



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:30 PM UTC

PDB ID : 5A9J / pdb_00005a9j
Title : Crystal structure of the Helicase domain of human DNA polymerase theta, apo-form
Authors : Newman, J.A.; Cooper, C.D.O.; Aitkenhead, H.; Pinkas, D.M.; Kupinska, K.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Gileadi, O.
Deposited on : 2015-07-21
Resolution : 3.55 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

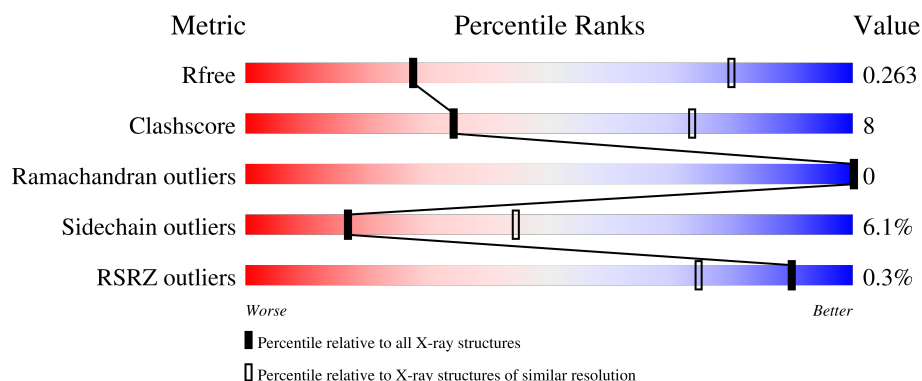
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

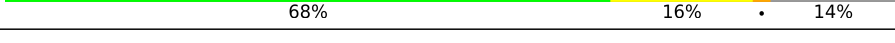
The reported resolution of this entry is 3.55 Å.

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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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	896	
1	B	896	
1	C	896	
1	D	896	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24408 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 DNA POLYMERASE THETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	805	Total	C	N	O	S	0	0	0
			6215	3974	1067	1134	40			
1	B	801	Total	C	N	O	S	0	0	0
			6168	3944	1058	1126	40			
1	C	780	Total	C	N	O	S	0	0	0
			6048	3870	1039	1102	37			
1	D	772	Total	C	N	O	S	0	0	0
			5977	3827	1025	1089	36			

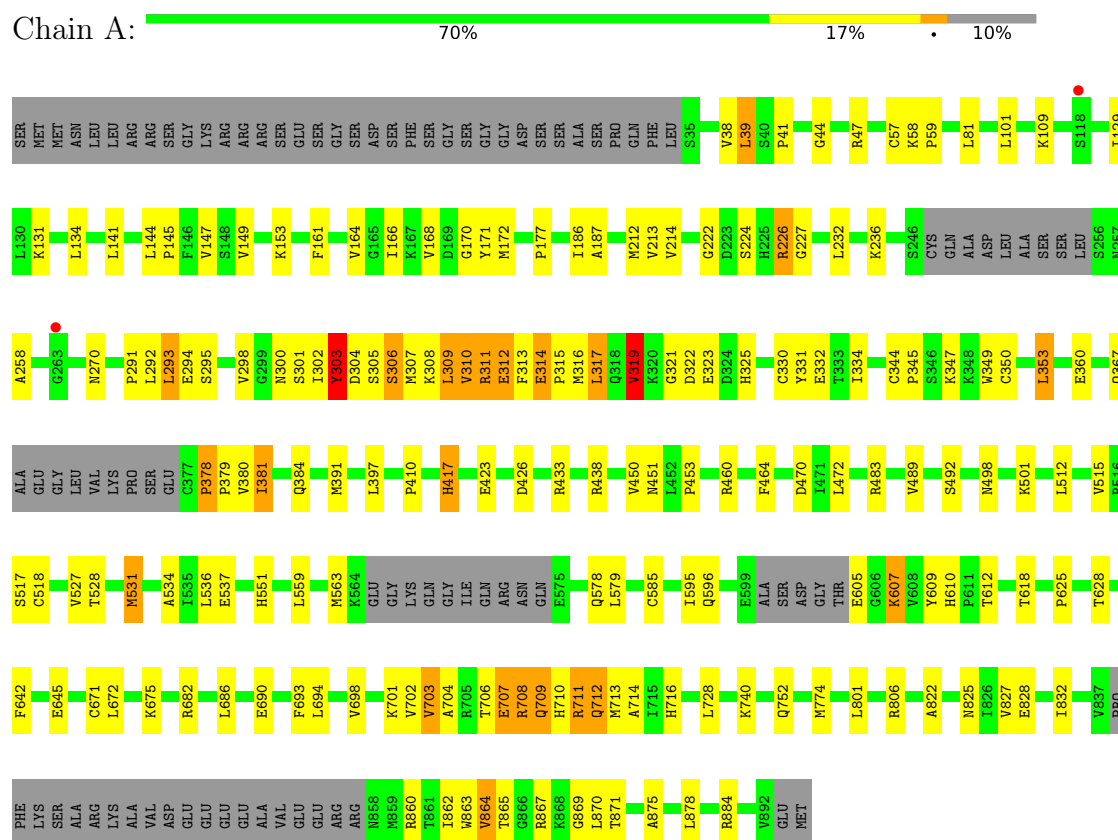
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP O75417
A	0	MET	-	expression tag	UNP O75417
B	-1	SER	-	expression tag	UNP O75417
B	0	MET	-	expression tag	UNP O75417
C	-1	SER	-	expression tag	UNP O75417
C	0	MET	-	expression tag	UNP O75417
D	-1	SER	-	expression tag	UNP O75417
D	0	MET	-	expression tag	UNP O75417

