



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:24 AM GMT

PDB ID : 3OWG
Title : Crystal structure of vaccinia virus Polyadenylate polymerase(vp55)
Authors : Li, C.; Li, H.; Zhou, S.; Gershon, P.D.; Poulos, T.L.
Deposited on : 2010-09-17
Resolution : 2.86 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 (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

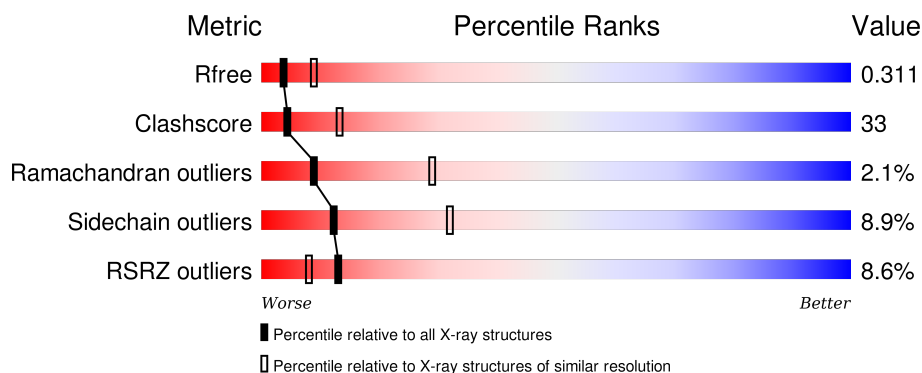
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	485	
1	B	485	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7436 atoms, of which 0 are hydrogens and 0 are deuteriums.

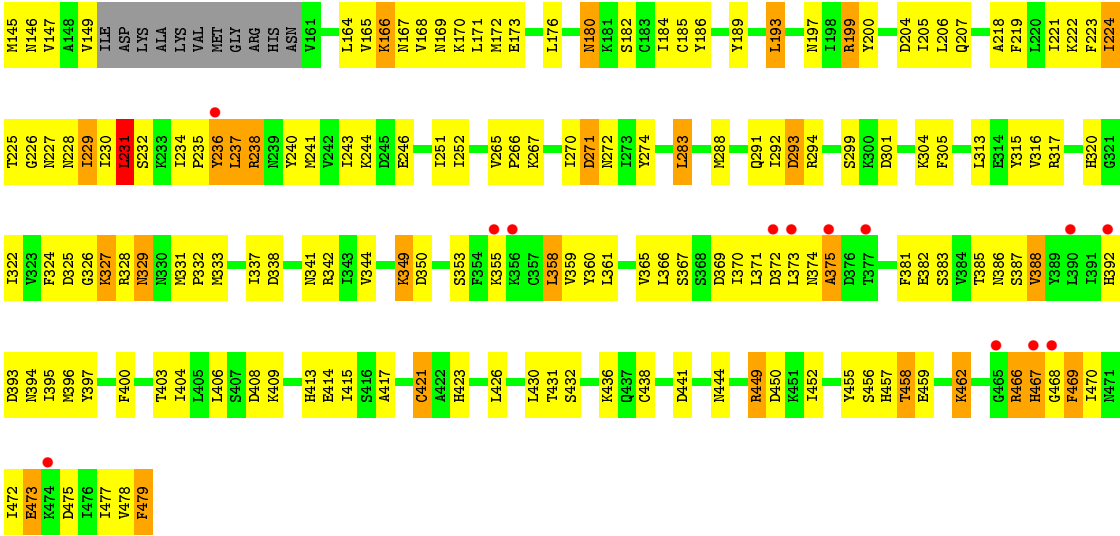
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Poly(A) polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3718	2377	620	697	24			
1	B	457	Total	C	N	O	S	0	0	0
			3718	2377	620	697	24			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP P23371
A	-4	HIS	-	EXPRESSION TAG	UNP P23371
A	-3	HIS	-	EXPRESSION TAG	UNP P23371
A	-2	HIS	-	EXPRESSION TAG	UNP P23371
A	-1	HIS	-	EXPRESSION TAG	UNP P23371
A	0	HIS	-	EXPRESSION TAG	UNP P23371
A	36	SER	LEU	ENGINEERED MUTATION	UNP P23371
B	-5	HIS	-	EXPRESSION TAG	UNP P23371
B	-4	HIS	-	EXPRESSION TAG	UNP P23371
B	-3	HIS	-	EXPRESSION TAG	UNP P23371
B	-2	HIS	-	EXPRESSION TAG	UNP P23371
B	-1	HIS	-	EXPRESSION TAG	UNP P23371
B	0	HIS	-	EXPRESSION TAG	UNP P23371
B	36	SER	LEU	ENGINEERED MUTATION	UNP P23371



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	80.13 Å 161.29 Å 97.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.77 – 2.86 41.77 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.77-2.86) 99.4 (41.77-2.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.86 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.253 , 0.316 0.252 , 0.311	Depositor DCC
R_{free} test set	1465 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 82.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 29693 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7436	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.53	1/3780 (0.0%)	0.71	0/5101
1	B	0.62	4/3780 (0.1%)	0.76	1/5101 (0.0%)
All	All	0.58	5/7560 (0.1%)	0.74	1/10202 (0.0%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	SER	CB-OG	10.97	1.56	1.42
1	A	124	SER	CB-OG	8.85	1.53	1.42
1	B	185	CYS	CB-SG	-6.84	1.70	1.82
1	B	125	SER	CB-OG	6.01	1.50	1.42
1	B	124	SER	CA-CB	5.11	1.60	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	LEU	CA-CB-CG	5.17	127.18	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	89	TYR	Sidechain

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	3718	0	3789	262	0
1	B	3718	0	3789	245	0
All	All	7436	0	7578	492	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 33.

