



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:27 PM UTC

PDB ID : 1OZ0 / pdb_00001oz0
Title : CRYSTAL STRUCTURE OF THE HOMODIMERIC BIFUNCTIONAL TRANSFORMYLASE AND CYCLOHYDROLASE ENZYME AVIAN ATIC IN COMPLEX WITH A MULTISUBSTRATE ADDUCT INHIBITOR BETA-DADF.
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Deposited on : 2003-04-07
Resolution : 2.50 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

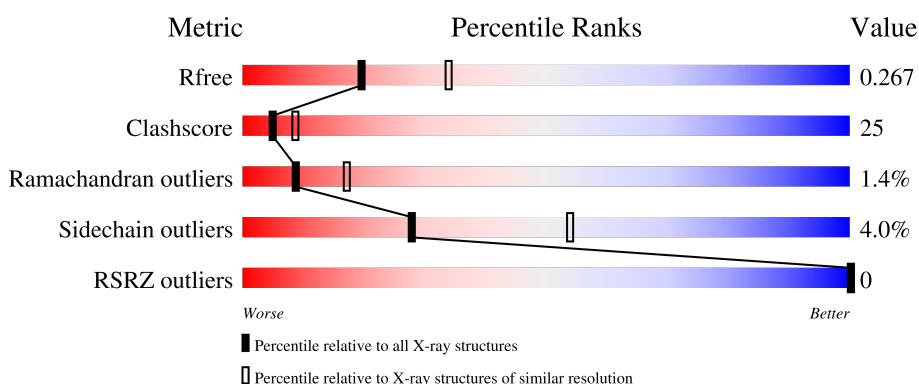
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	613	52% 41% . .
1	B	613	56% 36% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9526 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 Bifunctional purine biosynthesis protein PURH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	0
			4511	2843	800	849	19			
1	B	590	Total	C	N	O	S	4	0	0
			4511	2843	800	849	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P31335
A	-18	GLY	-	expression tag	UNP P31335
A	-17	SER	-	expression tag	UNP P31335
A	-16	SER	-	expression tag	UNP P31335
A	-15	HIS	-	expression tag	UNP P31335
A	-14	HIS	-	expression tag	UNP P31335
A	-13	HIS	-	expression tag	UNP P31335
A	-12	HIS	-	expression tag	UNP P31335
A	-11	HIS	-	expression tag	UNP P31335
A	-10	HIS	-	expression tag	UNP P31335
A	-9	SER	-	expression tag	UNP P31335
A	-8	SER	-	expression tag	UNP P31335
A	-7	GLY	-	expression tag	UNP P31335
A	-6	LEU	-	expression tag	UNP P31335
A	-5	VAL	-	expression tag	UNP P31335
A	-4	PRO	-	expression tag	UNP P31335
A	-3	ARG	-	expression tag	UNP P31335
A	-2	GLY	-	expression tag	UNP P31335
A	-1	SER	-	expression tag	UNP P31335
A	0	HIS	-	expression tag	UNP P31335
B	-19	MET	-	expression tag	UNP P31335
B	-18	GLY	-	expression tag	UNP P31335
B	-17	SER	-	expression tag	UNP P31335
B	-16	SER	-	expression tag	UNP P31335
B	-15	HIS	-	expression tag	UNP P31335

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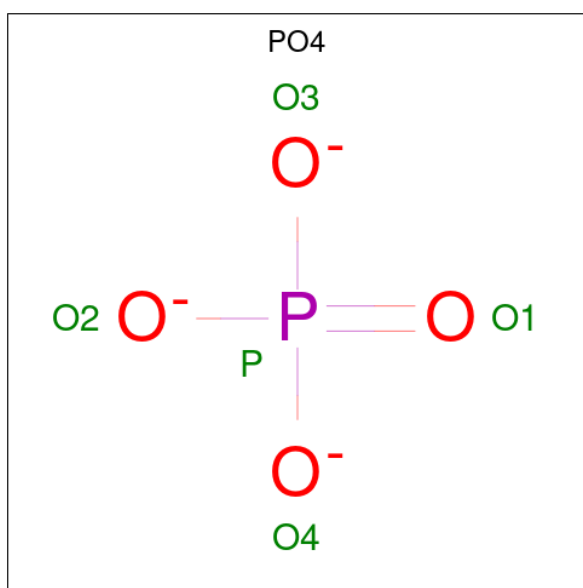
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P31335
B	-13	HIS	-	expression tag	UNP P31335
B	-12	HIS	-	expression tag	UNP P31335
B	-11	HIS	-	expression tag	UNP P31335
B	-10	HIS	-	expression tag	UNP P31335
B	-9	SER	-	expression tag	UNP P31335
B	-8	SER	-	expression tag	UNP P31335
B	-7	GLY	-	expression tag	UNP P31335
B	-6	LEU	-	expression tag	UNP P31335
B	-5	VAL	-	expression tag	UNP P31335
B	-4	PRO	-	expression tag	UNP P31335
B	-3	ARG	-	expression tag	UNP P31335
B	-2	GLY	-	expression tag	UNP P31335
B	-1	SER	-	expression tag	UNP P31335
B	0	HIS	-	expression tag	UNP P31335

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

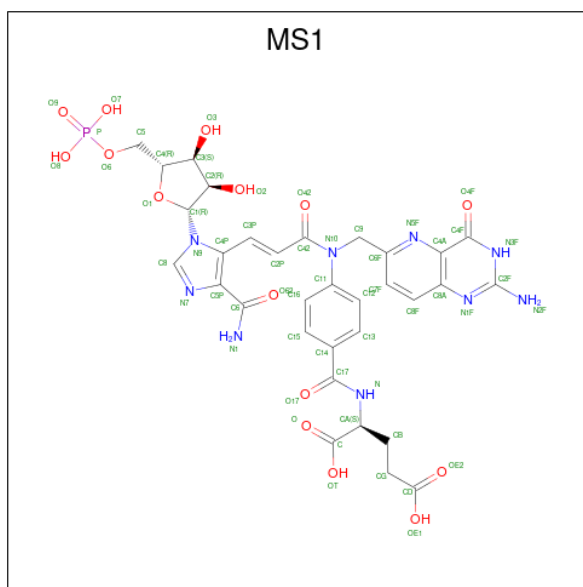
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is 2-[4-((2-AMINO-4-OXO-3,4-DIHYDRO-PYRIDO[3,2-D]PYRIMIDIN-6-YLM ETHYL)-{3-[5-CARBAMOYL-3-(3,4- DIHYDROXY-5-PHOSPHONOOXYMETHYL-TE TRAHYDRO-FURAN-2-YL)-3H-IMIDAZOL-4-YL]-ACRYLOYL}-AMINO)-BENZOYLAMINO]- PENTANEDIOIC ACID (CCD ID: MS1) (formula: C₃₂H₃₄N₉O₁₅P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 57 32 9 15 1	0	0
4	B	1	Total C N O P 57 32 9 15 1	0	0

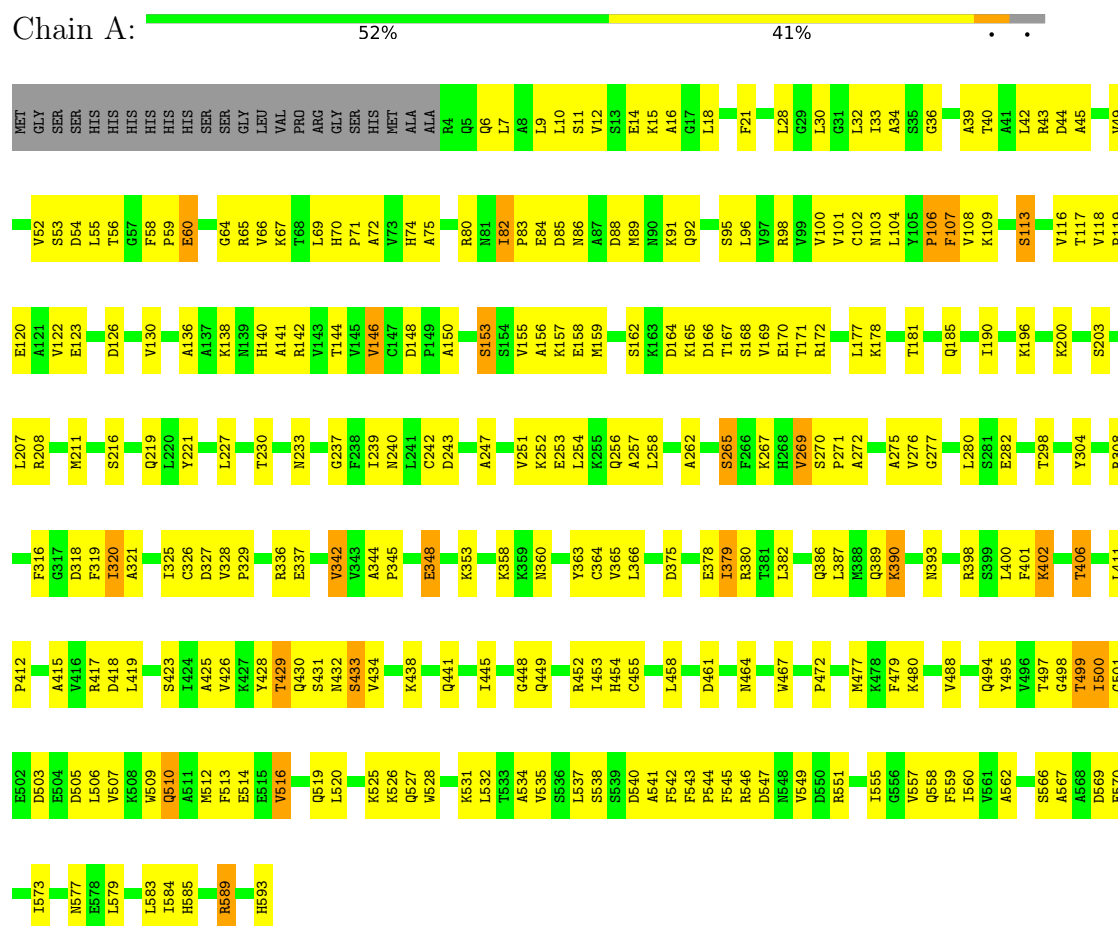
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	204	Total O 204 204	0	0
5	B	174	Total O 174 174	0	0

