



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:04 AM UTC

PDB ID : 3OWG / pdb_00003owg
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

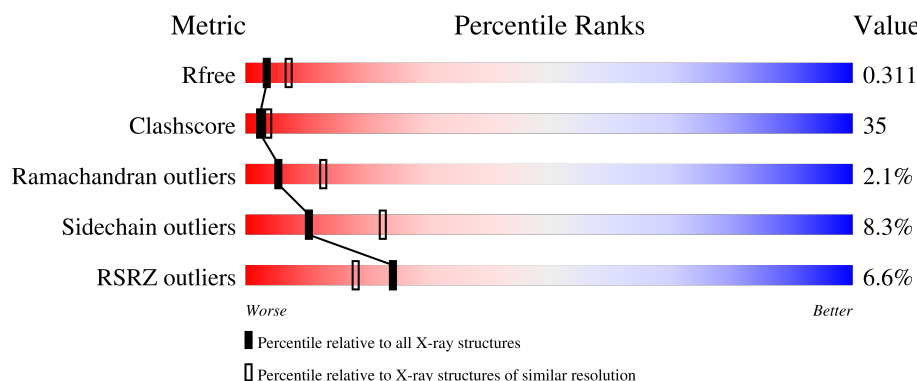
1 Overall quality at a glance

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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	485	9% 41% 43% 9% 6%
1	B	485	3% 43% 40% 10% 6%

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.

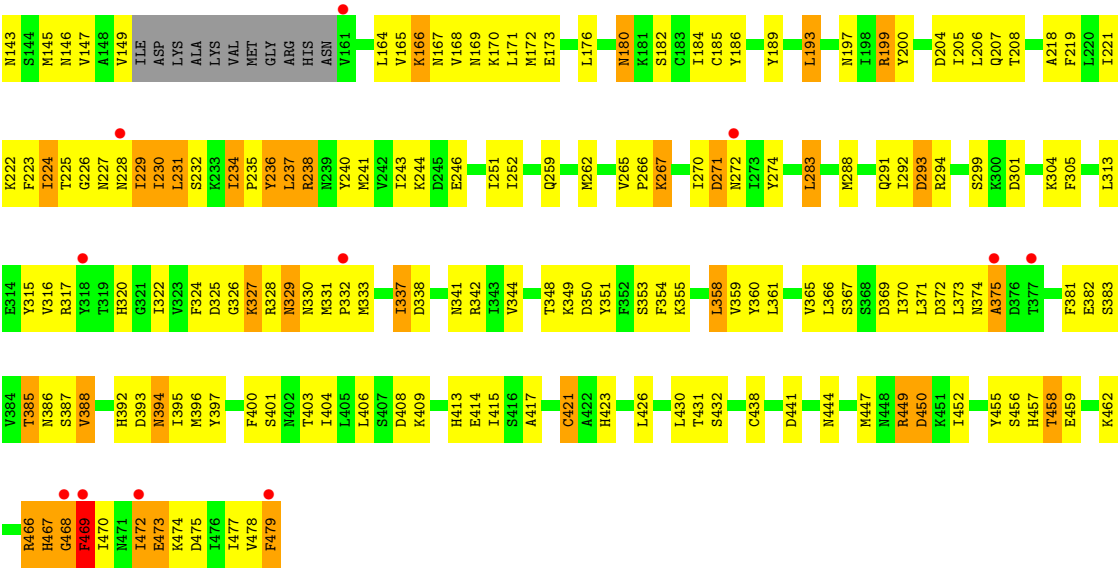
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.13Å 161.29Å 97.67Å 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 2.86Å)	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%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.63	2/3780 (0.1%)	1.10	21/5101 (0.4%)
1	B	0.76	1/3780 (0.0%)	1.14	24/5101 (0.5%)
All	All	0.70	3/7560 (0.0%)	1.12	45/10202 (0.4%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	SER	CB-OG	7.18	1.56	1.42
1	A	124	SER	CB-OG	5.80	1.53	1.42
1	A	103	VAL	CA-CB	-5.08	1.48	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	ILE	N-CA-C	10.18	122.37	108.11
1	A	208	THR	N-CA-C	-8.44	102.74	113.72
1	B	401	SER	N-CA-C	8.34	121.81	112.97
1	A	337	ILE	N-CA-C	8.28	119.76	108.17
1	A	475	ASP	N-CA-C	7.58	121.85	111.54
1	A	259	GLN	N-CA-C	-7.33	103.29	111.71
1	A	469	PHE	N-CA-C	7.09	119.17	108.46
1	A	401	SER	N-CA-C	6.91	120.38	112.57
1	B	126	LYS	N-CA-C	6.85	124.30	114.16
1	B	385	THR	N-CA-C	-6.85	105.48	114.31
1	B	234	ILE	CA-C-N	6.84	128.39	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	ILE	C-N-CA	6.84	128.39	119.84
1	B	330	ASN	N-CA-C	-6.82	103.36	113.72
1	B	394	ASN	N-CA-C	-6.75	104.34	112.58
1	B	469	PHE	N-CA-C	6.44	118.18	108.46
1	A	234	ILE	CA-C-N	6.39	127.83	119.84
1	A	234	ILE	C-N-CA	6.39	127.83	119.84
1	A	351	TYR	N-CA-C	6.39	120.28	112.23
1	A	468	GLY	N-CA-C	6.31	119.27	112.33
1	B	337	ILE	N-CA-C	6.30	116.99	108.17
1	A	272	ASN	N-CA-C	6.25	120.86	113.23
1	B	185	CYS	N-CA-C	6.22	119.78	110.14
1	B	105	VAL	N-CA-C	6.10	116.84	110.62
1	A	385	THR	N-CA-C	-6.03	106.53	114.31
1	B	208	THR	N-CA-C	-5.94	106.07	113.38
1	B	441	ASP	N-CA-C	-5.92	104.83	111.28
1	B	67	VAL	N-CA-C	5.81	117.11	108.46
1	A	185	CYS	N-CA-C	5.70	118.97	110.14
1	A	352	PHE	N-CA-C	5.65	118.27	109.52
1	B	450	ASP	N-CA-C	-5.61	102.97	110.55
1	B	259	GLN	N-CA-C	-5.58	105.30	111.71
1	A	192	TYR	N-CA-C	-5.57	105.75	112.54
1	B	468	GLY	N-CA-C	5.56	118.45	112.33
1	A	394	ASN	N-CA-C	-5.54	105.82	112.58
1	A	327	LYS	N-CA-C	5.44	118.80	110.20
1	B	230	ILE	N-CA-C	5.44	115.69	107.75
1	B	267	LYS	N-CA-C	5.44	117.95	109.52
1	B	94	LEU	N-CA-C	-5.42	105.46	111.36
1	A	231	LEU	N-CA-C	-5.38	100.40	108.96
1	A	67	VAL	N-CA-C	5.33	116.34	108.45
1	B	122	VAL	CA-C-N	-5.32	116.17	123.14
1	B	122	VAL	C-N-CA	-5.32	116.17	123.14
1	A	173	GLU	N-CA-C	-5.26	105.44	111.07
1	B	133	SER	N-CA-C	-5.16	105.84	111.82
1	A	472	ILE	N-CA-C	5.04	119.14	111.89