All (492) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:THR:HB	1:A:349:LYS:HD2	1.22	1.10
1:A:335:CYS:HA	1:A:346:VAL:HG12	1.32	1.08
1:A:225:THR:HG22	1:A:227:ASN:H	1.20	1.03
1:B:225:THR:HG22	1:B:227:ASN:H	1.16	1.03
1:B:238:ARG:HB3	1:B:238:ARG:NH1	1.74	1.02
1:A:27:SER:HB3	1:A:30:GLU:HG3	1.42	1.02
1:A:288:MET:HG2	1:A:294:ARG:HG3	1.42	1.02
1:A:222:LYS:HD2	1:A:472:ILE:CG2	1.90	1.01
1:A:324:PHE:HA	1:A:444:ASN:HD21	1.21	1.01
1:B:27:SER:HB3	1:B:30:GLU:HG3	1.43	1.01
1:B:304:LYS:HE3	1:B:305:PHE:HE1	1.28	0.99
1:A:328:ARG:HG3	1:A:329:ASN:H	1.28	0.98
1:B:238:ARG:HB3	1:B:238:ARG:HH11	1.27	0.96
1:A:328:ARG:CG	1:A:329:ASN:H	1.77	0.96
1:A:222:LYS:HD2	1:A:472:ILE:HG23	1.46	0.95
1:B:288:MET:HG2	1:B:294:ARG:HG3	1.51	0.93
1:A:238:ARG:NH1	1:A:238:ARG:HB3	1.83	0.92
1:B:222:LYS:HD2	1:B:472:ILE:HG21	1.53	0.88
1:A:238:ARG:HB3	1:A:238:ARG:HH11	1.40	0.87
1:A:469:PHE:H	1:A:478:VAL:HG23	1.37	0.86
1:A:196:PRO:HG2	1:B:197:ASN:HA	1.57	0.86
1:A:468:GLY:HA3	1:A:478:VAL:O	1.77	0.85
1:B:449:ARG:HH11	1:B:449:ARG:HG3	1.40	0.85
1:B:304:LYS:HE3	1:B:305:PHE:CE1	2.11	0.84
1:A:229:ILE:CD1	1:A:472:ILE:HG13	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LYS:HE3	1:A:305:PHE:HE1	1.43	0.84
1:B:222:LYS:HD2	1:B:472:ILE:CG2	2.07	0.84
1:B:31:TYR:O	1:B:35:LYS:HG3	1.78	0.83
1:A:328:ARG:HG3	1:A:329:ASN:N	1.93	0.83
1:A:347:THR:HB	1:A:349:LYS:CD	2.07	0.82
1:B:229:ILE:C	1:B:230:ILE:HD12	2.00	0.82
1:A:466:ARG:HG2	1:A:479:PHE:CG	2.14	0.82
1:A:229:ILE:HD11	1:A:472:ILE:HG13	1.60	0.81
1:A:139:ARG:HH21	1:B:166:LYS:HE2	1.45	0.81
1:A:196:PRO:CG	1:B:197:ASN:HA	2.10	0.80
1:A:316:VAL:HG22	1:A:322:ILE:HG13	1.62	0.80
1:A:343:ILE:HG22	1:A:344:VAL:H	1.44	0.80
1:A:333:MET:SD	1:A:421:CYS:SG	2.80	0.79
1:B:122:VAL:O	1:B:123:ILE:HD13	1.83	0.79
1:A:172:MET:HE2	1:A:205:ILE:HG21	1.64	0.79
1:B:329:ASN:HB2	1:B:331:MET:O	1.83	0.79
1:A:70:SER:HB3	1:A:73:GLU:HG3	1.64	0.78
1:B:225:THR:HG22	1:B:227:ASN:N	1.97	0.77
1:A:196:PRO:CB	1:B:197:ASN:HA	2.14	0.77
1:B:324:PHE:HA	1:B:444:ASN:HD21	1.48	0.77
1:B:366:LEU:O	1:B:370:ILE:HB	1.85	0.76
1:A:347:THR:CB	1:A:349:LYS:HD2	2.10	0.76
1:A:466:ARG:HG2	1:A:479:PHE:CB	2.16	0.76
1:B:238:ARG:CB	1:B:238:ARG:HH11	1.99	0.75
1:B:120:PRO:O	1:B:121:ASN:C	2.25	0.75
1:A:236:TYR:HB2	1:A:237:LEU:HD13	1.67	0.75
1:A:366:LEU:O	1:A:370:ILE:HB	1.85	0.75
1:B:413:HIS:HD2	1:B:415:ILE:H	1.34	0.75
1:A:320:HIS:HB3	1:A:436:LYS:HD2	1.69	0.74
1:A:266:PRO:HD3	1:A:430:LEU:HD23	1.69	0.74
1:B:218:ALA:HB1	1:B:229:ILE:HD11	1.67	0.74
1:B:131:VAL:HG23	1:B:131:VAL:O	1.85	0.74
1:B:468:GLY:HA3	1:B:478:VAL:O	1.88	0.74
1:A:324:PHE:CA	1:A:444:ASN:HD21	1.99	0.73
1:B:21:TYR:CZ	1:B:85:GLN:HG2	2.23	0.73
1:A:126:LYS:HE2	1:B:197:ASN:OD1	1.89	0.73
1:B:70:SER:HB3	1:B:73:GLU:HG3	1.69	0.73
1:A:304:LYS:HE3	1:A:305:PHE:CE1	2.22	0.73
1:A:466:ARG:HG2	1:A:479:PHE:HB2	1.71	0.73
1:B:49:LYS:O	1:B:53:VAL:HG23	1.89	0.73
1:B:316:VAL:HG22	1:B:322:ILE:HG13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:GLY:HA2	1:A:478:VAL:HB	1.70	0.72
1:A:21:TYR:CZ	1:A:85:GLN:HG2	2.24	0.72
1:A:49:LYS:O	1:A:53:VAL:HG23	1.88	0.72
1:B:93:LYS:HE2	1:B:475:ASP:HB2	1.71	0.72
1:B:349:LYS:HD2	1:B:350:ASP:N	2.05	0.71
1:A:164:LEU:HA	1:A:167:ASN:HD22	1.55	0.71
1:B:449:ARG:HG3	1:B:449:ARG:NH1	1.99	0.70
1:A:225:THR:HG22	1:A:227:ASN:N	2.03	0.70
1:B:349:LYS:HB3	1:B:355:LYS:HA	1.74	0.69
1:A:117:ILE:HG13	1:A:117:ILE:O	1.93	0.69
1:A:232:SER:HA	1:A:469:PHE:HB3	1.73	0.69
1:A:381:PHE:HB2	1:A:385:THR:OG1	1.93	0.69
1:B:48:ASN:OD1	1:B:51:ILE:HG22	1.92	0.69
1:B:172:MET:HE3	1:B:176:LEU:HG	1.75	0.69
1:A:48:ASN:OD1	1:A:51:ILE:HG22	1.92	0.69
1:B:236:TYR:HB2	1:B:237:LEU:HD13	1.75	0.69
