



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:06 pm GMT

PDB ID : 2HYD
Title : Multidrug ABC transporter SAV1866
Authors : Dawson, R.J.P.; Locher, K.P.
Deposited on : 2006-08-05
Resolution : 3.00 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

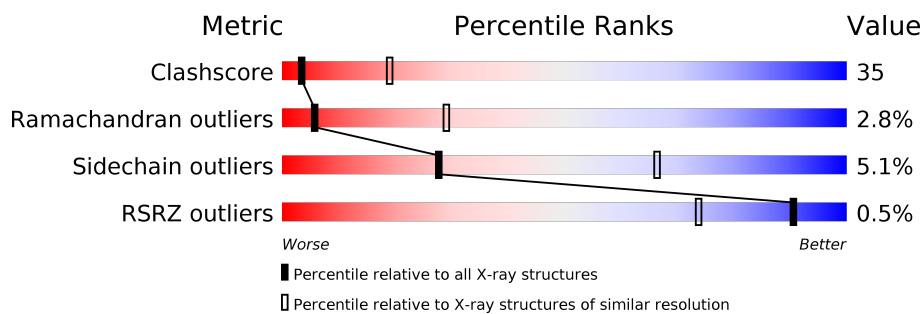
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	578	
1	B	578	

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	NA	B	910	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9240 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.

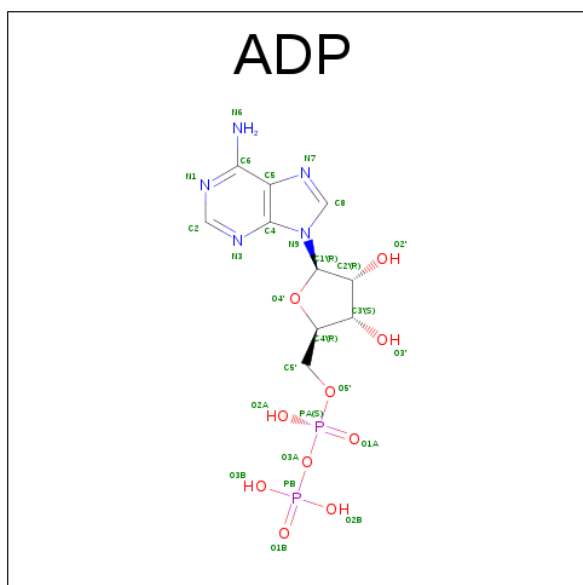
- Molecule 1 is a protein called ABC transporter homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	1	0	0
			4584	2967	774	834	9			
1	B	578	Total	C	N	O	S	1	0	0
			4584	2967	774	834	9			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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



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

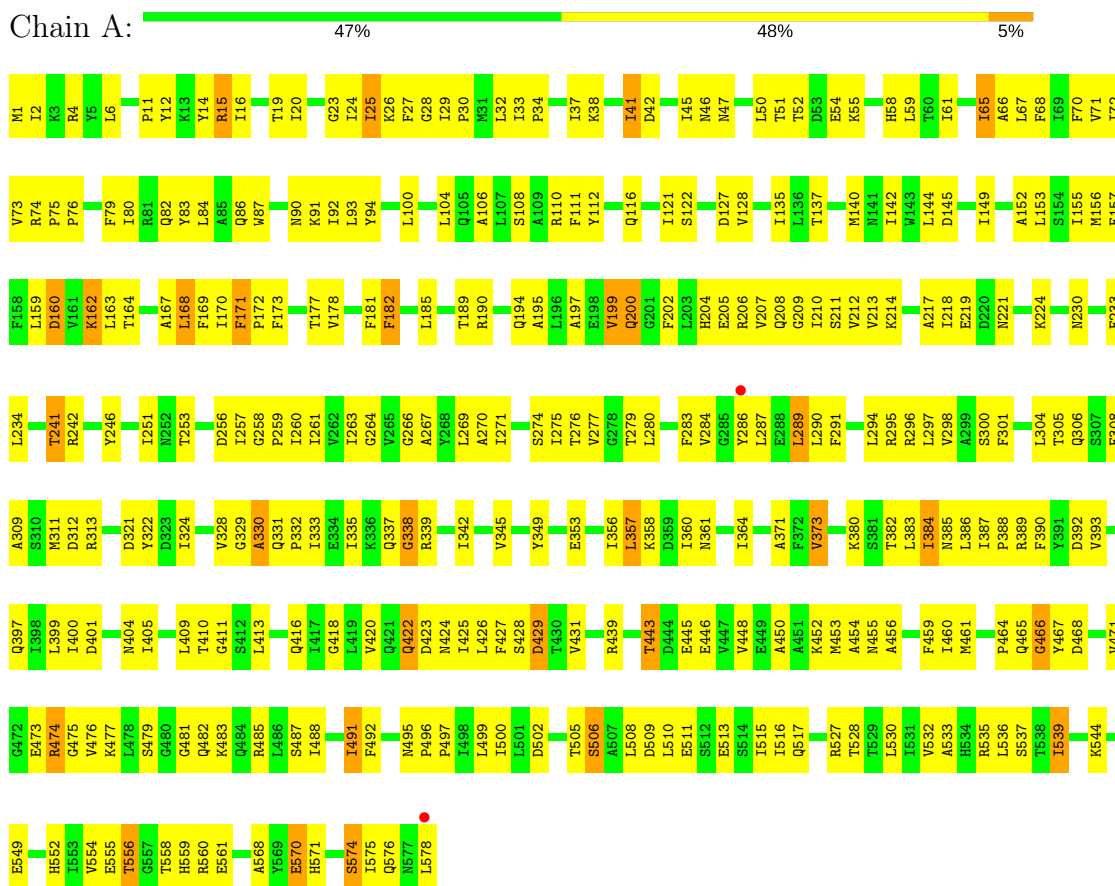
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	8	Total	O	0	0
			8	8		

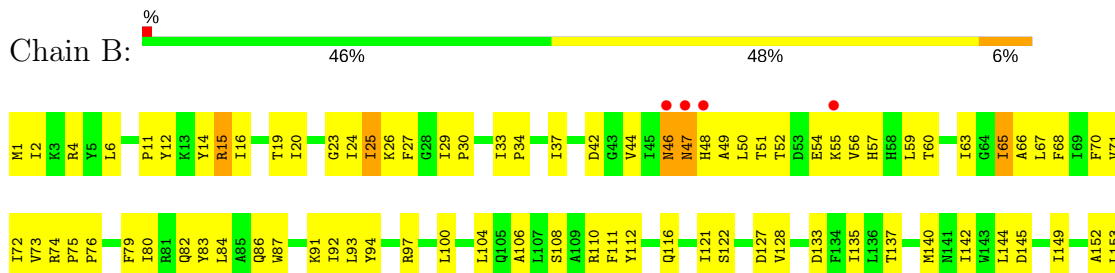
3 Residue-property plots

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: ABC transporter homolog



• Molecule 1: ABC transporter homolog



S154	L155	M156	F233	L234	F305	T241	R242	Y246	I251	N252	T253	D256	I257	G258	P259	I260	I261	V262	I263	G264	V265	G266	A267	Y268	L269	A270	I271	G272	S273	S274	I275	L276	V277	G278	V279	L280	F283	V284	G285	Y286	L287	E288	L289	G290	F291	L294	R295	R296	L297	V298	A299	I298	E299	F301	I302	N221	K224
T305	Q306	S307	F308	A309	S310	R311	D312	R313	D321	Y322	G323	I324	V328	G329	A330	Q331	P332	I333	E334	I335	K336	Q337	G338	R339	I342	V345	Y349	E353	I356	L357	K358	D359	I360	N361	I364	A371	F372	V373	K380	S381	T382	L383	I384	N385	L386	I387	P388	R389	F390								
Y391	D392	V393	Q397	I398	L399	I400	D401	N404	I405	L409	T410	G411	S412	L413	R414	R415	Q416	I417	G418	L419	V420	G421	Q422	D423	N424	I425	L426	F427	S428	D429	T430	V431	R439	T443	D444	E445	E446	V447	V448	E449	A450	A451	K452	M453	A454	M455	A456	F459	I460	M461	P464	Q465					
G466	Y467	D468	V471	G472	E473	R474	G475	V476	T477	L478	S479	G480	G481	Q482	K483	Q484	R485	T488	I489	F492	M495	P496	P497	L498	L499	I500	L501	D502	T505	S506	A507	L508	D509	L510	E511	S512	E513	S514	I515	I516	D517	R527	T528	T529	L530	I531	V532	A533	H534	R535	L536	S537	T538				
I539	K544	E549	H552	I553	V554	E555	T556	G557	S558	H559	R560	E561	A568	Y569	E570	H571	S574	I575	Q576	R577	L578																																				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.28Å 103.95Å 181.01Å 90.00° 97.99° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00 29.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 99.2 (29.88-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.272 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 74.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9240	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: NA, 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	0.41	0/4669	0.66	1/6328 (0.0%)
1	B	0.52	3/4669 (0.1%)	0.68	3/6328 (0.0%)
All	All	0.47	3/9338 (0.0%)	0.67	4/12656 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	ASN	CB-CG	15.97	1.87	1.51
1	B	46	ASN	C-N	-9.51	1.12	1.34
1	B	48	HIS	CA-CB	8.89	1.73	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ALA	CB-CA-C	5.39	118.18	110.10
1	A	357	LEU	N-CA-C	-5.15	97.09	111.00
1	B	46	ASN	O-C-N	5.12	130.89	122.70
1	B	357	LEU	N-CA-C	-5.01	97.47	111.00

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	4584	0	4713	346	0
1	B	4584	0	4712	373	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	7	0
3	B	27	0	12	5	0
4	A	8	0	0	3	0
4	B	8	0	0	2	0
All	All	9240	0	9449	658	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 35.

