



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1KY9 / pdb_00001ky9
Title : Crystal Structure of DegP (HtrA)
Authors : Krojer, T.; Garrido-Franco, M.; Huber, R.; Ehrmann, M.; Clausen, T.
Deposited on : 2002-02-04
Resolution : 2.80 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

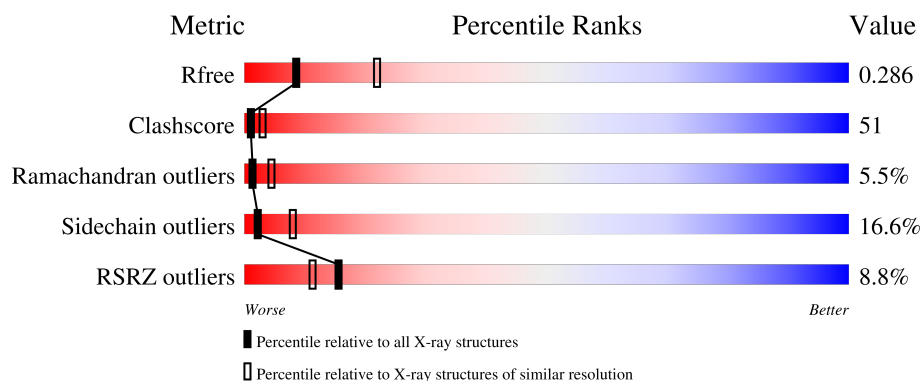
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	448	6% 29% 28% 10% 31%
1	B	448	7% 34% 41% 11% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5366 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 PROTEASE DO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	Se	0	0	0
			2282	1426	403	441	12			
1	B	396	Total	C	N	O	Se	0	0	0
			2918	1818	519	568	13			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MSE	MET	modified residue	UNP P0C0V0
A	18	MSE	MET	modified residue	UNP P0C0V0
A	23	MSE	MET	modified residue	UNP P0C0V0
A	42	MSE	MET	modified residue	UNP P0C0V0
A	85	MSE	MET	modified residue	UNP P0C0V0
A	127	MSE	MET	modified residue	UNP P0C0V0
A	152	MSE	MET	modified residue	UNP P0C0V0
A	210	ALA	SER	engineered mutation	UNP P0C0V0
A	246	MSE	MET	modified residue	UNP P0C0V0
A	254	MSE	MET	modified residue	UNP P0C0V0
A	268	MSE	MET	modified residue	UNP P0C0V0
A	280	MSE	MET	modified residue	UNP P0C0V0
A	331	MSE	MET	modified residue	UNP P0C0V0
A	376	MSE	MET	modified residue	UNP P0C0V0
A	447	MSE	MET	modified residue	UNP P0C0V0
B	12	MSE	MET	modified residue	UNP P0C0V0
B	18	MSE	MET	modified residue	UNP P0C0V0
B	23	MSE	MET	modified residue	UNP P0C0V0
B	42	MSE	MET	modified residue	UNP P0C0V0
B	85	MSE	MET	modified residue	UNP P0C0V0
B	127	MSE	MET	modified residue	UNP P0C0V0
B	152	MSE	MET	modified residue	UNP P0C0V0
B	210	ALA	SER	engineered mutation	UNP P0C0V0
B	246	MSE	MET	modified residue	UNP P0C0V0
B	254	MSE	MET	modified residue	UNP P0C0V0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	268	MSE	MET	modified residue	UNP P0C0V0
B	280	MSE	MET	modified residue	UNP P0C0V0
B	331	MSE	MET	modified residue	UNP P0C0V0
B	376	MSE	MET	modified residue	UNP P0C0V0
B	447	MSE	MET	modified residue	UNP P0C0V0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	77	Total O 77 77	0	0
2	B	89	Total O 89 89	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.37Å 121.37Å 233.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 99.2 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.275 0.228 , 0.286	Depositor DCC
R_{free} test set	2338 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 79.4	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	0.93	EDS
Total number of atoms	5366	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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	0.80	2/2295 (0.1%)	1.29	29/3078 (0.9%)
1	B	0.76	5/2932 (0.2%)	1.62	31/3934 (0.8%)
All	All	0.78	7/5227 (0.1%)	1.49	60/7012 (0.9%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	ILE	CA-CB	5.92	1.61	1.54
1	B	93	ILE	CA-CB	5.85	1.62	1.54
1	A	16	ALA	CA-CB	-5.70	1.48	1.54
1	B	229	LEU	CA-C	-5.43	1.45	1.53
1	A	113	ILE	CA-CB	5.30	1.62	1.54
1	B	230	ALA	CA-CB	-5.20	1.46	1.53
1	B	230	ALA	N-CA	-5.17	1.40	1.45

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	ALA	CA-C-N	47.68	179.44	119.84
1	B	230	ALA	C-N-CA	47.68	179.44	119.84
1	B	230	ALA	C-N-CD	-12.27	74.72	125.00
1	A	300	ALA	N-CA-C	-11.53	98.64	113.17
1	A	230	ALA	CA-C-N	10.24	151.57	127.00
1	A	230	ALA	C-N-CA	10.24	151.57	127.00
1	B	160	VAL	N-CA-C	10.17	121.04	110.36
1	A	230	ALA	C-N-CD	-9.74	99.18	120.60
1	B	111	THR	N-CA-C	-9.44	101.65	113.55
1	A	196	GLU	N-CA-C	-8.41	97.17	109.11
1	B	230	ALA	N-CA-C	8.14	118.97	109.60
1	A	170	PRO	N-CA-C	7.33	123.37	113.84
1	A	205	ILE	N-CA-C	7.29	118.51	108.89
1	B	174	GLY	N-CA-C	7.26	121.20	110.60
1	B	128	VAL	N-CA-C	-7.06	106.61	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	SER	N-CA-C	6.84	120.11	111.69
1	A	265	LEU	N-CA-C	6.80	118.54	107.32
1	A	268	MSE	N-CA-C	-6.74	96.44	110.80
1	A	213	ALA	N-CA-C	6.66	120.13	110.28
1	B	169	ASN	CA-C-N	6.48	127.94	119.84
1	B	169	ASN	C-N-CA	6.48	127.94	119.84
1	B	231	PRO	N-CA-C	-6.42	99.24	112.47
1	B	316	LYS	CA-C-N	6.31	126.26	119.76
1	B	316	LYS	C-N-CA	6.31	126.26	119.76
1	A	323	ALA	N-CA-C	-6.27	104.44	111.28
1	A	236	ILE	N-CA-C	-6.26	105.52	113.22
1	B	131	ASP	CA-C-N	6.19	126.66	119.47
1	B	131	ASP	C-N-CA	6.19	126.66	119.47
1	B	231	PRO	CB-CA-C	6.19	121.77	111.56
1	B	397	ALA	N-CA-C	-6.15	104.66	111.36
1	A	242	ILE	CA-C-N	-6.06	113.71	120.14
1	A	242	ILE	C-N-CA	-6.06	113.71	120.14
1	B	413	GLN	N-CA-C	5.96	118.52	109.63
1	B	235	ASN	N-CA-C	5.89	119.17	110.46
1	B	265	LEU	N-CA-C	-5.86	105.89	113.16
1	A	231	PRO	N-CA-C	5.86	127.33	112.10
1	B	232	ASP	N-CA-C	5.84	119.94	112.12
1	B	299	ALA	N-CA-C	-5.84	105.00	111.36
1	A	111	THR	N-CA-C	-5.75	106.92	114.04
1	B	256	GLU	N-CA-C	5.73	119.97	113.15
1	B	321	PHE	N-CA-C	-5.71	104.25	111.11
1	A	233	GLY	N-CA-C	-5.62	99.86	113.18
1	A	268	MSE	N-CA-CB	5.61	119.97	110.49
1	A	258	GLY	N-CA-C	-5.59	108.02	115.40
1	B	391	LYS	N-CA-C	5.44	117.74	109.63
1	A	267	ILE	CB-CA-C	5.42	120.17	111.29
1	B	106	VAL	CB-CA-C	-5.40	105.43	111.80
1	A	107	VAL	N-CA-CB	-5.38	105.32	112.26
1	A	22	VAL	CB-CA-C	-5.38	105.37	111.55
1	B	411	ASN	N-CA-C	-5.37	107.10	113.38
1	A	124	ASP	N-CA-C	-5.33	102.16	110.42
1	A	15	LEU	N-CA-C	-5.33	106.95	113.50
1	A	160	VAL	N-CA-C	5.26	120.28	109.34
1	B	28	SER	N-CA-C	-5.26	101.99	110.14
1	A	197	ASN	N-CA-C	5.26	122.00	110.80
1	B	93	ILE	CB-CA-C	5.24	115.78	110.65
1	A	95	ALA	N-CA-C	5.23	117.06	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	VAL	CB-CA-C	-5.22	106.46	111.06
1	B	249	ASN	N-CA-C	5.12	116.55	111.07
1	A	322	ALA	N-CA-C	-5.05	106.63	112.89

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	2282	0	2340	232	0
1	B	2918	0	3008	304	0
2	A	77	0	0	18	0
2	B	89	0	0	15	0
All	All	5366	0	5348	536	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 51.