1:A:139:ARG:NH2	1:B:166:LYS:HE2	2.08	0.68
1:A:336:ILE:HD12	1:A:336:ILE:H	1.58	0.68
1:B:469:PHE:H	1:B:478:VAL:HB	1.58	0.67
1:A:53:VAL:HG21	1:A:75:LYS:HG3	1.76	0.67
1:A:115:LEU:HD23	1:A:178:ARG:HG3	1.77	0.67
1:A:369:ASP:HA	1:A:372:ASP:OD2	1.95	0.67
1:B:468:GLY:CA	1:B:478:VAL:HB	2.25	0.67
1:A:228:ASN:CG	1:A:473:GLU:HB3	2.15	0.66
1:B:122:VAL:HG13	1:B:272:ASN:ND2	2.10	0.66
1:B:172:MET:HE2	1:B:205:ILE:HG21	1.76	0.66
1:A:131:VAL:HG23	1:A:131:VAL:O	1.96	0.66
1:A:324:PHE:HA	1:A:444:ASN:ND2	2.04	0.66
1:B:53:VAL:HG21	1:B:75:LYS:HG3	1.78	0.66
1:B:292:ILE:HG22	1:B:403:THR:HG21	1.77	0.66
1:A:122:VAL:HG11	1:A:272:ASN:ND2	2.10	0.66
1:B:468:GLY:HA2	1:B:478:VAL:HB	1.78	0.66
1:A:44:ILE:HD13	1:A:101:GLN:HE21	1.60	0.66
1:B:331:MET:HE1	1:B:438:CYS:SG	2.37	0.65
1:B:331:MET:HG2	1:B:333:MET:N	2.12	0.65
1:A:238:ARG:CB	1:A:238:ARG:HH11	2.09	0.65
1:B:70:SER:C	1:B:72:SER:H	2.00	0.65
1:A:189:TYR:O	1:A:193:LEU:HD22	1.97	0.65
1:A:343:ILE:HG22	1:A:344:VAL:N	2.11	0.65
1:B:466:ARG:CZ	1:B:466:ARG:HA	2.27	0.65
1:A:243:ILE:HD11	1:A:252:ILE:CG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:PHE:H	1:A:478:VAL:CG2	2.10	0.64
1:B:331:MET:HG2	1:B:332:PRO:C	2.17	0.64
1:A:236:TYR:N	1:A:236:TYR:CD2	2.62	0.64
1:B:462:LYS:O	1:B:462:LYS:HD2	1.97	0.64
1:A:243:ILE:HD11	1:A:252:ILE:HG22	1.78	0.64
1:B:349:LYS:N	1:B:355:LYS:O	2.30	0.64
1:A:288:MET:CG	1:A:294:ARG:HG3	2.24	0.64
1:A:84:LYS:HG3	1:A:97:ILE:HD13	1.79	0.64
1:B:393:ASP:O	1:B:394:ASN:HB2	1.97	0.64
1:A:379:CYS:O	1:A:388:VAL:HG22	1.98	0.64
1:B:164:LEU:HA	1:B:167:ASN:HD22	1.61	0.64
1:B:129:TYR:N	1:B:129:TYR:CD2	2.66	0.64
1:B:230:ILE:HD12	1:B:230:ILE:N	2.13	0.63
1:B:325:ASP:OD1	1:B:327:LYS:HE3	1.98	0.63
1:B:236:TYR:CD2	1:B:236:TYR:N	2.65	0.63
1:B:129:TYR:N	1:B:129:TYR:HD2	1.96	0.63
1:A:413:HIS:HD2	1:A:415:ILE:H	1.44	0.63
1:B:122:VAL:CG1	1:B:272:ASN:HD22	2.12	0.63
1:A:462:LYS:O	1:A:462:LYS:HD2	1.99	0.63
1:B:165:VAL:HG12	1:B:169:ASN:ND2	2.14	0.62
1:B:51:ILE:O	1:B:54:SER:HB3	1.99	0.62
1:B:117:ILE:O	1:B:117:ILE:HG13	1.98	0.62
1:B:165:VAL:HG12	1:B:169:ASN:HD21	1.65	0.62
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.65	0.62
1:B:301:ASP:OD2	1:B:304:LYS:HB2	2.00	0.62
1:B:199:ARG:HG2	1:B:199:ARG:HH11	1.64	0.62
1:A:346:VAL:HG23	1:A:346:VAL:O	1.99	0.61
1:A:31:TYR:O	1:A:35:LYS:HG3	2.00	0.61
1:A:229:ILE:HD13	1:A:229:ILE:H	1.64	0.61
1:A:229:ILE:C	1:A:230:ILE:HD12	2.21	0.61
1:B:221:ILE:O	1:B:225:THR:HB	1.99	0.61
1:B:326:GLY:O	1:B:328:ARG:N	2.34	0.61
1:B:413:HIS:HE1	1:B:452:ILE:O	1.84	0.61
1:A:468:GLY:CA	1:A:478:VAL:HB	2.30	0.61
1:A:165:VAL:HG12	1:A:169:ASN:ND2	2.15	0.61
1:A:337:ILE:HG13	1:A:344:VAL:HG22	1.83	0.61
1:A:197:ASN:HA	1:B:199:ARG:HH11	1.66	0.61
1:B:61:LYS:O	1:B:61:LYS:HD2	2.00	0.60
1:A:350:ASP:N	1:A:350:ASP:OD2	2.33	0.60
1:B:40:ASN:O	1:B:44:ILE:HG13	2.01	0.60
1:A:115:LEU:CD2	1:A:178:ARG:HG3	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:VAL:HG23	1:B:320:HIS:HD2	1.66	0.60
1:B:337:ILE:HG13	1:B:344:VAL:HG22	1.82	0.60
1:A:229:ILE:HD13	1:A:472:ILE:HG13	1.81	0.60
1:A:470:ILE:HG12	1:A:477:ILE:CD1	2.30	0.60
1:B:381:PHE:HB2	1:B:385:THR:OG1	2.02	0.59
1:B:186:TYR:CZ	1:B:204:ASP:HB3	2.38	0.59
1:A:122:VAL:HG11	1:A:272:ASN:HD21	1.66	0.59
1:B:331:MET:CB	1:B:332:PRO:HA	2.33	0.59
1:A:70:SER:H	1:A:73:GLU:CD	2.06	0.59
1:A:51:ILE:O	1:A:54:SER:HB3	2.02	0.59
1:B:367:SER:O	1:B:371:LEU:HD23	2.03	0.58
1:B:331:MET:CG	1:B:332:PRO:HA	2.34	0.58
1:A:186:TYR:CZ	1:A:204:ASP:HB3	2.38	0.58
1:B:466:ARG:NH1	1:B:466:ARG:HA	2.18	0.58
1:A:414:GLU:O	1:A:417:ALA:HB3	2.03	0.58
1:B:470:ILE:HG12	1:B:477:ILE:HD13	1.84	0.58
1:A:413:HIS:CE1	1:A:452:ILE:HB	2.38	0.58
1:B:369:ASP:HA	1:B:372:ASP:OD2	2.03	0.58
