W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:37 AM 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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865
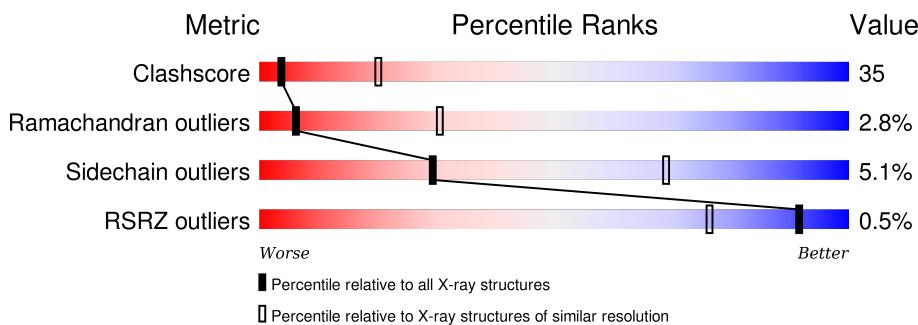
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
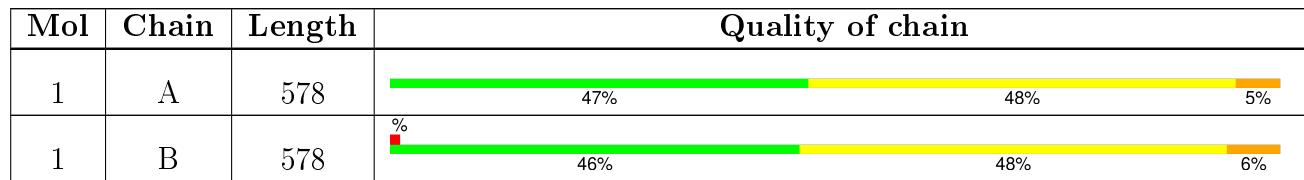
The reported resolution of this entry is 3.00 Å.

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	Percentile Ranks	Value
Clashscore		35
Ramachandran outliers		2.8%
Sidechain outliers		5.1%
RSRZ outliers		0.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 <=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	47%　　　48%　　　5%
1	B	578	%　46%　　　48%　　　6%

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.
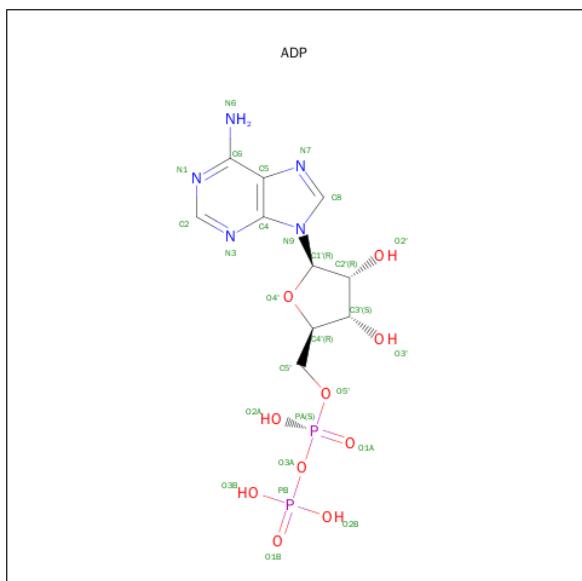
- Molecule 1 is a protein called ABC transporter homolog.

