3	1:B:190:PRO:HD3	1.80	0.62
1:A:220:GLU:O	1:A:223:LYS:HB3	1.98	0.62
1:A:379:CYS:O	1:A:382:MET:N	2.31	0.62
1:B:74:GLY:O	1:B:75:HIS:C	2.36	0.62
1:A:149:GLU:HB2	4:A:602:CTP:O2	1.99	0.61
1:A:396:MET:HE2	1:A:480:GLN:HG2	1.82	0.61
1:A:401:SER:HA	1:A:413:VAL:O	2.00	0.61
1:B:401:SER:HB2	1:B:413:VAL:CB	2.27	0.61
1:A:335:THR:HG22	1:A:336:ARG:N	2.12	0.61
1:B:197:GLU:HG3	5:B:1717:HOH:O	1.99	0.61
1:B:410:TYR:CE1	1:B:422:GLU:HB3	2.34	0.61
1:B:85:SER:OG	1:B:87:ARG:HB2	2.00	0.61
1:A:309:ILE:HG22	1:A:310:GLU:N	2.14	0.61
1:A:490:GLY:HA3	1:A:500:ILE:HD12	1.82	0.61
1:A:188:THR:N	4:B:1602:CTP:O2G	2.25	0.61
1:A:11:GLY:O	1:A:16:LEU:HD11	2.01	0.61
1:A:177:VAL:HG13	1:A:187:LYS:O	2.00	0.61
1:A:382:MET:HE3	1:A:499:GLU:O	2.00	0.61
1:A:42:ASP:HB3	1:A:44:TYR:CE2	2.36	0.61
1:B:460:ALA:HB1	1:B:461:PRO:HD2	1.83	0.61
1:B:192:GLN:HG2	1:B:227:PHE:CE2	2.36	0.61
1:B:396:MET:HE1	1:B:480:GLN:HB3	1.83	0.60
1:B:121:ASN:O	1:B:125:GLU:HG3	2.00	0.60
1:B:127:VAL:CG1	1:B:160:MET:HE1	2.30	0.60
1:B:257:ASP:OD1	1:B:257:ASP:N	2.35	0.60
1:B:383:GLN:HB3	1:B:413:VAL:HG21	1.84	0.60
1:A:9:THR:HG22	1:A:173:HIS:ND1	2.17	0.60
1:A:71:LEU:HD12	1:A:72:ASP:N	2.17	0.60
1:B:296:GLY:O	1:B:299:ILE:HD11	2.00	0.60
1:B:17:GLY:HA2	3:B:1601:ADP:PA	2.42	0.59
1:B:299:ILE:HG21	1:B:327:LEU:HB3	1.82	0.59
1:A:57:HIS:HB3	5:A:804:HOH:O	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:ARG:HB3	1:A:268:CYS:HB3	1.84	0.59
1:B:12:VAL:HG11	1:B:176:LEU:HB3	1.84	0.59
1:A:341:LEU:HD23	1:A:341:LEU:N	2.17	0.59
1:B:357:GLY:O	1:B:358:VAL:C	2.41	0.59
1:A:29:LEU:O	1:A:34:LEU:HB2	2.03	0.59
1:B:426:VAL:HG12	1:B:427:GLU:N	2.12	0.59
1:A:425:ASN:HD22	1:A:425:ASN:N	2.01	0.58
1:A:402:THR:CG2	1:A:414:ALA:HB2	2.32	0.58
1:A:373:ILE:HG23	1:A:374:PRO:HD2	1.86	0.58
1:A:454:VAL:HB	1:A:502:GLU:OE2	2.03	0.58
1:A:204:GLN:NE2	1:A:205:PRO:HD2	2.18	0.58
1:B:361:MET:O	1:B:364:THR:HB	2.04	0.58
3:B:1601:ADP:H5'2	5:B:1821:HOH:O	2.03	0.58
1:B:211:ARG:CD	1:B:238:LEU:HD23	2.34	0.58
1:A:252:LYS:HE3	1:A:271:ALA:HB3	1.84	0.58
1:B:6:ILE:HD11	1:B:260:ILE:HD13	1.84	0.58
1:B:502:GLU:HG2	1:B:510:VAL:HG22	1.85	0.58
1:B:494:ASP:CG	1:B:495:ASP:H	2.06	0.57
1:A:155:GLU:OE2	1:A:158:ARG:NH2	2.34	0.57
1:A:408:CYS:C	1:A:410:TYR:H	2.08	0.57
1:A:409:LYS:H	1:A:420:ARG:HH21	1.52	0.57
1:A:535:ALA:O	1:A:536:ALA:C	2.40	0.57
1:B:357:GLY:O	1:B:359:GLU:N	2.36	0.57
1:B:375:TYR:HB3	1:B:509:PHE:CD2	2.39	0.57
1:B:86:ARG:NH1	1:B:89:ASN:O	2.38	0.57
1:A:368:ALA:O	1:A:506:HIS:HE1	1.88	0.57
1:A:401:SER:HB2	1:A:413:VAL:HB	1.86	0.57
1:B:35:ASN:N	1:B:135:ASP:OD2	2.30	0.57
1:B:382:MET:SD	1:B:513:GLN:HG2	2.44	0.57
1:B:95:ILE:O	1:B:99:VAL:HG23	2.05	0.57
1:A:372:ASN:O	1:A:507:PRO:HG2	2.05	0.57
1:A:408:CYS:O	1:A:409:LYS:HB3	2.05	0.57
1:A:521:THR:HG23	1:A:522:PRO:CD	2.27	0.57
1:B:105:ARG:HD2	1:B:107:ASP:OD1	2.04	0.57
1:A:244:ILE:O	1:A:247:ILE:HG13	2.05	0.57
1:B:6:ILE:CD1	1:B:260:ILE:HD13	2.35	0.57
1:A:223:LYS:CA	1:A:227:PHE:HE1	2.18	0.56
1:A:285:ASN:O	1:A:320:ARG:NH1	2.29	0.56
1:A:346:ALA:C	1:A:347:ILE:HD12	2.25	0.56
1:A:439:MET:HE2	1:A:469:HIS:C	2.24	0.56
1:A:542:ARG:O	1:A:544:ALA:N	2.37	0.56
1:B:338:VAL:HG11	1:B:367:PHE:CE1	2.39	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:LYS:O	1:A:224:ILE:C	2.43	0.56
1:A:412:VAL:HA	1:A:477:LEU:HD12	1.88	0.56
1:A:453:LEU:O	1:A:453:LEU:HD12	2.04	0.56
1:B:491:ARG:HD3	5:B:1733:HOH:O	2.05	0.56
1:A:379:CYS:O	1:A:380:LEU:C	2.43	0.56
1:A:441:LEU:HA	1:A:467:HIS:O	2.06	0.56
1:B:355:TYR:CD1	1:B:404:PHE:HB3	2.41	0.56
1:B:101:ARG:O	1:B:102:LYS:C	2.39	0.56
1:B:174:LEU:HG	1:B:209:ILE:HB	1.86	0.56
1:A:243:SER:O	1:A:246:LYS:HG3	2.05	0.56
1:A:52:MET:CE	1:A:57:HIS:HB2	2.36	0.56
1:A:541:LYS:O	1:A:542:ARG:C	2.44	0.56