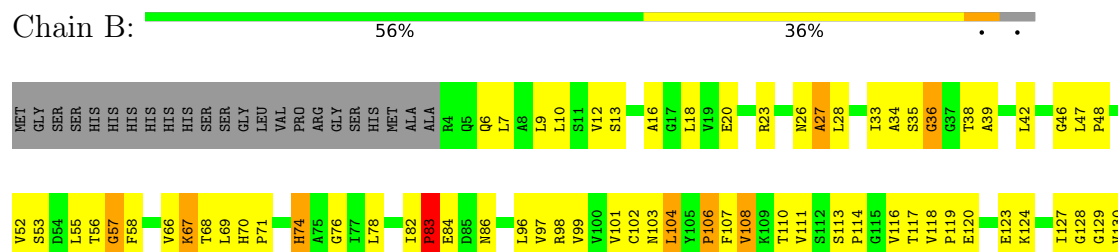
3 Residue-property plots

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: Bifunctional purine biosynthesis protein PURH



- Molecule 1: Bifunctional purine biosynthesis protein PURH



F543	G448	D327	Q219	A131
R546	Q449	V328	L220	L132
D547	Q450	P329	Y221	L133
N548	S451	V342	T222	R134
V549	R452	V343	P225	A135
D550	I453	A344	K226	A136
R551	H454	P345	L227	A137
A552	C455	E349	P228	K138
K553	K462	E350	L229	M139
R554	I555	M660	V143	V143
I555	A463	V365	T144	T144
G556	N464	L366	V145	V145
V557	R469	Y372	C147	V146
Q558	V474	I379	D148	C147
F559	M477	L382	Y152	D148
I560	K478	Q386	V155	Y152
V561	F479	L387	A156	V155
A562	K480	K388	K157	A156
P563	K481	K390	E158	K157
S564	A482	N393	M159	E158
G565	G483	A394	A160	M159
S566	V484	F401	A161	A160
A567	K484	T406	D164	A161
A568	E487	K407	K165	D164
D569	V488	N408	S168	K165
I573	S489	K409	V169	S168
A575	N490	L411	E170	V169
L579	Q494	A415	T171	E170
L583	Y495	V416	R172	T171
I584	V496	R417	R173	R172
H585	T497	D418	H174	R173
L588	I500	I420	L175	H174
F591	W509	V426	A176	L175
H592	Q510	S431	L177	A176
H593	A511	N432	K178	L177
	M512	S433	T181	K178
	F513	V436	Q185	T181
	E514	A437	R195	Q185
	E515	K438	S199	R195
	V516	D540	K200	S199
	P517	A541	S203	K200
	T521	F542	L207	S203
	E524		M211	L207
	V535		N212	M211
	S536		S216	N212
	L537			S216

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.41Å 108.10Å 102.36Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.1 (50.00-2.50) 92.8 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.269 0.215 , 0.267	Depositor DCC
R_{free} test set	3554 reflections (7.59%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.060 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9526	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, PO4, MS1

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	0.49	0/4595	0.98	13/6230 (0.2%)
1	B	0.49	0/4595	0.99	15/6230 (0.2%)
All	All	0.49	0/9190	0.98	28/12460 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	ALA	N-CA-C	-8.30	102.86	113.16
1	B	567	ALA	N-CA-C	-7.78	103.78	113.20
1	A	75	ALA	N-CA-C	-7.42	103.13	111.07
1	B	433	SER	N-CA-C	7.30	119.96	108.79
1	A	433	SER	N-CA-C	7.11	119.87	109.07
1	B	13	SER	N-CA-C	-6.79	104.89	113.72
1	B	431	SER	N-CA-C	6.46	119.06	110.53
1	B	441	GLN	N-CA-C	6.35	118.83	109.24
1	B	514	GLU	N-CA-C	-6.30	104.75	112.88
1	A	441	GLN	N-CA-C	6.16	118.54	109.24
1	B	320	ILE	N-CA-C	6.11	117.81	108.71
1	B	272	ALA	N-CA-C	-5.95	104.74	112.23
1	A	514	GLU	N-CA-C	-5.91	102.52	111.56
1	A	516	VAL	N-CA-C	5.68	115.21	108.96
1	B	462	LYS	N-CA-C	-5.64	105.28	111.82
1	A	272	ALA	N-CA-C	-5.63	105.52	112.90
1	B	74	HIS	N-CA-C	5.59	117.38	111.28
1	B	562	ALA	CA-C-N	-5.46	114.63	120.03
1	B	562	ALA	C-N-CA	-5.46	114.63	120.03
1	A	320	ILE	N-CA-C	5.35	116.69	108.71
1	B	390	LYS	N-CA-C	-5.29	101.84	110.20
1	B	57	GLY	N-CA-C	-5.28	108.33	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	LYS	N-CA-C	-5.28	101.87	110.20
1	A	107	PHE	N-CA-C	-5.23	106.60	112.87
1	A	319	PHE	N-CA-C	-5.15	100.77	109.07
1	B	228	PRO	N-CA-C	-5.09	107.77	114.03
1	A	275	ALA	N-CA-C	5.02	115.77	108.14
1	A	348	GLU	N-CA-C	-5.01	102.87	110.28

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	4511	0	4561	255	0
1	B	4511	0	4561	221	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	57	0	31	6	0
4	B	57	0	31	7	0
5	A	204	0	0	29	0
5	B	174	0	0	23	0
All	All	9526	0	9184	460	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 25.