1:B:15:LEU:HD11	1:B:26:PRO:HG2	1.85	0.58
1:A:165:VAL:HG12	1:A:169:ASN:HD21	1.67	0.58
1:A:93:LYS:HE2	1:A:475:ASP:HB2	1.85	0.58
1:A:337:ILE:HG13	1:A:343:ILE:O	2.04	0.58
1:B:331:MET:CE	1:B:438:CYS:SG	2.92	0.58
1:B:375:ALA:HB3	1:B:392:HIS:CE1	2.38	0.58
1:B:228:ASN:OD1	1:B:473:GLU:HG2	2.03	0.57
1:B:122:VAL:CG1	1:B:272:ASN:ND2	2.67	0.57
1:B:83:SER:HA	1:B:85:GLN:OE1	2.04	0.57
1:B:78:ILE:HA	1:B:223:PHE:CE2	2.38	0.57
1:A:236:TYR:HB2	1:A:237:LEU:CD1	2.34	0.57
1:B:331:MET:HB3	1:B:332:PRO:HA	1.86	0.57
1:A:301:ASP:OD2	1:A:304:LYS:HB2	2.03	0.57
1:A:375:ALA:HB3	1:A:392:HIS:CE1	2.40	0.57
1:A:393:ASP:O	1:A:394:ASN:HB2	2.04	0.57
1:A:13:ILE:O	1:A:17:ILE:HG13	2.04	0.57
1:A:166:LYS:O	1:A:170:LYS:HG3	2.05	0.57
1:B:431:THR:O	1:B:432:SER:HB2	2.05	0.56
1:A:331:MET:HG2	1:A:442:LEU:HA	1.87	0.56
1:A:333:MET:SD	1:A:333:MET:N	2.77	0.56
1:B:329:ASN:ND2	1:B:331:MET:O	2.36	0.56
1:A:367:SER:O	1:A:371:LEU:HD23	2.05	0.56
1:A:466:ARG:CZ	1:A:466:ARG:HA	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:C	1:A:72:SER:H	2.07	0.56
1:B:12:ASN:OD1	1:B:14:THR:HB	2.05	0.56
1:A:229:ILE:HB	1:A:244:LYS:O	2.05	0.56
1:A:222:LYS:HB2	1:A:472:ILE:HG21	1.87	0.56
1:A:230:ILE:N	1:A:230:ILE:HD12	2.20	0.56
1:A:224:ILE:HG22	1:A:225:THR:N	2.20	0.56
1:A:61:LYS:HD2	1:A:61:LYS:O	2.05	0.56
1:B:234:ILE:HD12	1:B:240:TYR:CE2	2.41	0.56
1:A:452:ILE:HG22	1:A:453:PRO:HD2	1.88	0.56
1:A:132:THR:HA	1:A:135:GLU:HG3	1.88	0.56
1:B:139:ARG:HB2	1:B:139:ARG:NH1	2.21	0.56
1:B:392:HIS:O	1:B:395:ILE:HB	2.07	0.55
1:A:17:ILE:HD13	1:A:42:GLN:HB2	1.89	0.55
1:B:44:ILE:HD13	1:B:101:GLN:HE21	1.72	0.55
1:A:339:GLU:HG3	1:A:409:LYS:NZ	2.21	0.55
1:B:70:SER:H	1:B:73:GLU:CD	2.09	0.55
1:B:47:PHE:CG	1:B:105:VAL:HG22	2.41	0.55
1:B:413:HIS:CD2	1:B:415:ILE:H	2.21	0.55
1:B:235:PRO:HG3	1:B:467:HIS:CE1	2.41	0.55
1:B:288:MET:CG	1:B:294:ARG:HG3	2.32	0.54
1:B:229:ILE:HB	1:B:244:LYS:O	2.06	0.54
1:B:331:MET:HG2	1:B:332:PRO:HA	1.88	0.54
1:A:392:HIS:O	1:A:395:ILE:HB	2.06	0.54
1:A:336:ILE:HD12	1:A:336:ILE:N	2.22	0.54
1:B:370:ILE:HG22	1:B:371:LEU:HD22	1.89	0.54
1:A:170:LYS:HA	1:A:173:GLU:HG3	1.88	0.54
1:B:17:ILE:HD13	1:B:42:GLN:HB2	1.90	0.54
1:A:258:ARG:HB2	1:A:260:ASP:HB3	1.88	0.54
1:A:345:THR:OG1	1:A:356:LYS:HD2	2.08	0.54
1:A:218:ALA:HB1	1:A:229:ILE:HD11	1.88	0.54
1:B:371:LEU:C	1:B:373:LEU:H	2.11	0.54
1:B:165:VAL:CG1	1:B:169:ASN:HD21	2.20	0.54
1:A:431:THR:O	1:A:432:SER:HB2	2.08	0.54
1:B:469:PHE:N	1:B:478:VAL:HB	2.22	0.54
1:B:266:PRO:HD3	1:B:430:LEU:HD23	1.89	0.54
1:B:329:ASN:C	1:B:331:MET:H	2.12	0.53
1:B:365:VAL:HG12	1:B:365:VAL:O	2.08	0.53
1:B:134:MET:HG2	1:B:313:LEU:HB2	1.89	0.53
1:B:342:ARG:HB3	1:B:361:LEU:HB2	1.90	0.53
1:B:131:VAL:CG2	1:B:131:VAL:O	2.57	0.53
1:B:331:MET:CB	1:B:332:PRO:CA	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:O	1:A:103:VAL:HG23	2.09	0.53
1:A:358:LEU:HD23	1:A:397:TYR:CE2	2.44	0.53
1:A:111:ILE:HG23	1:A:175:TYR:HE1	1.74	0.53
1:B:224:ILE:HG22	1:B:225:THR:N	2.23	0.52
1:B:172:MET:CE	1:B:205:ILE:HG21	2.38	0.52
1:B:69:THR:HG21	1:B:74:ILE:HG13	1.91	0.52
1:B:77:ARG:NE	1:B:226:GLY:HA2	2.24	0.52
1:A:328:ARG:CG	1:A:329:ASN:N	2.53	0.52
1:A:69:THR:HG21	1:A:74:ILE:HG13	1.92	0.52
1:A:180:ASN:ND2	1:A:272:ASN:O	2.42	0.52
1:B:125:SER:O	1:B:126:LYS:HG2	2.10	0.52
1:A:137:LEU:O	1:A:141:MET:HG3	2.10	0.52
1:B:104:LEU:HD11	1:B:219:PHE:CD2	2.44	0.52
1:A:15:LEU:HD11	1:A:26:PRO:HG2	1.92	0.52
1:A:236:TYR:N	1:A:236:TYR:HD2	2.08	0.52
1:B:125:SER:OG	1:B:271:ASP:HB3	2.10	0.52
1:B:84:LYS:HG3	1:B:97:ILE:HD13	1.91	0.52
1:B:137:LEU:O	1:B:141:MET:HG3	2.10	0.52
1:A:40:ASN:O	1:A:44:ILE:HG13	2.09	0.51
1:A:371:LEU:C	1:A:373:LEU:H	2.14	0.51
