



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:06 AM UTC

PDB ID : 3DJA / pdb_00003dja
Title : Crystal Structure of cpaf solved with MAD
Authors : Chai, J.; Huang, Z.
Deposited on : 2008-06-22
Resolution : 2.90 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
Mogul : 2022.3.0, CSD as543be (2022)
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

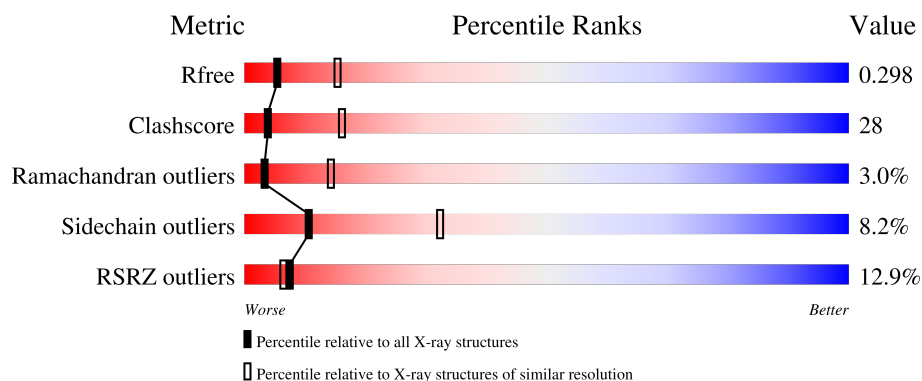
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	579	5% 52% 32% 7% 9%
1	B	579	18% 41% 42% 7% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8290 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 Protein CT_858.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	Se	0	0	0
			4145	2654	694	784	7	6			
1	B	527	Total	C	N	O	S	Se	0	0	0
			4145	2654	694	784	7	6			



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.87Å 124.87Å 241.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.00-2.90) 99.6 (20.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.290 0.256 , 0.298	Depositor DCC
R_{free} test set	2160 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8290	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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	0.60	4/4237 (0.1%)	1.06	20/5750 (0.3%)
1	B	0.57	7/4237 (0.2%)	1.00	19/5750 (0.3%)
All	All	0.59	11/8474 (0.1%)	1.03	39/11500 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	MSE	SE-CE	-5.99	1.77	1.95
1	B	338	MSE	CG-SE	-5.83	1.77	1.95
1	B	434	MSE	SE-CE	-5.78	1.78	1.95
1	B	136	MSE	SE-CE	-5.62	1.78	1.95
1	B	387	MSE	SE-CE	-5.45	1.79	1.95
1	A	186	MSE	SE-CE	-5.44	1.79	1.95
1	B	338	MSE	SE-CE	-5.25	1.79	1.95
1	B	434	MSE	CG-SE	-5.15	1.79	1.95
1	A	434	MSE	SE-CE	-5.13	1.80	1.95
1	B	186	MSE	CG-SE	-5.08	1.80	1.95
1	A	338	MSE	CG-SE	-5.05	1.80	1.95

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	598	ASP	N-CA-C	-11.60	88.29	108.23
1	B	600	THR	N-CA-C	-10.39	88.67	110.80
1	A	452	ARG	N-CA-C	-9.89	100.05	111.03
1	B	441	LEU	N-CA-C	-8.95	101.61	111.36
1	A	575	ILE	N-CA-C	7.70	117.77	110.53
1	A	402	LEU	N-CA-C	7.59	122.01	109.95
1	A	450	PHE	N-CA-C	-7.19	101.01	110.43
1	B	502	ASP	N-CA-C	-7.14	103.18	112.68
1	B	467	THR	N-CA-C	-7.14	100.77	109.83
1	B	126	SER	N-CA-C	7.11	120.85	111.75
1	A	285	TYR	N-CA-C	-6.95	104.37	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	GLU	N-CA-C	-6.72	104.83	113.16
1	A	330	ILE	N-CA-C	-6.61	101.54	107.56
1	A	217	ARG	N-CA-C	-6.46	99.85	109.15
1	B	217	ARG	N-CA-C	-6.34	99.55	109.25
1	B	192	LYS	N-CA-C	-5.80	100.38	109.25
1	A	528	VAL	CB-CA-C	-5.62	102.82	111.31
1	A	491	VAL	N-CA-C	5.61	116.18	107.99
1	B	330	ILE	N-CA-C	-5.60	102.01	107.55
1	A	233	ILE	CB-CA-C	-5.45	104.84	111.88
1	B	402	LEU	N-CA-C	5.38	118.26	109.59
1	A	348	PRO	N-CA-C	5.38	120.83	113.84
1	B	493	ILE	N-CA-C	5.36	116.38	108.45
1	B	313	SER	N-CA-C	5.34	117.21	108.55
1	A	139	SER	N-CA-C	-5.31	103.02	110.50
1	A	177	ALA	N-CA-C	-5.30	105.50	111.28
1	A	199	THR	N-CA-C	5.27	117.32	107.99
1	B	43	LEU	N-CA-C	-5.21	105.68	111.36
1	A	400	MSE	N-CA-C	5.20	118.58	110.32
1	B	351	GLU	N-CA-C	-5.19	105.71	111.36
1	A	117	TYR	N-CA-C	5.18	117.60	108.75
1	B	403	THR	N-CA-C	-5.18	101.54	109.41
1	B	589	LYS	N-CA-C	-5.18	105.06	111.33
1	A	552	GLU	N-CA-C	5.15	116.89	111.28
1	B	87	THR	N-CA-C	-5.11	105.71	111.28
1	B	399	ARG	N-CA-C	-5.11	100.83	108.96
1	A	401	ILE	N-CA-C	-5.09	101.07	108.36
1	A	358	VAL	N-CA-C	-5.09	105.53	110.42
1	B	528	VAL	CB-CA-C	-5.02	104.01	111.19

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	4145	0	4091	196	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4145	0	4091	293	0
All	All	8290	0	8182	469	1

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 28.