All (460) 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:501:GLY:HA3	1:A:505:ASP:HB2	1.45	0.97
1:A:401:PHE:HB3	1:A:584:ILE:HD13	1.48	0.94
1:B:350:GLU:HB2	5:B:1125:HOH:O	1.70	0.90
1:B:283:GLU:HG3	5:B:1067:HOH:O	1.69	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLY:HA3	1:A:67:LYS:HE3	1.55	0.88
1:A:426:VAL:HA	1:A:429:THR:CG2	2.02	0.88
1:B:464:ASN:OD1	1:B:555:ILE:HD13	1.74	0.86
1:A:7:LEU:HD13	1:A:33:ILE:HD11	1.59	0.84
1:B:211:MET:HE2	1:B:239:ILE:HG12	1.60	0.84
1:A:12:VAL:HB	1:A:103:ASN:ND2	1.91	0.83
1:A:411:LEU:HB3	5:A:1137:HOH:O	1.78	0.83
1:B:104:LEU:HD21	1:B:133:LEU:HD12	1.60	0.81
1:A:32:LEU:HD11	1:A:49:VAL:HG22	1.63	0.81
1:A:138:LYS:HD2	1:B:127:ILE:HD11	1.64	0.80
1:B:406:THR:HG23	1:B:583:LEU:HB3	1.64	0.80
1:A:200:LYS:HE2	5:A:1094:HOH:O	1.83	0.77
1:A:495:TYR:HA	1:A:500:ILE:HD11	1.67	0.76
1:A:510:GLN:OE1	1:A:516:VAL:HG11	1.85	0.76
1:A:98:ARG:HA	5:A:1199:HOH:O	1.86	0.76
1:A:88:ASP:HA	1:A:91:LYS:HE3	1.69	0.75
1:B:207:LEU:HD23	1:B:219:GLN:HA	1.69	0.75
1:B:452:ARG:NH2	1:B:541:ALA:HB3	2.03	0.74
1:A:118:VAL:HB	1:A:119:PRO:HD3	1.70	0.74
1:B:113:SER:HB2	1:B:114:PRO:HD2	1.68	0.73
1:A:379:ILE:HG22	5:B:1077:HOH:O	1.88	0.72
1:B:128:GLY:O	1:B:132:LEU:HG	1.89	0.72
1:B:200:LYS:NZ	5:B:1114:HOH:O	2.22	0.72
1:A:537:LEU:HD23	1:A:538:SER:N	2.05	0.71
1:B:118:VAL:HB	1:B:119:PRO:HD3	1.73	0.70
1:A:208:ARG:NH2	4:B:1001:MS1:O8	2.24	0.69
1:B:48:PRO:HD2	5:B:1096:HOH:O	1.92	0.69
1:A:138:LYS:CD	1:B:127:ILE:HD11	2.23	0.69
1:B:130:VAL:O	1:B:134:ARG:HG3	1.92	0.68
1:B:155:VAL:HG12	1:B:159:MET:HE2	1.75	0.68
1:A:32:LEU:HG	5:A:1012:HOH:O	1.94	0.68
1:B:110:THR:CG2	1:B:124:LYS:HD2	2.24	0.68
1:A:9:LEU:HD12	1:A:33:ILE:O	1.95	0.67
1:B:7:LEU:HB3	1:B:33:ILE:HD11	1.77	0.67
1:A:558:GLN:HB3	5:A:1158:HOH:O	1.94	0.67
1:B:207:LEU:HD11	1:B:241:LEU:HD11	1.76	0.67
1:A:452:ARG:NH2	1:A:541:ALA:HB3	2.09	0.67
1:B:113:SER:OG	1:B:116:VAL:HB	1.95	0.66
1:A:336:ARG:HG3	5:A:1173:HOH:O	1.95	0.66
1:B:46:GLY:O	1:B:47:LEU:HG	1.94	0.66
1:B:6:GLN:OE1	1:B:98:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:LYS:HB3	5:B:1178:HOH:O	1.96	0.66
1:A:12:VAL:HG23	1:A:15:LYS:HG3	1.79	0.65
1:A:181:THR:O	1:A:185:GLN:HG3	1.96	0.65
1:B:27:ALA:HB2	5:B:1123:HOH:O	1.95	0.65
1:B:479:PHE:CE2	1:B:488:VAL:HG13	2.31	0.64
1:A:7:LEU:HD13	1:A:33:ILE:CD1	2.28	0.64
1:A:82:ILE:HD13	1:A:82:ILE:H	1.61	0.64
1:A:83:PRO:HG2	1:A:84:GLU:OE1	1.97	0.64
1:A:498:GLY:C	1:A:500:ILE:H	2.05	0.64
1:A:401:PHE:HB3	1:A:584:ILE:CD1	2.26	0.64
1:B:110:THR:HG21	1:B:124:LYS:HD2	1.78	0.64
1:B:379:ILE:HD13	1:B:379:ILE:C	2.23	0.64
1:B:453:ILE:HD13	1:B:547:ASP:CG	2.23	0.64
4:A:1002:MS1:C12	4:A:1002:MS1:C2P	2.74	0.64
1:B:7:LEU:HB3	1:B:33:ILE:CD1	2.27	0.63
1:A:526:LYS:NZ	1:A:526:LYS:HB3	2.14	0.63
1:B:389:GLN:HG3	1:B:390:LYS:O	1.99	0.63
1:B:33:ILE:N	1:B:33:ILE:HD12	2.13	0.63
1:B:104:LEU:HD21	1:B:133:LEU:CD1	2.29	0.63
1:A:402:LYS:NZ	1:A:402:LYS:HA	2.14	0.62
1:A:434:VAL:HG13	1:A:537:LEU:HD21	1.80	0.62
1:A:98:ARG:CB	5:A:1199:HOH:O	2.47	0.62
1:A:153:SER:O	1:A:157:LYS:HG3	2.00	0.62
1:B:226:LYS:HB2	1:B:226:LYS:NZ	2.14	0.62
1:A:10:LEU:HD22	1:A:42:LEU:HD21	1.80	0.61
1:B:252:LYS:O	1:B:256:GLN:HG3	1.99	0.61
1:A:65:ARG:NH2	1:A:123:GLU:OE1	2.27	0.61
1:B:521:THR:HG23	1:B:524:GLU:OE1	1.99	0.61
1:A:247:ALA:HB1	1:A:321:ALA:HB2	1.81	0.61
1:B:120:GLU:O	1:B:124:LYS:HG3	2.00	0.61
1:B:280:LEU:CD1	1:B:302:SER:HB3	2.30	0.61
1:A:52:VAL:C	1:A:54:ASP:H	2.07	0.61
1:A:325:ILE:HD12	1:A:325:ILE:H	1.66	0.61
1:B:34:ALA:HB3	1:B:39:ALA:HB2	1.81	0.61
1:A:400:LEU:HB2	5:A:1038:HOH:O	2.00	0.61
1:B:426:VAL:CG1	1:B:540:ASP:HB3	2.31	0.61
4:A:1002:MS1:C2P	4:A:1002:MS1:H12	2.31	0.60
1:B:18:LEU:HG	1:B:42:LEU:HD21	1.83	0.60
1:A:219:GLN:HE21	1:B:388:MET:HE2	1.66	0.60
1:A:282:GLU:N	1:A:282:GLU:OE1	2.33	0.60
1:B:477:MET:HE2	1:B:513:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:MET:O	1:A:162:SER:HB3	2.01	0.60
1:B:181:THR:HG22	1:B:185:GLN:HE21	1.66	0.60
1:B:252:LYS:HG2	1:B:256:GLN:HE21	1.65	0.60
4:A:1002:MS1:H52	1:B:239:ILE:HB	1.83	0.60
1:B:211:MET:HE3	1:B:211:MET:HA	1.83	0.60
1:B:34:ALA:O	1:B:52:VAL:HG23	2.02	0.59
1:B:474:VAL:O	1:B:477:MET:HG3	2.01	0.59
1:A:117:THR:O	1:A:120:GLU:HB2	2.02	0.59
1:A:316:PHE:CG	4:B:1001:MS1:H7F	2.38	0.59
1:A:402:LYS:HA	1:A:402:LYS:HZ2	1.66	0.59
1:A:458:LEU:HD12	5:A:1046:HOH:O	2.03	0.59
1:A:33:ILE:HD13	1:A:55:LEU:HD22	1.82	0.59
1:B:408:ASN:HB3	5:B:1156:HOH:O	2.03	0.59
1:A:80:ARG:HB2	1:A:82:ILE:HD12	1.85	0.59
1:A:393:ASN:ND2	5:A:1131:HOH:O	2.36	0.58
1:B:386:GLN:NE2	5:B:1030:HOH:O	2.36	0.58
1:A:159:MET:O	1:A:165:LYS:HA	2.03	0.58
1:A:454:HIS:ND1	5:A:1081:HOH:O	2.32	0.58
1:A:549:VAL:HG12	1:A:579:LEU:HD12	1.86	0.58
1:A:230:THR:HG23	5:A:1024:HOH:O	2.01	0.58
1:A:242:CYS:HA	1:B:382:LEU:HD21	1.84	0.58
1:A:82:ILE:HD13	1:A:85:ASP:HB2	1.86	0.58
1:A:426:VAL:HA	1:A:429:THR:HG21	1.85	0.57
1:B:174:HIS:C	1:B:174:HIS:CD2	2.82	0.57
1:A:32:LEU:CD1	1:A:49:VAL:HG22	2.33	0.57
1:A:82:ILE:CD1	1:A:85:ASP:HB2	2.35	0.57
1:A:169:VAL:HG23	1:A:170:GLU:H	1.67	0.57
1:A:380:ARG:HB2	5:B:1113:HOH:O	2.04	0.57
1:A:159:MET:HE2	1:A:166:ASP:HA	1.85	0.57
1:B:28:LEU:HB3	1:B:165:LYS:HD3	1.87	0.57
1:B:129:GLY:HA2	1:B:132:LEU:HD12	1.87	0.56
1:B:379:ILE:HD11	1:B:386:GLN:OE1	2.05	0.56
1:A:433:SER:HA	1:A:455:CYS:SG	2.45	0.56
1:B:453:ILE:HD13	1:B:547:ASP:OD1	2.05	0.56
1:A:89:MET:HE2	1:A:96:LEU:HD23	1.86	0.56
1:A:425:ALA:O	1:A:429:THR:HG22	2.05	0.56
1:B:252:LYS:HG2	1:B:256:GLN:NE2	2.20	0.56
1:A:64:GLY:HA3	1:A:67:LYS:CE	2.32	0.56
1:A:98:ARG:CA	5:A:1199:HOH:O	2.51	0.56
1:B:480:LYS:O	1:B:483:VAL:HG23	2.05	0.56
1:B:82:ILE:HG23	1:B:83:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:SER:O	1:A:448:GLY:HA2	2.05	0.56
1:A:589:ARG:HD3	5:A:1130:HOH:O	2.05	0.56
1:A:526:LYS:HB3	1:A:526:LYS:HZ3	1.70	0.56
1:B:542:PHE:CD1	1:B:566:SER:HB2	2.41	0.56
1:A:122:VAL:O	1:B:138:LYS:HE3	2.06	0.56
1:A:169:VAL:HG23	1:A:170:GLU:N	2.21	0.55
1:A:382:LEU:HD21	1:B:242:CYS:HA	1.89	0.55
1:B:229:LEU:HD11	1:B:366:LEU:HB3	1.88	0.55
1:A:265:SER:OG	1:A:318:ASP:OD2	2.24	0.55
1:A:271:PRO:HG2	1:A:445:ILE:CD1	2.36	0.55
1:B:452:ARG:HH21	1:B:541:ALA:HB3	1.71	0.55
1:B:82:ILE:HG22	1:B:84:GLU:OE1	2.06	0.55
1:B:145:VAL:HG12	5:B:1022:HOH:O	2.06	0.55
1:A:12:VAL:O	1:A:15:LYS:HE3	2.06	0.55
1:B:509:TRP:HH2	1:B:517:PRO:HG2	1.70	0.55
1:A:32:LEU:HD12	1:A:49:VAL:HA	1.89	0.55
1:B:575:ALA:O	1:B:579:LEU:HG	2.07	0.55
1:B:12:VAL:HG12	1:B:102:CYS:HA	1.89	0.55
1:B:139:ASN:ND2	1:B:143:VAL:HG23	2.22	0.55
1:A:43:ARG:HE	1:A:49:VAL:HB	1.72	0.55
1:B:136:ALA:HB1	1:B:145:VAL:HB	1.89	0.55
1:B:127:ILE:N	1:B:127:ILE:HD12	2.22	0.54
1:B:211:MET:CE	1:B:239:ILE:HG12	2.35	0.54
1:A:537:LEU:HD23	1:A:537:LEU:C	2.33	0.54
1:B:123:GLU:HG2	5:B:1079:HOH:O	2.07	0.54
1:B:552:ALA:O	1:B:555:ILE:HG22	2.07	0.54