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	283	0
1	B	3718	0	3789	263	0
All	All	7436	0	7578	532	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 (532) 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:NH1	1:B:238:ARG:HB3	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:A:328:ARG:CG	1:A:329:ASN:H	1.77	0.96
1:B:238:ARG:HB3	1:B:238:ARG:HH11	1.27	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:HB3	1:A:238:ARG:NH1	1.83	0.92
1:B:331:MET:HE1	1:B:438:CYS:SG	2.10	0.91
1:B:222:LYS:HD2	1:B:472:ILE:HG21	1.53	0.88
1:B:229:ILE:C	1:B:230:ILE:HD12	2.00	0.87
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:HG3	1:B:449:ARG:HH11	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:172:MET:HE2	1:B:205:ILE:HG21	1.59	0.84
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:A:466:ARG:HG2	1:A:479:PHE:CG	2.14	0.82
1:A:137:LEU:HD11	1:A:447:MET:HE3	1.58	0.82
1:A:172:MET:HE2	1:A:205:ILE:HG21	1.62	0.81
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:B:120:PRO:O	1:B:121:ASN:C	2.25	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: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:A:236:TYR:HB2	1:A:237:LEU:HD13	1.67	0.75
1:B:238:ARG:HH11	1:B:238:ARG:CB	1.99	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:266:PRO:HD3	1:A:430:LEU:HD23	1.69	0.74
1:A:320:HIS:HB3	1:A:436:LYS:HD2	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:137:LEU:CD1	1:A:447:MET:HE3	2.17	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:184:ILE:HG23	1:B:262:MET:HE1	1.69	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:A:228:ASN:CG	1:A:473:GLU:HB3	2.15	0.71
1:B:184:ILE:CG2	1:B:262:MET:HE1	2.21	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:70:SER:C	1:B:72:SER:H	2.00	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:A:48:ASN:OD1	1:A:51:ILE:HG22	1.92	0.69
1:B:231:LEU:HD11	1:B:241:MET:HE2	1.74	0.69
1:B:236:TYR:HB2	1:B:237:LEU:HD13	1.75	0.69
1:B:331:MET:HG2	1:B:332:PRO:C	2.17	0.69
1:A:139:ARG:NH2	1:B:166:LYS:HE2	2.08	0.68
1:A:336:ILE:H	1:A:336:ILE:HD12	1.58	0.68
1:A:53:VAL:HG21	1:A:75:LYS:HG3	1.76	0.67
1:B:469:PHE:H	1:B:478:VAL:HB	1.58	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:B:122:VAL:HG13	1:B:272:ASN:ND2	2.10	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:A:184:ILE:CG2	1:A:262:MET:HE1	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:MET:HG2	1:B:333:MET:N	2.12	0.65
1:A:238:ARG:HH11	1:A:238:ARG:CB	2.09	0.65
1:A:189:TYR:O	1:A:193:LEU:HD22	1.97	0.65
1:A:243:ILE:HD11	1:A:252:ILE:CG2	2.27	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:229:ILE:C	1:A:230:ILE:HD12	2.21	0.64
1:A:469:PHE:H	1:A:478:VAL:CG2	2.10	0.64
1:A:236:TYR:N	1:A:236:TYR:CD2	2.62	0.64
1:B:462:LYS:HD2	1:B:462:LYS:O	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:A:379:CYS:O	1:A:388:VAL:HG22	1.98	0.64