All (658) 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:47:ASN:CG	1:B:47:ASN:CB	1.87	1.42
1:A:15:ARG:H	1:A:15:ARG:HD2	1.01	1.15
1:B:15:ARG:H	1:B:15:ARG:HD2	1.01	1.09
1:A:52:THR:HA	1:A:55:LYS:HE2	1.10	1.09
1:B:44:VAL:HG13	1:B:55:LYS:HB2	1.36	1.08
1:B:276:THR:HG22	1:B:278:GLY:H	1.22	1.03
1:B:464:PRO:HB2	1:B:465:GLN:NE2	1.80	0.97
1:A:263:ILE:HG22	1:B:63:ILE:HD11	1.45	0.97
1:A:455:ASN:HD22	1:A:515:ILE:HG21	1.28	0.96
1:A:464:PRO:HB2	1:A:465:GLN:NE2	1.80	0.95
1:B:455:ASN:HD22	1:B:515:ILE:HG21	1.30	0.94
1:A:15:ARG:N	1:A:15:ARG:HD2	1.83	0.93
1:A:558:THR:HB	1:A:561:GLU:HG3	1.51	0.92
1:A:276:THR:HG22	1:A:277:VAL:H	1.33	0.92
1:B:156:MET:HB3	1:B:164:THR:HG22	1.53	0.91
1:B:505:THR:HG21	1:B:513:GLU:OE2	1.71	0.90
1:B:15:ARG:N	1:B:15:ARG:HD2	1.83	0.90
1:A:505:THR:HG21	1:A:513:GLU:OE2	1.71	0.90
1:B:558:THR:HB	1:B:561:GLU:HG3	1.51	0.90
1:B:51:THR:HB	1:B:54:GLU:HG2	1.54	0.89
1:A:52:THR:HA	1:A:55:LYS:CE	2.01	0.89
1:A:234:LEU:CD2	1:B:94:TYR:HB2	2.04	0.87
1:B:75:PRO:HB2	1:B:76:PRO:HD3	1.57	0.87
1:A:52:THR:CA	1:A:55:LYS:HE2	2.00	0.86
1:A:75:PRO:HB2	1:A:76:PRO:HD3	1.57	0.86
1:A:121:ILE:HD13	1:B:204:HIS:CD2	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:VAL:HG11	1:B:287:LEU:HD21	1.59	0.85
1:A:142:ILE:HD11	1:A:304:LEU:HD11	1.59	0.84
1:A:473:GLU:O	1:A:476:VAL:HG23	1.78	0.84
1:B:142:ILE:HD11	1:B:304:LEU:HD11	1.59	0.83
1:B:51:THR:CB	1:B:54:GLU:HG2	2.10	0.81
1:B:473:GLU:O	1:B:476:VAL:HG23	1.81	0.81
1:A:162:LYS:H	1:A:162:LYS:HD3	1.45	0.81
1:A:485:ARG:HG2	1:A:516:ILE:HD11	1.63	0.80
1:B:485:ARG:HG2	1:B:516:ILE:HD11	1.63	0.79
1:B:397:GLN:HE21	1:B:399:LEU:HD11	1.48	0.79
1:A:94:TYR:HB2	1:B:234:LEU:HD13	1.65	0.79
1:A:260:ILE:HG21	1:B:67:LEU:HD21	1.63	0.78
1:B:276:THR:HG22	1:B:278:GLY:N	1.97	0.78
1:B:106:ALA:HB3	1:B:322:TYR:HE2	1.50	0.77
1:B:380:LYS:HE3	3:B:701:ADP:O2B	1.85	0.76
1:A:397:GLN:HE21	1:A:399:LEU:HD11	1.47	0.76
1:A:106:ALA:HB3	1:A:322:TYR:HE2	1.51	0.76
1:A:275:ILE:HG22	1:A:276:THR:H	1.49	0.75
1:A:67:LEU:HD21	1:B:260:ILE:HG21	1.66	0.75
1:B:387:ILE:HB	1:B:388:PRO:HD3	1.69	0.75
1:A:2:ILE:HD11	1:A:308:PHE:HE2	1.52	0.75
1:B:2:ILE:HD11	1:B:308:PHE:HE2	1.52	0.75
1:B:162:LYS:H	1:B:162:LYS:HD3	1.51	0.74
1:A:25:ILE:O	1:A:25:ILE:HG22	1.88	0.73
1:A:387:ILE:HB	1:A:388:PRO:HD3	1.69	0.73
1:B:155:ILE:HG21	1:B:286:TYR:CE2	2.24	0.73
1:B:25:ILE:HG22	1:B:25:ILE:O	1.87	0.72
1:A:45:ILE:HG21	1:B:277:VAL:HG11	1.72	0.72
1:A:455:ASN:ND2	1:A:515:ILE:HG21	2.03	0.72
1:B:12:TYR:OH	1:B:91:LYS:HG2	1.89	0.71
1:A:276:THR:HG22	1:A:277:VAL:N	2.05	0.71
1:B:455:ASN:ND2	1:B:515:ILE:HG21	2.05	0.71
1:A:443:THR:HG22	1:A:445:GLU:OE1	1.90	0.71
1:B:443:THR:HG22	1:B:445:GLU:OE1	1.90	0.71
1:A:12:TYR:OH	1:A:91:LYS:HG2	1.91	0.71
1:B:106:ALA:CB	1:B:322:TYR:HE2	2.03	0.71
1:B:364:ILE:HD13	1:B:530:LEU:HD21	1.73	0.71
1:A:330:ALA:O	1:A:331:GLN:HG2	1.91	0.70
1:B:258:GLY:HA3	1:B:291:PHE:CE2	2.27	0.70
1:B:358:LYS:HD2	1:B:552:HIS:NE2	2.06	0.70
1:A:358:LYS:HD2	1:A:552:HIS:NE2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ALA:CB	1:A:322:TYR:HE2	2.03	0.69
1:A:15:ARG:CD	1:A:15:ARG:H	1.92	0.69
1:B:380:LYS:HB2	3:B:701:ADP:O2B	1.91	0.69
1:A:364:ILE:HD13	1:A:530:LEU:HD21	1.74	0.69
1:A:260:ILE:HG21	1:B:67:LEU:CD2	2.23	0.69
1:A:258:GLY:HA3	1:A:291:PHE:CE2	2.27	0.69
1:A:555:GLU:OE1	1:A:568:ALA:HB3	1.92	0.69
1:B:15:ARG:H	1:B:15:ARG:CD	1.92	0.69
1:A:185:LEU:HB2	1:A:305:THR:HG21	1.75	0.68
1:B:185:LEU:HB2	1:B:305:THR:HG21	1.74	0.68
1:A:160:ASP:O	1:A:164:THR:HG23	1.94	0.68
1:B:330:ALA:O	1:B:331:GLN:HG2	1.93	0.67
1:A:337:GLN:O	1:A:401:ASP:OD2	2.12	0.67
1:B:549:GLU:HB2	1:B:554:VAL:HG21	1.76	0.67
1:A:549:GLU:HB2	1:A:554:VAL:HG21	1.77	0.67
1:B:337:GLN:O	1:B:401:ASP:OD2	2.12	0.67
1:B:555:GLU:OE1	1:B:568:ALA:HB3	1.94	0.66
1:B:410:THR:HG22	1:B:411:GLY:N	2.10	0.66
1:B:42:ASP:HA	1:B:46:ASN:HB2	1.77	0.66
1:A:37:ILE:CG1	1:B:263:ILE:HD11	2.25	0.66
1:B:495:ASN:CG	1:B:527:ARG:HH22	1.99	0.66
1:B:331:GLN:O	1:B:333:ILE:HG13	1.95	0.66
1:B:47:ASN:HD22	1:B:50:LEU:HD21	1.61	0.66
1:A:464:PRO:HB2	1:A:465:GLN:HE22	1.60	0.66
1:A:204:HIS:HD2	1:B:204:HIS:ND1	1.93	0.66
1:B:431:VAL:HG11	1:B:460:ILE:HD13	1.77	0.66
1:A:331:GLN:O	1:A:333:ILE:HG13	1.96	0.66
1:A:410:THR:HG22	1:A:411:GLY:N	2.10	0.66
1:A:387:ILE:C	1:A:389:ARG:H	1.99	0.66
1:B:162:LYS:HE2	1:B:275:ILE:HD11	1.76	0.66
1:A:431:VAL:HG11	1:A:460:ILE:HD13	1.79	0.65
1:A:304:LEU:O	1:A:308:PHE:HD1	1.79	0.65
1:B:464:PRO:HB2	1:B:465:GLN:HE22	1.59	0.65
1:B:428:SER:HB2	1:B:473:GLU:HA	1.79	0.65
1:A:256:ASP:HB3	1:B:70:PHE:HD2	1.60	0.65
1:B:47:ASN:ND2	1:B:50:LEU:HD21	2.12	0.65
1:A:156:MET:HB3	1:A:164:THR:HG22	1.78	0.65
1:A:495:ASN:CG	1:A:527:ARG:HH22	1.98	0.65
1:A:275:ILE:HG22	1:A:276:THR:N	2.12	0.65
1:A:384:ILE:HD12	1:A:532:VAL:CG2	2.27	0.65
1:B:209:GLY:O	1:B:212:VAL:HG12	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LEU:O	1:B:308:PHE:HD1	1.79	0.64