1:A:390:LYS:HG3	1:B:216:SER:O	2.08	0.54
1:B:394:ALA:CB	1:B:588:LEU:HD11	2.37	0.54
1:A:64:GLY:HA2	5:A:1133:HOH:O	2.07	0.54
1:B:143:VAL:O	1:B:172:ARG:HD2	2.07	0.54
1:B:454:HIS:HB3	5:B:1102:HOH:O	2.08	0.54
1:A:501:GLY:HA3	1:A:505:ASP:CB	2.31	0.53
1:B:211:MET:HE2	1:B:239:ILE:CG1	2.34	0.53
1:A:11:SER:O	1:A:102:CYS:HA	2.07	0.53
1:B:102:CYS:O	1:B:147:CYS:HA	2.09	0.53
1:A:82:ILE:HD11	1:A:85:ASP:CG	2.33	0.53
1:A:252:LYS:O	1:A:256:GLN:HG3	2.08	0.53
1:A:398:ARG:NH1	1:A:398:ARG:HB2	2.23	0.53
1:A:461:ASP:HA	1:A:464:ASN:ND2	2.24	0.53
1:A:432:ASN:ND2	1:A:449:GLN:O	2.42	0.53
1:A:426:VAL:HA	1:A:429:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:CD1	1:A:49:VAL:HA	2.39	0.53
1:A:106:PRO:C	1:A:108:VAL:N	2.64	0.53
1:A:555:ILE:HG13	1:A:555:ILE:O	2.08	0.53
1:B:551:ARG:HD3	1:B:554:ARG:HH21	1.74	0.53
1:A:438:LYS:NZ	1:A:534:ALA:HB3	2.24	0.52
1:B:203:SER:HA	1:B:227:LEU:HG	1.90	0.52
1:A:379:ILE:HD11	1:A:386:GLN:HG3	1.91	0.52
1:B:67:LYS:HE3	5:B:1088:HOH:O	2.09	0.52
1:B:207:LEU:HD11	1:B:241:LEU:CD1	2.39	0.52
1:A:34:ALA:C	1:A:39:ALA:HB2	2.34	0.52
1:A:498:GLY:O	1:A:500:ILE:N	2.43	0.52
1:B:111:VAL:HA	1:B:116:VAL:HG11	1.90	0.52
1:B:304:TYR:CE1	1:B:320:ILE:HG12	2.45	0.52
1:A:382:LEU:CD2	1:B:242:CYS:HA	2.40	0.52
1:A:544:PRO:HB2	1:A:545:PHE:CD2	2.45	0.52
1:A:28:LEU:HD22	1:A:165:LYS:HB3	1.91	0.52
1:A:542:PHE:CD1	1:A:566:SER:HB2	2.45	0.52
1:B:207:LEU:HD23	1:B:219:GLN:CA	2.39	0.52
1:B:26:ASN:C	1:B:28:LEU:H	2.16	0.52
1:B:394:ALA:HB1	1:B:588:LEU:HD11	1.92	0.51
1:A:242:CYS:HA	1:B:382:LEU:CD2	2.40	0.51
1:A:168:SER:HB3	5:A:1103:HOH:O	2.09	0.51
1:A:15:LYS:HA	5:A:1075:HOH:O	2.10	0.51
1:A:426:VAL:O	1:A:429:THR:HG23	2.10	0.51
1:B:280:LEU:N	1:B:280:LEU:HD12	2.24	0.51
1:A:98:ARG:HB2	5:A:1199:HOH:O	2.10	0.51
1:A:452:ARG:NH1	1:A:540:ASP:OD1	2.43	0.51
1:A:106:PRO:C	1:A:108:VAL:H	2.18	0.51
1:A:401:PHE:HA	1:A:584:ILE:HG21	1.93	0.51
1:B:10:LEU:O	1:B:38:THR:HG21	2.11	0.51
1:B:431:SER:O	1:B:448:GLY:HA2	2.10	0.51
1:B:117:THR:HG23	1:B:120:GLU:OE1	2.10	0.51
1:A:546:ARG:HG2	5:A:1090:HOH:O	2.11	0.51
1:A:569:ASP:O	1:A:573:ILE:HG13	2.11	0.51
1:B:23:ARG:HG2	1:B:47:LEU:HD21	1.93	0.51
1:B:546:ARG:O	1:B:549:VAL:HG13	2.10	0.51
1:A:178:LYS:HE2	1:B:225:PRO:HG3	1.93	0.51
1:B:549:VAL:HG22	1:B:579:LEU:HD12	1.92	0.51
1:B:411:LEU:HD12	1:B:415:ALA:HB3	1.93	0.50
1:B:480:LYS:HD2	1:B:481:ALA:H	1.76	0.50
1:A:88:ASP:O	1:A:91:LYS:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLN:HB3	1:A:500:ILE:HA	1.93	0.50
1:A:52:VAL:C	1:A:54:ASP:N	2.69	0.50
1:B:487:GLU:HB3	1:B:512:MET:CE	2.41	0.50
1:B:541:ALA:HB2	1:B:591:PHE:CE1	2.47	0.50
1:A:431:SER:HB2	1:A:593:HIS:CE1	2.45	0.50
1:B:35:SER:O	1:B:36:GLY:C	2.55	0.50
1:B:226:LYS:HB2	1:B:226:LYS:HZ2	1.75	0.50
1:A:162:SER:C	1:A:164:ASP:H	2.20	0.50
1:A:527:GLN:NE2	5:A:1207:HOH:O	2.45	0.50
1:A:477:MET:HE2	1:A:513:PHE:CE2	2.47	0.49
1:A:144:THR:HG21	1:A:167:THR:HG21	1.93	0.49
1:B:418:ASP:OD2	1:B:438:LYS:HA	2.12	0.49
1:A:308:ARG:CZ	1:A:337:GLU:HB3	2.41	0.49
1:A:21:PHE:CE1	1:A:156:ALA:HB2	2.46	0.49
1:A:237:GLY:H	1:A:240:ASN:HB2	1.78	0.49
1:B:394:ALA:HA	5:B:1074:HOH:O	2.13	0.49
1:A:500:ILE:HG13	1:A:519:GLN:OE1	2.12	0.49
1:A:558:GLN:NE2	5:A:1158:HOH:O	2.45	0.49
1:B:159:MET:C	1:B:161:ALA:H	2.20	0.49
1:B:431:SER:CB	1:B:432:ASN:HA	2.41	0.49
1:A:56:THR:HG22	1:A:72:ALA:HB3	1.94	0.49
5:A:1203:HOH:O	1:B:239:ILE:HG13	2.12	0.49
4:A:1002:MS1:H7F	1:B:316:PHE:CG	2.47	0.49
1:A:528:TRP:O	1:A:531:LYS:HB2	2.13	0.49
1:A:12:VAL:HB	1:A:103:ASN:HD21	1.73	0.48
1:A:74:HIS:HB3	1:B:69:LEU:HD13	1.95	0.48
1:B:107:PHE:CE2	1:B:111:VAL:HG11	2.48	0.48
1:B:496:VAL:HG23	1:B:497:THR:HG23	1.95	0.48
1:A:84:GLU:OE1	1:A:84:GLU:N	2.36	0.48
1:A:430:GLN:HG3	5:B:1103:HOH:O	2.12	0.48
1:B:247:ALA:HB1	1:B:321:ALA:HB2	1.96	0.48
1:A:267:LYS:HG2	1:B:450:GLN:HB3	1.94	0.48
1:A:418:ASP:OD2	1:A:438:LYS:HA	2.13	0.48
1:B:549:VAL:CG2	1:B:579:LEU:HD12	2.44	0.48
1:A:477:MET:HE2	1:A:513:PHE:HE2	1.78	0.48
1:B:344:ALA:HB1	1:B:345:PRO:HD2	1.94	0.48
1:A:66:VAL:HA	1:A:69:LEU:HD12	1.95	0.48
1:A:141:ALA:HB2	5:A:1088:HOH:O	2.13	0.48
1:B:207:LEU:N	1:B:207:LEU:HD22	2.29	0.48
1:B:469:ARG:NH1	5:B:1041:HOH:O	2.40	0.48
1:B:106:PRO:HB3	1:B:108:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ALA:CB	1:A:321:ALA:HB2	2.42	0.48
1:A:406:THR:HG22	1:A:577:ASN:OD1	2.14	0.48
1:A:562:ALA:O	1:A:585:HIS:HA	2.14	0.48
1:B:233:ASN:HB3	1:B:365:VAL:HG23	1.95	0.48
1:B:500:ILE:HD11	1:B:509:TRP:CG	2.49	0.48
1:A:326:CYS:O	1:A:348:GLU:HG3	2.13	0.47
1:B:82:ILE:C	1:B:86:ASN:ND2	2.72	0.47
1:A:344:ALA:HB1	1:A:345:PRO:HD2	1.95	0.47
1:A:251:VAL:HG23	1:A:252:LYS:N	2.29	0.47
1:A:98:ARG:HG3	5:A:1190:HOH:O	2.14	0.47
1:A:358:LYS:HB2	1:A:363:TYR:HB2	1.97	0.47
1:B:327:ASP:OD1	1:B:329:PRO:HD2	2.14	0.47
1:A:196:LYS:HE2	1:A:219:GLN:NE2	2.30	0.47
1:A:258:LEU:HD13	1:A:417:ARG:HG3	1.96	0.47
1:B:56:THR:HB	1:B:70:HIS:CD2	2.49	0.47
1:B:254:LEU:HD23	1:B:262:ALA:HB1	1.96	0.47
1:B:342:VAL:HG22	1:B:343:VAL:N	2.30	0.47
1:B:583:LEU:HD12	1:B:584:ILE:N	2.30	0.47
1:A:80:ARG:HB2	1:A:82:ILE:CD1	2.44	0.47
1:B:535:VAL:HB	1:B:557:VAL:HA	1.97	0.47
1:A:500:ILE:HG22	1:A:501:GLY:N	2.30	0.47
1:A:177:LEU:HD21	1:B:195:ARG:HG2	1.97	0.47
1:A:520:LEU:HB2	1:A:525:LYS:HE3	1.97	0.47
1:A:70:HIS:ND1	1:A:71:PRO:HD2	2.30	0.47
1:A:375:ASP:HB3	5:A:1204:HOH:O	2.15	0.47
1:B:70:HIS:CG	1:B:71:PRO:HD2	2.50	0.47
1:A:583:LEU:HD12	1:A:584:ILE:H	1.80	0.46
1:B:164:ASP:O	1:B:165:LYS:C	2.58	0.46
1:A:589:ARG:HB3	1:B:212:ASN:OD1	2.15	0.46
1:B:393:ASN:HA	5:B:1019:HOH:O	2.15	0.46
1:B:401:PHE:HE2	1:B:420:ILE:HG13	1.80	0.46
1:B:547:ASP:OD1	1:B:548:ASN:N	2.47	0.46
1:A:254:LEU:HD23	1:A:262:ALA:HB1	1.97	0.46
1:A:316:PHE:CD1	4:B:1001:MS1:H7F	2.51	0.46
1:A:364:CYS:SG	1:A:366:LEU:HD21	2.55	0.46
1:A:243:ASP:OD1	1:A:269:VAL:N	2.46	0.46
1:A:257:ALA:HB2	5:A:1051:HOH:O	2.16	0.46
1:A:423:SER:O	1:A:426:VAL:HG22	2.16	0.46
1:B:99:VAL:HG22	1:B:144:THR:HB	1.96	0.46
1:A:480:LYS:HE3	1:A:513:PHE:O	2.15	0.46
1:A:497:THR:C	1:A:499:THR:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLY:C	1:A:500:ILE:N	2.71	0.46
1:A:80:ARG:CB	1:A:82:ILE:HD12	2.46	0.46
1:A:10:LEU:HD23	1:A:18:LEU:HD11	1.97	0.45
1:A:40:THR:HG22	1:A:44:ASP:OD2	2.16	0.45
1:B:83:PRO:O	1:B:84:GLU:C	2.57	0.45
1:B:148:ASP:CB	1:B:178:LYS:HE2	2.46	0.45
1:B:156:ALA:C	1:B:158:GLU:H	2.24	0.45
1:B:278:ILE:HD11	1:B:417:ARG:CZ	2.46	0.45
1:B:558:GLN:O	1:B:558:GLN:HG2	2.16	0.45
1:A:7:LEU:HD11	1:A:95:SER:HB2	1.97	0.45
1:A:320:ILE:O	1:A:342:VAL:HA	2.17	0.45
1:A:542:PHE:CD1	1:A:542:PHE:C	2.94	0.45
1:A:233:ASN:HB3	1:A:365:VAL:HG23	1.97	0.45
1:A:316:PHE:HB3	4:B:1001:MS1:H7F	1.97	0.45
4:A:1002:MS1:C12	4:A:1002:MS1:H2P	2.46	0.45
1:B:26:ASN:C	1:B:28:LEU:N	2.75	0.45
1:B:247:ALA:HA	1:B:266:PHE:CE1	2.52	0.45
1:B:478:LYS:HB2	1:B:515:GLU:HB3	1.98	0.45
