



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:11 PM UTC

PDB ID : 4QC8 / pdb_00004qc8
Title : Structural annotation of pathogenic bovine Parvovirus-1
Authors : Kailasan, S.; Halder, S.; Gurda, B.L.; Bladek, H.; Chipman, P.R.; McKenna, R.; Brown, K.; Agbandje-McKenna, M.
Deposited on : 2014-05-09
Resolution : 3.20 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

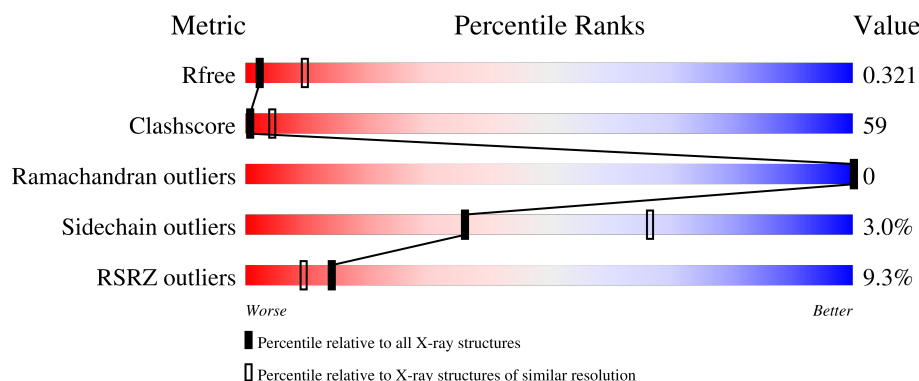
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	536	9% 43% 44% 6% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3950 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.

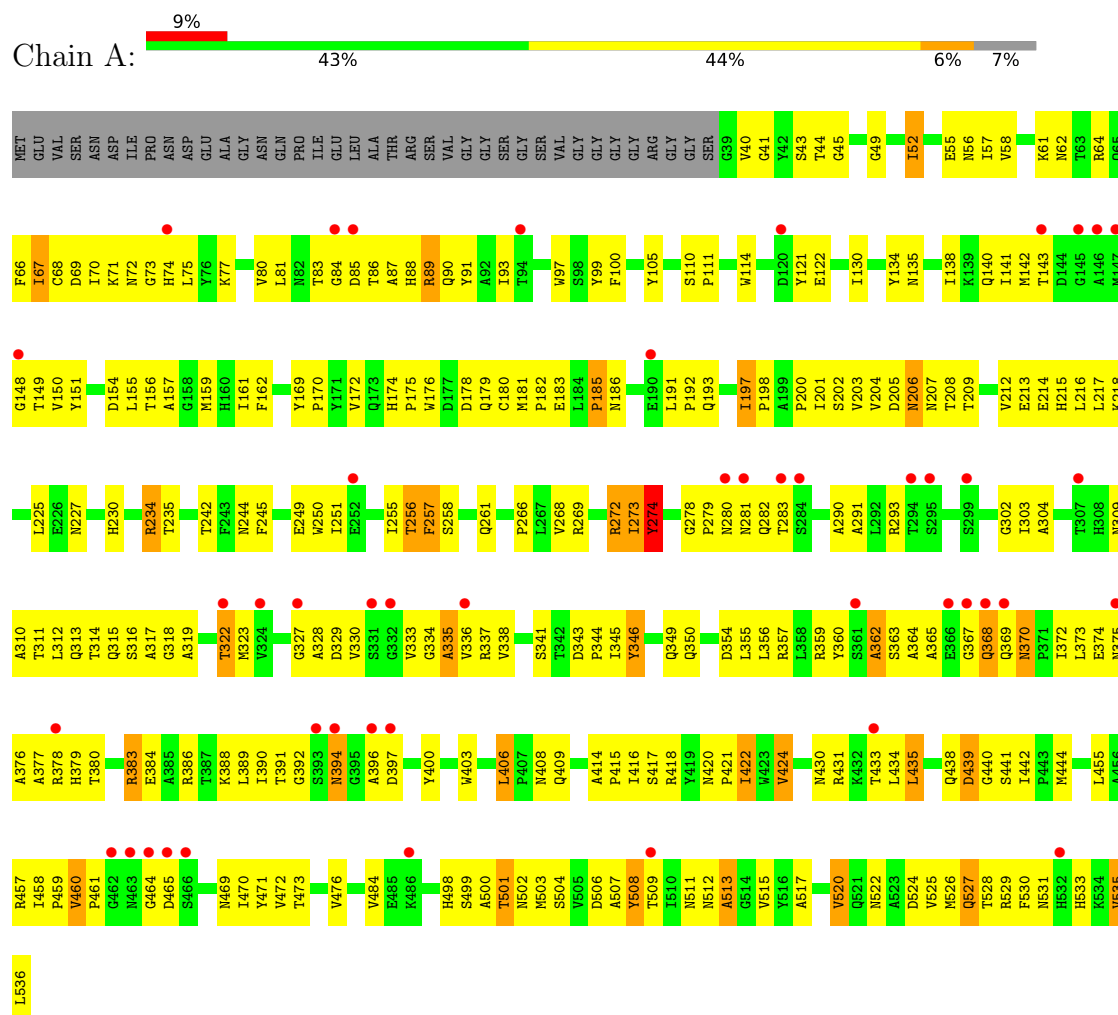
- Molecule 1 is a protein called VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	3950	2483	695	750	22	34	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: VP2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	323.45Å 381.23Å 376.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	82.1 (50.00-3.20) 82.1 (50.00-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.310 , 0.311 0.320 , 0.321	Depositor DCC
R_{free} test set	17020 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.18	EDS
Total number of atoms	3950	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.55	0/4059	1.15	40/5536 (0.7%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ALA	N-CA-C	-10.40	99.69	112.38
1	A	327	GLY	N-CA-C	-9.99	102.48	111.67
1	A	531	ASN	N-CA-C	9.65	125.52	112.68
1	A	356	LEU	N-CA-C	-9.03	101.08	112.90
1	A	272	ARG	N-CA-C	8.16	120.17	111.28
1	A	89	ARG	N-CA-C	8.00	122.08	111.28
1	A	88	HIS	N-CA-C	7.86	119.93	111.36
1	A	422	ILE	N-CA-C	7.58	118.35	110.62
1	A	256	THR	N-CA-C	7.51	122.92	112.93
1	A	501	THR	N-CA-C	-7.29	104.19	113.23
1	A	440	GLY	N-CA-C	-7.27	104.53	115.00
1	A	535	VAL	N-CA-C	7.03	117.60	111.90
1	A	438	GLN	N-CA-C	-6.96	104.05	112.54
1	A	110	SER	N-CA-C	-6.86	100.22	110.24
1	A	90	GLN	N-CA-C	6.60	119.81	110.50
1	A	322	THR	N-CA-C	6.54	120.41	111.39
1	A	273	ILE	N-CA-C	6.53	122.92	109.34
1	A	274	TYR	N-CA-C	6.21	119.26	110.50
1	A	185	PRO	N-CA-C	-6.18	102.14	111.41
1	A	508	TYR	N-CA-C	6.10	120.07	111.52
1	A	234	ARG	N-CA-C	-6.07	101.79	110.59
1	A	368	GLN	N-CA-C	6.03	123.64	110.80
1	A	319	ALA	N-CA-C	-5.99	104.75	111.28
1	A	460	VAL	O-C-N	5.91	125.41	121.69
1	A	435	LEU	N-CA-C	5.78	123.11	110.80
1	A	392	GLY	N-CA-C	5.74	118.53	111.93
1	A	362	ALA	N-CA-C	-5.70	105.07	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ASN	CA-C-N	-5.53	114.56	120.03
1	A	370	ASN	C-N-CA	-5.53	114.56	120.03
1	A	197	ILE	CA-C-N	5.43	125.26	119.28
1	A	197	ILE	C-N-CA	5.43	125.26	119.28
1	A	408	ASN	N-CA-C	5.38	119.14	112.58
1	A	513	ALA	N-CA-C	-5.34	102.58	110.48
1	A	509	THR	N-CA-C	5.25	116.96	109.14
1	A	460	VAL	CA-C-N	5.17	125.15	120.03
1	A	460	VAL	C-N-CA	5.17	125.15	120.03
1	A	257	PHE	N-CA-C	-5.13	106.97	113.23
1	A	383	ARG	N-CA-C	5.12	119.48	112.68
1	A	346	TYR	N-CA-C	5.08	116.81	111.28
1	A	281	ASN	N-CA-C	5.01	117.75	107.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3950	0	3755	449	0