1:B:266:GLY:HA3	1:B:280:LEU:HD11	1.78	0.64
1:A:70:PHE:HD2	1:B:256:ASP:HB3	1.61	0.64
1:B:384:ILE:HD12	1:B:532:VAL:CG2	2.27	0.64
1:A:170:ILE:HG13	1:A:258:GLY:HA2	1.80	0.64
1:A:380:LYS:HE3	3:A:700:ADP:O2B	1.96	0.64
1:A:418:GLY:HA3	1:A:496:PRO:HG3	1.79	0.64
1:A:353:GLU:HG2	1:B:464:PRO:HG3	1.80	0.64
1:A:234:LEU:HD21	1:B:94:TYR:HB2	1.80	0.64
1:B:418:GLY:HA3	1:B:496:PRO:HG3	1.80	0.64
1:A:47:ASN:HD22	1:A:50:LEU:HG	1.63	0.63
1:B:456:ALA:O	1:B:460:ILE:HG13	1.98	0.63
1:A:574:SER:O	1:A:578:LEU:HB2	1.98	0.63
1:A:234:LEU:HD22	1:B:94:TYR:HB2	1.80	0.63
1:B:387:ILE:C	1:B:389:ARG:H	2.00	0.63
1:B:495:ASN:ND2	1:B:527:ARG:HH22	1.97	0.63
1:B:160:ASP:OD2	1:B:163:LEU:HB2	1.99	0.63
1:B:210:ILE:HG22	1:B:214:LYS:HG2	1.80	0.63
1:A:67:LEU:CD2	1:B:260:ILE:HG21	2.28	0.62
1:B:170:ILE:HG13	1:B:258:GLY:HA2	1.80	0.62
1:A:271:ILE:HD13	1:B:56:VAL:HG22	1.79	0.62
1:A:309:ALA:O	1:A:312:ASP:HB2	2.00	0.62
1:A:479:SER:CB	3:B:701:ADP:O2A	2.47	0.62
1:A:122:SER:HB2	1:A:200:GLN:HG3	1.81	0.62
1:A:456:ALA:O	1:A:460:ILE:HG13	2.00	0.62
1:A:142:ILE:CD1	1:A:304:LEU:HD11	2.29	0.62
1:A:73:VAL:O	1:A:76:PRO:HD2	2.00	0.62
1:B:122:SER:HB2	1:B:200:GLN:HG3	1.81	0.62
1:A:464:PRO:HG3	1:B:353:GLU:HG2	1.82	0.62
1:B:19:THR:HG21	1:B:140:MET:HE3	1.81	0.62
1:B:116:GLN:HG2	4:B:803:HOH:O	1.99	0.62
1:A:209:GLY:O	1:A:212:VAL:HG12	2.00	0.62
1:A:389:ARG:HD2	1:A:405:ILE:HG22	1.82	0.62
1:A:448:VAL:O	1:A:452:LYS:HG3	2.00	0.62
1:A:47:ASN:HD22	1:A:50:LEU:CG	2.13	0.62
1:B:475:GLY:O	1:B:483:LYS:HE2	2.00	0.62
1:A:121:ILE:CD1	1:B:204:HIS:CD2	2.81	0.61
1:A:116:GLN:HA	1:B:473:GLU:OE1	2.00	0.61
1:A:495:ASN:ND2	1:A:527:ARG:HH22	1.99	0.61
1:A:202:PHE:CE2	1:A:206:ARG:HG3	2.35	0.61
1:B:142:ILE:CD1	1:B:304:LEU:HD11	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ILE:HD13	1:B:400:ILE:HG21	1.83	0.61
1:A:210:ILE:HG22	1:A:214:LYS:HG2	1.81	0.61
1:A:428:SER:HB2	1:A:473:GLU:HA	1.81	0.61
1:A:159:LEU:HD23	1:A:283:PHE:HD1	1.64	0.61
1:B:156:MET:HE3	1:B:283:PHE:CZ	2.35	0.61
3:A:700:ADP:O2A	1:B:479:SER:CB	2.49	0.61
1:A:137:THR:O	1:A:142:ILE:HG13	2.01	0.61
1:B:137:THR:O	1:B:142:ILE:HG13	2.00	0.60
1:A:269:LEU:HB3	1:A:274:SER:CB	2.31	0.60
1:A:475:GLY:O	1:A:483:LYS:HE2	2.01	0.60
1:A:37:ILE:HG12	1:B:263:ILE:HD11	1.82	0.60
1:A:19:THR:HG21	1:A:140:MET:HE3	1.81	0.60
1:A:275:ILE:HG21	1:A:279:THR:OG1	2.01	0.60
1:A:335:ILE:HD13	1:A:400:ILE:HG21	1.82	0.60
1:B:202:PHE:CE2	1:B:206:ARG:HG3	2.36	0.60
1:B:448:VAL:O	1:B:452:LYS:HG3	2.02	0.60
1:B:506:SER:O	1:B:535:ARG:NH2	2.34	0.60
1:B:389:ARG:HD2	1:B:405:ILE:HG22	1.82	0.60
1:B:309:ALA:O	1:B:312:ASP:HB2	2.01	0.60
1:A:324:ILE:HD13	1:A:389:ARG:O	2.02	0.60
1:A:380:LYS:HB2	3:A:700:ADP:O2B	2.01	0.59
1:A:506:SER:O	1:A:535:ARG:NH2	2.34	0.59
1:B:276:THR:HB	1:B:279:THR:OG1	2.02	0.59
1:B:73:VAL:O	1:B:76:PRO:HD2	2.02	0.59
1:A:178:VAL:HG13	1:A:301:PHE:CE1	2.37	0.59
1:A:41:ILE:HG22	1:A:42:ASP:N	2.17	0.59
1:B:324:ILE:HD13	1:B:389:ARG:O	2.02	0.59
1:A:479:SER:HB2	3:B:701:ADP:O2A	2.03	0.59
1:A:80:ILE:O	1:A:84:LEU:HB2	2.02	0.59
1:B:121:ILE:HD12	1:B:204:HIS:CE1	2.37	0.59
1:A:205:GLU:OE1	1:B:428:SER:N	2.34	0.59
1:A:167:ALA:O	1:A:169:PHE:N	2.36	0.58
1:B:80:ILE:O	1:B:84:LEU:HB2	2.03	0.58
1:A:106:ALA:CB	1:A:322:TYR:CE2	2.86	0.58
1:B:197:ALA:O	1:B:200:GLN:HB2	2.03	0.58
1:B:275:ILE:HG22	1:B:276:THR:N	2.18	0.58
1:B:106:ALA:CB	1:B:322:TYR:CE2	2.86	0.58
1:B:47:ASN:CG	1:B:47:ASN:CA	2.69	0.58
1:A:197:ALA:O	1:A:200:GLN:HB2	2.04	0.58
1:B:178:VAL:HG13	1:B:301:PHE:CE1	2.38	0.58
1:B:24:ILE:C	1:B:26:LYS:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASN:O	1:A:224:LYS:HB2	2.04	0.57
1:B:2:ILE:HD11	1:B:308:PHE:CE2	2.37	0.57
1:A:24:ILE:C	1:A:26:LYS:H	2.07	0.57
1:A:2:ILE:HD11	1:A:308:PHE:CE2	2.37	0.57
1:B:177:THR:HB	1:B:251:ILE:HD13	1.86	0.57
1:B:221:ASN:O	1:B:224:LYS:HB2	2.04	0.57
1:B:461:MET:CE	1:B:461:MET:HA	2.34	0.57
1:B:549:GLU:HB2	1:B:554:VAL:CG2	2.35	0.57
1:A:153:LEU:HD11	1:A:168:LEU:HD21	1.87	0.57
1:A:230:ASN:O	1:A:234:LEU:HG	2.04	0.57
1:A:384:ILE:HD13	1:A:500:ILE:CG2	2.34	0.57
1:B:371:ALA:CB	1:B:539:ILE:HG13	2.35	0.57
1:A:267:ALA:HA	1:A:280:LEU:HD21	1.87	0.57
1:B:384:ILE:HD13	1:B:500:ILE:CG2	2.34	0.57
1:A:349:TYR:CE1	1:A:356:ILE:HD12	2.40	0.57
1:B:26:LYS:O	1:B:30:PRO:HD2	2.05	0.57
1:A:26:LYS:O	1:A:30:PRO:HD2	2.05	0.56
1:B:108:SER:N	4:B:816:HOH:O	2.35	0.56
1:B:276:THR:C	1:B:278:GLY:H	2.09	0.56
1:A:428:SER:N	1:B:205:GLU:OE1	2.36	0.56
1:B:429:ASP:O	1:B:471:VAL:HG22	2.04	0.56
1:B:371:ALA:HB2	1:B:539:ILE:HG13	1.87	0.56
1:A:177:THR:HB	1:A:251:ILE:HD13	1.87	0.56
1:A:429:ASP:O	1:A:471:VAL:HG22	2.04	0.56
1:B:153:LEU:HD11	1:B:168:LEU:HD21	1.88	0.56
1:B:349:TYR:CE1	1:B:356:ILE:HD12	2.41	0.56
1:A:206:ARG:NH1	1:B:427:PHE:CE1	2.74	0.56
1:B:509:ASP:OD1	1:B:512:SER:OG	2.21	0.56
1:B:71:VAL:O	1:B:71:VAL:HG12	2.04	0.56