1:B:87:ARG:HB2	1:B:87:ARG:HH11	1.71	0.56
1:B:207:ILE:C	1:B:208:LEU:HD23	2.24	0.56
1:A:71:LEU:HD12	1:A:71:LEU:C	2.26	0.56
1:A:297:LYS:HE2	1:A:298:TYR:CE1	2.41	0.55
1:B:531:GLY:O	1:B:532:PHE:C	2.44	0.55
1:A:285:ASN:O	1:A:320:ARG:HD2	2.06	0.55
1:A:40:LYS:C	1:A:41:LEU:HD12	2.26	0.55
1:A:489:ALA:HB2	1:A:502:GLU:HG3	1.88	0.55
1:A:4:ASN:O	1:A:137:VAL:HG23	2.07	0.55
1:B:106:GLY:HA2	5:B:1799:HOH:O	2.07	0.55
1:B:19:GLY:HA2	1:B:140:GLU:OE1	2.06	0.55
1:A:373:ILE:CG2	1:A:374:PRO:HD2	2.37	0.55
1:A:383:GLN:O	1:A:384:VAL:C	2.45	0.55
1:A:69:THR:CB	1:A:73:LEU:HD22	2.37	0.55
1:B:336:ARG:HB2	1:B:340:ILE:HD11	1.88	0.55
1:B:401:SER:HB2	1:B:413:VAL:CG1	2.36	0.55
1:A:426:VAL:CG1	1:A:427:GLU:H	2.14	0.54
1:B:55:ILE:CD1	1:B:298:TYR:HB3	2.32	0.54
1:B:301:LEU:HD12	1:B:302:PRO:HD2	1.89	0.54
1:A:383:GLN:O	1:A:386:LEU:N	2.41	0.54
1:A:415:LEU:HD21	1:A:471:TYR:CE2	2.43	0.54
1:B:338:VAL:O	1:B:339:GLU:C	2.46	0.54
1:A:500:ILE:HG23	1:A:511:ALA:O	2.07	0.54
1:B:17:GLY:HA2	3:B:1601:ADP:O1A	2.08	0.54
1:B:71:LEU:HD12	1:B:72:ASP:N	2.23	0.54
1:B:401:SER:HA	1:B:413:VAL:O	2.08	0.54
1:A:32:ARG:HD2	1:A:268:CYS:CB	2.38	0.53
1:A:521:THR:HG22	1:A:523:ARG:N	2.23	0.53
1:B:71:LEU:C	1:B:71:LEU:HD12	2.28	0.53
1:A:439:MET:HE1	1:A:469:HIS:HA	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:213:ASP:HB2	1:B:214:ARG:HE	1.72	0.53
1:B:348:LEU:HD23	1:B:349:VAL:N	2.23	0.53
1:A:355:TYR:O	1:A:356:ARG:C	2.47	0.53
1:B:341:LEU:HB2	1:B:367:PHE:CE2	2.43	0.53
1:B:517:GLU:HG2	1:B:518:PHE:N	2.23	0.53
1:A:20:ILE:HG21	1:A:247:ILE:HD12	1.91	0.53
1:A:382:MET:O	1:A:385:ALA:HB3	2.08	0.53
1:B:382:MET:HE3	1:B:500:ILE:HA	1.89	0.53
1:B:60:VAL:HG11	1:B:68:GLU:HB3	1.90	0.53
1:A:177:VAL:HG12	1:A:186:VAL:HB	1.91	0.53
1:A:359:GLU:HA	1:A:362:ILE:HD12	1.90	0.53
1:B:295:VAL:HG13	1:B:328:ILE:CB	2.31	0.53
1:B:46:ASN:HB2	1:B:52:MET:HE2	1.90	0.53
1:A:297:LYS:HZ1	1:A:356:ARG:HG3	1.72	0.53
1:B:98:ASP:O	1:B:101:ARG:HG2	2.09	0.53
1:B:485:GLY:O	1:B:504:PRO:HG3	2.09	0.53
1:B:18:LYS:HG2	3:B:1601:ADP:O2B	2.09	0.53
1:B:330:SER:O	1:B:333:VAL:N	2.37	0.53
1:A:159:GLN:O	1:A:163:GLU:HG3	2.09	0.53
1:A:310:GLU:O	1:A:313:LYS:HB2	2.09	0.53
1:A:290:VAL:HG22	1:A:321:VAL:CG1	2.39	0.53
1:B:1:MET:HG3	5:B:1764:HOH:O	2.08	0.53
1:B:330:SER:O	1:B:331:GLN:C	2.47	0.53
1:B:440:ARG:HB2	1:B:469:HIS:CD2	2.44	0.53
1:A:473:VAL:HB	5:A:801:HOH:O	2.08	0.52
1:A:9:THR:HB	5:A:812:HOH:O	2.10	0.52
1:B:380:LEU:HA	1:B:383:GLN:HG3	1.90	0.52
1:A:12:VAL:HG11	1:A:176:LEU:HB3	1.92	0.52
1:B:281:PHE:O	1:B:282:GLU:C	2.46	0.52
1:A:348:LEU:HD23	1:A:348:LEU:C	2.30	0.52
1:A:521:THR:HG23	5:A:726:HOH:O	2.09	0.52
1:B:101:ARG:HA	5:B:1748:HOH:O	2.09	0.52
1:B:101:ARG:HG3	1:B:102:LYS:N	2.25	0.52
1:A:167:GLU:HB2	5:A:796:HOH:O	2.09	0.52
1:A:147:ASP:HB3	4:A:602:CTP:C2	2.44	0.52
1:A:295:VAL:O	1:A:350:PRO:HD2	2.10	0.52
1:A:382:MET:CE	1:A:500:ILE:HA	2.39	0.52
1:B:493:GLY:O	1:B:496:GLN:HG2	2.09	0.52
1:B:495:ASP:O	1:B:497:LEU:N	2.42	0.52
1:A:297:LYS:HZ3	1:A:353:PHE:C	2.13	0.52
1:A:223:LYS:O	1:A:226:LEU:N	2.40	0.52
1:A:37:THR:C	1:A:38:ILE:HG13	2.29	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:188:THR:O	1:B:191:THR:N	2.42	0.52
1:A:121:ASN:O	1:A:122:ALA:C	2.46	0.52
1:A:69:THR:OG1	1:A:73:LEU:HD22	2.10	0.52
1:B:402:THR:OG1	1:B:471:TYR:HE1	1.93	0.52
1:A:415:LEU:HD23	1:A:415:LEU:N	2.24	0.52
1:A:12:VAL:HG12	1:A:13:VAL:HG13	1.92	0.52
1:A:382:MET:HE3	1:A:512:CYS:HA	1.92	0.52
1:A:516:PRO:HD2	1:A:517:GLU:OE1	2.10	0.52
1:B:348:LEU:C	1:B:348:LEU:HD23	2.31	0.52
1:B:9:THR:HG23	5:B:1718:HOH:O	2.10	0.52
1:A:294:MET:HA	1:A:348:LEU:O	2.10	0.51
1:B:189:LYS:HB3	1:B:190:PRO:CD	2.40	0.51
1:B:539:PHE:O	1:B:543:GLN:HG2	2.11	0.51
1:A:299:ILE:C	1:A:299:ILE:HD12	2.30	0.51
1:A:323:VAL:HG12	1:A:325:ILE:HG13	1.93	0.51