1:A:117:ILE:CG1	1:A:178:ARG:HH21	2.23	0.51
1:A:189:TYR:CE2	1:A:193:LEU:HD21	2.45	0.51
1:A:131:VAL:O	1:A:135:GLU:HG3	2.10	0.51
1:A:172:MET:HE3	1:A:176:LEU:HG	1.92	0.51
1:A:270:ILE:HG22	1:A:271:ASP:OD1	2.11	0.51
1:A:473:GLU:CG	1:A:474:LYS:HD2	2.41	0.51
1:A:139:ARG:HB2	1:A:139:ARG:NH1	2.24	0.51
1:B:170:LYS:HA	1:B:173:GLU:HG3	1.92	0.51
1:B:232:SER:HA	1:B:469:PHE:HB3	1.93	0.51
1:A:197:ASN:HA	1:B:199:ARG:HG2	1.92	0.51
1:A:336:ILE:HB	1:A:345:THR:HG23	1.91	0.51
1:A:58:LYS:HB3	1:A:116:THR:HG21	1.92	0.51
1:B:228:ASN:O	1:B:246:GLU:HG3	2.11	0.50
1:B:53:VAL:O	1:B:57:LYS:HG3	2.11	0.50
1:B:63:PHE:O	1:B:167:ASN:HB3	2.11	0.50
1:A:77:ARG:HD2	1:A:223:PHE:O	2.11	0.50
1:B:413:HIS:CD2	1:B:414:GLU:N	2.79	0.50
1:A:53:VAL:O	1:A:57:LYS:HG3	2.11	0.50
1:A:48:ASN:CG	1:A:51:ILE:HG22	2.31	0.50
1:B:270:ILE:HG22	1:B:271:ASP:OD1	2.12	0.50
1:A:172:MET:CE	1:A:205:ILE:HG21	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:CD1	1:A:237:LEU:N	2.75	0.50
1:A:320:HIS:CB	1:A:436:LYS:HD2	2.38	0.50
1:B:115:LEU:HD12	1:B:171:LEU:HD11	1.93	0.50
1:B:406:LEU:HD12	1:B:457:HIS:HA	1.94	0.50
1:A:413:HIS:CD2	1:A:415:ILE:H	2.29	0.50
1:A:370:ILE:HG22	1:A:371:LEU:HD22	1.94	0.49
1:A:243:ILE:O	1:A:251:ILE:HB	2.11	0.49
1:B:180:ASN:ND2	1:B:272:ASN:O	2.45	0.49
1:B:70:SER:C	1:B:72:SER:N	2.64	0.49
1:A:12:ASN:OD1	1:A:14:THR:HB	2.12	0.49
1:B:331:MET:HG2	1:B:332:PRO:CA	2.42	0.49
1:A:231:LEU:O	1:A:469:PHE:HB2	2.12	0.49
1:B:409:LYS:HD3	1:B:455:TYR:HE2	1.78	0.49
1:A:352:PHE:HE1	1:A:434:GLU:O	1.96	0.49
1:A:228:ASN:ND2	1:A:473:GLU:HB3	2.26	0.49
1:A:69:THR:HG23	1:A:73:GLU:HB2	1.95	0.49
1:B:166:LYS:O	1:B:170:LYS:HG3	2.13	0.49
1:B:317:ARG:HG3	1:B:322:ILE:O	2.13	0.49
1:A:123:ILE:CD1	1:B:130:ASN:HD21	2.25	0.49
1:A:329:ASN:O	1:A:330:ASN:HB3	2.13	0.49
1:A:336:ILE:HB	1:A:345:THR:CG2	2.42	0.48
1:B:469:PHE:O	1:B:469:PHE:HD1	1.96	0.48
1:B:243:ILE:HD11	1:B:252:ILE:CG2	2.43	0.48
1:B:222:LYS:HD2	1:B:472:ILE:HG23	1.92	0.48
1:B:235:PRO:HG3	1:B:467:HIS:ND1	2.28	0.48
1:B:94:LEU:O	1:B:98:ILE:HG13	2.14	0.48
1:A:195:ASN:ND2	1:A:198:ILE:HG12	2.28	0.48
1:B:73:GLU:O	1:B:77:ARG:HG3	2.13	0.48
1:B:293:ASP:OD2	1:B:293:ASP:N	2.45	0.48
1:B:132:THR:HA	1:B:135:GLU:HG3	1.94	0.48
1:B:338:ASP:CG	1:B:341:ASN:HD22	2.16	0.48
1:B:291:GLN:OE1	1:B:403:THR:N	2.44	0.48
1:B:184:ILE:HG22	1:B:274:TYR:HB2	1.96	0.48
1:B:382:GLU:O	1:B:386:ASN:HA	2.14	0.48
1:B:358:LEU:HD23	1:B:397:TYR:CE2	2.49	0.48
1:A:395:ILE:HG22	1:A:396:MET:N	2.27	0.48
1:A:468:GLY:CA	1:A:478:VAL:O	2.57	0.48
1:B:236:TYR:HD2	1:B:236:TYR:N	2.12	0.47
1:A:337:ILE:HG23	1:A:337:ILE:O	2.13	0.47
1:B:329:ASN:C	1:B:331:MET:N	2.67	0.47
1:B:414:GLU:O	1:B:417:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ASN:HD21	1:B:299:SER:HA	1.79	0.47
1:A:473:GLU:OE1	1:A:474:LYS:HE3	2.15	0.47
1:A:231:LEU:HB3	1:A:470:ILE:HB	1.96	0.47
1:A:73:GLU:O	1:A:77:ARG:HG3	2.14	0.47
1:B:48:ASN:CG	1:B:51:ILE:HG22	2.34	0.47
1:A:235:PRO:HG2	1:A:236:TYR:CD2	2.49	0.47
1:A:134:MET:HA	1:A:134:MET:CE	2.43	0.47
1:B:265:VAL:O	1:B:267:LYS:HG3	2.15	0.47
1:B:243:ILE:HD11	1:B:252:ILE:HG22	1.96	0.47
1:A:57:LYS:HD2	1:A:71:ALA:HB1	1.97	0.47
1:B:99:GLU:O	1:B:103:VAL:HG23	2.14	0.47
1:A:360:TYR:CD1	1:A:366:LEU:HD13	2.50	0.47
1:B:69:THR:HG23	1:B:73:GLU:HB2	1.97	0.47
1:B:168:VAL:CG1	1:B:252:ILE:HD12	2.45	0.47
1:B:60:LYS:HA	1:B:224:ILE:CD1	2.44	0.47
1:A:317:ARG:HG3	1:A:322:ILE:O	2.15	0.47
1:B:373:LEU:O	1:B:374:ASN:HB2	2.15	0.47
1:A:339:GLU:HG3	1:A:409:LYS:HZ1	1.78	0.47
1:A:427:TYR:CE1	1:A:431:THR:HG21	2.50	0.47
1:A:145:MET:O	1:A:147:VAL:N	2.48	0.47
1:A:370:ILE:CG2	1:A:371:LEU:HD22	2.46	0.46
1:A:405:LEU:HD22	1:A:454:ILE:HD13	1.97	0.46
1:B:13:ILE:O	1:B:17:ILE:HG13	2.14	0.46