All (536) 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:266:GLY:O	1:A:267:ILE:HG13	1.38	1.21
1:B:267:ILE:HD11	1:B:321:PHE:HE1	1.15	1.08
1:A:309:VAL:HG23	1:A:342:LEU:HB3	1.33	1.06
1:B:246:MSE:HG2	2:B:476:HOH:O	1.56	1.05
1:A:265:LEU:HG	1:A:265:LEU:O	1.28	1.04
1:A:246:MSE:HG2	2:A:471:HOH:O	1.54	1.04
1:A:262:ARG:HH12	1:A:332:PRO:HG3	1.23	1.02
1:A:293:VAL:HG23	1:A:299:ALA:HB1	1.41	1.01
1:B:42:MSE:HE2	1:B:44:ARG:HD3	1.44	1.00
1:A:298:SER:HA	1:A:301:LYS:HB3	1.43	0.99
1:A:265:LEU:O	1:A:265:LEU:CG	2.10	0.98
1:A:195:TYR:HB3	1:A:336:LYS:O	1.62	0.97
1:B:367:ILE:HG23	1:B:368:PHE:H	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:MSE:HE2	1:B:44:ARG:CD	1.94	0.97
1:A:273:ASN:HA	1:A:278:LYS:HG2	1.43	0.97
1:B:93:ILE:HG13	1:B:152:MSE:HE2	1.46	0.97
1:B:18:MSE:HE1	1:B:165:VAL:HG11	1.47	0.95
1:B:409:GLY:HA3	1:B:435:ASN:HB2	1.46	0.95
1:A:187:ARG:HG3	1:A:195:TYR:HA	1.47	0.94
1:A:127:MSE:CG	2:A:490:HOH:O	2.14	0.94
1:A:261:LYS:O	1:A:333:VAL:HG23	1.68	0.94
1:A:343:ARG:HH11	1:A:346:LYS:HD2	1.31	0.93
1:B:382:ASP:HB3	1:B:416:LYS:HB2	1.51	0.92
1:A:313:LEU:HD11	1:A:337:LEU:HD12	1.50	0.91
1:B:302:ALA:CB	1:B:350:VAL:HG11	2.01	0.91
1:A:197:ASN:HD22	1:A:197:ASN:H	1.16	0.90
1:B:121:ARG:NH2	1:B:145:LYS:O	2.03	0.90
1:B:267:ILE:HD11	1:B:321:PHE:CE1	2.05	0.90
1:A:318:ILE:HG21	1:A:324:LEU:HG	1.54	0.89
1:A:337:LEU:HD21	1:A:352:LEU:HD11	1.54	0.89
1:A:197:ASN:HD22	1:A:197:ASN:N	1.63	0.89
1:B:268:MSE:HE2	1:B:294:LEU:HD11	1.54	0.88
1:B:302:ALA:HB1	1:B:350:VAL:HG11	1.55	0.88
1:B:396:ALA:O	1:B:399:ILE:HG22	1.73	0.87
1:B:443:ILE:HD12	1:B:445:LEU:HD21	1.58	0.86
1:A:293:VAL:HG21	1:A:304:ILE:O	1.75	0.86
1:A:290:VAL:HG21	1:A:310:ILE:HD13	1.58	0.85
1:A:304:ILE:HA	1:A:346:LYS:HZ3	1.42	0.83
1:B:367:ILE:HG23	1:B:368:PHE:N	1.95	0.81
1:B:266:GLY:O	1:B:294:LEU:HB2	1.79	0.81
1:B:276:LEU:HB3	1:B:280:MSE:HE2	1.63	0.81
1:B:304:ILE:HG12	1:B:341:LEU:HD11	1.61	0.81
1:B:399:ILE:HG23	1:B:401:LEU:HD13	1.63	0.80
1:B:42:MSE:CE	1:B:44:ARG:HD3	2.11	0.80
1:B:302:ALA:HB1	1:B:350:VAL:CG1	2.11	0.79
1:A:298:SER:O	1:A:302:ALA:HB2	1.81	0.79
1:A:341:LEU:HD22	1:A:346:LYS:HD3	1.65	0.79
1:B:402:LYS:HG2	1:B:403:LYS:H	1.48	0.78
1:A:321:PHE:HD2	1:A:321:PHE:H	1.31	0.78
1:B:268:MSE:CE	1:B:294:LEU:HD21	2.13	0.77
1:B:267:ILE:HD12	1:B:268:MSE:N	1.99	0.77
1:A:127:MSE:HG2	2:A:490:HOH:O	1.81	0.77
1:A:352:LEU:O	1:A:353:GLU:HB2	1.83	0.77
1:B:227:ALA:HA	2:B:507:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ILE:HG22	2:B:457:HOH:O	1.84	0.76
1:A:266:GLY:C	1:A:267:ILE:HG13	2.11	0.76
1:A:311:THR:HA	1:A:318:ILE:HB	1.66	0.76
1:A:127:MSE:HG3	2:A:490:HOH:O	1.83	0.75
1:B:169:ASN:C	1:B:169:ASN:HD22	1.94	0.75
1:B:247:VAL:O	1:B:251:THR:HB	1.86	0.75
1:A:313:LEU:HD23	1:A:327:GLN:HE21	1.52	0.75
1:A:271:GLU:HG2	1:A:272:LEU:N	2.00	0.75
1:B:339:LEU:HD12	1:B:339:LEU:H	1.51	0.75
1:B:41:ARG:C	1:B:42:MSE:HE3	2.13	0.74
1:A:205:ILE:HD12	1:A:205:ILE:H	1.50	0.74
1:B:229:LEU:O	1:B:232:ASP:HB3	1.87	0.74
1:A:29:ILE:HG23	1:A:113:ILE:HD13	1.69	0.74
1:A:107:VAL:HG13	1:A:127:MSE:HE1	1.70	0.74
1:A:197:ASN:H	1:A:197:ASN:ND2	1.78	0.73
1:B:41:ARG:O	1:B:42:MSE:HE3	1.88	0.73
1:A:29:ILE:HG23	1:A:113:ILE:CD1	2.19	0.73
1:A:246:MSE:HA	1:A:246:MSE:HE2	1.69	0.73
1:B:268:MSE:HE3	1:B:294:LEU:HD21	1.71	0.73
1:A:318:ILE:CG2	1:A:324:LEU:HG	2.18	0.72
1:A:42:MSE:HB3	1:A:43:PRO:HA	1.71	0.72
1:A:343:ARG:HH12	1:A:346:LYS:HZ2	1.37	0.72
1:B:348:VAL:HG12	1:B:349:ASN:H	1.54	0.72
1:B:226:THR:HG22	1:B:240:PHE:O	1.89	0.72
1:A:163:TYR:HB2	1:A:217:LEU:CD2	2.19	0.72
1:A:262:ARG:HH12	1:A:332:PRO:CG	1.99	0.72
1:A:87:LEU:C	1:A:87:LEU:HD23	2.15	0.72
1:A:312:SER:HB2	1:A:340:GLY:H	1.53	0.72
1:A:247:VAL:O	1:A:251:THR:HB	1.90	0.71
1:A:235:ASN:HB2	2:A:473:HOH:O	1.91	0.71
1:B:349:ASN:O	1:B:350:VAL:HG13	1.91	0.71
1:B:286:ARG:HD2	1:B:286:ARG:O	1.90	0.71
1:B:387:VAL:HG12	1:B:405:ASP:O	1.91	0.70
1:B:113:ILE:HG13	1:B:125:ALA:HB3	1.72	0.70
1:A:262:ARG:NH1	1:A:332:PRO:HG3	2.03	0.69