1:A:412:VAL:HG21	1:A:481:ILE:CD1	2.40	0.51
1:B:426:VAL:CG1	1:B:427:GLU:H	2.09	0.51
1:A:32:ARG:HD2	1:A:268:CYS:HB2	1.92	0.51
1:A:41:LEU:N	1:A:41:LEU:HD12	2.25	0.51
1:B:362:ILE:HG12	1:B:387:ILE:HG21	1.93	0.51
1:A:171:PHE:H	1:A:206:ASP:HB2	1.76	0.51
1:A:391:ARG:O	1:A:393:VAL:N	2.44	0.51
1:A:464:VAL:C	1:A:465:GLU:HG2	2.30	0.51
1:A:488:VAL:O	1:A:488:VAL:HG12	2.11	0.51
1:B:281:PHE:CE1	1:B:285:ASN:ND2	2.79	0.51
1:A:345:ASP:O	1:A:374:PRO:HG2	2.10	0.51
1:A:412:VAL:HG22	5:A:819:HOH:O	2.10	0.51
1:B:258:ASP:O	1:B:259:TYR:C	2.47	0.51
1:B:506:HIS:CG	1:B:509:PHE:HB2	2.46	0.51
1:A:425:ASN:O	1:A:476:MET:HE1	2.11	0.51
1:B:192:GLN:HA	1:B:227:PHE:HE2	1.77	0.51
1:A:132:GLU:HG3	1:A:132:GLU:O	2.11	0.50
1:A:341:LEU:HD12	1:A:367:PHE:CG	2.46	0.50
1:A:345:ASP:CG	1:A:540:GLN:HB2	2.32	0.50
1:B:149:GLU:OE1	4:B:1602:CTP:O3'	2.24	0.50
1:A:194:SER:O	1:A:197:GLU:HB2	2.11	0.50
1:A:301:LEU:CD1	1:A:302:PRO:HD2	2.24	0.50
1:B:178:PRO:HD2	1:B:187:LYS:O	2.11	0.50
1:A:115:VAL:O	1:A:119:ILE:HB	2.11	0.50
1:A:278:GLN:HE22	1:A:282:GLU:HG2	1.77	0.50
1:A:438:THR:OG1	1:A:439:MET:N	2.43	0.50
1:B:492:SER:O	1:B:494:ASP:OD1	2.29	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:9:THR:HG22	1:A:10:GLY:N	2.24	0.50
1:B:448:LEU:HD12	1:B:460:ALA:O	2.11	0.50
1:A:441:LEU:HD21	1:A:468:ARG:HG3	1.93	0.50
1:B:114:GLN:O	1:B:118:HIS:HB2	2.12	0.50
1:B:242:ASP:OD1	1:B:246:LYS:HE3	2.11	0.50
1:A:171:PHE:N	1:A:206:ASP:OD2	2.45	0.50
1:A:45:ILE:O	1:A:46:ASN:C	2.49	0.49
1:B:396:MET:HE2	1:B:480:GLN:HG2	1.94	0.49
1:B:40:LYS:NZ	1:B:42:ASP:OD1	2.45	0.49
1:B:542:ARG:C	1:B:544:ALA:H	2.16	0.49
1:B:55:ILE:HD11	1:B:298:TYR:CB	2.36	0.49
1:A:197:GLU:HA	1:A:197:GLU:OE1	2.11	0.49
1:A:276:TRP:O	1:A:280:ILE:HD12	2.12	0.49
1:B:362:ILE:HA	1:B:384:VAL:CG1	2.35	0.49
1:B:36:VAL:HG22	1:B:136:VAL:HB	1.95	0.49
1:B:405:VAL:HG12	1:B:405:VAL:O	2.12	0.49
1:A:151:LEU:HB2	1:A:152:PRO:HD3	1.93	0.49
1:A:9:THR:CG2	1:A:173:HIS:ND1	2.76	0.49
1:B:227:PHE:CE2	1:B:228:CYS:SG	3.06	0.49
1:A:224:ILE:O	1:A:225:ALA:C	2.48	0.49
1:B:382:MET:CE	1:B:500:ILE:HA	2.42	0.49
1:B:49:PRO:HG2	1:B:69:THR:HA	1.94	0.49
1:A:301:LEU:O	1:A:302:PRO:C	2.51	0.49
1:B:188:THR:O	1:B:191:THR:HB	2.13	0.49
1:B:37:THR:HG23	1:B:137:VAL:HG13	1.95	0.49
1:B:421:ASP:HB2	1:B:425:ASN:N	2.27	0.49
1:B:495:ASP:O	1:B:496:GLN:O	2.30	0.49
1:B:521:THR:HB	1:B:522:PRO:HD2	1.94	0.49
1:A:464:VAL:O	1:A:465:GLU:HG2	2.13	0.49
1:A:467:HIS:CD2	1:A:469:HIS:HE1	2.31	0.49
1:B:216:VAL:HG12	1:B:221:ARG:HG3	1.94	0.49
1:B:44:TYR:CE1	1:B:52:MET:HE2	2.48	0.49
1:A:151:LEU:N	1:A:152:PRO:CD	2.75	0.48
1:B:444:GLN:HB2	1:B:467:HIS:HD2	1.78	0.48
1:B:49:PRO:HA	1:B:52:MET:CE	2.42	0.48
1:A:347:ILE:HD12	1:A:347:ILE:N	2.28	0.48
1:B:305:TYR:O	1:B:306:LYS:C	2.51	0.48
1:B:494:ASP:C	1:B:496:GLN:H	2.17	0.48
1:A:336:ARG:HB2	1:A:340:ILE:HD11	1.95	0.48
1:B:338:VAL:HG22	1:B:341:LEU:HD12	1.95	0.48
1:B:373:ILE:HG23	1:B:374:PRO:HD2	1.96	0.48
1:A:372:ASN:HA	1:A:506:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:194:SER:O	1:B:197:GLU:HB2	2.13	0.48
1:B:506:HIS:CG	1:B:507:PRO:CD	2.90	0.48
1:B:93:GLY:O	1:B:94:ARG:C	2.50	0.48
1:A:147:ASP:OD1	1:B:193:HIS:HE1	1.97	0.48
1:A:20:ILE:CG2	1:A:247:ILE:HD12	2.44	0.48
1:A:494:ASP:C	1:A:496:GLN:H	2.17	0.48
1:A:473:VAL:CG2	1:A:498:VAL:HB	2.44	0.48
1:B:409:LYS:O	1:B:422:GLU:HA	2.14	0.48
1:A:17:GLY:HA2	3:A:601:ADP:PA	2.54	0.48
1:A:521:THR:CG2	1:A:522:PRO:HD2	2.28	0.48
1:A:20:ILE:HD13	3:A:601:ADP:H2'	1.94	0.48
1:A:401:SER:HB2	1:A:413:VAL:CG1	2.43	0.48
1:A:86:ARG:CD	1:A:86:ARG:H	2.25	0.48
1:A:412:VAL:HG21	1:A:481:ILE:HD11	1.96	0.48
1:A:47:VAL:HG12	1:A:48:ASP:N	2.29	0.48
1:B:396:MET:CE	1:B:480:GLN:HG2	2.44	0.48
1:A:358:VAL:HG12	1:A:362:ILE:HD11	1.94	0.48
