



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:34 pm GMT

PDB ID : 1Y4S
Title : Conformation rearrangement of heat shock protein 90 upon ADP binding
Authors : Huai, Q.; Wang, H.; Liu, Y.; Kim, H.; Toft, D.; Ke, H.
Deposited on : 2004-12-01
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

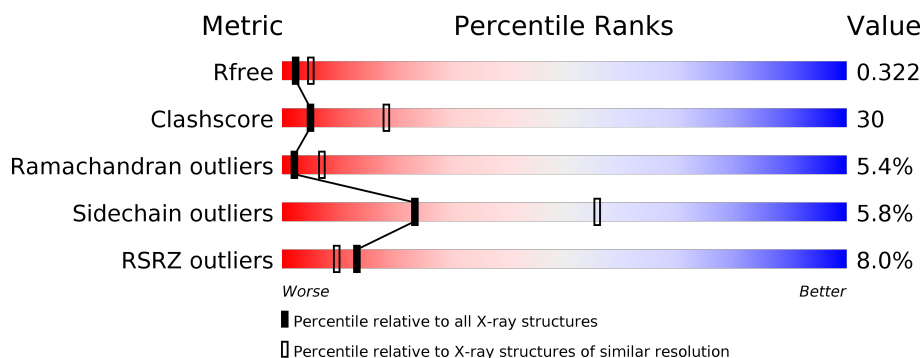
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	559	<div> <div>8%</div> <div>43%</div> <div>36%</div> <div>6%</div> <div>15%</div> </div>
1	B	559	<div> <div>6%</div> <div>37%</div> <div>43%</div> <div>15%</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
2	MG	A	703	-	-	-	X
2	MG	B	704	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7784 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.

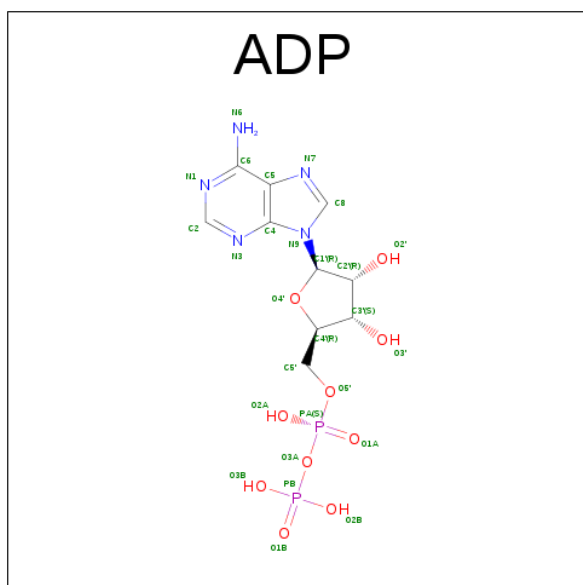
- Molecule 1 is a protein called Chaperone protein htpG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3864	2441	664	749	10			
1	B	475	Total	C	N	O	S	0	0	0
			3864	2441	664	749	10			

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

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

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

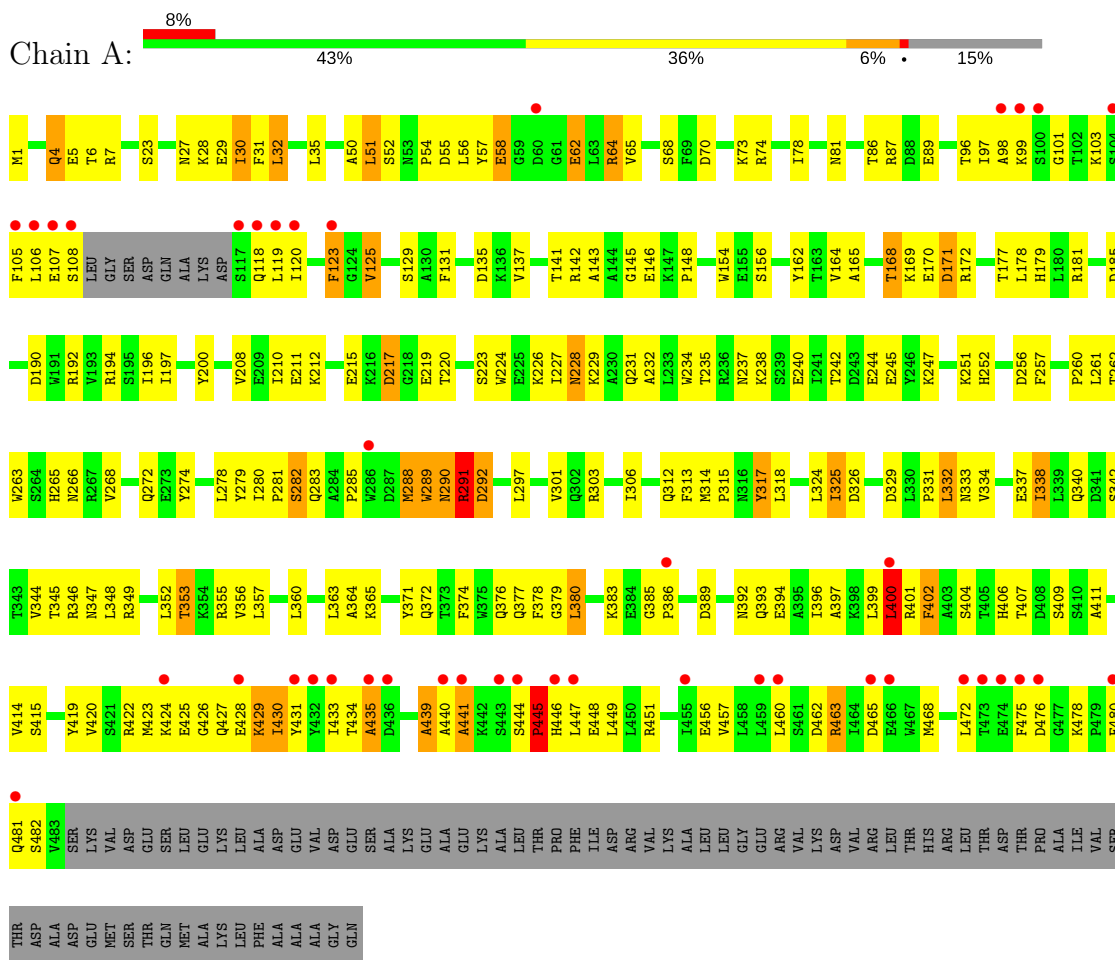


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

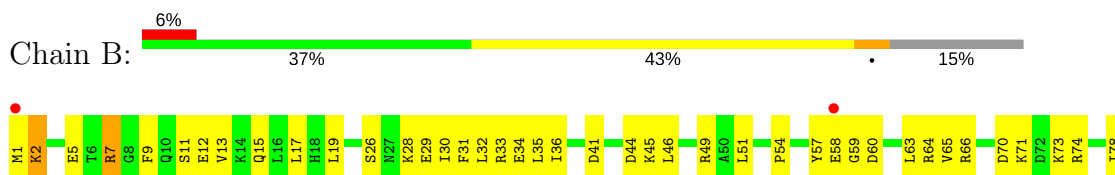
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: Chaperone protein htpG