1:B:393:ASP:O	1:B:394:ASN:HB2	1.97	0.64
1:A:70:SER:H	1:A:73:GLU:CD	2.06	0.64
1:B:129:TYR:CD2	1:B:129:TYR:N	2.66	0.64
1:B:164:LEU:HA	1:B:167:ASN:HD22	1.61	0.64
1:B:325:ASP:OD1	1:B:327:LYS:HE3	1.98	0.63
1:A:134:MET:HE3	1:A:134:MET:HA	1.80	0.63
1:B:236:TYR:N	1:B:236:TYR:CD2	2.65	0.63
1:B:137:LEU:HD11	1:B:447:MET:HE3	1.80	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:A:462:LYS:HD2	1:A:462:LYS:O	1.99	0.63
1:B:122:VAL:CG1	1:B:272:ASN:HD22	2.12	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:230:ILE:HD12	1:B:230:ILE:N	2.13	0.62
1:B:117:ILE:HG13	1:B:117:ILE:O	1.98	0.62
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.65	0.62
1:B:165:VAL:HG12	1:B:169:ASN:HD21	1.65	0.62
1:B:301:ASP:OD2	1:B:304:LYS:HB2	2.00	0.62
1:B:199:ARG:HH11	1:B:199:ARG:HG2	1.64	0.62
1:A:31:TYR:O	1:A:35:LYS:HG3	2.00	0.61
1:A:346:VAL:O	1:A:346:VAL:HG23	1.99	0.61
1:A:229:ILE:HD13	1:A:229:ILE:H	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:197:ASN:HA	1:B:199:ARG:HH11	1.66	0.61
1:A:337:ILE:HG13	1:A:344:VAL:HG22	1.83	0.61
1:A:70:SER:C	1:A:72:SER:H	2.07	0.60
1:A:350:ASP:OD2	1:A:350:ASP:N	2.33	0.60
1:B:61:LYS:HD2	1:B:61:LYS:O	2.00	0.60
1:A:115:LEU:CD2	1:A:178:ARG:HG3	2.30	0.60
1:B:40:ASN:O	1:B:44:ILE:HG13	2.01	0.60
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:70:SER:H	1:B:73:GLU:CD	2.09	0.59
1:B:137:LEU:CD1	1:B:447:MET:HE3	2.32	0.59
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:A:51:ILE:O	1:A:54:SER:HB3	2.02	0.59
1:B:331:MET:CB	1:B:332:PRO:HA	2.33	0.59
1:B:371:LEU:C	1:B:373:LEU:H	2.11	0.59
1:B:367:SER:O	1:B:371:LEU:HD23	2.03	0.58
1:A:186:TYR:CZ	1:A:204:ASP:HB3	2.38	0.58
1:B:331:MET:CG	1:B:332:PRO:HA	2.34	0.58
1:A:414:GLU:O	1:A:417:ALA:HB3	2.03	0.58
1:B:466:ARG:HA	1:B:466:ARG:NH1	2.18	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:231:LEU:HD11	1:A:241:MET:HE2	1.85	0.58
1:A:337:ILE:HG13	1:A:343:ILE:O	2.04	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:78:ILE:HA	1:B:223:PHE:CE2	2.38	0.57
1:B:83:SER:HA	1:B:85:GLN:OE1	2.04	0.57
1:B:329:ASN:C	1:B:331:MET:H	2.12	0.57
1:A:236:TYR:HB2	1:A:237:LEU:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:367:SER:O	1:A:371:LEU:HD23	2.05	0.56
1:B:329:ASN:ND2	1:B:331:MET:O	2.36	0.56
1:A:466:ARG:CZ	1:A:466:ARG:HA	2.36	0.56
1:A:184:ILE:HG23	1:A:262:MET:HE1	1.88	0.56
1:B:12:ASN:OD1	1:B:14:THR:HB	2.05	0.56
1:A:222:LYS:HB2	1:A:472:ILE:HG21	1.87	0.56
1:A:229:ILE:HB	1:A:244:LYS:O	2.05	0.56
1:A:230:ILE:HD12	1:A:230:ILE:N	2.20	0.56
1:A:61:LYS:HD2	1:A:61:LYS:O	2.05	0.56
1:A:224:ILE:HG22	1:A:225:THR:N	2.20	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:A:17:ILE:HD13	1:A:42:GLN:HB2	1.89	0.55
1:B:392:HIS:O	1:B:395:ILE:HB	2.07	0.55
1:B:331:MET:CE	1:B:438:CYS:SG	2.92	0.55
1:A:339:GLU:HG3	1:A:409:LYS:NZ	2.21	0.55
1:A:371:LEU:C	1:A:373:LEU:H	2.14	0.55
1:B:44:ILE:HD13	1:B:101:GLN:HE21	1.72	0.55