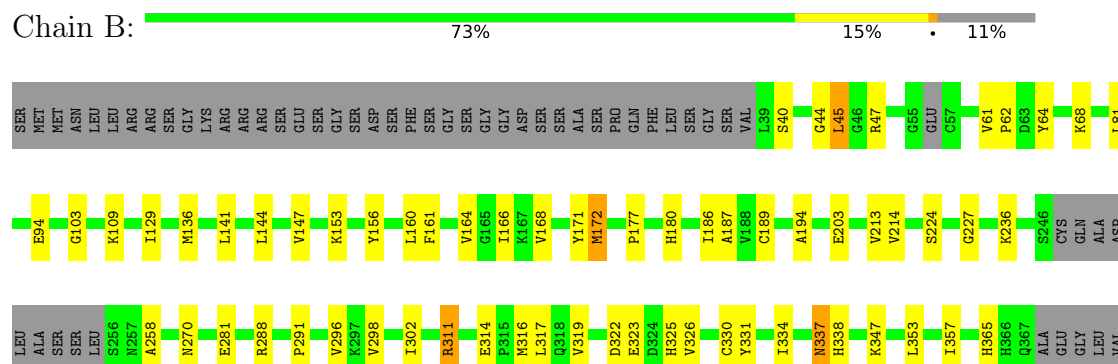
3 Residue-property plots

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: DNA POLYMERASE THETA



• Molecule 1: DNA POLYMERASE THETA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.02Å 130.53Å 160.91Å 90.00° 100.77° 90.00°	Depositor
Resolution (Å)	48.86 – 3.55 48.86 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.86-3.55) 99.1 (48.86-3.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.225 , 0.265 0.225 , 0.263	Depositor DCC
R_{free} test set	3060 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	130.6	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24408	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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	0.49	0/6324	0.92	16/8563 (0.2%)
1	B	0.35	0/6278	0.87	9/8507 (0.1%)
1	C	0.36	0/6154	0.89	16/8333 (0.2%)
1	D	0.35	0/6082	0.89	11/8236 (0.1%)
All	All	0.39	0/24838	0.89	52/33639 (0.2%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	VAL	N-CA-C	-10.38	92.84	107.99
1	D	526	GLU	N-CA-C	10.05	123.48	111.82
1	D	384	GLN	N-CA-C	9.06	121.16	111.28
1	B	384	GLN	N-CA-C	7.45	119.40	111.28
1	A	312	GLU	N-CA-C	-7.37	99.55	110.46
1	B	526	GLU	N-CA-C	6.95	119.89	111.82
1	D	378	PRO	N-CA-CB	6.95	109.82	103.08
1	A	294	GLU	N-CA-C	-6.93	98.39	109.76
1	A	378	PRO	N-CA-CB	6.93	109.80	103.08
1	A	703	VAL	N-CA-C	-6.82	103.83	110.72
1	C	41	PRO	CA-C-N	6.80	124.62	119.66
1	C	41	PRO	C-N-CA	6.80	124.62	119.66
1	A	712	GLN	N-CA-C	-6.77	103.54	112.34
1	C	871	THR	N-CA-C	-6.68	101.54	110.55
1	C	378	PRO	N-CA-CB	6.64	109.52	103.08
1	A	384	GLN	N-CA-C	6.36	118.21	111.28
1	C	875	ALA	N-CA-C	6.33	117.85	111.07
1	B	40	SER	CA-C-N	6.15	124.09	119.66
1	B	40	SER	C-N-CA	6.15	124.09	119.66
1	B	322	ASP	N-CA-C	-6.09	104.33	110.97
1	B	314	GLU	CA-C-N	5.98	126.92	119.98
1	B	314	GLU	C-N-CA	5.98	126.92	119.98
1	D	527	VAL	N-CA-C	5.93	118.16	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	826	ILE	N-CA-C	5.91	116.57	110.36
1	A	303	TYR	N-CA-C	5.86	118.77	109.50
1	A	711	ARG	N-CA-C	-5.80	105.30	112.38
1	C	873	ARG	N-CA-C	5.78	117.58	111.28
1	A	709	GLN	N-CA-C	-5.73	106.37	113.19
1	D	258	ALA	CB-CA-C	-5.72	109.44	117.23
1	B	515	VAL	N-CA-C	5.67	116.33	108.84
1	B	258	ALA	CB-CA-C	-5.66	109.53	117.23
1	C	711	ARG	N-CA-C	-5.66	106.36	113.20
1	A	258	ALA	CB-CA-C	-5.49	109.76	117.23
1	C	258	ALA	CB-CA-C	-5.49	109.77	117.23
1	A	862	ILE	N-CA-C	5.47	115.74	107.75
1	C	624	SER	CA-C-N	5.47	125.82	119.47
1	C	624	SER	C-N-CA	5.47	125.82	119.47
1	C	664	ILE	N-CA-C	5.44	116.07	108.89
1	C	119	ALA	N-CA-C	-5.32	106.73	114.12
1	C	384	GLN	N-CA-C	5.22	116.97	111.28
1	C	498	ASN	N-CA-C	5.21	117.86	111.82
1	C	836	ALA	N-CA-C	-5.17	106.97	113.28
1	A	314	GLU	CA-C-N	-5.16	114.25	119.83
1	A	314	GLU	C-N-CA	-5.16	114.25	119.83
1	D	624	SER	CA-C-N	5.09	125.38	119.47
1	D	624	SER	C-N-CA	5.09	125.38	119.47
1	C	562	SER	N-CA-C	5.08	118.73	112.54
1	D	288	ARG	CA-C-N	5.05	124.83	119.28
1	D	288	ARG	C-N-CA	5.05	124.83	119.28
1	A	41	PRO	O-C-N	5.04	123.52	121.15
1	A	708	ARG	N-CA-C	-5.02	106.85	112.87
1	D	887	LEU	CD1-CG-CD2	-5.01	99.78	110.80

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	6215	0	6282	164	0
1	B	6168	0	6197	63	0
1	C	6048	0	6114	72	0
1	D	5977	0	6030	89	0
All	All	24408	0	24623	373	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 8.