All	All	3950	0	3755	449	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 59.

All (449) 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:105:TYR:CE2	1:A:422:ILE:HD13	1.67	1.29
1:A:354:ASP:O	1:A:355:LEU:CG	1.79	1.26
1:A:255:ILE:HG21	1:A:529:ARG:O	1.43	1.16
1:A:312:LEU:HD12	1:A:313:GLN:N	1.62	1.14
1:A:203:VAL:CG1	1:A:216:LEU:HD13	1.77	1.14
1:A:203:VAL:HG11	1:A:216:LEU:HD13	1.19	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ASN:OD1	1:A:515:VAL:HG12	1.44	1.13
1:A:255:ILE:CG2	1:A:529:ARG:O	1.94	1.13
1:A:312:LEU:HB2	1:A:317:ALA:CB	1.79	1.13
1:A:278:GLY:HA3	1:A:282:GLN:NE2	1.61	1.12
1:A:417:SER:HB2	1:A:525:VAL:HG12	1.20	1.12
1:A:373:LEU:HD23	1:A:522:ASN:ND2	1.64	1.11
1:A:278:GLY:HA3	1:A:282:GLN:HE22	1.11	1.10
1:A:354:ASP:OD1	1:A:359:ARG:NH2	1.83	1.10
1:A:354:ASP:O	1:A:355:LEU:HG	0.94	1.09
1:A:309:ASN:HD22	1:A:336:VAL:HG11	1.09	1.09
1:A:370:ASN:HD21	1:A:520:VAL:HA	1.11	1.09
1:A:511:ASN:OD1	1:A:515:VAL:CG1	2.01	1.08
1:A:312:LEU:CB	1:A:317:ALA:HB2	1.83	1.07
1:A:203:VAL:CG1	1:A:216:LEU:CD1	2.34	1.05
1:A:373:LEU:HD23	1:A:522:ASN:HD21	0.91	1.05
1:A:105:TYR:CZ	1:A:422:ILE:HD13	1.92	1.05
1:A:417:SER:CB	1:A:525:VAL:HG12	1.86	1.05
1:A:460:VAL:HG13	1:A:461:PRO:HD2	1.37	1.03
1:A:208:THR:O	1:A:209:THR:OG1	1.77	1.02
1:A:105:TYR:CD2	1:A:422:ILE:HD13	1.94	1.02
1:A:72:ASN:OD1	1:A:193:GLN:NE2	1.93	1.01
1:A:373:LEU:H	1:A:522:ASN:ND2	1.59	1.00
1:A:433:THR:HG22	1:A:434:LEU:H	1.27	1.00
1:A:511:ASN:O	1:A:513:ALA:O	1.81	0.99
1:A:360:TYR:CE2	1:A:374:GLU:HG3	1.99	0.98
1:A:312:LEU:HB2	1:A:317:ALA:HB2	0.98	0.98
1:A:105:TYR:CE1	1:A:422:ILE:CD1	2.46	0.97
1:A:105:TYR:CG	1:A:422:ILE:HD11	1.98	0.96
1:A:105:TYR:CD1	1:A:422:ILE:CD1	2.48	0.96
1:A:134:TYR:HD2	1:A:135:ASN:OD1	1.49	0.95
1:A:179:GLN:OE1	1:A:192:PRO:HB3	1.64	0.95
1:A:134:TYR:CD2	1:A:135:ASN:OD1	2.20	0.95
1:A:309:ASN:ND2	1:A:336:VAL:HG11	1.81	0.95
1:A:105:TYR:CE1	1:A:422:ILE:HD12	2.03	0.94
1:A:370:ASN:ND2	1:A:520:VAL:HA	1.80	0.94
1:A:105:TYR:CZ	1:A:422:ILE:CD1	2.50	0.94
1:A:373:LEU:HG	1:A:376:ALA:HB2	1.49	0.94
1:A:416:ILE:N	1:A:528:THR:OG1	2.00	0.93
1:A:373:LEU:H	1:A:522:ASN:HD21	1.13	0.92
1:A:204:VAL:HG13	1:A:217:LEU:HB2	1.51	0.91
1:A:322:THR:O	1:A:322:THR:HG22	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ASP:C	1:A:355:LEU:HG	1.95	0.90
1:A:318:GLY:HA3	1:A:341:SER:HB3	1.51	0.89
1:A:365:ALA:O	1:A:369:GLN:NE2	2.05	0.89
1:A:503:MET:HB3	1:A:524:ASP:OD1	1.70	0.89
1:A:105:TYR:CE2	1:A:422:ILE:CD1	2.57	0.88
1:A:154:ASP:OD1	1:A:157:ALA:HB2	1.74	0.88
1:A:105:TYR:CG	1:A:422:ILE:CD1	2.56	0.88
1:A:105:TYR:CD1	1:A:422:ILE:HD11	2.08	0.87
1:A:203:VAL:O	1:A:213:GLU:HG2	1.73	0.87
1:A:272:ARG:O	1:A:273:ILE:HG22	1.74	0.87
1:A:105:TYR:CD2	1:A:422:ILE:CD1	2.59	0.86
1:A:373:LEU:CD2	1:A:522:ASN:HD21	1.85	0.86
1:A:279:PRO:O	1:A:280:ASN:OD1	1.93	0.86
1:A:417:SER:CB	1:A:525:VAL:CG1	2.53	0.86
1:A:148:GLY:O	1:A:149:THR:OG1	1.95	0.84
1:A:278:GLY:CA	1:A:282:GLN:NE2	2.40	0.84
1:A:417:SER:OG	1:A:525:VAL:CG1	2.25	0.83
1:A:114:TRP:CD1	1:A:526:MET:HG3	2.14	0.83
