



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:25 am GMT

PDB ID : 1KY9
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

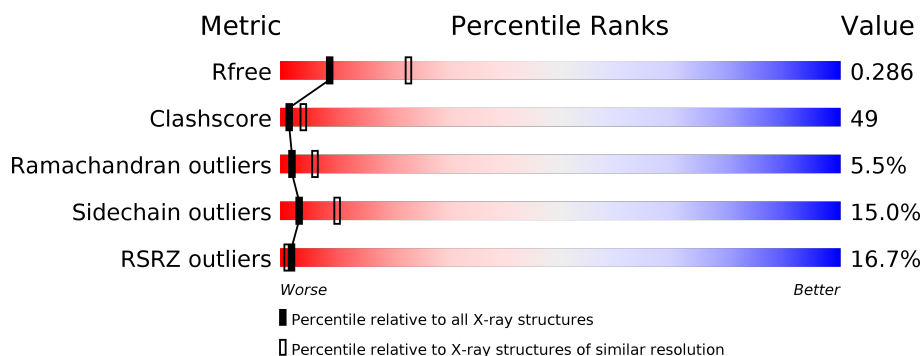
1 Overall quality at a glance

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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	448	

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	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	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 19.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 99.6 (19.93-2.80)	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	1273 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 83.2	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	0.61	0/2295	0.88	7/3078 (0.2%)
1	B	0.56	0/2932	0.90	4/3934 (0.1%)
All	All	0.58	0/5227	0.89	11/7012 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	ALA	C-N-CD	-20.86	74.72	120.60
1	B	230	ALA	C-N-CA	13.68	179.44	122.00
1	A	230	ALA	C-N-CD	-9.74	99.18	120.60
1	A	230	ALA	C-N-CA	7.04	151.57	122.00
1	B	87	LEU	CA-CB-CG	6.67	130.65	115.30
1	A	231	PRO	N-CA-C	5.86	127.33	112.10
1	A	268	MSE	N-CA-C	-5.39	96.44	111.00
1	A	233	GLY	N-CA-C	-5.30	99.86	113.10
1	B	250	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	268	MSE	N-CA-CB	5.21	119.97	110.60
1	A	196	GLU	N-CA-C	-5.12	97.17	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	225	0
1	B	2918	0	3008	290	0
2	A	77	0	0	18	0
2	B	89	0	0	15	0
All	All	5366	0	5348	515	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 49.