1:B:58:LYS:HB3	1:B:116:THR:HG21	1.97	0.46
1:A:102:SER:O	1:A:106:THR:HG23	2.15	0.46
1:B:333:MET:SD	1:B:421:CYS:SG	3.13	0.46
1:A:146:ASN:HD21	1:A:299:SER:HA	1.81	0.46
1:B:431:THR:O	1:B:432:SER:CB	2.63	0.46
1:A:64:PHE:O	1:A:67:VAL:HG23	2.14	0.46
1:A:137:LEU:HD11	1:A:447:MET:CE	2.45	0.46
1:B:338:ASP:OD2	1:B:341:ASN:ND2	2.37	0.46
1:B:238:ARG:HB3	1:B:238:ARG:CZ	2.44	0.46
1:A:469:PHE:N	1:A:478:VAL:HG23	2.19	0.46
1:A:466:ARG:NH1	1:A:466:ARG:HA	2.30	0.46
1:A:165:VAL:CG1	1:A:169:ASN:HD21	2.28	0.46
1:A:200:TYR:CD1	1:A:200:TYR:C	2.89	0.46
1:A:231:LEU:HD11	1:A:241:MET:CE	2.46	0.46
1:A:139:ARG:CB	1:A:139:ARG:NH1	2.79	0.46
1:B:466:ARG:HG2	1:B:479:PHE:CD1	2.50	0.46
1:B:423:HIS:HA	1:B:426:LEU:HD12	1.98	0.46
1:B:230:ILE:CD1	1:B:230:ILE:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:TYR:CD1	1:B:366:LEU:HD13	2.51	0.46
1:B:237:LEU:N	1:B:237:LEU:CD1	2.78	0.46
1:A:130:ASN:C	1:A:132:THR:H	2.19	0.45
1:B:271:ASP:O	1:B:272:ASN:HB2	2.15	0.45
1:B:457:HIS:HD2	1:B:458:THR:O	1.99	0.45
1:A:329:ASN:C	1:A:331:MET:H	2.19	0.45
1:A:470:ILE:HG12	1:A:477:ILE:HD12	1.98	0.45
1:A:427:TYR:CZ	1:A:431:THR:HG21	2.50	0.45
1:A:280:PHE:CZ	1:A:426:LEU:HD22	2.51	0.45
1:B:331:MET:HB3	1:B:332:PRO:CA	2.47	0.45
1:A:47:PHE:CG	1:A:105:VAL:HG22	2.51	0.45
1:A:228:ASN:O	1:A:246:GLU:HG3	2.17	0.45
1:B:120:PRO:O	1:B:122:VAL:N	2.48	0.45
1:A:21:TYR:OH	1:A:101:GLN:NE2	2.48	0.45
1:A:58:LYS:HB3	1:A:116:THR:CG2	2.46	0.45
1:A:222:LYS:HG3	1:A:228:ASN:HD22	1.82	0.45
1:A:70:SER:C	1:A:72:SER:N	2.70	0.45
1:A:117:ILE:O	1:A:117:ILE:CG1	2.64	0.45
1:A:452:ILE:CG2	1:A:453:PRO:HD2	2.46	0.45
1:A:342:ARG:NH2	1:A:362:ASP:OD1	2.44	0.45
1:A:344:VAL:O	1:A:346:VAL:HG13	2.16	0.45
1:A:128:SER:OG	1:B:126:LYS:HE3	2.16	0.45
1:A:83:SER:HA	1:A:85:GLN:OE1	2.17	0.45
1:B:404:ILE:HB	1:B:458:THR:CG2	2.46	0.45
1:A:123:ILE:CD1	1:B:130:ASN:ND2	2.80	0.45
1:A:473:GLU:HG2	1:A:474:LYS:HD2	1.98	0.45
1:B:123:ILE:HA	1:B:123:ILE:HD13	1.69	0.45
1:B:387:SER:OG	1:B:388:VAL:N	2.50	0.45
1:B:199:ARG:CG	1:B:199:ARG:HH11	2.30	0.44
1:A:265:VAL:HA	1:A:430:LEU:CD2	2.47	0.44
1:B:96:THR:HG23	1:B:477:ILE:HG12	1.99	0.44
1:B:58:LYS:HB3	1:B:116:THR:CG2	2.47	0.44
1:A:423:HIS:HA	1:A:426:LEU:HD12	1.99	0.44
1:A:470:ILE:HG12	1:A:477:ILE:HD13	2.00	0.44
1:A:58:LYS:CB	1:A:116:THR:HG21	2.47	0.44
1:B:64:PHE:O	1:B:67:VAL:HG23	2.17	0.44
1:A:48:ASN:HB3	1:A:51:ILE:CG2	2.48	0.44
1:B:235:PRO:HG2	1:B:236:TYR:CD2	2.53	0.44
1:B:395:ILE:HG22	1:B:396:MET:N	2.32	0.44
1:B:182:SER:O	1:B:207:GLN:HA	2.18	0.44
1:A:94:LEU:O	1:A:98:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LYS:HA	1:B:224:ILE:HD13	1.99	0.44
1:A:265:VAL:HA	1:A:430:LEU:HD23	1.99	0.44
1:A:303:GLU:OE1	1:B:166:LYS:NZ	2.48	0.44
1:B:122:VAL:HG11	1:B:272:ASN:HD22	1.83	0.44
1:B:408:ASP:OD1	1:B:409:LYS:N	2.51	0.44
1:B:243:ILE:O	1:B:251:ILE:HB	2.17	0.44
1:B:25:VAL:HA	1:B:26:PRO:HD2	1.82	0.44
1:A:340:ASN:C	1:A:342:ARG:H	2.20	0.44
1:B:131:VAL:O	1:B:135:GLU:HG3	2.18	0.44
1:A:413:HIS:CD2	1:A:414:GLU:N	2.85	0.43
1:B:189:TYR:O	1:B:193:LEU:HD22	2.18	0.43
1:A:365:VAL:HG12	1:A:365:VAL:O	2.17	0.43
1:B:231:LEU:HD11	1:B:241:MET:CE	2.47	0.43
1:A:147:VAL:HG12	1:A:451:LYS:HE2	2.01	0.43
1:A:359:VAL:CG1	1:A:400:PHE:HB2	2.48	0.43
1:B:44:ILE:HG21	1:B:101:GLN:NE2	2.33	0.43
1:A:269:PHE:CZ	1:A:272:ASN:HA	2.52	0.43
1:B:315:TYR:CD2	1:B:315:TYR:C	2.91	0.43
1:B:168:VAL:HG11	1:B:252:ILE:HB	2.01	0.43
1:B:58:LYS:O	1:B:62:ARG:HB2	2.19	0.43
1:A:129:TYR:CE2	1:A:194:ILE:HG23	2.54	0.43
1:A:413:HIS:O	1:A:414:GLU:C	2.55	0.43
1:A:466:ARG:HD2	1:A:479:PHE:CD2	2.53	0.43
1:A:373:LEU:O	1:A:374:ASN:HB2	2.19	0.43
1:B:292:ILE:CG2	1:B:403:THR:HG21	2.47	0.43
1:B:139:ARG:CB	1:B:139:ARG:NH1	2.82	0.43
