



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:31 pm BST

PDB ID : 3C7N  
Title : Structure of the Hsp110:Hsc70 Nucleotide Exchange Complex  
Authors : Schuermann, J.P.; Jiang, J.; Hart, P.J.; Sousa, R.  
Deposited on : 2008-02-07  
Resolution : 3.12 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

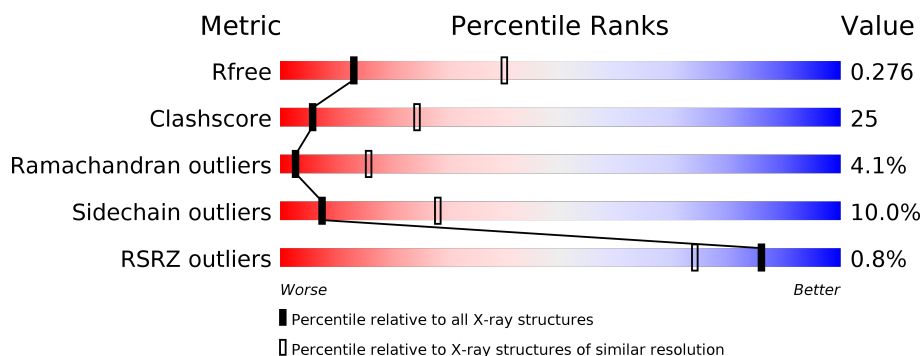
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.12 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))
$R_{free}$	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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 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	668	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>37%</div> <div>6%</div> <div>.</div> </div> </div>
2	B	554	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>40%</div> <div>9%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CL	B	555	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9368 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 Heat shock protein homolog SSE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	0
			5103	3227	853	1010	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P32589
A	0	PRO	-	EXPRESSION TAG	UNP P32589

- Molecule 2 is a protein called Heat shock cognate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	540	Total	C	N	O	S	0	0	0
			4182	2621	726	824	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

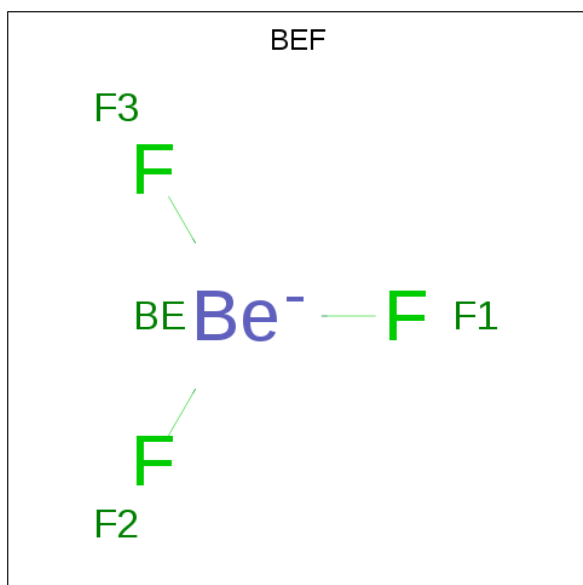
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



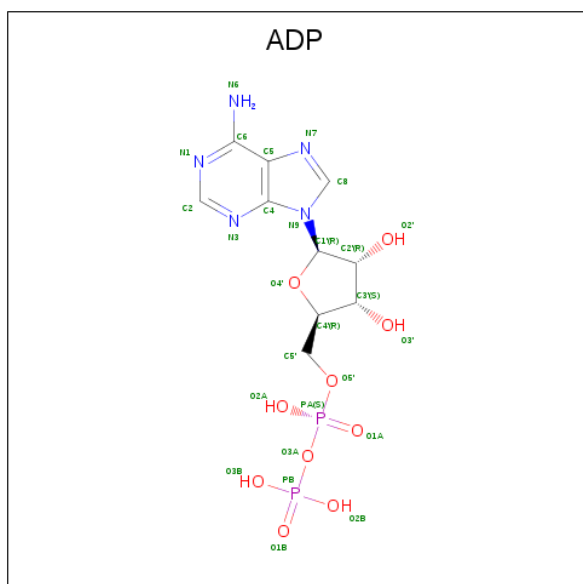
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Be	F	0	0
			4	1	3		

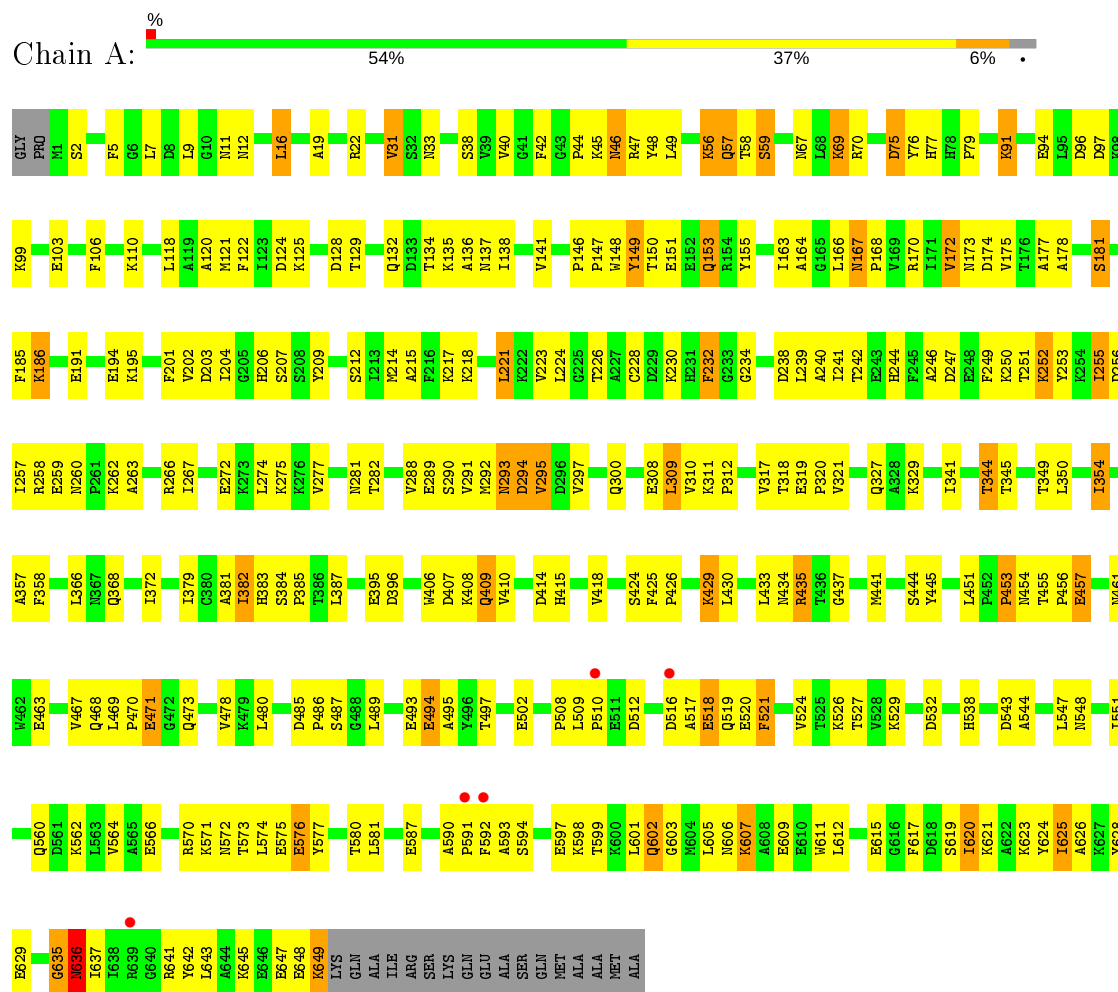
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



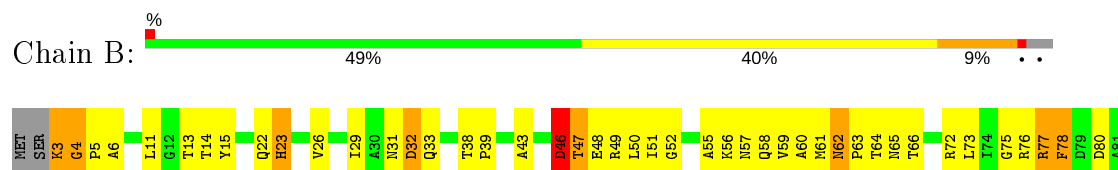
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Heat shock protein homolog SSE1



