



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:37 am BST

PDB ID : 5K1A
Title : Crystal structure of the UAF1-USP12 complex in C2 space group
Authors : Li, H.; D'Andrea, A.D.; Zheng, N.
Deposited on : 2016-05-18
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

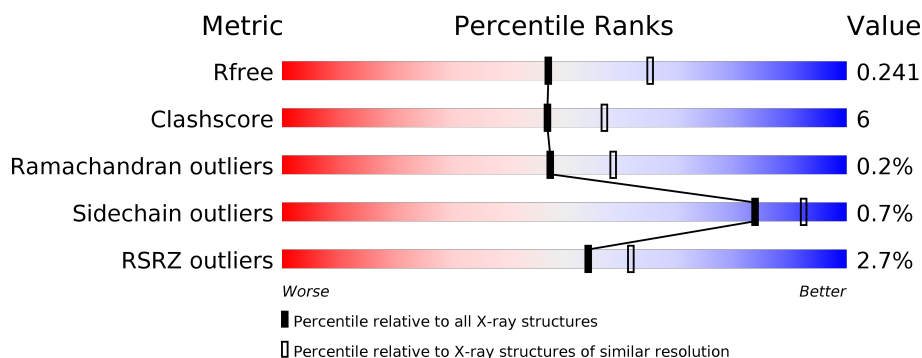
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	331	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>9%</div> <div>28%</div> </div> </div>
1	C	331	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>11%</div> <div>29%</div> </div> </div>
1	E	331	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>9%</div> <div>33%</div> </div> </div>
1	G	331	<div> <div>6%</div> <div> <div></div> <div>58%</div> <div>9%</div> <div>32%</div> </div> </div>
2	B	677	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>12%</div> </div> </div>
2	D	677	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>11%</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	677	<div><div></div><div>75%</div><div>13%</div><div>11%</div></div>
2	H	677	<div><div>2%</div><div></div><div>76%</div><div>11%</div><div>12%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27654 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 Ubiquitin carboxyl-terminal hydrolase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1886	1217	310	345	14			
1	C	236	Total	C	N	O	S	0	0	0
			1882	1215	308	345	14			
1	E	222	Total	C	N	O	S	0	0	0
			1747	1131	285	317	14			
1	G	224	Total	C	N	O	S	0	1	0
			1768	1136	290	328	14			

- Molecule 2 is a protein called WD repeat-containing protein 48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	595	Total	C	N	O	S	0	0	0
			4690	2973	818	872	27			
2	D	597	Total	C	N	O	S	0	0	0
			4701	2976	822	876	27			
2	F	600	Total	C	N	O	S	0	0	0
			4731	2994	825	885	27			
2	H	594	Total	C	N	O	S	0	0	0
			4664	2948	819	870	27			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		


- Molecule 4 is water.

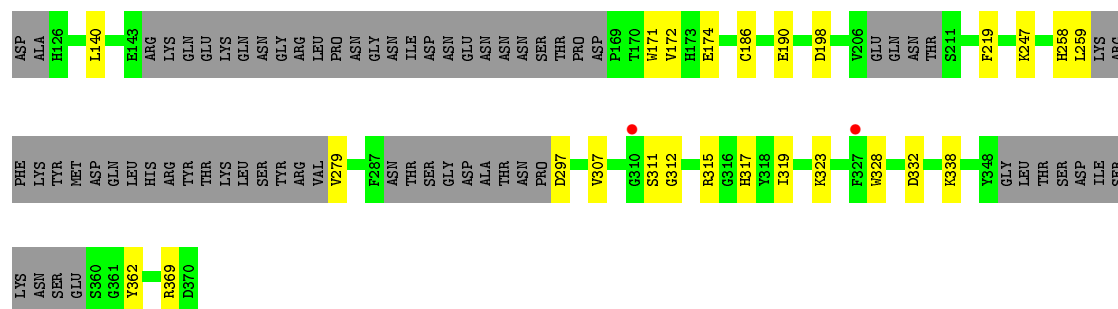
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total 81	O 81	0	0
4	B	286	Total 286	O 286	0	0
4	C	82	Total 82	O 82	0	0
4	D	334	Total 334	O 334	0	0
4	E	68	Total 68	O 68	0	0
4	F	364	Total 364	O 364	0	0
4	G	57	Total 57	O 57	0	0
4	H	309	Total 309	O 309	0	0

These plots are drawn for all protein, RNA and DNA 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.