1:A:399:LEU:HD23	1:A:404:ASN:HA	1.88	0.56
1:A:253:THR:OG1	1:B:75:PRO:HG3	2.06	0.56
1:A:371:ALA:CB	1:A:539:ILE:HG13	2.35	0.56
1:A:71:VAL:O	1:A:71:VAL:HG12	2.05	0.56
1:A:349:TYR:HE1	1:A:356:ILE:HD12	1.71	0.56
1:A:549:GLU:HB2	1:A:554:VAL:CG2	2.36	0.56
1:B:194:GLN:O	1:B:197:ALA:HB3	2.06	0.56
1:A:461:MET:HA	1:A:461:MET:CE	2.36	0.55
1:B:450:ALA:O	1:B:453:MET:HB2	2.06	0.55
1:A:324:ILE:HD11	1:A:390:PHE:C	2.27	0.55
1:A:33:ILE:HB	1:A:34:PRO:CD	2.36	0.55
1:A:479:SER:O	1:A:483:LYS:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:THR:OG1	1:B:54:GLU:HG2	2.05	0.55
1:A:450:ALA:O	1:A:453:MET:HB2	2.06	0.55
1:A:387:ILE:C	1:A:389:ARG:N	2.60	0.55
1:A:155:ILE:HD13	1:A:286:TYR:CE2	2.41	0.55
1:A:65:ILE:HG22	1:A:66:ALA:N	2.22	0.55
1:B:33:ILE:HB	1:B:34:PRO:CD	2.37	0.55
1:B:349:TYR:HE1	1:B:356:ILE:HD12	1.72	0.55
1:B:425:ILE:O	1:B:426:LEU:HD23	2.07	0.55
1:B:479:SER:O	1:B:483:LYS:HG3	2.06	0.55
1:A:371:ALA:HB2	1:A:539:ILE:HG13	1.88	0.55
1:A:162:LYS:N	1:A:162:LYS:HD3	2.19	0.55
1:B:491:ILE:HD13	1:B:499:LEU:HD22	1.89	0.55
1:B:63:ILE:O	1:B:63:ILE:HG22	2.07	0.55
1:A:145:ASP:OD1	1:A:296:ARG:HD2	2.07	0.54
1:A:75:PRO:HG3	1:B:253:THR:OG1	2.07	0.54
1:B:145:ASP:OD1	1:B:296:ARG:HD2	2.07	0.54
1:B:171:PHE:CE1	1:B:294:LEU:HD11	2.43	0.54
1:B:399:LEU:HD23	1:B:404:ASN:HA	1.88	0.54
1:A:157:PHE:HA	1:A:164:THR:HG21	1.90	0.54
1:A:194:GLN:O	1:A:197:ALA:HB3	2.06	0.54
1:B:384:ILE:HG22	1:B:385:ASN:N	2.22	0.54
1:B:60:THR:O	1:B:60:THR:HG22	2.07	0.54
1:A:491:ILE:HD13	1:A:499:LEU:HD22	1.89	0.54
1:A:439:ARG:NH2	1:A:446:GLU:OE2	2.40	0.54
1:A:373:VAL:HG13	1:A:533:ALA:O	2.07	0.54
1:B:387:ILE:C	1:B:389:ARG:N	2.60	0.54
1:B:488:ILE:CD1	1:B:516:ILE:HD13	2.38	0.54
1:B:106:ALA:HB3	1:B:322:TYR:CE2	2.38	0.54
1:B:12:TYR:HA	1:B:15:ARG:HD3	1.90	0.54
1:B:210:ILE:O	1:B:211:SER:C	2.46	0.54
1:B:324:ILE:HD11	1:B:390:PHE:C	2.28	0.54
1:B:52:THR:O	1:B:52:THR:HG22	2.08	0.54
1:A:12:TYR:HA	1:A:15:ARG:HD3	1.90	0.54
1:A:384:ILE:HG22	1:A:385:ASN:N	2.23	0.54
1:B:439:ARG:NH2	1:B:446:GLU:OE2	2.41	0.54
1:A:488:ILE:CD1	1:A:516:ILE:HD13	2.37	0.53
1:A:58:HIS:HA	1:A:61:ILE:HG12	1.90	0.53
1:A:210:ILE:O	1:A:211:SER:C	2.44	0.53
1:A:491:ILE:HG22	1:A:492:PHE:N	2.22	0.53
1:A:59:LEU:HD21	1:B:267:ALA:HB3	1.90	0.53
1:B:373:VAL:HG13	1:B:533:ALA:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:700:ADP:O2A	1:B:479:SER:HB2	2.09	0.53
1:A:466:GLY:O	1:A:468:ASP:N	2.41	0.53
1:B:213:VAL:HG13	1:B:218:ILE:HG13	1.90	0.53
1:B:181:PHE:O	1:B:182:PHE:C	2.47	0.53
1:B:420:VAL:HG23	1:B:491:ILE:CD1	2.39	0.53
1:A:217:ALA:HA	1:A:219:GLU:OE1	2.09	0.53
1:A:213:VAL:HG13	1:A:218:ILE:HG13	1.90	0.53
1:A:420:VAL:HG23	1:A:491:ILE:CD1	2.39	0.53
1:B:156:MET:CB	1:B:164:THR:HG22	2.34	0.53
1:B:24:ILE:O	1:B:26:LYS:N	2.41	0.53
1:B:330:ALA:HB1	1:B:409:LEU:CD2	2.39	0.53
1:B:491:ILE:HG22	1:B:492:PHE:N	2.24	0.53
1:B:571:HIS:O	1:B:575:ILE:HG13	2.09	0.53
1:A:159:LEU:HD23	1:A:283:PHE:CD1	2.44	0.53
1:A:171:PHE:CE1	1:A:294:LEU:HD11	2.44	0.53
1:B:269:LEU:HB3	1:B:274:SER:OG	2.09	0.53
1:B:328:VAL:HG23	1:B:329:GLY:N	2.23	0.53
1:B:357:LEU:HD22	1:B:360:ILE:HD11	1.91	0.52
1:A:181:PHE:O	1:A:182:PHE:C	2.47	0.52
1:A:571:HIS:O	1:A:575:ILE:HG13	2.09	0.52
1:B:163:LEU:O	1:B:166:ALA:HB3	2.09	0.52
1:B:337:GLN:O	1:B:339:ARG:N	2.43	0.52
1:B:466:GLY:O	1:B:468:ASP:N	2.42	0.52
1:B:65:ILE:HG22	1:B:66:ALA:N	2.23	0.52
1:A:425:ILE:O	1:A:426:LEU:HD23	2.07	0.52
1:A:328:VAL:HG23	1:A:329:GLY:N	2.25	0.52
1:A:330:ALA:HB1	1:A:409:LEU:CD2	2.40	0.52
1:B:217:ALA:HA	1:B:219:GLU:OE1	2.10	0.52
1:B:357:LEU:HB3	1:B:360:ILE:HD12	1.90	0.52
1:B:56:VAL:HG12	1:B:56:VAL:O	2.10	0.52
1:A:242:ARG:HG2	1:B:83:TYR:CE1	2.45	0.52
1:B:277:VAL:O	1:B:277:VAL:HG12	2.10	0.52
1:B:418:GLY:CA	1:B:496:PRO:HG3	2.40	0.52
1:B:384:ILE:CD1	1:B:532:VAL:HG23	2.40	0.52
1:B:536:LEU:HD23	1:B:536:LEU:N	2.25	0.52
1:A:269:LEU:HB3	1:A:274:SER:HB3	1.92	0.52
1:A:418:GLY:CA	1:A:496:PRO:HG3	2.39	0.52
1:A:427:PHE:CE1	1:B:206:ARG:NH1	2.78	0.51
1:A:337:GLN:O	1:A:339:ARG:N	2.43	0.51
1:A:357:LEU:HD22	1:A:360:ILE:HD11	1.92	0.51
1:A:558:THR:HG22	1:A:560:ARG:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ILE:HD11	1:B:257:ILE:HG22	1.93	0.51
1:B:59:LEU:O	1:B:59:LEU:HG	2.10	0.51
1:A:190:ARG:HH11	1:A:190:ARG:HG3	1.75	0.51
1:A:384:ILE:CD1	1:A:532:VAL:HG23	2.40	0.51
1:A:41:ILE:HA	1:A:45:ILE:HD12	1.93	0.51
1:B:405:ILE:HG23	1:B:413:LEU:CD2	2.41	0.51
1:B:276:THR:CG2	1:B:278:GLY:H	2.08	0.51
1:A:357:LEU:HB3	1:A:360:ILE:HD12	1.91	0.51
1:A:47:ASN:ND2	1:A:50:LEU:HG	2.26	0.51
1:A:51:THR:OG1	1:A:54:GLU:HG2	2.11	0.51
1:B:267:ALA:C	1:B:269:LEU:H	2.13	0.51
1:A:332:PRO:HD3	1:A:409:LEU:HD12	1.91	0.50
1:B:212:VAL:HG13	1:B:213:VAL:N	2.26	0.50
1:A:169:PHE:HD2	1:A:261:ILE:HD13	1.77	0.50
1:A:170:ILE:HD11	1:A:257:ILE:HG22	1.93	0.50
3:A:700:ADP:O2A	1:B:479:SER:HB3	2.10	0.50
1:A:159:LEU:O	1:A:160:ASP:HB2	2.12	0.50