#### • Molecule 2: Heat shock cognate



V82	A161	H249	K328	V409	T502
D86	I164	K250	S329	T419	I503
N87	I173	K251	Q330	T420	T504
K88	I174	D252	D333	P421	N505
H89	N175	I253	L336	T425	D506
W90	P176	S254	G337	F428	K507
P91	T177	E255	G338	T429	G508
P92	A178	K256	G339	T430	R509
V95	I181	R257	S340	T431	L510
N96	A182	A259	T341	S432	S511
D97	I183	V260	R342	D433	K312
A98	G184	R261	I343	Q434	E513
G99	G185	C267	F344	Q435	D514
R100	L186	E268	I346	P436	R517
P101	D186	K271	I354	Q437	K526
K102	K187	R272	G351	V438	A527
V103	G190	T278	G352	L439	E528
Q104	A191	Q279	R361	V442	D529
V105	E192	A280	N364	V447	K531
E106	R193	E283	P365	R448	Q532
Y107	N194	I284	L359	M449	K535
K108	V195	D285	R360	T450	S538
G109	L196	S286	R361	K451	K539
E110	I197	I291	N364	D452	N540
T111	F198	D292	P365	P459	S541
K112	D199	T295	A368	E460	L542
S113	L200	S296	Y371	L461	E543
F114	G203	I297	G372	T462	S544
Y115	I212	T298	V375	G463	Y545
P116	S221	R299	Q376	L464	A546
E117	T222	A300	A377	A467	F547
S121	T226	R301	A378	P468	ASN
M122	K127	F302	D383	R469	MET
V123	K128	E303	K384	G470	LYS
L124	E129	L304	SER	V471	ALA
T125	I130	L305	GLU	P472	THR
K126	A131	N306	ASN	T477	VAL
M127	E132	L309	VAL	I480	GLU
K128	K137	F310	GLN	I485	
E129	T138	L314	D390	V486	
I130	V139	D315	L391	V491	
A131	T140	F316	L392	T495	
E132	F150	K319	L393	G496	
K137	Q154	A320	D395	K497	
T138	R155	L321	I403	T405	
V139	Q156	A324	E404	K500	
T140	A157	L326	A406	I501	
F150	D160	D327			



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.53 Å   169.50 Å   87.72 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	42.38 – 3.12 42.38 – 3.12	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.38-3.12) 96.6 (42.38-3.12)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 3.12 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.224   ,   0.283 0.216   ,   0.276	Depositor DCC
$R_{free}$ test set	1652 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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, 0.333 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: MG, BEF, SO4, ADP, CL

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	0.56	0/5199	0.70	0/7037
2	B	0.56	1/4242 (0.0%)	0.70	1/5728 (0.0%)
All	All	0.56	1/9441 (0.0%)	0.70	1/12765 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ARG	CG-CD	5.82	1.66	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ARG	NE-CZ-NH2	-5.67	117.47	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	420	ILE	Peptide