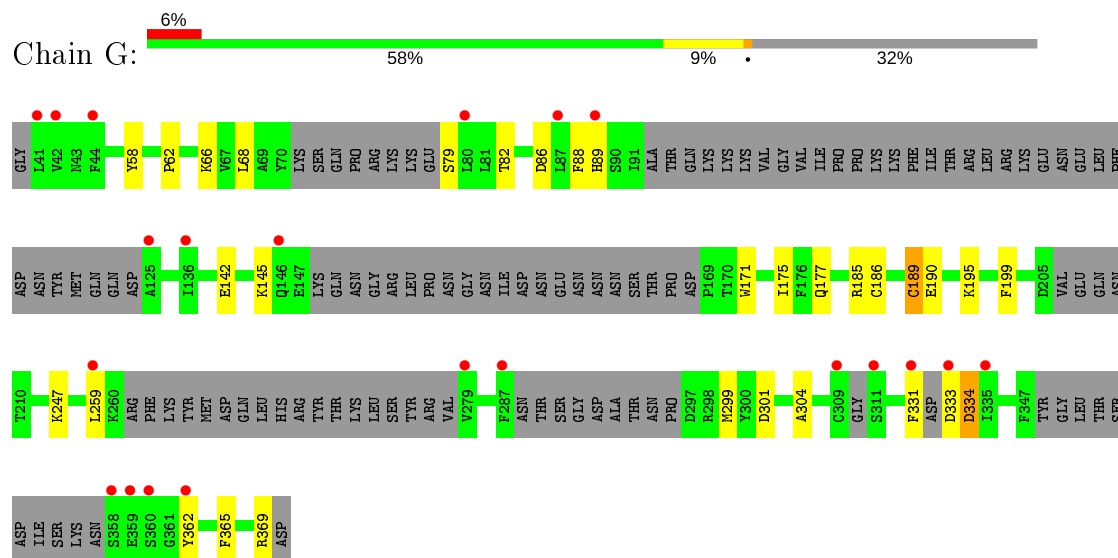
- Chain A:
-
- 4% 63% 9% 28%
- GLY L41 F63 V67 Y70 LYS SER GLN PRO ARG LYS LYS ASP ASN GLU L80 F88 H89 A92 T93 GLN LYS LYS LYS VAL GLY VAL ILE P102 P103 K104 K105 T108 R109 L110 ARG LYS GLU ASN ASN GLU LEU PHE ASP ASN MET TYR MET GLN GLN ASP A125 L132 I136
- L140 L147 LYS GLN ASN GLY ANG LEU PRO ASN GLY ILE ASP ASN GLU ASN ASN ASN SER THR PRO ASP P169 T170 M171 V172 H173 E174 D205 VAL GLU GLN ASN T210 L225 L226 Y228 V230 Y231 L259 L260 ARG PHE LYS TYR MET ASP GLN LEU HIS T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T195 T196 T197 T198 T199 T200 T201 T202 T203 T204 T205 T206 T207 T208 T209 T210 T211 T212 T213 T214 T215 T216 T217 T218 T219 T220 T221 T222 T223 T224 T225 T226 T227 T228 T229 T230 T231 T232 T233 T234 T235 T236 T237 T238 T239 T240 T241 T242 T243 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255 T256 T257 T258 T259 T260 T261 T262 T263 T264 T265 T266 T267 T268 T269 T270 T271 T272 T273 T274 T275 T276 T277 T278 T279 T280 T281 T282 T283 T284 T285 T286 T287 T288 T289 T290 T291 T292 T293 T294 T295 T296 T297 T298 T299 T300 T301 T302 T303 T304 T305 T306 T307 T308 T309 T310 T311 T312 T313 T314 T315 T316 T317 T318 T319 T320 T321 T322 T323 T324 T325 T326 T327 T328 T329 T330 T331 T332 T333 T334 T335 T336 T337 T338 T339 T340 T341 T342 T343 T344 T345 T346 T347 T348 T349 T350 T351 T352 T353 T354 T355 T356 T357 T358 T359 T360 T361 T362 T363 T364 T365 T366 T367 T368 T369 T370 T371 T372 T373 T374 T375 T376 T377 T378 T379 T380 T381 T382 T383 T384 T385 T386 T387 T388 T389 T390 T391 T392 T393 T394 T395 T396 T397 T398 T399 T400
- SER TYR ARG VAL V279 E283 F287 A288 THR SER GLY ASP ASP ALA THR ASN PRO D297 D301 G309 G310 S311 N314 R315 I319 F327 W328 L329 I335 V336 Q342 Y348 GLY LEU THR SER ASP ILE SER LYS N357 S358 E359 Y362 R369 ASP

- Chain C: 

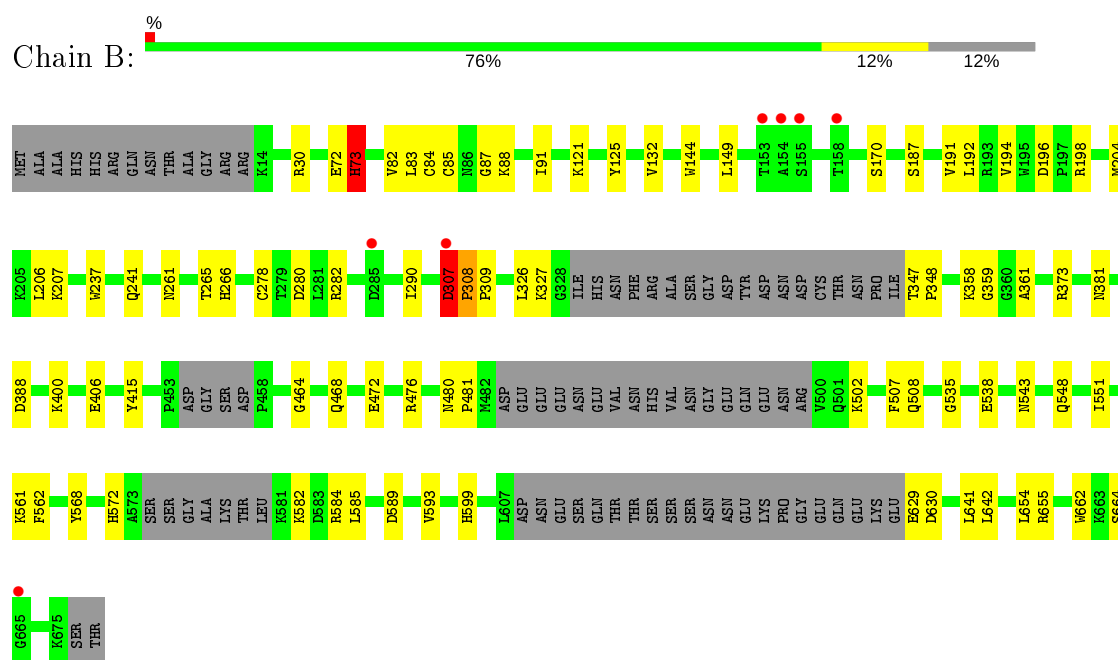
- Chain E: 