All (469) 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:204:ARG:HB3	1:A:204:ARG:NH1	1.61	1.14
1:A:204:ARG:HB3	1:A:204:ARG:HH11	1.14	1.05
1:B:359:PHE:O	1:B:363:THR:HG22	1.64	0.97
1:B:516:ILE:H	1:B:565:HIS:HD2	1.08	0.95
1:B:297:ILE:HD11	1:B:313:SER:HB2	1.49	0.94
1:A:186:MSE:H	1:A:191:HIS:HD2	1.16	0.90
1:B:433:ASN:ND2	1:B:436:GLY:H	1.70	0.89
1:B:433:ASN:HD22	1:B:436:GLY:H	1.18	0.87
1:B:149:LEU:HD11	1:B:203:ARG:HB2	1.56	0.87
1:B:186:MSE:H	1:B:191:HIS:HD2	1.18	0.87
1:A:151:VAL:HB	1:A:159:VAL:HG21	1.56	0.86
1:A:502:ASP:O	1:A:506:VAL:HG23	1.76	0.85
1:A:33:SER:O	1:A:37:LYS:HG3	1.77	0.85
1:B:238:LEU:HD13	1:B:239:GLN:H	1.41	0.85
1:B:82:GLN:HG3	1:B:89:PHE:CE2	2.12	0.84
1:A:432:ASP:HA	1:A:439:VAL:HB	1.60	0.83
1:B:427:ARG:HG2	1:B:432:ASP:HA	1.60	0.83
1:B:302:TRP:HB3	1:B:312:ILE:HG12	1.59	0.83
1:A:404:GLN:HG3	1:B:538:GLY:HA2	1.60	0.82
1:A:197:ARG:NH1	1:A:213:ARG:HE	1.76	0.82
1:A:366:LEU:HD13	1:A:368:ILE:HD11	1.62	0.82
1:B:143:ARG:HH22	1:B:204:ARG:HD2	1.44	0.82
1:A:516:ILE:H	1:A:565:HIS:HD2	1.26	0.81
1:A:493:ILE:HD11	1:A:564:PRO:HB3	1.62	0.81
1:B:516:ILE:H	1:B:565:HIS:CD2	1.97	0.81
1:A:192:LYS:HB2	1:A:192:LYS:NZ	1.95	0.81
1:A:367:ILE:HD11	1:A:591:VAL:HG21	1.61	0.80
1:B:567:ASP:OD1	1:B:569:PRO:HD3	1.81	0.80
1:B:297:ILE:HD11	1:B:313:SER:CB	2.11	0.79
1:B:509:LYS:HB2	1:B:516:ILE:HD12	1.64	0.79
1:B:120:TYR:HB2	1:B:183:PHE:CD1	2.18	0.79
1:B:335:TRP:HB2	1:B:348:PRO:HG3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:MSE:H	1:B:191:HIS:CD2	2.01	0.78
1:A:366:LEU:HD22	1:A:368:ILE:HD12	1.65	0.77
1:B:297:ILE:HD12	1:B:311:TYR:HE1	1.49	0.77
1:A:186:MSE:H	1:A:191:HIS:CD2	2.01	0.77
1:B:59:TRP:HE1	1:B:559:ASN:HD22	1.33	0.76
1:A:192:LYS:HB2	1:A:192:LYS:HZ2	1.48	0.76
1:B:160:LEU:HD21	1:B:182:LEU:HG	1.68	0.76
1:B:517:VAL:HG13	1:B:566:ILE:HB	1.67	0.76
1:B:367:ILE:HD13	1:B:490:CYS:HB3	1.68	0.75
1:A:534:PRO:HG2	1:B:49:LEU:HD22	1.68	0.75
1:A:404:GLN:NE2	1:A:404:GLN:H	1.85	0.75
1:B:82:GLN:HG3	1:B:89:PHE:CZ	2.22	0.75
1:A:515:LEU:HG	1:A:601:ILE:HD11	1.69	0.75
1:A:538:GLY:HA2	1:B:404:GLN:HG3	1.68	0.74
1:A:594:LEU:HD21	1:A:601:ILE:HD11	1.68	0.74
1:B:182:LEU:HD13	1:B:183:PHE:CE2	2.22	0.73
1:B:321:LYS:HE2	1:B:323:HIS:HE1	1.54	0.73
1:B:54:TYR:CZ	1:B:56:PRO:HG2	2.24	0.72
1:B:122:VAL:HG12	1:B:123:GLN:N	2.04	0.72
1:A:395:LEU:HD21	1:A:477:ILE:HD13	1.71	0.71
1:B:197:ARG:HG2	1:B:215:LYS:HB2	1.72	0.71
1:A:594:LEU:HD22	1:A:599:GLY:HA2	1.72	0.71
1:A:368:ILE:HD13	1:A:489:ILE:HG23	1.73	0.71
1:B:302:TRP:HB3	1:B:312:ILE:CG1	2.20	0.70
1:B:297:ILE:HD12	1:B:311:TYR:CE1	2.26	0.70
1:A:602:ILE:HG22	1:A:603:LEU:H	1.55	0.70
1:B:332:THR:HA	1:B:373:ASN:OD1	1.92	0.69
1:A:515:LEU:HG	1:A:601:ILE:CD1	2.22	0.69
1:B:352:PHE:HD2	1:B:387:MSE:HE3	1.57	0.69
1:B:568:LEU:HD13	1:B:583:TYR:CD1	2.27	0.69
1:A:404:GLN:CG	1:B:538:GLY:HA2	2.23	0.69
1:B:536:ARG:HG3	1:B:536:ARG:HH11	1.55	0.69
1:B:160:LEU:CD2	1:B:182:LEU:HG	2.23	0.68
1:B:238:LEU:HD13	1:B:239:GLN:N	2.09	0.68
1:B:535:ASN:HD21	1:B:539:ILE:HB	1.58	0.68
1:B:54:TYR:CE2	1:B:56:PRO:HG2	2.29	0.68
1:B:334:SER:O	1:B:336:GLN:N	2.27	0.68
1:A:204:ARG:HH11	1:A:204:ARG:CB	1.99	0.68
1:A:395:LEU:HD11	1:A:477:ILE:HD12	1.74	0.68
1:B:316:THR:HG22	1:B:322:SER:OG	1.94	0.67
1:B:509:LYS:HB2	1:B:516:ILE:CD1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ILE:N	1:B:565:HIS:HD2	1.88	0.67
1:A:123:GLN:HE21	1:A:133:VAL:HG11	1.60	0.66
1:B:155:PRO:HG2	1:B:158:ASP:OD2	1.95	0.66
1:B:591:VAL:O	1:B:595:ILE:HD12	1.95	0.66
1:A:470:PRO:HG2	1:A:473:GLY:HA2	1.76	0.66
1:B:284:GLY:N	1:B:289:SER:HG	1.95	0.65
1:B:297:ILE:CD1	1:B:311:TYR:HE1	2.09	0.64
1:A:516:ILE:H	1:A:565:HIS:CD2	2.12	0.64
1:B:114:GLU:HG2	1:B:193:VAL:HG21	1.79	0.64
1:A:67:ASP:HB3	1:A:70:GLN:HB2	1.79	0.64
1:A:103:ASP:HB3	1:A:106:ALA:HB3	1.80	0.64
1:B:499:SER:O	1:B:502:ASP:HB2	1.99	0.63
1:A:432:ASP:CA	1:A:439:VAL:HB	2.28	0.63
1:A:404:GLN:HG3	1:B:538:GLY:CA	2.30	0.62
1:A:204:ARG:NH1	1:A:205:PRO:HD2	2.15	0.62
1:B:151:VAL:HG13	1:B:200:LEU:HD23	1.80	0.62
1:A:413:TRP:CZ3	1:A:447:LEU:HD13	2.34	0.62
1:A:499:SER:O	1:A:502:ASP:HB2	1.99	0.62
1:A:602:ILE:HG22	1:A:603:LEU:N	2.14	0.62