1:B:60:VAL:CG1	1:B:68:GLU:HB3	2.44	0.48
1:A:155:GLU:OE1	1:A:155:GLU:HA	2.13	0.47
1:A:412:VAL:HG13	1:A:413:VAL:HG23	1.96	0.47
1:A:506:HIS:CD2	1:A:507:PRO:HD2	2.48	0.47
1:B:127:VAL:HB	1:B:160:MET:HE2	1.95	0.47
1:B:486:LEU:HD12	1:B:487:ARG:H	1.78	0.47
1:B:374:PRO:HA	1:B:508:TRP:O	2.14	0.47
1:A:172:MET:SD	1:A:209:ILE:HD11	2.54	0.47
1:A:9:THR:HG22	1:A:173:HIS:CE1	2.49	0.47
1:B:39:MET:CE	1:B:90:PHE:HE2	2.27	0.47
1:B:164:ILE:CG2	1:B:168:HIS:HB2	2.44	0.47
1:B:207:ILE:HG23	1:B:234:ALA:O	2.14	0.47
1:B:243:SER:O	1:B:246:LYS:HG3	2.14	0.47
1:A:52:MET:HE3	1:A:57:HIS:HB2	1.96	0.47
1:B:295:VAL:HA	1:B:328:ILE:O	2.14	0.47
1:A:223:LYS:HG3	1:A:227:PHE:CZ	2.49	0.47
1:A:499:GLU:C	1:A:500:ILE:HG13	2.34	0.47
1:A:506:HIS:CD2	1:A:509:PHE:HB2	2.49	0.47
1:A:506:HIS:HD2	1:A:508:TRP:N	2.10	0.47
1:B:151:LEU:HB2	1:B:152:PRO:HD3	1.96	0.47
1:B:359:GLU:HA	1:B:362:ILE:HD12	1.97	0.47
1:B:68:GLU:HG2	1:B:468:ARG:NE	2.29	0.47
1:A:159:GLN:O	1:A:162:VAL:HB	2.14	0.47
1:A:40:LYS:HE2	1:A:72:ASP:OD2	2.14	0.47
1:B:516:PRO:HB2	1:B:529:PHE:HE1	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:147:ASP:HB3	4:A:602:CTP:O2	2.14	0.47
1:A:30:GLU:HG3	5:A:791:HOH:O	2.14	0.47
1:A:383:GLN:O	1:A:385:ALA:N	2.48	0.47
1:B:493:GLY:CA	1:B:496:GLN:HE21	2.27	0.47
1:A:389:TYR:O	1:A:390:ALA:C	2.52	0.47
1:A:52:MET:HE1	5:A:804:HOH:O	2.13	0.47
1:B:335:THR:HG22	1:B:336:ARG:CG	2.43	0.47
1:B:361:MET:HB2	1:B:384:VAL:HG21	1.95	0.47
4:B:1602:CTP:HO3'	4:B:1602:CTP:HO2'	1.41	0.47
1:B:230:VAL:HG13	1:B:231:PRO:HD2	1.97	0.47
1:A:109:LEU:N	1:A:109:LEU:HD23	2.29	0.47
1:A:115:VAL:HG12	1:A:116:ILE:HG13	1.97	0.47
1:A:345:ASP:O	1:A:536:ALA:HA	2.14	0.47
1:A:469:HIS:HB2	5:A:817:HOH:O	2.15	0.47
1:A:45:ILE:O	1:A:93:GLY:HA3	2.15	0.47
1:A:297:LYS:NZ	1:A:356:ARG:HG3	2.30	0.47
1:B:256:LEU:HD12	1:B:256:LEU:O	2.15	0.47
1:B:39:MET:CE	1:B:127:VAL:HA	2.44	0.46
1:B:14:SER:O	1:B:15:SER:HB2	2.15	0.46
1:B:279:VAL:HG12	1:B:280:ILE:N	2.31	0.46
1:B:493:GLY:O	1:B:496:GLN:N	2.47	0.46
1:B:66:GLY:HA2	1:B:442:GLY:CA	2.45	0.46
1:A:338:VAL:CG1	1:A:367:PHE:CD2	2.98	0.46
1:B:78:ARG:HB3	1:B:522:PRO:HD3	1.97	0.46
1:A:312:LEU:O	1:A:313:LYS:C	2.53	0.46
1:A:409:LYS:C	1:A:411:PRO:HD3	2.35	0.46
1:B:272:ASN:O	1:B:273:LEU:HB2	2.15	0.46
1:B:363:THR:O	1:B:366:ARG:HB3	2.14	0.46
1:A:41:LEU:N	1:A:41:LEU:CD1	2.79	0.46
1:B:263:ARG:HG3	1:B:263:ARG:O	2.15	0.46
1:B:449:VAL:O	1:B:452:SER:OG	2.27	0.46
1:B:46:ASN:ND2	1:B:46:ASN:N	2.44	0.46
1:A:222:ALA:O	1:A:223:LYS:O	2.33	0.46
1:B:211:ARG:HD3	1:B:238:LEU:HD23	1.97	0.46
1:B:421:ASP:HB3	1:B:423:ASN:H	1.79	0.46
1:A:154:LEU:HD13	1:A:201:ILE:CD1	2.46	0.46
1:A:400:ASN:OD1	1:A:401:SER:N	2.29	0.46
1:A:415:LEU:HD21	1:A:471:TYR:CZ	2.51	0.46
1:B:338:VAL:CG1	1:B:367:PHE:CE1	2.99	0.46
1:B:42:ASP:O	1:B:91:THR:HA	2.15	0.46
1:B:521:THR:HB	1:B:522:PRO:CD	2.46	0.46
1:A:355:TYR:CD1	1:A:404:PHE:CB	2.99	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:458:TYR:CE2	1:B:528:LEU:CD1	2.97	0.46
1:A:297:LYS:O	1:A:299:ILE:N	2.49	0.46
1:A:492:SER:HG	1:A:493:GLY:H	1.61	0.46
1:A:539:PHE:O	1:A:540:GLN:C	2.53	0.46
1:B:299:ILE:HD13	1:B:329:ASP:HA	1.98	0.46
1:A:411:PRO:HG3	1:A:420:ARG:CZ	2.46	0.46
1:A:413:VAL:O	1:A:414:ALA:HB2	2.15	0.46
1:A:63:THR:OG1	1:A:67:ALA:HB3	2.15	0.46
1:B:349:VAL:O	1:B:381:GLY:HA3	2.15	0.46
1:A:367:PHE:CE1	1:A:373:ILE:CD1	3.00	0.45
1:B:331:GLN:O	1:B:334:GLU:HG2	2.15	0.45
1:A:278:GLN:NE2	1:A:282:GLU:CG	2.79	0.45
1:B:400:ASN:HD22	1:B:401:SER:N	1.91	0.45
1:A:106:GLY:O	1:A:109:LEU:HD23	2.17	0.45
1:A:124:LYS:CA	1:A:160:MET:HE2	2.40	0.45
1:A:36:VAL:HG12	1:A:37:THR:N	2.32	0.45
1:A:410:TYR:N	1:A:411:PRO:HD3	2.30	0.45
1:A:537:SER:O	1:A:541:LYS:HG3	2.16	0.45
1:A:346:ALA:HB2	1:A:374:PRO:HG2	1.97	0.45