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 12

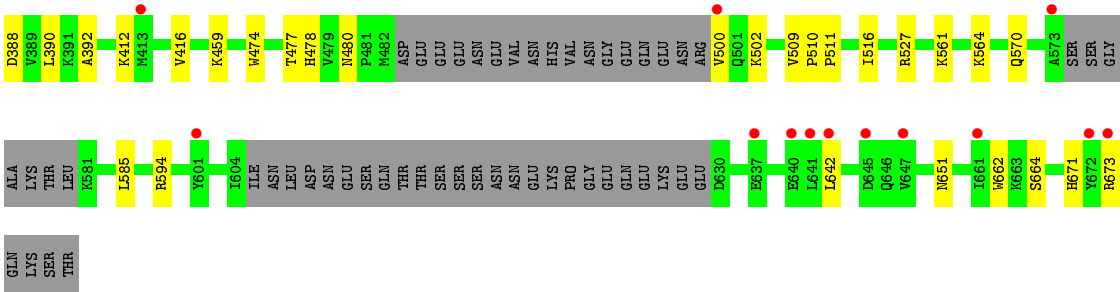


- Molecule 2: WD repeat-containing protein 48



- Molecule 2: WD repeat-containing protein 48





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	262.43 Å 103.30 Å 178.47 Å 90.00° 117.47° 90.00°	Depositor
Resolution (Å)	49.10 – 2.30 49.10 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.10-2.30) 92.4 (49.10-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.29 Å)	Xtriage
Refinement program	PHENIX dev_1760	Depositor
R, R_{free}	0.188 , 0.239 0.191 , 0.241	Depositor DCC
R_{free} test set	9518 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27654	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.41	0/1923	0.56	0/2601
1	C	0.42	0/1918	0.66	4/2591 (0.2%)
1	E	0.40	0/1782	0.59	0/2408
1	G	0.44	1/1803 (0.1%)	0.56	0/2435
2	B	0.50	2/4783 (0.0%)	0.63	4/6485 (0.1%)
2	D	0.49	1/4795 (0.0%)	0.64	4/6502 (0.1%)
2	F	0.51	1/4825 (0.0%)	0.64	3/6543 (0.0%)
2	H	0.50	1/4757 (0.0%)	0.63	4/6452 (0.1%)
All	All	0.48	6/26586 (0.0%)	0.63	19/36017 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	189	CYS	CB-SG	-8.79	1.67	1.82
2	D	84	CYS	CB-SG	-6.10	1.71	1.82
2	F	84	CYS	CB-SG	-6.05	1.72	1.82
2	H	84	CYS	CB-SG	-5.82	1.72	1.81
2	B	84	CYS	CB-SG	-5.16	1.73	1.81
2	B	309	PRO	N-CD	5.08	1.54	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	340	ASP	O-C-N	-13.95	100.37	122.70
2	F	73	HIS	N-CA-CB	10.34	129.21	110.60
2	B	73	HIS	N-CA-C	7.95	132.47	111.00
2	B	72	GLU	N-CA-C	7.00	129.90	111.00
1	C	340	ASP	CA-C-N	6.96	132.51	117.20
1	C	341	ALA	O-C-N	6.27	132.74	122.70
1	C	341	ALA	C-N-CA	-6.01	106.68	121.70
2	D	73	HIS	N-CA-C	6.00	127.19	111.00
2	D	307	ASP	CB-CG-OD1	5.92	123.63	118.30
2	D	307	ASP	C-N-CD	5.71	140.40	128.40
2	H	308	PRO	C-N-CD	5.71	140.39	128.40
2	F	307	ASP	C-N-CD	5.57	140.11	128.40
2	F	308	PRO	C-N-CD	5.51	139.98	128.40
2	B	307	ASP	C-N-CD	5.47	139.88	128.40
2	H	307	ASP	C-N-CD	5.37	139.68	128.40
2	D	308	PRO	C-N-CD	5.29	139.51	128.40
2	H	114	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	B	308	PRO	C-N-CD	5.22	139.37	128.40
2	H	307	ASP	N-CA-C	-5.12	97.18	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	GLN	Peptide
2	B	599	HIS	Sidechain