All (515) 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:CG	1:A:265:LEU:O	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:197:ASN:H	1:A:197:ASN:ND2	1.78	0.82
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
1:B:236:ILE:HG22	2:B:457:HOH:O	1.84	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: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:A:205:ILE:H	1:A:205:ILE:HD12	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: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:HE2	1:A:246:MSE:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:HH12	1:A:346:LYS:HZ2	1.37	0.72
1:A:42:MSE:HB3	1:A:43:PRO:HA	1.71	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: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:A:266:GLY:C	1:A:267:ILE:HG13	2.11	0.71
1:B:349:ASN:O	1:B:350:VAL:HG13	1.91	0.71
1:B:169:ASN:C	1:B:169:ASN:HD22	1.94	0.71
1:B:286:ARG:O	1:B:286:ARG:HD2	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:B:41:ARG:C	1:B:42:MSE:HE3	2.13	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:355:GLN:HG2	1:B:357:SER:H	1.57	0.69
1:B:93:ILE:HG13	1:B:152:MSE:CE	2.20	0.69
1:A:104:ASN:HD22	1:A:130:LYS:HB2	1.57	0.69
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:O	1:B:415:VAL:HG12	1.94	0.67
1:A:87:LEU:HD23	1:A:87:LEU:C	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:O	1:B:330:THR:HG22	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:A:282:VAL:O	1:A:282:VAL:HG12	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:393:GLY:C	1:B:395:PRO:HD3	2.22	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:HA	1:A:175:GLU:OE2	2.02	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:B:41:ARG:HH11	1:B:41:ARG:HG3	1.65	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:A:169:ASN:HD22	1:A:169:ASN:C	2.04	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:HH11	1:B:438:ARG:HG3	1.68	0.58
1:A:311:THR:CA	1:A:318:ILE:HB	2.34	0.58
1:A:321:PHE:N	1:A:321:PHE:CD2	2.63	0.58
1:B:265:LEU:HD21	1:B:339:LEU:HD21	1.85	0.58
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:O	1:B:113:ILE:HG13	2.04	0.57
1:B:185:LEU:O	1:B:187:ARG:N	2.38	0.57
1:B:381:LYS:HD3	1:B:381:LYS:N	2.20	0.56
1:A:154:ASP:HA	1:A:245:ASN:HD21	1.69	0.56
1:A:133:ARG:HD3	1:A:330:THR:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ARG:HG3	1:B:262:ARG:HH11	1.70	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:298:SER:HA	1:A:301:LYS:CB	2.28	0.56
1:A:91:VAL:CG2	1:A:213:ALA:HB2	2.35	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:415:VAL:CG1	1:B:421:LEU:HB2	2.36	0.55
1:A:114:LYS:HE2	1:A:124:ASP:OD1	2.07	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
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:HH11	1:B:286:ARG:HG2	1.72	0.55
1:B:330:THR:O	1:B:331:MSE:HG3	2.07	0.54
1:B:412:GLN:HG2	1:B:413:GLN:N	2.21	0.54
1:B:185:LEU:O	1:B:186:GLY:C	2.46	0.54
1:A:136:ILE:O	1:A:254:MSE:HE1	2.08	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: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:B:301:LYS:C	1:B:301:LYS:HD3	2.29	0.53
1:A:281:LYS:HD2	1:A:281:LYS:H	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:N	1:B:310:ILE:HD12	2.23	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:410:ALA:CB	1:B:415:VAL:HG23	2.37	0.52
1:B:82:GLN:HA	1:B:82:GLN:OE1	2.09	0.52
1:A:264:GLU:HG3	2:A:521:HOH:O	2.08	0.52
1:A:337:LEU:N	1:A:337:LEU:HD23	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:268:MSE:HE2	1:B:294:LEU:CD1	2.33	0.52
1:B:349:ASN:C	1:B:350:VAL:HG13	2.30	0.52
1:B:37:VAL:HG11	1:B:82:GLN:HE21	1.75	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:282:VAL:HG23	1:B:285:GLN:CD	2.30	0.52
1:B:386:VAL:CG2	1:B:406:VAL:HG22	2.40	0.52
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:HD22	1:B:445:LEU:N	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:160:VAL:O	1:B:182:VAL:O	2.26	0.51
1:B:44:ARG:NE	1:B:44:ARG:HA	2.24	0.51
1:B:310:ILE:H	1:B:310:ILE:HD12	1.76	0.51
1:B:204:ALA:C	1:B:205:ILE:HG13	2.31	0.51
1:B:411:ASN:HD21	1:B:428:LYS:NZ	2.08	0.51
1:B:11:GLN:CD	1:B:11:GLN:N	2.64	0.51
1:B:236:ILE:HG12	1:B:236:ILE:O	2.11	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:104:ASN:O	1:B:108:ASP:HB2	2.11	0.51
1:B:23:MSE:HE2	2:B:473:HOH:O	2.10	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:169:ASN:C	1:B:169:ASN:ND2	2.64	0.50
1:B:151:LYS:HD3	1:B:220:GLU:OE2	2.12	0.50
1:A:281:LYS:CD	1:A:281:LYS:H	2.25	0.50
1:B:127:MSE:HE1	1:B:129:GLY:C	2.31	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:B:427:SER:C	1:B:429:PRO:HD3	2.31	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:318:ILE:HG13	1:A:324:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:MSE:HE1	2:A:505:HOH:O	2.11	0.49
1:B:405:ASP:CA	1:B:438:ARG:HB3	2.41	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:B:126:LYS:NZ	2:B:518:HOH:O	2.45	0.49
1:B:41:ARG:HH11	1:B:41:ARG:CG	2.25	0.49
1:B:416:LYS:HD3	1:B:420:GLU:OE1	2.12	0.49
1:B:330:THR:C	1:B:331:MSE:HG3	2.32	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
1:B:267:ILE:HD12	1:B:267:ILE:C	2.33	0.49
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:CD	1:B:381:LYS:H	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:410:ALA:C	1:B:412:GLN:H	2.16	0.48
1:B:411:ASN:O	1:B:412:GLN:HB3	2.13	0.48
1:A:311:THR:HG23	1:A:318:ILE:O	2.13	0.48
1:A:133:ARG:HH11	1:A:330:THR:C	2.16	0.48
1:A:187:ARG:HH12	1:A:336:LYS:NZ	2.11	0.48
1:B:432:LEU:O	1:B:446:LEU:HA	2.13	0.48
1:B:82:GLN:HG2	2:B:472:HOH:O	2.13	0.48
1:A:85:MSE:HB3	2:A:479:HOH:O	2.14	0.48