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

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

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

- Molecule 3 is A D E N O S I N E - 5' - D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
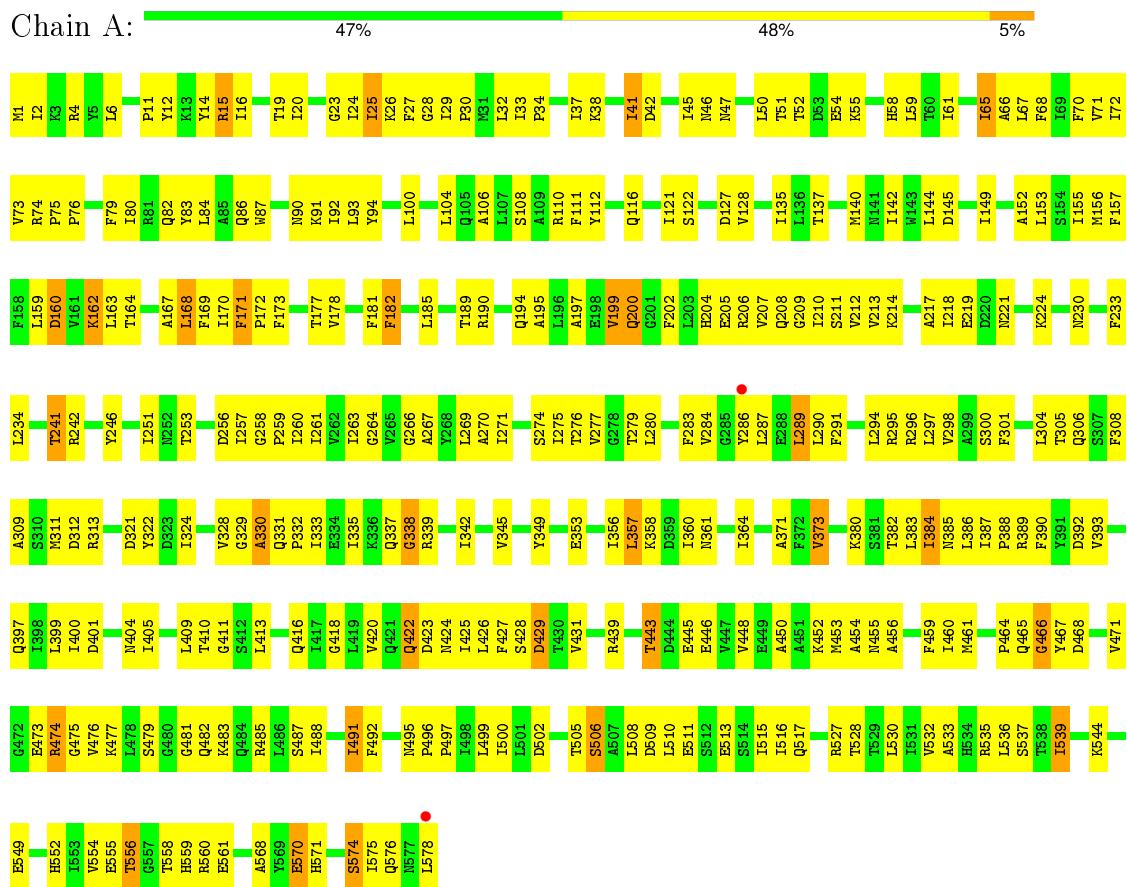
- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total 8	O 8	0	0
4	B	8	Total 8	O 8	0	0
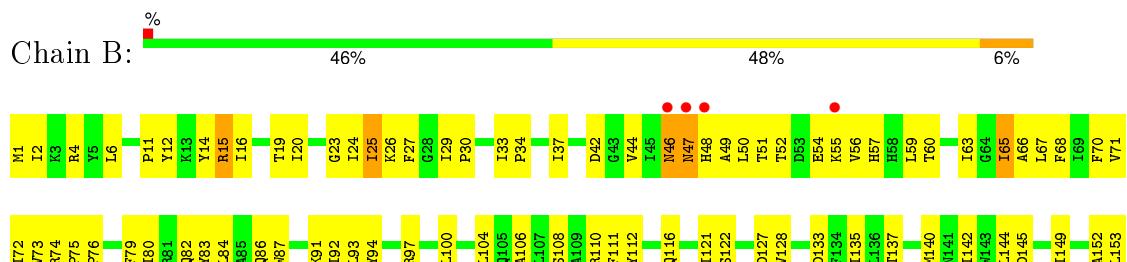
3 Residue-property plots ⓘ
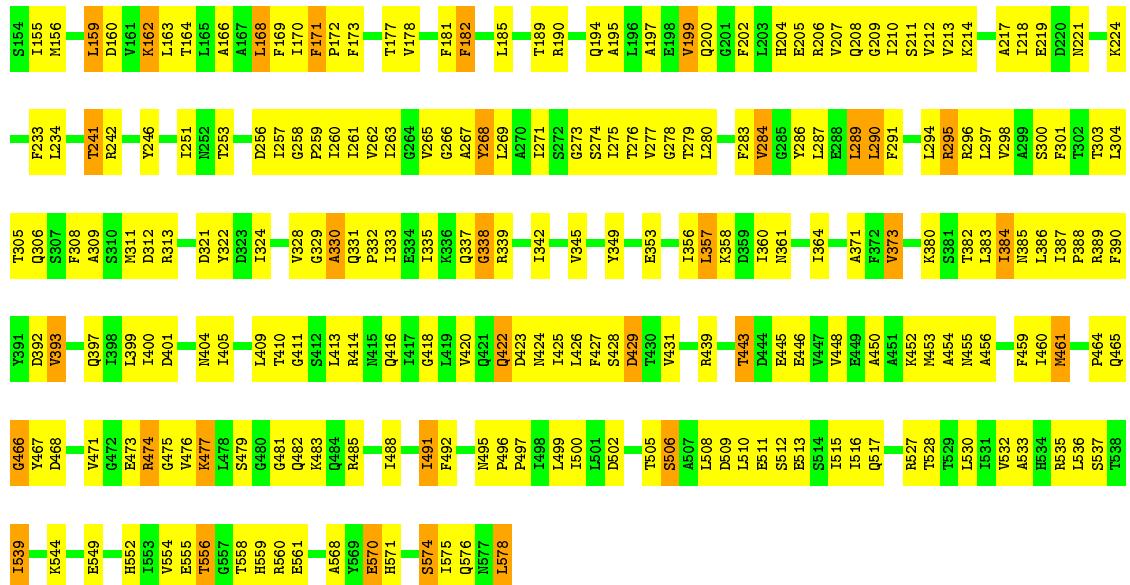
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