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	1886	0	1796	29	0
1	C	1882	0	1825	34	0
1	E	1747	0	1656	27	1
1	G	1768	0	1659	17	0
2	B	4690	0	4693	56	0
2	D	4701	0	4698	57	1
2	F	4731	0	4732	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	4664	0	4649	54	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	81	0	0	0	0
4	B	286	0	0	9	0
4	C	82	0	0	4	0
4	D	334	0	0	11	0
4	E	68	0	0	7	0
4	F	364	0	0	7	0
4	G	57	0	0	1	0
4	H	309	0	0	8	0
All	All	27654	0	25708	319	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (319) 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:C:284:LEU:HD13	1:C:366:TYR:CE1	1.81	1.16
1:A:314:ASN:HB3	1:A:319:ILE:CD1	1.84	1.07
1:A:314:ASN:HB3	1:A:319:ILE:HD11	1.45	0.95
1:C:284:LEU:CD1	1:C:366:TYR:CE1	2.49	0.95
2:F:30:ARG:NH1	2:F:361:ALA:O	2.05	0.89
2:H:474:TRP:O	2:H:477:THR:OG1	1.88	0.88
1:A:314:ASN:HB3	1:A:319:ILE:HD13	1.56	0.87
2:B:241:GLN:OE1	4:B:701:HOH:O	1.92	0.86
2:H:30:ARG:NH1	2:H:361:ALA:O	2.10	0.85
1:C:284:LEU:HD11	1:C:366:TYR:CZ	2.14	0.83
1:A:314:ASN:CB	1:A:319:ILE:CD1	2.58	0.81
2:D:159:VAL:HG12	2:D:160:THR:O	1.79	0.81
1:A:309:CYS:SG	1:A:348:TYR:CD1	2.73	0.81
2:H:307:ASP:HB3	2:H:308:PRO:HD3	1.63	0.80
2:F:327:LYS:H	2:F:349:LEU:HD21	1.46	0.80
2:H:478:HIS:HB3	2:H:500:VAL:HG23	1.63	0.79
2:F:536:GLU:OE1	4:F:701:HOH:O	2.02	0.78
2:D:83:LEU:HD22	2:D:87:GLY:HA2	1.68	0.76
1:E:307:VAL:O	1:E:319:ILE:HG12	1.86	0.76
1:C:284:LEU:CD1	1:C:366:TYR:CZ	2.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:592:GLN:OE1	2:D:594:ARG:NH1	2.20	0.75
2:H:594:ARG:NH2	2:H:651:ASN:OD1	2.21	0.73
1:A:309:CYS:SG	1:A:348:TYR:HD1	2.12	0.73
2:D:117:LYS:HD3	2:D:523:ARG:HH21	1.53	0.72
1:A:309:CYS:SG	1:A:348:TYR:CE1	2.83	0.72
1:E:198:ASP:O	4:E:501:HOH:O	2.08	0.72
1:G:86:ASP:HA	1:G:89:HIS:CE1	2.24	0.72
1:C:104:LYS:O	1:C:104:LYS:HG2	1.90	0.71
1:E:315:ARG:HH11	1:E:315:ARG:HG3	1.53	0.71
1:A:314:ASN:CB	1:A:319:ILE:HD13	2.20	0.70
1:C:101:ILE:N	4:C:503:HOH:O	2.23	0.70
2:H:170:SER:O	2:H:187:SER:HB2	1.92	0.70
1:E:297:ASP:O	4:E:502:HOH:O	2.09	0.70
2:B:388:ASP:OD2	4:B:702:HOH:O	2.09	0.69
2:B:373:ARG:NH1	2:B:388:ASP:OD1	2.25	0.69
2:B:406:GLU:OE1	4:B:703:HOH:O	2.10	0.69
1:A:314:ASN:O	1:A:319:ILE:HD11	1.93	0.68
2:D:307:ASP:HB3	2:D:308:PRO:CD	2.23	0.68
2:F:373:ARG:NH2	2:F:448:ALA:O	2.27	0.68
2:H:459:LYS:N	2:H:459:LYS:HD2	2.09	0.68
1:C:284:LEU:HD13	1:C:366:TYR:CD1	2.29	0.68
1:E:297:ASP:N	4:E:504:HOH:O	2.27	0.67
2:B:307:ASP:HB3	2:B:308:PRO:CD	2.24	0.67
2:F:673:ARG:NH2	4:F:708:HOH:O	2.26	0.67
1:E:258:HIS:ND1	4:E:506:HOH:O	2.28	0.67
2:D:159:VAL:HG12	2:D:160:THR:N	2.09	0.66
2:H:241:GLN:NE2	4:H:703:HOH:O	2.28	0.65
2:B:415:TYR:HD2	2:B:655:ARG:HG2	1.61	0.65
2:D:523:ARG:NH1	4:D:704:HOH:O	2.30	0.65
1:C:125:ALA:N	4:C:506:HOH:O	2.29	0.65
1:E:171:TRP:HA	1:E:174:GLU:HG2	1.79	0.64
1:A:314:ASN:CB	1:A:319:ILE:HD11	2.23	0.64
2:B:30:ARG:NH1	4:B:709:HOH:O	2.32	0.63
1:E:307:VAL:HG23	1:E:319:ILE:CG1	2.29	0.63
1:G:79:SER:O	1:G:82:THR:OG1	2.15	0.63
1:A:140:LEU:HD12	1:A:172:VAL:HG23	1.81	0.62
2:H:192:LEU:HB2	2:H:206:LEU:HB2	1.83	0.61
2:F:91:ILE:HD13	2:F:132:VAL:HG21	1.81	0.61
1:G:185:ARG:NH1	4:G:501:HOH:O	2.17	0.61
2:H:373:ARG:NH1	2:H:390:LEU:HB3	2.16	0.61
2:D:327:LYS:H	2:D:349:LEU:HD21	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:53:ILE:HG12	2:D:72:GLU:HG2	1.82	0.60
1:E:311:SER:O	4:E:503:HOH:O	2.16	0.60
2:D:13:ARG:N	4:D:708:HOH:O	2.33	0.60
2:D:153:THR:HG23	2:D:156:ASN:H	1.67	0.60
2:B:30:ARG:NH1	2:B:361:ALA:O	2.35	0.59
2:F:127:LYS:NZ	4:F:716:HOH:O	2.36	0.59
2:B:507:PHE:O	4:B:704:HOH:O	2.16	0.59
1:E:315:ARG:HG3	1:E:315:ARG:NH1	2.16	0.59
2:B:373:ARG:HD2	4:B:940:HOH:O	2.01	0.59
2:B:83:LEU:HD22	2:B:87:GLY:HA2	1.85	0.59
2:D:114:ARG:NH2	4:D:703:HOH:O	2.29	0.59
2:F:248:TYR:CD1	2:F:284:PRO:HB3	2.37	0.59
2:F:476:ARG:NH1	2:F:543:ASN:OD1	2.35	0.59
2:F:248:TYR:HD1	2:F:284:PRO:HB3	1.68	0.59
2:H:196:ASP:OD1	2:H:198:ARG:HD3	2.03	0.58
2:B:373:ARG:HG2	2:B:373:ARG:HH11	1.69	0.58
2:F:18:SER:HB2	2:F:516:ILE:HB	1.85	0.58
1:C:52:SER:HB3	1:C:306:VAL:HG13	1.84	0.58
2:F:82:VAL:HG11	2:F:125:TYR:HB2	1.85	0.58
1:C:301:ASP:OD2	1:C:369:ARG:HD3	2.04	0.58
1:G:62:PRO:HB2	1:G:175:ILE:HD12	1.86	0.58
2:H:91:ILE:HD13	2:H:132:VAL:HG21	1.85	0.57
2:F:283:ASN:HB3	2:F:286:ILE:HD13	1.86	0.57
1:C:104:LYS:HG3	4:C:572:HOH:O	2.04	0.57
2:D:170:SER:O	2:D:187:SER:HB2	2.03	0.57
2:B:170:SER:O	2:B:187:SER:HB2	2.04	0.57
2:D:478:HIS:CD2	2:D:502:LYS:HG3	2.40	0.57
2:B:307:ASP:HB3	2:B:308:PRO:HD3	1.87	0.57
1:E:307:VAL:HG23	1:E:319:ILE:HD11	1.85	0.57
2:F:662:TRP:CH2	2:F:664:SER:HB2	2.40	0.57
2:H:307:ASP:HB3	2:H:308:PRO:CD	2.32	0.57
2:D:91:ILE:HD13	2:D:132:VAL:HG21	1.87	0.56
2:B:280:ASP:OD1	2:B:282:ARG:HG3	2.05	0.56
1:A:259:LEU:HD12	1:A:362:TYR:CZ	2.40	0.56
2:B:476:ARG:NH1	2:B:543:ASN:OD1	2.38	0.56
2:B:191:VAL:HG22	2:B:207:LYS:HG3	1.87	0.56
2:F:500:VAL:N	4:F:721:HOH:O	2.38	0.56