## 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	5103	0	5079	245	0
2	B	4182	0	4209	243	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	0	0	0	0
4	B	5	0	0	0	0
5	A	4	0	0	0	0
6	A	27	0	12	1	0
6	B	27	0	12	5	0
7	B	3	0	0	2	0
All	All	9368	0	9312	473	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 (473) 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)
2:B:420:ILE:HG23	2:B:421:PRO:CD	1.75	1.15
1:A:594:SER:HB3	1:A:597:GLU:HG2	1.32	1.11
1:A:601:LEU:O	1:A:603:GLY:HA3	1.53	1.09
1:A:141:VAL:HG21	1:A:166:LEU:HD13	1.40	1.03
2:B:405:THR:HB	2:B:409:VAL:HG23	1.44	0.97
1:A:47:ARG:NH1	1:A:121:MET:HG2	1.80	0.95
1:A:408:LYS:HB2	1:A:414:ASP:HB3	1.48	0.94
2:B:420:ILE:HG23	2:B:421:PRO:HD2	1.48	0.94
1:A:75:ASP:OD1	1:A:99:LYS:HE2	1.70	0.91
2:B:508:GLY:HA2	2:B:509:ARG:HB2	1.52	0.90
2:B:542:LEU:HD12	2:B:543:GLU:H	1.36	0.89
2:B:439:LEU:HB2	2:B:544:SER:HA	1.53	0.89
1:A:594:SER:HB3	1:A:597:GLU:CG	2.03	0.89
1:A:174:ASP:HB2	1:A:372:ILE:HG21	1.56	0.88
1:A:572:ASN:HD21	2:B:300:ALA:H	1.19	0.88
2:B:420:ILE:HG23	2:B:421:PRO:HD3	1.53	0.88
2:B:376:GLN:HE21	2:B:376:GLN:HA	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:PHE:CD2	1:A:642:TYR:HA	2.12	0.85
1:A:470:PRO:HB2	1:A:473:GLN:HG3	1.58	0.82
1:A:593:ALA:HA	1:A:641:ARG:HH21	1.45	0.82
2:B:258:ARG:HH21	2:B:261:ARG:HH22	1.27	0.82
1:A:575:GLU:HG2	2:B:300:ALA:HB3	1.62	0.82
2:B:110:GLU:HG2	2:B:111:THR:N	1.93	0.81
2:B:110:GLU:HG2	2:B:111:THR:H	1.46	0.81
1:A:244:HIS:HB2	1:A:309:LEU:HD21	1.64	0.80
1:A:434:ASN:C	1:A:435:ARG:HD2	2.02	0.80
2:B:405:THR:HB	2:B:409:VAL:CG2	2.11	0.80
2:B:195:VAL:HG23	2:B:333:ASP:HB2	1.62	0.79
1:A:575:GLU:OE2	2:B:301:ARG:HG3	1.82	0.79
1:A:238:ASP:OD1	1:A:275:LYS:HE2	1.83	0.78
2:B:46:ASP:HA	2:B:108:LYS:HA	1.66	0.77
1:A:602:GLN:HG3	1:A:603:GLY:CA	2.14	0.77
2:B:102:LYS:HE3	2:B:113:SER:OG	1.84	0.77
2:B:237:MET:HE3	2:B:267:CYS:HB3	1.66	0.76
1:A:395:GLU:HB3	1:A:424:SER:HB3	1.68	0.75
1:A:202:VAL:HG11	1:A:354:ILE:HD12	1.67	0.75
2:B:177:THR:HG22	2:B:210:LEU:HD13	1.68	0.75
1:A:350:LEU:O	1:A:354:ILE:HG22	1.86	0.75
2:B:546:ALA:O	2:B:547:PHE:HB2	1.86	0.75
1:A:260:ASN:HB3	1:A:263:ALA:HB3	1.69	0.74
2:B:430:THR:HG21	2:B:472:PRO:HG2	1.69	0.74
1:A:407:ASP:O	1:A:435:ARG:NH2	2.20	0.73
2:B:6:ALA:H	2:B:384:LYS:HE3	1.53	0.73
2:B:340:SER:O	2:B:343:ILE:HG12	1.87	0.73
1:A:2:SER:HB3	1:A:137:ASN:HB3	1.71	0.73
2:B:542:LEU:HD12	2:B:543:GLU:N	2.03	0.72
1:A:636:ASN:H	1:A:636:ASN:ND2	1.87	0.72
2:B:542:LEU:HG	2:B:545:TYR:HB3	1.71	0.72
1:A:147:PRO:HA	1:A:173:ASN:OD1	1.90	0.72
1:A:602:GLN:HG3	1:A:603:GLY:HA3	1.72	0.72
1:A:574:LEU:HD23	1:A:612:LEU:HD11	1.70	0.72
2:B:38:THR:HB	2:B:127:MET:CE	2.19	0.72
2:B:244:GLU:OE2	2:B:295:THR:HG21	1.90	0.72
1:A:209:TYR:CE1	1:A:320:PRO:HG2	2.25	0.71
1:A:76:TYR:CD2	1:A:94:GLU:HB2	2.25	0.71
2:B:435:GLN:HG3	2:B:543:GLU:HB3	1.73	0.71
1:A:426:PRO:HG3	1:A:486:PRO:HA	1.71	0.71
1:A:590:ALA:HB3	1:A:591:PRO:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:THR:HB	2:B:127:MET:HE3	1.72	0.71
2:B:76:ARG:O	2:B:101:PRO:HD3	1.91	0.70
2:B:88:LYS:HE2	2:B:89:HIS:ND1	2.06	0.70
2:B:90:TRP:HB3	2:B:92:PHE:CE2	2.27	0.69
2:B:73:LEU:CD1	2:B:116:PRO:HG3	2.23	0.69
1:A:191:GLU:OE1	1:A:218:LYS:HE3	1.93	0.69
1:A:480:LEU:HD23	1:A:495:ALA:HB2	1.72	0.69
1:A:91:LYS:HD3	1:A:103:GLU:OE1	1.93	0.68
2:B:246:LYS:HG3	2:B:252:ASP:HB2	1.74	0.68
1:A:47:ARG:HH11	1:A:121:MET:HG2	1.55	0.68
2:B:268:GLU:OE1	2:B:272:ARG:HD3	1.93	0.68
2:B:43:ALA:HB2	2:B:66:THR:HG23	1.76	0.68
1:A:444:SER:HB2	1:A:457:GLU:O	1.94	0.68
1:A:434:ASN:O	1:A:435:ARG:HD2	1.94	0.68
1:A:601:LEU:C	1:A:603:GLY:HA3	2.13	0.68
2:B:505:ASN:O	2:B:506:ASP:HB2	1.94	0.68
1:A:194:GLU:O	1:A:217:LYS:HE2	1.94	0.67
1:A:234:GLY:HA2	1:A:344:THR:HG21	1.76	0.67
2:B:64:THR:HA	2:B:91:PRO:O	1.95	0.67
1:A:517:ALA:O	1:A:518:GLU:HB3	1.94	0.67
1:A:575:GLU:HG2	2:B:300:ALA:CB	2.25	0.67
1:A:572:ASN:ND2	2:B:300:ALA:H	1.90	0.67
2:B:174:ASN:HB3	2:B:176:PRO:HD2	1.77	0.67
1:A:560:GLN:O	1:A:564:VAL:HG23	1.95	0.67
1:A:518:GLU:HG3	1:A:518:GLU:O	1.94	0.66
1:A:645:LYS:O	1:A:649:LYS:HB2	1.95	0.66
1:A:611:TRP:HE3	1:A:612:LEU:HD12	1.57	0.66
2:B:51:ILE:HD13	2:B:122:MET:O	1.96	0.66
1:A:574:LEU:CD2	1:A:612:LEU:HD11	2.25	0.66
1:A:456:PRO:O	1:A:457:GLU:CB	2.44	0.66
2:B:532:GLN:HA	2:B:535:LYS:HD3	1.78	0.66
2:B:77:ARG:O	2:B:80:ASP:HB2	1.94	0.66
1:A:118:LEU:HA	1:A:121:MET:HE3	1.77	0.65
2:B:117:GLU:O	2:B:121:SER:HB3	1.96	0.65
2:B:11:LEU:HD13	2:B:124:LEU:HD11	1.78	0.65
1:A:341:ILE:HD12	1:A:372:ILE:HD11	1.79	0.65
2:B:395:ASP:HB2	2:B:420:ILE:HG21	1.77	0.65
1:A:385:PRO:HG3	2:B:512:LYS:N	2.11	0.65
2:B:299:ARG:O	2:B:303:GLU:HG3	1.96	0.65
1:A:445:TYR:CD1	1:A:451:LEU:HD21	2.32	0.64
2:B:132:GLU:HG3	2:B:139:VAL:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LEU:HD13	2:B:116:PRO:HG3	1.79	0.64
2:B:539:LYS:HG3	2:B:539:LYS:O	1.97	0.64
2:B:376:GLN:NE2	2:B:376:GLN:HA	2.13	0.63
1:A:445:TYR:CE1	1:A:451:LEU:HD21	2.32	0.63
1:A:547:LEU:O	1:A:551:ILE:HG13	1.99	0.62
1:A:253:TYR:HB3	1:A:255:ILE:HD13	1.82	0.62
2:B:50:LEU:O	2:B:55:ALA:HB2	1.99	0.62
2:B:246:LYS:HA	2:B:251:LYS:O	1.99	0.62
2:B:191:ALA:HB3	7:B:555:CL:CL	2.37	0.61
2:B:90:TRP:HB3	2:B:92:PHE:CZ	2.35	0.61
2:B:78:PHE:CD2	2:B:96:ASN:HB2	2.36	0.61
1:A:562:LYS:O	1:A:566:GLU:HB2	1.99	0.61
2:B:86:ASP:O	2:B:88:LYS:N	2.34	0.61
2:B:73:LEU:HD23	2:B:90:TRP:CZ3	2.36	0.61
1:A:594:SER:CB	1:A:597:GLU:HG2	2.21	0.60
2:B:279:GLN:HG2	2:B:280:ALA:H	1.66	0.60
2:B:531:LYS:HD3	2:B:531:LYS:O	2.01	0.60
1:A:636:ASN:H	1:A:636:ASN:HD22	1.48	0.60
1:A:435:ARG:HG2	1:A:478:VAL:HG22	1.83	0.60
1:A:625:ILE:O	1:A:629:GLU:HG2	2.02	0.60
2:B:467:ALA:HB1	2:B:468:PRO:CD	2.32	0.60
1:A:19:ALA:HB1	2:B:393:LEU:HD11	1.83	0.60
1:A:310:VAL:C	1:A:312:PRO:HD2	2.22	0.60
1:A:529:LYS:HE2	1:A:532:ASP:OD2	2.01	0.60
2:B:102:LYS:HD2	2:B:115:TYR:CE1	2.37	0.60
2:B:11:LEU:HD13	2:B:124:LEU:CD1	2.31	0.60
2:B:96:ASN:HD21	2:B:99:GLY:H	1.50	0.60
1:A:385:PRO:HG3	2:B:512:LYS:H	1.67	0.59
2:B:430:THR:CG2	2:B:472:PRO:HG2	2.32	0.59
1:A:519:GLN:HE21	1:A:520:GLU:N	2.00	0.59
1:A:203:ASP:HA	1:A:341:ILE:O	2.02	0.59
2:B:78:PHE:C	2:B:78:PHE:CD1	2.75	0.59
1:A:575:GLU:OE1	2:B:298:THR:HG21	2.03	0.59
2:B:508:GLY:CA	2:B:509:ARG:HB2	2.29	0.59
1:A:478:VAL:HG12	1:A:497:THR:CG2	2.33	0.59
1:A:291:VAL:HG23	1:A:292:MET:N	2.18	0.58
1:A:12:ASN:HB2	1:A:206:HIS:CG	2.38	0.58
2:B:439:LEU:CB	2:B:544:SER:HA	2.31	0.58
2:B:73:LEU:HD23	2:B:90:TRP:CH2	2.38	0.58
2:B:60:ALA:O	2:B:61:MET:HG3	2.02	0.58
2:B:110:GLU:CG	2:B:111:THR:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ASN:OD1	1:A:67:ASN:HA	2.03	0.58
2:B:117:GLU:HG2	2:B:157:ALA:HB1	1.84	0.58
2:B:248:LYS:C	2:B:249:HIS:CD2	2.77	0.58
2:B:539:LYS:CG	2:B:539:LYS:O	2.52	0.58
1:A:581:LEU:HD23	1:A:605:LEU:HD11	1.86	0.57
1:A:70:ARG:NH2	1:A:230:LYS:O	2.34	0.57
1:A:317:VAL:O	1:A:320:PRO:HD2	2.04	0.57
1:A:46:ASN:HB3	1:A:564:VAL:HG21	1.85	0.57
1:A:253:TYR:HB3	1:A:255:ILE:CD1	2.35	0.57
1:A:344:THR:HG23	6:A:672:ADP:H1'	1.86	0.57
1:A:221:LEU:C	1:A:221:LEU:HD12	2.25	0.57
1:A:456:PRO:O	1:A:457:GLU:HB3	2.03	0.57