- Molecule 1: Chaperone protein htpG



ASP	ARG	VAL	LYS	ALA	LEU	LEU	GLY	GLU	ARG	VAL	LYS	ASP	VAL	ARG	LEU	THR	HIS	ARG	LEU	THR	ASP	THR	PRO	ALA	ILE	VAL	SER	THR	ASP	ALA	ASP	GLU	MET	SER	THR	GLN	LYS	ASP	GLY	GLN													
H446	L447	E448	L449	L450	R451	G454	L455	E456	R463	L464	D465	E466	R467	L472	T473	E474	F475	D476	G477	K478	P479	S482	V483	SER	LYS	VAL	ASP	GLU	THR	GLN	ALA	ASP	GLU	THR	GLN	ALA	LYS	PHE	ALA	ALA	GLY	GLN											
Q372	W375	Q376	Q377	F378	G379	L380	V381	L382	K383	E384	G385	P386	A387	E388	D389	E394	A395	I396	L399	L400	R401	F402	A403	S404	T405	D408	V414	S415	D418	Y419	V420	S421	R422	M423	K424	E425	G426	Q427	E428	K429	Y432	I433	T434	A435	Y438	A441	K442	S443	S444	P445			
L299	Y300	V301	Q302	F305	I306	M307	D308	E311	Q312	F313	M314	P315	N316	Y317	L318	R319	F320	V321	R322	G323	L324	I325	D326	L330	P331	L332	N333	V334	I338	L339	Q340	D341	S342	T345	R346	N347	L348	K354	R355	Q358	M359	L360	E361	K362	L363	A364	K365	D366	D367	K370	Y371		
K226	I227	N228	K229	A230	Q231	A232	L233	W234	T235	K238	S239	E240	D243	E244	E245	Y246	K247	E248	F249	Y250	K251	H252	L253	D256	F257	N258	D259	P260	L261	T262	H265	E269	G270	K271	Q272	S276	L277	L278	Y279	I280	P281	S282	P285	W286	D287	M288	R291	D292	L297	K298			
V152	F153	W154	E155	S156	G160	E161	Y162	T163	V164	A165	D166	I167	T168	D171	R172	G173	T174	E175	I176	T177	L178	H179	L180	L188	D189	D190	W191	R192	V193	R194	S195	I196	I197	D202	H203	I204	A205	L206	P207	V208	E209	I210	E211	K216	D217	Q218	E219	T220	V221	L222	S223	W224	E225
N81	G82	V83	G84	M85	T86	E89	L94	G95	T96	I97	A98	K99	S100	G101	T102	K103	S104	F105	L106	E107	S108	LEU	GLY	SER	ASP	GLN	ALA	LYS	ASP	S117	Q118	L119	I120	G121	Q122	F123	G124	V125	G126	F127	Y128	V133	A134	V139	R140	T141	R142	A143	E146	K147	P148	E149	

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	72.50Å 84.18Å 212.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 78.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 88.4 (78.28-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.82Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.269 , 0.314 0.275 , 0.322	Depositor DCC
R_{free} test set	2728 reflections (9.72%)	DCC
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7784	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5801e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/3941	0.78	3/5314 (0.1%)
1	B	0.48	0/3941	0.71	2/5314 (0.0%)
All	All	0.50	0/7882	0.75	5/10628 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	GLY	N-CA-C	-8.81	91.07	113.10
1	B	426	GLY	N-CA-C	-6.12	97.81	113.10
1	A	123	PHE	N-CA-C	5.89	126.89	111.00
1	B	447	LEU	CA-CB-CG	5.61	128.19	115.30
1	A	400	LEU	CA-CB-CG	5.46	127.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3864	0	3786	215	0
1	B	3864	0	3786	245	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	12	0	0
3	B	27	0	12	0	0
All	All	7784	0	7596	460	1

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 30.