1:A:511:ASN:CG	1:A:515:VAL:CG1	2.53	0.82
1:A:499:SER:CB	1:A:501:THR:HG22	2.10	0.81
1:A:272:ARG:HG2	1:A:274:TYR:CZ	2.15	0.81
1:A:204:VAL:HG11	1:A:217:LEU:HD23	1.59	0.81
1:A:416:ILE:H	1:A:528:THR:HG1	1.25	0.81
1:A:499:SER:HB3	1:A:501:THR:HG22	1.63	0.81
1:A:312:LEU:CB	1:A:317:ALA:CB	2.53	0.81
1:A:73:GLY:O	1:A:74:HIS:HB2	1.82	0.80
1:A:100:PHE:CE1	1:A:476:VAL:HG21	2.16	0.80
1:A:511:ASN:ND2	1:A:515:VAL:HG13	1.94	0.80
1:A:360:TYR:HE2	1:A:374:GLU:HG3	1.46	0.80
1:A:354:ASP:OD1	1:A:355:LEU:N	2.14	0.80
1:A:363:SER:HB2	1:A:364:ALA:HA	1.62	0.79
1:A:178:ASP:OD1	1:A:179:GLN:N	2.17	0.78
1:A:349:GLN:HE21	1:A:403:TRP:CD1	2.02	0.78
1:A:433:THR:HG22	1:A:434:LEU:N	1.95	0.78
1:A:111:PRO:HB3	1:A:508:TYR:CE1	2.19	0.77
1:A:303:ILE:HB	1:A:345:ILE:CG2	2.14	0.77
1:A:155:LEU:HD22	1:A:235:THR:HG21	1.66	0.77
1:A:203:VAL:O	1:A:213:GLU:CG	2.33	0.77
1:A:389:LEU:HD23	1:A:391:THR:H	1.49	0.77
1:A:70:ILE:HG21	1:A:74:HIS:CD2	2.20	0.76
1:A:360:TYR:OH	1:A:374:GLU:CG	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:SER:HB2	1:A:364:ALA:CA	2.16	0.76
1:A:203:VAL:CG1	1:A:216:LEU:HD12	2.16	0.76
1:A:360:TYR:CZ	1:A:374:GLU:HG3	2.21	0.76
1:A:374:GLU:OE1	1:A:416:ILE:HA	1.86	0.75
1:A:323:MET:HE3	1:A:338:VAL:HG11	1.68	0.75
1:A:335:ALA:C	1:A:337:ARG:H	1.92	0.75
1:A:330:VAL:HG12	1:A:330:VAL:O	1.87	0.74
1:A:272:ARG:HG2	1:A:274:TYR:CE2	2.23	0.74
1:A:506:ASP:HB2	1:A:520:VAL:HG11	1.69	0.74
1:A:315:GLN:NE2	1:A:337:ARG:HD3	2.01	0.74
1:A:272:ARG:O	1:A:273:ILE:CG2	2.36	0.73
1:A:420:ASN:ND2	1:A:421:PRO:HD2	2.02	0.73
1:A:528:THR:O	1:A:529:ARG:HB2	1.88	0.73
1:A:155:LEU:C	1:A:156:THR:HG23	2.14	0.73
1:A:255:ILE:HD12	1:A:379:HIS:HB3	1.71	0.73
1:A:43:SER:OG	1:A:45:GLY:O	2.07	0.72
1:A:373:LEU:CD2	1:A:522:ASN:ND2	2.48	0.72
1:A:500:ALA:HA	1:A:503:MET:HG3	1.71	0.72
1:A:138:ILE:HG12	1:A:472:VAL:HG22	1.72	0.72
1:A:140:GLN:CG	1:A:142:MET:HE3	2.19	0.72
1:A:433:THR:CG2	1:A:434:LEU:H	2.01	0.72
1:A:511:ASN:ND2	1:A:515:VAL:CG1	2.52	0.72
1:A:334:GLY:C	1:A:336:VAL:N	2.42	0.72
1:A:114:TRP:HD1	1:A:526:MET:HG3	1.54	0.72
1:A:334:GLY:C	1:A:336:VAL:H	1.97	0.72
1:A:69:ASP:H	1:A:71:LYS:NZ	1.87	0.72
1:A:430:ASN:O	1:A:431:ARG:HD2	1.90	0.71
1:A:185:PRO:O	1:A:186:ASN:HB3	1.88	0.71
1:A:208:THR:O	1:A:209:THR:CB	2.37	0.71
1:A:279:PRO:O	1:A:280:ASN:CG	2.34	0.70
1:A:460:VAL:CG1	1:A:461:PRO:HD2	2.19	0.69
1:A:499:SER:OG	1:A:501:THR:HG22	1.91	0.69
1:A:203:VAL:HG13	1:A:216:LEU:CD1	2.20	0.69
1:A:511:ASN:HD21	1:A:515:VAL:CG1	2.05	0.69
1:A:43:SER:O	1:A:44:THR:HG22	1.92	0.69
1:A:91:TYR:HB2	1:A:201:ILE:CD1	2.23	0.69
1:A:322:THR:O	1:A:322:THR:CG2	2.42	0.68
1:A:460:VAL:HG13	1:A:461:PRO:CD	2.21	0.68
1:A:391:THR:OG1	1:A:396:ALA:O	2.12	0.67
1:A:70:ILE:CG2	1:A:74:HIS:CD2	2.77	0.67
1:A:511:ASN:HD21	1:A:515:VAL:HG13	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ALA:C	1:A:337:ARG:N	2.51	0.67
1:A:360:TYR:OH	1:A:374:GLU:HG3	1.94	0.67
1:A:323:MET:CE	1:A:338:VAL:HG11	2.25	0.67
1:A:155:LEU:CD2	1:A:235:THR:HG21	2.25	0.66
1:A:323:MET:HE3	1:A:338:VAL:CG1	2.25	0.66