1:B:224:ILE:O	1:B:225:ALA:C	2.53	0.45
1:B:346:ALA:HB2	1:B:536:ALA:HB2	1.98	0.45
1:B:355:TYR:O	1:B:356:ARG:C	2.54	0.45
1:A:299:ILE:HB	1:A:327:LEU:HD13	1.98	0.45
1:A:66:GLY:HA2	1:A:442:GLY:CA	2.47	0.45
1:B:216:VAL:HA	1:B:217:PRO:HD2	1.78	0.45
1:B:274:SER:HA	1:B:277:GLU:OE1	2.16	0.45
1:B:44:TYR:CE1	1:B:52:MET:CE	2.99	0.45
1:A:252:LYS:CE	1:A:271:ALA:HB3	2.46	0.45
1:A:329:ASP:OD1	1:A:331:GLN:HB2	2.17	0.45
1:A:339:GLU:HG3	1:A:340:ILE:N	2.31	0.45
1:A:441:LEU:CD2	1:A:468:ARG:HG3	2.47	0.45
1:B:236:ILE:N	1:B:236:ILE:CD1	2.80	0.45
1:B:411:PRO:HD2	1:B:477:LEU:HD11	1.98	0.45
1:A:124:LYS:HG2	1:A:160:MET:HE2	1.98	0.45
1:B:310:GLU:O	1:B:313:LYS:HB2	2.16	0.45
1:A:36:VAL:CG1	1:A:37:THR:N	2.80	0.45
1:A:86:ARG:HG2	1:A:87:ARG:N	2.31	0.45
1:A:90:PHE:CD1	1:A:95:ILE:HD11	2.51	0.45
1:B:23:ALA:HB1	1:B:79:PHE:HB2	1.98	0.45
1:B:284:ALA:C	1:B:286:PRO:HD3	2.36	0.45
1:A:338:VAL:HG12	1:A:367:PHE:CD2	2.52	0.45
1:B:115:VAL:O	1:B:119:ILE:HB	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:503:VAL:HG13	1:B:504:PRO:HD2	1.99	0.45
1:A:415:LEU:HD23	1:A:471:TYR:CD2	2.52	0.45
1:A:495:ASP:OD2	1:A:497:LEU:HD11	2.17	0.45
1:A:520:SER:HA	1:A:526:HIS:HB2	1.99	0.45
1:B:220:GLU:H	1:B:220:GLU:HG2	1.50	0.45
1:B:32:ARG:HG3	1:B:271:ALA:HB2	1.98	0.45
1:B:515:HIS:HB3	1:B:517:GLU:CD	2.37	0.45
1:A:172:MET:HG2	1:A:209:ILE:HD12	1.99	0.44
1:A:503:VAL:HB	1:A:509:PHE:HB3	1.99	0.44
1:B:231:PRO:O	1:B:232:GLU:C	2.54	0.44
1:B:343:GLY:O	1:B:344:LEU:HD23	2.17	0.44
1:B:394:ALA:HB3	1:B:396:MET:HG3	1.98	0.44
1:A:391:ARG:HB2	1:A:392:HIS:H	1.39	0.44
1:B:373:ILE:CG2	1:B:374:PRO:HD2	2.47	0.44
1:B:209:ILE:HG23	1:B:209:ILE:HD12	1.81	0.44
1:A:9:THR:CG2	1:A:10:GLY:N	2.80	0.44
1:A:124:LYS:O	1:A:128:LEU:HD12	2.18	0.44
1:A:28:ILE:HD11	1:A:251:LEU:HB2	2.00	0.44
1:A:46:ASN:N	1:A:46:ASN:ND2	2.62	0.44
1:A:532:PHE:O	1:A:535:ALA:HB3	2.18	0.44
1:B:102:LYS:O	1:B:105:ARG:HG3	2.17	0.44
1:B:230:VAL:CG1	1:B:234:ALA:HB3	2.47	0.44
1:A:301:LEU:O	1:A:304:ALA:N	2.29	0.44
1:A:362:ILE:HA	1:A:384:VAL:CG1	2.39	0.44
1:A:42:ASP:HA	1:A:43:PRO:HD3	1.90	0.44
1:B:331:GLN:HE21	1:B:331:GLN:HA	1.83	0.44
1:B:459:ASN:O	1:B:460:ALA:HB2	2.18	0.44
1:B:478:LEU:HA	1:B:478:LEU:HD12	1.86	0.44
1:A:403:GLU:HG3	1:A:471:TYR:CZ	2.52	0.44
1:B:319:ASN:O	1:B:321:VAL:HG23	2.17	0.44
1:B:450:ASP:O	1:B:451:ASP:HB2	2.17	0.44
1:A:309:ILE:O	1:A:312:LEU:HB2	2.18	0.44
1:A:312:LEU:HA	1:A:312:LEU:HD23	1.63	0.44
1:A:297:LYS:NZ	1:A:353:PHE:O	2.50	0.44
1:A:399:ALA:O	1:A:400:ASN:HB2	2.16	0.44
1:A:419:TRP:CZ3	1:A:475:ASN:HB2	2.53	0.44
1:A:290:VAL:HG11	1:A:537:SER:HA	2.00	0.44
1:A:453:LEU:HD12	1:A:453:LEU:C	2.37	0.44
1:A:345:ASP:HA	1:A:539:PHE:CD1	2.52	0.44
1:B:192:GLN:HA	1:B:227:PHE:CE2	2.53	0.44
1:B:80:ILE:HD12	1:B:82:THR:HB	1.99	0.44
1:A:32:ARG:HD2	1:A:268:CYS:HB3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:421:ASP:OD1	1:A:424:GLY:N	2.46	0.44
1:B:236:ILE:N	1:B:236:ILE:HD12	2.33	0.44
1:B:410:TYR:CE1	1:B:422:GLU:CB	3.01	0.44
1:A:305:TYR:CE1	1:A:350:PRO:HB2	2.53	0.43
1:A:396:MET:O	1:A:397:GLU:C	2.56	0.43
1:A:421:ASP:OD2	1:A:425:ASN:HB2	2.17	0.43
1:A:382:MET:HA	1:A:511:ALA:HB1	2.00	0.43
1:A:349:VAL:CG1	1:A:381:GLY:HA2	2.47	0.43
1:A:425:ASN:ND2	1:A:425:ASN:N	2.65	0.43
1:A:500:ILE:HG22	1:A:501:ILE:N	2.33	0.43
1:B:131:GLY:HA2	1:B:137:VAL:HG21	2.00	0.43
1:B:131:GLY:O	1:B:134:HIS:HD2	2.00	0.43
1:B:151:LEU:N	1:B:152:PRO:CD	2.81	0.43
1:B:332:ASP:HA	1:B:335:THR:HB	2.00	0.43
1:A:231:PRO:O	1:A:234:ALA:N	2.41	0.43
1:B:46:ASN:HD22	1:B:46:ASN:N	2.01	0.43
1:B:53:SER:OG	1:B:54:PRO:HD2	2.18	0.43
1:B:235:VAL:C	1:B:236:ILE:HD12	2.38	0.43
1:B:382:MET:HA	1:B:511:ALA:HB1	2.01	0.43
1:B:355:TYR:HB2	1:B:404:PHE:HD1	1.83	0.43