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:B:402:PHE:HD1	1:B:460:LEU:HD21	1.11	1.14
1:A:463:ARG:H	1:A:463:ARG:HD2	1.17	1.06
1:B:402:PHE:CD1	1:B:460:LEU:HD21	1.92	1.02
1:B:2:LYS:H	1:B:2:LYS:HD3	1.25	0.98
1:A:242:THR:HG22	1:A:244:GLU:H	1.27	0.96
1:A:407:THR:HG22	1:A:409:SER:H	1.36	0.89
1:A:29:GLU:HG3	1:A:192:ARG:HH22	1.38	0.88
1:A:97:ILE:HG22	1:A:98:ALA:H	1.37	0.88
1:A:107:GLU:HG2	1:A:108:SER:H	1.39	0.86
1:A:314:MET:HE1	1:A:356:VAL:HG21	1.56	0.86
1:A:96:THR:HG22	1:A:97:ILE:H	1.40	0.86
1:A:460:LEU:HD13	1:A:465:ASP:HB3	1.59	0.85
1:A:419:TYR:HE2	1:A:430:ILE:HA	1.41	0.85
1:A:62:GLU:HA	1:A:62:GLU:OE1	1.74	0.85
1:B:203:HIS:H	1:B:203:HIS:CD2	1.93	0.84
1:B:331:PRO:O	1:B:334:VAL:HG23	1.76	0.84
1:A:346:ARG:HG3	1:A:349:ARG:HH21	1.42	0.83
1:A:386:PRO:HD3	1:A:396:ILE:HG21	1.61	0.81
1:A:444:SER:HB3	1:A:445:PRO:HD2	1.61	0.81
1:A:419:TYR:CE2	1:A:430:ILE:HA	2.15	0.81
1:B:152:VAL:HG12	1:B:153:PHE:H	1.47	0.80
1:A:99:LYS:NZ	1:A:123:PHE:HB2	1.97	0.79
1:B:97:ILE:HD11	1:B:125:VAL:HG21	1.62	0.79
1:B:420:VAL:HG22	1:B:423:MET:HE2	1.66	0.77
1:B:285:PRO:HG2	1:B:288:MET:HB2	1.66	0.76
1:A:266:ASN:ND2	1:A:355:ARG:HD3	2.01	0.76
1:A:397:ALA:HA	1:A:400:LEU:HD11	1.67	0.76
1:A:401:ARG:HG2	1:A:415:SER:HA	1.65	0.76
1:B:190:ASP:O	1:B:194:ARG:HB2	1.86	0.75
1:B:372:GLN:O	1:B:376:GLN:HG3	1.86	0.75
1:B:30:ILE:HD11	1:B:257:PHE:CE1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:GLN:O	1:B:428:GLU:HB2	1.89	0.72
1:B:332:LEU:HD23	1:B:332:LEU:O	1.88	0.72
1:A:463:ARG:H	1:A:463:ARG:CD	1.99	0.71
1:B:238:LYS:HE2	1:B:265:HIS:O	1.89	0.71
1:B:96:THR:HG22	1:B:97:ILE:H	1.54	0.71
1:B:203:HIS:H	1:B:203:HIS:HD2	1.39	0.71
1:B:334:VAL:CG1	1:B:339:LEU:HG	2.22	0.70
1:B:297:LEU:N	1:B:297:LEU:HD12	2.07	0.70
1:A:463:ARG:HD2	1:A:463:ARG:N	2.00	0.69
1:A:99:LYS:HZ1	1:A:123:PHE:HB2	1.55	0.69
1:A:431:TYR:HE2	1:A:481:GLN:HE21	1.38	0.69
1:B:36:ILE:HG22	1:B:204:ILE:CD1	2.22	0.69
1:A:397:ALA:HA	1:A:400:LEU:CD1	2.23	0.69
1:A:247:LYS:HG2	1:A:260:PRO:HD2	1.73	0.68
1:A:301:VAL:HB	1:A:306:ILE:CD1	2.23	0.68
1:A:419:TYR:HE1	1:A:456:GLU:HB2	1.58	0.68
1:A:97:ILE:HG22	1:A:98:ALA:N	2.08	0.68
1:B:2:LYS:N	1:B:2:LYS:HD3	2.02	0.68
1:B:152:VAL:HG12	1:B:153:PHE:N	2.08	0.68
1:A:106:LEU:HD13	1:A:106:LEU:O	1.94	0.67
1:B:396:ILE:O	1:B:400:LEU:HG	1.93	0.67
1:B:423:MET:HE1	1:B:478:LYS:HG3	1.76	0.67
1:A:50:ALA:HB1	1:A:57:TYR:CE1	2.30	0.67
1:B:104:SER:HB2	1:B:286:TRP:NE1	2.09	0.67
1:B:262:THR:CG2	1:B:363:LEU:HD13	2.25	0.67
1:B:74:ARG:HG2	1:B:74:ARG:HH11	1.59	0.67
1:A:192:ARG:NH1	1:A:196:ILE:HD11	2.09	0.67
1:A:426:GLY:O	1:A:427:GLN:HB3	1.96	0.66
1:A:324:LEU:C	1:A:324:LEU:HD12	2.16	0.66
1:B:74:ARG:HA	1:B:188:LEU:HD11	1.77	0.66
1:B:375:TRP:HZ2	1:B:383:LYS:HE3	1.58	0.66
1:A:318:LEU:HD13	1:A:356:VAL:HG11	1.77	0.65
1:B:35:LEU:CD1	1:B:78:ILE:HD12	2.25	0.65
1:A:242:THR:HB	1:A:245:GLU:HG3	1.79	0.65
1:A:428:GLU:HG3	1:A:428:GLU:O	1.96	0.65
1:B:104:SER:HA	1:B:107:GLU:OE1	1.96	0.65
1:A:242:THR:HG22	1:A:244:GLU:N	2.06	0.64
1:B:297:LEU:HD11	1:B:314:MET:HG2	1.77	0.64
1:B:121:GLY:O	1:B:122:GLN:HG3	1.96	0.64
1:B:97:ILE:CD1	1:B:125:VAL:HG21	2.28	0.64
1:B:278:LEU:HD12	1:B:278:LEU:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:HB	1:B:89:GLU:HG3	1.81	0.63
1:B:297:LEU:HD11	1:B:314:MET:CG	2.28	0.63
1:A:344:VAL:O	1:A:348:LEU:HG	1.98	0.63
1:B:1:MET:HG3	1:B:167:ILE:CG2	2.29	0.63
1:A:407:THR:CG2	1:A:409:SER:H	2.09	0.63
1:A:331:PRO:C	1:A:333:ASN:H	2.02	0.63
1:B:375:TRP:CZ2	1:B:383:LYS:HE3	2.33	0.62
1:B:276:SER:HB2	1:B:278:LEU:CD1	2.29	0.62
1:B:388:GLU:O	1:B:388:GLU:HG2	1.98	0.62
1:A:261:LEU:HD12	1:A:280:ILE:HG22	1.82	0.62
1:B:49:ARG:HH11	1:B:49:ARG:HG2	1.63	0.62
1:A:192:ARG:O	1:A:196:ILE:HG13	2.00	0.62
1:A:434:THR:HG22	1:A:435:ALA:N	2.14	0.62
1:B:318:LEU:O	1:B:321:VAL:HG23	1.99	0.62
1:B:106:LEU:O	1:B:107:GLU:HG3	2.00	0.62
1:B:234:TRP:CE3	1:B:324:LEU:HD21	2.35	0.62
1:B:194:ARG:HG3	1:B:227:ILE:HD11	1.81	0.62
1:A:210:ILE:CG2	1:A:227:ILE:HD11	2.30	0.61
1:B:262:THR:HG21	1:B:363:LEU:HD13	1.82	0.61
1:A:210:ILE:HG21	1:A:227:ILE:HD11	1.83	0.61
1:A:190:ASP:O	1:A:194:ARG:HB2	2.01	0.61
1:A:29:GLU:H	1:A:29:GLU:CD	2.04	0.61
1:A:261:LEU:HD21	1:A:282:SER:HA	1.82	0.61
1:B:319:ARG:NH1	1:B:381:VAL:HG22	2.15	0.60
1:B:30:ILE:HD11	1:B:257:PHE:HE1	1.65	0.60
1:B:441:ALA:O	1:B:459:LEU:HD22	2.01	0.60
1:A:23:SER:HB3	1:A:119:LEU:O	2.02	0.60
1:A:145:GLY:O	1:A:146:GLU:HG2	2.02	0.60
1:B:191:TRP:O	1:B:195:SER:HB2	2.02	0.60
1:B:104:SER:HB2	1:B:286:TRP:CE2	2.37	0.60
1:B:297:LEU:HD22	1:B:325:ILE:HD11	1.82	0.60
1:B:70:ASP:OD1	1:B:73:LYS:N	2.32	0.60
1:A:234:TRP:NE1	1:A:326:ASP:HB2	2.17	0.59
1:A:435:ALA:HB3	1:A:441:ALA:HB2	1.84	0.59
1:B:192:ARG:O	1:B:196:ILE:HG13	2.02	0.59
1:B:272:GLN:NE2	1:B:347:ASN:HB3	2.17	0.59
1:B:473:THR:O	1:B:474:GLU:CB	2.51	0.59
1:A:325:ILE:HD12	1:A:352:LEU:HD11	1.83	0.59
1:A:346:ARG:HG3	1:A:349:ARG:NH2	2.16	0.59
1:B:281:PRO:HG2	1:B:378:PHE:CE1	2.38	0.59
1:A:272:GLN:NE2	1:A:347:ASN:HB3	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HD12	1:A:313:PHE:HB2	1.85	0.59