1:B:169:PHE:HD2	1:B:261:ILE:HD13	1.77	0.50
1:A:443:THR:HB	1:A:446:GLU:HG3	1.93	0.50
1:A:24:ILE:O	1:A:26:LYS:N	2.40	0.50
1:A:536:LEU:HD23	1:A:536:LEU:N	2.25	0.50
1:A:169:PHE:CD2	1:A:261:ILE:HD13	2.47	0.50
1:B:332:PRO:HD3	1:B:409:LEU:HD12	1.92	0.50
1:A:276:THR:CG2	1:A:277:VAL:H	2.12	0.50
1:A:473:GLU:O	1:A:474:ARG:HB3	2.11	0.50
1:B:190:ARG:HG3	1:B:190:ARG:HH11	1.75	0.50
1:A:37:ILE:HG13	1:B:263:ILE:HD11	1.92	0.50
1:A:459:PHE:CZ	1:A:482:GLN:HG2	2.47	0.50
1:B:558:THR:HG22	1:B:560:ARG:H	1.76	0.50
1:A:459:PHE:C	1:A:459:PHE:CD1	2.86	0.50
1:A:106:ALA:HB3	1:A:322:TYR:CE2	2.38	0.49
1:A:83:TYR:CE1	1:B:242:ARG:HG2	2.47	0.49
1:B:169:PHE:CD2	1:B:261:ILE:HD13	2.47	0.49
1:A:121:ILE:HD11	1:B:204:HIS:HA	1.94	0.49
1:A:405:ILE:HG23	1:A:413:LEU:CD2	2.42	0.49
1:A:2:ILE:O	1:A:6:LEU:HG	2.12	0.49
1:B:459:PHE:CZ	1:B:482:GLN:HG2	2.48	0.49
1:B:384:ILE:HD12	1:B:532:VAL:HG21	1.94	0.49
1:A:269:LEU:HB3	1:A:274:SER:OG	2.12	0.49
1:A:384:ILE:HD12	1:A:532:VAL:HG23	1.93	0.49
1:A:75:PRO:CB	1:A:76:PRO:HD3	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:GLU:O	1:B:474:ARG:HB3	2.12	0.49
1:A:267:ALA:HA	1:A:280:LEU:CD2	2.42	0.49
1:B:51:THR:HB	1:B:54:GLU:CG	2.35	0.49
1:B:459:PHE:CD1	1:B:459:PHE:C	2.86	0.49
1:A:195:ALA:HB1	1:A:233:PHE:HA	1.95	0.49
1:A:206:ARG:NH1	1:B:427:PHE:CD1	2.80	0.49
1:A:24:ILE:O	1:A:27:PHE:HD1	1.96	0.49
1:A:422:GLN:HG3	1:A:423:ASP:N	2.28	0.49
1:A:443:THR:C	1:A:445:GLU:N	2.66	0.49
1:B:24:ILE:O	1:B:27:PHE:HD1	1.95	0.49
1:B:422:GLN:HG3	1:B:423:ASP:N	2.27	0.49
1:B:443:THR:HB	1:B:446:GLU:HG3	1.93	0.49
1:A:297:LEU:HA	1:A:300:SER:HB2	1.95	0.49
1:B:160:ASP:O	1:B:164:THR:HG23	2.12	0.49
1:A:479:SER:HB3	3:B:701:ADP:O2A	2.13	0.49
1:B:262:VAL:HG12	1:B:263:ILE:N	2.27	0.49
1:B:16:ILE:O	1:B:20:ILE:HG13	2.13	0.48
1:A:90:ASN:O	1:B:234:LEU:HD11	2.13	0.48
1:B:266:GLY:O	1:B:280:LEU:HD22	2.12	0.48
1:B:384:ILE:HD12	1:B:532:VAL:HG23	1.92	0.48
1:A:108:SER:HB3	4:A:805:HOH:O	2.13	0.48
1:A:106:ALA:HB1	1:A:322:TYR:CE2	2.48	0.48
1:B:2:ILE:O	1:B:6:LEU:HG	2.12	0.48
1:B:297:LEU:HA	1:B:300:SER:HB2	1.94	0.48
1:A:505:THR:HG22	1:A:505:THR:O	2.13	0.48
1:B:34:PRO:HA	1:B:37:ILE:HD12	1.95	0.48
1:A:284:VAL:HG11	1:B:37:ILE:HG23	1.94	0.48
1:B:152:ALA:HB2	1:B:289:LEU:HD13	1.95	0.48
1:A:284:VAL:HG11	1:B:37:ILE:CG2	2.43	0.48
1:B:443:THR:C	1:B:445:GLU:N	2.67	0.48
1:A:284:VAL:HA	1:A:287:LEU:HG	1.96	0.48
1:B:155:ILE:HD13	1:B:286:TYR:HE2	1.79	0.48
1:B:502:ASP:HA	1:B:532:VAL:HB	1.96	0.48
1:A:439:ARG:NH2	1:A:446:GLU:CD	2.67	0.48
1:B:106:ALA:HB1	1:B:322:TYR:CE2	2.48	0.48
1:B:275:ILE:CG2	1:B:276:THR:N	2.77	0.48
1:B:488:ILE:HG22	1:B:492:PHE:HE1	1.79	0.48
1:B:195:ALA:HB1	1:B:233:PHE:HA	1.95	0.47
1:B:439:ARG:NH2	1:B:446:GLU:CD	2.68	0.47
1:A:384:ILE:HD12	1:A:532:VAL:HG21	1.94	0.47
1:B:474:ARG:HH11	1:B:474:ARG:CG	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ARG:HH11	1:A:474:ARG:CG	2.27	0.47
1:B:25:ILE:O	1:B:25:ILE:CG2	2.59	0.47
1:A:33:ILE:HB	1:A:34:PRO:HD3	1.96	0.47
1:A:460:ILE:O	1:A:466:GLY:HA2	2.15	0.47
1:A:502:ASP:HA	1:A:532:VAL:HB	1.96	0.47
1:A:510:LEU:HD13	1:B:576:GLN:HG3	1.96	0.47
1:A:16:ILE:O	1:A:20:ILE:HG13	2.13	0.47
1:A:90:ASN:O	1:B:234:LEU:CD1	2.62	0.47
1:B:159:LEU:HD23	1:B:283:PHE:HA	1.96	0.47
1:A:260:ILE:CD1	1:B:67:LEU:HD23	2.44	0.47
1:A:481:GLY:CA	1:A:508:LEU:HD23	2.45	0.47
1:A:488:ILE:HD12	1:A:516:ILE:HD13	1.97	0.47
1:A:212:VAL:CG1	1:A:213:VAL:N	2.77	0.47
1:A:1:MET:O	1:A:4:ARG:HB2	2.15	0.47
1:B:481:GLY:CA	1:B:508:LEU:HD23	2.45	0.47
1:A:212:VAL:HG13	1:A:213:VAL:N	2.28	0.47
1:A:481:GLY:HA2	1:A:508:LEU:HD23	1.96	0.47
1:B:212:VAL:CG1	1:B:213:VAL:N	2.77	0.47
1:B:27:PHE:O	1:B:30:PRO:HG2	2.15	0.47
1:A:93:LEU:HD22	1:A:128:VAL:HG12	1.97	0.47
1:A:488:ILE:HG22	1:A:492:PHE:HE1	1.80	0.47
1:B:170:ILE:HG13	1:B:258:GLY:CA	2.44	0.47
1:B:259:PRO:HD3	1:B:291:PHE:CD2	2.51	0.47
1:B:173:PHE:H	1:B:173:PHE:HD1	1.63	0.46
1:B:508:LEU:CD1	1:B:516:ILE:HD12	2.46	0.46
1:B:474:ARG:O	1:B:474:ARG:HG3	2.15	0.46
1:A:153:LEU:CD1	1:A:168:LEU:HD21	2.45	0.46
1:B:481:GLY:HA2	1:B:508:LEU:HD23	1.96	0.46
1:A:142:ILE:HD11	1:A:304:LEU:CD1	2.38	0.46
1:B:163:LEU:HG	1:B:283:PHE:CE2	2.50	0.46
1:B:405:ILE:HG23	1:B:413:LEU:HD21	1.98	0.46
1:A:427:PHE:CD1	1:B:206:ARG:NH1	2.84	0.46
1:A:170:ILE:HG13	1:A:258:GLY:CA	2.43	0.46
1:A:51:THR:CB	1:A:54:GLU:HG2	2.46	0.46
1:A:556:THR:O	1:A:556:THR:HG22	2.16	0.46
1:B:110:ARG:O	1:B:111:PHE:C	2.52	0.46
1:B:544:LYS:HE3	1:B:556:THR:HG23	1.97	0.46
1:A:152:ALA:HB2	1:A:289:LEU:HD13	1.96	0.46
1:A:568:ALA:O	1:A:571:HIS:HB3	2.16	0.46
1:A:38:LYS:HG3	1:A:42:ASP:OD2	2.16	0.46
1:A:479:SER:OG	1:A:482:GLN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LYS:HE3	1:A:556:THR:HG23	1.98	0.46
1:B:33:ILE:HB	1:B:34:PRO:HD3	1.97	0.46
1:A:208:GLN:OE1	1:B:208:GLN:NE2	2.25	0.45
1:B:162:LYS:CD	1:B:162:LYS:H	2.25	0.45
1:B:505:THR:HG22	1:B:505:THR:O	2.14	0.45