1:A:87:LEU:HD23	1:A:88:GLY:N	2.07	0.69
1:A:293:VAL:HG11	1:A:305:LYS:HA	1.73	0.69
1:B:206:ASN:OD1	1:B:207:ARG:HG3	1.92	0.69
1:B:93:ILE:HG13	1:B:152:MSE:CE	2.20	0.69
1:B:355:GLN:HG2	1:B:357:SER:H	1.57	0.69
1:A:104:ASN:HD22	1:A:130:LYS:HB2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ALA:HB2	1:B:415:VAL:HG23	1.73	0.69
1:B:384:GLY:HA3	1:B:408:ILE:HD13	1.73	0.69
1:B:169:ASN:HD21	1:B:172:GLY:CA	2.05	0.69
1:A:341:LEU:HD23	1:A:342:LEU:N	2.08	0.68
1:B:361:GLN:HG3	1:B:375:GLU:HG2	1.74	0.68
1:B:381:LYS:HD3	1:B:381:LYS:H	1.57	0.68
1:B:276:LEU:HB3	1:B:280:MSE:CE	2.22	0.68
1:A:343:ARG:HH11	1:A:346:LYS:CD	2.04	0.68
1:A:343:ARG:NH1	1:A:346:LYS:HD2	2.08	0.68
1:A:293:VAL:HG23	1:A:299:ALA:CB	2.20	0.68
1:B:302:ALA:CB	1:B:350:VAL:CG1	2.70	0.68
1:B:410:ALA:N	1:B:413:GLN:O	2.21	0.68
1:A:160:VAL:O	1:A:182:VAL:O	2.12	0.68
1:B:405:ASP:HA	1:B:438:ARG:HB3	1.75	0.68
1:B:415:VAL:HG12	1:B:415:VAL:O	1.94	0.67
1:B:324:LEU:O	1:B:328:VAL:HG22	1.94	0.67
1:A:264:GLU:HA	1:A:329:GLY:HA2	1.78	0.67
1:B:18:MSE:CE	1:B:165:VAL:HG11	2.24	0.67
1:B:415:VAL:HG13	1:B:421:LEU:HB2	1.77	0.67
1:B:184:ALA:HB3	1:B:200:GLN:HB2	1.77	0.66
1:B:360:ASN:ND2	1:B:418:ILE:HD13	2.11	0.66
1:B:169:ASN:ND2	1:B:172:GLY:H	1.93	0.66
1:A:342:LEU:HD23	1:A:343:ARG:N	2.09	0.66
1:A:269:GLY:HA2	1:A:291:SER:OG	1.95	0.66
1:A:343:ARG:NH1	1:A:346:LYS:HZ2	1.93	0.65
1:A:93:ILE:HG13	1:A:152:MSE:HE2	1.77	0.65
1:A:19:LEU:HD21	1:A:177:VAL:HG21	1.77	0.65
1:A:169:ASN:C	1:A:169:ASN:HD22	2.04	0.65
1:A:304:ILE:HA	1:A:346:LYS:NZ	2.10	0.65
1:B:304:ILE:CG1	1:B:341:LEU:HD11	2.27	0.65
1:B:304:ILE:HG12	1:B:341:LEU:CD1	2.27	0.65
1:B:393:GLY:C	1:B:395:PRO:HD3	2.22	0.64
1:A:289:PHE:HA	1:A:309:VAL:HG12	1.79	0.64
1:A:163:TYR:HB2	1:A:217:LEU:HD21	1.80	0.64
1:B:243:PRO:O	1:B:247:VAL:HG23	1.98	0.64
1:B:379:LYS:HB2	1:B:386:VAL:HB	1.80	0.64
1:A:187:ARG:CG	1:A:195:TYR:HA	2.24	0.63
1:A:266:GLY:O	1:A:267:ILE:CG1	2.32	0.63
1:B:232:ASP:OD1	1:B:233:GLY:O	2.16	0.63
1:B:284:ALA:HB1	1:B:286:ARG:NH2	2.14	0.63
1:B:411:ASN:HA	1:B:433:ALA:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:NH1	1:A:330:THR:HG23	2.12	0.63
1:A:305:LYS:HB2	1:A:305:LYS:NZ	2.14	0.63
1:A:85:MSE:HE2	2:A:479:HOH:O	1.99	0.62
1:B:363:ASP:OD1	1:B:422:ARG:NH1	2.26	0.62
1:B:330:THR:HG22	1:B:330:THR:O	1.99	0.62
1:B:386:VAL:HG22	1:B:406:VAL:HG22	1.82	0.62
1:A:268:MSE:O	1:A:292:GLN:HB2	2.00	0.62
1:B:165:VAL:CG1	1:B:215:VAL:HG12	2.30	0.62
1:B:303:GLY:O	1:B:304:ILE:HG13	2.00	0.61
1:B:420:GLU:O	1:B:423:LYS:HB3	2.00	0.61
1:A:337:LEU:HD21	1:A:352:LEU:CD1	2.28	0.61
1:B:94:ASP:HB3	1:B:99:TYR:HB2	1.82	0.61
1:A:235:ASN:N	2:A:473:HOH:O	2.31	0.61
1:B:267:ILE:HD12	1:B:268:MSE:CA	2.31	0.61
1:B:354:LEU:HD13	1:B:355:GLN:N	2.16	0.61
1:A:343:ARG:HH12	1:A:346:LYS:NZ	1.99	0.60
1:B:384:GLY:HA2	1:B:415:VAL:O	2.01	0.60
1:A:312:SER:HB2	1:A:340:GLY:N	2.16	0.60
1:A:335:SER:HB2	1:A:352:LEU:HD13	1.82	0.60
1:B:313:LEU:HD21	1:B:337:LEU:HD12	1.84	0.60
1:A:133:ARG:NH1	1:A:331:MSE:HA	2.17	0.59
1:B:334:GLY:HA2	1:B:351:ASN:HD21	1.66	0.59
1:A:175:GLU:OE2	1:A:175:GLU:HA	2.02	0.59
1:B:41:ARG:HG3	1:B:41:ARG:HH11	1.65	0.59
1:B:185:LEU:O	1:B:186:GLY:C	2.46	0.59
1:B:409:GLY:HA3	1:B:435:ASN:CB	2.27	0.59
1:B:411:ASN:OD1	1:B:433:ALA:N	2.25	0.59
1:A:135:ASP:HB3	1:A:226:THR:OG1	2.02	0.59
1:B:113:ILE:CG1	1:B:125:ALA:HB3	2.32	0.59
1:A:318:ILE:HG21	1:A:324:LEU:CG	2.29	0.59
1:B:348:VAL:HG12	1:B:349:ASN:N	2.18	0.59
1:B:226:THR:OG1	1:B:227:ALA:N	2.36	0.59
1:A:133:ARG:HH11	1:A:330:THR:HG23	1.68	0.58
1:B:340:GLY:HA2	1:B:347:GLN:HG3	1.83	0.58
1:B:339:LEU:HD12	1:B:339:LEU:N	2.18	0.58
1:B:438:ARG:HG3	1:B:438:ARG:HH11	1.68	0.58
1:B:301:LYS:HD3	1:B:301:LYS:C	2.29	0.58
1:A:282:VAL:HG12	1:A:282:VAL:O	2.01	0.58
1:A:311:THR:CA	1:A:318:ILE:HB	2.34	0.58
1:A:321:PHE:CD2	1:A:321:PHE:N	2.63	0.58
1:B:265:LEU:HD21	1:B:339:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ASN:O	1:B:350:VAL:CG1	2.51	0.58