1:A:372:GLN:O	1:A:376:GLN:HG3	2.03	0.59
1:A:35:LEU:CD1	1:A:78:ILE:HD12	2.32	0.59
1:B:280:ILE:HG13	1:B:359:MET:HE3	1.84	0.59
1:A:211:GLU:HG2	1:A:212:LYS:N	2.18	0.58
1:A:57:TYR:O	1:A:58:GLU:C	2.40	0.58
1:B:96:THR:HG22	1:B:97:ILE:N	2.18	0.58
1:A:219:GLU:HG2	1:A:220:THR:N	2.19	0.58
1:A:232:ALA:O	1:A:235:THR:HB	2.04	0.58
1:A:346:ARG:CG	1:A:349:ARG:HH21	2.14	0.58
1:B:51:LEU:HD13	1:B:332:LEU:HD21	1.84	0.58
1:A:64:ARG:HD3	1:A:81:ASN:OD1	2.02	0.58
1:B:36:ILE:HG22	1:B:204:ILE:HD13	1.85	0.58
1:A:234:TRP:HE1	1:A:326:ASP:HB2	1.68	0.58
1:A:211:GLU:HB2	1:A:224:TRP:CZ3	2.39	0.58
1:B:380:LEU:HD12	1:B:380:LEU:H	1.69	0.58
1:A:27:ASN:O	1:A:30:ILE:HB	2.03	0.57
1:B:35:LEU:HD13	1:B:78:ILE:HD12	1.86	0.57
1:B:387:ALA:HB1	1:B:467:TRP:CH2	2.39	0.57
1:A:263:TRP:HB3	1:A:279:TYR:CD2	2.39	0.57
1:A:301:VAL:HB	1:A:306:ILE:HD11	1.86	0.57
1:A:107:GLU:CG	1:A:108:SER:H	2.13	0.57
1:B:194:ARG:HG3	1:B:227:ILE:CD1	2.34	0.57
1:B:334:VAL:HG13	1:B:339:LEU:HG	1.87	0.57
1:B:64:ARG:HG3	1:B:64:ARG:HH11	1.70	0.57
1:A:449:LEU:O	1:A:449:LEU:HD23	2.05	0.57
1:A:29:GLU:CG	1:A:192:ARG:HH22	2.13	0.56
1:B:250:TYR:HB2	1:B:279:TYR:CE2	2.40	0.56
1:B:446:HIS:O	1:B:449:LEU:HG	2.05	0.56
1:B:203:HIS:HB2	1:B:249:PHE:HD1	1.71	0.56
1:B:216:LYS:HB2	1:B:221:VAL:HG21	1.88	0.56
1:B:299:LEU:HD23	1:B:300:TYR:N	2.21	0.56
1:B:312:GLN:HA	1:B:312:GLN:OE1	2.05	0.56
1:A:290:ASN:O	1:A:292:ASP:N	2.39	0.56
1:A:125:VAL:CG1	1:A:129:SER:HB3	2.36	0.56
1:A:70:ASP:OD2	1:A:73:LYS:HB2	2.06	0.56
1:A:103:LYS:HB3	1:A:105:PHE:CD2	2.40	0.56
1:A:281:PRO:HG2	1:A:378:PHE:CZ	2.41	0.55
1:A:142:ARG:HB2	1:A:169:LYS:HB3	1.88	0.55
1:A:178:LEU:N	1:A:178:LEU:HD12	2.21	0.55
1:A:317:TYR:OH	1:A:357:LEU:HD21	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:SER:HB2	1:B:278:LEU:HD11	1.87	0.55
1:A:73:LYS:O	1:A:74:ARG:HB2	2.06	0.55
1:A:107:GLU:HG2	1:A:108:SER:N	2.17	0.55
1:B:32:LEU:CD1	1:B:78:ILE:HD11	2.36	0.55
1:A:389:ASP:CG	1:A:392:ASN:HD22	2.10	0.55
1:B:34:GLU:HG3	1:B:126:GLY:HA2	1.87	0.55
1:B:306:ILE:HG22	1:B:307:MET:N	2.22	0.55
1:B:122:GLN:O	1:B:123:PHE:O	2.25	0.55
1:B:64:ARG:NH1	1:B:64:ARG:HG3	2.22	0.55
1:B:12:GLU:HA	1:B:15:GLN:HE21	1.70	0.55
1:A:5:GLU:OE2	1:A:87:ARG:NH2	2.40	0.55
1:A:212:LYS:HB2	1:A:223:SER:HB2	1.89	0.54
1:A:96:THR:HG22	1:A:97:ILE:N	2.18	0.54
1:B:297:LEU:CD1	1:B:297:LEU:N	2.70	0.54
1:A:103:LYS:HD3	1:A:105:PHE:HE2	1.71	0.54
1:B:435:ALA:HB3	1:B:441:ALA:HB2	1.89	0.54
1:B:7:ARG:HD3	1:B:162:TYR:OH	2.07	0.54
1:A:431:TYR:HE2	1:A:481:GLN:NE2	2.05	0.54
1:A:211:GLU:HG2	1:A:212:LYS:H	1.72	0.54
1:A:261:LEU:O	1:A:262:THR:HG23	2.08	0.54
1:A:29:GLU:HG3	1:A:192:ARG:NH2	2.16	0.54
1:A:460:LEU:HD22	1:A:465:ASP:OD1	2.08	0.54
1:B:261:LEU:HG	1:B:281:PRO:O	2.08	0.54
1:B:301:VAL:HG12	1:B:302:GLN:HG3	1.89	0.54
1:A:383:LYS:C	1:A:385:GLY:H	2.11	0.53
1:B:419:TYR:CE1	1:B:456:GLU:HB3	2.43	0.53
1:A:420:VAL:HA	1:A:423:MET:HE3	1.89	0.53
1:A:280:ILE:HD13	1:A:360:LEU:HD21	1.89	0.53
1:A:103:LYS:CD	1:A:105:PHE:HE2	2.21	0.53
1:A:433:ILE:HD11	1:A:457:VAL:HG11	1.90	0.53
1:B:330:LEU:HB3	1:B:334:VAL:HG21	1.91	0.53
1:B:316:ASN:O	1:B:319:ARG:HG3	2.09	0.53
1:B:380:LEU:HD12	1:B:380:LEU:N	2.23	0.53
1:A:317:TYR:CE1	1:A:318:LEU:HG	2.43	0.53
1:A:99:LYS:O	1:A:99:LYS:HD3	2.08	0.53
1:B:211:GLU:HB2	1:B:224:TRP:CZ3	2.44	0.53
1:B:433:ILE:HD11	1:B:447:LEU:HB3	1.89	0.53
1:A:406:HIS:CE1	1:A:422:ARG:HH11	2.26	0.52
1:B:104:SER:HB2	1:B:286:TRP:HE1	1.74	0.52
1:B:176:ILE:HG22	1:B:178:LEU:CD1	2.40	0.52
1:B:209:GLU:HA	1:B:226:LYS:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASP:H	1:B:203:HIS:HD2	1.57	0.52
1:B:2:LYS:CD	1:B:2:LYS:H	2.11	0.52
1:B:272:GLN:HE21	1:B:347:ASN:HB3	1.72	0.52
1:B:423:MET:HE1	1:B:478:LYS:NZ	2.24	0.52
1:B:94:LEU:HD22	1:B:127:PHE:CE2	2.45	0.52
1:B:133:VAL:HG12	1:B:180:LEU:CD2	2.40	0.52
1:B:330:LEU:CD1	1:B:339:LEU:HD21	2.39	0.52
1:B:311:GLU:CD	1:B:311:GLU:H	2.13	0.52
1:B:420:VAL:HA	1:B:423:MET:HE2	1.91	0.52
1:A:135:ASP:HB3	1:A:181:ARG:HG2	1.91	0.52
1:A:261:LEU:CD2	1:A:282:SER:HA	2.40	0.52
1:B:361:GLU:HG3	1:B:365:LYS:HE3	1.91	0.52
1:B:97:ILE:O	1:B:97:ILE:HG23	2.09	0.52
1:B:30:ILE:O	1:B:33:ARG:N	2.42	0.52
1:A:99:LYS:HZ1	1:A:123:PHE:CB	2.22	0.51
1:A:238:LYS:HE2	1:A:265:HIS:O	2.09	0.51
1:A:97:ILE:CG2	1:A:98:ALA:H	2.17	0.51
1:B:2:LYS:CD	1:B:2:LYS:N	2.73	0.51
1:A:434:THR:O	1:A:435:ALA:HB2	2.11	0.51
1:B:172:ARG:HG2	1:B:173:GLY:N	2.26	0.51
1:B:420:VAL:HG13	1:B:423:MET:CE	2.41	0.51
1:A:331:PRO:O	1:A:333:ASN:N	2.44	0.51
1:B:428:GLU:C	1:B:429:LYS:HG3	2.29	0.51
1:A:235:THR:HG21	1:A:303:ARG:NH2	2.26	0.51
1:A:31:PHE:CG	1:A:32:LEU:N	2.79	0.51
1:B:432:TYR:O	1:B:483:VAL:HG23	2.10	0.51
1:B:7:ARG:HG2	1:B:7:ARG:HH11	1.75	0.51
1:A:169:LYS:NZ	1:A:171:ASP:HB2	2.25	0.50
1:A:434:THR:CG2	1:A:435:ALA:N	2.73	0.50
1:B:248:GLU:OE1	1:B:251:LYS:HE3	2.11	0.50
1:A:106:LEU:O	1:A:106:LEU:HD22	2.11	0.50
1:A:62:GLU:OE1	1:A:62:GLU:CA	2.53	0.50
1:A:404:SER:HB2	1:A:414:VAL:HG21	1.92	0.50
1:A:86:THR:H	1:A:89:GLU:HB2	1.76	0.50
1:B:321:VAL:HG12	1:B:322:ARG:N	2.27	0.50
