



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 12, 2022 – 02:02 PM EST

PDB ID : 7S1T
Title : Structure of the human POT1-TPP1 complex
Authors : Aramburu, T.; Skordalakes, E.
Deposited on : 2021-09-02
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.25
buster-report : 1.1.7 (2018)
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) : 2.25

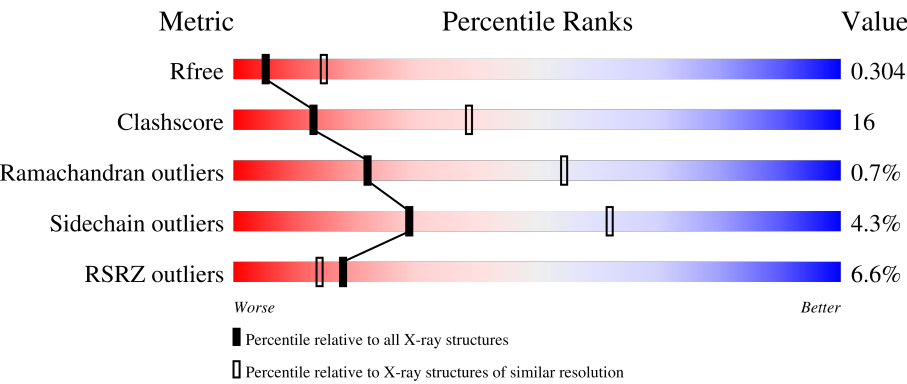
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	313	
1	D	313	
1	G	313	
1	J	313	
2	B	93	

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Mol	Chain	Length	Quality of chain
2	E	93	<div><div><div></div><div></div><div></div><div></div></div><div>3%48%29%•20%</div></div>
2	H	93	<div><div><div></div><div></div><div></div><div></div></div><div>6%46%30%•20%</div></div>
2	K	93	<div><div><div></div><div></div><div></div><div></div></div><div>2%59%19%•20%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11776 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 Protection of telomeres protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2393	1528	398	451	16			
1	D	302	Total	C	N	O	S	0	0	0
			2393	1528	398	451	16			
1	G	302	Total	C	N	O	S	0	0	0
			2393	1528	398	451	16			
1	J	302	Total	C	N	O	S	0	0	0
			2393	1528	398	451	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	SER	-	expression tag	UNP Q9NUX5
A	323	ASN	-	expression tag	UNP Q9NUX5
A	324	ILE	-	expression tag	UNP Q9NUX5
D	322	SER	-	expression tag	UNP Q9NUX5
D	323	ASN	-	expression tag	UNP Q9NUX5
D	324	ILE	-	expression tag	UNP Q9NUX5
G	322	SER	-	expression tag	UNP Q9NUX5
G	323	ASN	-	expression tag	UNP Q9NUX5
G	324	ILE	-	expression tag	UNP Q9NUX5
J	322	SER	-	expression tag	UNP Q9NUX5
J	323	ASN	-	expression tag	UNP Q9NUX5
J	324	ILE	-	expression tag	UNP Q9NUX5

- Molecule 2 is a protein called Adrenocortical dysplasia protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	74	Total	C	N	O	S	0	0	0
			550	338	91	114	7			
2	E	74	Total	C	N	O	S	0	0	0
			550	338	91	114	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	74	Total	C	N	O	S	0	0	0
			550	338	91	114	7			
2	K	74	Total	C	N	O	S	0	0	0
			550	338	91	114	7			

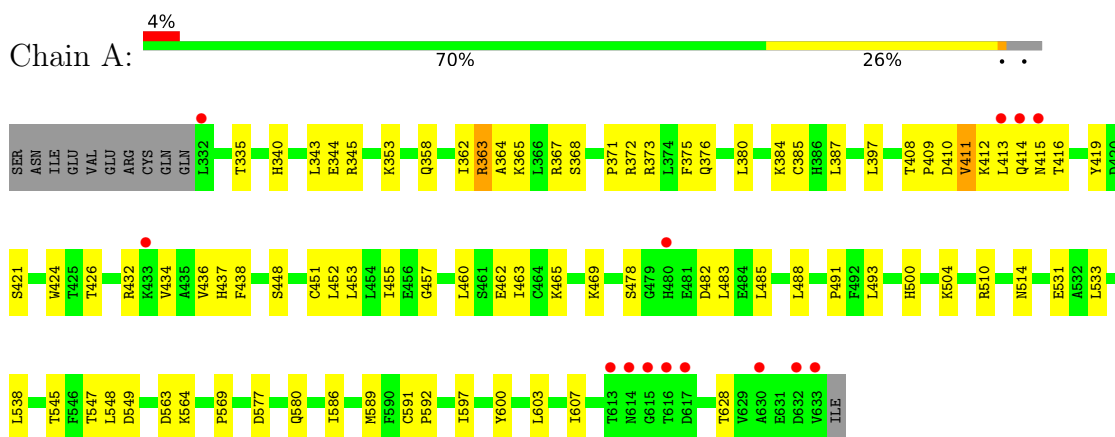
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		