4 Data and refinement statistics (i)

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
$<I/\sigma(I)>$ [1]	2.83 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.272 0.254 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	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 , 74.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|>$ = 0.50, $<L^2>$ = 0.33	Xtriage
Outliers	0 of 58973 reflections	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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(^{o})	Ideal(^{o})
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 (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	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:HD2	1:A:15:ARG:H	1.01	1.15
1:B:15:ARG:HD2	1:B:15:ARG:H	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:HD2	1:B:15:ARG:N	1.83	0.90
1:B:558:THR:HB	1:B:561:GLU:HG3	1.51	0.90
1:A:505:THR:HG21	1:A:513:GLU:OE2	1.71	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:455:ASN:ND2	1:A:515:ILE:HG21	2.03	0.72
1:A:45:ILE:HG21	1:B:277:VAL:HG11	1.72	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:260:ILE:HG21	1:B:67:LEU:CD2	2.23	0.69
1:A:364:ILE:HD13	1:A:530:LEU:HD21	1.74	0.69
1:A:555:GLU:OE1	1:A:568:ALA:HB3	1.92	0.69
1:A:258:GLY:HA3	1:A:291:PHE:CE2	2.27	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:42:ASP:HA	1:B:46:ASN:HB2	1.77	0.66
1:B:410:THR:HG22	1:B:411:GLY:N	2.10	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:47:ASN:HD22	1:B:50:LEU:HD21	1.61	0.66
1:B:331:GLN:O	1:B:333:ILE:HG13	1.95	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:B:464:PRO:HB2	1:B:465:GLN:HE22	1.59	0.65
1:A:304:LEU:O	1:A:308:PHE:HD1	1.79	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:B:456:ALA:O	1:B:460:ILE:HG13	1.98	0.63
1:A:47:ASN:HD22	1:A:50:LEU:HG	1.63	0.63
1:A:234:LEU:HD22	1:B:94:TYR:HB2	1.80	0.63
1:A:574:SER:O	1:A:578:LEU:HB2	1.98	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:479:SER:CB	3:B:701:ADP:O2A	2.47	0.62
1:A:309:ALA:O	1:A:312:ASP:HB2	2.00	0.62
1:A:456:ALA:O	1:A:460:ILE:HG13	2.00	0.62
1:A:122:SER:HB2	1:A:200:GLN:HG3	1.81	0.62
1:A:73:VAL:O	1:A:76:PRO:HD2	2.00	0.62
1:A:142:ILE:CD1	1:A:304:LEU:HD11	2.29	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:389:ARG:HD2	1:A:405:ILE:HG22	1.82	0.62
1:A:209:GLY:O	1:A:212:VAL:HG12	2.00	0.62
1:B:475:GLY:O	1:B:483:LYS:HE2	2.00	0.62
1:A:47:ASN:HD22	1:A:50:LEU:CG	2.13	0.62
1:A:448:VAL:O	1:A:452:LYS:HG3	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:428:SER:HB2	1:A:473:GLU:HA	1.81	0.61
1:A:210:ILE:HG22	1:A:214:LYS:HG2	1.81	0.61
1:B:156:MET:HE3	1:B:283:PHE:CZ	2.35	0.61
1:A:159:LEU:HD23	1:A:283:PHE:HD1	1.64	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:37:ILE:HG12	1:B:263:ILE:HD11	1.82	0.60
1:A:475:GLY:O	1:A:483:LYS:HE2	2.01	0.60
1:A:275:ILE:HG21	1:A:279:THR:OG1	2.01	0.60
1:A:19:THR:HG21	1:A:140:MET:HE3	1.81	0.60
1:A:335:ILE:HD13	1:A:400:ILE:HG21	1.82	0.60
1:B:448:VAL:O	1:B:452:LYS:HG3	2.02	0.60
1:B:202:PHE:CE2	1:B:206:ARG:HG3	2.36	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: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:506:SER:O	1:A:535:ARG:NH2	2.34	0.59
1:A:479:SER:HB2	3:B:701:ADP:O2A	2.03	0.59
1:B:324:ILE:HD13	1:B:389:ARG:O	2.02	0.59
1:A:41:ILE:HG22	1:A:42:ASP:N	2.17	0.59
1:A:178:VAL:HG13	1:A:301:PHE:CE1	2.37	0.59
1:B:121:ILE:HD12	1:B:204:HIS:CE1	2.37	0.59
1:A:80:ILE:O	1:A:84:LEU:HB2	2.02	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:47:ASN:CG	1:B:47:ASN:CA	2.69	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: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:B:2:ILE:HD11	1:B:308:PHE:CE2	2.37	0.57
1:A:221:ASN:O	1:A:224:LYS:HB2	2.04	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:461:MET:CE	1:B:461:MET:HA	2.34	0.57