1:B:558:THR:O	1:B:559:HIS:C	2.55	0.45
1:A:308:PHE:HA	1:A:311:MET:HG2	1.99	0.45
1:A:474:ARG:HG3	1:A:474:ARG:O	2.16	0.45
1:B:153:LEU:CD1	1:B:168:LEU:HD21	2.47	0.45
1:A:209:GLY:HA2	1:B:425:ILE:HD13	1.99	0.45
1:A:173:PHE:HD1	1:A:173:PHE:H	1.63	0.45
1:A:27:PHE:O	1:A:30:PRO:HG2	2.16	0.45
1:B:1:MET:O	1:B:4:ARG:HB2	2.15	0.45
1:B:488:ILE:HD12	1:B:516:ILE:HD13	1.98	0.45
1:B:75:PRO:CB	1:B:76:PRO:HD3	2.38	0.45
1:A:47:ASN:HD22	1:A:50:LEU:CD2	2.29	0.45
1:A:67:LEU:HD23	1:B:260:ILE:CD1	2.46	0.45
1:B:460:ILE:O	1:B:466:GLY:HA2	2.16	0.45
1:A:260:ILE:HD13	1:B:67:LEU:HD23	1.97	0.45
1:A:453:MET:HB3	1:A:492:PHE:CE2	2.52	0.45
1:B:568:ALA:O	1:B:571:HIS:HB3	2.16	0.45
1:A:163:LEU:HG	1:A:283:PHE:CE2	2.52	0.45
1:A:474:ARG:NH1	1:A:474:ARG:CG	2.79	0.45
1:A:536:LEU:HG	1:B:510:LEU:HD11	1.98	0.45
1:A:110:ARG:O	1:A:111:PHE:C	2.53	0.45
1:A:167:ALA:C	1:A:169:PHE:N	2.70	0.45
1:B:93:LEU:HD22	1:B:128:VAL:HG12	1.99	0.45
1:B:276:THR:C	1:B:278:GLY:N	2.70	0.45
1:B:27:PHE:HZ	1:B:144:LEU:HB3	1.82	0.45
1:A:185:LEU:CB	1:A:305:THR:HG21	2.45	0.45
1:A:405:ILE:HG23	1:A:413:LEU:HD21	1.99	0.45
1:A:508:LEU:CD1	1:A:516:ILE:HD12	2.46	0.45
1:B:284:VAL:HA	1:B:287:LEU:HG	1.98	0.45
1:B:308:PHE:HA	1:B:311:MET:HG2	1.99	0.45
1:B:453:MET:HB3	1:B:492:PHE:CE2	2.52	0.45
1:B:92:ILE:HD12	1:B:135:ILE:HD13	1.99	0.45
1:A:108:SER:N	4:A:806:HOH:O	2.45	0.44
1:A:167:ALA:C	1:A:169:PHE:H	2.19	0.44
1:B:181:PHE:CE2	1:B:246:TYR:HD2	2.35	0.44
1:B:364:ILE:HD13	1:B:530:LEU:CD2	2.45	0.44
1:A:181:PHE:CE2	1:A:246:TYR:HD2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:THR:O	1:A:559:HIS:C	2.55	0.44
1:B:474:ARG:NH1	1:B:474:ARG:CG	2.79	0.44
1:A:259:PRO:HD3	1:A:291:PHE:CD2	2.52	0.44
1:A:275:ILE:CG2	1:A:276:THR:H	2.26	0.44
1:A:29:ILE:N	1:A:30:PRO:HD2	2.32	0.44
1:B:260:ILE:C	1:B:262:VAL:H	2.21	0.44
1:A:270:ALA:HA	1:A:275:ILE:O	2.17	0.44
1:A:45:ILE:HG22	1:A:46:ASN:OD1	2.16	0.44
1:B:338:GLY:HA3	1:B:528:THR:OG1	2.17	0.44
1:A:68:PHE:CD1	1:A:72:ILE:HD12	2.53	0.44
1:A:92:ILE:HD12	1:A:135:ILE:HD13	2.00	0.44
1:A:264:GLY:HA2	1:B:63:ILE:HG13	1.99	0.44
1:B:479:SER:OG	1:B:482:GLN:HB2	2.16	0.44
1:A:267:ALA:HB3	1:B:59:LEU:HD21	2.00	0.44
1:A:338:GLY:HA3	1:A:528:THR:OG1	2.18	0.44
1:A:576:GLN:HG3	1:B:510:LEU:HD13	2.00	0.44
1:A:66:ALA:HB1	1:B:260:ILE:HD11	2.00	0.44
1:B:574:SER:O	1:B:578:LEU:HB2	2.17	0.44
1:B:75:PRO:HB2	1:B:76:PRO:CD	2.38	0.44
1:A:127:ASP:OD1	1:A:313:ARG:HD3	2.17	0.44
1:A:517:GLN:HA	1:A:517:GLN:OE1	2.18	0.44
1:B:268:TYR:O	1:B:268:TYR:CD2	2.71	0.44
1:B:294:LEU:O	1:B:298:VAL:HG23	2.17	0.44
1:B:68:PHE:CD1	1:B:72:ILE:HD12	2.52	0.44
1:A:329:GLY:O	1:A:330:ALA:C	2.56	0.43
1:B:153:LEU:HD21	1:B:168:LEU:HD21	2.00	0.43
1:B:195:ALA:O	1:B:199:VAL:HG13	2.17	0.43
1:A:27:PHE:HZ	1:A:144:LEU:HB3	1.82	0.43
1:B:100:LEU:O	1:B:104:LEU:HG	2.17	0.43
1:B:260:ILE:O	1:B:262:VAL:N	2.52	0.43
1:B:260:ILE:C	1:B:262:VAL:N	2.70	0.43
1:B:383:LEU:O	1:B:386:LEU:HB2	2.18	0.43
1:A:100:LEU:O	1:A:104:LEU:HG	2.18	0.43
1:A:266:GLY:HA3	1:A:280:LEU:HD11	1.99	0.43
1:A:51:THR:HB	1:A:54:GLU:HG2	2.00	0.43
1:A:260:ILE:O	1:A:263:ILE:N	2.51	0.43
1:A:204:HIS:HA	1:B:121:ILE:HD11	2.00	0.43
1:B:251:ILE:CG2	1:B:298:VAL:HG22	2.48	0.43
1:A:67:LEU:HD23	1:B:260:ILE:HD13	2.00	0.43
1:A:383:LEU:O	1:A:386:LEU:HB2	2.18	0.43
1:A:464:PRO:O	1:A:465:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ILE:HD11	1:B:304:LEU:CD1	2.39	0.43
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.83	0.43
1:B:357:LEU:HB3	1:B:360:ILE:CD1	2.48	0.43
1:B:51:THR:HG22	1:B:52:THR:N	2.33	0.43
1:A:294:LEU:O	1:A:298:VAL:HG23	2.17	0.43
1:A:510:LEU:HD11	1:B:536:LEU:HG	2.00	0.43
1:B:357:LEU:HD22	1:B:360:ILE:CD1	2.49	0.43
1:B:464:PRO:O	1:B:465:GLN:HB2	2.19	0.43
1:B:517:GLN:OE1	1:B:517:GLN:HA	2.19	0.43
1:A:153:LEU:HD21	1:A:168:LEU:HD21	2.00	0.43
1:A:241:THR:HG22	1:A:242:ARG:N	2.34	0.43
1:B:280:LEU:HD12	1:B:280:LEU:HA	1.85	0.43
1:B:163:LEU:HD23	1:B:283:PHE:CG	2.54	0.43
1:B:329:GLY:O	1:B:330:ALA:C	2.57	0.43
1:B:342:ILE:HG23	1:B:345:VAL:HG21	2.01	0.43
1:A:157:PHE:N	1:A:164:THR:HG21	2.34	0.43
1:A:34:PRO:HA	1:A:37:ILE:HD12	2.01	0.43
1:A:349:TYR:OH	1:A:382:THR:HG23	2.18	0.43
1:A:357:LEU:HD11	1:A:383:LEU:HA	2.01	0.43
1:B:349:TYR:OH	1:B:382:THR:HG23	2.19	0.43
1:A:189:THR:HG21	1:A:306:GLN:HA	2.00	0.43
1:A:94:TYR:CG	1:B:234:LEU:HD22	2.54	0.43
1:B:189:THR:HG21	1:B:306:GLN:HA	2.00	0.43
1:A:14:TYR:HB2	1:A:15:ARG:NH1	2.34	0.42
1:A:195:ALA:O	1:A:199:VAL:HG13	2.18	0.42
1:A:61:ILE:O	1:A:65:ILE:HB	2.19	0.42
1:B:177:THR:CG2	1:B:251:ILE:HD13	2.49	0.42
1:B:268:TYR:CG	1:B:268:TYR:O	2.71	0.42
1:B:357:LEU:HD11	1:B:383:LEU:HA	2.01	0.42
1:B:454:ALA:O	1:B:455:ASN:HB3	2.19	0.42
1:A:91:LYS:O	1:A:94:TYR:HB3	2.19	0.42
1:B:276:THR:HG22	1:B:278:GLY:CA	2.49	0.42
1:B:29:ILE:N	1:B:30:PRO:HD2	2.34	0.42
1:B:509:ASP:OD2	1:B:511:GLU:HB3	2.19	0.42
1:B:556:THR:HG22	1:B:556:THR:O	2.18	0.42