1:A:453:ILE:HD13	1:A:547:ASP:CG	2.42	0.45
1:B:74:HIS:O	1:B:78:LEU:N	2.42	0.45
1:B:490:ASN:O	1:B:494:GLN:HG2	2.17	0.45
1:A:570:GLU:HB2	5:A:1079:HOH:O	2.16	0.45
1:B:34:ALA:C	1:B:52:VAL:HG23	2.42	0.45
1:B:108:VAL:HA	1:B:111:VAL:HG22	1.99	0.45
1:B:139:ASN:HD22	1:B:143:VAL:HG23	1.81	0.45
1:A:253:GLU:OE2	1:A:428:TYR:OH	2.27	0.45
1:A:86:ASN:N	1:A:86:ASN:HD22	2.13	0.45
1:A:401:PHE:CB	1:A:584:ILE:HD13	2.34	0.45
1:B:172:ARG:HG3	1:B:172:ARG:HH11	1.82	0.45
1:A:126:ASP:OD1	1:A:130:VAL:HG23	2.17	0.45
1:A:140:HIS:C	1:A:142:ARG:N	2.72	0.45
1:A:148:ASP:OD2	1:A:150:ALA:HB3	2.16	0.45
1:B:7:LEU:HD13	1:B:33:ILE:HD11	1.97	0.45
1:A:159:MET:CE	1:A:166:ASP:HA	2.47	0.45
1:A:304:TYR:OH	1:A:308:ARG:NH1	2.49	0.45
1:B:406:THR:CG2	1:B:583:LEU:HB3	2.43	0.45
1:A:56:THR:C	1:A:58:PHE:H	2.24	0.44
1:B:320:ILE:HG22	1:B:342:VAL:HG23	1.99	0.44
1:A:14:GLU:OE2	1:A:16:ALA:HB2	2.17	0.44
1:A:130:VAL:HG21	1:B:134:ARG:NH1	2.32	0.44
1:B:484:LYS:HB2	1:B:487:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:THR:HB	1:A:70:HIS:CD2	2.53	0.44
1:B:76:GLY:C	1:B:97:VAL:HG23	2.42	0.44
1:A:328:VAL:N	1:A:329:PRO:HD2	2.32	0.44
1:B:543:PHE:HE2	1:B:560:ILE:HG21	1.83	0.44
1:A:82:ILE:HD13	1:A:82:ILE:N	2.29	0.44
1:A:258:LEU:HD12	1:A:276:VAL:HG11	2.00	0.44
1:A:327:ASP:HB2	1:A:329:PRO:HD2	1.99	0.44
1:B:173:ARG:O	1:B:176:ALA:HB3	2.17	0.44
1:B:278:ILE:HD11	1:B:417:ARG:NH1	2.33	0.44
1:B:407:LYS:O	1:B:409:LYS:HG3	2.18	0.44
1:B:401:PHE:HB3	1:B:584:ILE:HD13	1.99	0.44
1:A:452:ARG:HH21	1:A:541:ALA:HB3	1.79	0.44
1:B:53:SER:O	1:B:57:GLY:N	2.46	0.44
1:B:158:GLU:OE2	1:B:168:SER:N	2.50	0.44
1:A:271:PRO:HG2	1:A:445:ILE:HD13	2.00	0.44
1:A:389:GLN:HB3	1:B:238:PHE:CE2	2.53	0.44
1:B:537:LEU:HB3	1:B:560:ILE:HG12	1.99	0.43
1:B:555:ILE:O	1:B:555:ILE:HG13	2.18	0.43
1:A:64:GLY:CA	1:A:67:LYS:HG3	2.48	0.43
1:B:16:ALA:O	1:B:152:TYR:HE2	2.01	0.43
1:A:69:LEU:O	1:B:71:PRO:HD3	2.19	0.43
1:A:104:LEU:HD22	1:A:126:ASP:CG	2.44	0.43
1:A:431:SER:HB3	1:A:432:ASN:HA	1.98	0.43
1:A:464:ASN:HD21	1:A:551:ARG:HH22	1.67	0.43
1:A:43:ARG:C	1:A:45:ALA:H	2.26	0.43
1:A:43:ARG:C	1:A:45:ALA:N	2.71	0.43
1:A:535:VAL:HB	1:A:557:VAL:HA	2.01	0.43
1:B:26:ASN:O	1:B:28:LEU:N	2.51	0.43
1:B:98:ARG:C	1:B:99:VAL:HG23	2.43	0.43
1:A:219:GLN:NE2	1:B:388:MET:HE2	2.32	0.43
1:B:379:ILE:HA	1:B:387:LEU:O	2.19	0.43
1:A:9:LEU:HD12	1:A:10:LEU:N	2.34	0.43
1:B:20:GLU:H	1:B:20:GLU:CD	2.26	0.43
1:B:67:LYS:HE2	5:B:1139:HOH:O	2.19	0.43
1:A:168:SER:O	1:A:172:ARG:HG3	2.19	0.43
4:A:1002:MS1:H7F	1:B:316:PHE:CD1	2.54	0.43
1:A:12:VAL:HB	1:A:103:ASN:HD22	1.79	0.43
1:A:16:ALA:C	1:A:18:LEU:H	2.27	0.43
1:A:58:PHE:CD1	1:A:59:PRO:HD2	2.54	0.43
1:A:426:VAL:CA	1:A:429:THR:CG2	2.87	0.43
1:A:320:ILE:HB	1:A:342:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLU:OE2	1:A:389:GLN:NE2	2.49	0.43
1:B:104:LEU:CD2	1:B:133:LEU:HD12	2.42	0.43
1:B:311:ASP:HB3	5:B:1111:HOH:O	2.19	0.43
1:A:64:GLY:O	1:A:67:LYS:HG3	2.19	0.42
1:A:101:VAL:HG22	1:A:146:VAL:HG13	2.01	0.42
1:A:107:PHE:CE2	1:A:190:ILE:HA	2.54	0.42
1:A:230:THR:CG2	5:A:1024:HOH:O	2.63	0.42
1:B:222:THR:HG22	1:B:227:LEU:HD23	2.00	0.42
1:B:433:SER:HA	1:B:455:CYS:SG	2.59	0.42
1:A:207:LEU:HG	1:A:219:GLN:HA	2.01	0.42
1:A:379:ILE:C	1:A:379:ILE:HD13	2.44	0.42
1:B:431:SER:HB3	1:B:432:ASN:HA	2.01	0.42
1:A:91:LYS:NZ	1:A:92:GLN:HG2	2.35	0.42
1:A:177:LEU:O	1:A:177:LEU:HD12	2.20	0.42
1:B:9:LEU:C	1:B:10:LEU:HD12	2.45	0.42
1:B:10:LEU:HD23	1:B:18:LEU:HD11	2.01	0.42
1:B:564:SER:HB3	1:B:585:HIS:CG	2.54	0.42
1:A:52:VAL:O	1:A:54:ASP:N	2.52	0.42
1:A:60:GLU:OE2	1:A:67:LYS:HE2	2.19	0.42
1:A:113:SER:O	1:A:116:VAL:HG12	2.19	0.42
1:B:203:SER:HB3	1:B:226:LYS:HA	2.00	0.42
1:A:239:ILE:HB	4:B:1001:MS1:H51	2.01	0.42
1:B:99:VAL:HG12	1:B:101:VAL:HG23	2.02	0.42
1:A:431:SER:CB	1:A:432:ASN:HA	2.49	0.42
1:A:467:TRP:NE1	1:A:532:LEU:HB2	2.35	0.42
1:B:360:ASN:C	5:B:1097:HOH:O	2.62	0.42
1:A:415:ALA:O	1:A:419:LEU:HG	2.19	0.42
1:A:510:GLN:HE21	1:A:510:GLN:HB2	1.50	0.42
1:B:170:GLU:O	1:B:173:ARG:N	2.52	0.42
1:B:500:ILE:HD12	1:B:500:ILE:HA	1.92	0.42
1:A:6:GLN:O	1:A:30:LEU:HD23	2.19	0.41
1:A:461:ASP:HA	1:A:464:ASN:HD22	1.85	0.41
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.91	0.41
1:B:510:GLN:HG2	1:B:516:VAL:HG11	2.02	0.41
4:B:1001:MS1:H1	4:B:1001:MS1:H3P	1.75	0.41
1:A:74:HIS:CB	1:B:69:LEU:HD13	2.50	0.41
1:B:569:ASP:O	1:B:573:ILE:HG13	2.21	0.41
1:A:203:SER:HA	1:A:227:LEU:HG	2.03	0.41
1:A:479:PHE:CE2	1:A:488:VAL:HG13	2.55	0.41
1:B:247:ALA:CB	1:B:321:ALA:HB2	2.50	0.41
1:A:14:GLU:O	1:A:14:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ALA:C	1:A:18:LEU:N	2.77	0.41
1:A:106:PRO:HB2	1:A:109:LYS:HG3	2.03	0.41
1:B:294:HIS:HA	1:B:297:LEU:HD12	2.01	0.41
1:A:7:LEU:CD1	1:A:33:ILE:HD11	2.40	0.41
1:A:506:LEU:O	1:A:510:GLN:HB2	2.20	0.41
1:B:103:ASN:HB3	1:B:147:CYS:O	2.20	0.41
1:B:247:ALA:HB2	1:B:266:PHE:CD1	2.54	0.41
1:B:436:TYR:CE2	1:B:555:ILE:HG21	2.55	0.41
1:A:211:MET:N	1:B:389:GLN:OE1	2.52	0.41
1:A:379:ILE:CG2	5:B:1077:HOH:O	2.60	0.41
1:A:509:TRP:CZ2	1:A:513:PHE:CZ	3.08	0.41
1:B:320:ILE:O	1:B:342:VAL:HA	2.21	0.41
1:B:66:VAL:O	1:B:68:THR:N	2.53	0.41
1:A:528:TRP:HH2	5:A:1196:HOH:O	2.03	0.41
1:B:78:LEU:HD21	1:B:135:ALA:HB1	2.03	0.41
1:B:278:ILE:CD1	1:B:417:ARG:CZ	2.99	0.41
1:A:100:VAL:HG21	1:A:136:ALA:HB2	2.01	0.41
1:A:555:ILE:O	1:A:555:ILE:CG1	2.69	0.41
1:B:66:VAL:O	1:B:67:LYS:C	2.64	0.41
1:B:68:THR:OG1	5:B:1086:HOH:O	2.22	0.41
1:B:349:GLU:OE1	1:B:349:GLU:N	2.54	0.41
1:B:379:ILE:C	1:B:379:ILE:CD1	2.91	0.41
1:A:140:HIS:C	1:A:142:ARG:H	2.26	0.41
1:A:353:LYS:HE3	1:A:353:LYS:HB2	1.95	0.41
1:A:543:PHE:HE2	1:A:560:ILE:HG21	1.86	0.41
1:A:583:LEU:HD12	1:A:584:ILE:N	2.36	0.41
1:B:28:LEU:CB	1:B:165:LYS:HD3	2.51	0.41
1:B:372:TYR:CD1	1:B:372:TYR:C	2.99	0.41
1:B:494:GLN:HG2	1:B:494:GLN:H	1.73	0.41
1:A:155:VAL:O	1:A:158:GLU:N	2.52	0.40
1:B:47:LEU:HA	1:B:48:PRO:HD3	1.85	0.40
1:B:243:ASP:OD1	1:B:269:VAL:N	2.49	0.40
1:A:86:ASN:N	1:A:86:ASN:ND2	2.69	0.40
1:A:316:PHE:CB	4:B:1001:MS1:H7F	2.51	0.40
1:A:472:PRO:HD3	1:A:528:TRP:CZ3	2.56	0.40
1:B:111:VAL:C	1:B:116:VAL:HG11	2.46	0.40
1:B:113:SER:CB	1:B:114:PRO:HD2	2.45	0.40
1:A:221:TYR:CD1	1:A:221:TYR:C	2.99	0.40
1:B:237:GLY:H	1:B:240:ASN:HB2	1.85	0.40
1:B:406:THR:O	1:B:407:LYS:C	2.63	0.40
1:A:170:GLU:O	1:A:171:THR:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:THR:HG23	1:A:329:PRO:HG3	2.04	0.40
1:A:379:ILE:HA	1:A:387:LEU:O	2.21	0.40
1:A:412:PRO:HD2	1:A:559:PHE:CE2	2.56	0.40
1:B:159:MET:C	1:B:161:ALA:N	2.80	0.40
1:B:221:TYR:CD1	1:B:221:TYR:C	3.00	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	588/613 (96%)	542 (92%)	39 (7%)	7 (1%)	10	20
1	B	588/613 (96%)	541 (92%)	38 (6%)	9 (2%)	8	16
All	All	1176/1226 (96%)	1083 (92%)	77 (6%)	16 (1%)	9	17