1:A:187:ARG:NH1	1:A:336:LYS:HD2	2.29	0.48
1:A:184:ALA:HB3	1:A:200:GLN:HB2	1.96	0.48
1:A:310:ILE:HD12	1:A:310:ILE:N	2.29	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: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:A:266:GLY:C	1:A:267:ILE:CG1	2.78	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LYS:NZ	1:A:282:VAL:HG11	2.28	0.47
1:B:265:LEU:O	1:B:299:ALA:HB2	2.14	0.47
1:B:320:SER:O	1:B:321:PHE:C	2.52	0.47
1:B:382:ASP:OD2	1:B:416:LYS:HE2	2.14	0.47
1:B:42:MSE:HG3	1:B:43:PRO:HA	1.96	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:A:232:ASP:O	1:A:233:GLY:C	2.53	0.47
1:A:293:VAL:O	1:A:293:VAL:HG22	2.14	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:B:424:VAL:C	1:B:426:ASP:H	2.18	0.47
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:248:LYS:O	1:B:251:THR:HG22	2.15	0.47
1:B:42:MSE:HE2	1:B:44:ARG:CG	2.43	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:267:ILE:HD12	1:B:268:MSE:C	2.34	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: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:87:LEU:HD23	1:B:87:LEU:C	2.35	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:312:SER:HA	1:B:318:ILE:HG12	1.97	0.46
1:B:37:VAL:HG11	1:B:82:GLN:NE2	2.31	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:A:36:THR:HG22	1:A:36:THR:O	2.15	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:410:ALA:C	1:B:412:GLN:N	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:205:ILE:HD12	2.25	0.45
1:B:99:TYR:CD2	1:B:140:GLN:HG3	2.51	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:133:ARG:NE	1:B:325:ARG:NH1	2.65	0.45
1:B:337:LEU:N	1:B:337:LEU:HD23	2.30	0.45
1:B:333:VAL:HG21	1:B:354:LEU:HD23	1.98	0.45
1:A:298:SER:O	1:A:302:ALA:CB	2.58	0.45
1:A:313:LEU:HD11	1:A:337:LEU:CD1	2.35	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:42:MSE:HE2	1:B:44:ARG:HD2	1.93	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: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:B:408:ILE:H	1:B:437:GLN:NE2	2.15	0.45
1:A:232:ASP:O	1:A:234:GLY:N	2.49	0.45
1:B:133:ARG:HG3	1:B:262:ARG:NH1	2.29	0.45
1:B:128:VAL:HG13	1:B:138:LEU:HB3	1.98	0.45
1:B:365:SER:C	1:B:367:ILE:N	2.70	0.45
1:A:169:ASN:C	1:A:169:ASN:ND2	2.69	0.45
1:A:262:ARG:HH11	1:A:331:MSE:C	2.20	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:135:ASP:O	1:B:135:ASP:CG	2.54	0.45
1:B:365:SER:CB	1:B:367:ILE:HG22	2.47	0.45
1:B:259:GLN:HE22	1:B:377:SER:HB2	1.82	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:142:GLN:O	1:A:143:ASN:HB2	2.18	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:365:SER:C	1:B:367:ILE:H	2.21	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:168:GLY:C	1:B:170:PRO:HD3	2.39	0.44
1:B:286:ARG:HH11	1:B:286:ARG:CG	2.30	0.44
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:281:LYS:O	1:A:282:VAL:HB	2.17	0.43
1:A:133:ARG:NH1	1:A:330:THR:O	2.51	0.43
1:A:41:ARG:HD3	1:A:41:ARG:C	2.38	0.43
1:A:11:GLN:HB2	2:A:512:HOH:O	2.18	0.43
1:B:405:ASP:CG	1:B:438:ARG:HB3	2.39	0.43
1:A:264:GLU:CA	1:A:329:GLY:HA2	2.47	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:257:TYR:C	1:A:259:GLN:H	2.22	0.43
1:A:307:GLY:O	1:A:308:ASP:O	2.35	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:293:VAL:O	1:B:293:VAL:HG13	2.19	0.43
1:B:399:ILE:O	1:B:399:ILE:HG23	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:405:ASP:N	1:B:405:ASP:OD1	2.52	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:B:435:ASN:OD1	1:B:435:ASN:N	2.52	0.42
1:B:434:LEU:O	1:B:436:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG2	1:A:343:ARG:HH11	1.84	0.42
1:B:384:GLY:HA3	1:B:408:ILE:CD1	2.45	0.42
1:B:42:MSE:HA	1:B:43:PRO:O	2.18	0.42
1:B:410:ALA:HB3	1:B:413:GLN:HB2	2.02	0.42
1:A:11:GLN:NE2	1:A:11:GLN:N	2.68	0.42
1:A:270:THR:O	1:A:271:GLU:O	2.38	0.42
1:A:278:LYS:HZ2	1:A:282:VAL:HG11	1.85	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: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: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: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:B:41:ARG:NH1	1:B:41:ARG:CG	2.84	0.41
1:A:185:LEU:CD1	1:A:188:SER:HB2	2.50	0.41
1:A:29:ILE:CG2	1:A:113:ILE:HD13	2.47	0.41
1:A:19:LEU:HA	1:A:19:LEU:HD12	1.96	0.41
1:A:280:MSE:HB3	1:A:281:LYS:H	1.60	0.41
1:B:169:ASN:O	1:B:169:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:229:LEU:HA	1:B:229:LEU:HD23	1.80	0.41
1:B:365:SER:HB3	1:B:367:ILE:HG22	2.03	0.41
1:A:11:GLN:CD	1:A:11:GLN:N	2.73	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:B:187:ARG:NH1	2:B:521:HOH:O	2.54	0.41
1:A:154:ASP:OD2	1:A:154:ASP:C	2.57	0.41
1:A:228:ILE:HG13	1:A:229:LEU:CD2	2.51	0.41
1:B:185:LEU:HA	1:B:185:LEU:HD12	1.81	0.41
1:B:368:PHE:O	1:B:369:ASN:OD1	2.39	0.41
1:B:364:SER:HA	1:B:422:ARG:HD3	2.03	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:164:THR:HG23	1:B:214:LEU:HD21	2.01	0.40
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:368:PHE:CD1	1:B:369:ASN:N	2.90	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:HD12	1:B:205:ILE:N	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:240:PHE:N	1:B:240:PHE:CD1	2.89	0.40
1:B:272:LEU:CD1	1:B:287:GLY:H	2.34	0.40
1:B:259:GLN:NE2	1:B:358:SER:O	2.54	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
1:A:97:LYS:HA	1:A:97:LYS:HD3	1.77	0.40
1:B:108:ASP:CG	1:B:130:LYS:NZ	2.75	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%)	2	6
1	B	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	6
All	All	693/896 (77%)	577 (83%)	78 (11%)	38 (6%)	2	6