1:G:304:ALA:HB3	1:G:365:PHE:HB2	1.88	0.56
2:D:159:VAL:CG1	2:D:160:THR:N	2.69	0.55
2:F:390:LEU:HD22	2:F:507:PHE:CZ	2.41	0.55
2:D:480:ASN:HB2	2:D:500:VAL:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:LYS:HG2	1:G:171:TRP:CD2	2.41	0.55
2:H:261:ASN:HD21	2:H:265:THR:CG2	2.18	0.55
2:H:373:ARG:HH11	2:H:373:ARG:HG3	1.72	0.55
1:A:171:TRP:HA	1:A:174:GLU:HG2	1.89	0.55
2:D:480:ASN:HB3	2:F:585:LEU:HD23	1.89	0.55
2:B:629:GLU:HG2	2:B:630:ASP:H	1.70	0.54
2:D:373:ARG:NH1	2:D:448:ALA:O	2.39	0.54
1:E:259:LEU:HD12	1:E:362:TYR:CZ	2.42	0.54
2:F:501:GLN:OE1	4:F:703:HOH:O	2.18	0.54
2:F:638:LYS:HE2	2:F:674:GLN:OE1	2.06	0.54
2:D:71:MET:HB3	2:D:102:TRP:CZ3	2.42	0.54
1:E:140:LEU:HD11	1:E:171:TRP:CE2	2.42	0.54
1:E:83:SER:O	1:E:86:THR:OG1	2.21	0.54
2:F:663:LYS:NZ	4:F:720:HOH:O	2.40	0.54
2:D:593:VAL:HG13	2:D:641:LEU:HD12	1.89	0.54
1:G:68:LEU:HD22	1:G:89:HIS:HB3	1.90	0.54
2:H:642:LEU:HD21	2:H:673:ARG:HH21	1.72	0.54
1:A:105:LYS:O	1:A:108:THR:OG1	2.24	0.53
2:B:265:THR:HG23	2:B:266:HIS:ND1	2.24	0.53
2:F:570:GLN:OE1	2:F:582:LYS:NZ	2.37	0.53
1:C:47:THR:OG1	2:F:160:THR:HG23	2.08	0.53
1:C:171:TRP:HA	1:C:174:GLU:HG2	1.91	0.53
1:C:341:ALA:O	1:C:342:GLN:C	2.47	0.52
2:D:30:ARG:NH1	2:D:361:ALA:O	2.42	0.52
2:F:272:ARG:HA	2:F:296:PRO:HB3	1.91	0.52
2:H:147:ASN:ND2	4:H:717:HOH:O	2.41	0.52
2:F:192:LEU:HB2	2:F:206:LEU:HB2	1.92	0.52
2:H:83:LEU:HD22	2:H:87:GLY:HA2	1.92	0.52
2:B:82:VAL:HG11	2:B:125:TYR:HB2	1.92	0.52
1:C:340:ASP:O	1:C:342:GLN:N	2.43	0.52
1:G:259:LEU:HD12	1:G:362:TYR:CE2	2.44	0.52
1:A:311:SER:HA	1:A:315:ARG:HD3	1.91	0.52
2:D:347:THR:N	4:D:721:HOH:O	2.41	0.52
2:D:20:VAL:HB	2:D:514:PRO:HG2	1.92	0.52
2:D:327:LYS:O	2:D:349:LEU:HD11	2.09	0.52
2:B:381:ASN:O	2:B:400:LYS:HE3	2.09	0.51
2:D:558:ASN:ND2	2:F:562:PHE:O	2.42	0.51
2:D:72:GLU:OE1	4:D:701:HOH:O	2.19	0.51
2:D:261:ASN:HD21	2:D:265:THR:CG2	2.23	0.51
2:F:472:GLU:HG2	2:F:502:LYS:HE2	1.92	0.51
2:H:306:ALA:O	2:H:307:ASP:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:374:HIS:NE2	4:H:709:HOH:O	2.34	0.51
2:D:584:ARG:NH1	4:D:723:HOH:O	2.42	0.51
2:B:280:ASP:OD1	2:B:282:ARG:CG	2.58	0.51
1:A:259:LEU:HD12	1:A:362:TYR:CE2	2.46	0.50
2:F:170:SER:O	2:F:187:SER:HB2	2.09	0.50
2:H:372:LYS:NZ	2:H:416:VAL:O	2.41	0.50
1:C:280:PHE:HD1	1:C:364:LEU:HD21	1.77	0.50
2:H:412:LYS:NZ	4:H:719:HOH:O	2.43	0.50
1:A:225:LEU:HD12	1:A:231:TYR:HB2	1.93	0.50
2:D:542:LEU:O	2:D:546:VAL:HG13	2.12	0.50
1:G:331:PHE:C	1:G:333:ASP:N	2.65	0.50
1:G:333:ASP:O	1:G:334:ASP:HB2	2.11	0.50
2:F:568:TYR:CD1	2:F:582:LYS:HE3	2.46	0.50
2:H:145:ASP:OD2	2:H:148:THR:HG23	2.12	0.50
2:D:114:ARG:NE	4:D:703:HOH:O	2.40	0.50
2:B:196:ASP:OD1	2:B:198:ARG:HD3	2.12	0.49
1:E:317:HIS:NE2	1:E:332:ASP:OD1	2.41	0.49
1:G:177:GLN:HA	1:G:199:PHE:O	2.12	0.49
2:H:18:SER:HB2	2:H:516:ILE:HB	1.94	0.49
2:B:585:LEU:HD23	2:H:480:ASN:HB3	1.94	0.49
1:G:171:TRP:O	1:G:175:ILE:HG12	2.12	0.49
2:B:480:ASN:HB3	2:H:585:LEU:HD23	1.95	0.49
1:A:41:LEU:HA	2:H:157:ASN:HB2	1.94	0.49
1:E:323:LYS:HD3	1:E:328:TRP:CE2	2.47	0.49
2:H:106:LYS:NZ	4:H:722:HOH:O	2.46	0.49
2:H:478:HIS:CD2	2:H:502:LYS:HG2	2.47	0.49
1:A:132:LEU:O	1:A:136:ILE:HG13	2.13	0.49
2:D:196:ASP:OD1	2:D:198:ARG:HD3	2.13	0.49
1:C:300:TYR:CZ	1:C:368:SER:HB3	2.48	0.48
1:E:307:VAL:HG23	1:E:319:ILE:CD1	2.43	0.48
2:H:306:ALA:O	2:H:307:ASP:O	2.31	0.48
1:C:52:SER:CB	1:C:306:VAL:HG13	2.44	0.48
1:G:299:MET:HG2	1:G:369:ARG:NH2	2.27	0.48
1:C:52:SER:HB3	1:C:306:VAL:CG1	2.43	0.48
2:F:460:LEU:HB3	2:F:465:LEU:HD11	1.96	0.48
2:B:662:TRP:CZ2	2:B:664:SER:HB2	2.49	0.48
2:H:14:LYS:HE3	2:H:14:LYS:HB2	1.56	0.48
2:B:548:GLN:HA	2:B:551:ILE:HD12	1.96	0.48
1:C:280:PHE:CD1	1:C:364:LEU:HD21	2.49	0.47
2:B:278:CYS:HB2	2:B:290:ILE:HD11	1.95	0.47
1:E:312:GLY:O	1:E:315:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:PHE:HE1	1:A:329:LEU:HD21	1.79	0.47
2:D:527:ARG:C	2:D:527:ARG:HD3	2.35	0.47
2:H:392:ALA:HB3	2:H:509:VAL:HG22	1.97	0.47
1:A:283:GLU:OE2	1:A:369:ARG:NH2	2.40	0.47
1:A:309:CYS:SG	1:A:348:TYR:HE1	2.34	0.47
2:D:570:GLN:O	2:D:671:HIS:HA	2.15	0.47
2:F:196:ASP:OD1	2:F:198:ARG:HD3	2.14	0.47
2:H:261:ASN:HD21	2:H:265:THR:HG22	1.78	0.47
2:H:570:GLN:O	2:H:671:HIS:HA	2.13	0.47
1:A:140:LEU:HD11	1:A:171:TRP:CE2	2.49	0.47
1:G:58:TYR:HA	1:G:88:PHE:CE2	2.50	0.47
2:F:597:MET:CE	2:F:636:GLU:HA	2.45	0.47
2:D:460:LEU:HD13	2:D:465:LEU:HD11	1.97	0.47
1:E:140:LEU:HD12	1:E:172:VAL:HG23	1.96	0.46
2:B:589:ASP:O	2:B:655:ARG:HB2	2.14	0.46
2:F:184:VAL:HG12	2:F:218:LEU:HD11	1.98	0.46
2:F:478:HIS:NE2	2:F:502:LYS:HG3	2.30	0.46
2:B:326:LEU:O	2:B:327:LYS:HD3	2.15	0.46
2:B:502:LYS:HB3	2:B:502:LYS:HE2	1.56	0.46
1:C:259:LEU:HD12	1:C:362:TYR:CE2	2.51	0.46
2:D:35:ALA:HA	2:D:299:LYS:HG2	1.96	0.46
2:D:54:ILE:HB	2:D:71:MET:HB2	1.98	0.46
1:E:279:VAL:HG12	4:E:543:HOH:O	2.15	0.46
2:H:163:SER:HB2	4:H:888:HOH:O	2.16	0.46
1:A:309:CYS:HG	1:A:348:TYR:HE1	1.47	0.46
2:D:192:LEU:HB2	2:D:206:LEU:HB2	1.98	0.46