1:B:359:VAL:CG1	1:B:400:PHE:HB2	2.49	0.43
1:A:231:LEU:HD11	1:A:241:MET:HE1	2.01	0.43
1:B:459:GLU:OE1	1:B:459:GLU:HA	2.19	0.43
1:A:228:ASN:OD1	1:A:473:GLU:HB3	2.19	0.43
1:A:214:LEU:HB3	1:A:231:LEU:CD2	2.49	0.43
1:B:69:THR:CG2	1:B:74:ILE:HG13	2.48	0.43
1:A:366:LEU:HD22	1:A:399:TYR:HB2	2.01	0.42
1:B:57:LYS:HD2	1:B:71:ALA:HB1	2.01	0.42
1:A:112:LEU:HD13	1:A:220:LEU:HD22	2.02	0.42
1:B:70:SER:O	1:B:72:SER:N	2.53	0.42
1:B:125:SER:O	1:B:126:LYS:CG	2.66	0.42
1:A:186:TYR:CE2	1:A:204:ASP:HB3	2.54	0.42
1:A:198:ILE:HD13	1:A:307:ALA:HB1	2.00	0.42
1:B:370:ILE:CG2	1:B:371:LEU:HD22	2.49	0.42
1:A:359:VAL:HG11	1:A:400:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PRO:O	1:B:199:ARG:CG	2.68	0.42
1:A:199:ARG:CG	1:A:199:ARG:HH11	2.30	0.42
1:A:348:THR:OG1	1:A:354:PHE:O	2.37	0.42
1:A:139:ARG:CB	1:A:139:ARG:HH11	2.33	0.42
1:A:373:LEU:HB3	1:A:392:HIS:CD2	2.55	0.42
1:B:21:TYR:OH	1:B:85:GLN:HG2	2.19	0.42
1:B:145:MET:O	1:B:147:VAL:N	2.53	0.42
1:B:291:GLN:HE22	1:B:403:THR:HG23	1.85	0.42
1:A:466:ARG:HD2	1:A:479:PHE:CE2	2.55	0.41
1:B:83:SER:CA	1:B:85:GLN:OE1	2.67	0.41
1:B:205:ILE:O	1:B:206:LEU:HD23	2.20	0.41
1:B:291:GLN:OE1	1:B:403:THR:HG23	2.20	0.41
1:A:122:VAL:O	1:A:122:VAL:HG13	2.21	0.41
1:A:469:PHE:HD1	1:A:469:PHE:O	2.03	0.41
1:A:395:ILE:CG2	1:A:396:MET:N	2.83	0.41
1:A:21:TYR:OH	1:A:85:GLN:HG2	2.19	0.41
1:B:200:TYR:CD1	1:B:200:TYR:C	2.94	0.41
1:B:283:LEU:HD12	1:B:283:LEU:HA	1.89	0.41
1:B:238:ARG:CB	1:B:238:ARG:NH1	2.62	0.41
1:A:75:LYS:O	1:A:79:LEU:HG	2.20	0.41
1:B:48:ASN:HB3	1:B:51:ILE:CG2	2.51	0.41
1:A:81:TYR:CE2	1:A:219:PHE:CE2	3.08	0.41
1:B:75:LYS:O	1:B:79:LEU:HG	2.21	0.41
1:A:117:ILE:HD11	1:A:178:ARG:NH2	2.36	0.41
1:A:165:VAL:O	1:A:169:ASN:ND2	2.54	0.41
1:B:406:LEU:HD12	1:B:456:SER:O	2.20	0.41
1:B:409:LYS:HD3	1:B:455:TYR:CE2	2.53	0.41
1:A:293:ASP:OD2	1:A:293:ASP:N	2.52	0.41
1:A:343:ILE:O	1:A:344:VAL:CG2	2.69	0.41
1:A:336:ILE:CD1	1:A:336:ILE:H	2.32	0.41
1:A:123:ILE:HD13	1:B:130:ASN:ND2	2.36	0.41
1:A:382:GLU:O	1:A:386:ASN:HA	2.21	0.41
1:A:282:LEU:HD21	1:A:443:LEU:HD21	2.03	0.41
1:A:330:ASN:O	1:A:330:ASN:ND2	2.53	0.41
1:B:236:TYR:HB2	1:B:237:LEU:CD1	2.48	0.41
1:A:346:VAL:O	1:A:346:VAL:CG2	2.68	0.41
1:B:329:ASN:CB	1:B:331:MET:O	2.61	0.41
1:B:73:GLU:HG3	1:B:73:GLU:H	1.70	0.41
1:A:25:VAL:HA	1:A:26:PRO:HD2	1.86	0.41
1:B:166:LYS:HG3	1:B:167:ASN:H	1.86	0.41
1:B:100:LEU:HD21	1:B:470:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:VAL:HG11	1:B:400:PHE:HB2	2.02	0.41
1:B:326:GLY:H	1:B:444:ASN:ND2	2.18	0.40
1:B:58:LYS:CB	1:B:116:THR:HG21	2.51	0.40
1:A:64:PHE:C	1:A:66:ASP:N	2.73	0.40
1:A:129:TYR:CD2	1:A:194:ILE:HG22	2.56	0.40
1:A:135:GLU:OE2	1:B:170:LYS:HE2	2.21	0.40
1:A:69:THR:HA	1:A:73:GLU:OE2	2.21	0.40
1:B:189:TYR:CE2	1:B:193:LEU:HD21	2.55	0.40
1:A:316:VAL:HG23	1:A:320:HIS:HD2	1.87	0.40
1:A:117:ILE:HG13	1:A:178:ARG:HH21	1.87	0.40
1:A:449:ARG:HA	1:A:449:ARG:HD3	1.92	0.40
1:A:114:VAL:O	1:A:114:VAL:HG12	2.21	0.40
1:A:131:VAL:CG2	1:A:131:VAL:O	2.67	0.40
1:B:21:TYR:HE1	1:B:101:GLN:HE22	1.68	0.40
1:A:164:LEU:HA	1:A:167:ASN:ND2	2.31	0.40
1:B:404:ILE:HB	1:B:458:THR:HG23	2.03	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	453/485 (93%)	391 (86%)	53 (12%)	9 (2%)	9	30
1	B	453/485 (93%)	396 (87%)	47 (10%)	10 (2%)	8	27
All	All	906/970 (93%)	787 (87%)	100 (11%)	19 (2%)	9	29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	VAL
1	A	344	VAL

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Mol	Chain	Res	Type
1	A	355	LYS
1	B	131	VAL
1	B	327	LYS
1	A	146	ASN
1	A	467	HIS
1	A	126	LYS
1	A	375	ALA
1	B	27	SER
1	B	121	ASN
1	B	271	ASP
1	B	375	ALA
1	B	467	HIS
1	B	71	ALA
1	B	124	SER