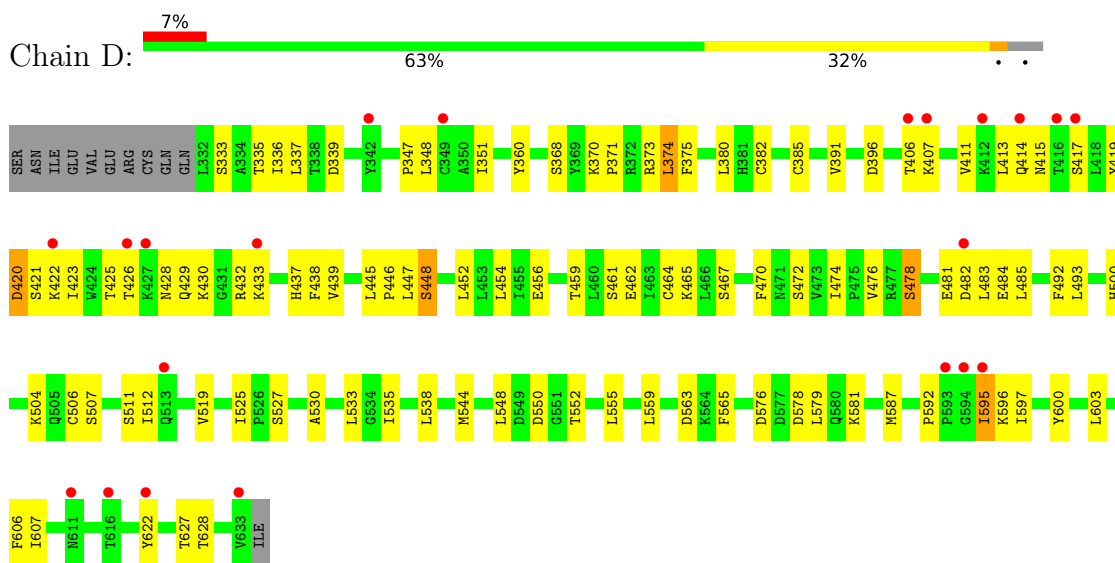
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protection of telomeres protein 1