1:B:120:TYR:HB2	1:B:183:PHE:HD1	1.62	0.62
1:B:591:VAL:O	1:B:594:LEU:HB2	2.00	0.62
1:B:123:GLN:HE22	1:B:285:TYR:HE2	1.48	0.61
1:B:335:TRP:HB2	1:B:348:PRO:CG	2.31	0.61
1:B:503:PHE:HA	1:B:506:VAL:HG12	1.82	0.61
1:B:543:SER:O	1:B:544:LEU:HD23	2.00	0.61
1:A:335:TRP:HB2	1:A:348:PRO:HG3	1.83	0.60
1:A:538:GLY:HA2	1:B:404:GLN:CG	2.31	0.60
1:B:33:SER:O	1:B:37:LYS:HG3	2.00	0.60
1:B:64:LEU:HD23	1:B:169:LYS:HD2	1.83	0.60
1:A:399:ARG:HD2	1:A:466:SER:O	2.01	0.60
1:A:427:ARG:HD3	1:A:432:ASP:HB2	1.83	0.60
1:A:82:GLN:HG3	1:A:89:PHE:CE2	2.37	0.60
1:B:330:ILE:HD11	1:B:352:PHE:CE1	2.37	0.59
1:A:53:LYS:HB3	1:A:529:PHE:HZ	1.67	0.59
1:A:321:LYS:HE3	1:A:323:HIS:HE1	1.66	0.59
1:B:297:ILE:HD13	1:B:298:GLY:N	2.18	0.59
1:B:535:ASN:ND2	1:B:539:ILE:HB	2.18	0.59
1:B:586:LYS:O	1:B:590:LEU:HG	2.01	0.59
1:B:392:PRO:HA	1:B:477:ILE:O	2.03	0.59
1:A:538:GLY:CA	1:B:404:GLN:HG3	2.32	0.59
1:A:321:LYS:HE3	1:A:323:HIS:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASN:HD22	1:A:496:GLN:HB2	1.67	0.58
1:B:143:ARG:HH22	1:B:204:ARG:CD	2.11	0.58
1:B:157:GLN:OE1	1:B:157:GLN:N	2.35	0.58
1:B:499:SER:OG	1:B:500:CYS:N	2.36	0.58
1:B:504:PHE:HB3	1:B:505:PRO:CD	2.34	0.58
1:B:198:THR:N	1:B:214:VAL:O	2.33	0.58
1:B:423:ASN:OD1	1:B:441:LEU:HB2	2.03	0.58
1:A:534:PRO:HG2	1:B:49:LEU:CD2	2.34	0.58
1:B:503:PHE:O	1:B:506:VAL:HG12	2.03	0.58
1:A:336:GLN:H	1:A:336:GLN:CD	2.11	0.58
1:A:520:ARG:HA	1:A:562:VAL:O	2.04	0.58
1:B:122:VAL:CG1	1:B:123:GLN:N	2.67	0.58
1:B:150:GLU:OE1	1:B:201:LYS:HD3	2.04	0.58
1:A:204:ARG:HB3	1:A:204:ARG:CZ	2.32	0.58
1:A:597:ASN:O	1:A:598:ASP:HB2	2.04	0.58
1:B:60:LYS:HZ3	1:B:558:GLU:HG3	1.69	0.58
1:B:156:VAL:O	1:B:159:VAL:HB	2.03	0.58
1:B:111:PHE:CE1	1:B:540:LYS:HA	2.38	0.57
1:B:587:VAL:O	1:B:591:VAL:HG23	2.04	0.57
1:B:339:GLU:O	1:B:340:ASP:HB2	2.04	0.57
1:A:127:ASP:OD1	1:A:129:ARG:NH2	2.38	0.57
1:A:206:PHE:HE1	1:A:208:THR:HG1	1.52	0.57
1:B:367:ILE:HD11	1:B:591:VAL:CG2	2.34	0.57
1:A:402:LEU:HB2	1:A:463:ILE:HB	1.87	0.57
1:B:536:ARG:HG3	1:B:536:ARG:NH1	2.20	0.57
1:B:122:VAL:HG12	1:B:123:GLN:H	1.69	0.57
1:B:143:ARG:NH2	1:B:204:ARG:HD2	2.18	0.57
1:A:427:ARG:CD	1:A:432:ASP:HB2	2.35	0.57
1:B:87:THR:O	1:B:91:GLN:HG3	2.04	0.57
1:B:367:ILE:HD11	1:B:591:VAL:HG22	1.86	0.57
1:A:390:ASP:OD1	1:A:391:ARG:HG2	2.06	0.56
1:A:594:LEU:HD21	1:A:601:ILE:CD1	2.35	0.56
1:B:201:LYS:HE3	1:B:209:THR:HG21	1.86	0.56
1:B:352:PHE:CD2	1:B:387:MSE:HE3	2.39	0.56
1:B:492:LEU:HD22	1:B:583:TYR:OH	2.06	0.56
1:A:509:LYS:HG3	1:A:516:ILE:HD13	1.88	0.56
1:B:401:ILE:HG12	1:B:464:GLU:O	2.05	0.56
1:B:122:VAL:HB	1:B:179:LEU:HD21	1.86	0.56
1:B:209:THR:O	1:B:210:ARG:HD3	2.06	0.56
1:A:602:ILE:CG2	1:A:603:LEU:H	2.13	0.56
1:B:192:LYS:O	1:B:194:PRO:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:NH1	1:A:213:ARG:NE	2.51	0.55
1:A:498:PHE:CD1	1:A:498:PHE:N	2.73	0.55
1:B:122:VAL:CG1	1:B:123:GLN:H	2.20	0.55
1:A:70:GLN:HE21	1:A:70:GLN:N	2.05	0.55
1:A:168:HIS:CE1	1:A:170:GLY:HA2	2.42	0.55
1:B:316:THR:HA	1:B:321:LYS:O	2.06	0.55
1:B:119:PRO:HG3	1:B:217:ARG:HH22	1.70	0.55
1:A:54:TYR:CZ	1:A:56:PRO:HG2	2.41	0.55
1:A:404:GLN:H	1:A:404:GLN:CD	2.12	0.55
1:A:487:LYS:HB3	1:A:488:PRO:HD2	1.88	0.55
1:A:105:HIS:CE1	1:A:528:VAL:HG22	2.41	0.54
1:B:182:LEU:O	1:B:183:PHE:HD2	1.90	0.54
1:B:450:PHE:O	1:B:454:VAL:HG23	2.07	0.54
1:B:53:LYS:HB3	1:B:529:PHE:CZ	2.42	0.54
1:B:204:ARG:HB2	1:B:208:THR:HG22	1.89	0.54
1:B:314:SER:O	1:B:315:VAL:HG23	2.08	0.54
1:B:329:ARG:HH11	1:B:369:ASP:CG	2.16	0.54
1:B:138:PHE:O	1:B:139:SER:C	2.50	0.54
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.72	0.54
1:B:375:GLY:HA3	1:B:499:SER:OG	2.08	0.54
1:B:600:THR:O	1:B:602:ILE:N	2.41	0.54
1:A:192:LYS:NZ	1:A:192:LYS:CB	2.70	0.54
1:A:599:GLY:O	1:A:600:THR:C	2.49	0.53
1:B:159:VAL:HG11	1:B:182:LEU:HD21	1.91	0.53
1:B:157:GLN:H	1:B:157:GLN:CD	2.15	0.53
1:B:197:ARG:HA	1:B:215:LYS:HA	1.89	0.53
1:A:399:ARG:HD3	1:A:468:PRO:HD3	1.91	0.53
1:B:182:LEU:HD13	1:B:183:PHE:HE2	1.72	0.53
1:A:602:ILE:O	1:A:603:LEU:C	2.51	0.53
1:A:206:PHE:HE1	1:A:208:THR:OG1	1.92	0.53
1:A:333:TYR:CE2	1:A:381:LEU:HD23	2.44	0.53