1:B:407:ILE:HG12	1:B:436:ILE:HG22	1.85	0.58
1:A:335:SER:HB2	1:A:352:LEU:HD22	1.85	0.58
1:A:169:ASN:ND2	1:A:172:GLY:H	2.01	0.58
1:B:169:ASN:HD21	1:B:172:GLY:N	2.02	0.58
1:B:311:THR:HB	2:B:484:HOH:O	2.03	0.57
1:A:293:VAL:HG11	1:A:305:LYS:HD3	1.86	0.57
1:B:360:ASN:O	1:B:375:GLU:HA	2.04	0.57
1:B:405:ASP:OD2	1:B:438:ARG:HD3	2.04	0.57
1:B:161:GLY:N	2:B:533:HOH:O	2.20	0.57
1:B:405:ASP:HA	1:B:438:ARG:CB	2.35	0.57
1:A:267:ILE:HG22	1:A:295:PRO:HD2	1.86	0.57
1:A:272:LEU:HG	1:A:289:PHE:HB2	1.86	0.57
1:B:119:ASP:OD2	1:B:121:ARG:HD3	2.04	0.57
1:B:113:ILE:HG13	1:B:113:ILE:O	2.04	0.57
1:A:266:GLY:C	1:A:267:ILE:CG1	2.78	0.57
1:B:185:LEU:O	1:B:187:ARG:N	2.38	0.57
1:B:349:ASN:C	1:B:350:VAL:HG13	2.30	0.56
1:B:381:LYS:HD3	1:B:381:LYS:N	2.20	0.56
1:A:133:ARG:HD3	1:A:330:THR:O	2.05	0.56
1:A:154:ASP:HA	1:A:245:ASN:HD21	1.69	0.56
1:B:133:ARG:HG3	1:B:262:ARG:HH11	1.70	0.56
1:B:282:VAL:HG23	1:B:285:GLN:CD	2.30	0.56
1:A:91:VAL:HG21	1:A:213:ALA:HB2	1.87	0.56
1:B:394:THR:N	1:B:395:PRO:HD3	2.20	0.56
1:A:271:GLU:HB2	1:A:321:PHE:CE1	2.41	0.56
1:B:337:LEU:HD23	1:B:337:LEU:H	1.70	0.56
1:A:91:VAL:CG2	1:A:213:ALA:HB2	2.35	0.56
1:A:298:SER:HA	1:A:301:LYS:CB	2.28	0.56
1:A:272:LEU:O	1:A:273:ASN:HB2	2.05	0.56
1:A:206:ASN:OD1	1:A:207:ARG:HG3	2.06	0.55
1:A:334:GLY:N	1:A:352:LEU:HB2	2.21	0.55
1:B:11:GLN:CD	1:B:11:GLN:N	2.64	0.55
1:B:415:VAL:CG1	1:B:421:LEU:HB2	2.36	0.55
1:B:204:ALA:C	1:B:205:ILE:HG13	2.31	0.55
1:A:114:LYS:HE2	1:A:124:ASP:OD1	2.07	0.55
1:B:169:ASN:C	1:B:169:ASN:ND2	2.64	0.55
1:A:337:LEU:HD23	1:A:337:LEU:H	1.72	0.55
1:B:127:MSE:HE1	1:B:129:GLY:O	2.07	0.55
1:A:234:GLY:HA3	2:A:462:HOH:O	2.06	0.55
1:A:283:ASP:O	1:A:284:ALA:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLN:O	1:B:82:GLN:OE1	2.24	0.55
1:B:365:SER:O	1:B:367:ILE:N	2.40	0.55
1:B:286:ARG:HG2	1:B:286:ARG:HH11	1.72	0.55
1:B:330:THR:O	1:B:331:MSE:HG3	2.07	0.54
1:B:427:SER:C	1:B:429:PRO:HD3	2.31	0.54
1:A:136:ILE:O	1:A:254:MSE:HE1	2.08	0.54
1:B:127:MSE:HE1	1:B:129:GLY:C	2.31	0.54
1:B:412:GLN:HG2	1:B:413:GLN:N	2.21	0.54
1:B:336:LYS:HG2	1:B:351:ASN:HB2	1.90	0.54
1:A:283:ASP:O	1:A:284:ALA:CB	2.55	0.54
1:B:267:ILE:HD12	1:B:267:ILE:C	2.33	0.54
1:B:330:THR:C	1:B:331:MSE:HG3	2.32	0.54
1:B:164:THR:HG21	1:B:201:THR:OG1	2.08	0.54
1:B:438:ARG:HG3	1:B:438:ARG:NH1	2.23	0.54
1:A:343:ARG:NH1	1:A:346:LYS:NZ	2.54	0.54
1:B:355:GLN:OE1	1:B:357:SER:HB2	2.08	0.54
1:B:184:ALA:HB3	1:B:200:GLN:CB	2.39	0.53
1:A:133:ARG:HH11	1:A:330:THR:C	2.16	0.53
1:A:281:LYS:H	1:A:281:LYS:HD2	1.73	0.53
1:A:267:ILE:HG21	1:A:299:ALA:CB	2.37	0.53
1:B:262:ARG:HG3	1:B:355:GLN:NE2	2.24	0.53
1:B:310:ILE:HD12	1:B:310:ILE:N	2.23	0.53
1:B:410:ALA:C	1:B:412:GLN:H	2.16	0.53
1:B:259:GLN:HG2	1:B:378:ASN:HD22	1.74	0.52
1:A:305:LYS:HG3	1:A:306:ALA:H	1.73	0.52
1:B:82:GLN:OE1	1:B:82:GLN:HA	2.09	0.52
1:B:410:ALA:CB	1:B:415:VAL:HG23	2.37	0.52
1:A:264:GLU:HG3	2:A:521:HOH:O	2.08	0.52
1:B:320:SER:O	1:B:321:PHE:C	2.52	0.52
1:A:337:LEU:HD23	1:A:337:LEU:N	2.25	0.52
1:B:169:ASN:ND2	1:B:172:GLY:N	2.58	0.52
1:B:212:GLY:O	1:B:225:ASN:N	2.35	0.52
1:B:437:GLN:HA	1:B:441:SER:O	2.10	0.52
1:A:232:ASP:O	1:A:233:GLY:C	2.53	0.52
1:B:37:VAL:HG11	1:B:82:GLN:HE21	1.75	0.52
1:B:268:MSE:HE2	1:B:294:LEU:CD1	2.33	0.52
1:A:185:LEU:HD13	1:A:188:SER:HB2	1.90	0.52
1:A:337:LEU:HG	1:A:350:VAL:HG22	1.90	0.52
1:B:204:ALA:O	1:B:205:ILE:HG13	2.09	0.52
1:B:272:LEU:HD13	1:B:285:GLN:CA	2.40	0.52
1:B:386:VAL:CG2	1:B:406:VAL:HG22	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLY:H	1:A:352:LEU:HB2	1.75	0.51
1:B:259:GLN:OE1	1:B:354:LEU:HG	2.10	0.51
1:B:445:LEU:N	1:B:445:LEU:HD22	2.25	0.51
1:A:107:VAL:HG13	1:A:127:MSE:CE	2.39	0.51
1:A:42:MSE:HB3	1:A:43:PRO:CA	2.40	0.51
1:B:44:ARG:HA	1:B:44:ARG:NE	2.24	0.51
1:B:160:VAL:O	1:B:182:VAL:O	2.26	0.51
1:B:267:ILE:HD12	1:B:268:MSE:C	2.34	0.51
1:B:87:LEU:C	1:B:87:LEU:HD23	2.35	0.51
1:B:310:ILE:HD12	1:B:310:ILE:H	1.76	0.51
1:B:411:ASN:HD21	1:B:428:LYS:NZ	2.08	0.51