1:B:221:ASN:O	1:B:224:LYS:HB2	2.04	0.57
1:A:24:ILE:C	1:A:26:LYS:H	2.07	0.57
1:B:549:GLU:HB2	1:B:554:VAL:CG2	2.35	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:A:153:LEU:HD11	1:A:168:LEU:HD21	1.87	0.57
1:B:371:ALA:CB	1:B:539:ILE:HG13	2.35	0.57
1:B:384:ILE:HD13	1:B:500:ILE:CG2	2.34	0.57
1:A:267:ALA:HA	1:A:280:LEU:HD21	1.87	0.57
1:B:26:LYS:O	1:B:30:PRO:HD2	2.05	0.57
1:A:349:TYR:CE1	1:A:356:ILE:HD12	2.40	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:371:ALA:HB2	1:B:539:ILE:HG13	1.87	0.56
1:B:429:ASP:O	1:B:471:VAL:HG22	2.04	0.56
1:A:206:ARG:NH1	1:B:427:PHE:CE1	2.74	0.56
1:B:349:TYR:CE1	1:B:356:ILE:HD12	2.41	0.56
1:A:429:ASP:O	1:A:471:VAL:HG22	2.04	0.56
1:B:71:VAL:O	1:B:71:VAL:HG12	2.04	0.56
1:B:509:ASP:OD1	1:B:512:SER:OG	2.21	0.56
1:B:153:LEU:HD11	1:B:168:LEU:HD21	1.88	0.56
1:A:177:THR:HB	1:A:251:ILE:HD13	1.87	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:71:VAL:HG12	1:A:71:VAL:O	2.05	0.56
1:A:371:ALA:CB	1:A:539:ILE:HG13	2.35	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:349:TYR:HE1	1:A:356:ILE:HD12	1.71	0.56
1:B:450:ALA:O	1:B:453:MET:HB2	2.06	0.55
1:A:461:MET:HA	1:A:461:MET:CE	2.36	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
1:A:324:ILE:HD11	1:A:390:PHE:C	2.27	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: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:A:155:ILE:HD13	1:A:286:TYR:CE2	2.41	0.55
1:B:479:SER:O	1:B:483:LYS:HG3	2.06	0.55
1:B:425:ILE:O	1:B:426:LEU:HD23	2.07	0.55
1:B:349:TYR:HE1	1:B:356:ILE:HD12	1.72	0.55
1:A:371:ALA:HB2	1:A:539:ILE:HG13	1.88	0.55
1:B:63:ILE:O	1:B:63:ILE:HG22	2.07	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:A:75:PRO:HG3	1:B:253:THR:OG1	2.07	0.54
1:A:145:ASP:OD1	1:A:296:ARG:HD2	2.07	0.54
1:B:399:LEU:HD23	1:B:404:ASN:HA	1.88	0.54
1:B:171:PHE:CE1	1:B:294:LEU:HD11	2.43	0.54
1:B:145:ASP:OD1	1:B:296:ARG:HD2	2.07	0.54
1:A:157:PHE:HA	1:A:164:THR:HG21	1.90	0.54
1:B:384:ILE:HG22	1:B:385:ASN:N	2.22	0.54
1:A:194:GLN:O	1:A:197:ALA:HB3	2.06	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:B:488:ILE:CD1	1:B:516:ILE:HD13	2.38	0.54
1:B:387:ILE:C	1:B:389:ARG:N	2.60	0.54
1:A:373:VAL:HG13	1:A:533:ALA:O	2.07	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:52:THR:O	1:B:52:THR:HG22	2.08	0.54
1:B:324:ILE:HD11	1:B:390:PHE:C	2.28	0.54
1:B:210:ILE:O	1:B:211:SER:C	2.46	0.54
1:A:12:TYR:HA	1:A:15:ARG:HD3	1.90	0.54
1:B:439:ARG:NH2	1:B:446:GLU:OE2	2.41	0.54
1:A:384:ILE:HG22	1:A:385:ASN:N	2.23	0.54
1:A:58:HIS:HA	1:A:61:ILE:HG12	1.90	0.53
1:A:488:ILE:CD1	1:A:516:ILE:HD13	2.37	0.53
1:A:491:ILE:HG22	1:A:492:PHE:N	2.22	0.53
1:A:210:ILE:O	1:A:211:SER:C	2.44	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:420:VAL:HG23	1:B:491:ILE:CD1	2.39	0.53
1:B:181:PHE:O	1:B:182:PHE:C	2.47	0.53
1:B:156:MET:CB	1:B:164:THR:HG22	2.34	0.53
1:A:420:VAL:HG23	1:A:491:ILE:CD1	2.39	0.53
1:B:491:ILE:HG22	1:B:492:PHE:N	2.24	0.53
1:B:330:ALA:HB1	1:B:409:LEU:CD2	2.39	0.53
1:B:571:HIS:O	1:B:575:ILE:HG13	2.09	0.53
1:A:213:VAL:HG13	1:A:218:ILE:HG13	1.90	0.53
1:B:24:ILE:O	1:B:26:LYS:N	2.41	0.53
1:A:217:ALA:HA	1:A:219:GLU:OE1	2.09	0.53
1:A:159:LEU:HD23	1:A:283:PHE:CD1	2.44	0.53
1:B:328:VAL:HG23	1:B:329:GLY:N	2.23	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:357:LEU:HD22	1:B:360:ILE:HD11	1.91	0.52
1:A:571:HIS:O	1:A:575:ILE:HG13	2.09	0.52
1:A:181:PHE:O	1:A:182:PHE:C	2.47	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:357:LEU:HB3	1:B:360:ILE:HD12	1.90	0.52
1:B:217:ALA:HA	1:B:219:GLU:OE1	2.10	0.52
1:B:56:VAL:O	1:B:56:VAL:HG12	2.10	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:242:ARG:HG2	1:B:83:TYR:CE1	2.45	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:558:THR:HG22	1:A:560:ARG:H	1.75	0.51