1:A:415:THR:HA	1:A:418:GLU:HG3	1.90	0.53
1:B:330:ILE:HD11	1:B:352:PHE:HE1	1.72	0.53
1:A:516:ILE:N	1:A:516:ILE:HD12	2.23	0.53
1:B:149:LEU:O	1:B:155:PRO:HA	2.08	0.53
1:B:363:THR:HG23	1:B:485:TYR:OH	2.09	0.53
1:B:596:ASN:O	1:B:597:ASN:HB3	2.08	0.52
1:B:57:LYS:O	1:B:61:GLU:HG3	2.09	0.52
1:B:143:ARG:NH2	1:B:204:ARG:CZ	2.72	0.52
1:B:156:VAL:HB	1:B:157:GLN:OE1	2.09	0.52
1:B:329:ARG:HD2	1:B:369:ASP:OD1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:O	1:A:61:GLU:HG3	2.10	0.52
1:A:515:LEU:HD23	1:A:565:HIS:CD2	2.45	0.52
1:B:105:HIS:CG	1:B:528:VAL:HG13	2.45	0.52
1:A:316:THR:HA	1:A:321:LYS:O	2.09	0.52
1:B:515:LEU:HD13	1:B:517:VAL:HG22	1.91	0.52
1:B:150:GLU:HB3	1:B:154:ALA:O	2.10	0.52
1:B:163:LEU:HD11	1:B:185:ARG:HH21	1.74	0.52
1:A:493:ILE:HD13	1:A:519:THR:O	2.10	0.52
1:B:328:LEU:C	1:B:328:LEU:HD13	2.35	0.52
1:B:566:ILE:HD12	1:B:590:LEU:CD1	2.40	0.52
1:A:64:LEU:HD23	1:A:169:LYS:HD2	1.92	0.52
1:B:64:LEU:CD2	1:B:169:LYS:HD2	2.39	0.52
1:B:155:PRO:CG	1:B:158:ASP:OD2	2.58	0.51
1:A:432:ASP:OD1	1:A:432:ASP:C	2.53	0.51
1:B:155:PRO:O	1:B:156:VAL:C	2.53	0.51
1:B:574:ASP:OD1	1:B:582:GLU:HB2	2.11	0.51
1:B:494:ASN:C	1:B:494:ASN:HD22	2.17	0.51
1:B:494:ASN:ND2	1:B:496:GLN:H	2.08	0.51
1:A:204:ARG:NH1	1:A:206:PHE:CE2	2.78	0.51
1:A:230:ALA:N	1:A:231:PRO:HD2	2.26	0.51
1:A:577:TYR:O	1:A:579:GLY:N	2.44	0.51
1:B:134:ASP:O	1:B:135:ILE:HD13	2.10	0.51
1:A:142:ILE:HD12	1:A:202:ILE:HG21	1.93	0.51
1:A:536:ARG:HA	1:B:404:GLN:NE2	2.26	0.51
1:A:551:ARG:HG3	1:A:557:ILE:HD11	1.92	0.51
1:B:88:SER:O	1:B:92:GLN:HG3	2.11	0.51
1:B:487:LYS:HB3	1:B:488:PRO:HD2	1.92	0.51
1:B:563:GLU:O	1:B:563:GLU:HG2	2.09	0.51
1:A:600:THR:O	1:A:600:THR:HG22	2.11	0.51
1:B:197:ARG:HA	1:B:214:VAL:O	2.11	0.51
1:B:503:PHE:HA	1:B:506:VAL:CG1	2.41	0.51
1:B:506:VAL:HB	1:B:562:VAL:HG21	1.91	0.51
1:B:356:ILE:O	1:B:357:GLN:C	2.52	0.51
1:A:155:PRO:O	1:A:158:ASP:HB2	2.12	0.50
1:B:480:HIS:ND1	1:B:481:PRO:HD2	2.27	0.50
1:A:382:TYR:CD1	1:A:477:ILE:HD11	2.46	0.50
1:A:393:LEU:HD21	1:A:513:ARG:HG3	1.93	0.50
1:A:427:ARG:HB3	1:A:432:ASP:HB3	1.93	0.50
1:A:593:GLN:OE1	1:A:603:LEU:O	2.29	0.50
1:B:117:TYR:CG	1:B:118:LEU:N	2.78	0.50
1:A:161:ALA:HA	1:A:164:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LEU:HB2	1:A:485:TYR:CE2	2.47	0.50
1:A:499:SER:OG	1:A:500:CYS:N	2.38	0.50
1:B:66:TRP:CZ2	1:B:101:LEU:HD21	2.47	0.50
1:B:297:ILE:HD13	1:B:297:ILE:N	2.27	0.50
1:B:417:LEU:HB2	1:B:448:LYS:HD2	1.94	0.50
1:A:489:ILE:HG22	1:A:490:CYS:N	2.26	0.50
1:B:149:LEU:C	1:B:150:GLU:HG3	2.37	0.50
1:A:325:VAL:CG1	1:A:367:ILE:HD13	2.40	0.50
1:A:499:SER:H	1:A:524:ALA:HB3	1.77	0.50
1:A:537:THR:HG22	1:A:537:THR:O	2.12	0.50
1:B:182:LEU:C	1:B:183:PHE:HD2	2.19	0.50
1:B:516:ILE:O	1:B:565:HIS:N	2.42	0.50
1:B:517:VAL:CG1	1:B:566:ILE:HB	2.39	0.49
1:A:548:LEU:HD22	1:A:556:PHE:HD2	1.77	0.49
1:B:297:ILE:HD13	1:B:298:GLY:H	1.76	0.49
1:B:103:ASP:OD1	1:B:105:HIS:HB2	2.12	0.49
1:A:376:GLY:O	1:A:500:CYS:SG	2.64	0.49
1:B:566:ILE:HD12	1:B:590:LEU:HD13	1.94	0.49
1:A:49:LEU:CD2	1:B:534:PRO:HG2	2.42	0.49
1:A:105:HIS:HB3	1:A:528:VAL:HG13	1.95	0.49
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.77	0.49
1:B:470:PRO:HG2	1:B:473:GLY:HA2	1.95	0.49
1:A:302:TRP:CH2	1:A:304:SER:HB3	2.47	0.49
1:B:126:SER:OG	1:B:571:THR:HG22	2.12	0.49
1:B:545:THR:HG22	1:B:547:SER:H	1.77	0.49
1:B:89:PHE:O	1:B:93:VAL:HG23	2.13	0.49
1:B:504:PHE:HB3	1:B:505:PRO:HD3	1.95	0.49
1:A:60:LYS:NZ	1:A:559:ASN:HD21	2.11	0.48
1:A:366:LEU:HD22	1:A:368:ILE:CD1	2.38	0.48
1:B:118:LEU:HD22	1:B:120:TYR:CE1	2.48	0.48
1:B:230:ALA:N	1:B:231:PRO:HD2	2.27	0.48
1:A:48:HIS:O	1:A:52:VAL:HG22	2.13	0.48
1:B:290:THR:O	1:B:329:ARG:HD3	2.12	0.48
1:A:353:ALA:O	1:A:357:GLN:HG3	2.14	0.48
1:B:370:GLN:HE21	1:B:370:GLN:HB3	1.49	0.48
1:A:83:GLU:O	1:A:84:ASN:C	2.56	0.48
1:A:105:HIS:CE1	1:A:499:SER:HB3	2.48	0.48
1:B:43:LEU:HD23	1:B:43:LEU:O	2.13	0.48
1:B:329:ARG:HB2	1:B:369:ASP:HB3	1.95	0.48
1:B:53:LYS:HB3	1:B:529:PHE:HZ	1.75	0.48
1:B:499:SER:H	1:B:524:ALA:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TRP:HE1	1:A:559:ASN:HD22	1.60	0.48
1:A:182:LEU:HD13	1:A:183:PHE:CZ	2.49	0.48