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	LYS
1	A	36	GLY
1	A	53	SER
1	A	499	THR
1	A	500	ILE
1	B	27	ALA
1	B	36	GLY
1	A	277	GLY
1	A	512	MET
1	B	157	LYS
1	B	515	GLU
1	B	83	PRO
1	B	106	PRO

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Mol	Chain	Res	Type
1	B	165	LYS
1	A	106	PRO
1	B	277	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/502 (96%)	464 (96%)	20 (4%)	27	53
1	B	484/502 (96%)	465 (96%)	19 (4%)	28	55
All	All	968/1004 (96%)	929 (96%)	39 (4%)	28	54

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	82	ILE
1	A	113	SER
1	A	146	VAL
1	A	153	SER
1	A	216	SER
1	A	265	SER
1	A	269	VAL
1	A	270	SER
1	A	280	LEU
1	A	342	VAL
1	A	360	ASN
1	A	379	ILE
1	A	402	LYS
1	A	406	THR
1	A	429	THR
1	A	503	ASP
1	A	507	VAL
1	A	510	GLN
1	A	589	ARG

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Mol	Chain	Res	Type
1	B	55	LEU
1	B	58	PHE
1	B	83	PRO
1	B	96	LEU
1	B	104	LEU
1	B	108	VAL
1	B	174	HIS
1	B	177	LEU
1	B	199	SER
1	B	211	MET
1	B	226	LYS
1	B	235	SER
1	B	269	VAL
1	B	350	GLU
1	B	360	ASN
1	B	379	ILE
1	B	494	GLN
1	B	537	LEU
1	B	549	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	26	ASN
1	A	81	ASN
1	A	86	ASN
1	A	139	ASN
1	A	215	GLN
1	A	219	GLN
1	A	408	ASN
1	A	464	ASN
1	A	527	GLN
1	B	5	GLN
1	B	81	ASN
1	B	86	ASN
1	B	139	ASN
1	B	174	HIS
1	B	185	GLN
1	B	215	GLN
1	B	256	GLN
1	B	367	GLN