1:B:236:ILE:HG12	1:B:236:ILE:O	2.11	0.51
1:B:410:ALA:C	1:B:412:GLN:N	2.67	0.51
1:B:410:ALA:HB1	1:B:424:VAL:HG21	1.93	0.51
1:A:271:GLU:HG3	1:A:321:PHE:CE2	2.46	0.51
1:B:23:MSE:HE2	2:B:473:HOH:O	2.10	0.51
1:B:104:ASN:O	1:B:108:ASP:HB2	2.11	0.51
1:B:424:VAL:C	1:B:426:ASP:H	2.18	0.51
1:A:335:SER:CB	1:A:352:LEU:HD22	2.41	0.50
1:A:348:VAL:HG12	1:A:349:ASN:N	2.26	0.50
1:B:151:LYS:HD3	1:B:220:GLU:OE2	2.12	0.50
1:A:281:LYS:H	1:A:281:LYS:CD	2.25	0.50
1:A:308:ASP:OD1	1:A:343:ARG:NH1	2.44	0.50
1:A:16:ALA:HB3	1:A:17:PRO:HD3	1.93	0.50
1:A:271:GLU:HB2	1:A:321:PHE:CD1	2.46	0.50
1:B:313:LEU:HD13	1:B:327:GLN:HE21	1.76	0.50
1:A:23:MSE:N	1:A:24:PRO:CD	2.74	0.50
1:A:42:MSE:HE1	2:A:505:HOH:O	2.11	0.49
1:A:318:ILE:HG13	1:A:324:LEU:HD21	1.94	0.49
1:B:365:SER:C	1:B:367:ILE:N	2.70	0.49
1:B:405:ASP:CA	1:B:438:ARG:HB3	2.41	0.49
1:A:262:ARG:HH11	1:A:331:MSE:C	2.20	0.49
1:A:335:SER:HB2	1:A:352:LEU:CD1	2.43	0.49
1:B:333:VAL:HG12	1:B:334:GLY:N	2.27	0.49
1:A:169:ASN:C	1:A:169:ASN:ND2	2.69	0.49
1:B:41:ARG:HH11	1:B:41:ARG:CG	2.25	0.49
1:B:126:LYS:NZ	2:B:518:HOH:O	2.45	0.49
1:B:416:LYS:HD3	1:B:420:GLU:OE1	2.12	0.49
1:B:135:ASP:CG	1:B:135:ASP:O	2.54	0.49
1:B:410:ALA:CA	1:B:415:VAL:HG23	2.42	0.49
1:A:290:VAL:CG2	1:A:310:ILE:HD13	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:MSE:HE2	1:B:294:LEU:HD21	1.90	0.49
1:A:278:LYS:HD3	1:A:282:VAL:HG21	1.94	0.49
1:B:142:GLN:HG3	2:B:486:HOH:O	2.11	0.49
1:B:416:LYS:HG2	1:B:420:GLU:OE2	2.12	0.49
1:A:323:ALA:O	1:A:327:GLN:HG3	2.13	0.49
1:B:381:LYS:H	1:B:381:LYS:CD	2.19	0.49
1:B:411:ASN:ND2	1:B:412:GLN:OE1	2.45	0.49
1:A:89:SER:HB2	2:A:502:HOH:O	2.13	0.49
1:B:160:VAL:HB	2:B:533:HOH:O	2.11	0.48
1:A:243:PRO:O	1:A:247:VAL:HG23	2.13	0.48
1:B:365:SER:C	1:B:367:ILE:H	2.21	0.48
1:B:411:ASN:O	1:B:412:GLN:HB3	2.13	0.48
1:A:187:ARG:HH12	1:A:336:LYS:NZ	2.11	0.48
1:A:311:THR:HG23	1:A:318:ILE:O	2.13	0.48
1:B:82:GLN:HG2	2:B:472:HOH:O	2.13	0.48
1:B:432:LEU:O	1:B:446:LEU:HA	2.13	0.48
1:A:41:ARG:HD3	1:A:41:ARG:C	2.38	0.48
1:A:85:MSE:HB3	2:A:479:HOH:O	2.14	0.48
1:A:184:ALA:HB3	1:A:200:GLN:HB2	1.96	0.48
1:A:187:ARG:NH1	1:A:336:LYS:HD2	2.29	0.48
1:A:310:ILE:N	1:A:310:ILE:HD12	2.29	0.48
1:B:405:ASP:CG	1:B:438:ARG:HB3	2.39	0.48
1:A:304:ILE:HG23	1:A:308:ASP:OD2	2.13	0.48
1:A:308:ASP:OD1	1:A:341:LEU:HD21	2.13	0.48
1:B:290:VAL:HG23	1:B:308:ASP:O	2.14	0.48
1:B:354:LEU:HD13	1:B:355:GLN:H	1.77	0.48
1:A:257:TYR:C	1:A:259:GLN:H	2.22	0.48
1:B:334:GLY:HA2	1:B:351:ASN:ND2	2.28	0.48
1:A:207:ARG:CG	1:A:207:ARG:HH11	2.27	0.48
1:B:360:ASN:ND2	1:B:418:ILE:CD1	2.77	0.47
1:A:133:ARG:HH12	1:A:331:MSE:HG2	1.79	0.47
1:A:278:LYS:NZ	1:A:282:VAL:HG11	2.28	0.47
1:B:42:MSE:HG3	1:B:43:PRO:HA	1.96	0.47
1:B:265:LEU:O	1:B:299:ALA:HB2	2.14	0.47
1:B:382:ASP:OD2	1:B:416:LYS:HE2	2.14	0.47
1:A:200:GLN:HA	1:A:239:GLY:O	2.14	0.47
1:B:41:ARG:O	1:B:44:ARG:NH1	2.47	0.47
1:B:168:GLY:C	1:B:170:PRO:HD3	2.39	0.47
1:B:272:LEU:HD13	1:B:285:GLN:HA	1.96	0.47
1:A:335:SER:HB2	1:A:352:LEU:CD2	2.44	0.47
1:A:87:LEU:C	1:A:87:LEU:CD2	2.86	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:O	1:A:235:ASN:ND2	2.48	0.47
1:A:298:SER:CA	1:A:301:LYS:HB3	2.30	0.47
1:A:325:ARG:HG2	1:A:325:ARG:HH11	1.78	0.47
1:B:399:ILE:O	1:B:445:LEU:HG	2.15	0.47
1:A:290:VAL:HG21	1:A:310:ILE:CD1	2.36	0.47
1:B:42:MSE:HE2	1:B:44:ARG:CG	2.43	0.47
1:B:248:LYS:O	1:B:251:THR:HG22	2.15	0.47
1:B:412:GLN:HG2	1:B:413:GLN:H	1.80	0.46
1:A:259:GLN:HG3	2:A:495:HOH:O	2.15	0.46
1:B:45:ASN:HB3	1:B:48:GLN:HB3	1.96	0.46
1:A:205:ILE:HD11	2:A:451:HOH:O	2.15	0.46
1:A:293:VAL:HG22	1:A:293:VAL:O	2.14	0.46
1:A:294:LEU:O	1:A:296:ASN:ND2	2.48	0.46
1:B:409:GLY:HA2	1:B:413:GLN:O	2.15	0.46
1:B:410:ALA:H	1:B:413:GLN:C	2.18	0.46
1:A:214:LEU:HG	1:A:225:ASN:HD21	1.80	0.46
1:A:272:LEU:O	1:A:273:ASN:CB	2.63	0.46
1:B:37:VAL:HG11	1:B:82:GLN:NE2	2.31	0.46
1:B:312:SER:HA	1:B:318:ILE:HG12	1.97	0.46
1:A:36:THR:O	1:A:36:THR:HG22	2.15	0.46