2:B:132:GLU:HG2	2:B:138:THR:HA	1.85	0.57
2:B:185:LEU:CD1	2:B:195:VAL:HG21	2.33	0.57
2:B:343:ILE:CD1	6:B:560:ADP:H2	2.18	0.57
2:B:62:ASN:N	2:B:63:PRO:CD	2.67	0.57
1:A:42:PHE:HB3	1:A:106:PHE:HB2	1.86	0.57
1:A:599:THR:HG22	1:A:599:THR:O	2.05	0.57
2:B:185:LEU:C	2:B:187:LYS:H	2.08	0.56
2:B:96:ASN:HD22	2:B:97:ASP:N	2.03	0.56
1:A:91:LYS:HG2	1:A:103:GLU:HB3	1.85	0.56
1:A:478:VAL:HG12	1:A:497:THR:HG22	1.86	0.56
1:A:621:LYS:O	1:A:625:ILE:HG12	2.05	0.56
1:A:426:PRO:HG3	1:A:486:PRO:CA	2.36	0.56
1:A:262:LYS:O	1:A:266:ARG:HG3	2.06	0.56
1:A:396:ASP:HB3	1:A:425:PHE:CE2	2.39	0.56
1:A:572:ASN:HD21	2:B:300:ALA:N	1.96	0.56
1:A:469:LEU:HD12	1:A:469:LEU:N	2.20	0.56
1:A:590:ALA:HA	1:A:598:LYS:NZ	2.21	0.56
1:A:150:THR:H	1:A:153:GLN:HG3	1.71	0.56
1:A:406:TRP:CE2	1:A:433:LEU:HD21	2.42	0.55
2:B:405:THR:HG23	2:B:540:ASN:H	1.72	0.55
1:A:451:LEU:CD2	1:A:455:THR:HG21	2.36	0.55
2:B:78:PHE:C	2:B:78:PHE:HD1	2.10	0.55
2:B:430:THR:HG22	2:B:472:PRO:HD2	1.88	0.55
1:A:601:LEU:O	1:A:602:GLN:CG	2.55	0.55
1:A:266:ARG:NH1	1:A:289:GLU:O	2.37	0.54
1:A:76:TYR:CG	1:A:94:GLU:HB2	2.42	0.54
2:B:395:ASP:CB	2:B:420:ILE:HG21	2.36	0.54
1:A:509:LEU:N	1:A:510:PRO:HD3	2.23	0.54
1:A:641:ARG:O	1:A:645:LYS:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:437:GLY:O	2:B:543:GLU:HA	2.07	0.54
2:B:248:LYS:O	2:B:249:HIS:CD2	2.61	0.54
2:B:286:SER:N	2:B:292:ASP:OD2	2.34	0.54
2:B:460:GLU:HG2	2:B:462:THR:CG2	2.38	0.54
1:A:137:ASN:O	1:A:138:ILE:HD13	2.08	0.54
2:B:3:LYS:HB2	2:B:137:LYS:HE3	1.88	0.54
2:B:436:PRO:O	2:B:464:ILE:HG13	2.08	0.54
1:A:246:ALA:HB2	1:A:257:ILE:HD11	1.90	0.54
1:A:451:LEU:HD22	1:A:455:THR:HG21	1.89	0.54
2:B:338:GLY:HA2	6:B:560:ADP:O2A	2.08	0.54
2:B:429:THR:CG2	2:B:540:ASN:HB3	2.38	0.54
1:A:290:SER:HA	1:A:295:VAL:O	2.07	0.54
1:A:134:THR:C	1:A:136:ALA:H	2.11	0.53
1:A:257:ILE:C	1:A:259:GLU:H	2.10	0.53
1:A:150:THR:H	1:A:153:GLN:CG	2.21	0.53
1:A:385:PRO:CD	2:B:509:ARG:HH22	2.20	0.53
1:A:433:LEU:HB3	1:A:435:ARG:HD3	1.91	0.53
2:B:351:GLN:HB2	2:B:359:LEU:HD11	1.90	0.53
1:A:571:LYS:HE2	1:A:617:PHE:O	2.07	0.53
1:A:141:VAL:CG2	1:A:166:LEU:HD13	2.25	0.53
1:A:408:LYS:HG2	1:A:408:LYS:O	2.06	0.53
1:A:636:ASN:N	1:A:636:ASN:ND2	2.51	0.53
2:B:86:ASP:C	2:B:88:LYS:H	2.12	0.53
1:A:384:SER:CB	1:A:387:LEU:HD12	2.39	0.53
1:A:623:LYS:HA	1:A:626:ALA:HB3	1.91	0.53
2:B:31:ASN:C	2:B:33:GLN:H	2.12	0.53
2:B:438:VAL:HG23	2:B:461:LEU:HB3	1.91	0.53
2:B:429:THR:HG22	2:B:540:ASN:HB3	1.90	0.53
2:B:183:TYR:OH	2:B:361:LYS:HA	2.09	0.52
1:A:311:LYS:N	1:A:312:PRO:CD	2.73	0.52
1:A:643:LEU:O	1:A:647:GLU:HB2	2.08	0.52
2:B:240:HIS:CB	2:B:305:LEU:HD21	2.39	0.52
2:B:29:ILE:HD13	2:B:131:ALA:HA	1.91	0.52
2:B:221:SER:OG	2:B:324:ALA:HB2	2.09	0.52
2:B:229:GLY:O	2:B:230:GLY:C	2.47	0.52
2:B:240:HIS:O	2:B:243:ALA:HB3	2.10	0.52
1:A:201:PHE:HE1	1:A:366:LEU:HD11	1.73	0.52
2:B:90:TRP:C	2:B:92:PHE:H	2.12	0.52
1:A:91:LYS:HD3	1:A:103:GLU:CD	2.30	0.52
1:A:150:THR:OG1	1:A:153:GLN:HG2	2.10	0.52
1:A:260:ASN:HB3	1:A:263:ALA:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:ALA:O	2:B:371:TYR:HB3	2.10	0.52
1:A:170:ARG:HE	1:A:383:HIS:HE1	1.57	0.52
1:A:635:GLY:O	1:A:636:ASN:C	2.48	0.52
1:A:341:ILE:HA	1:A:368:GLN:HB2	1.91	0.51
2:B:106:GLU:O	2:B:106:GLU:HG3	2.08	0.51
2:B:253:ILE:O	2:B:255:GLU:N	2.43	0.51
2:B:96:ASN:HD21	2:B:99:GLY:N	2.07	0.51
1:A:256:ASP:HB3	1:A:259:GLU:CG	2.40	0.51
1:A:7:LEU:HD21	1:A:9:LEU:HD12	1.92	0.51
2:B:185:LEU:HD12	2:B:195:VAL:HG21	1.91	0.51
2:B:279:GLN:HG2	2:B:280:ALA:N	2.26	0.51
2:B:75:GLY:HA3	2:B:154:GLN:HA	1.93	0.51
2:B:86:ASP:HB3	2:B:90:TRP:CH2	2.45	0.51
2:B:248:LYS:HB3	2:B:249:HIS:CD2	2.45	0.51
2:B:405:THR:HG22	2:B:406:ALA:N	2.25	0.51
2:B:503:ILE:C	2:B:505:ASN:H	2.14	0.51
2:B:117:GLU:CG	2:B:157:ALA:HB1	2.41	0.51
1:A:649:LYS:HB3	1:A:649:LYS:NZ	2.26	0.50
1:A:214:MET:HG2	1:A:223:VAL:HG22	1.92	0.50
2:B:315:ASP:HB2	2:B:316:PRO:HD3	1.93	0.50
2:B:238:VAL:O	2:B:242:ILE:HD12	2.10	0.50
1:A:146:PRO:HB2	1:A:148:TRP:CD1	2.46	0.50
1:A:291:VAL:CG2	1:A:292:MET:H	2.24	0.50
2:B:197:ILE:N	2:B:197:ILE:HD13	2.27	0.50
2:B:430:THR:CG2	2:B:472:PRO:HD2	2.42	0.50
2:B:542:LEU:HD21	2:B:545:TYR:HD1	1.77	0.50
1:A:291:VAL:CG2	1:A:292:MET:N	2.75	0.50
1:A:470:PRO:CB	1:A:473:GLN:HG3	2.35	0.50
2:B:22:GLN:O	2:B:23:HIS:HB2	2.12	0.50
2:B:343:ILE:HD13	6:B:560:ADP:H2	1.76	0.50
1:A:212:SER:HB2	1:A:226:THR:OG1	2.12	0.50
1:A:318:THR:HG22	1:A:357:ALA:HB2	1.93	0.50
1:A:379:ILE:O	1:A:382:ILE:HB	2.12	0.50
2:B:6:ALA:HB1	2:B:377:ALA:HB1	1.93	0.50
1:A:174:ASP:HB2	1:A:372:ILE:CG2	2.34	0.49
1:A:620:ILE:HD11	1:A:623:LYS:HG2	1.94	0.49
1:A:70:ARG:NH1	1:A:207:SER:OG	2.44	0.49
2:B:106:GLU:HA	2:B:110:GLU:O	2.11	0.49
2:B:132:GLU:CG	2:B:139:VAL:HG23	2.43	0.49
2:B:324:ALA:O	2:B:326:LEU:HG	2.12	0.49
2:B:375:VAL:O	2:B:378:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ARG:HH12	2:B:226:THR:HG22	1.76	0.49
1:A:544:ALA:O	1:A:548:ASN:ND2	2.46	0.49
2:B:121:SER:HB2	2:B:161:ALA:O	2.12	0.49
2:B:298:THR:CG2	2:B:301:ARG:H	2.24	0.49
1:A:292:MET:O	1:A:294:ASP:N	2.46	0.49
2:B:471:VAL:HB	2:B:472:PRO:HD3	1.94	0.49
1:A:204:ILE:HD13	1:A:345:THR:HG22	1.93	0.48
1:A:128:ASP:O	1:A:129:THR:C	2.52	0.48
2:B:286:SER:HA	2:B:291:ILE:O	2.13	0.48
1:A:9:LEU:O	1:A:69:LYS:HE2	2.14	0.48
2:B:102:LYS:HD2	2:B:115:TYR:CZ	2.49	0.48
2:B:62:ASN:H	2:B:63:PRO:CD	2.25	0.48
1:A:256:ASP:O	1:A:259:GLU:CG	2.62	0.48
1:A:451:LEU:N	1:A:451:LEU:HD12	2.29	0.48
1:A:607:LYS:O	1:A:611:TRP:HB2	2.13	0.48
2:B:32:ASP:OD2	2:B:32:ASP:N	2.46	0.48
1:A:2:SER:HB2	1:A:137:ASN:O	2.12	0.48
1:A:56:LYS:O	1:A:58:THR:N	2.47	0.48
1:A:150:THR:N	1:A:153:GLN:HG3	2.29	0.48
2:B:238:VAL:HG12	2:B:242:ILE:HD11	1.96	0.48
2:B:26:VAL:HB	2:B:371:TYR:CE2	2.48	0.48
2:B:460:GLU:HG2	2:B:462:THR:HG23	1.96	0.48
1:A:134:THR:C	1:A:136:ALA:N	2.66	0.48
1:A:75:ASP:HA	1:A:99:LYS:HD3	1.96	0.48
2:B:110:GLU:CG	2:B:111:THR:N	2.66	0.48
2:B:198:PHE:CD1	2:B:198:PHE:O	2.67	0.47
2:B:467:ALA:HB1	2:B:468:PRO:HD3	1.97	0.47
2:B:38:THR:HB	2:B:127:MET:HE1	1.96	0.47
2:B:500:LYS:HG3	2:B:501:ILE:N	2.29	0.47
1:A:385:PRO:HD2	2:B:509:ARG:HH22	1.79	0.47
1:A:601:LEU:O	1:A:602:GLN:HG2	2.14	0.47
2:B:364:ASN:HA	2:B:365:PRO:HD2	1.74	0.47
2:B:228:LEU:HD22	2:B:229:GLY:N	2.30	0.47
2:B:425:THR:HG23	2:B:477:THR:OG1	2.14	0.47
1:A:396:ASP:O	1:A:424:SER:HA	2.15	0.47
1:A:623:LYS:HA	1:A:626:ALA:CB	2.44	0.47
1:A:38:SER:HA	1:A:122:PHE:CE1	2.50	0.47
1:A:178:ALA:O	1:A:181:SER:HB2	2.14	0.47
2:B:298:THR:HG22	2:B:301:ARG:HB2	1.97	0.47
1:A:461:ASN:ND2	1:A:538:HIS:HD2	2.13	0.47
1:A:485:ASP:HB2	1:A:486:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:VAL:HG21	2:B:488:VAL:HG21	1.97	0.47
1:A:97:ASP:OD1	1:A:99:LYS:HB2	2.15	0.46
1:A:59:SER:OG	2:B:283:GLU:OE1	2.28	0.46
2:B:543:GLU:O	2:B:545:TYR:N	2.49	0.46
2:B:107:TYR:O	2:B:108:LYS:HB2	2.15	0.46
2:B:31:ASN:HB3	2:B:130:ILE:HD13	1.97	0.46
2:B:249:HIS:ND1	2:B:291:ILE:HG21	2.31	0.46
1:A:288:VAL:H	1:A:297:VAL:HG23	1.81	0.46
1:A:327:GLN:C	1:A:329:LYS:H	2.18	0.46
2:B:233:PHE:CD1	2:B:310:PHE:HE1	2.34	0.46
2:B:328:LYS:HE3	2:B:353:PHE:O	2.16	0.46