All (373) 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:708:ARG:NH2	1:D:708:ARG:CB	1.73	1.47
1:A:708:ARG:NH2	1:D:708:ARG:HB2	1.16	1.42
1:A:708:ARG:HH22	1:D:708:ARG:N	1.21	1.34
1:A:708:ARG:NH2	1:D:708:ARG:H	1.25	1.34
1:A:708:ARG:HH21	1:D:708:ARG:CB	1.33	1.25
1:A:708:ARG:NH2	1:D:708:ARG:CA	2.13	1.12
1:C:830:GLU:OE1	1:C:873:ARG:HD3	1.50	1.11
1:A:708:ARG:NH2	1:D:708:ARG:N	1.85	1.08
1:A:708:ARG:HH21	1:D:708:ARG:HB3	1.21	1.04
1:A:708:ARG:HH22	1:D:708:ARG:CA	1.72	1.01
1:A:707:GLU:OE1	1:A:707:GLU:N	1.93	0.99
1:A:693:PHE:HE1	1:A:710:HIS:CE1	1.85	0.93
1:A:309:LEU:HD12	1:A:310:VAL:N	1.83	0.92
1:A:298:VAL:HG11	1:A:501:LYS:HD3	1.50	0.91
1:C:830:GLU:OE1	1:C:873:ARG:CD	2.17	0.91
1:A:693:PHE:HE1	1:A:710:HIS:HE1	1.20	0.88
1:D:338:HIS:HD2	1:D:455:ARG:HH11	1.23	0.86
1:A:693:PHE:CE1	1:A:710:HIS:CE1	2.63	0.86
1:A:711:ARG:O	1:A:714:ALA:N	2.12	0.82
1:A:559:LEU:HD21	1:A:578:GLN:HG2	1.61	0.82
1:A:693:PHE:CE1	1:A:710:HIS:HE1	1.98	0.80
1:A:317:LEU:HD23	1:A:317:LEU:O	1.82	0.80
1:C:498:ASN:HA	1:C:501:LYS:HG3	1.62	0.79
1:D:521:ARG:H	1:D:578:GLN:HE22	1.31	0.79
1:B:801:LEU:O	1:B:806:ARG:NH1	2.15	0.78
1:B:298:VAL:HG11	1:B:501:LYS:HD3	1.64	0.78
1:A:708:ARG:CZ	1:D:708:ARG:HB2	2.10	0.77
1:D:801:LEU:O	1:D:806:ARG:NH1	2.19	0.76
1:D:288:ARG:NH2	1:D:481:ALA:O	2.19	0.75
1:A:293:LEU:HD23	1:A:293:LEU:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:LEU:O	1:A:806:ARG:NH1	2.22	0.73
1:A:317:LEU:HD23	1:A:317:LEU:C	2.14	0.73
1:C:801:LEU:HD11	1:C:878:LEU:HD22	1.69	0.72
1:B:801:LEU:HD11	1:B:878:LEU:HD22	1.71	0.72
1:C:41:PRO:HB3	1:C:101:LEU:HD21	1.72	0.71
1:A:309:LEU:HD12	1:A:309:LEU:C	2.16	0.71
1:A:609:TYR:O	1:A:610:HIS:CG	2.44	0.71
1:D:801:LEU:HD11	1:D:878:LEU:HD22	1.72	0.70
1:A:321:GLY:O	1:A:322:ASP:C	2.33	0.70
1:A:708:ARG:HH22	1:D:708:ARG:H	0.80	0.69
1:A:309:LEU:HD11	1:A:311:ARG:C	2.17	0.69
1:D:298:VAL:HG11	1:D:501:LYS:HD3	1.75	0.69
1:C:319:VAL:HB	1:C:323:GLU:HG3	1.75	0.68
1:A:314:GLU:HA	1:A:314:GLU:OE1	1.93	0.68
1:A:304:ASP:OD2	1:A:306:SER:OG	2.11	0.68
1:C:801:LEU:O	1:C:806:ARG:NH1	2.27	0.68
1:A:607:LYS:N	1:A:607:LYS:HD2	2.09	0.68
1:A:236:LYS:NZ	1:A:537:GLU:OE1	2.25	0.68
1:A:708:ARG:CZ	1:D:708:ARG:H	2.04	0.67
1:A:292:LEU:C	1:A:293:LEU:HD23	2.19	0.67
1:D:830:GLU:OE1	1:D:873:ARG:NH1	2.28	0.67
1:A:306:SER:O	1:A:307:MET:HB2	1.93	0.66
1:A:321:GLY:O	1:A:323:GLU:N	2.29	0.66
1:B:168:VAL:HG22	1:B:186:ILE:HB	1.76	0.66
1:A:291:PRO:HG2	1:A:489:VAL:HG12	1.78	0.66
1:B:319:VAL:HB	1:B:323:GLU:HG3	1.77	0.65
1:C:707:GLU:H	1:C:707:GLU:CD	2.04	0.65
1:C:396:ARG:HE	1:C:837:VAL:HG13	1.61	0.65
1:A:300:ASN:O	1:A:313:PHE:HB3	1.96	0.65
1:A:145:PRO:O	1:A:226:ARG:NH2	2.29	0.64
1:C:288:ARG:NH2	1:C:481:ALA:O	2.30	0.64
1:A:607:LYS:HD2	1:A:607:LYS:H	1.63	0.64
1:A:161:PHE:HB3	1:A:166:ILE:HB	1.79	0.64
1:A:498:ASN:HA	1:A:501:LYS:HG3	1.79	0.64
1:D:559:LEU:HD22	1:D:578:GLN:HG2	1.81	0.63
1:A:316:MET:HE2	1:A:331:TYR:CD2	2.33	0.63
1:C:236:LYS:NZ	1:C:537:GLU:OE1	2.31	0.63
1:A:311:ARG:NH2	1:A:332:GLU:OE1	2.32	0.63
1:A:472:LEU:HD13	1:A:512:LEU:HD21	1.79	0.63
1:D:171:TYR:CZ	1:D:177:PRO:HG3	2.34	0.63
1:C:806:ARG:NH2	1:C:863:TRP:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ILE:HD12	1:B:311:ARG:HD2	1.79	0.62
1:A:311:ARG:HG2	1:A:312:GLU:O	2.00	0.61
1:A:702:VAL:O	1:A:702:VAL:HG13	1.98	0.61
1:A:801:LEU:HD23	1:A:864:VAL:HG11	1.81	0.61
1:A:313:PHE:HE2	1:A:325:HIS:HB3	1.65	0.61
1:D:498:ASN:HA	1:D:501:LYS:HG3	1.81	0.61
1:B:870:LEU:HD13	1:B:875:ALA:HA	1.83	0.61
1:C:161:PHE:HB3	1:C:166:ILE:HB	1.82	0.61
1:B:161:PHE:HB3	1:B:166:ILE:HB	1.83	0.60
1:A:147:VAL:HG13	1:A:172:MET:HB3	1.81	0.60
1:A:309:LEU:HD12	1:A:311:ARG:N	2.17	0.60
1:B:291:PRO:HG2	1:B:489:VAL:HG12	1.82	0.60
1:B:334:ILE:HD12	1:B:438:ARG:HB3	1.82	0.60
1:D:291:PRO:HG2	1:D:489:VAL:HG12	1.84	0.60
1:A:860:ARG:HG2	1:A:871:THR:HG22	1.84	0.59
1:D:453:PRO:O	1:D:483:ARG:NH1	2.36	0.59
1:D:399:SER:O	1:D:735:ARG:NH1	2.36	0.59
1:A:303:TYR:CD1	1:A:303:TYR:N	2.71	0.59
1:A:703:VAL:HG13	1:A:704:ALA:N	2.17	0.58
1:A:596:GLN:HG3	1:A:612:THR:HG22	1.85	0.58
1:D:342:LEU:HD21	1:D:353:LEU:HD23	1.85	0.58
1:A:312:GLU:HG3	1:A:313:PHE:N	2.18	0.58
1:A:690:GLU:OE1	1:A:712:GLN:NE2	2.36	0.58
1:A:870:LEU:HD13	1:A:875:ALA:HA	1.86	0.58
1:C:298:VAL:HG11	1:C:501:LYS:HD3	1.84	0.58
1:B:671:CYS:O	1:B:675:LYS:HD3	2.04	0.58
1:A:301:SER:CB	1:A:303:TYR:HE1	2.17	0.58
1:D:355:ASP:OD1	1:D:407:LYS:NZ	2.36	0.57
1:B:396:ARG:HE	1:B:837:VAL:HG12	1.69	0.57
1:A:708:ARG:HH22	1:D:708:ARG:HB2	1.38	0.57
1:A:319:VAL:O	1:A:321:GLY:N	2.35	0.57
1:D:168:VAL:HG22	1:D:186:ILE:HB	1.86	0.57
1:C:311:ARG:HH22	1:C:332:GLU:CD	2.12	0.57
1:D:222:GLY:O	1:D:518:CYS:HB2	2.05	0.57
1:C:144:LEU:HD13	1:C:150:ALA:HA	1.87	0.57
1:D:870:LEU:HD13	1:D:875:ALA:HA	1.87	0.56
1:A:301:SER:CB	1:A:303:TYR:CE1	2.88	0.56
1:D:806:ARG:NH2	1:D:863:TRP:O	2.38	0.56
1:A:311:ARG:HD3	1:A:312:GLU:O	2.04	0.56
1:D:433:ARG:NH1	1:D:451:ASN:O	2.39	0.56
1:B:129:ILE:HD11	1:B:214:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:THR:HG22	1:C:608:VAL:HG22	1.88	0.56
1:B:596:GLN:HG3	1:B:612:THR:HG22	1.88	0.56
1:B:830:GLU:OE1	1:B:873:ARG:HD3	2.05	0.56
1:B:559:LEU:HD22	1:B:578:GLN:HG2	1.88	0.55
1:A:806:ARG:NH2	1:A:863:TRP:O	2.38	0.55
1:D:472:LEU:HB2	1:D:512:LEU:HD21	1.88	0.55
1:B:288:ARG:NH2	1:B:481:ALA:O	2.39	0.55
1:D:129:ILE:HD11	1:D:214:VAL:HG21	1.89	0.55
1:A:171:TYR:CZ	1:A:177:PRO:HG3	2.42	0.55
1:A:301:SER:HB2	1:A:303:TYR:HE1	1.72	0.55
1:A:380:VAL:C	1:A:381:ILE:HG13	2.32	0.55
1:A:302:ILE:C	1:A:303:TYR:CD1	2.85	0.54
1:A:311:ARG:HG2	1:A:312:GLU:N	2.23	0.54
1:B:224:SER:HB3	1:B:227:GLY:H	1.72	0.54
1:A:303:TYR:N	1:A:303:TYR:HD1	2.05	0.54
1:A:645:GLU:OE2	1:A:682:ARG:NH1	2.40	0.54