1:A:48:ASN:CG	1:A:51:ILE:HG22	2.31	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:229:ILE:HB	1:B:244:LYS:O	2.06	0.54
1:B:288:MET:CG	1:B:294:ARG:HG3	2.32	0.54
1:B:331:MET:HG2	1:B:332:PRO:HA	1.88	0.54
1:A:336:ILE:HD12	1:A:336:ILE:N	2.22	0.54
1:A:392:HIS:O	1:A:395:ILE:HB	2.06	0.54
1:A:170:LYS:HA	1:A:173:GLU:HG3	1.88	0.54
1:A:258:ARG:HB2	1:A:260:ASP:HB3	1.88	0.54
1:B:17:ILE:HD13	1:B:42:GLN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ILE:HG22	1:B:371:LEU:HD22	1.89	0.54
1:B:70:SER:C	1:B:72:SER:N	2.64	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:A:431:THR:O	1:A:432:SER:HB2	2.08	0.54
1:B:165:VAL:CG1	1:B:169:ASN:HD21	2.20	0.54
1:B:266:PRO:HD3	1:B:430:LEU:HD23	1.89	0.54
1:B:469:PHE:N	1:B:478:VAL:HB	2.22	0.54
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:365:VAL:HG12	1:B:365:VAL:O	2.08	0.53
1:B:131:VAL:O	1:B:131:VAL:CG2	2.57	0.53
1:B:338:ASP:CG	1:B:341:ASN:HD22	2.16	0.53
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:B:331:MET:CB	1:B:332:PRO:CA	2.86	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: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:B:134:MET:HE3	1:B:134:MET:HA	1.91	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:A:328:ARG:CG	1:A:329:ASN:N	2.53	0.52
1:A:137:LEU:O	1:A:141:MET:HG3	2.10	0.52
1:B:48:ASN:CG	1:B:51:ILE:HG22	2.34	0.52
1:B:125:SER:O	1:B:126:LYS:HG2	2.10	0.52
1:A:15:LEU:HD11	1:A:26:PRO:HG2	1.92	0.52
1:B:104:LEU:HD11	1:B:219:PHE:CD2	2.44	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: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:B:329:ASN:C	1:B:331:MET:N	2.67	0.51
1:A:131:VAL:O	1:A:135:GLU:HG3	2.10	0.51
1:A:331:MET:HE2	1:A:333:MET:SD	2.50	0.51
1:A:270:ILE:HG22	1:A:271:ASP:OD1	2.11	0.51
1:B:354:PHE:CZ	1:B:396:MET:HE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:NH1	1:A:139:ARG:HB2	2.24	0.51
1:A:473:GLU:CG	1:A:474:LYS:HD2	2.41	0.51
1:B:170:LYS:HA	1:B:173:GLU:HG3	1.92	0.51
1:B:172:MET:CE	1:B:205:ILE:HG21	2.38	0.51
1:B:232:SER:HA	1:B:469:PHE:HB3	1.93	0.51
1:A:58:LYS:HB3	1:A:116:THR:HG21	1.92	0.51
1:A:197:ASN:HA	1:B:199:ARG:HG2	1.92	0.51
1:A:200:TYR:CD1	1:A:200:TYR:C	2.89	0.51
1:A:336:ILE:HB	1:A:345:THR:HG23	1.91	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:A:77:ARG:HD2	1:A:223:PHE:O	2.11	0.50
1:B:63:PHE:O	1:B:167:ASN:HB3	2.11	0.50
1:A:53:VAL:O	1:A:57:LYS:HG3	2.11	0.50
1:A:130:ASN:C	1:A:132:THR:H	2.19	0.50
1:B:413:HIS:CD2	1:B:414:GLU:N	2.79	0.50
1:A:172:MET:CE	1:A:205:ILE:HG21	2.40	0.50
1:B:270:ILE:HG22	1:B:271:ASP:OD1	2.12	0.50
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:231:LEU:CD1	1:B:241:MET:HE2	2.40	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:B:172:MET:HE3	1:B:176:LEU:HG	1.92	0.50
1:A:243:ILE:O	1:A:251:ILE:HB	2.11	0.49
1:A:370:ILE:HG22	1:A:371:LEU:HD22	1.94	0.49
1:A:70:SER:C	1:A:72:SER:N	2.70	0.49
1:B:180:ASN:ND2	1:B:272:ASN:O	2.45	0.49