2:F:121:LYS:HD2	2:F:137:LEU:HD21	1.98	0.46
2:B:472:GLU:OE2	2:B:508:GLN:HG2	2.15	0.45
2:D:303:ASP:O	2:D:310:PRO:HD2	2.15	0.45
2:D:233:THR:HG21	2:D:249:ARG:HH11	1.82	0.45
2:D:261:ASN:HD21	2:D:265:THR:HG22	1.81	0.45
1:C:286:LEU:O	1:C:287:PHE:HB2	2.16	0.45
2:D:307:ASP:HB3	2:D:308:PRO:HD3	1.95	0.45
2:D:601:TYR:HD1	2:D:639:ILE:HD11	1.82	0.45
2:B:261:ASN:HD21	2:B:265:THR:HG22	1.82	0.45
1:C:284:LEU:HD11	1:C:366:TYR:OH	2.16	0.45
2:B:192:LEU:HB2	2:B:206:LEU:HB2	1.98	0.45
2:D:381:ASN:O	2:D:400:LYS:HE3	2.16	0.45
2:F:260:VAL:O	2:F:304:ARG:NH2	2.50	0.45
2:H:326:LEU:O	2:H:327:LYS:HD2	2.17	0.45
2:D:153:THR:CG2	2:D:156:ASN:H	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:ASP:HB2	2:H:83:LEU:HD11	1.99	0.45
2:H:459:LYS:N	2:H:459:LYS:CD	2.79	0.45
2:F:261:ASN:HD21	2:F:265:THR:CG2	2.29	0.45
1:A:102:PRO:HA	1:A:103:PRO:HD3	1.87	0.45
1:A:309:CYS:HG	1:A:348:TYR:HD1	1.34	0.45
2:B:561:LYS:HG2	2:B:562:PHE:O	2.17	0.45
1:C:140:LEU:HD11	1:C:171:TRP:CZ2	2.52	0.44
2:F:54:ILE:HB	2:F:71:MET:HB2	1.99	0.44
1:C:170:THR:HB	1:C:173:HIS:ND1	2.31	0.44
2:H:510:PRO:HA	2:H:511:PRO:HD3	1.86	0.44
2:D:439:PHE:CE1	2:D:553:ILE:HG13	2.51	0.44
2:F:133:ALA:HB2	2:F:143:LEU:HD23	1.99	0.44
2:B:91:ILE:HD13	2:B:132:VAL:HG21	2.00	0.44
1:E:297:ASP:N	4:E:511:HOH:O	2.49	0.44
2:F:15:VAL:HG22	2:F:547:PRO:HG3	1.98	0.44
2:H:71:MET:HB3	2:H:102:TRP:CZ3	2.52	0.44
2:B:261:ASN:HD21	2:B:265:THR:CG2	2.30	0.44
2:D:30:ARG:NH2	4:D:740:HOH:O	2.51	0.44
1:E:307:VAL:HG23	1:E:319:ILE:HG13	1.98	0.44
2:H:561:LYS:HE3	2:H:561:LYS:HB3	1.71	0.44
1:C:300:TYR:CE2	1:C:368:SER:HB3	2.53	0.43
2:B:144:TRP:HB3	2:B:149:LEU:HD11	2.00	0.43
2:H:347:THR:CG2	2:H:348:PRO:HD2	2.48	0.43
2:B:194:VAL:HB	2:B:204:MET:HG2	2.01	0.43
1:E:67:PHE:O	1:E:71:VAL:HG13	2.19	0.43
2:H:373:ARG:NH1	2:H:388:ASP:OD1	2.51	0.43
2:B:593:VAL:HG13	2:B:641:LEU:HD12	2.00	0.43
2:D:552:ASP:HB3	4:D:702:HOH:O	2.19	0.43
1:E:186:CYS:O	1:E:190:GLU:HA	2.19	0.43
2:F:561:LYS:HG2	2:F:562:PHE:O	2.19	0.43
1:G:186:CYS:O	1:G:190:GLU:HA	2.18	0.43
2:H:248:TYR:CE2	2:H:284:PRO:HG3	2.54	0.43
1:A:301:ASP:OD2	1:A:369:ARG:HD3	2.19	0.43
1:C:185:ARG:NH1	4:C:509:HOH:O	2.38	0.43
1:C:305:VAL:HG12	1:C:307:VAL:CG2	2.49	0.43
1:E:219:PHE:CE1	1:E:247:LYS:HB2	2.54	0.43
2:B:206:LEU:HB3	2:B:237:TRP:CZ3	2.55	0.42
2:B:282:ARG:HG2	2:B:282:ARG:H	1.54	0.42
2:B:373:ARG:NH2	4:B:724:HOH:O	2.46	0.42
1:C:227:SER:O	1:C:230:LYS:HG3	2.19	0.42
2:B:535:GLY:HA3	2:B:538:GLU:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:CYS:O	2:B:88:LYS:HE3	2.19	0.42
2:H:88:LYS:HB3	2:H:88:LYS:HE2	1.88	0.42
2:H:378:LYS:NZ	4:H:727:HOH:O	2.49	0.42
1:C:143:GLU:HA	1:C:146:GLN:HE21	1.84	0.42
2:D:191:VAL:HG22	2:D:207:LYS:HG2	2.01	0.42
2:D:211:ASP:OD1	2:D:212:ASN:N	2.39	0.42
2:B:464:GLY:O	2:B:468:GLN:HG3	2.19	0.42
1:C:201:ASP:OD1	1:C:201:ASP:N	2.53	0.42
2:D:44:ARG:HA	2:D:57:TRP:O	2.20	0.42
1:E:311:SER:OG	1:E:312:GLY:N	2.52	0.42
2:B:568:TYR:CG	2:B:582:LYS:HE3	2.54	0.42
2:D:558:ASN:HD21	2:F:562:PHE:C	2.22	0.42
1:G:301:ASP:OD2	1:G:369:ARG:HD3	2.20	0.42
2:B:121:LYS:HE2	4:B:761:HOH:O	2.20	0.42
2:F:629:GLU:HG2	2:F:630:ASP:N	2.35	0.41
2:B:358:LYS:HD2	2:B:359:GLY:H	1.84	0.41
2:F:194:VAL:HB	2:F:204:MET:HG2	2.02	0.41
1:A:67:VAL:HG21	1:A:88:PHE:CD2	2.56	0.41
2:B:307:ASP:CB	2:B:308:PRO:CD	2.96	0.41
2:B:358:LYS:HD2	2:B:358:LYS:HA	1.76	0.41
2:D:27:LYS:NZ	4:D:716:HOH:O	2.54	0.41
2:H:307:ASP:CB	2:H:308:PRO:CD	2.98	0.41
2:B:347:THR:HA	2:B:348:PRO:HD3	1.75	0.41
2:F:261:ASN:HD21	2:F:265:THR:HG23	1.85	0.41
2:F:367:HIS:CD2	2:F:369:LEU:HD13	2.55	0.41
2:H:662:TRP:CZ2	2:H:664:SER:HB2	2.55	0.41
1:C:196:ASP:OD2	1:C:249:LYS:NZ	2.40	0.41
2:D:114:ARG:CZ	4:D:703:HOH:O	2.67	0.41
1:E:68:ARG:O	1:E:72:LEU:HG	2.20	0.41
2:F:527:ARG:NH2	4:F:725:HOH:O	2.40	0.41
2:F:83:LEU:HD22	2:F:87:GLY:HA2	2.03	0.41
2:D:19:TYR:CE1	2:D:466:LEU:HD21	2.56	0.41
2:D:527:ARG:HD3	2:D:528:LEU:N	2.36	0.41
1:G:142:GLU:HA	1:G:145:LYS:HB3	2.02	0.41
1:C:63:PHE:O	1:C:67:VAL:HG13	2.20	0.41
2:D:662:TRP:CZ2	2:D:664:SER:HB2	2.56	0.41
2:F:283:ASN:HA	2:F:284:PRO:HD2	1.84	0.41
2:H:82:VAL:HG11	2:H:125:TYR:HB2	2.03	0.41
2:F:510:PRO:HA	2:F:511:PRO:HD3	1.87	0.41
2:B:481:PRO:HB3	2:H:564:LYS:NZ	2.35	0.41
2:B:584:ARG:HD3	4:B:864:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:649:ASP:HA	2:F:650:PRO:HD2	1.89	0.40
2:F:640:GLU:HG3	2:F:675:LYS:HD3	2.04	0.40
2:B:654:LEU:HA	2:B:654:LEU:HD23	1.91	0.40
2:H:265:THR:OG1	2:H:282:ARG:HD2	2.21	0.40
2:H:39:ASP:OD1	4:H:701:HOH:O	2.22	0.40
1:C:79:SER:OG	1:C:80:LEU:N	2.55	0.40
2:F:287:ARG:HE	2:F:287:ARG:HB3	1.72	0.40
1:A:63:PHE:O	1:A:67:VAL:HG22	2.20	0.40
2:B:572:HIS:CD2	2:B:642:LEU:HD22	2.57	0.40
2:F:593:VAL:HG12	2:F:650:PRO:HA	2.02	0.40
2:H:184:VAL:HG12	2:H:218:LEU:HD11	2.03	0.40
2:H:347:THR:HG23	2:H:348:PRO:HD2	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:249:ARG:NH2	1:E:338:LYS:O[2_555]	2.11	0.09