1:B:36:VAL:CG1	1:B:37:THR:N	2.81	0.43
1:A:290:VAL:HG22	1:A:321:VAL:HG11	2.00	0.43
1:A:179:TYR:HA	1:A:186:VAL:HA	2.01	0.43
1:B:490:GLY:HA3	1:B:500:ILE:HD12	2.01	0.43
1:A:297:LYS:HZ1	1:A:356:ARG:CG	2.31	0.43
1:B:25:LEU:HD21	1:B:260:ILE:CD1	2.49	0.43
1:B:477:LEU:HD23	1:B:477:LEU:N	2.34	0.43
1:B:188:THR:O	1:B:189:LYS:C	2.55	0.43
1:B:479:LYS:HA	1:B:482:GLU:HG3	1.99	0.43
1:A:103:GLU:HA	1:A:108:TYR:CD2	2.53	0.43
1:A:124:LYS:CB	1:A:160:MET:HE2	2.49	0.43
1:A:332:ASP:HA	1:A:335:THR:HB	2.01	0.43
1:A:415:LEU:CD2	1:A:471:TYR:CE2	3.01	0.43
1:B:299:ILE:N	1:B:299:ILE:HD12	2.13	0.43
1:B:503:VAL:HB	1:B:509:PHE:HB3	2.00	0.43
1:B:533:VAL:O	1:B:534:LYS:C	2.57	0.43
1:A:105:ARG:O	1:A:107:ASP:OD1	2.37	0.42
1:A:318:LYS:HD3	1:A:318:LYS:HA	1.69	0.42
1:A:373:ILE:O	1:A:374:PRO:C	2.57	0.42
1:A:4:ASN:OD1	1:A:168:HIS:ND1	2.43	0.42
1:B:39:MET:HE1	1:B:127:VAL:HA	2.00	0.42
1:B:396:MET:HE1	1:B:480:GLN:CG	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:539:PHE:CE1	1:B:543:GLN:HG3	2.53	0.42
1:A:262:LYS:HG2	1:A:263:ARG:N	2.34	0.42
1:A:515:HIS:HB3	1:A:517:GLU:OE1	2.18	0.42
1:B:164:ILE:HG21	1:B:169:THR:HG23	2.01	0.42
1:B:319:ASN:O	1:B:320:ARG:C	2.54	0.42
1:A:160:MET:O	1:A:161:ALA:C	2.54	0.42
1:A:204:GLN:HG3	1:A:204:GLN:O	2.19	0.42
1:A:257:ASP:N	1:A:257:ASP:OD1	2.52	0.42
1:A:292:ILE:HG12	1:A:346:ALA:HB3	2.01	0.42
1:A:42:ASP:C	1:A:44:TYR:H	2.22	0.42
1:A:487:ARG:O	1:A:501:ILE:HA	2.18	0.42
1:B:361:MET:CB	1:B:384:VAL:HG21	2.49	0.42
1:A:247:ILE:O	1:A:248:PRO:C	2.57	0.42
1:B:338:VAL:O	1:B:341:LEU:N	2.47	0.42
1:B:389:TYR:CE2	1:B:486:LEU:HB2	2.54	0.42
1:B:26:ALA:HB1	1:B:80:ILE:HG21	2.01	0.42
1:A:543:GLN:O	1:A:544:ALA:HB2	2.19	0.42
1:B:218:ALA:HA	1:B:221:ARG:CZ	2.49	0.42
1:A:467:HIS:HA	5:A:704:HOH:O	2.19	0.42
1:A:358:VAL:HG12	1:A:362:ILE:CD1	2.50	0.42
1:A:386:LEU:O	1:A:387:ILE:C	2.57	0.42
1:A:99:VAL:HG13	1:A:108:TYR:OH	2.20	0.42
1:B:179:TYR:CE2	1:B:181:ALA:HA	2.53	0.42
1:B:355:TYR:CG	1:B:404:PHE:HB3	2.55	0.42
1:A:101:ARG:HG2	1:A:102:LYS:N	2.34	0.42
1:A:399:ALA:HA	1:A:410:TYR:HB3	2.02	0.42
1:A:481:ILE:HG12	1:A:481:ILE:H	1.30	0.42
1:B:151:LEU:HA	1:B:151:LEU:HD23	1.82	0.42
1:B:338:VAL:HG11	1:B:367:PHE:CD1	2.54	0.42
1:B:532:PHE:O	1:B:535:ALA:HB3	2.20	0.42
1:A:308:VAL:O	1:A:309:ILE:C	2.57	0.42
1:A:452:SER:HB2	1:A:502:GLU:OE2	2.19	0.42
1:A:345:ASP:HA	1:A:539:PHE:CE1	2.55	0.42
1:B:349:VAL:HA	1:B:350:PRO:HD3	1.84	0.42
1:B:389:TYR:OH	1:B:485:GLY:HA3	2.20	0.42
1:B:465:GLU:HB3	1:B:514:PHE:CD1	2.54	0.42
1:A:152:PRO:HG2	5:A:813:HOH:O	2.19	0.42
1:A:495:ASP:O	1:A:496:GLN:O	2.38	0.42
1:A:18:LYS:HG3	3:A:601:ADP:O2B	2.20	0.42
1:B:465:GLU:CB	1:B:514:PHE:CD1	3.03	0.42
1:B:68:GLU:HG2	1:B:468:ARG:HE	1.84	0.42
1:A:367:PHE:HE1	1:A:373:ILE:CD1	2.33	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:386:LEU:HA	1:A:386:LEU:HD12	1.78	0.41
1:A:408:CYS:SG	1:A:411:PRO:HA	2.60	0.41
1:B:230:VAL:HG13	1:B:234:ALA:HB3	2.02	0.41
1:A:114:GLN:O	1:A:118:HIS:HB2	2.20	0.41
1:A:339:GLU:CG	1:A:340:ILE:N	2.83	0.41
1:A:86:ARG:HD2	1:A:86:ARG:H	1.84	0.41
1:B:211:ARG:HD2	1:B:238:LEU:HD23	2.02	0.41
1:B:387:ILE:O	1:B:388:ASP:C	2.58	0.41
1:B:474:ASN:HB3	5:B:1802:HOH:O	2.19	0.41
1:B:467:HIS:CE1	1:B:514:PHE:HB3	2.54	0.41
1:B:62:VAL:HA	1:B:67:ALA:O	2.20	0.41
1:A:117:PRO:O	1:A:118:HIS:C	2.59	0.41
1:A:401:SER:C	1:A:403:GLU:H	2.23	0.41
1:A:355:TYR:CD1	1:A:404:PHE:CG	3.08	0.41
1:A:515:HIS:HB3	1:A:517:GLU:CD	2.41	0.41
1:B:247:ILE:N	1:B:248:PRO:CD	2.83	0.41
1:B:453:LEU:HD12	1:B:453:LEU:HA	1.66	0.41
1:A:247:ILE:O	1:A:251:LEU:HG	2.20	0.41
1:A:366:ARG:O	1:A:367:PHE:C	2.58	0.41
1:B:127:VAL:HB	1:B:160:MET:CE	2.50	0.41
1:A:231:PRO:HB2	1:A:233:LYS:HG3	2.02	0.41
1:B:289:GLU:CB	1:B:322:SER:HB3	2.44	0.41
1:B:116:ILE:HA	1:B:117:PRO:HA	1.85	0.41