1:A:135:ASP:OD1	1:A:179:HIS:ND1	2.32	0.50
1:B:342:SER:HB3	1:B:345:THR:OG1	2.12	0.50
1:B:35:LEU:HD12	1:B:78:ILE:HD12	1.92	0.50
1:B:428:GLU:O	1:B:479:PRO:HD2	2.11	0.50
1:A:118:GLN:HG3	1:A:120:ILE:HG13	1.94	0.50
1:A:154:TRP:CH2	1:A:156:SER:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:THR:CG2	1:A:363:LEU:HD13	2.42	0.50
1:A:35:LEU:HD13	1:A:78:ILE:HD12	1.94	0.50
1:B:9:PHE:HB3	1:B:13:VAL:HB	1.93	0.50
1:A:324:LEU:HD12	1:A:325:ILE:N	2.26	0.50
1:B:383:LYS:C	1:B:385:GLY:H	2.14	0.50
1:A:28:LYS:C	1:A:30:ILE:H	2.15	0.49
1:B:298:LYS:O	1:B:324:LEU:HA	2.12	0.49
1:B:464:ILE:O	1:B:464:ILE:HG12	2.10	0.49
1:B:278:LEU:H	1:B:278:LEU:HD12	1.76	0.49
1:B:74:ARG:NH1	1:B:74:ARG:HG2	2.25	0.49
1:B:234:TRP:NE1	1:B:326:ASP:HB2	2.27	0.49
1:A:427:GLN:NE2	1:A:431:TYR:OH	2.45	0.49
1:B:41:ASP:O	1:B:45:LYS:HG2	2.13	0.49
1:A:177:THR:C	1:A:178:LEU:HD12	2.33	0.49
1:A:148:PRO:HB3	1:A:170:GLU:HA	1.95	0.49
1:B:96:THR:CG2	1:B:97:ILE:H	2.17	0.49
1:A:312:GLN:NE2	1:A:340:GLN:OE1	2.46	0.49
1:B:234:TRP:HE1	1:B:326:ASP:HB2	1.78	0.49
1:B:249:PHE:CE2	1:B:253:ILE:HD13	2.48	0.48
1:B:44:ASP:HB3	1:B:305:PHE:CB	2.43	0.48
1:B:152:VAL:CG1	1:B:153:PHE:H	2.23	0.48
1:B:104:SER:HB2	1:B:286:TRP:CZ2	2.47	0.48
1:B:253:ILE:HG22	1:B:298:LYS:HD2	1.95	0.48
1:A:125:VAL:HG12	1:A:129:SER:HB3	1.94	0.48
1:A:393:GLN:HE21	1:A:472:LEU:HA	1.79	0.48
1:A:301:VAL:HG12	1:A:332:LEU:HD23	1.95	0.48
1:B:26:SER:HB2	1:B:118:GLN:HG2	1.94	0.48
1:A:406:HIS:ND1	1:A:422:ARG:NH1	2.62	0.48
1:A:397:ALA:HB2	1:A:472:LEU:HD21	1.94	0.48
1:B:281:PRO:HG2	1:B:378:PHE:CZ	2.48	0.48
1:A:272:GLN:HE21	1:A:347:ASN:HB3	1.77	0.48
1:B:288:MET:O	1:B:288:MET:HG2	2.13	0.48
1:B:44:ASP:HB3	1:B:305:PHE:HB3	1.95	0.48
1:A:226:LYS:HG3	1:A:228:ASN:H	1.78	0.48
1:A:449:LEU:C	1:A:449:LEU:HD23	2.34	0.48
1:B:15:GLN:HB3	1:B:105:PHE:CZ	2.49	0.48
1:B:299:LEU:HD23	1:B:300:TYR:O	2.13	0.48
1:B:203:HIS:N	1:B:203:HIS:CD2	2.71	0.48
1:B:361:GLU:OE1	1:B:361:GLU:HA	2.13	0.47
1:A:251:LYS:HE2	1:A:257:PHE:O	2.14	0.47
1:A:342:SER:HB3	1:A:345:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LYS:HA	1:B:188:LEU:HD13	1.96	0.47
1:B:278:LEU:N	1:B:278:LEU:CD1	2.78	0.47
1:A:6:THR:HG22	1:A:7:ARG:N	2.29	0.47
1:B:319:ARG:HH11	1:B:381:VAL:HG22	1.78	0.47
1:B:206:LEU:O	1:B:228:ASN:ND2	2.48	0.47
1:A:360:LEU:O	1:A:363:LEU:HB3	2.15	0.47
1:B:217:ASP:O	1:B:218:GLY:C	2.53	0.47
1:B:280:ILE:HG13	1:B:359:MET:CE	2.45	0.47
1:A:444:SER:CB	1:A:445:PRO:HD2	2.32	0.47
1:B:367:ASP:OD2	1:B:370:LYS:HG3	2.15	0.47
1:A:317:TYR:CD1	1:A:318:LEU:HG	2.50	0.47
1:A:56:LEU:C	1:A:58:GLU:H	2.18	0.47
1:A:219:GLU:HG2	1:A:220:THR:H	1.79	0.47
1:B:11:SER:O	1:B:15:GLN:HG3	2.15	0.47
1:A:103:LYS:HB3	1:A:105:PHE:CE2	2.50	0.46
1:A:148:PRO:O	1:A:168:THR:HA	2.14	0.46
1:B:232:ALA:O	1:B:235:THR:HB	2.14	0.46
1:B:120:ILE:HD13	1:B:257:PHE:HE2	1.80	0.46
1:B:259:ASP:HB3	1:B:260:PRO:HD2	1.97	0.46
1:A:363:LEU:C	1:A:365:LYS:H	2.17	0.46
1:A:462:ASP:HB2	1:A:465:ASP:OD2	2.15	0.46
1:B:423:MET:CE	1:B:478:LYS:HG3	2.42	0.46
1:A:99:LYS:HZ2	1:A:123:PHE:HB2	1.78	0.46
1:A:439:ALA:O	1:A:441:ALA:N	2.49	0.46
1:B:280:ILE:HA	1:B:281:PRO:HD2	1.81	0.46
1:B:28:LYS:C	1:B:30:ILE:H	2.19	0.46
1:A:65:VAL:CG1	1:A:208:VAL:HG22	2.46	0.46
1:B:280:ILE:O	1:B:281:PRO:O	2.34	0.46
1:A:268:VAL:HG21	1:A:274:TYR:CZ	2.50	0.46
1:A:280:ILE:HD13	1:A:360:LEU:CD2	2.45	0.46
1:A:315:PRO:HD3	1:A:353:THR:OG1	2.15	0.46
1:B:250:TYR:HB2	1:B:279:TYR:CD2	2.51	0.46
1:B:297:LEU:HD11	1:B:314:MET:HG3	1.98	0.46
1:B:46:LEU:N	1:B:83:VAL:HG13	2.31	0.46
1:B:141:THR:HB	1:B:174:THR:HG23	1.97	0.46
1:B:386:PRO:HD3	1:B:396:ILE:HG21	1.97	0.46
1:A:289:TRP:O	1:A:290:ASN:HB2	2.15	0.46
1:A:481:GLN:HG2	1:A:482:SER:N	2.30	0.46
1:B:229:LYS:O	1:B:230:ALA:HB3	2.15	0.46
1:B:29:GLU:CG	1:B:192:ARG:HH22	2.28	0.46
1:A:103:LYS:HD3	1:A:105:PHE:CE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:C	1:B:30:ILE:N	2.70	0.45
1:B:262:THR:HG23	1:B:363:LEU:HD13	1.97	0.45
1:A:427:GLN:HG3	1:A:429:LYS:CG	2.46	0.45
1:B:155:GLU:HG3	1:B:156:SER:N	2.31	0.45
1:B:7:ARG:NH1	1:B:7:ARG:HG2	2.30	0.45
1:A:291:ARG:O	1:A:292:ASP:HB2	2.16	0.45
1:A:389:ASP:OD1	1:A:392:ASN:HB2	2.17	0.45
1:B:133:VAL:HG12	1:B:180:LEU:HD22	1.99	0.45
1:B:133:VAL:CG1	1:B:180:LEU:HD22	2.46	0.45
1:A:229:LYS:HE2	1:A:231:GLN:OE1	2.17	0.45
1:A:329:ASP:HB2	1:A:344:VAL:HG11	1.98	0.45
1:A:402:PHE:CD2	1:A:402:PHE:N	2.84	0.45
1:B:103:LYS:HG2	1:B:103:LYS:O	2.17	0.45
1:B:15:GLN:OE1	1:B:105:PHE:CE2	2.69	0.45
1:A:268:VAL:HG12	1:A:272:GLN:O	2.16	0.45
1:B:278:LEU:H	1:B:278:LEU:CD1	2.30	0.45
1:B:434:THR:HG21	1:B:466:GLU:HB2	1.99	0.45
1:A:331:PRO:C	1:A:333:ASN:N	2.69	0.45
1:A:448:GLU:O	1:A:451:ARG:HB3	2.17	0.45
1:B:49:ARG:HG2	1:B:49:ARG:NH1	2.32	0.45
1:A:28:LYS:C	1:A:30:ILE:N	2.70	0.45
1:A:283:GLN:HA	1:A:377:GLN:HG3	1.98	0.45
1:A:435:ALA:CB	1:A:441:ALA:HB2	2.47	0.45
1:B:256:ASP:OD1	1:B:258:ASN:ND2	2.50	0.45
1:B:321:VAL:O	1:B:322:ARG:HG2	2.17	0.45
1:A:289:TRP:CZ2	1:A:380:LEU:HD23	2.51	0.44
1:A:318:LEU:HD13	1:A:356:VAL:CG1	2.46	0.44