1:D:596:GLN:HG3	1:D:612:THR:HG22	1.90	0.54
1:C:559:LEU:O	1:C:562:SER:OG	2.21	0.53
1:A:170:GLY:HA3	1:A:172:MET:HE3	1.91	0.53
1:A:319:VAL:HG13	1:A:360:GLU:HG3	1.90	0.53
1:D:141:LEU:HD12	1:D:187:ALA:HB3	1.89	0.53
1:D:329:LEU:HD12	1:D:495:ILE:HD11	1.91	0.53
1:B:863:TRP:HD1	1:B:867:ARG:HE	1.57	0.53
1:B:433:ARG:NH1	1:B:451:ASN:O	2.42	0.53
1:D:144:LEU:HD13	1:D:150:ALA:HA	1.91	0.53
1:A:309:LEU:HD11	1:A:311:ARG:O	2.08	0.53
1:A:309:LEU:CD1	1:A:311:ARG:N	2.72	0.53
1:D:326:VAL:HG21	1:D:460:ARG:NE	2.24	0.53
1:A:301:SER:HB3	1:A:303:TYR:CE1	2.44	0.52
1:A:141:LEU:HB3	1:A:213:VAL:HG12	1.91	0.52
1:A:302:ILE:C	1:A:303:TYR:HD1	2.17	0.52
1:C:645:GLU:OE2	1:C:682:ARG:NH1	2.43	0.52
1:B:396:ARG:HD2	1:B:861:THR:HB	1.91	0.52
1:A:706:THR:HG23	1:A:707:GLU:CD	2.34	0.52
1:B:147:VAL:HG13	1:B:172:MET:HB2	1.91	0.52
1:B:860:ARG:HG2	1:B:871:THR:HG22	1.92	0.52
1:D:300:ASN:O	1:D:313:PHE:HB3	2.10	0.51
1:A:316:MET:HE2	1:A:331:TYR:CE2	2.45	0.51
1:B:496:CYS:HB3	1:B:500:GLU:HG3	1.92	0.51
1:A:702:VAL:HG22	1:A:704:ALA:HB2	1.92	0.51
1:B:45:LEU:HG	1:B:68:LYS:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ARG:C	1:A:710:HIS:H	2.19	0.51
1:C:830:GLU:OE1	1:C:873:ARG:HD2	2.09	0.51
1:C:596:GLN:HG3	1:C:612:THR:HG22	1.92	0.51
1:A:149:VAL:HG12	1:A:450:VAL:HA	1.93	0.51
1:C:131:LYS:NZ	1:C:135:GLU:OE2	2.41	0.51
1:C:302:ILE:HD12	1:C:311:ARG:HD3	1.92	0.51
1:D:453:PRO:HB2	1:D:483:ARG:HG2	1.92	0.51
1:C:860:ARG:HB3	1:C:869:GLY:O	2.11	0.51
1:B:236:LYS:NZ	1:B:537:GLU:OE1	2.42	0.50
1:A:391:MET:SD	1:A:410:PRO:HG3	2.51	0.50
1:A:707:GLU:CD	1:A:707:GLU:H	1.97	0.50
1:A:607:LYS:N	1:A:607:LYS:CD	2.73	0.50
1:D:242:ARG:HD2	1:D:556:CYS:SG	2.51	0.50
1:A:39:LEU:HG	1:A:131:LYS:HD2	1.94	0.50
1:A:316:MET:HE2	1:A:331:TYR:HD2	1.76	0.50
1:A:144:LEU:HD11	1:A:153:LYS:HG2	1.94	0.50
1:D:668:ARG:HD3	1:D:740:LYS:O	2.11	0.50
1:D:540:VAL:HG22	1:D:611:PRO:HB3	1.94	0.49
1:A:711:ARG:C	1:A:713:MET:N	2.60	0.49
1:A:319:VAL:C	1:A:321:GLY:H	2.20	0.49
1:C:171:TYR:CZ	1:C:177:PRO:HG3	2.47	0.49
1:A:453:PRO:HB2	1:A:483:ARG:HG2	1.94	0.49
1:A:706:THR:HG23	1:A:707:GLU:N	2.28	0.49
1:A:300:ASN:O	1:A:313:PHE:N	2.46	0.49
1:A:870:LEU:HB3	1:A:875:ALA:HB2	1.94	0.49
1:D:79:ALA:HB3	1:D:164:VAL:HG22	1.95	0.49
1:A:301:SER:HB2	1:A:303:TYR:CE1	2.48	0.49
1:C:828:GLU:O	1:C:832:ILE:HG13	2.13	0.49
1:A:822:ALA:HB1	1:A:884:ARG:HG2	1.94	0.49
1:C:224:SER:HB3	1:C:227:GLY:HA3	1.94	0.49
1:A:433:ARG:NH1	1:A:451:ASN:O	2.45	0.49
1:B:144:LEU:HD11	1:B:153:LYS:HG2	1.94	0.49
1:B:863:TRP:CD1	1:B:867:ARG:HE	2.31	0.49
1:C:129:ILE:HD11	1:C:214:VAL:HG21	1.93	0.49
1:C:711:ARG:HE	1:C:715:ILE:HD11	1.77	0.48
1:C:37:SER:HA	1:C:135:GLU:OE1	2.12	0.48
1:A:559:LEU:CD2	1:A:578:GLN:HG2	2.38	0.48
1:B:643:VAL:H	1:B:649:HIS:HD2	1.58	0.48
1:C:218:LEU:H	1:C:265:SER:HB3	1.78	0.48
1:C:863:TRP:CD1	1:C:867:ARG:HE	2.31	0.48
1:C:643:VAL:H	1:C:649:HIS:HD2	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:707:GLU:H	1:D:707:GLU:HG3	1.39	0.48
1:A:129:ILE:HD11	1:A:214:VAL:HG21	1.95	0.48
1:B:270:ASN:HD21	1:B:515:VAL:H	1.62	0.48
1:A:345:PRO:HA	1:A:464:PHE:CD2	2.49	0.48
1:B:64:TYR:OH	1:B:94:GLU:OE1	2.31	0.48
1:D:867:ARG:HG2	1:D:869:GLY:H	1.79	0.48
1:A:347:LYS:HB3	1:A:417:HIS:CD2	2.49	0.47
1:A:334:ILE:HD12	1:A:438:ARG:HB3	1.96	0.47
1:D:224:SER:HB3	1:D:227:GLY:HA3	1.95	0.47
1:A:423:GLU:OE2	1:A:423:GLU:N	2.47	0.47
1:D:402:ASP:OD1	1:D:745:ARG:NH2	2.41	0.47
1:A:319:VAL:C	1:A:321:GLY:N	2.73	0.47
1:A:706:THR:HG23	1:A:707:GLU:HG3	1.95	0.47
1:B:44:GLY:HA2	1:B:47:ARG:HD3	1.96	0.47
1:A:708:ARG:HD2	1:D:708:ARG:HB3	1.96	0.47
1:A:825:ASN:OD1	1:A:827:VAL:HG12	2.15	0.47
1:D:792:GLU:HB3	1:D:811:TYR:CE1	2.49	0.47
1:A:44:GLY:HA2	1:A:47:ARG:HG3	1.97	0.47
1:A:706:THR:CG2	1:A:707:GLU:CD	2.88	0.47
1:B:801:LEU:HD23	1:B:864:VAL:HG11	1.97	0.47
1:D:780:GLN:HE22	1:D:791:ARG:HD3	1.78	0.47
1:A:224:SER:HB3	1:A:227:GLY:HA3	1.96	0.46
1:A:618:THR:OG1	1:A:628:THR:HG21	2.15	0.46
1:D:643:VAL:H	1:D:649:HIS:HD2	1.63	0.46
1:B:331:TYR:OH	1:B:377:CYS:HB3	2.15	0.46
1:D:559:LEU:HD12	1:D:560:ALA:N	2.30	0.46
1:D:727:ASP:OD2	1:D:741:TYR:OH	2.32	0.46
1:C:224:SER:HB3	1:C:227:GLY:H	1.79	0.46
1:B:298:VAL:HG21	1:B:501:LYS:HG2	1.98	0.46
1:A:531:MET:HG2	1:A:585:CYS:SG	2.55	0.46
1:D:326:VAL:HG21	1:D:460:ARG:CZ	2.46	0.46
1:A:609:TYR:C	1:A:610:HIS:CG	2.94	0.45
1:B:171:TYR:CZ	1:B:177:PRO:HG3	2.51	0.45
1:A:291:PRO:CG	1:A:489:VAL:HG12	2.44	0.45
1:A:708:ARG:C	1:A:710:HIS:N	2.73	0.45
1:D:218:LEU:H	1:D:265:SER:HB3	1.81	0.45
1:C:222:GLY:O	1:C:518:CYS:HB3	2.16	0.45
1:A:330:CYS:O	1:A:334:ILE:HG12	2.15	0.45
1:B:867:ARG:HG2	1:B:869:GLY:H	1.81	0.45
1:A:58:LYS:HG3	1:A:59:PRO:HD2	1.98	0.45
1:C:342:LEU:HD21	1:C:353:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:828:GLU:O	1:D:832:ILE:HG13	2.17	0.45
1:A:313:PHE:HE2	1:A:325:HIS:CB	2.29	0.45
1:B:156:TYR:O	1:B:160:LEU:HD13	2.17	0.45
1:A:319:VAL:HG13	1:A:360:GLU:CD	2.42	0.45
1:A:864:VAL:HG12	1:A:865:THR:H	1.82	0.45
1:A:706:THR:HG23	1:A:707:GLU:CG	2.47	0.44
1:B:357:ILE:HD13	1:B:439:VAL:HG11	1.98	0.44
1:C:232:LEU:O	1:C:236:LYS:HB2	2.17	0.44
1:A:344:CYS:HB2	1:A:350:CYS:SG	2.58	0.44
1:C:396:ARG:HD3	1:C:861:THR:HB	1.99	0.44
1:A:801:LEU:HD11	1:A:878:LEU:HD22	2.00	0.44
1:C:733:PRO:HB2	1:C:736:GLU:HG3	1.99	0.44
1:D:353:LEU:HD12	1:D:353:LEU:HA	1.78	0.44
1:D:472:LEU:HD13	1:D:512:LEU:HD11	1.99	0.44
1:A:559:LEU:O	1:A:563:MET:HE2	2.18	0.44
1:C:531:MET:HG2	1:C:585:CYS:SG	2.57	0.44
1:A:349:TRP:HZ3	1:A:460:ARG:HD2	1.82	0.44
1:B:141:LEU:HD12	1:B:187:ALA:HB3	1.98	0.44
1:D:234:LEU:HD22	1:D:261:ILE:HD13	1.99	0.44
1:D:338:HIS:CD2	1:D:455:ARG:HH11	2.16	0.44
1:D:521:ARG:H	1:D:578:GLN:NE2	2.09	0.44
1:D:645:GLU:OE2	1:D:682:ARG:NH1	2.50	0.44