1:A:511:ASN:CG	1:A:515:VAL:HG13	2.19	0.66
1:A:360:TYR:OH	1:A:374:GLU:HG2	1.92	0.66
1:A:202:SER:O	1:A:205:ASP:CG	2.37	0.66
1:A:318:GLY:CA	1:A:341:SER:HB3	2.25	0.66
1:A:500:ALA:CB	1:A:503:MET:HE2	2.26	0.66
1:A:86:THR:HA	1:A:337:ARG:NH1	2.11	0.66
1:A:202:SER:HB2	1:A:330:VAL:HG22	1.78	0.65
1:A:354:ASP:O	1:A:355:LEU:CD1	2.43	0.65
1:A:303:ILE:HB	1:A:345:ILE:HG21	1.78	0.65
1:A:377:ALA:HB3	1:A:527:GLN:OE1	1.96	0.65
1:A:40:VAL:HG22	1:A:41:GLY:N	2.11	0.65
1:A:69:ASP:H	1:A:71:LYS:HZ2	1.44	0.65
1:A:204:VAL:HG11	1:A:217:LEU:CD2	2.27	0.65
1:A:418:ARG:NH1	1:A:508:TYR:HE1	1.95	0.65
1:A:155:LEU:O	1:A:156:THR:OG1	2.12	0.65
1:A:460:VAL:HG12	1:A:461:PRO:O	1.96	0.64
1:A:535:VAL:O	1:A:536:LEU:HB2	1.97	0.64
1:A:360:TYR:OH	1:A:525:VAL:HG11	1.98	0.64
1:A:105:TYR:OH	1:A:251:ILE:HD11	1.97	0.63
1:A:162:PHE:HB2	1:A:230:HIS:CB	2.28	0.63
1:A:140:GLN:CD	1:A:142:MET:HE3	2.23	0.63
1:A:528:THR:O	1:A:529:ARG:CB	2.44	0.63
1:A:394:ASN:H	1:A:394:ASN:ND2	1.96	0.63
1:A:349:GLN:NE2	1:A:403:TRP:CD1	2.66	0.63
1:A:155:LEU:O	1:A:156:THR:HG23	1.99	0.63
1:A:417:SER:OG	1:A:525:VAL:HG11	1.99	0.63
1:A:373:LEU:CG	1:A:376:ALA:HB2	2.27	0.63
1:A:66:PHE:CD2	1:A:476:VAL:HG23	2.34	0.62
1:A:370:ASN:ND2	1:A:520:VAL:CA	2.58	0.62
1:A:176:TRP:NE1	1:A:439:ASP:OD1	2.28	0.62
1:A:208:THR:C	1:A:209:THR:HG23	2.25	0.62
1:A:303:ILE:HB	1:A:345:ILE:HG22	1.80	0.62
1:A:362:ALA:O	1:A:363:SER:OG	2.15	0.62
1:A:315:GLN:O	1:A:316:SER:C	2.43	0.62
1:A:156:THR:HA	1:A:234:ARG:HD2	1.80	0.62
1:A:333:VAL:HG12	1:A:337:ARG:HH21	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HG22	1:A:380:THR:HB	1.81	0.62
1:A:49:GLY:HA2	1:A:61:LYS:O	1.99	0.61
1:A:314:THR:HG23	1:A:315:GLN:HG3	1.81	0.61
1:A:140:GLN:HG3	1:A:142:MET:HE3	1.82	0.61
1:A:256:THR:O	1:A:257:PHE:HB2	2.00	0.61
1:A:435:LEU:HG	1:A:435:LEU:O	2.00	0.61
1:A:420:ASN:CG	1:A:421:PRO:HD2	2.24	0.61
1:A:312:LEU:HD12	1:A:313:GLN:H	1.60	0.61
1:A:273:ILE:HG13	1:A:273:ILE:O	2.01	0.61
1:A:255:ILE:CG2	1:A:529:ARG:C	2.74	0.60
1:A:455:LEU:HD22	1:A:470:ILE:HG13	1.83	0.60
1:A:52:ILE:HD12	1:A:52:ILE:N	2.17	0.60
1:A:349:GLN:HE21	1:A:403:TRP:HD1	1.48	0.60
1:A:183:GLU:CG	1:A:418:ARG:HH22	2.14	0.60
1:A:272:ARG:C	1:A:273:ILE:HG22	2.27	0.60
1:A:204:VAL:HG12	1:A:204:VAL:O	2.00	0.60
1:A:318:GLY:HA3	1:A:341:SER:CB	2.30	0.60
1:A:89:ARG:O	1:A:89:ARG:HG2	2.00	0.60
1:A:312:LEU:HD12	1:A:312:LEU:C	2.23	0.59
1:A:525:VAL:O	1:A:526:MET:HB2	2.01	0.59
1:A:312:LEU:HD12	1:A:313:GLN:CA	2.32	0.59
1:A:363:SER:HB2	1:A:364:ALA:CB	2.33	0.59
1:A:458:ILE:HD13	1:A:470:ILE:CD1	2.32	0.59
1:A:389:LEU:HD23	1:A:391:THR:N	2.17	0.59
1:A:91:TYR:HB2	1:A:201:ILE:HD13	1.84	0.59
1:A:335:ALA:O	1:A:337:ARG:N	2.36	0.59
1:A:415:PRO:HB3	1:A:528:THR:O	2.03	0.59
1:A:458:ILE:HD13	1:A:470:ILE:HD13	1.83	0.58
1:A:525:VAL:O	1:A:526:MET:CB	2.50	0.58
1:A:74:HIS:CB	1:A:457:ARG:HH21	2.16	0.58
1:A:91:TYR:HB2	1:A:201:ILE:HD12	1.86	0.58
1:A:40:VAL:CG2	1:A:41:GLY:N	2.67	0.57
1:A:155:LEU:O	1:A:156:THR:CB	2.52	0.57
1:A:251:ILE:HD13	1:A:416:ILE:HD13	1.86	0.57
1:A:304:ALA:CB	1:A:386:ARG:HH22	2.16	0.57