1:A:12:ASN:OD1	1:A:14:THR:HB	2.12	0.49
1:A:331:MET:HE1	1:A:351:TYR:HE2	1.77	0.49
1:A:329:ASN:C	1:A:331:MET:H	2.19	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:A:352:PHE:HE1	1:A:434:GLU:O	1.96	0.49
1:B:409:LYS:HD3	1:B:455:TYR:HE2	1.78	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:A:339:GLU:HG3	1:A:409:LYS:HZ3	1.78	0.49
1:A:123:ILE:CD1	1:B:130:ASN:HD21	2.25	0.49
1:A:340:ASN:C	1:A:342:ARG:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:243:ILE:HD11	1:B:252:ILE:CG2	2.43	0.48
1:B:469:PHE:HD1	1:B:469:PHE:O	1.96	0.48
1:B:94:LEU:O	1:B:98:ILE:HG13	2.14	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: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:N	1:B:293:ASP:OD2	2.45	0.48
1:B:132:THR:HA	1:B:135:GLU:HG3	1.94	0.48
1:B:184:ILE:HG22	1:B:274:TYR:HB2	1.96	0.48
1:B:291:GLN:OE1	1:B:403:THR:N	2.44	0.48
1:B:315:TYR:C	1:B:315:TYR:CD2	2.91	0.48
1:B:358:LEU:HD23	1:B:397:TYR:CE2	2.49	0.48
1:B:382:GLU:O	1:B:386:ASN:HA	2.14	0.48
1:A:395:ILE:HG22	1:A:396:MET:N	2.27	0.48
1:A:413:HIS:O	1:A:414:GLU:C	2.55	0.48
1:A:468:GLY:CA	1:A:478:VAL:O	2.57	0.48
1:B:236:TYR:N	1:B:236:TYR:HD2	2.12	0.47
1:A:337:ILE:HG23	1:A:337:ILE:O	2.13	0.47
1:B:146:ASN:HD21	1:B:299:SER:HA	1.79	0.47
1:B:414:GLU:O	1:B:417:ALA:HB3	2.14	0.47
1:A:231:LEU:HB3	1:A:470:ILE:HB	1.96	0.47
1:A:473:GLU:OE1	1:A:474:LYS:HE3	2.15	0.47
1:A:73:GLU:O	1:A:77:ARG:HG3	2.14	0.47
1:A:172:MET:HE3	1:A:176:LEU:HG	1.96	0.47
1:A:235:PRO:HG2	1:A:236:TYR:CD2	2.49	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:A:317:ARG:HG3	1:A:322:ILE:O	2.15	0.47
1:B:60:LYS:HA	1:B:224:ILE:CD1	2.44	0.47
1:B:373:LEU:O	1:B:374:ASN:HB2	2.15	0.47
1:A:134:MET:HA	1:A:134:MET:CE	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:MET:O	1:A:147:VAL:N	2.48	0.47
1:A:427:TYR:CE1	1:A:431:THR:HG21	2.50	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:A:102:SER:O	1:A:106:THR:HG23	2.15	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:146:ASN:HD21	1:A:299:SER:HA	1.81	0.46
1:B:333:MET:SD	1:B:421:CYS:SG	3.13	0.46
1:A:64:PHE:O	1:A:67:VAL:HG23	2.14	0.46
1:B:431:THR:O	1:B:432:SER:CB	2.63	0.46
1:B:200:TYR:C	1:B:200:TYR:CD1	2.94	0.46
1:B:338:ASP:OD2	1:B:341:ASN:ND2	2.37	0.46
1:A:165:VAL:CG1	1:A:169:ASN:HD21	2.28	0.46
1:A:466:ARG:HA	1:A:466:ARG:NH1	2.30	0.46
1:A:469:PHE:N	1:A:478:VAL:HG23	2.19	0.46
1:B:238:ARG:HB3	1:B:238:ARG:CZ	2.44	0.46
1:A:231:LEU:HD11	1:A:241:MET:CE	2.46	0.46
1:A:139:ARG:NH1	1:A:139:ARG:CB	2.79	0.46
1:B:423:HIS:HA	1:B:426:LEU:HD12	1.98	0.46
1:B:466:ARG:HG2	1:B:479:PHE:CD1	2.50	0.46
1:B:230:ILE:N	1:B:230:ILE:CD1	2.78	0.46
1:B:237:LEU:N	1:B:237:LEU:CD1	2.78	0.46
1:B:360:TYR:CD1	1:B:366:LEU:HD13	2.51	0.46
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:427:TYR:CZ	1:A:431:THR:HG21	2.50	0.45
1:A:470:ILE:HG12	1:A:477:ILE:HD12	1.98	0.45
1:A:280:PHE:CZ	1:A:426:LEU:HD22	2.51	0.45