1:A:300:ASN:O	1:A:313:PHE:CB	2.64	0.44
1:A:708:ARG:O	1:A:708:ARG:HG2	2.17	0.44
1:B:61:VAL:HA	1:B:62:PRO:HD2	1.84	0.44
1:C:559:LEU:HD12	1:C:560:ALA:N	2.32	0.44
1:C:864:VAL:HG12	1:C:865:THR:H	1.82	0.44
1:A:703:VAL:CG1	1:A:704:ALA:N	2.81	0.44
1:C:366:HIS:O	1:C:366:HIS:ND1	2.51	0.44
1:D:236:LYS:NZ	1:D:537:GLU:OE1	2.40	0.44
1:D:643:VAL:H	1:D:649:HIS:CD2	2.36	0.44
1:D:864:VAL:HG12	1:D:865:THR:H	1.83	0.44
1:A:671:CYS:O	1:A:675:LYS:HD3	2.18	0.44
1:A:694:LEU:O	1:A:698:VAL:HG23	2.18	0.44
1:A:168:VAL:HG22	1:A:186:ILE:HB	2.00	0.43
1:C:330:CYS:O	1:C:334:ILE:HG12	2.18	0.43
1:A:141:LEU:HD12	1:A:187:ALA:HB3	2.01	0.43
1:A:317:LEU:C	1:A:317:LEU:CD2	2.85	0.43
1:A:728:LEU:HD21	1:A:752:GLN:HB3	1.99	0.43
1:B:707:GLU:H	1:B:707:GLU:HG3	1.46	0.43
1:C:316:MET:HE2	1:C:316:MET:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:873:ARG:HG2	1:C:873:ARG:HH11	1.84	0.43
1:A:222:GLY:O	1:A:518:CYS:HB2	2.18	0.43
1:A:309:LEU:C	1:A:309:LEU:CD1	2.86	0.43
1:A:378:PRO:HA	1:A:379:PRO:HD3	1.82	0.43
1:A:426:ASP:OD2	1:A:863:TRP:NE1	2.50	0.43
1:B:224:SER:HB3	1:B:227:GLY:HA3	2.00	0.43
1:B:559:LEU:HD12	1:B:560:ALA:N	2.33	0.43
1:C:141:LEU:HD12	1:C:187:ALA:HB3	2.00	0.43
1:C:464:PHE:CD1	1:C:469:LEU:HD13	2.53	0.43
1:A:38:VAL:HG21	1:A:134:LEU:HD12	1.99	0.43
1:A:536:LEU:HD22	1:A:625:PRO:HG3	2.00	0.43
1:A:867:ARG:HG2	1:A:869:GLY:H	1.82	0.43
1:B:337:ASN:HA	1:B:438:ARG:NH2	2.33	0.43
1:B:792:GLU:HB3	1:B:811:TYR:CE1	2.53	0.43
1:C:345:PRO:HA	1:C:464:PHE:CD2	2.53	0.43
1:C:783:LYS:HE3	1:C:783:LYS:HB2	1.86	0.43
1:A:391:MET:HE2	1:A:391:MET:HB3	1.92	0.43
1:A:551:HIS:ND1	1:A:579:LEU:HD21	2.34	0.43
1:D:338:HIS:CD2	1:D:455:ARG:HD3	2.54	0.43
1:A:609:TYR:O	1:A:610:HIS:CD2	2.71	0.43
1:D:337:ASN:HA	1:D:438:ARG:NH2	2.33	0.43
1:B:655:THR:HA	1:B:656:PRO:HD3	1.79	0.43
1:C:396:ARG:CD	1:C:861:THR:HB	2.48	0.43
1:C:408:THR:HB	1:C:413:VAL:HB	2.01	0.43
1:D:360:GLU:O	1:D:364:LEU:HD23	2.18	0.43
1:A:312:GLU:HG3	1:A:313:PHE:H	1.80	0.43
1:B:531:MET:HG2	1:B:585:CYS:SG	2.59	0.43
1:D:347:LYS:HG2	1:D:417:HIS:CD2	2.54	0.43
1:D:393:GLN:O	1:D:397:LEU:HD13	2.19	0.43
1:B:189:CYS:HB2	1:B:194:ALA:HB2	2.01	0.43
1:C:387:LEU:HD21	1:C:409:VAL:O	2.18	0.43
1:D:330:CYS:O	1:D:334:ILE:HG12	2.19	0.42
1:D:822:ALA:HB1	1:D:884:ARG:HG2	2.01	0.42
1:A:315:PRO:HG3	1:A:325:HIS:CE1	2.54	0.42
1:B:860:ARG:HB3	1:B:869:GLY:O	2.19	0.42
1:D:801:LEU:HD22	1:D:864:VAL:HG11	2.01	0.42
1:A:708:ARG:HH21	1:D:708:ARG:CA	2.00	0.42
1:A:709:GLN:HG3	1:A:709:GLN:O	2.19	0.42
1:B:864:VAL:HG12	1:B:865:THR:H	1.85	0.42
1:D:297:LYS:NZ	1:D:299:GLY:O	2.51	0.42
1:D:345:PRO:HA	1:D:464:PHE:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:ARG:NH2	1:D:491:GLU:OE1	2.52	0.42
1:D:517:SER:OG	1:D:559:LEU:HB3	2.19	0.42
1:D:767:ASN:HD22	1:D:775:GLU:CD	2.27	0.42
1:D:405:LEU:O	1:D:409:VAL:HB	2.19	0.42
1:D:789:ILE:HD13	1:D:797:VAL:HG11	2.01	0.42
1:B:752:GLN:NE2	1:B:785:LEU:O	2.51	0.42
1:B:822:ALA:HB1	1:B:884:ARG:HG2	2.01	0.42
1:C:423:GLU:OE2	1:C:423:GLU:N	2.53	0.42
1:C:629:LEU:HD23	1:C:629:LEU:HA	1.89	0.42
1:C:809:VAL:O	1:C:813:SER:OG	2.34	0.42
1:A:353:LEU:HA	1:A:353:LEU:HD12	1.78	0.42
1:D:470:ASP:OD1	1:D:472:LEU:N	2.46	0.42
1:A:470:ASP:OD1	1:A:472:LEU:N	2.47	0.42
1:A:316:MET:CE	1:A:331:TYR:CE2	3.03	0.42
1:A:712:GLN:O	1:A:716:HIS:ND1	2.41	0.42
1:B:399:SER:O	1:B:735:ARG:NH1	2.53	0.42
1:C:867:ARG:HG2	1:C:869:GLY:H	1.85	0.41
1:A:129:ILE:HA	1:A:212:MET:SD	2.60	0.41
1:A:642:PHE:CE1	1:A:774:MET:HE1	2.55	0.41
1:B:103:GLY:HA3	1:B:281:GLU:OE1	2.20	0.41
1:B:330:CYS:O	1:B:334:ILE:HG12	2.21	0.41
1:C:433:ARG:NH1	1:C:451:ASN:O	2.53	0.41
1:A:517:SER:OG	1:A:559:LEU:HB2	2.21	0.41
1:C:42:PRO:HG2	1:C:68:LYS:O	2.19	0.41
1:B:326:VAL:HG21	1:B:460:ARG:NE	2.36	0.41
1:B:792:GLU:HB3	1:B:811:TYR:CZ	2.55	0.41
1:B:338:HIS:ND1	1:B:455:ARG:HD3	2.36	0.41
1:C:168:VAL:HG22	1:C:186:ILE:HB	2.02	0.41
1:D:423:GLU:OE2	1:D:423:GLU:N	2.54	0.41
1:A:672:LEU:HD11	1:A:740:LYS:HG2	2.03	0.41
1:B:423:GLU:OE2	1:B:423:GLU:N	2.54	0.41
1:C:323:GLU:C	1:C:325:HIS:H	2.28	0.41
1:C:521:ARG:H	1:C:578:GLN:CD	2.27	0.41
1:D:825:ASN:OD1	1:D:827:VAL:HG12	2.21	0.41
1:A:295:SER:OG	1:A:492:SER:O	2.35	0.41
1:C:655:THR:HA	1:C:656:PRO:HD3	1.81	0.41
1:C:79:ALA:HB3	1:C:164:VAL:HG22	2.03	0.41
1:C:518:CYS:SG	1:C:519:LEU:HD12	2.61	0.41
1:B:323:GLU:C	1:B:325:HIS:H	2.29	0.41
1:B:373:LYS:N	1:B:374:PRO:HD2	2.36	0.41
1:C:219:HIS:ND1	1:C:265:SER:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:LEU:HD12	1:C:353:LEU:HA	1.83	0.41
1:C:357:ILE:HD13	1:C:439:VAL:HG11	2.03	0.41
1:C:643:VAL:H	1:C:649:HIS:CD2	2.38	0.41
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.85	0.41
1:A:347:LYS:HB3	1:A:417:HIS:HD2	1.85	0.41
1:C:304:ASP:HB3	1:C:310:VAL:HG11	2.01	0.40
1:A:232:LEU:HG	1:A:534:ALA:HB2	2.02	0.40
1:B:316:MET:HE2	1:B:316:MET:HB3	1.82	0.40
1:D:298:VAL:HG21	1:D:501:LYS:HG2	2.04	0.40
1:D:684:ALA:HB2	1:D:719:PHE:CZ	2.57	0.40
1:A:270:ASN:HD21	1:A:515:VAL:H	1.67	0.40
1:C:423:GLU:HG3	1:C:863:TRP:CH2	2.56	0.40
1:A:863:TRP:HD1	1:A:867:ARG:HE	1.69	0.40
1:A:828:GLU:O	1:A:832:ILE:HG13	2.22	0.40
1:C:676:LEU:HA	1:C:677:PRO:HD3	1.95	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	793/896 (88%)	754 (95%)	39 (5%)	0	100	100
1	B	787/896 (88%)	746 (95%)	41 (5%)	0	100	100
1	C	766/896 (86%)	726 (95%)	40 (5%)	0	100	100
1	D	758/896 (85%)	720 (95%)	38 (5%)	0	100	100
All	All	3104/3584 (87%)	2946 (95%)	158 (5%)	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	668/768 (87%)	637 (95%)	31 (5%)	24	50
1	B	659/768 (86%)	618 (94%)	41 (6%)	16	44
1	C	652/768 (85%)	609 (93%)	43 (7%)	15	42
1	D	642/768 (84%)	597 (93%)	45 (7%)	14	40
All	All	2621/3072 (85%)	2461 (94%)	160 (6%)	17	44