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Mol	Chain	Res	Type
1	B	408	ASN
1	B	430	GLN
1	B	494	GLN
1	B	510	GLN
1	B	558	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	$\# Z > 2$
4	MS1	B	1001	-	60,61,61	2.31	23 (38%)	78,89,89	2.93	37 (47%)
4	MS1	A	1002	-	60,61,61	3.50	21 (35%)	78,89,89	3.03	32 (41%)
3	PO4	B	1006	-	4,4,4	1.69	1 (25%)	6,6,6	0.45	0
3	PO4	A	1005	-	4,4,4	1.69	0	6,6,6	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MS1	B	1001	-	-	12/48/64/64	0/5/5/5
4	MS1	A	1002	-	-	13/48/64/64	0/5/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	MS1	C42-N10	-19.44	1.11	1.36
4	A	1002	MS1	C11-N10	8.63	1.60	1.43
4	B	1001	MS1	C11-N10	7.32	1.57	1.43
4	A	1002	MS1	C2P-C42	5.49	1.56	1.48
4	A	1002	MS1	C13-C14	4.89	1.46	1.39
4	B	1001	MS1	C4P-N9	-4.67	1.32	1.38
4	A	1002	MS1	OE2-CD	4.60	1.37	1.22
4	B	1001	MS1	OE2-CD	4.59	1.37	1.22
4	A	1002	MS1	C12-C11	4.47	1.47	1.39
4	B	1001	MS1	C4A-C4F	4.31	1.55	1.47
4	A	1002	MS1	C9-N10	4.10	1.53	1.46
4	A	1002	MS1	C16-C11	4.04	1.46	1.39
4	B	1001	MS1	C16-C11	3.80	1.46	1.39
4	B	1001	MS1	C15-C14	3.79	1.45	1.39
4	B	1001	MS1	C8A-N1F	3.78	1.46	1.39
4	B	1001	MS1	C2F-N3F	3.72	1.46	1.37
4	A	1002	MS1	C2F-N3F	3.71	1.46	1.37
4	A	1002	MS1	C12-C13	3.58	1.44	1.38
4	A	1002	MS1	P-O9	3.53	1.61	1.50
4	A	1002	MS1	C4A-C4F	3.44	1.54	1.47
4	B	1001	MS1	P-O9	3.40	1.61	1.50
4	A	1002	MS1	C4P-C5P	3.29	1.43	1.39
4	B	1001	MS1	C9-N10	3.27	1.52	1.46
4	B	1001	MS1	C2P-C42	3.25	1.53	1.48
4	A	1002	MS1	C15-C16	3.15	1.43	1.38
4	A	1002	MS1	C15-C14	2.91	1.43	1.39
4	B	1001	MS1	C12-C11	2.85	1.44	1.39
4	B	1001	MS1	C12-C13	2.68	1.43	1.38
4	B	1001	MS1	C7F-C8F	2.67	1.43	1.38
4	A	1002	MS1	C5P-C6	2.66	1.55	1.47
4	B	1001	MS1	C7F-C6F	2.59	1.44	1.38
4	B	1001	MS1	C15-C16	2.51	1.42	1.38
4	B	1001	MS1	OT-C	2.40	1.38	1.30
4	B	1001	MS1	C3P-C2P	2.28	1.39	1.33
4	B	1001	MS1	C4P-C5P	2.24	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	MS1	C42-N10	-2.23	1.33	1.36
4	A	1002	MS1	C3P-C2P	2.22	1.39	1.33
4	B	1001	MS1	CB-CA	2.20	1.58	1.53
4	A	1002	MS1	C8A-N1F	2.19	1.43	1.39
4	A	1002	MS1	OT-C	2.19	1.37	1.30
4	A	1002	MS1	C8-N7	2.14	1.38	1.32
4	A	1002	MS1	C17-N	-2.10	1.29	1.34
4	B	1001	MS1	CA-N	2.08	1.50	1.45
4	B	1001	MS1	C13-C14	2.06	1.42	1.39
3	B	1006	PO4	P-O3	-2.04	1.48	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	MS1	C8-N9-C4P	-12.66	96.51	107.30
4	A	1002	MS1	C3P-C2P-C42	11.13	151.85	121.53
4	B	1001	MS1	C3P-C2P-C42	11.03	151.57	121.53
4	B	1001	MS1	C8-N9-C4P	-8.24	100.28	107.30
4	A	1002	MS1	C11-N10-C42	-7.27	115.72	123.53
4	B	1001	MS1	C2P-C3P-C4P	6.91	147.42	127.53
4	A	1002	MS1	C2P-C3P-C4P	6.65	146.69	127.53
4	B	1001	MS1	O1-C1-C2	6.64	120.82	106.62
4	B	1001	MS1	CG-CB-CA	5.46	123.23	113.16
4	A	1002	MS1	O42-C42-N10	-5.42	113.61	120.66
4	A	1002	MS1	O1-C1-C2	5.03	117.39	106.62
4	B	1001	MS1	CA-N-C17	-5.02	109.53	121.56
4	B	1001	MS1	O42-C42-C2P	-4.85	112.22	122.02
4	A	1002	MS1	O42-C42-C2P	-4.80	112.34	122.02
4	B	1001	MS1	O42-C42-N10	4.76	126.85	120.66
4	B	1001	MS1	C3P-C4P-N9	-4.69	111.64	123.80
4	A	1002	MS1	N9-C8-N7	4.62	121.98	113.40
4	A	1002	MS1	C6F-C9-N10	4.60	119.76	112.73
4	B	1001	MS1	C4-O1-C1	-4.12	100.37	109.47
4	A	1002	MS1	C16-C11-N10	3.81	125.66	120.18
4	A	1002	MS1	C3P-C4P-N9	-3.79	113.97	123.80
4	B	1001	MS1	C16-C11-N10	3.73	125.55	120.18
4	B	1001	MS1	C6F-C9-N10	3.67	118.33	112.73
4	B	1001	MS1	CB-CA-N	3.55	117.93	110.91
4	A	1002	MS1	OE2-CD-CG	-3.40	112.32	123.09
4	B	1001	MS1	OE2-CD-CG	-3.34	112.50	123.09
4	B	1001	MS1	C3-C2-C1	-3.33	95.17	101.46
4	B	1001	MS1	C5-C4-C3	-3.23	103.58	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	MS1	C4P-C5P-N7	-3.14	107.58	110.14
4	B	1001	MS1	C2-C1-N9	-3.13	104.53	113.25
4	A	1002	MS1	OE1-CD-CG	3.13	123.89	114.00
4	A	1002	MS1	C4-O1-C1	-3.05	102.72	109.47
4	B	1001	MS1	C16-C11-C12	-3.03	113.39	119.18
4	A	1002	MS1	CA-N-C17	-2.96	114.46	121.56
4	B	1001	MS1	OE1-CD-CG	2.93	123.27	114.00
4	B	1001	MS1	N9-C8-N7	2.84	118.66	113.40
4	A	1002	MS1	O62-C6-N1	-2.83	116.55	122.89
4	B	1001	MS1	O62-C6-N1	-2.80	116.61	122.89
4	B	1001	MS1	C11-N10-C42	2.80	126.54	123.53
4	B	1001	MS1	C1-N9-C8	2.79	134.65	126.73
4	A	1002	MS1	C8-N7-C5P	-2.76	99.34	104.26
4	B	1001	MS1	C15-C16-C11	2.75	123.79	120.30
4	B	1001	MS1	O2-C2-C3	2.73	120.57	111.82
4	B	1001	MS1	C8A-N1F-C2F	2.69	121.65	118.05
4	A	1002	MS1	O2-C2-C3	2.69	120.43	111.82
4	B	1001	MS1	C5P-C6-N1	2.68	121.46	116.73
4	A	1002	MS1	CB-CA-N	-2.68	105.61	110.91
4	A	1002	MS1	C8A-C4A-N5F	-2.63	119.55	121.46
4	A	1002	MS1	C2-C1-N9	-2.62	105.95	113.25
4	A	1002	MS1	C8A-N1F-C2F	2.61	121.55	118.05
4	B	1001	MS1	C8F-C8A-N1F	2.60	121.91	118.61
4	B	1001	MS1	C13-C12-C11	2.54	123.52	120.30
4	B	1001	MS1	O4F-C4F-N3F	-2.52	117.62	120.62
4	A	1002	MS1	C8F-C8A-N1F	2.52	121.82	118.61
4	A	1002	MS1	C5P-C6-N1	2.50	121.14	116.73
4	B	1001	MS1	O1-C4-C3	2.47	110.05	105.15
4	A	1002	MS1	C12-C13-C14	2.41	123.38	120.80
4	A	1002	MS1	O4F-C4F-N3F	-2.38	117.79	120.62
4	B	1001	MS1	C2-C3-C4	2.35	107.16	102.61
4	B	1001	MS1	C8-N7-C5P	-2.33	100.10	104.26
4	A	1002	MS1	C15-C16-C11	2.33	123.25	120.30
4	B	1001	MS1	C14-C17-N	2.32	121.35	117.04
4	A	1002	MS1	O1-C4-C3	2.31	109.74	105.15
4	A	1002	MS1	C15-C14-C13	-2.28	115.67	118.57
4	B	1001	MS1	C4F-C4A-N5F	2.23	122.58	118.17
4	A	1002	MS1	C16-C11-C12	-2.14	115.10	119.18
4	B	1001	MS1	O17-C17-N	-2.14	118.40	122.47
4	A	1002	MS1	C4F-C4A-N5F	2.13	122.39	118.17
4	A	1002	MS1	O1-C1-N9	2.08	113.06	108.36

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	MS1	C4P-C5P-C6-O62
4	A	1002	MS1	N7-C5P-C6-O62
4	A	1002	MS1	N7-C5P-C6-N1
4	A	1002	MS1	C5-O6-P-O8
4	B	1001	MS1	C5-O6-P-O8
4	B	1001	MS1	C5-O6-P-O7
4	B	1001	MS1	N-CA-CB-CG
4	B	1001	MS1	C-CA-CB-CG
4	B	1001	MS1	O1-C4-C5-O6
4	B	1001	MS1	C3-C4-C5-O6
4	A	1002	MS1	C12-C11-N10-C42
4	A	1002	MS1	C4P-C5P-C6-N1
4	B	1001	MS1	C3P-C2P-C42-O42
4	A	1002	MS1	O42-C42-N10-C9
4	A	1002	MS1	C3P-C2P-C42-O42
4	B	1001	MS1	C3P-C2P-C42-N10
4	A	1002	MS1	C16-C11-N10-C42
4	A	1002	MS1	C6F-C9-N10-C42
4	A	1002	MS1	OE1-CD-CG-CB
4	B	1001	MS1	N7-C5P-C6-N1
4	B	1001	MS1	C5-O6-P-O9
4	A	1002	MS1	OE2-CD-CG-CB
4	B	1001	MS1	C4P-C5P-C6-N1
4	B	1001	MS1	N7-C5P-C6-O62
4	A	1002	MS1	C12-C11-N10-C9

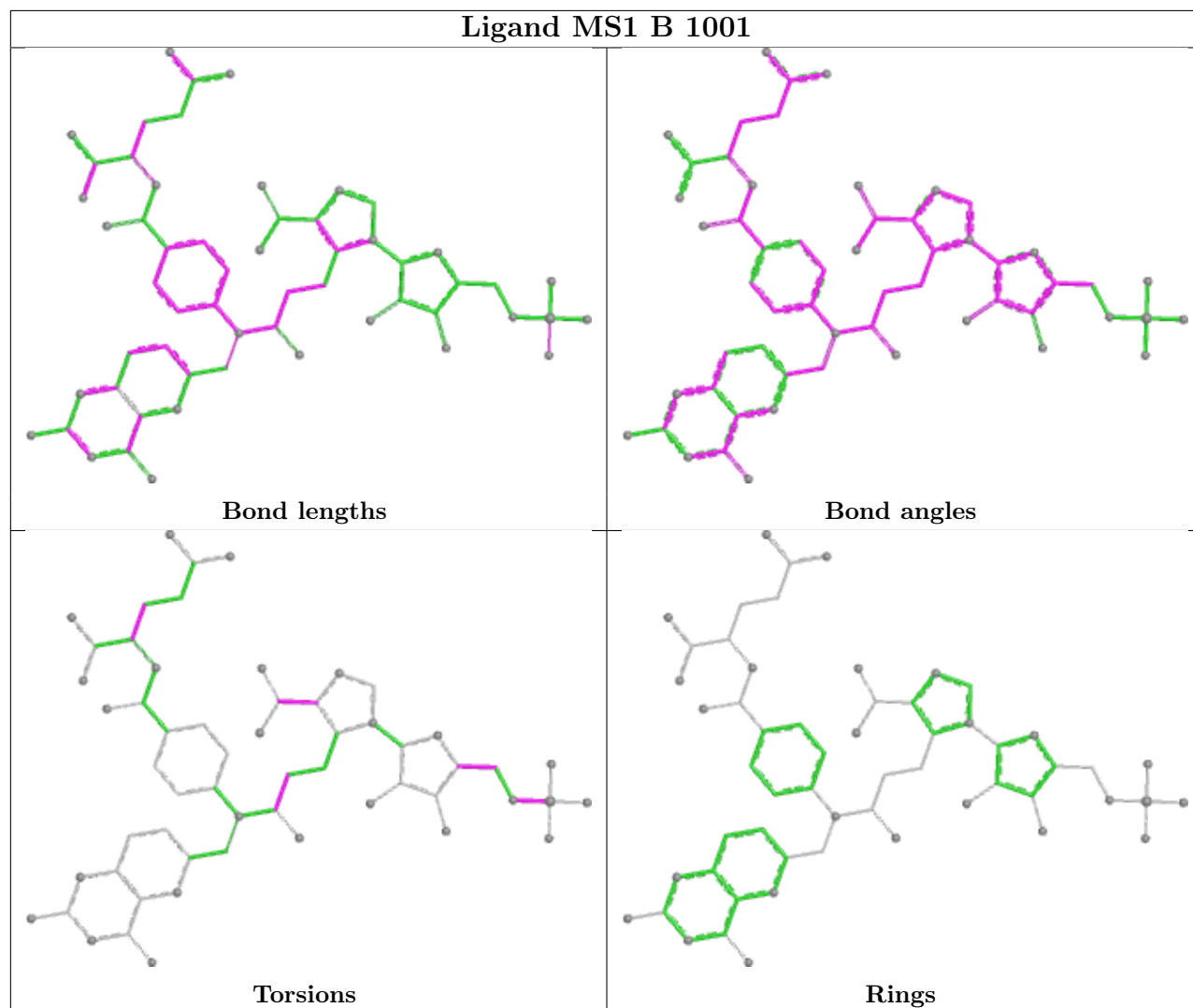
There are no ring outliers.