2:B:531:LYS:CD	2:B:531:LYS:O	2.64	0.46
1:A:132:GLN:O	1:A:135:LYS:HE3	2.16	0.46
1:A:256:ASP:O	1:A:259:GLU:HG2	2.16	0.46
1:A:281:ASN:HD21	2:B:57:ASN:HB2	1.80	0.46
1:A:592:PHE:CE2	1:A:642:TYR:HA	2.49	0.46
2:B:301:ARG:O	2:B:305:LEU:CD1	2.64	0.46
2:B:339:GLY:N	6:B:560:ADP:O2A	2.45	0.46
2:B:303:GLU:OE2	2:B:345:LYS:HB2	2.16	0.46
2:B:191:ALA:CB	7:B:555:CL:CL	3.01	0.45
2:B:420:ILE:CG2	2:B:421:PRO:CD	2.69	0.45
2:B:200:LEU:HD11	2:B:228:LEU:HD13	1.99	0.45
2:B:526:LYS:O	2:B:530:GLU:HB2	2.16	0.45
2:B:339:GLY:O	2:B:342:ARG:HG3	2.17	0.45
2:B:49:ARG:O	2:B:50:LEU:HD23	2.15	0.45
1:A:174:ASP:OD1	1:A:175:VAL:N	2.45	0.45
1:A:232:PHE:C	1:A:232:PHE:CD2	2.90	0.45
1:A:204:ILE:HG13	1:A:209:TYR:CD2	2.51	0.45
1:A:606:ASN:O	1:A:609:GLU:HB3	2.17	0.45
2:B:436:PRO:HG2	2:B:437:GLY:H	1.81	0.45
1:A:602:GLN:HG3	1:A:603:GLY:HA2	1.93	0.45
1:A:487:SER:HB2	1:A:489:LEU:HG	1.98	0.45
2:B:480:ILE:HA	2:B:485:ILE:O	2.17	0.45
1:A:16:LEU:N	1:A:16:LEU:CD1	2.79	0.45
1:A:172:VAL:HG21	1:A:379:ILE:CD1	2.46	0.45
2:B:459:PHE:CE1	2:B:501:ILE:HG22	2.52	0.45
2:B:249:HIS:C	2:B:251:LYS:H	2.20	0.44
1:A:291:VAL:HG23	1:A:292:MET:H	1.79	0.44
2:B:392:LEU:C	2:B:392:LEU:HD12	2.38	0.44
1:A:203:ASP:C	1:A:203:ASP:OD2	2.56	0.44
1:A:381:ALA:O	1:A:382:ILE:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG22	1:A:49:LEU:HD22	2.00	0.44
2:B:508:GLY:HA2	2:B:509:ARG:CB	2.34	0.44
1:A:31:VAL:CG2	1:A:33:ASN:ND2	2.80	0.44
1:A:418:VAL:O	1:A:429:LYS:HE3	2.17	0.44
1:A:577:TYR:HA	1:A:580:THR:HG22	2.00	0.44
2:B:279:GLN:NE2	2:B:296:SER:HB2	2.33	0.44
2:B:449:MET:O	2:B:451:LYS:N	2.51	0.44
1:A:249:PHE:O	1:A:255:ILE:O	2.35	0.44
1:A:406:TRP:O	1:A:414:ASP:HB2	2.18	0.44
2:B:46:ASP:CA	2:B:108:LYS:HA	2.43	0.44
2:B:256:ASN:HB3	2:B:259:ALA:HB3	2.00	0.44
1:A:56:LYS:O	1:A:57:GLN:C	2.56	0.44
1:A:48:TYR:CD2	1:A:56:LYS:HG2	2.53	0.44
2:B:469:ARG:HG2	2:B:469:ARG:O	2.18	0.44
2:B:542:LEU:HG	2:B:545:TYR:CB	2.42	0.44
1:A:310:VAL:C	1:A:312:PRO:CD	2.86	0.43
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.74	0.43
2:B:405:THR:CG2	2:B:406:ALA:N	2.81	0.43
2:B:435:GLN:CG	2:B:543:GLU:HB3	2.45	0.43
1:A:146:PRO:HG2	1:A:149:TYR:CD1	2.53	0.43
2:B:104:GLN:HG3	2:B:113:SER:HB3	2.00	0.43
1:A:110:LYS:HA	1:A:110:LYS:HD3	1.80	0.43
1:A:167:ASN:HA	1:A:168:PRO:HD3	1.83	0.43
1:A:174:ASP:O	1:A:177:ALA:N	2.50	0.43
1:A:560:GLN:O	1:A:560:GLN:HG2	2.17	0.43
1:A:573:THR:HG22	1:A:628:TYR:CE1	2.54	0.43
1:A:647:GLU:HB3	1:A:648:GLU:OE2	2.18	0.43
2:B:174:ASN:HB2	2:B:177:THR:OG1	2.18	0.43
1:A:151:GLU:O	1:A:155:TYR:HD1	2.01	0.43
2:B:505:ASN:O	2:B:506:ASP:CB	2.64	0.43
1:A:135:LYS:HE2	1:A:135:LYS:HA	1.99	0.43
1:A:239:LEU:O	1:A:240:ALA:C	2.57	0.43
1:A:406:TRP:HB3	1:A:441:MET:HG2	2.01	0.43
2:B:185:LEU:C	2:B:187:LYS:N	2.72	0.43
2:B:511:SER:O	2:B:514:ASP:N	2.51	0.43
1:A:469:LEU:N	1:A:469:LEU:CD1	2.81	0.43
2:B:178:ALA:O	2:B:372:GLY:HA3	2.19	0.43
2:B:510:LEU:HD22	2:B:514:ASP:HB3	2.01	0.43
1:A:247:ASP:O	1:A:250:LYS:HB3	2.18	0.43
1:A:453:PRO:O	1:A:454:ASN:HB2	2.19	0.43
1:A:521:PHE:CD1	1:A:521:PHE:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PHE:O	1:A:186:LYS:C	2.57	0.43
1:A:425:PHE:HA	1:A:426:PRO:C	2.40	0.43
2:B:240:HIS:HB2	2:B:305:LEU:HD21	2.01	0.43
1:A:463:GLU:OE2	1:A:538:HIS:NE2	2.33	0.42
2:B:319:LYS:O	2:B:319:LYS:HG3	2.18	0.42
2:B:301:ARG:O	2:B:305:LEU:HD12	2.19	0.42
2:B:343:ILE:HD11	6:B:560:ADP:H2	1.84	0.42
2:B:59:VAL:O	2:B:60:ALA:HB3	2.19	0.42
1:A:22:ARG:HH11	2:B:394:LEU:HD12	1.84	0.42
1:A:435:ARG:HG2	1:A:478:VAL:CG2	2.49	0.42
2:B:181:ILE:O	2:B:184:GLY:N	2.47	0.42
2:B:31:ASN:O	2:B:33:GLN:N	2.52	0.42
2:B:251:LYS:HA	2:B:251:LYS:HD3	1.89	0.42
2:B:309:LEU:HD23	2:B:309:LEU:HA	1.80	0.42
2:B:403:ILE:HD11	2:B:428:PHE:CZ	2.54	0.42
1:A:120:ALA:O	1:A:164:ALA:HB2	2.20	0.42
2:B:238:VAL:HG12	2:B:242:ILE:CD1	2.49	0.42
2:B:459:PHE:CD1	2:B:501:ILE:HG22	2.55	0.42
2:B:513:GLU:HG2	2:B:517:ARG:NH2	2.34	0.42
2:B:543:GLU:O	2:B:544:SER:C	2.58	0.42
1:A:395:GLU:HB3	1:A:424:SER:CB	2.44	0.42
1:A:576:GLU:O	1:A:580:THR:HG22	2.19	0.42
1:A:249:PHE:N	1:A:249:PHE:CD1	2.86	0.42
2:B:238:VAL:O	2:B:239:ASN:C	2.58	0.42
2:B:237:MET:HE1	2:B:271:LYS:HB2	2.01	0.42
1:A:564:VAL:O	1:A:564:VAL:HG12	2.20	0.42
2:B:237:MET:CE	2:B:267:CYS:HB3	2.42	0.42
2:B:505:ASN:HB3	2:B:507:LYS:HD3	2.01	0.42
2:B:5:PRO:HB3	2:B:384:LYS:CE	2.50	0.42
2:B:86:ASP:C	2:B:88:LYS:N	2.72	0.42
1:A:251:THR:HG22	1:A:252:LYS:N	2.35	0.42
2:B:65:ASN:OD1	2:B:106:GLU:HB3	2.20	0.42
1:A:274:LEU:O	1:A:277:VAL:HB	2.20	0.41
1:A:414:ASP:O	1:A:415:HIS:HB3	2.20	0.41
1:A:437:GLY:HA2	1:A:467:VAL:HG11	2.02	0.41
1:A:46:ASN:N	1:A:46:ASN:HD22	2.18	0.41
1:A:602:GLN:CG	1:A:603:GLY:HA3	2.45	0.41
1:A:77:HIS:CD2	1:A:94:GLU:OE1	2.73	0.41
2:B:291:ILE:HG22	2:B:292:ASP:N	2.35	0.41
2:B:78:PHE:CE2	2:B:96:ASN:HB2	2.55	0.41
1:A:571:LYS:HA	1:A:624:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:GLU:CD	2:B:272:ARG:HH11	2.23	0.41
2:B:495:THR:OG1	2:B:497:LYS:HG2	2.20	0.41
1:A:103:GLU:OE2	1:A:110:LYS:HD2	2.20	0.41
1:A:409:GLN:HG3	1:A:435:ARG:NH2	2.33	0.41
2:B:336:LEU:HD11	2:B:359:LEU:HD22	2.03	0.41
2:B:150:PHE:O	2:B:155:ARG:NH2	2.51	0.41
2:B:193:ARG:O	2:B:211:THR:HA	2.20	0.41
1:A:215:ALA:HB2	1:A:224:LEU:HD11	2.02	0.41
2:B:39:PRO:O	2:B:52:GLY:HA2	2.21	0.41
2:B:56:LYS:O	2:B:59:VAL:HG12	2.20	0.41
1:A:120:ALA:HB1	1:A:163:ILE:CG2	2.51	0.41
1:A:45:LYS:O	1:A:564:VAL:HG21	2.20	0.41
1:A:502:GLU:HA	1:A:524:VAL:O	2.20	0.41
1:A:623:LYS:HA	1:A:623:LYS:HD3	1.74	0.41
1:A:203:ASP:HB2	1:A:341:ILE:HG13	2.03	0.41
1:A:252:LYS:HG3	1:A:252:LYS:O	2.21	0.41
2:B:15:TYR:CE2	2:B:39:PRO:HG3	2.56	0.41
2:B:543:GLU:C	2:B:545:TYR:N	2.73	0.41
1:A:241:ILE:O	1:A:242:THR:C	2.58	0.41
1:A:251:THR:C	1:A:253:TYR:H	2.24	0.41
1:A:251:THR:O	1:A:253:TYR:N	2.52	0.41
1:A:321:VAL:HG22	1:A:358:PHE:CE2	2.56	0.41
1:A:350:LEU:HD12	1:A:350:LEU:O	2.20	0.41
1:A:526:LYS:HA	1:A:526:LYS:HD3	1.74	0.41
2:B:125:THR:O	2:B:128:LYS:HB3	2.21	0.41
2:B:459:PHE:CD1	2:B:501:ILE:CG2	3.03	0.41
2:B:508:GLY:CA	2:B:509:ARG:CB	2.95	0.41
1:A:611:TRP:CE2	1:A:615:GLU:O	2.75	0.41
2:B:160:ASP:C	2:B:164:ILE:HD12	2.42	0.41
2:B:321:LEU:HD23	2:B:321:LEU:HA	1.74	0.41
1:A:516:ASP:O	1:A:517:ALA:HB2	2.21	0.40
2:B:198:PHE:O	2:B:198:PHE:HD1	2.04	0.40
1:A:125:LYS:O	1:A:128:ASP:HB3	2.20	0.40
1:A:194:GLU:O	1:A:217:LYS:CE	2.65	0.40
1:A:267:ILE:HD13	1:A:288:VAL:HG21	2.03	0.40
1:A:570:ARG:C	1:A:572:ASN:N	2.74	0.40
2:B:419:THR:O	2:B:420:ILE:O	2.40	0.40
2:B:447:ARG:HG3	2:B:452:ASP:HB3	2.03	0.40
1:A:493:GLU:O	1:A:494:GLU:HB2	2.21	0.40
2:B:302:PHE:O	2:B:306:ASN:ND2	2.55	0.40
2:B:343:ILE:HB	2:B:346:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:GLY:HA2	2:B:5:PRO:HD3	1.78	0.40
1:A:12:ASN:HB2	1:A:206:HIS:CB	2.52	0.40
1:A:571:LYS:O	1:A:571:LYS:HG2	2.20	0.40
2:B:194:ASN:HB2	2:B:330:GLN:O	2.21	0.40
2:B:354:PHE:O	2:B:355:ASN:HB2	2.22	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	647/668 (97%)	546 (84%)	80 (12%)	21 (3%)	4	21
2	B	536/554 (97%)	442 (82%)	67 (12%)	27 (5%)	2	13
All	All	1183/1222 (97%)	988 (84%)	147 (12%)	48 (4%)	3	16