1:A:480:PHE:O	1:A:481:GLN:HB2	2.16	0.44
1:A:424:LYS:C	1:A:426:GLY:H	2.20	0.44
1:A:434:THR:CG2	1:A:435:ALA:H	2.30	0.44
1:B:147:LYS:C	1:B:149:GLU:H	2.21	0.44
1:B:300:TYR:O	1:B:301:VAL:HG23	2.17	0.44
1:A:178:LEU:N	1:A:178:LEU:CD1	2.80	0.44
1:A:237:ASN:ND2	1:A:240:GLU:OE1	2.47	0.44
1:B:194:ARG:NH2	1:B:225:GLU:OE2	2.46	0.44
1:B:279:TYR:N	1:B:322:ARG:O	2.47	0.44
1:B:354:LYS:O	1:B:358:GLN:HG3	2.18	0.44
1:B:85:MET:O	1:B:143:ALA:HB2	2.17	0.44
1:B:447:LEU:HD12	1:B:448:GLU:N	2.32	0.44
1:B:154:TRP:HA	1:B:163:THR:O	2.17	0.44
1:B:312:GLN:OE1	1:B:312:GLN:CA	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:TYR:OH	1:B:442:LYS:HD2	2.18	0.44
1:A:378:PHE:O	1:A:379:GLY:C	2.54	0.44
1:A:427:GLN:HG3	1:A:429:LYS:HG3	1.98	0.44
1:B:194:ARG:NH2	1:B:225:GLU:CD	2.71	0.44
1:A:406:HIS:CE1	1:A:422:ARG:NH1	2.86	0.43
1:B:414:VAL:HG13	1:B:418:ASP:HB2	2.00	0.43
1:A:262:THR:HG21	1:A:363:LEU:HD13	2.01	0.43
1:A:345:THR:O	1:A:348:LEU:N	2.47	0.43
1:A:261:LEU:HD13	1:A:374:PHE:HB2	1.99	0.43
1:B:1:MET:HG2	1:B:1:MET:O	2.17	0.43
1:B:207:PRO:HA	1:B:228:ASN:HD22	1.84	0.43
1:B:330:LEU:HD13	1:B:339:LEU:HD21	2.00	0.43
1:B:389:ASP:O	1:B:389:ASP:OD1	2.35	0.43
1:A:278:LEU:N	1:A:278:LEU:HD12	2.34	0.43
1:A:414:VAL:HG13	1:A:422:ARG:NH2	2.33	0.43
1:B:231:GLN:O	1:B:232:ALA:C	2.56	0.43
1:B:243:ASP:O	1:B:247:LYS:HG3	2.18	0.43
1:B:404:SER:OG	1:B:405:THR:N	2.52	0.43
1:A:7:ARG:HD3	1:A:162:TYR:OH	2.18	0.43
1:A:35:LEU:HD12	1:A:78:ILE:HD12	1.99	0.43
1:B:197:ILE:HD12	1:B:210:ILE:HD12	2.00	0.43
1:B:360:LEU:HB3	1:B:399:LEU:HD22	2.00	0.43
1:B:202:ASP:H	1:B:203:HIS:CD2	2.37	0.43
1:B:473:THR:O	1:B:474:GLU:HB2	2.18	0.43
1:B:5:GLU:CD	1:B:7:ARG:HE	2.22	0.43
1:A:68:SER:HB3	1:A:211:GLU:HB2	2.01	0.43
1:B:463:ARG:O	1:B:463:ARG:NE	2.43	0.43
1:A:6:THR:CG2	1:A:7:ARG:N	2.82	0.43
1:B:57:TYR:HA	1:B:172:ARG:HH12	1.84	0.43
1:B:396:ILE:O	1:B:396:ILE:HG22	2.19	0.43
1:B:65:VAL:CG1	1:B:208:VAL:HG22	2.49	0.43
1:B:203:HIS:HB3	1:B:249:PHE:HB2	2.00	0.42
1:A:164:VAL:CG1	1:A:165:ALA:N	2.82	0.42
1:A:232:ALA:HB1	1:A:234:TRP:CZ3	2.54	0.42
1:B:139:VAL:HG22	1:B:176:ILE:HG12	1.99	0.42
1:B:31:PHE:CG	1:B:32:LEU:N	2.87	0.42
1:A:217:ASP:C	1:A:219:GLU:H	2.23	0.42
1:A:422:ARG:HG2	1:A:456:GLU:OE2	2.19	0.42
1:A:143:ALA:O	1:A:146:GLU:HB2	2.19	0.42
1:A:423:MET:SD	1:A:478:LYS:HG3	2.60	0.42
1:B:316:ASN:C	1:B:318:LEU:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LEU:O	1:B:450:LEU:HB2	2.20	0.42
1:A:371:TYR:OH	1:A:399:LEU:HB3	2.20	0.42
1:A:419:TYR:O	1:A:423:MET:HB2	2.19	0.42
1:A:397:ALA:CB	1:A:472:LEU:HD21	2.49	0.42
1:B:400:LEU:O	1:B:401:ARG:HD3	2.20	0.42
1:A:74:ARG:HH12	1:A:185:ASP:CG	2.22	0.41
1:A:28:LYS:O	1:A:30:ILE:N	2.53	0.41
1:B:1:MET:HG3	1:B:167:ILE:HG22	2.01	0.41
1:A:51:LEU:O	1:A:54:PRO:HD3	2.20	0.41
1:B:195:SER:O	1:B:198:SER:HB3	2.19	0.41
1:A:383:LYS:C	1:A:385:GLY:N	2.73	0.41
1:A:81:ASN:HA	1:A:172:ARG:O	2.20	0.41
1:B:66:ARG:NE	1:B:209:GLU:OE1	2.50	0.41
1:B:57:TYR:O	1:B:59:GLY:N	2.54	0.41
1:A:393:GLN:NE2	1:A:472:LEU:HA	2.35	0.41
1:B:94:LEU:HD22	1:B:127:PHE:CZ	2.55	0.41
1:B:153:PHE:O	1:B:164:VAL:HA	2.20	0.41
1:B:423:MET:O	1:B:424:LYS:HG2	2.20	0.41
1:B:401:ARG:HA	1:B:401:ARG:HD3	1.88	0.41
1:B:63:LEU:HD22	1:B:81:ASN:O	2.20	0.41
1:A:337:GLU:O	1:A:338:ILE:C	2.58	0.41
1:B:94:LEU:O	1:B:128:TYR:OH	2.37	0.41
1:A:447:LEU:HD23	1:A:447:LEU:O	2.21	0.41
1:B:19:LEU:HD22	1:B:105:PHE:CE1	2.55	0.41
1:B:164:VAL:HG12	1:B:165:ALA:N	2.35	0.41
1:B:415:SER:O	1:B:418:ASP:HB2	2.21	0.41
1:B:444:SER:N	1:B:445:PRO:HD3	2.36	0.41
1:A:131:PHE:CE2	1:A:137:VAL:HG23	2.56	0.41
1:A:197:ILE:O	1:A:200:TYR:N	2.54	0.41
1:A:317:TYR:O	1:A:318:LEU:HD23	2.21	0.41
1:A:333:ASN:O	1:A:334:VAL:C	2.59	0.41
1:B:134:ALA:HB2	1:B:178:LEU:HB3	2.03	0.41
1:B:230:ALA:O	1:B:231:GLN:HG3	2.21	0.41
1:B:288:MET:CG	1:B:288:MET:O	2.69	0.41
1:B:355:ARG:HG2	1:B:355:ARG:HH11	1.86	0.41
1:B:423:MET:HE1	1:B:478:LYS:HZ2	1.86	0.41
1:A:169:LYS:HZ3	1:A:171:ASP:HB2	1.86	0.41
1:B:101:GLY:HA2	1:B:286:TRP:CZ3	2.55	0.41
1:A:1:MET:HE2	1:A:4:GLN:HE22	1.84	0.40
1:B:208:VAL:HB	1:B:228:ASN:HB2	2.02	0.40
1:B:313:PHE:CE2	1:B:348:LEU:HD23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:NH2	1:B:456:GLU:OE1	2.55	0.40
1:B:60:ASP:O	1:B:60:ASP:OD2	2.39	0.40
1:A:285:PRO:HG2	1:A:288:MET:HB2	2.03	0.40
1:A:409:SER:HB3	1:A:411:ALA:H	1.85	0.40
1:A:74:ARG:NH1	1:A:185:ASP:OD1	2.54	0.40
1:B:202:ASP:HB2	1:B:245:GLU:OE1	2.21	0.40
1:B:321:VAL:HG12	1:B:322:ARG:H	1.85	0.40
1:A:428:GLU:H	1:A:428:GLU:HG2	1.60	0.40
1:B:197:ILE:CD1	1:B:210:ILE:HD12	2.51	0.40
1:B:208:VAL:H	1:B:228:ASN:CB	2.35	0.40
1:B:29:GLU:H	1:B:29:GLU:CD	2.23	0.40
1:B:299:LEU:HD13	1:B:307:MET:HG2	2.03	0.40
1:B:354:LYS:HB3	1:B:354:LYS:HE2	1.92	0.40
1:B:383:LYS:C	1:B:385:GLY:N	2.75	0.40
1:B:420:VAL:CG2	1:B:423:MET:HE2	2.44	0.40
1:A:428:GLU:CG	1:A:428:GLU:O	2.67	0.40
1:B:190:ASP:O	1:B:194:ARG:CB	2.65	0.40
1:A:334:VAL:HA	1:A:338:ILE:HD12	2.04	0.40
1:B:384:GLU:HA	1:B:464:ILE:HD11	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ILE:CD1	1:B:338:ILE:CD1[2_655]	2.15	0.05