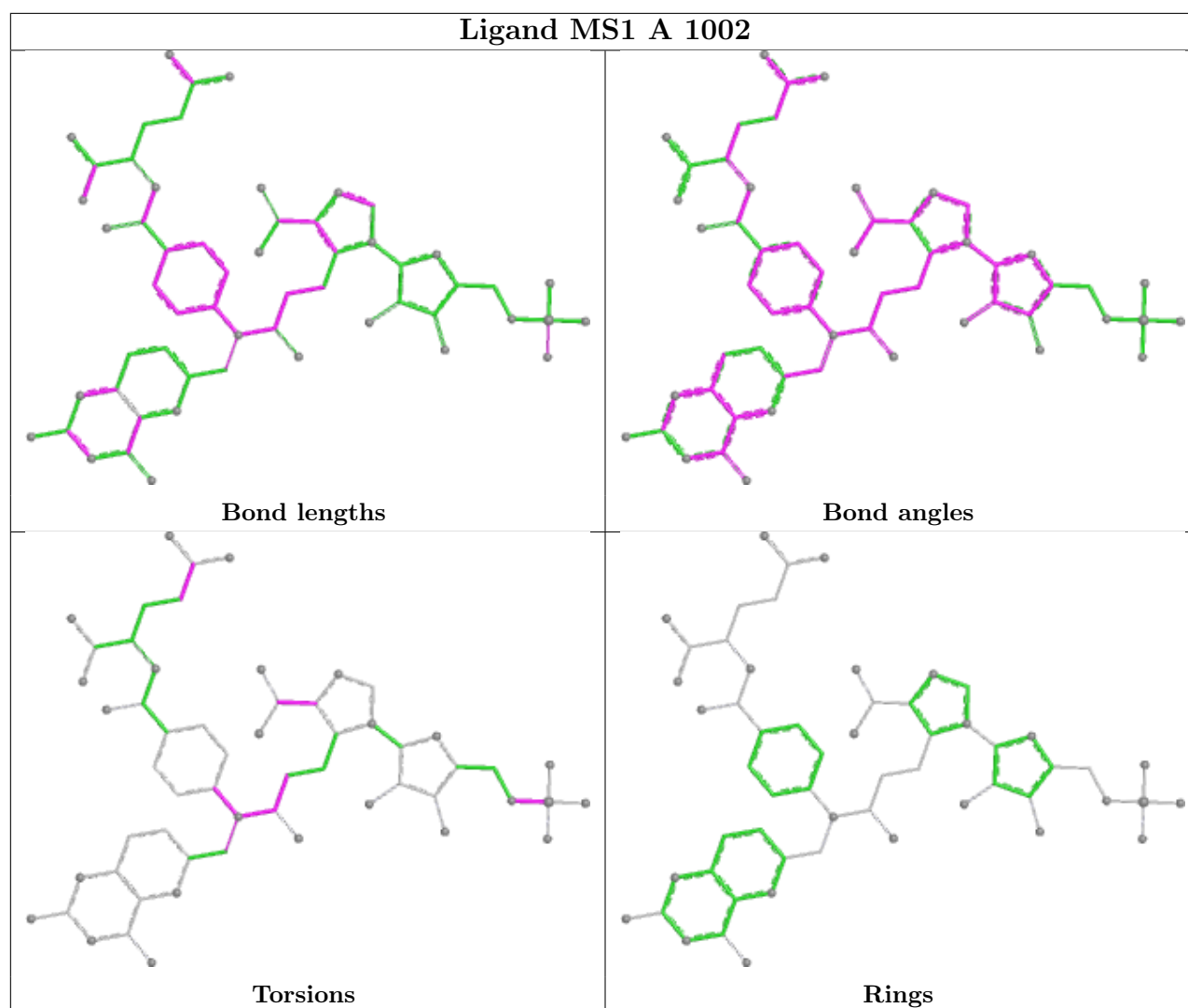
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	MS1	7	0
4	A	1002	MS1	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	590/613 (96%)	-0.21	0 100 100	21, 40, 70, 87	0
1	B	590/613 (96%)	-0.18	0 100 100	21, 39, 68, 82	1 (0%)
All	All	1180/1226 (96%)	-0.20	0 100 100	21, 40, 69, 87	1 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

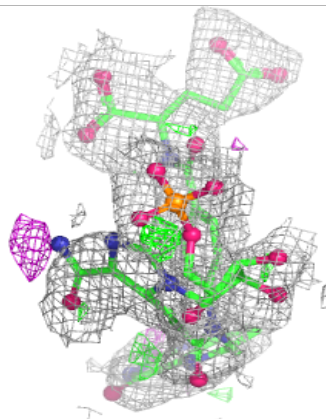
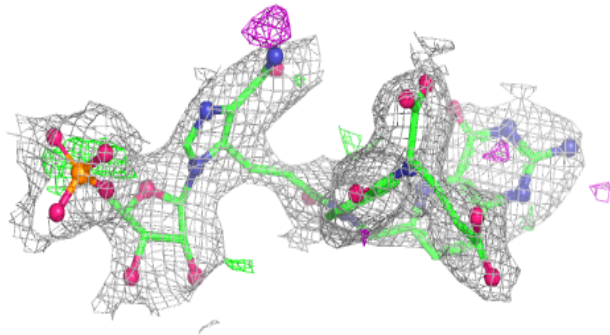
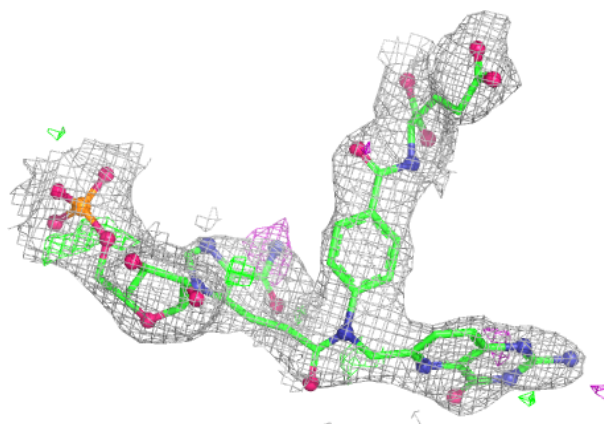
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	B	1006	5/5	0.78	0.12	81,81,81,82	0
3	PO4	A	1005	5/5	0.83	0.12	97,97,97,98	0
4	MS1	B	1001	57/57	0.86	0.12	47,57,65,66	0
4	MS1	A	1002	57/57	0.92	0.09	38,50,58,58	0
2	K	A	1004	1/1	0.95	0.06	42,42,42,42	0
2	K	B	1003	1/1	0.95	0.05	35,35,35,35	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.

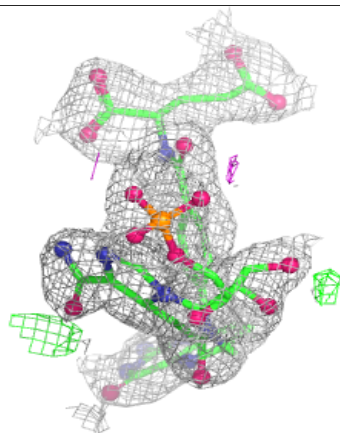
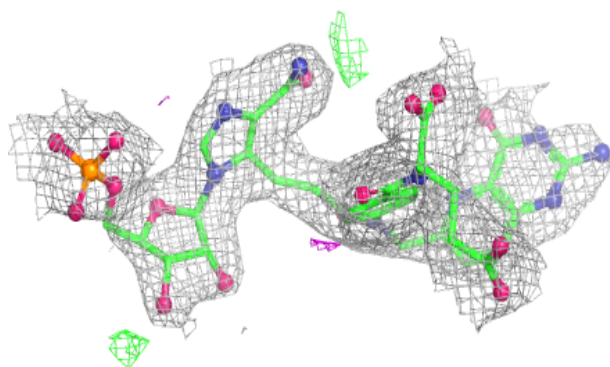
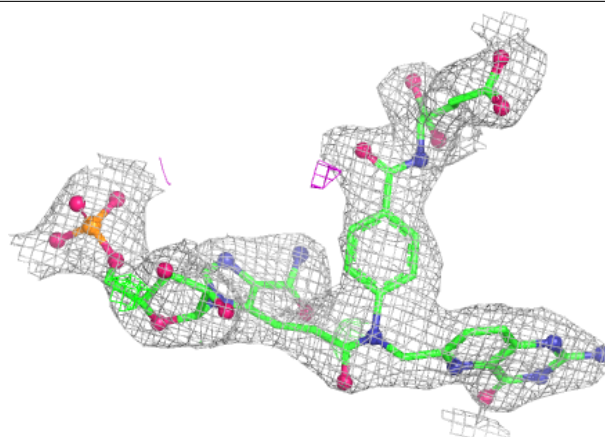
Electron density around MS1 B 1001:

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



Electron density around MS1 A 1002:

$2mF_o-DF_c$ (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.