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	57	CYS
1	A	81	LEU
1	A	109	LYS
1	A	164	VAL
1	A	226	ARG
1	A	293	LEU
1	A	303	TYR
1	A	305	SER
1	A	306	SER
1	A	308	LYS
1	A	309	LEU
1	A	310	VAL
1	A	311	ARG
1	A	317	LEU
1	A	319	VAL
1	A	353	LEU
1	A	367	GLN
1	A	381	ILE
1	A	397	LEU
1	A	417	HIS
1	A	527	VAL
1	A	528	THR
1	A	531	MET

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Mol	Chain	Res	Type
1	A	595	ILE
1	A	605	GLU
1	A	607	LYS
1	A	686	LEU
1	A	701	LYS
1	A	707	GLU
1	A	864	VAL
1	B	45	LEU
1	B	81	LEU
1	B	109	LYS
1	B	136	MET
1	B	164	VAL
1	B	172	MET
1	B	180	HIS
1	B	203	GLU
1	B	213	VAL
1	B	296	VAL
1	B	311	ARG
1	B	317	LEU
1	B	337	ASN
1	B	347	LYS
1	B	353	LEU
1	B	365	HIS
1	B	375	SER
1	B	381	ILE
1	B	382	LEU
1	B	388	LEU
1	B	391	MET
1	B	397	LEU
1	B	417	HIS
1	B	527	VAL
1	B	528	THR
1	B	531	MET
1	B	548	GLN
1	B	559	LEU
1	B	587	MET
1	B	595	ILE
1	B	660	ASP
1	B	664	ILE
1	B	678	THR
1	B	686	LEU
1	B	698	VAL