1:B:91:LYS:O	1:B:94:TYR:HB3	2.19	0.42
1:A:24:ILE:C	1:A:26:LYS:N	2.72	0.42
1:A:284:VAL:CG1	1:B:37:ILE:HD13	2.49	0.42
1:A:342:ILE:HG23	1:A:345:VAL:HG21	2.00	0.42
1:A:357:LEU:HB3	1:A:360:ILE:CD1	2.48	0.42
1:B:416:GLN:HB3	1:B:497:PRO:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLU:O	1:B:57:HIS:HB3	2.19	0.42
1:B:86:GLN:O	1:B:87:TRP:C	2.58	0.42
1:A:251:ILE:CG2	1:A:298:VAL:HG22	2.49	0.42
1:A:466:GLY:C	1:A:468:ASP:N	2.72	0.42
1:A:505:THR:O	1:A:505:THR:CG2	2.67	0.42
1:A:74:ARG:NH2	1:B:295:ARG:NH2	2.66	0.42
1:B:539:ILE:HA	1:B:539:ILE:HD12	1.71	0.42
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.88	0.42
1:A:357:LEU:HD11	1:A:383:LEU:CA	2.49	0.42
1:A:496:PRO:O	1:A:527:ARG:NH1	2.53	0.42
1:B:495:ASN:HD21	1:B:527:ARG:HH22	1.68	0.42
1:A:171:PHE:HB2	1:A:172:PRO:HD3	2.02	0.42
1:A:177:THR:CG2	1:A:251:ILE:HD13	2.50	0.42
1:A:364:ILE:HD13	1:A:530:LEU:CD2	2.46	0.42
1:B:24:ILE:C	1:B:26:LYS:N	2.73	0.42
1:B:127:ASP:OD1	1:B:313:ARG:HD3	2.19	0.42
1:A:27:PHE:H	1:A:27:PHE:HD1	1.67	0.42
1:A:291:PHE:N	1:A:291:PHE:CD1	2.88	0.42
1:A:454:ALA:O	1:A:455:ASN:HB3	2.19	0.42
1:B:145:ASP:O	1:B:149:ILE:HG13	2.20	0.42
1:B:185:LEU:CB	1:B:305:THR:HG21	2.44	0.42
1:A:145:ASP:O	1:A:149:ILE:HG13	2.20	0.42
1:B:241:THR:HG22	1:B:242:ARG:N	2.34	0.42
1:B:271:ILE:C	1:B:273:GLY:H	2.22	0.42
1:B:474:ARG:HH11	1:B:474:ARG:HG3	1.85	0.42
1:A:207:VAL:HG13	1:B:112:TYR:CE2	2.55	0.42
1:A:570:GLU:OE1	1:A:574:SER:HB2	2.20	0.42
1:B:570:GLU:OE1	1:B:574:SER:HB2	2.20	0.42
1:A:233:PHE:HE2	1:B:97:ARG:HH12	1.68	0.42
1:A:178:VAL:HG13	1:A:301:PHE:CD1	2.55	0.42
1:A:274:SER:OG	1:A:275:ILE:N	2.53	0.42
1:B:171:PHE:HB2	1:B:172:PRO:HD3	2.02	0.42
1:B:461:MET:HE3	1:B:461:MET:HA	2.02	0.42
3:A:700:ADP:C5	1:B:477:LYS:HA	2.54	0.42
1:A:263:ILE:CG2	1:B:63:ILE:HD11	2.33	0.42
1:A:455:ASN:OD1	1:A:455:ASN:O	2.38	0.41
1:A:536:LEU:H	1:A:536:LEU:HD23	1.85	0.41
3:A:700:ADP:N1	1:B:477:LYS:HG2	2.35	0.41
1:B:357:LEU:HD11	1:B:383:LEU:CA	2.49	0.41
1:B:65:ILE:CG2	1:B:66:ALA:N	2.83	0.41
1:A:23:GLY:O	1:A:26:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLN:O	1:A:87:TRP:C	2.58	0.41
1:B:505:THR:CG2	1:B:505:THR:O	2.67	0.41
1:B:14:TYR:HB2	1:B:15:ARG:NH1	2.34	0.41
1:B:160:ASP:OD2	1:B:163:LEU:N	2.49	0.41
1:B:178:VAL:HG13	1:B:301:PHE:CD1	2.56	0.41
1:A:171:PHE:CB	1:A:172:PRO:HD3	2.50	0.41
1:A:357:LEU:HD22	1:A:360:ILE:CD1	2.50	0.41
1:B:265:VAL:O	1:B:269:LEU:HG	2.21	0.41
1:B:466:GLY:C	1:B:468:ASP:N	2.72	0.41
1:B:558:THR:HB	1:B:561:GLU:CG	2.37	0.41
1:B:71:VAL:CG1	1:B:71:VAL:O	2.68	0.41
1:A:453:MET:HA	1:A:453:MET:CE	2.50	0.41
1:A:509:ASP:OD2	1:A:511:GLU:HB3	2.20	0.41
1:B:397:GLN:NE2	1:B:399:LEU:HD11	2.25	0.41
1:A:416:GLN:HB3	1:A:497:PRO:CG	2.50	0.41
1:B:291:PHE:CD1	1:B:291:PHE:N	2.88	0.41
1:A:28:GLY:O	1:A:32:LEU:HG	2.20	0.41
1:A:425:ILE:HG22	1:A:426:LEU:N	2.36	0.41
1:B:536:LEU:HD23	1:B:536:LEU:H	1.84	0.41
1:A:170:ILE:HD11	1:A:257:ILE:CG2	2.50	0.41
1:A:251:ILE:HG21	1:A:298:VAL:HG22	2.03	0.41
1:A:74:ARG:HB3	1:A:75:PRO:HD3	2.03	0.41
1:B:345:VAL:HG13	1:B:393:VAL:CG2	2.51	0.41
1:B:153:LEU:HA	1:B:153:LEU:HD23	1.84	0.41
1:B:339:ARG:O	1:B:400:ILE:HA	2.21	0.41
1:B:425:ILE:HG22	1:B:426:LEU:N	2.35	0.41
1:B:508:LEU:HD13	1:B:516:ILE:HD12	2.03	0.41
1:B:266:GLY:O	1:B:280:LEU:HD13	2.21	0.41
1:B:455:ASN:O	1:B:455:ASN:OD1	2.38	0.41
1:A:169:PHE:CD2	1:A:261:ILE:CD1	3.04	0.41
1:A:342:ILE:O	1:A:361:ASN:HA	2.21	0.41
1:A:425:ILE:HD13	1:B:209:GLY:HA2	2.03	0.41
1:B:171:PHE:CB	1:B:172:PRO:HD3	2.51	0.41
1:A:112:TYR:CE2	1:B:207:VAL:HG13	2.56	0.41
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.92	0.41
1:B:342:ILE:O	1:B:361:ASN:HA	2.21	0.41
1:A:448:VAL:HG12	1:A:452:LYS:HE3	2.03	0.40
1:B:170:ILE:HD11	1:B:257:ILE:CG2	2.50	0.40
1:A:260:ILE:HG22	1:A:261:ILE:N	2.36	0.40
1:B:133:ASP:HB3	1:B:303:THR:CG2	2.51	0.40
1:B:12:TYR:CZ	1:B:91:LYS:HG2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ARG:O	1:A:400:ILE:HA	2.22	0.40
1:A:47:ASN:HD22	1:A:50:LEU:HD21	1.85	0.40
1:A:12:TYR:CZ	1:A:91:LYS:HG2	2.57	0.40
1:A:70:PHE:CD2	1:B:256:ASP:HB3	2.49	0.40
1:B:267:ALA:O	1:B:269:LEU:N	2.55	0.40
1:B:251:ILE:HG21	1:B:298:VAL:HG22	2.02	0.40
1:B:558:THR:HG22	1:B:560:ARG:N	2.36	0.40
1:B:74:ARG:HB3	1:B:75:PRO:HD3	2.03	0.40
1:A:207:VAL:O	1:A:210:ILE:HG13	2.20	0.40
1:B:289:LEU:HD23	1:B:289:LEU:HA	1.76	0.40
1:B:461:MET:HE2	1:B:461:MET:HA	2.03	0.40
1:B:496:PRO:O	1:B:527:ARG:NH1	2.54	0.40
1:B:570:GLU:OE1	1:B:570:GLU:C	2.60	0.40
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.92	0.40
1:B:23:GLY:O	1:B:26:LYS:HB2	2.20	0.40
1:B:266:GLY:CA	1:B:280:LEU:HD11	2.50	0.40
4:A:807:HOH:O	1:B:414:ARG:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	576/578 (100%)	487 (84%)	73 (13%)	16 (3%)	6	29
1	B	576/578 (100%)	480 (83%)	80 (14%)	16 (3%)	6	29
All	All	1152/1156 (100%)	967 (84%)	153 (13%)	32 (3%)	6	29