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

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Mol	Chain	Res	Type
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
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%)	207 (84%)	39 (16%)	3	9
1	B	319/342 (93%)	273 (86%)	46 (14%)	4	11
All	All	565/684 (83%)	480 (85%)	85 (15%)	3	10

All (85) 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	41	ARG
1	A	49	PHE
1	A	87	LEU
1	A	93	ILE
1	A	107	VAL
1	A	113	ILE

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Mol	Chain	Res	Type
1	A	114	LYS
1	A	133	ARG
1	A	138	LEU
1	A	147	LEU
1	A	165	VAL
1	A	169	ASN
1	A	177	VAL
1	A	195	TYR
1	A	196	GLU
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	232	ASP
1	A	236	ILE
1	A	251	THR
1	A	259	GLN
1	A	267	ILE
1	A	268	MSE
1	A	272	LEU
1	A	280	MSE
1	A	305	LYS
1	A	321	PHE
1	A	325	ARG
1	A	337	LEU
1	A	343	ARG
1	B	12	MSE
1	B	18	MSE
1	B	42	MSE
1	B	44	ARG
1	B	49	PHE
1	B	50	PHE
1	B	80	GLN
1	B	87	LEU
1	B	93	ILE
1	B	96	ASP
1	B	113	ILE
1	B	128	VAL
1	B	138	LEU

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Mol	Chain	Res	Type
1	B	147	LEU
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	205	ILE
1	B	214	LEU
1	B	215	VAL
1	B	217	LEU
1	B	231	PRO
1	B	235	ASN
1	B	251	THR
1	B	261	LYS
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	351	ASN
1	B	352	LEU
1	B	354	LEU
1	B	363	ASP
1	B	381	LYS
1	B	405	ASP
1	B	413	GLN
1	B	435	ASN
1	B	437	GLN

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

Mol	Chain	Res	Type
1	A	11	GLN
1	A	80	GLN
1	A	104	ASN
1	A	140	GLN
1	A	142	GLN

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Mol	Chain	Res	Type
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	146	ASN
1	B	169	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

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.