1:B:132:PHE:CZ	1:B:148:LEU:HD13	2.49	0.48
1:B:143:ARG:NH2	1:B:204:ARG:NE	2.61	0.48
1:A:548:LEU:HD22	1:A:556:PHE:CD2	2.49	0.48
1:B:143:ARG:HB2	1:B:143:ARG:NH1	2.28	0.48
1:B:537:THR:O	1:B:537:THR:HG22	2.13	0.48
1:A:359:PHE:O	1:A:363:THR:HG22	2.14	0.48
1:B:355:ILE:HG22	1:B:359:PHE:CE1	2.49	0.47
1:B:494:ASN:C	1:B:494:ASN:ND2	2.72	0.47
1:A:572:ALA:O	1:A:576:ARG:HB2	2.13	0.47
1:B:114:GLU:HA	1:B:219:VAL:O	2.14	0.47
1:A:197:ARG:CZ	1:A:213:ARG:HE	2.27	0.47
1:B:98:ILE:N	1:B:98:ILE:HD12	2.29	0.47
1:B:173:ALA:HA	1:B:495:GLU:HB2	1.96	0.47
1:B:366:LEU:HB2	1:B:485:TYR:CE2	2.50	0.47
1:A:321:LYS:HG2	1:A:323:HIS:CE1	2.49	0.47
1:A:494:ASN:O	1:A:521:THR:HA	2.14	0.47
1:B:201:LYS:HE3	1:B:209:THR:CG2	2.44	0.47
1:A:70:GLN:HE21	1:A:70:GLN:CA	2.27	0.47
1:B:148:LEU:HG	1:B:156:VAL:CG2	2.45	0.47
1:A:53:LYS:HB3	1:A:529:PHE:CZ	2.46	0.47
1:B:179:LEU:HD23	1:B:179:LEU:O	2.15	0.47
1:A:229:ILE:HD13	1:B:458:TRP:O	2.14	0.47
1:B:370:GLN:O	1:B:497:ASP:OD1	2.31	0.47
1:B:297:ILE:CD1	1:B:297:ILE:N	2.78	0.47
1:B:579:GLY:C	1:B:581:SER:H	2.21	0.47
1:B:297:ILE:CD1	1:B:297:ILE:H	2.28	0.47
1:A:335:TRP:C	1:A:337:ASP:H	2.23	0.46
1:B:449:SER:O	1:B:453:GLN:HG3	2.15	0.46
1:B:94:LEU:O	1:B:98:ILE:HD13	2.15	0.46
1:B:579:GLY:C	1:B:581:SER:N	2.70	0.46
1:A:371:THR:HA	1:A:494:ASN:HB2	1.98	0.46
1:A:407:VAL:O	1:A:410:ALA:HB3	2.15	0.46
1:B:60:LYS:HZ3	1:B:558:GLU:CG	2.27	0.46
1:B:118:LEU:O	1:B:120:TYR:N	2.48	0.46
1:A:304:SER:O	1:A:306:GLY:N	2.49	0.46
1:A:601:ILE:HD12	1:A:601:ILE:H	1.81	0.46
1:B:55:ALA:N	1:B:56:PRO:HD2	2.30	0.46
1:B:333:TYR:CE2	1:B:381:LEU:HD23	2.50	0.46
1:B:395:LEU:HD11	1:B:477:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LEU:HD11	1:A:477:ILE:CD1	2.43	0.46
1:A:363:THR:CG2	1:A:485:TYR:OH	2.64	0.46
1:A:381:LEU:C	1:A:381:LEU:HD13	2.41	0.46
1:B:123:GLN:NE2	1:B:285:TYR:HE2	2.11	0.46
1:B:503:PHE:O	1:B:504:PHE:C	2.59	0.46
1:B:571:THR:O	1:B:572:ALA:C	2.59	0.46
1:A:516:ILE:N	1:A:565:HIS:HD2	2.05	0.45
1:B:310:ALA:HA	1:B:327:PHE:O	2.16	0.45
1:B:317:ASP:CG	1:B:321:LYS:HB3	2.41	0.45
1:B:325:VAL:HG12	1:B:326:GLY:N	2.30	0.45
1:A:70:GLN:HE21	1:A:70:GLN:H	1.63	0.45
1:A:404:GLN:NE2	1:B:536:ARG:HA	2.31	0.45
1:A:519:THR:O	1:A:520:ARG:C	2.59	0.45
1:B:72:SER:O	1:B:76:GLN:HG3	2.16	0.45
1:B:214:VAL:HG12	1:B:215:LYS:N	2.30	0.45
1:A:380:TYR:CE1	1:A:384:LEU:HD21	2.52	0.45
1:A:370:GLN:HE21	1:A:370:GLN:HB3	1.51	0.45
1:B:294:LEU:HD13	1:B:584:LEU:HD21	1.99	0.45
1:B:471:LEU:O	1:B:472:PHE:HB2	2.17	0.45
1:A:56:PRO:O	1:A:60:LYS:HG2	2.16	0.45
1:A:239:GLN:HE21	1:A:239:GLN:HA	1.81	0.45
1:B:132:PHE:CE1	1:B:148:LEU:HD13	2.52	0.45
1:B:55:ALA:HA	1:B:401:ILE:HD11	1.98	0.45
1:B:165:GLY:H	1:B:168:HIS:HB2	1.81	0.45
1:B:366:LEU:HD23	1:B:367:ILE:N	2.32	0.45
1:B:69:VAL:O	1:B:73:VAL:HG23	2.17	0.44
1:B:506:VAL:HB	1:B:562:VAL:CG2	2.48	0.44
1:B:579:GLY:O	1:B:581:SER:N	2.50	0.44
1:B:595:ILE:HD12	1:B:595:ILE:H	1.82	0.44
1:A:504:PHE:HB3	1:A:505:PRO:CD	2.47	0.44
1:B:493:ILE:O	1:B:493:ILE:HG13	2.16	0.44
1:B:515:LEU:CD1	1:B:517:VAL:HG22	2.48	0.44
1:A:391:ARG:NH2	1:A:511:ASN:O	2.48	0.44
1:B:195:SER:HB3	1:B:218:TYR:CD1	2.53	0.44
1:B:568:LEU:HA	1:B:568:LEU:HD23	1.80	0.44
1:A:558:GLU:O	1:A:559:ASN:HB2	2.17	0.44
1:B:117:TYR:O	1:B:118:LEU:HG	2.17	0.44
1:B:137:THR:HG23	1:B:138:PHE:N	2.33	0.44
1:B:59:TRP:HE1	1:B:559:ASN:ND2	2.09	0.44
1:B:126:SER:OG	1:B:571:THR:HA	2.18	0.44
1:A:335:TRP:C	1:A:337:ASP:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:VAL:HG13	1:A:455:LEU:CD2	2.47	0.44
1:A:408:VAL:HG21	1:B:111:PHE:HB3	1.99	0.44
1:B:168:HIS:CE1	1:B:170:GLY:H	2.36	0.44
1:B:286:ASN:O	1:B:287:ILE:C	2.61	0.44
1:A:43:LEU:HD13	1:A:43:LEU:C	2.42	0.44
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.89	0.44
1:A:328:LEU:HD11	1:A:352:PHE:HE1	1.83	0.44
1:A:285:TYR:HE2	1:A:580:TYR:HH	1.67	0.43
1:A:408:VAL:CG2	1:B:111:PHE:HB3	2.48	0.43
1:A:451:GLY:O	1:A:455:LEU:HG	2.18	0.43
1:A:493:ILE:HD12	1:A:519:THR:H	1.83	0.43
1:B:328:LEU:O	1:B:368:ILE:HA	2.18	0.43
1:B:352:PHE:HD2	1:B:387:MSE:CE	2.29	0.43
1:B:33:SER:HB3	1:B:36:CYS:HB3	2.01	0.43
1:B:541:THR:HG22	1:B:542:CYS:N	2.33	0.43
1:B:558:GLU:O	1:B:559:ASN:HB2	2.19	0.43