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	221/331 (67%)	211 (96%)	10 (4%)	0	100	100
1	C	218/331 (66%)	212 (97%)	6 (3%)	0	100	100
1	E	204/331 (62%)	197 (97%)	7 (3%)	0	100	100
1	G	205/331 (62%)	198 (97%)	6 (3%)	1 (0%)	29	35
2	B	583/677 (86%)	558 (96%)	23 (4%)	2 (0%)	41	50
2	D	587/677 (87%)	570 (97%)	17 (3%)	0	100	100
2	F	590/677 (87%)	570 (97%)	19 (3%)	1 (0%)	47	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	584/677 (86%)	563 (96%)	20 (3%)	1 (0%)	47	58
All	All	3192/4032 (79%)	3079 (96%)	108 (3%)	5 (0%)	47	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	334	ASP
2	B	73	HIS
2	F	73	HIS
2	B	307	ASP
2	H	307	ASP

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	202/305 (66%)	202 (100%)	0	100	100
1	C	207/305 (68%)	207 (100%)	0	100	100
1	E	186/305 (61%)	185 (100%)	1 (0%)	88	95
1	G	188/305 (62%)	185 (98%)	3 (2%)	62	78
2	B	518/597 (87%)	517 (100%)	1 (0%)	93	97
2	D	519/597 (87%)	514 (99%)	5 (1%)	76	87
2	F	525/597 (88%)	522 (99%)	3 (1%)	86	94
2	H	514/597 (86%)	508 (99%)	6 (1%)	71	84
All	All	2859/3608 (79%)	2840 (99%)	19 (1%)	84	92