1:A:138:ILE:HD12	1:A:157:ALA:O	2.03	0.57
1:A:140:GLN:CD	1:A:142:MET:CE	2.77	0.57
1:A:316:SER:HB3	1:A:341:SER:OG	2.05	0.57
1:A:334:GLY:O	1:A:336:VAL:N	2.38	0.57
1:A:504:SER:OG	1:A:520:VAL:HG22	2.05	0.57
1:A:256:THR:HG22	1:A:258:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ILE:HG21	1:A:525:VAL:CG2	2.35	0.57
1:A:302:GLY:HA3	1:A:346:TYR:O	2.04	0.56
1:A:169:TYR:OH	1:A:227:ASN:HB3	2.05	0.56
1:A:111:PRO:HB3	1:A:508:TYR:CD1	2.39	0.56
1:A:373:LEU:HD23	1:A:373:LEU:H	1.70	0.56
1:A:282:GLN:OE1	1:A:283:THR:C	2.48	0.56
1:A:179:GLN:OE1	1:A:192:PRO:CB	2.48	0.56
1:A:359:ARG:NH1	1:A:373:LEU:HD13	2.21	0.56
1:A:178:ASP:OD2	1:A:364:ALA:N	2.38	0.56
1:A:390:ILE:O	1:A:391:THR:OG1	2.21	0.56
1:A:58:VAL:HG23	1:A:484:VAL:HG21	1.88	0.56
1:A:141:ILE:HG23	1:A:151:TYR:CE1	2.40	0.56
1:A:507:ALA:HB2	1:A:524:ASP:OD2	2.06	0.56
1:A:185:PRO:O	1:A:186:ASN:CB	2.54	0.56
1:A:334:GLY:O	1:A:335:ALA:C	2.48	0.56
1:A:251:ILE:HD11	1:A:442:ILE:HD11	1.88	0.56
1:A:69:ASP:N	1:A:71:LYS:HZ2	2.04	0.55
1:A:422:ILE:O	1:A:442:ILE:HD13	2.06	0.55
1:A:178:ASP:O	1:A:179:GLN:HB2	2.06	0.55
1:A:268:VAL:O	1:A:293:ARG:NH2	2.39	0.55
1:A:71:LYS:CG	1:A:193:GLN:HB2	2.37	0.55
1:A:373:LEU:N	1:A:522:ASN:ND2	2.42	0.54
1:A:64:ARG:NE	1:A:185:PRO:HA	2.22	0.54
1:A:434:LEU:O	1:A:435:LEU:HB3	2.07	0.54
1:A:134:TYR:CE2	1:A:135:ASN:OD1	2.60	0.54
1:A:389:LEU:CD2	1:A:391:THR:H	2.17	0.54
1:A:373:LEU:N	1:A:522:ASN:HD21	1.94	0.54
1:A:363:SER:HB2	1:A:364:ALA:HB2	1.89	0.54
1:A:499:SER:O	1:A:500:ALA:HB3	2.07	0.54
1:A:84:GLY:O	1:A:85:ASP:HB3	2.08	0.54
1:A:499:SER:OG	1:A:501:THR:CG2	2.55	0.54
1:A:455:LEU:HG	1:A:472:VAL:HG23	1.89	0.54
1:A:498:HIS:CE1	1:A:527:GLN:N	2.76	0.54
1:A:43:SER:O	1:A:135:ASN:ND2	2.41	0.53
1:A:74:HIS:CE1	1:A:457:ARG:HA	2.43	0.53
1:A:100:PHE:CD1	1:A:191:LEU:HD11	2.43	0.53
1:A:389:LEU:HD23	1:A:390:ILE:N	2.24	0.53
1:A:312:LEU:CD1	1:A:313:GLN:N	2.54	0.53
1:A:84:GLY:H	1:A:87:ALA:HB3	1.74	0.53
1:A:500:ALA:HB2	1:A:503:MET:HE2	1.91	0.53
1:A:370:ASN:OD1	1:A:370:ASN:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:HIS:CG	1:A:457:ARG:HG3	2.43	0.53
1:A:97:TRP:CD2	1:A:225:LEU:HD12	2.44	0.52
1:A:439:ASP:HB3	1:A:441:SER:OG	2.08	0.52
1:A:251:ILE:HD13	1:A:416:ILE:CD1	2.39	0.52
1:A:457:ARG:O	1:A:459:PRO:HD3	2.09	0.52
1:A:245:PHE:HD2	1:A:444:MET:HE1	1.75	0.52
1:A:290:ALA:O	1:A:291:ALA:HB3	2.10	0.52
1:A:44:THR:HG23	1:A:135:ASN:H	1.75	0.52
1:A:74:HIS:HB3	1:A:457:ARG:HH21	1.74	0.52
1:A:121:TYR:CD1	1:A:484:VAL:CG1	2.93	0.52
1:A:183:GLU:CG	1:A:418:ARG:NH2	2.73	0.52
1:A:363:SER:CB	1:A:364:ALA:CA	2.84	0.52
1:A:370:ASN:HD21	1:A:520:VAL:CA	2.02	0.51
1:A:309:ASN:HD22	1:A:336:VAL:CG1	2.01	0.51
1:A:375:ASN:O	1:A:378:ARG:NH1	2.43	0.51
1:A:71:LYS:HG2	1:A:193:GLN:HB2	1.93	0.51
1:A:83:THR:HG22	1:A:89:ARG:HG3	1.92	0.51
1:A:442:ILE:N	1:A:442:ILE:HD12	2.26	0.51
1:A:62:ASN:HB3	1:A:64:ARG:NH2	2.26	0.51
1:A:75:LEU:HD12	1:A:75:LEU:C	2.35	0.51
1:A:372:ILE:HG21	1:A:525:VAL:HG21	1.93	0.51
1:A:81:LEU:O	1:A:89:ARG:HA	2.11	0.51
1:A:249:GLU:HG2	1:A:250:TRP:N	2.24	0.51