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	471/559 (84%)	368 (78%)	78 (17%)	25 (5%)	2 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	471/559 (84%)	366 (78%)	79 (17%)	26 (6%)	2	7
All	All	942/1118 (84%)	734 (78%)	157 (17%)	51 (5%)	2	7

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	125	VAL
1	A	288	MET
1	A	290	ASN
1	A	292	ASP
1	A	435	ALA
1	A	439	ALA
1	A	445	PRO
1	A	475	PHE
1	A	476	ASP
1	B	58	GLU
1	B	97	ILE
1	B	123	PHE
1	B	281	PRO
1	B	291	ARG
1	B	445	PRO
1	B	463	ARG
1	B	474	GLU
1	A	332	LEU
1	A	425	GLU
1	A	430	ILE
1	A	446	HIS
1	A	463	ARG
1	B	17	LEU
1	B	126	GLY
1	B	218	GLY
1	B	282	SER
1	B	292	ASP
1	B	317	TYR
1	B	320	PHE
1	A	51	LEU
1	A	291	ARG
1	A	441	ALA
1	B	101	GLY
1	B	160	GLY
1	B	427	GLN

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Mol	Chain	Res	Type
1	B	444	SER
1	A	217	ASP
1	A	252	HIS
1	A	364	ALA
1	A	440	ALA
1	B	99	LYS
1	B	146	GLU
1	B	219	GLU
1	B	421	SER
1	A	289	TRP
1	A	380	LEU
1	B	54	PRO
1	A	338	ILE
1	B	148	PRO
1	B	270	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	419/488 (86%)	395 (94%)	24 (6%)	24	56
1	B	419/488 (86%)	394 (94%)	25 (6%)	22	54
All	All	838/976 (86%)	789 (94%)	49 (6%)	23	56