1:A:129:GLY:HA3	1:A:254:MSE:HB3	1.98	0.46
1:A:160:VAL:N	2:A:511:HOH:O	2.48	0.46
1:A:305:LYS:HB2	1:A:305:LYS:HZ3	1.79	0.46
1:B:385:VAL:HG11	1:B:418:ILE:HG12	1.97	0.46
1:A:37:VAL:HG22	1:A:38:ASN:N	2.30	0.46
1:A:207:ARG:HG3	1:A:207:ARG:HH11	1.79	0.46
1:A:263:GLY:O	1:A:265:LEU:HD22	2.15	0.46
1:B:367:ILE:CG2	1:B:368:PHE:H	2.05	0.46
1:B:282:VAL:HG23	1:B:285:GLN:HG2	1.98	0.46
1:A:318:ILE:O	1:A:318:ILE:HG22	2.16	0.46
1:B:108:ASP:O	1:B:109:ASN:HB2	2.14	0.46
1:A:205:ILE:HD12	1:A:205:ILE:N	2.25	0.45
1:B:99:TYR:CD2	1:B:140:GLN:HG3	2.51	0.45
1:B:133:ARG:NE	1:B:325:ARG:NH1	2.65	0.45
1:B:271:GLU:OE2	1:B:321:PHE:N	2.46	0.45
1:B:272:LEU:CD1	1:B:286:ARG:N	2.79	0.45
1:B:333:VAL:HG21	1:B:354:LEU:HD23	1.98	0.45
1:B:337:LEU:HD23	1:B:337:LEU:N	2.30	0.45
1:A:11:GLN:N	1:A:11:GLN:CD	2.73	0.45
1:A:154:ASP:C	1:A:154:ASP:OD2	2.57	0.45
1:A:298:SER:O	1:A:302:ALA:CB	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HD11	1:A:337:LEU:CD1	2.35	0.45
1:B:42:MSE:HE2	1:B:44:ARG:HD2	1.93	0.45
1:B:282:VAL:HG23	1:B:285:GLN:CG	2.47	0.45
1:B:402:LYS:CG	1:B:403:LYS:H	2.20	0.45
1:B:141:ILE:HD12	1:B:147:LEU:HD21	1.97	0.45
1:B:308:ASP:HA	1:B:342:LEU:O	2.15	0.45
1:B:16:ALA:HB3	1:B:17:PRO:HD3	1.99	0.45
1:B:408:ILE:H	1:B:437:GLN:NE2	2.15	0.45
1:B:411:ASN:ND2	1:B:428:LYS:NZ	2.65	0.45
1:B:433:ALA:HA	1:B:445:LEU:O	2.17	0.45
1:A:232:ASP:O	1:A:234:GLY:N	2.49	0.45
1:B:128:VAL:HG13	1:B:138:LEU:HB3	1.98	0.45
1:B:133:ARG:HG3	1:B:262:ARG:NH1	2.29	0.45
1:B:108:ASP:CG	1:B:130:LYS:NZ	2.75	0.45
1:A:112:VAL:HG13	2:A:487:HOH:O	2.17	0.45
1:A:267:ILE:O	1:A:295:PRO:HG2	2.17	0.45
1:B:108:ASP:OD1	1:B:130:LYS:NZ	2.50	0.45
1:B:259:GLN:HE22	1:B:377:SER:HB2	1.82	0.45
1:B:365:SER:CB	1:B:367:ILE:HG22	2.47	0.45
1:A:113:ILE:HD12	1:A:114:LYS:N	2.31	0.44
1:A:308:ASP:HB3	1:A:341:LEU:HD21	1.99	0.44
1:A:187:ARG:HD2	1:A:195:TYR:CD2	2.52	0.44
1:B:119:ASP:OD1	1:B:119:ASP:C	2.60	0.44
1:A:262:ARG:HA	1:A:262:ARG:HD3	1.72	0.44
1:B:338:THR:HA	1:B:349:ASN:HA	1.99	0.44
1:B:92:ILE:HD13	1:B:147:LEU:HG	2.00	0.44
1:A:196:GLU:OE1	1:A:331:MSE:HE2	2.17	0.44
1:A:341:LEU:HD13	1:A:346:LYS:HD3	1.99	0.44
1:A:342:LEU:HD23	1:A:342:LEU:C	2.43	0.44
1:B:46:PHE:CD1	1:B:46:PHE:C	2.95	0.44
1:B:152:MSE:HE2	2:B:519:HOH:O	2.17	0.44
1:B:259:GLN:HG2	1:B:378:ASN:ND2	2.32	0.44
1:A:100:VAL:HB	1:A:139:ILE:HG13	1.98	0.44
1:A:187:ARG:HH11	1:A:336:LYS:HD2	1.82	0.44
1:B:201:THR:O	1:B:238:ILE:HG12	2.16	0.44
1:B:405:ASP:HA	1:B:438:ARG:HA	1.99	0.44
1:A:331:MSE:HA	1:A:332:PRO:HD3	1.79	0.44
1:B:333:VAL:HG13	1:B:353:GLU:HA	2.00	0.44
1:B:410:ALA:HB3	1:B:413:GLN:CB	2.48	0.44
1:A:312:SER:HB2	1:A:340:GLY:CA	2.48	0.44
1:B:286:ARG:HH11	1:B:286:ARG:CG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:PHE:HE2	1:B:307:GLY:HA2	1.82	0.44
1:B:391:LYS:HB3	1:B:392:THR:H	1.68	0.44
1:A:133:ARG:NH1	1:A:330:THR:O	2.51	0.43
1:A:281:LYS:O	1:A:282:VAL:HB	2.17	0.43
1:A:11:GLN:HB2	2:A:512:HOH:O	2.18	0.43
1:A:133:ARG:NH1	1:A:330:THR:C	2.75	0.43
1:A:264:GLU:CA	1:A:329:GLY:HA2	2.47	0.43
1:A:311:THR:C	1:A:318:ILE:H	2.26	0.43
1:B:368:PHE:C	1:B:369:ASN:OD1	2.60	0.43
1:B:404:GLY:O	1:B:438:ARG:HB2	2.17	0.43
1:B:172:GLY:O	1:B:174:GLY:N	2.52	0.43
1:B:313:LEU:HD21	1:B:337:LEU:HB2	2.00	0.43
1:A:142:GLN:O	1:A:143:ASN:HB2	2.18	0.43
1:A:294:LEU:C	1:A:296:ASN:N	2.75	0.43
1:B:113:ILE:C	1:B:113:ILE:HD12	2.44	0.43
1:A:307:GLY:O	1:A:308:ASP:O	2.35	0.43
1:B:169:ASN:HD21	1:B:172:GLY:C	2.25	0.43
1:B:256:GLU:O	1:B:257:TYR:CD2	2.71	0.43
1:B:277:ALA:O	1:B:282:VAL:HG22	2.18	0.43
1:A:253:GLN:OE1	1:A:260:VAL:HG23	2.19	0.43
1:B:258:GLY:HA3	1:B:418:ILE:HB	2.01	0.43
1:B:399:ILE:HG23	1:B:399:ILE:O	2.19	0.43
1:B:406:VAL:HG11	1:B:408:ILE:HD11	1.99	0.43
1:B:210:ALA:O	1:B:211:GLY:O	2.36	0.43
1:B:334:GLY:O	1:B:351:ASN:ND2	2.48	0.43
1:B:402:LYS:HG2	1:B:403:LYS:N	2.25	0.43
1:B:406:VAL:HG12	1:B:407:ILE:N	2.34	0.43
1:A:216:ASN:OD1	1:A:216:ASN:C	2.62	0.42
1:B:434:LEU:O	1:B:436:ILE:HG23	2.20	0.42
1:B:435:ASN:OD1	1:B:435:ASN:N	2.52	0.42