1:B:170:ILE:HD11	1:B:257:ILE:HG22	1.93	0.51
1:A:337:GLN:O	1:A:339:ARG:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LEU:HD22	1:A:360:ILE:HD11	1.92	0.51
1:B:59:LEU:O	1:B:59:LEU:HG	2.10	0.51
1:A:384:ILE:CD1	1:A:532:VAL:HG23	2.40	0.51
1:A:190:ARG:HH11	1:A:190:ARG:HG3	1.75	0.51
1:B:405:ILE:HG23	1:B:413:LEU:CD2	2.41	0.51
1:A:41:ILE:HA	1:A:45:ILE:HD12	1.93	0.51
1:B:276:THR:CG2	1:B:278:GLY:H	2.08	0.51
1:A:47:ASN:ND2	1:A:50:LEU:HG	2.26	0.51
1:A:357:LEU:HB3	1:A:360:ILE:HD12	1.91	0.51
1:B:267:ALA:C	1:B:269:LEU:H	2.13	0.51
1:A:51:THR:OG1	1:A:54:GLU:HG2	2.11	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:B:558:THR:HG22	1:B:560:ARG:H	1.76	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:A:459:PHE:C	1:A:459:PHE:CD1	2.86	0.50
1:A:121:ILE:HD11	1:B:204:HIS:HA	1.94	0.49
1:A:106:ALA:HB3	1:A:322:TYR:CE2	2.38	0.49
1:B:169:PHE:CD2	1:B:261:ILE:HD13	2.47	0.49
1:A:83:TYR:CE1	1:B:242:ARG:HG2	2.47	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:384:ILE:HD12	1:B:532:VAL:HG21	1.94	0.49
1:B:459:PHE:CZ	1:B:482:GLN:HG2	2.48	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:B:51:THR:HB	1:B:54:GLU:CG	2.35	0.49
1:A:267:ALA:HA	1:A:280:LEU:CD2	2.42	0.49
1:B:459:PHE:CD1	1:B:459:PHE:C	2.86	0.49
1:A:443:THR:C	1:A:445:GLU:N	2.66	0.49
1:B:443:THR:HB	1:B:446:GLU:HG3	1.93	0.49
1:A:206:ARG:NH1	1:B:427:PHE:CD1	2.80	0.49
1:B:24:ILE:O	1:B:27:PHE:HD1	1.95	0.49
1:A:24:ILE:O	1:A:27:PHE:HD1	1.96	0.49
1:A:195:ALA:HB1	1:A:233:PHE:HA	1.95	0.49
1:A:422:GLN:HG3	1:A:423:ASP:N	2.28	0.49
1:B:422:GLN:HG3	1:B:423:ASP:N	2.27	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:A:297:LEU:HA	1:A:300:SER:HB2	1.95	0.49
1:B:262:VAL:HG12	1:B:263:ILE:N	2.27	0.49
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:16:ILE:O	1:B:20:ILE:HG13	2.13	0.48
1:B:384:ILE:HD12	1:B:532:VAL:HG23	1.92	0.48
1:B:2:ILE:O	1:B:6:LEU:HG	2.12	0.48
1:A:106:ALA:HB1	1:A:322:TYR:CE2	2.48	0.48
1:A:108:SER:HB3	4:A:805:HOH:O	2.13	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:B:443:THR:C	1:B:445:GLU:N	2.67	0.48
1:A:284:VAL:HG11	1:B:37:ILE:CG2	2.43	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: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:284:VAL:HA	1:A:287:LEU:HG	1.96	0.48
1:B:106:ALA:HB1	1:B:322:TYR:CE2	2.48	0.48
1:A:439:ARG:NH2	1:A:446:GLU:CD	2.67	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:439:ARG:NH2	1:B:446:GLU:CD	2.68	0.47
1:B:195:ALA:HB1	1:B:233:PHE:HA	1.95	0.47
1:B:474:ARG:HH11	1:B:474:ARG:CG	2.27	0.47
1:A:384:ILE:HD12	1:A:532:VAL:HG21	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ARG:CG	1:A:474:ARG:HH11	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:90:ASN:O	1:B:234:LEU:CD1	2.62	0.47
1:A:260:ILE:CD1	1:B:67:LEU:HD23	2.44	0.47
1:B:159:LEU:HD23	1:B:283:PHE:HA	1.96	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:16:ILE:O	1:A:20:ILE:HG13	2.13	0.47
1:B:481:GLY:CA	1:B:508:LEU:HD23	2.45	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: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:A:212:VAL:HG13	1:A:213:VAL:N	2.28	0.47
1:B:27:PHE:O	1:B:30:PRO:HG2	2.15	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:A:93:LEU:HD22	1:A:128:VAL:HG12	1.97	0.47
1:B:508:LEU:CD1	1:B:516:ILE:HD12	2.46	0.46
1:B:173:PHE:H	1:B:173:PHE:HD1	1.63	0.46
1:B:474:ARG:O	1:B:474:ARG:HG3	2.15	0.46
1:B:481:GLY:HA2	1:B:508:LEU:HD23	1.96	0.46
1:A:153:LEU:CD1	1:A:168:LEU:HD21	2.45	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:544:LYS:HE3	1:B:556:THR:HG23	1.97	0.46
1:B:110:ARG:O	1:B:111:PHE:C	2.52	0.46
1:A:568:ALA:O	1:A:571:HIS:HB3	2.16	0.46
1:A:152:ALA:HB2	1:A:289:LEU:HD13	1.96	0.46
1:A:479:SER:OG	1:A:482:GLN:HB2	2.15	0.46
1:A:38:LYS:HG3	1:A:42:ASP:OD2	2.16	0.46