1:A:66:PHE:HD2	1:A:476:VAL:HG23	1.75	0.51
1:A:256:THR:CG2	1:A:258:SER:HB3	2.41	0.51
1:A:64:ARG:NH1	1:A:182:PRO:O	2.44	0.51
1:A:208:THR:O	1:A:209:THR:HG23	2.10	0.51
1:A:383:ARG:CZ	1:A:414:ALA:HA	2.40	0.51
1:A:212:VAL:HG11	1:A:328:ALA:H	1.76	0.50
1:A:417:SER:HB2	1:A:525:VAL:CG1	2.09	0.50
1:A:130:ILE:N	1:A:130:ILE:HD12	2.26	0.50
1:A:535:VAL:O	1:A:536:LEU:CB	2.59	0.50
1:A:498:HIS:CE1	1:A:527:GLN:H	2.29	0.50
1:A:508:TYR:HA	1:A:517:ALA:O	2.10	0.50
1:A:406:LEU:O	1:A:409:GLN:HG3	2.10	0.50
1:A:272:ARG:CG	1:A:274:TYR:CZ	2.92	0.50
1:A:162:PHE:HB2	1:A:230:HIS:HB2	1.93	0.49
1:A:500:ALA:HA	1:A:503:MET:HE2	1.94	0.49
1:A:80:VAL:CG1	1:A:89:ARG:CG	2.89	0.49
1:A:204:VAL:CG1	1:A:217:LEU:HB2	2.31	0.49
1:A:374:GLU:O	1:A:527:GLN:CD	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ALA:O	1:A:515:VAL:N	2.45	0.49
1:A:255:ILE:CD1	1:A:379:HIS:HB3	2.40	0.49
1:A:455:LEU:HD21	1:A:471:TYR:CA	2.41	0.49
1:A:274:TYR:CD1	1:A:274:TYR:N	2.78	0.49
1:A:334:GLY:O	1:A:337:ARG:N	2.46	0.49
1:A:183:GLU:CD	1:A:418:ARG:HH22	2.19	0.49
1:A:203:VAL:HG13	1:A:216:LEU:HD12	1.87	0.49
1:A:208:THR:O	1:A:209:THR:CG2	2.59	0.49
1:A:336:VAL:HG12	1:A:336:VAL:O	2.13	0.49
1:A:500:ALA:HA	1:A:503:MET:CG	2.41	0.49
1:A:363:SER:CB	1:A:364:ALA:HA	2.31	0.49
1:A:86:THR:O	1:A:337:ARG:HD3	2.12	0.48
1:A:172:VAL:CG1	1:A:172:VAL:O	2.60	0.48
1:A:525:VAL:C	1:A:526:MET:HG2	2.38	0.48
1:A:312:LEU:C	1:A:312:LEU:CD1	2.86	0.48
1:A:506:ASP:O	1:A:507:ALA:C	2.56	0.48
1:A:455:LEU:N	1:A:455:LEU:HD12	2.28	0.48
1:A:155:LEU:O	1:A:156:THR:CG2	2.60	0.48
1:A:455:LEU:HD12	1:A:455:LEU:H	1.77	0.47
1:A:390:ILE:O	1:A:396:ALA:O	2.32	0.47
1:A:91:TYR:O	1:A:197:ILE:HG23	2.14	0.47
1:A:169:TYR:O	1:A:170:PRO:C	2.57	0.47
1:A:255:ILE:HG23	1:A:529:ARG:C	2.39	0.47
1:A:455:LEU:HD21	1:A:471:TYR:HA	1.96	0.47
1:A:205:ASP:OD1	1:A:206:ASN:OD1	2.32	0.47
1:A:511:ASN:O	1:A:512:ASN:C	2.56	0.47
1:A:67:ILE:HG13	1:A:68:CYS:N	2.30	0.47
1:A:373:LEU:HD23	1:A:373:LEU:N	2.30	0.47
1:A:455:LEU:CG	1:A:472:VAL:HG23	2.44	0.47
1:A:213:GLU:HG3	1:A:328:ALA:HA	1.97	0.47
1:A:464:GLY:O	1:A:465:ASP:HB3	2.15	0.47
1:A:203:VAL:HG12	1:A:216:LEU:CD1	2.39	0.47
1:A:311:THR:O	1:A:314:THR:HG22	2.15	0.47
1:A:318:GLY:H	1:A:341:SER:CB	2.28	0.47
1:A:330:VAL:HG13	1:A:338:VAL:HG21	1.96	0.47
1:A:394:ASN:H	1:A:394:ASN:HD22	1.61	0.47
1:A:357:ARG:NH2	1:A:384:GLU:OE2	2.48	0.46
1:A:255:ILE:HG23	1:A:529:ARG:O	2.04	0.46
1:A:472:VAL:HG12	1:A:473:THR:N	2.30	0.46
1:A:501:THR:HG23	1:A:502:ASN:OD1	2.15	0.46
1:A:93:ILE:CD1	1:A:198:PRO:HG3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:TYR:HH	1:A:374:GLU:HG2	1.80	0.46
1:A:55:GLU:OE2	1:A:55:GLU:HA	2.15	0.46
1:A:149:THR:O	1:A:150:VAL:C	2.58	0.46
1:A:200:PRO:O	1:A:201:ILE:C	2.57	0.46
1:A:66:PHE:HB2	1:A:191:LEU:HD21	1.98	0.46
1:A:80:VAL:HG12	1:A:89:ARG:HG3	1.97	0.46
1:A:312:LEU:CB	1:A:317:ALA:HB1	2.45	0.46
1:A:455:LEU:HG	1:A:472:VAL:CG2	2.45	0.46
1:A:141:ILE:HD12	1:A:469:ASN:OD1	2.16	0.45
1:A:203:VAL:O	1:A:213:GLU:CB	2.64	0.45
1:A:204:VAL:HG11	1:A:217:LEU:CG	2.46	0.45
1:A:415:PRO:CB	1:A:528:THR:O	2.65	0.45