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	457	GLU
1	A	471	GLU
1	A	636	ASN
1	A	637	ILE
2	B	46	ASP
2	B	190	GLY
2	B	230	GLY
2	B	420	ILE
2	B	421	PRO
2	B	543	GLU
1	A	57	GLN
1	A	252	LYS

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Mol	Chain	Res	Type
1	A	508	PRO
1	A	518	GLU
1	A	635	GLY
2	B	62	ASN
2	B	186	ASP
2	B	191	ALA
2	B	254	SER
2	B	469	ARG
2	B	506	ASP
2	B	508	GLY
2	B	538	SER
2	B	23	HIS
2	B	32	ASP
2	B	87	MET
2	B	450	THR
2	B	504	THR
2	B	507	LYS
1	A	44	PRO
1	A	258	ARG
1	A	409	GLN
1	A	602	GLN
2	B	47	THR
2	B	305	LEU
1	A	494	GLU
1	A	619	SER
2	B	203	GLY
2	B	378	ALA
2	B	532	GLN
1	A	56	LYS
1	A	294	ASP
1	A	453	PRO
2	B	4	GLY
2	B	91	PRO
1	A	79	PRO
1	A	382	ILE

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was



analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	560/573 (98%)	511 (91%)	49 (9%)	10	35
2	B	455/468 (97%)	403 (89%)	52 (11%)	5	23
All	All	1015/1041 (98%)	914 (90%)	101 (10%)	7	28