1:A:207:ARG:CG	1:A:207:ARG:NH1	2.81	0.42
1:A:228:ILE:HD11	1:A:236:ILE:HG21	2.00	0.42
1:B:293:VAL:O	1:B:293:VAL:HG13	2.19	0.42
1:A:163:TYR:HB2	1:A:217:LEU:HD22	2.01	0.42
1:A:345:GLY:O	1:A:346:LYS:HB2	2.19	0.42
1:A:256:GLU:O	1:A:256:GLU:HG3	2.19	0.42
1:A:343:ARG:HH11	1:A:343:ARG:HG2	1.84	0.42
1:B:42:MSE:HA	1:B:43:PRO:O	2.18	0.42
1:B:363:ASP:OD1	1:B:363:ASP:C	2.62	0.42
1:B:384:GLY:HA3	1:B:408:ILE:CD1	2.45	0.42
1:B:410:ALA:HB3	1:B:413:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLN:N	1:A:11:GLN:NE2	2.68	0.42
1:A:270:THR:O	1:A:271:GLU:O	2.38	0.42
1:B:142:GLN:O	1:B:143:ASN:HB2	2.20	0.42
1:B:165:VAL:HG12	1:B:215:VAL:O	2.20	0.42
1:B:298:SER:HB2	1:B:353:GLU:OE1	2.20	0.42
1:A:348:VAL:HG12	1:A:349:ASN:H	1.84	0.42
1:B:169:ASN:HB2	1:B:175:GLU:OE1	2.20	0.42
1:B:405:ASP:HA	1:B:438:ARG:CA	2.50	0.42
1:A:41:ARG:HD3	1:A:41:ARG:O	2.19	0.42
1:B:42:MSE:HA	1:B:43:PRO:C	2.45	0.42
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.85	0.42
1:B:35:THR:O	1:B:81:GLN:HA	2.20	0.42
1:A:228:ILE:HD11	1:A:236:ILE:CG2	2.50	0.41
1:A:246:MSE:HA	1:A:246:MSE:CE	2.45	0.41
1:B:126:LYS:HG3	1:B:142:GLN:CD	2.44	0.41
1:B:204:ALA:C	1:B:205:ILE:CG1	2.93	0.41
1:B:340:GLY:HA2	1:B:347:GLN:CG	2.50	0.41
1:B:175:GLU:HG3	2:B:464:HOH:O	2.20	0.41
1:B:432:LEU:HD11	1:B:434:LEU:HD11	2.02	0.41
1:A:144:PRO:HB2	1:A:147:LEU:HD22	2.01	0.41
1:A:274:SER:O	1:A:278:LYS:HB2	2.20	0.41
1:B:138:LEU:HA	1:B:138:LEU:HD23	1.78	0.41
1:B:196:GLU:O	1:B:198:PHE:N	2.49	0.41
1:B:262:ARG:HG3	1:B:355:GLN:HE21	1.84	0.41
1:B:302:ALA:HB1	1:B:350:VAL:HG12	1.96	0.41
1:A:211:GLY:HA2	2:A:502:HOH:O	2.20	0.41
1:B:41:ARG:CG	1:B:41:ARG:NH1	2.84	0.41
1:B:103:ASN:HB2	1:B:106:VAL:HG23	2.03	0.41
1:B:302:ALA:HB3	1:B:350:VAL:HG11	1.93	0.41
1:A:185:LEU:CD1	1:A:188:SER:HB2	2.50	0.41
1:B:196:GLU:N	1:B:196:GLU:CD	2.79	0.41
1:B:405:ASP:OD1	1:B:405:ASP:N	2.52	0.41
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.96	0.41
1:A:29:ILE:CG2	1:A:113:ILE:HD13	2.47	0.41
1:A:130:LYS:C	1:A:254:MSE:HE2	2.46	0.41
1:A:280:MSE:HB3	1:A:281:LYS:H	1.60	0.41
1:B:169:ASN:ND2	1:B:169:ASN:O	2.54	0.41
1:B:198:PHE:HE2	1:B:226:THR:HG21	1.85	0.41
1:B:410:ALA:HA	1:B:415:VAL:CG2	2.51	0.41
1:B:411:ASN:OD1	1:B:432:LEU:HA	2.21	0.41
1:A:311:THR:C	1:A:318:ILE:HB	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.80	0.41
1:B:365:SER:HB3	1:B:367:ILE:HG22	2.03	0.41
1:A:187:ARG:HB2	1:A:197:ASN:HB3	2.02	0.41
1:A:228:ILE:HG13	1:A:229:LEU:HD23	2.03	0.41
1:A:228:ILE:HG13	1:A:229:LEU:CD2	2.51	0.41
1:B:185:LEU:HD12	1:B:185:LEU:HA	1.81	0.41
1:B:187:ARG:NH1	2:B:521:HOH:O	2.54	0.41
1:B:301:LYS:C	1:B:301:LYS:CD	2.93	0.41
1:B:364:SER:HA	1:B:422:ARG:HD3	2.03	0.41
1:B:368:PHE:O	1:B:369:ASN:OD1	2.39	0.41
1:A:18:MSE:O	1:A:22:VAL:HG23	2.21	0.41
1:B:154:ASP:HA	1:B:245:ASN:HD21	1.85	0.41
1:B:379:LYS:HB2	1:B:386:VAL:CB	2.50	0.41
1:B:91:VAL:CG2	1:B:213:ALA:HB2	2.51	0.40
1:B:129:GLY:HA3	1:B:254:MSE:HB3	2.03	0.40
1:B:164:THR:HG23	1:B:214:LEU:HD21	2.01	0.40
1:B:368:PHE:CD1	1:B:369:ASN:N	2.90	0.40
1:B:421:LEU:HD13	1:B:421:LEU:C	2.46	0.40
1:A:262:ARG:NH1	1:A:332:PRO:N	2.69	0.40
1:B:175:GLU:HB2	2:B:473:HOH:O	2.20	0.40
1:B:205:ILE:N	1:B:205:ILE:HD12	2.36	0.40
1:A:31:VAL:HG21	1:A:106:VAL:O	2.21	0.40
1:B:152:MSE:CE	2:B:519:HOH:O	2.69	0.40
1:B:172:GLY:C	1:B:174:GLY:H	2.29	0.40
1:B:240:PHE:CD1	1:B:240:PHE:N	2.89	0.40
1:B:259:GLN:NE2	1:B:358:SER:O	2.54	0.40
1:B:272:LEU:CD1	1:B:287:GLY:H	2.34	0.40
1:A:97:LYS:HD3	1:A:97:LYS:HA	1.77	0.40
1:A:119:ASP:OD1	1:A:121:ARG:HG3	2.21	0.40
1:A:131:ASP:OD1	1:A:262:ARG:NH2	2.54	0.40
1:A:285:GLN:O	1:A:286:ARG:HB3	2.21	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	305/448 (68%)	259 (85%)	29 (10%)	17 (6%)	1	4
1	B	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	1	4
All	All	693/896 (77%)	577 (83%)	78 (11%)	38 (6%)	1	4

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	267	ILE
1	A	268	MSE
1	A	271	GLU
1	A	281	LYS
1	A	284	ALA