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Mol	Chain	Res	Type
1	B	699	LYS
1	B	702	VAL
1	B	706	THR
1	B	707	GLU
1	B	776	LEU
1	B	864	VAL
1	C	81	LEU
1	C	109	LYS
1	C	164	VAL
1	C	174	SER
1	C	203	GLU
1	C	213	VAL
1	C	217	GLU
1	C	220	MET
1	C	221	LEU
1	C	226	ARG
1	C	296	VAL
1	C	317	LEU
1	C	319	VAL
1	C	347	LYS
1	C	353	LEU
1	C	364	LEU
1	C	381	ILE
1	C	387	LEU
1	C	388	LEU
1	C	391	MET
1	C	397	LEU
1	C	417	HIS
1	C	455	ARG
1	C	517	SER
1	C	518	CYS
1	C	520	GLN
1	C	531	MET
1	C	550	MET
1	C	559	LEU
1	C	595	ILE
1	C	660	ASP
1	C	678	THR
1	C	686	LEU
1	C	699	LYS
1	C	702	VAL
1	C	707	GLU

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Mol	Chain	Res	Type
1	C	710	HIS
1	C	813	SER
1	C	818	VAL
1	C	864	VAL
1	C	865	THR
1	C	870	LEU
1	C	889	GLN
1	D	39	LEU
1	D	81	LEU
1	D	109	LYS
1	D	131	LYS
1	D	164	VAL
1	D	172	MET
1	D	180	HIS
1	D	203	GLU
1	D	213	VAL
1	D	226	ARG
1	D	296	VAL
1	D	317	LEU
1	D	323	GLU
1	D	347	LYS
1	D	353	LEU
1	D	364	LEU
1	D	366	HIS
1	D	367	GLN
1	D	379	PRO
1	D	381	ILE
1	D	383	GLU
1	D	384	GLN
1	D	388	LEU
1	D	397	LEU
1	D	409	VAL
1	D	417	HIS
1	D	520	GLN
1	D	527	VAL
1	D	531	MET
1	D	548	GLN
1	D	559	LEU
1	D	595	ILE
1	D	660	ASP
1	D	664	ILE
1	D	686	LEU