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	30	ILE
1	A	32	LEU
1	A	52	SER
1	A	55	ASP
1	A	62	GLU
1	A	64	ARG
1	A	141	THR

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Mol	Chain	Res	Type
1	A	168	THR
1	A	171	ASP
1	A	215	GLU
1	A	228	ASN
1	A	256	ASP
1	A	282	SER
1	A	291	ARG
1	A	317	TYR
1	A	325	ILE
1	A	353	THR
1	A	394	GLU
1	A	400	LEU
1	A	402	PHE
1	A	429	LYS
1	A	445	PRO
1	A	468	MET
1	B	2	LYS
1	B	7	ARG
1	B	86	THR
1	B	161	GLU
1	B	163	THR
1	B	168	THR
1	B	171	ASP
1	B	174	THR
1	B	202	ASP
1	B	203	HIS
1	B	223	SER
1	B	240	GLU
1	B	260	PRO
1	B	269	GLU
1	B	278	LEU
1	B	291	ARG
1	B	292	ASP
1	B	299	LEU
1	B	308	ASP
1	B	319	ARG
1	B	341	ASP
1	B	408	ASP
1	B	447	LEU
1	B	472	LEU
1	B	482	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	228	ASN
1	A	266	ASN
1	A	272	GLN
1	A	290	ASN
1	A	393	GLN
1	A	427	GLN
1	A	481	GLN
1	B	4	GLN
1	B	15	GLN
1	B	203	HIS
1	B	228	ASN
1	B	266	ASN
1	B	272	GLN
1	B	350	ASN
1	B	358	GLN
1	B	427	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	A	701	2	25,29,29	0.66	0	24,45,45	0.65	0
3	ADP	B	702	2	25,29,29	0.74	0	24,45,45	0.60	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
3	ADP	A	701	2	-	0/12/32/32	0/3/3/3
3	ADP	B	702	2	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	475/559 (84%)	0.58	42 (8%) 11 7	9, 58, 100, 100	0
1	B	475/559 (84%)	0.53	34 (7%) 16 11	33, 70, 98, 100	0
All	All	950/1118 (84%)	0.55	76 (8%) 13 10	9, 65, 100, 100	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	SER	13.2
1	A	108	SER	8.1
1	A	107	GLU	7.6
1	B	105	PHE	7.3
1	A	118	GLN	6.6
1	B	100	SER	6.6
1	B	99	LYS	6.1
1	A	117	SER	5.7
1	A	99	LYS	5.5
1	A	119	LEU	5.3
1	A	475	PHE	5.1
1	A	106	LEU	5.1
1	A	480	PHE	4.9
1	B	108	SER	4.8
1	B	118	GLN	4.8
1	A	98	ALA	4.7
1	A	440	ALA	4.7
1	B	119	LEU	4.7
1	B	98	ALA	4.7
1	A	104	SER	4.6
1	B	220	THR	4.0
1	B	219	GLU	4.0
1	B	454	GLY	3.9
1	A	105	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	424	LYS	3.9
1	A	459	LEU	3.9
1	B	476	ASP	3.7
1	A	432	TYR	3.7
1	A	472	LEU	3.6
1	B	104	SER	3.5
1	A	447	LEU	3.5
1	B	455	ILE	3.4
1	A	428	GLU	3.4
1	A	441	ALA	3.3
1	A	455	ILE	3.3
1	A	444	SER	3.2
1	A	481	GLN	3.2
1	A	400	LEU	3.2
1	A	433	ILE	3.2
1	A	476	ASP	3.2
1	A	100	SER	3.2
1	A	473	THR	3.1
1	A	286	TRP	3.0
1	B	478	LYS	2.9
1	B	106	LEU	2.8
1	B	441	ALA	2.8
1	A	465	ASP	2.8
1	A	466	GLU	2.7
1	B	428	GLU	2.6
1	B	386	PRO	2.6
1	A	436	ASP	2.5
1	B	465	ASP	2.5
1	B	414	VAL	2.5
1	A	123	PHE	2.4
1	B	477	GLY	2.4
1	B	1	MET	2.4
1	B	445	PRO	2.3
1	A	446	HIS	2.3
1	A	120	ILE	2.3
1	A	460	LEU	2.3
1	B	394	GLU	2.3
1	A	60	ASP	2.3
1	A	443	SER	2.2
1	B	103	LYS	2.2
1	B	366	ASP	2.2
1	A	386	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	447	LEU	2.2
1	B	58	GLU	2.2
1	A	435	ALA	2.2
1	B	451	ARG	2.2
1	B	443	SER	2.1
1	B	422	ARG	2.1
1	B	444	SER	2.1
1	A	431	TYR	2.0
1	B	286	TRP	2.0
1	A	474	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	MG	B	704	1/1	0.94	0.31	7.78	28,28,28,28	0
2	MG	A	703	1/1	0.99	0.32	4.13	26,26,26,26	0
3	ADP	A	701	27/27	0.96	0.19	-0.48	22,26,28,29	0
3	ADP	B	702	27/27	0.96	0.16	-1.43	27,35,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.