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ILE

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Mol	Chain	Res	Type
1	A	41	ILE
1	A	338	GLY
1	B	25	ILE
1	B	338	GLY
1	A	160	ASP
1	A	168	LEU
1	A	182	PHE
1	A	466	GLY
1	A	467	TYR
1	A	506	SER
1	B	182	PHE
1	B	466	GLY
1	B	506	SER
1	A	79	PHE
1	A	330	ALA
1	A	574	SER
1	B	79	PHE
1	B	330	ALA
1	B	467	TYR
1	B	574	SER
1	A	477	LYS
1	A	537	SER
1	B	168	LEU
1	B	268	TYR
1	B	477	LYS
1	B	537	SER
1	B	11	PRO
1	A	11	PRO
1	B	171	PHE
1	B	284	VAL
1	A	171	PHE

5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/499 (100%)	474 (95%)	25 (5%)	28	67
1	B	499/499 (100%)	473 (95%)	26 (5%)	27	65
All	All	998/998 (100%)	947 (95%)	51 (5%)	28	66

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	65	ILE
1	A	82	GLN
1	A	162	LYS
1	A	199	VAL
1	A	200	GLN
1	A	241	THR
1	A	289	LEU
1	A	290	LEU
1	A	295	ARG
1	A	321	ASP
1	A	373	VAL
1	A	384	ILE
1	A	392	ASP
1	A	393	VAL
1	A	422	GLN
1	A	424	ASN
1	A	429	ASP
1	A	443	THR
1	A	474	ARG
1	A	487	SER
1	A	491	ILE
1	A	539	ILE
1	A	556	THR
1	A	570	GLU
1	B	15	ARG
1	B	65	ILE
1	B	82	GLN
1	B	159	LEU
1	B	162	LYS
1	B	199	VAL
1	B	241	THR

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Mol	Chain	Res	Type
1	B	289	LEU
1	B	290	LEU
1	B	295	ARG
1	B	321	ASP
1	B	373	VAL
1	B	384	ILE
1	B	392	ASP
1	B	393	VAL
1	B	422	GLN
1	B	424	ASN
1	B	429	ASP
1	B	443	THR
1	B	461	MET
1	B	474	ARG
1	B	491	ILE
1	B	539	ILE
1	B	556	THR
1	B	570	GLU
1	B	578	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	105	GLN
1	A	126	ASN
1	A	200	GLN
1	A	204	HIS
1	A	306	GLN
1	A	397	GLN
1	A	455	ASN
1	A	465	GLN
1	B	47	ASN
1	B	105	GLN
1	B	126	ASN
1	B	200	GLN
1	B	306	GLN
1	B	397	GLN
1	B	465	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	700	-	25,29,29	1.18	2 (8%)	24,45,45	2.00	3 (12%)
3	ADP	B	701	-	25,29,29	1.15	2 (8%)	24,45,45	2.04	3 (12%)

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	700	-	-	0/12/32/32	0/3/3/3
3	ADP	B	701	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	ADP	C8-N7	-2.53	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	ADP	C8-N7	-2.51	1.30	1.34
3	B	701	ADP	O4'-C1'	3.43	1.46	1.41
3	A	700	ADP	O4'-C1'	3.67	1.46	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	ADP	N3-C2-N1	-8.30	121.63	128.86
3	A	700	ADP	N3-C2-N1	-8.11	121.80	128.86
3	B	701	ADP	C4-C5-N7	-2.25	107.23	109.41
3	A	700	ADP	C4-C5-N7	-2.13	107.35	109.41
3	B	701	ADP	C2'-C3'-C4'	2.33	107.15	102.62
3	A	700	ADP	C2'-C3'-C4'	2.41	107.31	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	ADP	7	0
3	B	701	ADP	5	0

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	578/578 (100%)	-0.52	2 (0%) 93 82	56, 97, 162, 200	2 (0%)
1	B	578/578 (100%)	-0.48	4 (0%) 87 67	54, 95, 162, 200	2 (0%)
All	All	1156/1156 (100%)	-0.50	6 (0%) 90 74	54, 96, 162, 200	4 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	ASN	5.9
1	B	46	ASN	4.5
1	B	48	HIS	3.0
1	A	286	TYR	2.7
1	A	578	LEU	2.6
1	B	55	LYS	2.5

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(\AA^2)	Q<0.9
2	NA	B	910	1/1	0.90	0.28	2.46	31,31,31,31	0
2	NA	A	900	1/1	0.96	0.23	0.93	24,24,24,24	0
3	ADP	B	701	27/27	0.91	0.20	0.47	78,83,84,85	0
3	ADP	A	700	27/27	0.91	0.19	0.35	80,83,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.