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Mol	Chain	Res	Type
1	D	698	VAL
1	D	702	VAL
1	D	706	THR
1	D	707	GLU
1	D	710	HIS
1	D	864	VAL
1	D	872	GLU
1	D	873	ARG
1	D	886	ILE
1	D	887	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	610	HIS
1	A	710	HIS
1	A	752	GLN
1	A	767	ASN
1	B	199	ASN
1	B	548	GLN
1	B	709	GLN
1	B	710	HIS
1	B	752	GLN
1	B	858	ASN
1	C	199	ASN
1	C	434	GLN
1	C	767	ASN
1	D	338	HIS
1	D	417	HIS
1	D	434	GLN
1	D	578	GLN
1	D	710	HIS
1	D	752	GLN
1	D	767	ASN

5.3.3 RNA ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	805/896 (89%)	-0.35	2 (0%) 91 80	70, 124, 178, 203	0
1	B	801/896 (89%)	-0.32	0 100 100	88, 149, 211, 255	0
1	C	780/896 (87%)	-0.32	3 (0%) 88 70	78, 144, 195, 217	0
1	D	772/896 (86%)	-0.15	4 (0%) 87 66	78, 178, 243, 264	0
All	All	3158/3584 (88%)	-0.29	9 (0%) 90 74	70, 146, 218, 264	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	704	ALA	3.2
1	C	794	CYS	2.7
1	A	118	SER	2.5
1	A	263	GLY	2.5
1	C	377	CYS	2.5
1	D	99	CYS	2.4
1	C	263	GLY	2.2
1	D	708	ARG	2.1
1	D	881	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.