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	73	HIS
2	D	73	HIS
2	D	249	ARG

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Mol	Chain	Res	Type
2	D	527	ARG
2	D	561	LYS
2	D	594	ARG
1	E	369	ARG
2	F	73	HIS
2	F	169	ASP
2	F	282	ARG
1	G	189	CYS
1	G	195	LYS
1	G	247	LYS
2	H	73	HIS
2	H	84	CYS
2	H	169	ASP
2	H	282	ARG
2	H	307	ASP
2	H	527	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	146	GLN
2	D	283	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	239/331 (72%)	0.06	12 (5%)	28 35	25, 49, 80, 92	0
1	C	236/331 (71%)	0.17	10 (4%)	36 43	27, 53, 84, 95	0
1	E	222/331 (67%)	0.25	8 (3%)	42 49	25, 54, 84, 89	0
1	G	224/331 (67%)	0.49	21 (9%)	8 11	24, 55, 87, 97	0
2	B	595/677 (87%)	-0.15	7 (1%)	79 83	23, 35, 57, 90	0
2	D	597/677 (88%)	-0.15	11 (1%)	68 74	21, 33, 60, 81	0
2	F	600/677 (88%)	-0.26	3 (0%)	91 94	22, 31, 58, 73	0
2	H	594/677 (87%)	-0.11	16 (2%)	54 62	20, 32, 70, 87	0
All	All	3307/4032 (82%)	-0.05	88 (2%)	54 62	20, 37, 73, 97	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	44	PHE	5.4
2	H	500	VAL	5.1
1	G	358	SER	4.3
1	G	359	GLU	4.3
1	C	206	VAL	4.2
1	G	125	ALA	4.0
2	B	153	THR	4.0
1	G	331	PHE	3.7
2	B	154	ALA	3.7
1	C	146	GLN	3.6
2	H	286	ILE	3.5
1	G	279	VAL	3.5
1	E	103	PRO	3.5
1	C	280	PHE	3.5
1	C	65	GLU	3.5
1	C	169	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	285	ASP	3.4
2	D	159	VAL	3.3
1	G	360	SER	3.3
1	A	279	VAL	3.3
2	H	285	ASP	3.2
1	C	210	THR	3.2
1	G	333	ASP	3.2
2	H	641	LEU	3.1
1	G	89	HIS	3.0
2	B	158	THR	3.0
2	H	642	LEU	3.0
1	E	91	LEU	2.9
1	G	42	VAL	2.9
2	H	673	ARG	2.8
1	E	102	PRO	2.8
2	B	155	SER	2.7
2	D	639	ILE	2.7
2	D	665	GLY	2.7
1	C	360	SER	2.7
1	C	343	ALA	2.7
2	D	645	ASP	2.6
2	D	64	GLN	2.6
2	H	413	MET	2.6
2	H	645	ASP	2.6
1	A	358	SER	2.5
2	H	573	ALA	2.5
1	A	80	LEU	2.5
1	E	48	PHE	2.5
1	G	80	LEU	2.5
1	E	84	LEU	2.5
1	A	102	PRO	2.4
1	G	309	CYS	2.4
2	H	640	GLU	2.4
2	F	664	SER	2.4
1	G	87	LEU	2.4
2	H	601	TYR	2.4
2	H	661	ILE	2.4
1	G	259	LEU	2.4
1	A	336	VAL	2.4
2	B	307	ASP	2.3
2	D	286	ILE	2.3
1	G	362	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	287	ARG	2.3
2	D	581	LYS	2.3
1	E	327	PHE	2.3
2	D	634	LEU	2.3
1	A	327	PHE	2.3
1	A	89	HIS	2.3
1	A	335	ILE	2.3
2	D	307	ASP	2.3
1	A	92	ALA	2.3
2	D	72	GLU	2.3
1	C	339	ILE	2.3
2	F	286	ILE	2.3
1	G	41	LEU	2.2
1	A	359	GLU	2.2
1	G	287	PHE	2.2
1	G	146	GLN	2.2
1	A	210	THR	2.2
1	G	335	ILE	2.2
2	B	665	GLY	2.2
1	A	229	TYR	2.1
2	H	347	THR	2.1
1	C	142	GLU	2.1
2	H	647	VAL	2.1
1	E	106	PHE	2.1
2	H	672	TYR	2.1
1	G	136	ILE	2.0
1	E	310	GLY	2.0
2	H	637	GLU	2.0
2	D	158	THR	2.0
1	G	311	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	G	401	1/1	0.97	0.22	45,45,45,45	0
3	ZN	C	401	1/1	0.99	0.11	30,30,30,30	0
3	ZN	A	401	1/1	1.00	0.17	38,38,38,38	0
3	ZN	E	401	1/1	1.00	0.15	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.