1:B:334:GLU:H	1:B:334:GLU:HG2	1.56	0.41
1:B:347:ILE:CG2	1:B:348:LEU:N	2.80	0.41
1:B:421:ASP:HB2	1:B:425:ASN:H	1.85	0.41
1:B:458:TYR:CZ	1:B:528:LEU:HD12	2.55	0.41
1:B:386:LEU:HA	1:B:386:LEU:HD12	1.78	0.41
1:A:17:GLY:HA3	3:A:601:ADP:C8	2.55	0.41
1:B:354:GLY:O	1:B:355:TYR:HB2	2.21	0.41
1:B:402:THR:CG2	1:B:414:ALA:CB	2.99	0.41
1:A:394:ALA:HB3	1:A:396:MET:HG3	2.03	0.41
1:A:478:LEU:HD12	1:A:478:LEU:HA	1.77	0.41
1:A:71:LEU:O	1:A:72:ASP:C	2.58	0.41
1:A:76:TYR:N	1:A:76:TYR:CD1	2.86	0.41
1:B:198:LEU:O	1:B:201:ILE:HG12	2.20	0.41
1:A:362:ILE:CA	1:A:384:VAL:HG13	2.44	0.41
1:B:117:PRO:O	1:B:118:HIS:C	2.59	0.41
1:B:45:ILE:O	1:B:46:ASN:C	2.56	0.41
1:B:4:ASN:OD1	1:B:168:HIS:ND1	2.46	0.41
1:B:372:ASN:HA	1:B:506:HIS:CD2	2.56	0.41
1:A:372:ASN:HD22	1:A:372:ASN:N	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:412:VAL:HG23	1:A:477:LEU:HB2	2.03	0.41
1:A:448:LEU:HB2	1:A:461:PRO:O	2.21	0.41
1:A:86:ARG:N	1:A:86:ARG:CD	2.84	0.41
1:B:486:LEU:HD21	1:B:501:ILE:HD12	2.03	0.41
1:A:126:ARG:O	1:A:127:VAL:C	2.58	0.40
1:A:298:TYR:O	1:A:300:GLU:N	2.54	0.40
1:A:442:GLY:O	1:A:466:ARG:HA	2.22	0.40
1:A:495:ASP:OD1	1:A:495:ASP:N	2.45	0.40
1:B:379:CYS:O	1:B:380:LEU:C	2.58	0.40
1:B:385:ALA:O	1:B:386:LEU:C	2.60	0.40
1:A:215:ALA:O	1:A:217:PRO:HD3	2.21	0.40
1:A:409:LYS:HG3	1:A:409:LYS:O	2.09	0.40
1:B:215:ALA:O	1:B:217:PRO:HD3	2.21	0.40
1:A:268:CYS:HA	1:A:269:PRO:HD2	1.83	0.40
1:A:312:LEU:O	1:A:315:GLY:N	2.55	0.40
1:A:338:VAL:HG11	1:A:367:PHE:HD2	1.86	0.40
1:A:349:VAL:HG12	1:A:381:GLY:HA2	2.03	0.40
1:A:493:GLY:O	1:A:496:GLN:HG2	2.21	0.40
1:B:396:MET:CE	1:B:480:GLN:CG	2.99	0.40
1:B:402:THR:CG2	1:B:414:ALA:HB2	2.52	0.40
1:A:396:MET:HE1	1:A:480:GLN:CB	2.28	0.40
1:A:537:SER:O	1:A:538:GLU:C	2.59	0.40
1:B:380:LEU:HD12	1:B:380:LEU:HA	1.78	0.40
1:A:4:ASN:N	1:A:135:ASP:O	2.50	0.40
1:A:506:HIS:CG	1:A:507:PRO:CD	3.02	0.40
1:B:28:ILE:HD12	1:B:257:ASP:HB3	2.04	0.40
1:B:426:VAL:HG12	1:B:427:GLU:HG2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:1724:HOH:O	5:B:1724:HOH:O[2_555]	0.81	1.39

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/545 (97%)	445 (84%)	66 (12%)	19 (4%)	5	16
1	B	532/545 (98%)	461 (87%)	60 (11%)	11 (2%)	10	32
All	All	1062/1090 (97%)	906 (85%)	126 (12%)	30 (3%)	7	23

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	TYR
1	A	335	THR
1	A	356	ARG
1	A	391	ARG
1	A	392	HIS
1	A	504	PRO
1	B	358	VAL
1	B	397	GLU
1	B	494	ASP
1	A	223	LYS
1	A	224	ILE
1	A	302	PRO
1	A	306	LYS
1	A	408	CYS
1	A	492	SER
1	A	496	GLN
1	A	543	GLN
1	B	132	GLU
1	B	355	TYR
1	B	493	GLY
1	B	496	GLN
1	B	544	ALA
1	A	478	LEU
1	B	306	LYS
1	A	397	GLU
1	A	409	LYS
1	A	299	ILE
1	A	384	VAL
1	B	387	ILE
1	B	426	VAL

### 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	451/461 (98%)	396 (88%)	55 (12%)	7	20
1	B	453/461 (98%)	398 (88%)	55 (12%)	7	20
All	All	904/922 (98%)	794 (88%)	110 (12%)	7	20

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	52	MET
1	A	53	SER
1	A	57	HIS
1	A	81	ARG
1	A	86	ARG
1	A	94	ARG
1	A	97	SER
1	A	112	THR
1	A	128	LEU
1	A	132	GLU
1	A	135	ASP
1	A	163	GLU
1	A	166	ARG
1	A	183	SER
1	A	219	ASN
1	A	220	GLU
1	A	224	ILE
1	A	229	ASN
1	A	230	VAL
1	A	243	SER
1	A	250	LEU
1	A	253	SER
1	A	262	LYS
1	A	272	ASN
1	A	274	SER
1	A	278	GLN
1	A	289	GLU
1	A	294	MET

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Mol	Chain	Res	Type
1	A	298	TYR
1	A	300	GLU
1	A	301	LEU
1	A	309	ILE
1	A	326	LYS
1	A	327	LEU
1	A	338	VAL
1	A	356	ARG
1	A	372	ASN
1	A	397	GLU
1	A	401	SER
1	A	408	CYS
1	A	409	LYS
1	A	412	VAL
1	A	420	ARG
1	A	427	GLU
1	A	438	THR
1	A	439	MET
1	A	454	VAL
1	A	455	ARG
1	A	480	GLN
1	A	481	ILE
1	A	495	ASP
1	A	501	ILE
1	A	521	THR
1	A	542	ARG
1	B	1	MET