1	A	285	GLN
1	A	308	ASP
1	A	343	ARG
1	B	231	PRO
1	B	281	LYS
1	B	304	ILE
1	B	333	VAL
1	B	367	ILE
1	B	412	GLN
1	A	264	GLU
1	A	293	VAL
1	A	319	SER
1	B	50	PHE
1	B	173	LEU
1	B	186	GLY
1	B	197	ASN
1	B	211	GLY
1	B	345	GLY
1	B	366	SER
1	B	381	LYS
1	A	211	GLY
1	B	210	ALA
1	B	284	ALA
1	B	286	ARG
1	A	282	VAL
1	B	274	SER
1	B	389	ASN

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Mol	Chain	Res	Type
1	B	402	LYS
1	A	333	VAL
1	B	212	GLY
1	A	309	VAL
1	A	231	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	246/342 (72%)	201 (82%)	45 (18%)	2	6
1	B	319/342 (93%)	270 (85%)	49 (15%)	2	10
All	All	565/684 (83%)	471 (83%)	94 (17%)	2	8

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	18	MSE
1	A	19	LEU
1	A	36	THR
1	A	49	PHE
1	A	87	LEU
1	A	93	ILE
1	A	107	VAL
1	A	113	ILE
1	A	114	LYS
1	A	128	VAL
1	A	133	ARG
1	A	138	LEU
1	A	147	LEU
1	A	165	VAL
1	A	177	VAL
1	A	195	TYR
1	A	196	GLU

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Mol	Chain	Res	Type
1	A	197	ASN
1	A	198	PHE
1	A	200	GLN
1	A	205	ILE
1	A	214	LEU
1	A	215	VAL
1	A	217	LEU
1	A	224	ILE
1	A	231	PRO
1	A	232	ASP
1	A	235	ASN
1	A	236	ILE
1	A	246	MSE
1	A	251	THR
1	A	259	GLN
1	A	267	ILE
1	A	268	MSE
1	A	272	LEU
1	A	275	GLU
1	A	305	LYS
1	A	311	THR
1	A	321	PHE
1	A	325	ARG
1	A	328	VAL
1	A	337	LEU
1	A	343	ARG
1	A	350	VAL
1	B	12	MSE
1	B	27	VAL
1	B	30	ASN
1	B	42	MSE
1	B	44	ARG
1	B	50	PHE
1	B	82	GLN
1	B	87	LEU
1	B	93	ILE
1	B	96	ASP
1	B	113	ILE
1	B	128	VAL
1	B	136	ILE
1	B	138	LEU
1	B	147	LEU

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Mol	Chain	Res	Type
1	B	164	THR
1	B	169	ASN
1	B	173	LEU
1	B	177	VAL
1	B	185	LEU
1	B	187	ARG
1	B	196	GLU
1	B	200	GLN
1	B	205	ILE
1	B	214	LEU
1	B	215	VAL
1	B	217	LEU
1	B	231	PRO
1	B	235	ASN
1	B	236	ILE
1	B	251	THR
1	B	268	MSE
1	B	281	LYS
1	B	286	ARG
1	B	292	GLN
1	B	301	LYS
1	B	304	ILE
1	B	313	LEU
1	B	316	LYS
1	B	324	LEU
1	B	339	LEU
1	B	348	VAL
1	B	351	ASN
1	B	352	LEU
1	B	354	LEU
1	B	363	ASP
1	B	381	LYS
1	B	386	VAL
1	B	413	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	48	GLN
1	A	80	GLN
1	A	104	ASN

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Mol	Chain	Res	Type
1	A	116	GLN
1	A	140	GLN
1	A	142	GLN
1	A	169	ASN
1	A	197	ASN
1	A	225	ASN
1	A	235	ASN
1	A	245	ASN
1	A	327	GLN
1	A	347	GLN
1	B	48	GLN
1	B	80	GLN
1	B	104	ASN
1	B	116	GLN
1	B	140	GLN
1	B	143	ASN
1	B	146	ASN
1	B	169	ASN
1	B	197	ASN
1	B	245	ASN
1	B	292	GLN
1	B	296	ASN
1	B	327	GLN
1	B	347	GLN
1	B	351	ASN
1	B	355	GLN
1	B	360	ASN
1	B	378	ASN
1	B	383	GLN
1	B	388	ASN
1	B	411	ASN
1	B	413	GLN
1	B	437	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	299/448 (66%)	0.29	28 (9%) 14 10	35, 68, 175, 186	0
1	B	383/448 (85%)	0.37	32 (8%) 17 12	37, 102, 163, 169	0
All	All	682/896 (76%)	0.34	60 (8%) 15 11	35, 83, 167, 186	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	272	LEU	5.4
1	A	266	GLY	5.1
1	B	230	ALA	4.4
1	A	233	GLY	4.4
1	B	232	ASP	4.2
1	A	276	LEU	4.2
1	A	339	LEU	4.1
1	B	233	GLY	3.8
1	A	350	VAL	3.7
1	B	51	GLY	3.7
1	A	274	SER	3.5
1	B	323	ALA	3.4
1	B	236	ILE	3.3
1	B	390	VAL	3.3
1	A	277	ALA	3.2
1	A	337	LEU	3.2
1	B	403	LYS	3.0
1	B	443	ILE	3.0
1	A	188	SER	3.0
1	A	273	ASN	2.9
1	B	50	PHE	2.9
1	A	281	LYS	2.9
1	A	348	VAL	2.8
1	B	385	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	265	LEU	2.8
1	B	360	ASN	2.8
1	A	283	ASP	2.8
1	B	337	LEU	2.7
1	B	434	LEU	2.6
1	A	290	VAL	2.6
1	A	282	VAL	2.6
1	B	446	LEU	2.5
1	B	369	ASN	2.5
1	B	49	PHE	2.5
1	B	330	THR	2.5
1	B	267	ILE	2.4
1	B	407	ILE	2.4
1	B	393	GLY	2.4
1	A	189	GLY	2.4
1	A	270	THR	2.4
1	B	304	ILE	2.4
1	A	278	LYS	2.3
1	A	322	ALA	2.3
1	A	294	LEU	2.3
1	A	352	LEU	2.3
1	B	231	PRO	2.3
1	B	408	ILE	2.2
1	A	328	VAL	2.2
1	B	282	VAL	2.2
1	B	410	ALA	2.2
1	A	49	PHE	2.2
1	A	324	LEU	2.2
1	B	358	SER	2.2
1	B	79	GLY	2.2
1	B	340	GLY	2.2
1	B	439	GLY	2.2
1	A	232	ASP	2.1
1	B	338	THR	2.1
1	B	425	LEU	2.0
1	A	236	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.