5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/448 (66%)	0.74	54 (18%)  	35, 68, 175, 186	0
1	B	383/448 (85%)	0.65	60 (15%)  	37, 102, 163, 169	0
All	All	682/896 (76%)	0.69	114 (16%)  	35, 83, 167, 186	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	439	GLY	10.9
1	A	345	GLY	8.3
1	A	274	SER	8.1
1	A	271	GLU	7.9
1	A	276	LEU	7.8
1	B	232	ASP	7.5
1	B	392	THR	7.2
1	A	348	VAL	6.9
1	A	266	GLY	6.9
1	A	287	GLY	6.8
1	A	277	ALA	6.7
1	B	273	ASN	6.6
1	A	292	GLN	6.4
1	B	403	LYS	6.3
1	A	267	ILE	6.2
1	A	349	ASN	6.2
1	B	323	ALA	6.1
1	B	438	ARG	5.9
1	B	393	GLY	5.8
1	B	443	ILE	5.6
1	A	275	GLU	5.6
1	A	195	TYR	5.6
1	A	50	PHE	5.6
1	A	281	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	272	LEU	5.4
1	A	344	ASP	5.3
1	B	431	VAL	5.0
1	B	296	ASN	5.0
1	B	427	SER	4.9
1	A	273	ASN	4.9
1	B	285	GLN	4.9
1	B	391	LYS	4.8
1	A	188	SER	4.8
1	A	286	ARG	4.8
1	A	288	ALA	4.7
1	B	233	GLY	4.6
1	A	189	GLY	4.6
1	B	446	LEU	4.5
1	A	282	VAL	4.4
1	B	394	THR	4.3
1	A	330	THR	4.3
1	B	231	PRO	4.2
1	A	293	VAL	4.1
1	A	323	ALA	4.1
1	B	230	ALA	4.1
1	B	288	ALA	4.1
1	A	347	GLN	4.0
1	B	11	GLN	4.0
1	B	286	ARG	3.9
1	B	444	TYR	3.9
1	B	51	GLY	3.9
1	A	283	ASP	3.8
1	A	291	SER	3.7
1	A	315	GLY	3.7
1	B	408	ILE	3.6
1	B	44	ARG	3.5
1	B	402	LYS	3.4
1	A	336	LYS	3.3
1	B	383	GLN	3.3
1	B	338	THR	3.3
1	B	322	ALA	3.3
1	A	265	LEU	3.3
1	B	275	GLU	3.2
1	B	290	VAL	3.2
1	B	196	GLU	3.1
1	A	350	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	271	GLU	3.1
1	B	440	ASP	3.1
1	A	290	VAL	3.0
1	B	274	SER	3.0
1	B	345	GLY	3.0
1	A	231	PRO	3.0
1	A	294	LEU	3.0
1	B	426	ASP	3.0
1	A	317	PRO	2.9
1	B	320	SER	2.9
1	A	335	SER	2.8
1	A	321	PHE	2.8
1	B	343	ARG	2.8
1	B	356	GLN	2.8
1	A	329	GLY	2.7
1	B	278	LYS	2.7
1	A	51	GLY	2.7
1	B	289	PHE	2.7
1	A	339	LEU	2.7
1	B	413	GLN	2.7
1	B	442	THR	2.7
1	B	279	ALA	2.6
1	A	289	PHE	2.6
1	A	319	SER	2.6
1	B	380	GLY	2.5
1	A	343	ARG	2.5
1	A	305	LYS	2.4
1	A	316	LYS	2.4
1	A	38	ASN	2.4
1	B	43	PRO	2.4
1	B	346	LYS	2.4
1	A	264	GLU	2.3
1	B	49	PHE	2.3
1	B	50	PHE	2.3
1	B	381	LYS	2.2
1	A	49	PHE	2.2
1	B	385	VAL	2.2
1	B	308	ASP	2.2
1	A	232	ASP	2.2
1	B	270	THR	2.1
1	B	79	GLY	2.1
1	B	389	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	295	PRO	2.1
1	B	368	PHE	2.1
1	A	346	LYS	2.1
1	A	307	GLY	2.0
1	B	369	ASN	2.0
1	B	418	ILE	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 carbohydrates 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.