1	B	2	THR
1	B	20	ILE
1	B	32	ARG
1	B	40	LYS
1	B	46	ASN
1	B	86	ARG
1	B	87	ARG
1	B	89	ASN
1	B	94	ARG
1	B	97	SER
1	B	104	ARG
1	B	105	ARG
1	B	109	LEU
1	B	132	GLU
1	B	166	ARG

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Mol	Chain	Res	Type
1	B	180	MET
1	B	208	LEU
1	B	238	LEU
1	B	239	LYS
1	B	253	SER
1	B	257	ASP
1	B	263	ARG
1	B	265	SER
1	B	267	ASN
1	B	273	LEU
1	B	274	SER
1	B	288	SER
1	B	295	VAL
1	B	299	ILE
1	B	300	GLU
1	B	306	LYS
1	B	326	LYS
1	B	330	SER
1	B	331	GLN
1	B	340	ILE
1	B	379	CYS
1	B	383	GLN
1	B	387	ILE
1	B	388	ASP
1	B	392	HIS
1	B	397	GLU
1	B	400	ASN
1	B	409	LYS
1	B	421	ASP
1	B	427	GLU
1	B	428	VAL
1	B	444	GLN
1	B	469	HIS
1	B	479	LYS
1	B	492	SER
1	B	519	THR
1	B	528	LEU
1	B	540	GLN
1	B	542	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	272	ASN
1	A	278	GLN
1	A	285	ASN
1	A	319	ASN
1	A	372	ASN
1	A	425	ASN
1	A	469	HIS
1	A	506	HIS
1	B	46	ASN
1	B	134	HIS
1	B	193	HIS
1	B	229	ASN
1	B	285	ASN
1	B	331	GLN
1	B	400	ASN
1	B	425	ASN
1	B	467	HIS
1	B	469	HIS
1	B	480	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - 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	ADP	A	601	2	29,29,29	0.91	2 (6%)	45,45,45	1.49	4 (8%)
4	CTP	A	602	-	30,30,30	1.93	6 (20%)	44,47,47	1.70	5 (11%)
3	ADP	B	1601	2	29,29,29	0.99	3 (10%)	45,45,45	0.91	1 (2%)
4	CTP	B	1602	-	30,30,30	1.63	4 (13%)	44,47,47	1.86	7 (15%)

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	ADP	A	601	2	-	0/16/32/32	0/3/3/3
4	CTP	A	602	-	-	0/20/38/38	0/2/2/2
3	ADP	B	1601	2	-	0/16/32/32	0/3/3/3
4	CTP	B	1602	-	-	0/20/38/38	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	CTP	C2-N1	4.94	1.43	1.38
4	A	602	CTP	PG-O3B	4.68	1.68	1.60
4	A	602	CTP	PB-O3A	4.26	1.67	1.59
4	B	1602	CTP	PB-O3B	4.15	1.67	1.59
4	B	1602	CTP	PG-O3B	3.55	1.66	1.60
4	A	602	CTP	O4'-C1'	3.47	1.45	1.41
4	A	602	CTP	C2'-C1'	-2.84	1.49	1.53
3	B	1601	ADP	PA-O3A	2.72	1.64	1.59
4	B	1602	CTP	O4'-C1'	2.57	1.44	1.41
3	B	1601	ADP	PB-O3A	2.28	1.64	1.60
3	A	601	ADP	PA-O5'	-2.19	1.49	1.59
3	B	1601	ADP	PA-O5'	-2.08	1.49	1.59
4	A	602	CTP	C4-N3	2.06	1.39	1.35
4	B	1602	CTP	C5'-C4'	2.01	1.58	1.51
3	A	601	ADP	PA-O3A	2.00	1.63	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	CTP	C6-C5-C4	7.30	120.99	117.51
4	B	1602	CTP	O4'-C1'-N1	-6.40	94.05	108.08
3	A	601	ADP	C8-N9-C1'	5.89	137.24	126.15
3	A	601	ADP	C1'-N9-C4	-5.53	117.08	126.64
4	A	602	CTP	C4'-O4'-C1'	-5.25	103.95	109.72
4	B	1602	CTP	C4'-O4'-C1'	-4.43	104.85	109.72
4	B	1602	CTP	C6-C5-C4	4.35	119.59	117.51
4	B	1602	CTP	C2'-C1'-N1	3.84	123.85	113.34
4	B	1602	CTP	O4'-C1'-C2'	-3.38	101.76	106.69
3	A	601	ADP	PA-O3A-PB	-2.83	124.09	131.93
4	A	602	CTP	O4'-C1'-C2'	-2.78	102.65	106.69
4	A	602	CTP	C2-N3-C4	2.75	119.61	115.65
4	B	1602	CTP	PB-O3A-PA	-2.65	124.59	131.93
4	B	1602	CTP	C2-N3-C4	2.59	119.37	115.65
4	A	602	CTP	O4'-C1'-N1	-2.21	103.23	108.08
3	B	1601	ADP	C1'-N9-C4	2.20	130.44	126.64
3	A	601	ADP	O3B-PB-O2B	2.14	115.42	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	534/545 (97%)	-0.57	4 (0%)	84 86	30, 58, 93, 99	5 (0%)
1	B	536/545 (98%)	-0.56	4 (0%)	84 86	25, 56, 92, 100	3 (0%)
All	All	1070/1090 (98%)	-0.57	8 (0%)	84 86	25, 57, 92, 100	8 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.2
1	B	494	ASP	3.1
1	B	545	LYS	2.7
1	A	339	GLU	2.4
1	B	495	ASP	2.4
1	A	394	ALA	2.2
1	A	504	PRO	2.1
1	A	408	CYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	1701	1/1	0.14	0.59	45,45,45,45	0
3	ADP	B	1601	27/27	0.14	0.05	45,78,94,100	0
3	ADP	A	601	27/27	0.12	-0.13	38,72,98,100	0
4	CTP	A	602	29/29	0.13	-0.28	29,41,48,52	0
4	CTP	B	1602	29/29	0.13	-0.70	39,44,48,50	0
2	MG	A	701	1/1	0.09	-0.83	32,32,32,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.