1:A:99:TYR:O	1:A:191:LEU:HD12	2.16	0.45
1:A:172:VAL:O	1:A:172:VAL:HG12	2.14	0.45
1:A:206:ASN:OD1	1:A:213:GLU:OE1	2.34	0.45
1:A:225:LEU:C	1:A:227:ASN:H	2.24	0.45
1:A:354:ASP:C	1:A:355:LEU:CG	2.68	0.45
1:A:105:TYR:CZ	1:A:422:ILE:HD12	2.34	0.45
1:A:360:TYR:HH	1:A:525:VAL:HG11	1.81	0.45
1:A:417:SER:H	1:A:420:ASN:HB2	1.81	0.45
1:A:71:LYS:HG3	1:A:193:GLN:HB2	1.99	0.45
1:A:121:TYR:CD1	1:A:484:VAL:HG11	2.52	0.45
1:A:180:CYS:O	1:A:181:MET:C	2.58	0.45
1:A:207:ASN:O	1:A:214:GLU:HB2	2.17	0.45
1:A:360:TYR:HH	1:A:374:GLU:CG	2.28	0.45
1:A:416:ILE:N	1:A:528:THR:HG1	2.01	0.45
1:A:86:THR:HA	1:A:337:ARG:HH11	1.79	0.45
1:A:389:LEU:HD12	1:A:400:TYR:OH	2.17	0.45
1:A:93:ILE:HD13	1:A:198:PRO:HG3	1.99	0.44
1:A:121:TYR:CG	1:A:484:VAL:CG1	3.00	0.44
1:A:416:ILE:HG12	1:A:528:THR:HG21	1.99	0.44
1:A:439:ASP:HB3	1:A:441:SER:H	1.82	0.44
1:A:312:LEU:HB3	1:A:317:ALA:CB	2.46	0.44
1:A:380:THR:CG2	1:A:383:ARG:CG	2.95	0.44
1:A:388:LYS:HB3	1:A:397:ASP:HB2	2.00	0.44
1:A:455:LEU:HD21	1:A:471:TYR:C	2.42	0.44
1:A:179:GLN:CD	1:A:192:PRO:HB3	2.39	0.44
1:A:225:LEU:C	1:A:227:ASN:N	2.75	0.44
1:A:372:ILE:HG23	1:A:522:ASN:HA	1.99	0.44
1:A:256:THR:HG22	1:A:258:SER:N	2.32	0.44
1:A:44:THR:HG23	1:A:44:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:H	1:A:269:ARG:HG2	1.65	0.44
1:A:343:ASP:OD1	1:A:344:PRO:HA	2.17	0.44
1:A:162:PHE:HB2	1:A:230:HIS:HB3	1.99	0.43
1:A:527:GLN:HB2	1:A:530:PHE:HB2	1.98	0.43
1:A:204:VAL:HG13	1:A:217:LEU:CB	2.35	0.43
1:A:350:GLN:O	1:A:386:ARG:NH2	2.51	0.43
1:A:386:ARG:HE	1:A:386:ARG:HA	1.84	0.43
1:A:183:GLU:HG3	1:A:418:ARG:NH2	2.33	0.43
1:A:256:THR:HG22	1:A:258:SER:CB	2.47	0.43
1:A:390:ILE:C	1:A:391:THR:OG1	2.62	0.43
1:A:172:VAL:O	1:A:174:HIS:N	2.51	0.43
1:A:215:HIS:HA	1:A:218:LYS:HD2	2.00	0.43
1:A:255:ILE:O	1:A:533:HIS:HA	2.18	0.43
1:A:333:VAL:HG12	1:A:337:ARG:NH2	2.33	0.43
1:A:330:VAL:O	1:A:330:VAL:CG1	2.60	0.43
1:A:149:THR:O	1:A:151:TYR:CD2	2.71	0.43
1:A:266:PRO:HA	1:A:291:ALA:HA	2.01	0.43
1:A:355:LEU:C	1:A:355:LEU:HD12	2.43	0.43
1:A:527:GLN:CB	1:A:530:PHE:HB2	2.49	0.43
1:A:148:GLY:C	1:A:149:THR:HG1	2.08	0.42
1:A:176:TRP:CZ3	1:A:360:TYR:CG	3.07	0.42
1:A:56:ASN:O	1:A:57:ILE:HD13	2.19	0.42
1:A:335:ALA:O	1:A:338:VAL:N	2.24	0.42
1:A:213:GLU:CG	1:A:328:ALA:HA	2.48	0.42
1:A:417:SER:O	1:A:418:ARG:C	2.59	0.42
1:A:204:VAL:O	1:A:205:ASP:C	2.62	0.42
1:A:273:ILE:O	1:A:273:ILE:HG23	2.19	0.42
1:A:207:ASN:ND2	1:A:208:THR:HG23	2.34	0.42
1:A:213:GLU:OE2	1:A:329:ASP:N	2.50	0.42
1:A:309:ASN:OD1	1:A:310:ALA:N	2.53	0.42
1:A:422:ILE:O	1:A:442:ILE:CD1	2.67	0.42
1:A:155:LEU:C	1:A:156:THR:CG2	2.82	0.42
1:A:204:VAL:CG1	1:A:217:LEU:CG	2.98	0.42
1:A:269:ARG:HB3	1:A:269:ARG:NH2	2.35	0.42
1:A:311:THR:O	1:A:312:LEU:C	2.63	0.42
1:A:315:GLN:HB3	1:A:336:VAL:HG12	2.02	0.42
1:A:460:VAL:CG1	1:A:461:PRO:CD	2.89	0.42
1:A:318:GLY:N	1:A:341:SER:OG	2.42	0.42
1:A:374:GLU:O	1:A:527:GLN:OE1	2.37	0.42
1:A:500:ALA:CA	1:A:503:MET:HE2	2.50	0.42
1:A:130:ILE:HG23	1:A:242:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:CG1	1:A:338:VAL:HG21	2.51	0.41