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	16	LEU
1	A	31	VAL
1	A	46	ASN
1	A	59	SER
1	A	69	LYS
1	A	75	ASP
1	A	91	LYS
1	A	96	ASP
1	A	124	ASP
1	A	149	TYR
1	A	153	GLN
1	A	167	ASN
1	A	172	VAL
1	A	181	SER
1	A	186	LYS
1	A	195	LYS
1	A	221	LEU
1	A	228	CYS
1	A	232	PHE
1	A	255	ILE
1	A	272	GLU
1	A	282	THR
1	A	293	ASN
1	A	295	VAL
1	A	300	GLN
1	A	308	GLU
1	A	309	LEU
1	A	319	GLU
1	A	344	THR
1	A	349	THR
1	A	354	ILE
1	A	410	VAL
1	A	429	LYS

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Mol	Chain	Res	Type
1	A	430	LEU
1	A	435	ARG
1	A	468	GLN
1	A	471	GLU
1	A	512	ASP
1	A	521	PHE
1	A	527	THR
1	A	543	ASP
1	A	576	GLU
1	A	587	GLU
1	A	607	LYS
1	A	620	ILE
1	A	625	ILE
1	A	636	ASN
1	A	649	LYS
2	B	3	LYS
2	B	13	THR
2	B	14	THR
2	B	46	ASP
2	B	47	THR
2	B	48	GLU
2	B	58	GLN
2	B	77	ARG
2	B	78	PHE
2	B	82	VAL
2	B	88	LYS
2	B	89	HIS
2	B	96	ASN
2	B	105	VAL
2	B	121	SER
2	B	137	LYS
2	B	140	THR
2	B	173	ILE
2	B	193	ARG
2	B	211	THR
2	B	212	ILE
2	B	222	THR
2	B	226	THR
2	B	228	LEU
2	B	250	LYS
2	B	278	THR
2	B	285	ASP

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Mol	Chain	Res	Type
2	B	298	THR
2	B	314	LEU
2	B	319	LYS
2	B	328	LYS
2	B	361	LYS
2	B	364	ASN
2	B	376	GLN
2	B	392	LEU
2	B	394	LEU
2	B	430	THR
2	B	432	SER
2	B	433	ASP
2	B	438	VAL
2	B	447	ARG
2	B	491	VAL
2	B	497	LYS
2	B	501	ILE
2	B	504	THR
2	B	507	LYS
2	B	528	GLU
2	B	531	LYS
2	B	535	LYS
2	B	539	LYS
2	B	544	SER
2	B	545	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	46	ASN
1	A	77	HIS
1	A	87	HIS
1	A	153	GLN
1	A	244	HIS
1	A	281	ASN
1	A	300	GLN
1	A	383	HIS
1	A	415	HIS
1	A	461	ASN
1	A	519	GLN
1	A	572	ASN

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Mol	Chain	Res	Type
1	A	606	ASN
1	A	636	ASN
2	B	57	ASN
2	B	84	GLN
2	B	96	ASN
2	B	227	HIS
2	B	249	HIS
2	B	279	GLN
2	B	376	GLN
2	B	505	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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$
6	ADP	A	672	3,5	24,29,29	0.97	1 (4%)	29,45,45	1.39	4 (13%)
4	SO4	A	670	-	4,4,4	0.16	0	6,6,6	0.42	0
4	SO4	A	669	-	4,4,4	0.16	0	6,6,6	0.39	0
4	SO4	A	668	-	4,4,4	0.15	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BEF	A	671	6	0,3,3	0.00	-	-		
6	ADP	B	560	-	24,29,29	1.01	1 (4%)	29,45,45	1.85	8 (27%)
4	SO4	B	559	-	4,4,4	0.09	0	6,6,6	0.29	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
6	ADP	A	672	3,5	-	2/12/32/32	0/3/3/3
6	ADP	B	560	-	-	6/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	672	ADP	C5-C4	2.69	1.48	1.40
6	B	560	ADP	C5-C4	2.39	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	560	ADP	C4-C5-N7	-4.32	104.89	109.40
6	B	560	ADP	N3-C2-N1	-3.80	122.74	128.68
6	B	560	ADP	PA-O3A-PB	-3.34	121.36	132.83
6	B	560	ADP	C2-N1-C6	3.08	124.03	118.75
6	A	672	ADP	N3-C2-N1	-3.02	123.96	128.68
6	A	672	ADP	PA-O3A-PB	-2.96	122.68	132.83
6	A	672	ADP	C3'-C2'-C1'	2.84	105.25	100.98
6	B	560	ADP	O3B-PB-O2B	2.42	116.90	107.64
6	A	672	ADP	C4-C5-N7	-2.39	106.91	109.40
6	B	560	ADP	C5-C6-N6	2.18	123.67	120.35
6	B	560	ADP	C5-C6-N1	-2.04	115.73	120.35
6	B	560	ADP	C1'-N9-C4	-2.03	123.07	126.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	672	ADP	PA-O3A-PB-O2B

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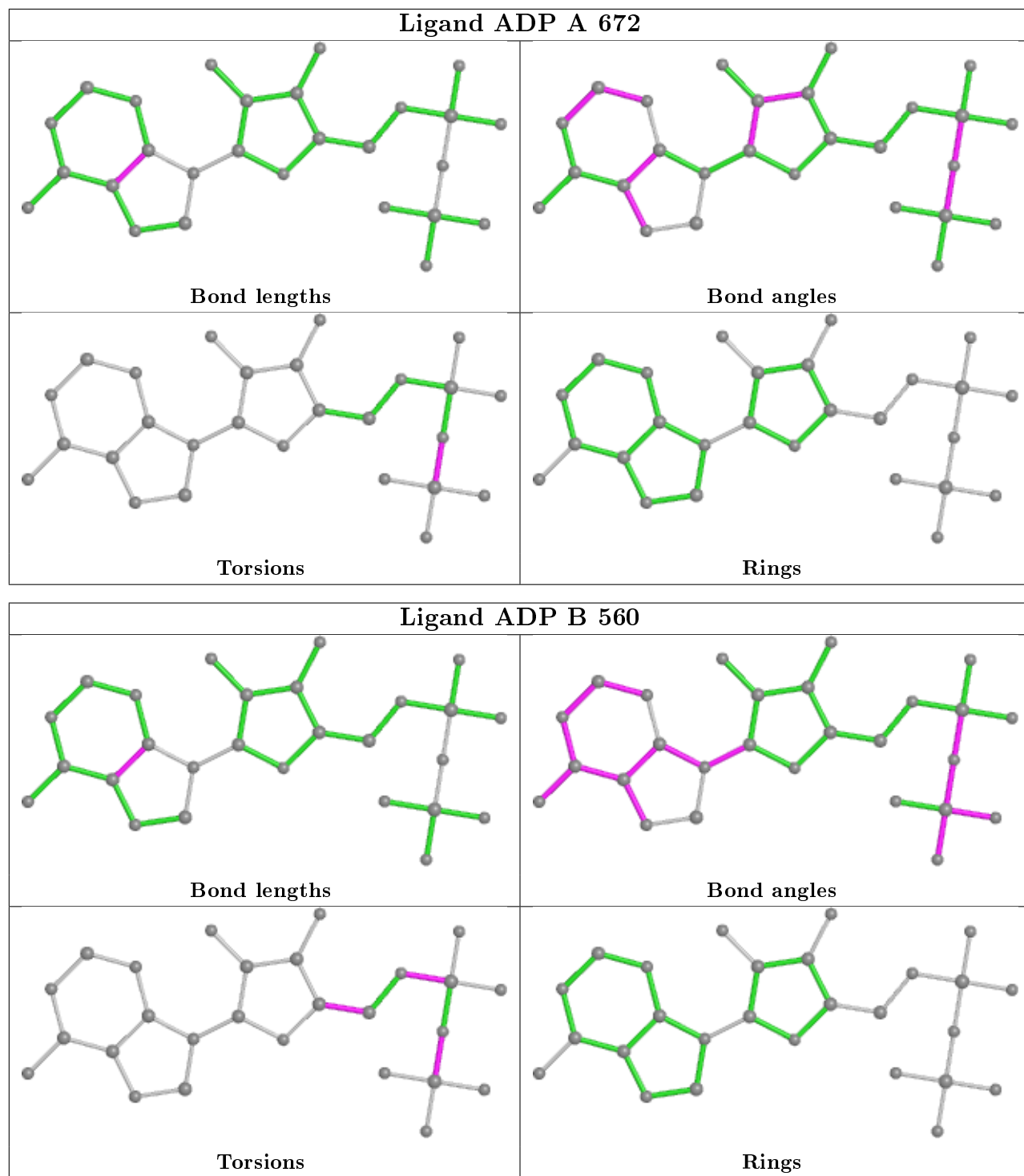
Mol	Chain	Res	Type	Atoms
6	B	560	ADP	PA-O3A-PB-O2B
6	B	560	ADP	C5'-O5'-PA-O1A
6	B	560	ADP	C5'-O5'-PA-O3A
6	B	560	ADP	O4'-C4'-C5'-O5'
6	B	560	ADP	C3'-C4'-C5'-O5'
6	B	560	ADP	C5'-O5'-PA-O2A
6	A	672	ADP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	672	ADP	1	0
6	B	560	ADP	5	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	649/668 (97%)	-0.28	5 (0%)	86 74	10, 42, 114, 147	0
2	B	540/554 (97%)	-0.23	4 (0%)	87 77	22, 50, 99, 136	0
All	All	1189/1222 (97%)	-0.26	9 (0%)	86 74	10, 47, 107, 147	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	508	GLY	3.5
1	A	591	PRO	2.9
1	A	516	ASP	2.8
2	B	109	GLY	2.6
2	B	383	ASP	2.3
2	B	95	VAL	2.2
1	A	639	ARG	2.2
1	A	510	PRO	2.1
1	A	592	PHE	2.0