1:A:368:ILE:HD12	1:A:368:ILE:N	2.33	0.43
1:A:368:ILE:HD13	1:A:489:ILE:CG2	2.46	0.43
1:A:427:ARG:HB3	1:A:432:ASP:CB	2.49	0.43
1:B:363:THR:HG23	1:B:485:TYR:HH	1.83	0.43
1:B:433:ASN:ND2	1:B:436:GLY:N	2.53	0.43
1:A:576:ARG:O	1:A:577:TYR:CD2	2.72	0.43
1:A:603:LEU:C	1:A:603:LEU:HD23	2.43	0.43
1:B:342:ASP:HA	1:B:343:PRO:HD2	1.77	0.43
1:A:534:PRO:CG	1:B:49:LEU:HD22	2.43	0.43
1:A:530:ASN:HB3	1:A:541:THR:CG2	2.49	0.43
1:B:55:ALA:HA	1:B:401:ILE:HG13	2.01	0.43
1:B:359:PHE:O	1:B:363:THR:CG2	2.52	0.43
1:A:35:VAL:HG21	1:A:227:ALA:HB2	2.01	0.43
1:A:335:TRP:HB2	1:A:348:PRO:CG	2.46	0.43
1:B:393:LEU:HB2	1:B:477:ILE:HB	2.00	0.43
1:B:516:ILE:HG22	1:B:564:PRO:HA	2.00	0.43
1:B:589:LYS:O	1:B:593:GLN:HG3	2.19	0.43
1:A:111:PHE:CE1	1:B:405:ASP:HB2	2.54	0.42
1:B:164:TYR:HB3	1:B:168:HIS:CG	2.54	0.42
1:B:210:ARG:O	1:B:211:GLU:HG2	2.19	0.42
1:A:142:ILE:HD13	1:A:202:ILE:HD13	2.00	0.42
1:A:304:SER:C	1:A:306:GLY:H	2.27	0.42
1:A:366:LEU:HB2	1:A:485:TYR:CZ	2.54	0.42
1:A:461:GLY:HA2	1:B:229:ILE:CG2	2.49	0.42
1:B:119:PRO:HG3	1:B:217:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLU:OE1	1:B:201:LYS:CD	2.66	0.42
1:A:392:PRO:HA	1:A:477:ILE:O	2.19	0.42
1:A:382:TYR:CG	1:A:477:ILE:HD11	2.54	0.42
1:A:504:PHE:HB3	1:A:505:PRO:HD3	2.02	0.42
1:B:474:PHE:N	1:B:474:PHE:CD1	2.88	0.42
1:A:105:HIS:ND1	1:A:528:VAL:HG22	2.35	0.42
1:B:159:VAL:CG1	1:B:182:LEU:HD21	2.50	0.42
1:B:210:ARG:O	1:B:211:GLU:CG	2.67	0.42
1:B:182:LEU:C	1:B:183:PHE:CD2	2.98	0.42
1:A:355:ILE:HG22	1:A:359:PHE:CE1	2.54	0.42
1:B:149:LEU:HD11	1:B:203:ARG:CB	2.40	0.42
1:B:352:PHE:CD2	1:B:384:LEU:HD22	2.54	0.42
1:B:382:TYR:CD1	1:B:477:ILE:HD11	2.55	0.42
1:A:404:GLN:HE22	1:B:536:ARG:HA	1.85	0.42
1:A:449:SER:OG	1:A:453:GLN:NE2	2.50	0.42
1:B:150:GLU:HB3	1:B:154:ALA:C	2.44	0.42
1:A:236:PRO:HB3	1:B:464:GLU:HB3	2.02	0.42
1:B:317:ASP:OD2	1:B:321:LYS:HB3	2.20	0.42
1:B:339:GLU:O	1:B:340:ASP:CB	2.68	0.42
1:B:464:GLU:OE2	1:B:464:GLU:HA	2.19	0.42
1:B:498:PHE:HA	1:B:502:ASP:OD2	2.20	0.42
1:A:602:ILE:O	1:A:603:LEU:O	2.38	0.41
1:B:67:ASP:HB3	1:B:70:GLN:HB3	2.02	0.41
1:B:186:MSE:N	1:B:191:HIS:HD2	2.00	0.41
1:B:520:ARG:HG3	1:B:520:ARG:HH11	1.84	0.41
1:A:238:LEU:O	1:A:239:GLN:C	2.62	0.41
1:A:431:GLY:C	1:A:433:ASN:H	2.26	0.41
1:B:111:PHE:CZ	1:B:540:LYS:HG3	2.55	0.41
1:B:130:PHE:CD1	1:B:130:PHE:N	2.88	0.41
1:B:342:ASP:O	1:B:344:SER:N	2.54	0.41
1:A:33:SER:HB3	1:A:36:CYS:HB3	2.01	0.41
1:A:82:GLN:HG3	1:A:89:PHE:CZ	2.56	0.41
1:B:118:LEU:HD22	1:B:120:TYR:HE1	1.85	0.41
1:B:325:VAL:CG1	1:B:326:GLY:N	2.84	0.41
1:A:471:LEU:O	1:A:472:PHE:HB2	2.20	0.41
1:B:46:LEU:HD13	1:B:98:ILE:HD11	2.02	0.41
1:B:143:ARG:NH2	1:B:204:ARG:CD	2.79	0.41
1:B:143:ARG:HH11	1:B:143:ARG:CB	2.34	0.41
1:B:148:LEU:HG	1:B:156:VAL:HG22	2.03	0.41
1:B:433:ASN:HB2	1:B:437:TYR:O	2.21	0.41
1:A:53:LYS:HD3	1:A:53:LYS:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ILE:H	1:A:516:ILE:HD12	1.84	0.41
1:B:135:ILE:CG2	1:B:137:THR:HG22	2.50	0.41
1:A:432:ASP:C	1:A:439:VAL:HB	2.45	0.41
1:B:333:TYR:C	1:B:376:GLY:HA3	2.45	0.41
1:B:492:LEU:HA	1:B:517:VAL:O	2.21	0.41
1:B:592:CYS:C	1:B:594:LEU:N	2.75	0.41
1:A:163:LEU:HD13	1:A:181:THR:HG22	2.03	0.41
1:A:476:LYS:HE2	1:A:476:LYS:HB3	1.91	0.41
1:A:483:VAL:C	1:A:484:GLN:HG2	2.46	0.41
1:B:353:ALA:O	1:B:354:LYS:C	2.64	0.41
1:B:370:GLN:OE1	1:B:501:ALA:HA	2.21	0.41
1:B:503:PHE:CA	1:B:506:VAL:HG12	2.49	0.41
1:B:532:GLN:HE21	1:B:532:GLN:HB2	1.59	0.41
1:A:133:VAL:O	1:A:578:LYS:HD3	2.21	0.41
1:A:407:VAL:HG11	1:B:223:VAL:HG13	2.03	0.41
1:B:317:ASP:HB3	1:B:592:CYS:SG	2.61	0.41
1:B:494:ASN:HA	1:B:519:THR:OG1	2.21	0.41
1:B:592:CYS:O	1:B:593:GLN:C	2.64	0.41
1:A:43:LEU:HD23	1:A:94:LEU:CD2	2.52	0.40
1:A:89:PHE:O	1:A:93:VAL:HG23	2.21	0.40
1:B:575:ILE:O	1:B:576:ARG:C	2.65	0.40
1:B:351:GLU:O	1:B:355:ILE:HG13	2.20	0.40
1:A:478:HIS:O	1:A:479:PRO:C	2.63	0.40
1:B:114:GLU:O	1:B:193:VAL:HG21	2.20	0.40
1:B:135:ILE:HG22	1:B:137:THR:HG22	2.04	0.40
1:B:363:THR:CG2	1:B:485:TYR:OH	2.69	0.40
1:B:586:LYS:O	1:B:586:LYS:HD3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:NH1	1:A:204:ARG:NH2[7_465]	2.19	0.01