1:A:47:PHE:CG	1:A:105:VAL:HG22	2.51	0.45
1:A:64:PHE:C	1:A:66:ASP:N	2.73	0.45
1:B:331:MET:HB3	1:B:332:PRO:CA	2.47	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:117:ILE:O	1:A:117:ILE:CG1	2.64	0.45
1:A:222:LYS:HG3	1:A:228:ASN:HD22	1.82	0.45
1:A:342:ARG:NH2	1:A:362:ASP:OD1	2.44	0.45
1:A:452:ILE:CG2	1:A:453:PRO:HD2	2.46	0.45
1:A:83:SER:HA	1:A:85:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:CD1	1:B:130:ASN:ND2	2.80	0.45
1:A:128:SER:OG	1:B:126:LYS:HE3	2.16	0.45
1:A:344:VAL:O	1:A:346:VAL:HG13	2.16	0.45
1:B:404:ILE:HB	1:B:458:THR:CG2	2.46	0.45
1:A:473:GLU:HG2	1:A:474:LYS:HD2	1.98	0.45
1:B:123:ILE:HD13	1:B:123:ILE:HA	1.69	0.45
1:B:387:SER:OG	1:B:388:VAL:N	2.50	0.45
1:A:134:MET:HE3	1:A:134:MET:CA	2.47	0.44
1:A:265:VAL:HA	1:A:430:LEU:CD2	2.47	0.44
1:B:199:ARG:HH11	1:B:199:ARG:CG	2.30	0.44
1:A:81:TYR:C	1:A:83:SER:H	2.25	0.44
1:A:423:HIS:HA	1:A:426:LEU:HD12	1.99	0.44
1:B:58:LYS:HB3	1:B:116:THR:CG2	2.47	0.44
1:B:96:THR:HG23	1:B:477:ILE:HG12	1.99	0.44
1:A:58:LYS:CB	1:A:116:THR:HG21	2.47	0.44
1:A:148:ALA:O	1:A:149:VAL:C	2.59	0.44
1:A:470:ILE:HG12	1:A:477:ILE:HD13	2.00	0.44
1:B:64:PHE:O	1:B:67:VAL:HG23	2.17	0.44
1:B:371:LEU:C	1:B:373:LEU:N	2.75	0.44
1:A:48:ASN:HB3	1:A:51:ILE:CG2	2.48	0.44
1:A:90:ASN:CG	1:A:93:LYS:HG3	2.43	0.44
1:A:94:LEU:O	1:A:98:ILE:HG13	2.17	0.44
1:B:182:SER:O	1:B:207:GLN:HA	2.18	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:A:265:VAL:HA	1:A:430:LEU:HD23	1.99	0.44
1:A:343:ILE:C	1:A:344:VAL:HG23	2.43	0.44
1:A:466:ARG:C	1:A:468:GLY:H	2.26	0.44
1:B:60:LYS:HA	1:B:224:ILE:HD13	1.99	0.44
1:A:231:LEU:CD1	1:A:241:MET:HE2	2.47	0.44
1:B:122:VAL:HG11	1:B:272:ASN:HD22	1.83	0.44
1:B:243:ILE:O	1:B:251:ILE:HB	2.17	0.44
1:B:408:ASP:OD1	1:B:409:LYS:N	2.51	0.44
1:B:25:VAL:HA	1:B:26:PRO:HD2	1.82	0.44
1:B:131:VAL:O	1:B:135:GLU:HG3	2.18	0.44
1:A:365:VAL:HG12	1:A:365:VAL:O	2.17	0.43
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: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:A:269:PHE:CZ	1:A:272:ASN:HA	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:HG21	1:B:101:GLN:NE2	2.33	0.43
1:B:291:GLN:HE21	1:B:293:ASP:CG	2.26	0.43
1:A:329:ASN:C	1:A:331:MET:N	2.77	0.43
1:A:129:TYR:CE2	1:A:194:ILE:HG23	2.54	0.43
1:B:58:LYS:O	1:B:62:ARG:HB2	2.19	0.43
1:B:168:VAL:HG11	1:B:252:ILE:HB	2.01	0.43
1:A:373:LEU:O	1:A:374:ASN:HB2	2.19	0.43
1:A:466:ARG:HD2	1:A:479:PHE:CD2	2.53	0.43
1:B:139:ARG:NH1	1:B:139:ARG:CB	2.82	0.43
1:B:292:ILE:CG2	1:B:403:THR:HG21	2.47	0.43
1:B:359:VAL:CG1	1:B:400:PHE:HB2	2.49	0.43
1:B:459:GLU:OE1	1:B:459:GLU:HA	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:466:ARG:C	1:B:468:GLY:H	2.27	0.42
1:A:112:LEU:HD13	1:A:220:LEU:HD22	2.02	0.42
1:B:57:LYS:HD2	1:B:71:ALA:HB1	2.01	0.42
1:B:70:SER:O	1:B:72:SER:N	2.53	0.42
1:B:325:ASP:CG	1:B:327:LYS:HB2	2.44	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:A:371:LEU:C	1:A:373:LEU:N	2.77	0.42