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ARG:NH1	1:B:474:ARG:CG	2.79	0.44
1:A:181:PHE:CE2	1:A:246:TYR:HD2	2.35	0.44
1:A:275:ILE:CG2	1:A:276:THR:H	2.26	0.44
1:B:260:ILE:C	1:B:262:VAL:H	2.21	0.44
1:A:259:PRO:HD3	1:A:291:PHE:CD2	2.52	0.44
1:A:29:ILE:N	1:A:30:PRO:HD2	2.32	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:264:GLY:HA2	1:B:63:ILE:HG13	1.99	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: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:66:ALA:HB1	1:B:260:ILE:HD11	2.00	0.44
1:A:576:GLN:HG3	1:B:510:LEU:HD13	2.00	0.44
1:A:338:GLY:HA3	1:A:528:THR:OG1	2.18	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:B:294:LEU:O	1:B:298:VAL:HG23	2.17	0.44
1:A:517:GLN:HA	1:A:517:GLN:OE1	2.18	0.44
1:B:268:TYR:CD2	1:B:268:TYR:O	2.71	0.44
1:A:127:ASP:OD1	1:A:313:ARG:HD3	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:B:260:ILE:C	1:B:262:VAL:N	2.70	0.43
1:B:260:ILE:O	1:B:262:VAL:N	2.52	0.43
1:A:27:PHE:HZ	1:A:144:LEU:HB3	1.82	0.43
1:B:383:LEU:O	1:B:386:LEU:HB2	2.18	0.43
1:B:100:LEU:O	1:B:104:LEU:HG	2.17	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:100:LEU:O	1:A:104:LEU:HG	2.18	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:A:67:LEU:HD23	1:B:260:ILE:HD13	2.00	0.43
1:B:251:ILE:CG2	1:B:298:VAL:HG22	2.48	0.43
1:A:464:PRO:O	1:A:465:GLN:HB2	2.18	0.43
1:B:51:THR:HG22	1:B:52:THR:N	2.33	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:357:LEU:HB3	1:B:360:ILE:CD1	2.48	0.43
1:A:383:LEU:O	1:A:386:LEU:HB2	2.18	0.43
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.83	0.43
1:B:464:PRO:O	1:B:465:GLN:HB2	2.19	0.43
1:A:294:LEU:O	1:A:298:VAL:HG23	2.17	0.43
1:B:357:LEU:HD22	1:B:360:ILE:CD1	2.49	0.43
1:A:510:LEU:HD11	1:B:536:LEU:HG	2.00	0.43
1:B:517:GLN:OE1	1:B:517:GLN:HA	2.19	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:280:LEU:HD12	1:B:280:LEU:HA	1.85	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:342:ILE:HG23	1:B:345:VAL:HG21	2.01	0.43
1:A:34:PRO:HA	1:A:37:ILE:HD12	2.01	0.43
1:A:157:PHE:N	1:A:164:THR:HG21	2.34	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: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:189:THR:HG21	1:A:306:GLN:HA	2.00	0.43
1:A:14:TYR:HB2	1:A:15:ARG:NH1	2.34	0.42
1:B:454:ALA:O	1:B:455:ASN:HB3	2.19	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:357:LEU:HD11	1:B:383:LEU:HA	2.01	0.42
1:A:195:ALA:O	1:A:199:VAL:HG13	2.18	0.42
1:B:268:TYR:CG	1:B:268:TYR:O	2.71	0.42
1:A:91:LYS:O	1:A:94:TYR:HB3	2.19	0.42
1:B:91:LYS:O	1:B: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:54:GLU:O	1:B:57:HIS: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:357:LEU:HB3	1:A:360:ILE:CD1	2.48	0.42
1:B:86:GLN:O	1:B:87:TRP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLN:HB3	1:B:497:PRO:CG	2.49	0.42
1:A:342:ILE:HG23	1:A:345:VAL:HG21	2.00	0.42
1:A:505:THR:CG2	1:A:505:THR:O	2.67	0.42
1:A:74:ARG:NH2	1:B:295:ARG:NH2	2.66	0.42
1:A:466:GLY:C	1:A:468:ASP:N	2.72	0.42
1:B:539:ILE:HA	1:B:539:ILE:HD12	1.71	0.42
1:A:251:ILE:CG2	1:A:298:VAL:HG22	2.49	0.42
1:B:495:ASN:HD21	1:B:527:ARG:HH22	1.68	0.42
1:A:496:PRO:O	1:A:527:ARG:NH1	2.53	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: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: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:B:127:ASP:OD1	1:B:313:ARG:HD3	2.19	0.42
1:A:454:ALA:O	1:A:455:ASN:HB3	2.19	0.42
1:A:291:PHE:N	1:A:291:PHE:CD1	2.88	0.42
1:B:185:LEU:CB	1:B:305:THR:HG21	2.44	0.42
1:A:27:PHE:H	1:A:27:PHE:HD1	1.67	0.42
1:B:145:ASP:O	1:B:149:ILE:HG13	2.20	0.42
1:B:474:ARG:HH11	1:B:474:ARG:HG3	1.85	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:A:570:GLU:OE1	1:A:574:SER:HB2	2.20	0.42
1:A:207:VAL:HG13	1:B:112:TYR:CE2	2.55	0.42
1:A:233:PHE:HE2	1:B:97:ARG:HH12	1.68	0.42
1:B:570:GLU:OE1	1:B:574:SER:HB2	2.20	0.42
1:A:263:ILE:CG2	1:B:63:ILE:HD11	2.33	0.42
1:A:274:SER:OG	1:A:275:ILE:N	2.53	0.42
3:A:700:ADP:C5	1:B:477:LYS:HA	2.54	0.42
1:A:178:VAL:HG13	1:A:301:PHE:CD1	2.55	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
1:A:455:ASN:OD1	1:A:455:ASN:O	2.38	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:536:LEU:H	1:A:536:LEU:HD23	1.85	0.41
1:B:505:THR:CG2	1:B:505:THR:O	2.67	0.41