1	A	224	ILE
1	A	349	LYS
1	B	224	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	433/459 (94%)	395 (91%)	38 (9%)	12	33
1	B	433/459 (94%)	394 (91%)	39 (9%)	12	31
All	All	866/918 (94%)	789 (91%)	77 (9%)	12	32

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	51	ILE
1	A	61	LYS
1	A	62	ARG
1	A	68	ASN
1	A	85	GLN

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Mol	Chain	Res	Type
1	A	124	SER
1	A	134	MET
1	A	149	VAL
1	A	166	LYS
1	A	180	ASN
1	A	193	LEU
1	A	229	ILE
1	A	231	LEU
1	A	236	TYR
1	A	237	LEU
1	A	238	ARG
1	A	254	SER
1	A	283	LEU
1	A	293	ASP
1	A	331	MET
1	A	333	MET
1	A	339	GLU
1	A	341	ASN
1	A	349	LYS
1	A	350	ASP
1	A	358	LEU
1	A	383	SER
1	A	388	VAL
1	A	421	CYS
1	A	436	LYS
1	A	441	ASP
1	A	458	THR
1	A	462	LYS
1	A	469	PHE
1	A	473	GLU
1	A	474	LYS
1	A	478	VAL
1	B	42	GLN
1	B	51	ILE
1	B	61	LYS
1	B	62	ARG
1	B	85	GLN
1	B	102	SER
1	B	127	ILE
1	B	129	TYR
1	B	131	VAL
1	B	134	MET

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Mol	Chain	Res	Type
1	B	149	VAL
1	B	166	LYS
1	B	180	ASN
1	B	193	LEU
1	B	199	ARG
1	B	229	ILE
1	B	231	LEU
1	B	236	TYR
1	B	237	LEU
1	B	238	ARG
1	B	283	LEU
1	B	293	ASP
1	B	329	ASN
1	B	349	LYS
1	B	353	SER
1	B	358	LEU
1	B	383	SER
1	B	388	VAL
1	B	421	CYS
1	B	436	LYS
1	B	441	ASP
1	B	449	ARG
1	B	450	ASP
1	B	458	THR
1	B	462	LYS
1	B	466	ARG
1	B	469	PHE
1	B	473	GLU
1	B	479	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	42	GLN
1	A	101	GLN
1	A	130	ASN
1	A	167	ASN
1	A	169	ASN
1	A	179	HIS
1	A	207	GLN
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	249	ASN
1	A	272	ASN
1	A	306	ASN
1	A	330	ASN
1	A	340	ASN
1	A	392	HIS
1	A	413	HIS
1	A	444	ASN
1	A	457	HIS
1	B	32	HIS
1	B	42	GLN
1	B	101	GLN
1	B	130	ASN
1	B	167	ASN
1	B	169	ASN
1	B	179	HIS
1	B	207	GLN
1	B	227	ASN
1	B	228	ASN
1	B	249	ASN
1	B	272	ASN
1	B	340	ASN
1	B	392	HIS
1	B	413	HIS
1	B	428	GLN
1	B	444	ASN
1	B	457	HIS

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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	457/485 (94%)	0.76	62 (13%) 4 2	49, 106, 176, 200	0
1	B	457/485 (94%)	0.08	17 (3%) 45 38	37, 71, 147, 200	0
All	All	914/970 (94%)	0.42	79 (8%) 13 8	37, 88, 167, 200	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	467	HIS	9.6
1	A	465	GLY	9.3
1	A	373	LEU	8.1
1	A	370	ILE	7.8
1	A	467	HIS	7.1
1	A	464	PRO	6.6
1	A	56	VAL	6.0
1	A	366	LEU	5.8
1	A	391	ILE	5.5
1	A	360	TYR	5.4
1	A	367	SER	5.4
1	B	124	SER	5.3
1	A	392	HIS	5.1
1	A	374	ASN	4.9
1	A	462	LYS	4.8
1	A	64	PHE	4.4
1	A	477	ILE	4.3
1	A	333	MET	4.2
1	B	373	LEU	4.2
1	B	468	GLY	3.8
1	A	463	LYS	3.8
1	A	375	ALA	3.8
1	B	372	ASP	3.7
1	A	332	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	142	LEU	3.5
1	A	61	LYS	3.5
1	A	372	ASP	3.3
1	A	476	ILE	3.3
1	B	392	HIS	3.3
1	A	300	LYS	3.2
1	B	356	LYS	3.2
1	A	454	ILE	3.2
1	A	335	CYS	3.1
1	B	465	GLY	3.1
1	A	71	ALA	2.9
1	A	447	MET	2.9
1	A	395	ILE	2.9
1	B	355	LYS	2.8
1	A	369	ASP	2.8
1	B	377	THR	2.8
1	A	468	GLY	2.8
1	B	127	ILE	2.8
1	A	128	SER	2.7
1	B	121	ASN	2.7
1	A	223	PHE	2.7
1	B	390	LEU	2.7
1	A	390	LEU	2.7
1	B	375	ALA	2.7
1	A	65	SER	2.6
1	A	389	TYR	2.6
1	A	368	SER	2.5
1	A	143	ASN	2.5
1	A	75	LYS	2.5
1	A	330	ASN	2.5
1	A	361	LEU	2.5
1	A	460	ARG	2.5
1	A	344	VAL	2.4
1	A	52	PHE	2.4
1	A	359	VAL	2.3
1	A	475	ASP	2.3
1	A	478	VAL	2.3
1	A	446	MET	2.3
1	A	168	VAL	2.3
1	A	115	LEU	2.2
1	A	58	LYS	2.2
1	A	46	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	400	PHE	2.1
1	A	404	ILE	2.1
1	A	199	ARG	2.1
1	A	131	VAL	2.1
1	B	474	LYS	2.1
1	A	120	PRO	2.1
1	B	71	ALA	2.1
1	A	337	ILE	2.0
1	A	79	LEU	2.0
1	A	474	LYS	2.0
1	A	108	TYR	2.0
1	B	236	TYR	2.0
1	A	67	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.