1:A:367:GLY:O	1:A:368:GLN:HB3	2.20	0.41
1:A:70:ILE:HD13	1:A:74:HIS:NE2	2.35	0.41
1:A:75:LEU:HD12	1:A:77:LYS:HG3	2.03	0.41
1:A:80:VAL:CG1	1:A:89:ARG:HG2	2.50	0.41
1:A:149:THR:O	1:A:151:TYR:CE2	2.73	0.41
1:A:511:ASN:HD21	1:A:515:VAL:HG11	1.82	0.41
1:A:442:ILE:HD12	1:A:442:ILE:H	1.85	0.41
1:A:67:ILE:HD11	1:A:471:TYR:CE2	2.56	0.41
1:A:458:ILE:HD12	1:A:458:ILE:N	2.36	0.41
1:A:181:MET:HA	1:A:182:PRO:HD2	1.85	0.41
1:A:178:ASP:O	1:A:179:GLN:CB	2.69	0.41
1:A:74:HIS:HB2	1:A:457:ARG:HH21	1.83	0.41
1:A:279:PRO:C	1:A:280:ASN:CG	2.88	0.41
1:A:72:ASN:HB3	1:A:73:GLY:H	1.78	0.41
1:A:80:VAL:CG1	1:A:89:ARG:HG3	2.50	0.41
1:A:282:GLN:CD	1:A:282:GLN:C	2.89	0.41
1:A:315:GLN:HB3	1:A:336:VAL:O	2.21	0.41
1:A:74:HIS:ND1	1:A:457:ARG:HG3	2.36	0.40
1:A:191:LEU:HD22	1:A:191:LEU:N	2.36	0.40
1:A:416:ILE:CG1	1:A:528:THR:HG21	2.51	0.40
1:A:143:THR:HA	1:A:149:THR:H	1.86	0.40
1:A:330:VAL:HG11	1:A:338:VAL:HG11	2.04	0.40
1:A:205:ASP:OD1	1:A:205:ASP:N	2.55	0.40
1:A:362:ALA:C	1:A:363:SER:HG	2.22	0.40
1:A:45:GLY:HA3	1:A:134:TYR:CD2	2.56	0.40
1:A:175:PRO:CG	1:A:424:VAL:HG13	2.51	0.40
1:A:203:VAL:HG12	1:A:216:LEU:HD12	1.99	0.40
1:A:74:HIS:HB3	1:A:457:ARG:HD2	2.02	0.40
1:A:140:GLN:HA	1:A:470:ILE:HA	2.04	0.40
1:A:159:MET:HE3	1:A:161:ILE:HB	2.03	0.40
1:A:304:ALA:HB1	1:A:386:ARG:HH22	1.87	0.40
1:A:390:ILE:O	1:A:390:ILE:HG22	2.22	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	496/536 (92%)	448 (90%)	48 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	429/455 (94%)	416 (97%)	13 (3%)	36	66

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ILE
1	A	67	ILE
1	A	122	GLU
1	A	206	ASN
1	A	244	ASN
1	A	261	GLN
1	A	274	TYR
1	A	394	ASN
1	A	406	LEU
1	A	424	VAL
1	A	439	ASP
1	A	520	VAL
1	A	527	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	135	ASN
1	A	140	GLN
1	A	160	HIS
1	A	173	GLN
1	A	207	ASN
1	A	288	GLN
1	A	446	HIS
1	A	521	GLN
1	A	522	ASN

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 [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	497/536 (92%)	0.94	46 (9%) 14 9	21, 45, 74, 117	9 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	GLY	10.4
1	A	143	THR	6.7
1	A	464	GLY	6.0
1	A	367	GLY	5.5
1	A	366	GLU	4.5
1	A	147	MET	4.2
1	A	332	GLY	4.1
1	A	84	GLY	4.1
1	A	463	ASN	3.9
1	A	368	GLN	3.7
1	A	148	GLY	3.4
1	A	369	GLN	3.3
1	A	295	SER	3.2
1	A	375	ASN	3.1
1	A	393	SER	3.1
1	A	324	VAL	3.0
1	A	280	ASN	2.9
1	A	397	ASP	2.8
1	A	299	SER	2.8
1	A	466	SER	2.8
1	A	361	SER	2.8
1	A	307	THR	2.8
1	A	281	ASN	2.7
1	A	465	ASP	2.7
1	A	462	GLY	2.6
1	A	331	SER	2.6
1	A	74	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	433	THR	2.5
1	A	486	LYS	2.3
1	A	190	GLU	2.3
1	A	322	THR	2.3
1	A	336	VAL	2.3
1	A	394	ASN	2.3
1	A	327	GLY	2.2
1	A	120	ASP	2.2
1	A	85	ASP	2.2
1	A	94	THR	2.1
1	A	283	THR	2.1
1	A	294	THR	2.1
1	A	509	THR	2.1
1	A	146	ALA	2.1
1	A	284	SER	2.1
1	A	378	ARG	2.1
1	A	532	HIS	2.1
1	A	396	ALA	2.1
1	A	252	GLU	2.1

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 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.