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLY:O	1:A:26:LYS:HB2	2.20	0.41
1:A:86:GLN:O	1:A:87:TRP:C	2.58	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:B:558:THR:HB	1:B:561:GLU:CG	2.37	0.41
1:B:466:GLY:C	1:B:468:ASP:N	2.72	0.41
1:B:71:VAL:CG1	1:B:71:VAL:O	2.68	0.41
1:A:171:PHE:CB	1:A:172:PRO:HD3	2.50	0.41
1:B:265:VAL:O	1:B:269:LEU:HG	2.21	0.41
1:A:357:LEU:HD22	1:A:360:ILE:CD1	2.50	0.41
1:A:453:MET:CE	1:A:453:MET:HA	2.50	0.41
1:B:397:GLN:NE2	1:B:399:LEU:HD11	2.25	0.41
1:A:509:ASP:OD2	1:A:511:GLU:HB3	2.20	0.41
1:B:291:PHE:N	1:B:291:PHE:CD1	2.88	0.41
1:A:416:GLN:HB3	1:A:497:PRO:CG	2.50	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:28:GLY:O	1:A:32:LEU:HG	2.20	0.41
1:A:74:ARG:HB3	1:A:75:PRO:HD3	2.03	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:B:345:VAL:HG13	1:B:393:VAL:CG2	2.51	0.41
1:B:455:ASN:OD1	1:B:455:ASN:O	2.38	0.41
1:B:508:LEU:HD13	1:B:516:ILE:HD12	2.03	0.41
1:B:339:ARG:O	1:B:400:ILE:HA	2.21	0.41
1:B:266:GLY:O	1:B:280:LEU:HD13	2.21	0.41
1:B:425:ILE:HG22	1:B:426:LEU:N	2.35	0.41
1:B:153:LEU:HA	1:B:153:LEU:HD23	1.84	0.41
1:A:169:PHE:CD2	1:A:261:ILE:CD1	3.04	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: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:342:ILE:O	1:A:361:ASN:HA	2.21	0.41
1:A:112:TYR:CE2	1:B:207:VAL:HG13	2.56	0.41
1:B:170:ILE:HD11	1:B:257:ILE:CG2	2.50	0.40
1:A:448:VAL:HG12	1:A:452:LYS:HE3	2.03	0.40
1:B:12:TYR:CZ	1:B:91:LYS:HG2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:TYR:CZ	1:A:91:LYS:HG2	2.57	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:339:ARG:O	1:A:400:ILE:HA	2.22	0.40
1:A:70:PHE:CD2	1:B:256:ASP:HB3	2.49	0.40
1:A:47:ASN:HD22	1:A:50:LEU:HD21	1.85	0.40
1:B:251:ILE:HG21	1:B:298:VAL:HG22	2.02	0.40
1:B:267:ALA:O	1:B:269:LEU:N	2.55	0.40
1:B:496:PRO:O	1:B:527:ARG:NH1	2.54	0.40
1:A:207:VAL:O	1:A:210:ILE:HG13	2.20	0.40
1:B:461:MET:HE2	1:B:461:MET:HA	2.03	0.40
1:B:289:LEU:HD23	1:B:289:LEU:HA	1.76	0.40
1:B:570:GLU:OE1	1:B:570:GLU:C	2.60	0.40
1:B:266:GLY:CA	1:B:280:LEU:HD11	2.50	0.40
1:B:23:GLY:O	1:B:26:LYS:HB2	2.20	0.40
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.92	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 (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	576/578 (100%)	487 (84%)	73 (13%)	16 (3%)	6	30
1	B	576/578 (100%)	480 (83%)	80 (14%)	16 (3%)	6	30
All	All	1152/1156 (100%)	967 (84%)	153 (13%)	32 (3%)	6	30