### 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 carbohydrates in this entry.

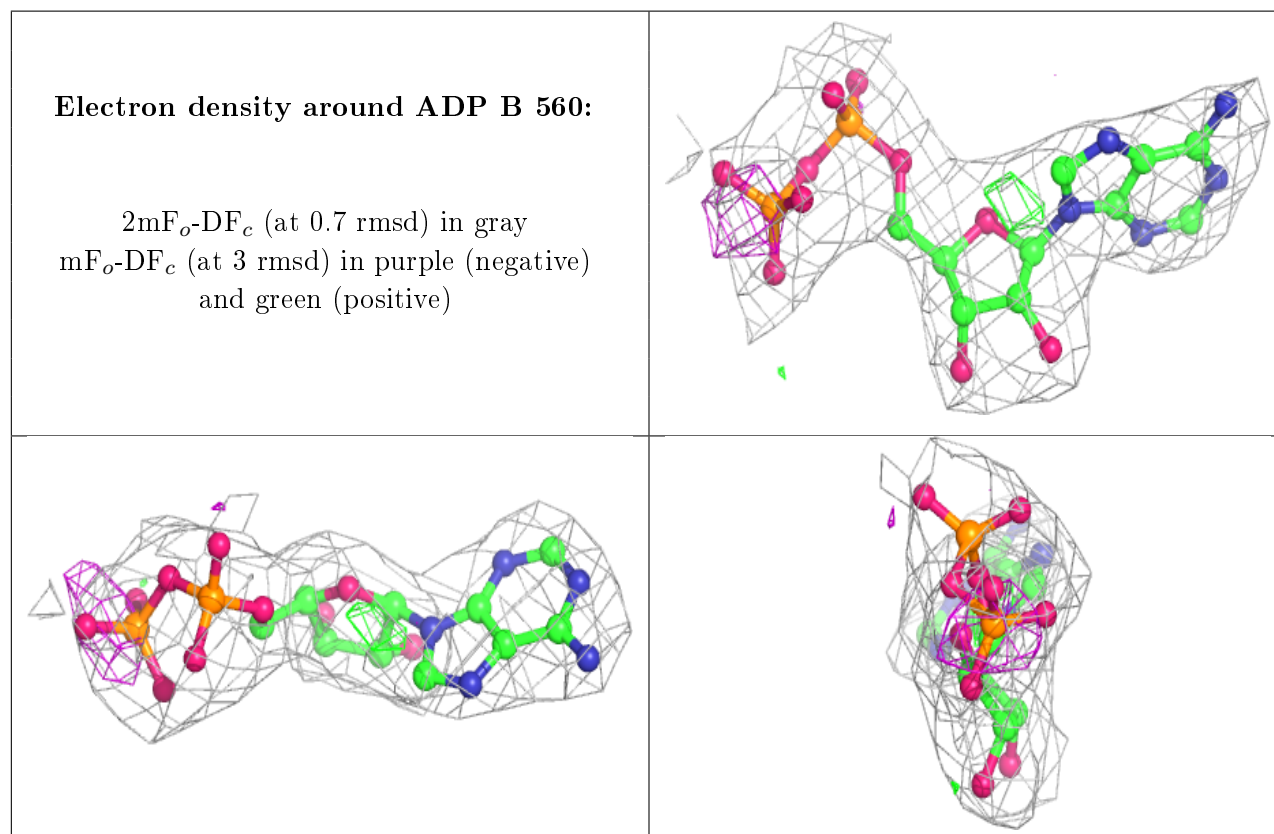
### 6.4 Ligands [i](#)

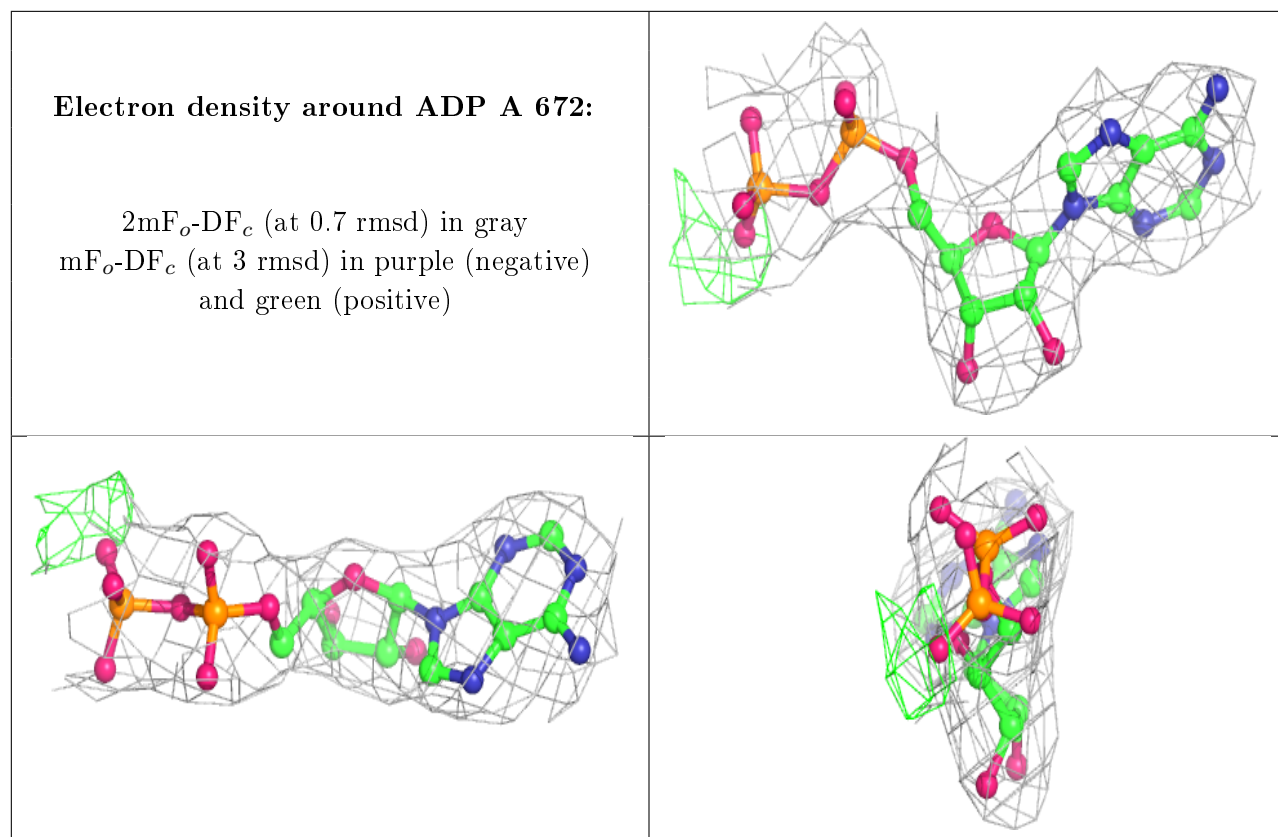
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	CL	B	555	1/1	0.85	0.15	69,69,69,69	0
7	CL	B	556	1/1	0.86	0.22	65,65,65,65	0
4	SO4	A	670	5/5	0.87	0.28	103,106,108,109	0
4	SO4	A	669	5/5	0.91	0.33	76,79,80,82	0
6	ADP	B	560	27/27	0.93	0.23	60,60,60,60	0
3	MG	B	558	1/1	0.94	0.34	27,27,27,27	0
6	ADP	A	672	27/27	0.96	0.23	44,44,44,44	0
4	SO4	B	559	5/5	0.96	0.24	70,72,74,75	0
5	BEF	A	671	4/4	0.97	0.34	39,39,39,39	0
7	CL	B	557	1/1	0.97	0.15	48,48,48,48	0
3	MG	A	667	1/1	0.97	0.41	14,14,14,14	0
4	SO4	A	668	5/5	0.97	0.34	81,83,85,86	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.