1:B:125:SER:O	1:B:126:LYS:CG	2.66	0.42
1:A:340:ASN:C	1:A:342:ARG:N	2.77	0.42
1:A:359:VAL:HG11	1:A:400:PHE:HB2	2.01	0.42
1:B:370:ILE:CG2	1:B:371:LEU:HD22	2.49	0.42
1:A:196:PRO:O	1:B:199:ARG:CG	2.68	0.42
1:A:199:ARG:HH11	1:A:199:ARG:CG	2.30	0.42
1:A:348:THR:OG1	1:A:354:PHE:O	2.37	0.42
1:B:128:SER:C	1:B:129:TYR:HD2	2.27	0.42
1:A:64:PHE:C	1:A:66:ASP:H	2.28	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:231:LEU:HD11	1:B:241:MET:CE	2.47	0.42
1:B:143:ASN:C	1:B:145:MET:N	2.77	0.42
1:B:145:MET:O	1:B:147:VAL:N	2.53	0.42
1:B:331:MET:HE3	1:B:351:TYR:CZ	2.55	0.42
1:B:291:GLN:HE22	1:B:403:THR:HG23	1.85	0.42
1:A:343:ILE:C	1:A:344:VAL:CG2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:107:THR:O	1:A:108:TYR:C	2.62	0.41
1:A:21:TYR:OH	1:A:85:GLN:HG2	2.19	0.41
1:A:395:ILE:CG2	1:A:396:MET:N	2.83	0.41
1:A:469:PHE:HD1	1:A:469:PHE:O	2.03	0.41
1:B:283:LEU:HD12	1:B:283:LEU:HA	1.89	0.41
1:A:75:LYS:O	1:A:79:LEU:HG	2.20	0.41
1:A:81:TYR:CE2	1:A:219:PHE:CE2	3.08	0.41
1:B:48:ASN:HB3	1:B:51:ILE:CG2	2.51	0.41
1:B:238:ARG:NH1	1:B:238:ARG:CB	2.62	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:75:LYS:O	1:B:79:LEU:HG	2.21	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:B:327:LYS:O	1:B:328:ARG:C	2.64	0.41
1:A:123:ILE:HD13	1:B:130:ASN:ND2	2.36	0.41
1:A:282:LEU:HD21	1:A:443:LEU:HD21	2.03	0.41
1:A:315:TYR:CD2	1:A:315:TYR:C	2.98	0.41
1:A:336:ILE:H	1:A:336:ILE:CD1	2.32	0.41
1:A:343:ILE:O	1:A:344:VAL:CG2	2.69	0.41
1:A:382:GLU:O	1:A:386:ASN:HA	2.21	0.41
1:B:123:ILE:O	1:B:124:SER:C	2.62	0.41
1:A:330:ASN:ND2	1:A:330:ASN:O	2.53	0.41
1:B:236:TYR:HB2	1:B:237:LEU:CD1	2.48	0.41
1:A:25:VAL:HA	1:A:26:PRO:HD2	1.86	0.41
1:A:228:ASN:OD1	1:A:473:GLU:HB3	2.19	0.41
1:A:346:VAL:O	1:A:346:VAL:CG2	2.68	0.41
1:A:348:THR:C	1:A:350:ASP:OD2	2.64	0.41
1:B:73:GLU:HG3	1:B:73:GLU:H	1.70	0.41
1:B:329:ASN:CB	1:B:331:MET:O	2.61	0.41
1:A:52:PHE:C	1:A:54:SER:N	2.79	0.41
1:B:100:LEU:HD21	1:B:470:ILE:HD13	2.03	0.41
1:B:166:LYS:HG3	1:B:167:ASN:H	1.86	0.41
1:B:359:VAL:HG11	1:B:400:PHE:HB2	2.02	0.41
1:A:129:TYR:CD2	1:A:194:ILE:HG22	2.56	0.40
1:B:58:LYS:CB	1:B:116:THR:HG21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLY:H	1:B:444:ASN:ND2	2.18	0.40
1:A:69:THR:HA	1:A:73:GLU:OE2	2.21	0.40
1:A:135:GLU:OE2	1:B:170:LYS:HE2	2.21	0.40
1:B:189:TYR:CE2	1:B:193:LEU:HD21	2.55	0.40
1:B:348:THR:C	1:B:350:ASP:N	2.78	0.40
1:A:195:ASN:OD1	1:A:195:ASN:C	2.65	0.40
1:A:316:VAL:HG23	1:A:320:HIS:HD2	1.87	0.40
1:A:114:VAL:O	1:A:114:VAL:HG12	2.21	0.40
1:A:117:ILE:HG13	1:A:178:ARG:HH21	1.87	0.40
1:A:449:ARG:HD3	1:A:449:ARG:HA	1.92	0.40
1:A:131:VAL:O	1:A:131:VAL:CG2	2.67	0.40
1:A:164:LEU:HA	1:A:167:ASN:ND2	2.31	0.40
1:B:21:TYR:HE1	1:B:101:GLN:HE22	1.68	0.40
1:B:61:LYS:HD2	1:B:61:LYS:C	2.45	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