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/499 (100%)	474 (95%)	25 (5%)	30	70
1	B	499/499 (100%)	473 (95%)	26 (5%)	29	68
All	All	998/998 (100%)	947 (95%)	51 (5%)	29	69

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	-	22,29,29	1.31	2 (9%)	27,45,45	2.77	6 (22%)
3	ADP	B	701	-	22,29,29	1.27	2 (9%)	27,45,45	2.79	6 (22%)

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	-2.44	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	ADP	C8-N7	-2.42	1.30	1.34
3	B	701	ADP	O4'-C1'	3.80	1.46	1.41
3	A	700	ADP	O4'-C1'	4.06	1.46	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	ADP	N3-C2-N1	-9.49	121.63	128.89
3	A	700	ADP	N3-C2-N1	-9.27	121.80	128.89
3	A	700	ADP	PA-O3A-PB	-8.17	105.28	132.67
3	B	701	ADP	PA-O3A-PB	-8.16	105.31	132.67
3	A	700	ADP	C2'-C1'-N9	-3.66	108.71	114.29
3	B	701	ADP	C2'-C1'-N9	-3.39	109.11	114.29
3	B	701	ADP	C4-C5-N7	-2.44	107.23	109.48
3	A	700	ADP	C4-C5-N7	-2.32	107.35	109.48
3	A	700	ADP	O2A-PA-O3A	2.08	114.55	105.09
3	B	701	ADP	O2A-PA-O3A	2.09	114.59	105.09
3	B	701	ADP	C2'-C3'-C4'	2.21	107.15	102.61
3	A	700	ADP	C2'-C3'-C4'	2.29	107.31	102.61

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%)	-0.51	2 (0%)	94	84	56, 97, 162, 200	2 (0%)
1	B	578/578 (100%)	-0.47	4 (0%)	89	70	54, 95, 162, 200	2 (0%)
All	All	1156/1156 (100%)	-0.49	6 (0%)	91	76	54, 96, 162, 200	4 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	ASN	6.0
1	B	46	ASN	4.6
1	B	48	HIS	3.1
1	A	286	TYR	2.8
1	A	578	LEU	2.7
1	B	55	LYS	2.6

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	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.