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	523/579 (90%)	477 (91%)	32 (6%)	14 (3%)	4	16
1	B	523/579 (90%)	449 (86%)	57 (11%)	17 (3%)	3	13
All	All	1046/1158 (90%)	926 (88%)	89 (8%)	31 (3%)	3	14

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	GLU
1	A	466	SER
1	A	578	LYS
1	A	602	ILE
1	B	83	GLU
1	B	156	VAL
1	B	335	TRP
1	B	466	SER
1	B	600	THR
1	A	306	GLY
1	A	335	TRP
1	B	141	GLU
1	B	166	SER
1	B	170	GLY
1	B	601	ILE
1	A	315	VAL
1	B	139	SER
1	B	343	PRO
1	B	499	SER
1	B	576	ARG
1	A	600	THR
1	B	119	PRO
1	B	580	TYR
1	B	597	ASN
1	A	499	SER
1	A	597	ASN
1	B	299	PRO
1	A	56	PRO
1	A	465	LEU
1	A	156	VAL
1	A	479	PRO

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	456/495 (92%)	415 (91%)	41 (9%)	9	28
1	B	438/495 (88%)	406 (93%)	32 (7%)	13	38
All	All	894/990 (90%)	821 (92%)	73 (8%)	10	32

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	70	GLN
1	A	87	THR
1	A	175	GLU
1	A	179	LEU
1	A	182	LEU
1	A	192	LYS
1	A	203	ARG
1	A	204	ARG
1	A	213	ARG
1	A	226	LEU
1	A	239	GLN
1	A	328	LEU
1	A	361	SER
1	A	363	THR
1	A	366	LEU
1	A	370	GLN
1	A	384	LEU
1	A	394	GLU
1	A	404	GLN
1	A	416	LEU
1	A	432	ASP
1	A	433	ASN
1	A	448	LYS
1	A	463	ILE
1	A	467	THR
1	A	477	ILE