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	453/485 (93%)	391 (86%)	53 (12%)	9 (2%)	6	13
1	B	453/485 (93%)	396 (87%)	47 (10%)	10 (2%)	5	12
All	All	906/970 (93%)	787 (87%)	100 (11%)	19 (2%)	5	13

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	VAL
1	A	344	VAL
1	A	355	LYS

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Mol	Chain	Res	Type
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%)	397 (92%)	36 (8%)	10	22
1	B	433/459 (94%)	397 (92%)	36 (8%)	10	22
All	All	866/918 (94%)	794 (92%)	72 (8%)	10	22

All (72) 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	85	GLN
1	A	134	MET
1	A	149	VAL

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Mol	Chain	Res	Type
1	A	166	LYS
1	A	180	ASN
1	A	193	LEU
1	A	199	ARG
1	A	225	THR
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	361	LEU
1	A	383	SER
1	A	388	VAL
1	A	421	CYS
1	A	458	THR
1	A	466	ARG
1	A	469	PHE
1	A	473	GLU
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	127	ILE
1	B	129	TYR
1	B	131	VAL
1	B	134	MET
1	B	149	VAL
1	B	166	LYS
1	B	180	ASN
1	B	193	LEU

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Mol	Chain	Res	Type
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	353	SER
1	B	358	LEU
1	B	383	SER
1	B	388	VAL
1	B	421	CYS
1	B	449	ARG
1	B	450	ASP
1	B	458	THR
1	B	466	ARG
1	B	469	PHE
1	B	472	ILE
1	B	473	GLU
1	B	474	LYS
1	B	479	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
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	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

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Mol	Chain	Res	Type
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	272	ASN
1	B	306	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

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%)	0.83	44 (9%) 13 11	48, 106, 176, 200	0
1	B	457/485 (94%)	0.11	16 (3%) 47 37	37, 71, 147, 200	0
All	All	914/970 (94%)	0.47	60 (6%) 24 18	37, 88, 167, 200	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	ILE	5.6
1	A	366	LEU	4.3
1	A	332	PRO	4.2
1	A	128	SER	4.0
1	A	442	LEU	3.5
1	B	124	SER	3.5
1	B	272	ASN	3.5
1	A	425	LEU	3.4
1	B	377	THR	3.2
1	B	332	PRO	3.2
1	B	469	PHE	3.1
1	A	477	ILE	3.1
1	B	130	ASN	3.1
1	A	131	VAL	3.1
1	A	168	VAL	3.1
1	A	143	ASN	3.0
1	B	128	SER	3.0
1	A	421	CYS	3.0
1	A	149	VAL	3.0
1	A	194	ILE	3.0
1	A	443	LEU	2.9
1	A	367	SER	2.9
1	A	478	VAL	2.9
1	A	148	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	228	ASN	2.8
1	A	196	PRO	2.7
1	A	460	ARG	2.7
1	A	223	PHE	2.6
1	B	121	ASN	2.6
1	B	375	ALA	2.6
1	A	199	ARG	2.6
1	A	315	TYR	2.6
1	B	468	GLY	2.6
1	A	286	ILE	2.6
1	A	56	VAL	2.5
1	A	119	ALA	2.5
1	B	479	PHE	2.5
1	A	313	LEU	2.4
1	A	64	PHE	2.4
1	A	467	HIS	2.4
1	B	161	VAL	2.4
1	B	318	TYR	2.3
1	B	127	ILE	2.3
1	A	71	ALA	2.3
1	A	202	ASP	2.3
1	A	142	LEU	2.2
1	A	65	SER	2.2
1	A	354	PHE	2.2
1	A	375	ALA	2.2
1	A	454	ILE	2.2
1	A	185	CYS	2.2
1	A	373	LEU	2.2
1	B	472	ILE	2.1
1	A	193	LEU	2.1
1	A	189	TYR	2.1
1	A	83	SER	2.1
1	A	333	MET	2.1
1	A	288	MET	2.1
1	A	138	ALA	2.1
1	A	446	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.