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Mol	Chain	Res	Type
1	A	483	VAL
1	A	484	GLN
1	A	495	GLU
1	A	498	PHE
1	A	513	ARG
1	A	515	LEU
1	A	528	VAL
1	A	548	LEU
1	A	553	HIS
1	A	562	VAL
1	A	568	LEU
1	A	589	LYS
1	A	593	GLN
1	A	603	LEU
1	B	41	GLN
1	B	58	THR
1	B	72	SER
1	B	88	SER
1	B	136	MSE
1	B	157	GLN
1	B	182	LEU
1	B	209	THR
1	B	238	LEU
1	B	297	ILE
1	B	301	ILE
1	B	312	ILE
1	B	328	LEU
1	B	366	LEU
1	B	370	GLN
1	B	381	LEU
1	B	404	GLN
1	B	416	LEU
1	B	421	ASP
1	B	424	VAL
1	B	441	LEU
1	B	483	VAL
1	B	494	ASN
1	B	513	ARG
1	B	517	VAL
1	B	528	VAL
1	B	532	GLN
1	B	568	LEU

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Mol	Chain	Res	Type
1	B	586	LYS
1	B	592	CYS
1	B	596	ASN
1	B	603	LEU

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

Mol	Chain	Res	Type
1	A	48	HIS
1	A	62	GLN
1	A	70	GLN
1	A	84	ASN
1	A	92	GLN
1	A	102	ASN
1	A	123	GLN
1	A	168	HIS
1	A	191	HIS
1	A	239	GLN
1	A	323	HIS
1	A	404	GLN
1	A	442	GLN
1	A	453	GLN
1	A	494	ASN
1	A	559	ASN
1	A	565	HIS
1	A	593	GLN
1	A	596	ASN
1	B	38	ASN
1	B	84	ASN
1	B	102	ASN
1	B	123	GLN
1	B	167	ASN
1	B	168	HIS
1	B	191	HIS
1	B	239	GLN
1	B	286	ASN
1	B	323	HIS
1	B	357	GLN
1	B	404	GLN
1	B	494	ASN
1	B	530	ASN
1	B	532	GLN

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Mol	Chain	Res	Type
1	B	559	ASN
1	B	565	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 [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	521/579 (89%)	0.15	27 (5%) 33 26	18, 36, 68, 119	0
1	B	521/579 (89%)	1.03	107 (20%) 2 2	23, 54, 105, 159	0
All	All	1042/1158 (89%)	0.59	134 (12%) 7 6	18, 43, 94, 159	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	577	TYR	8.8
1	B	603	LEU	8.1
1	A	603	LEU	7.7
1	B	206	PHE	6.7
1	B	137	THR	6.4
1	B	602	ILE	6.4
1	B	600	THR	6.3
1	B	205	PRO	6.2
1	B	142	ILE	6.2
1	A	602	ILE	6.1
1	B	204	ARG	6.1
1	B	239	GLN	5.7
1	B	571	THR	5.7
1	A	305	GLU	5.5
1	B	209	THR	5.4
1	A	206	PHE	5.3
1	B	599	GLY	5.3
1	B	196	GLY	5.1
1	B	120	TYR	5.0
1	A	306	GLY	4.9
1	B	138	PHE	4.9
1	B	149	LEU	4.9
1	B	212	VAL	4.8
1	B	139	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	141	GLU	4.5
1	A	601	ILE	4.4
1	B	202	ILE	4.4
1	B	322	SER	4.4
1	B	208	THR	4.4
1	B	117	TYR	4.4
1	A	140	SER	4.3
1	A	599	GLY	4.3
1	B	199	THR	4.3
1	B	570	PHE	4.3
1	A	600	THR	4.3
1	B	213	ARG	4.2
1	B	200	LEU	4.2
1	B	575	ILE	4.1
1	A	70	GLN	4.0
1	B	217	ARG	3.9
1	A	598	ASP	3.9
1	B	210	ARG	3.9
1	B	143	ARG	3.8
1	B	148	LEU	3.7
1	B	214	VAL	3.7
1	B	145	GLY	3.6
1	B	318	GLY	3.6
1	B	601	ILE	3.6
1	B	155	PRO	3.5
1	B	572	ALA	3.5
1	B	125	SER	3.5
1	B	207	GLY	3.5
1	B	150	GLU	3.4
1	B	154	ALA	3.4
1	B	146	ASP	3.4
1	B	118	LEU	3.3
1	B	131	TYR	3.3
1	B	134	ASP	3.3
1	B	580	TYR	3.3
1	A	139	SER	3.2
1	B	127	ASP	3.2
1	A	239	GLN	3.2
1	A	319	ASP	3.1
1	B	295	PRO	3.1
1	A	315	VAL	3.0
1	B	577	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	320	GLY	3.0
1	B	364	GLU	3.0
1	B	219	VAL	3.0
1	B	147	GLU	2.9
1	B	297	ILE	2.9
1	A	204	ARG	2.9
1	B	211	GLU	2.9
1	B	123	GLN	2.9
1	A	421	ASP	2.9
1	B	122	VAL	2.8
1	A	336	GLN	2.8
1	B	440	ASP	2.8
1	A	138	PHE	2.7
1	B	183	PHE	2.7
1	B	151	VAL	2.7
1	B	140	SER	2.7
1	B	133	VAL	2.6
1	B	316	THR	2.6
1	B	130	PHE	2.6
1	B	157	GLN	2.6
1	B	285	TYR	2.5
1	B	198	THR	2.5
1	B	305	GLU	2.5
1	A	141	GLU	2.5
1	B	313	SER	2.5
1	B	153	GLY	2.5
1	B	132	PHE	2.5
1	B	193	VAL	2.5
1	B	597	ASN	2.5
1	B	144	VAL	2.4
1	B	563	GLU	2.4
1	B	197	ARG	2.4
1	B	583	TYR	2.4
1	B	135	ILE	2.4
1	B	598	ASP	2.4
1	B	215	LYS	2.4
1	B	582	GLU	2.4
1	A	440	ASP	2.4
1	B	317	ASP	2.4
1	B	361	SER	2.4
1	B	160	LEU	2.4
1	A	314	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	578	LYS	2.3
1	B	574	ASP	2.3
1	B	306	GLY	2.3
1	A	442	GLN	2.3
1	B	319	ASP	2.2
1	B	299	PRO	2.2
1	B	532	GLN	2.2
1	B	284	GLY	2.2
1	B	568	LEU	2.2
1	A	77	GLN	2.2
1	B	589	LYS	2.2
1	B	579	GLY	2.1
1	B	495	GLU	2.1
1	B	70	GLN	2.1
1	B	286	ASN	2.1
1	B	345	GLY	2.1
1	B	83	GLU	2.1
1	B	315	VAL	2.1
1	B	581	SER	2.1
1	B	584	LEU	2.1
1	B	293	PHE	2.1
1	A	432	ASP	2.1
1	A	553	HIS	2.0
1	B	300	VAL	2.0
1	B	596	ASN	2.0
1	B	585	ASP	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.