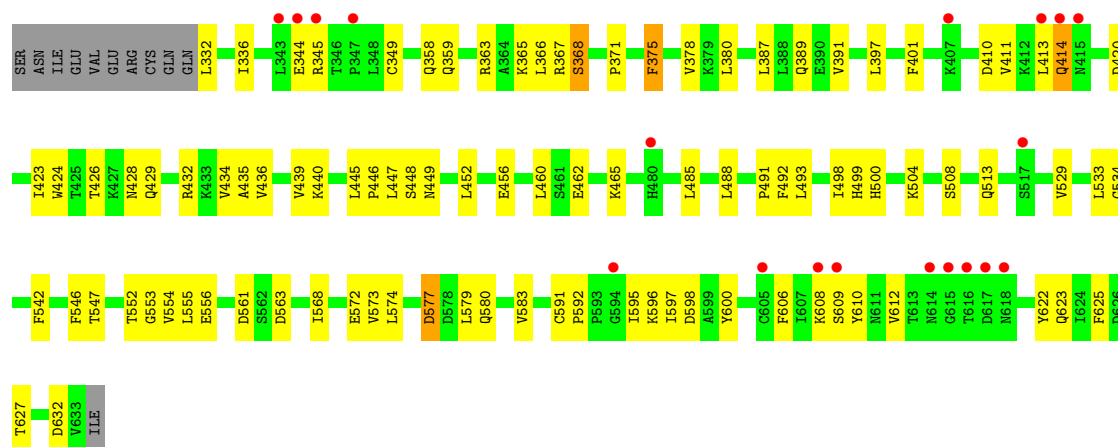


• Molecule 1: Protection of telomeres protein 1

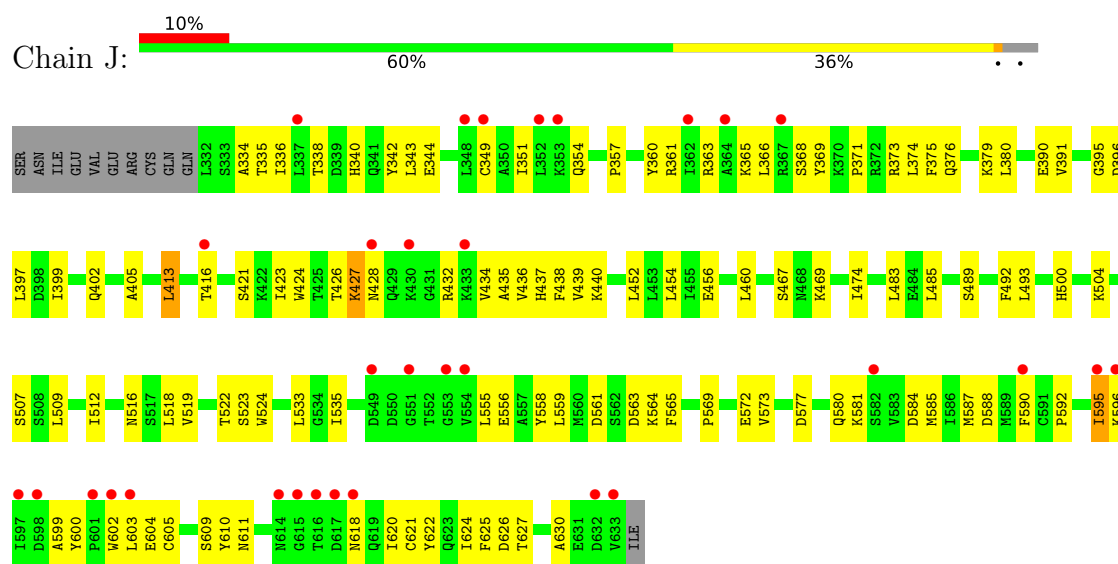


• Molecule 1: Protection of telomeres protein 1

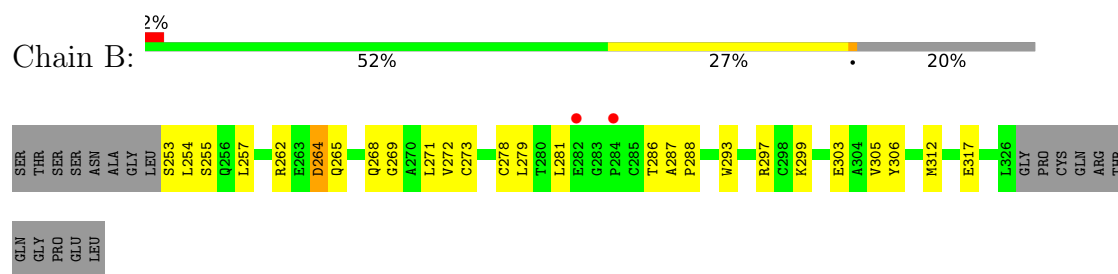




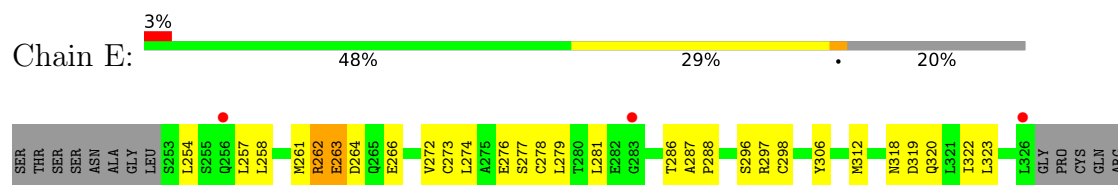
• Molecule 1: Protection of telomeres protein 1



• Molecule 2: Adrenocortical dysplasia protein homolog



• Molecule 2: Adrenocortical dysplasia protein homolog



THR
GLN
GLY
PRO
GLU
LEU

● Molecule 2: Adrenocortical dysplasia protein homolog



SER THR SER SER ASN ALA GLY LEU S253 L254 L257 L258 D259 E260 M261 R262 E263 D264 Q265 E266 H267 Q268 G269 A270 L271 V272 C273 E276 S277 C278 L279 T280 L281 E282 G283 P284 C285 T291 H292 W293 R297 Y306 P309 S310 S311 M312 E317 N318 L321 L326 GLY

PRO
CYS
GLN
ARG
THR
GLN
GLY
PRO
GLU
LEU

● Molecule 2: Adrenocortical dysplasia protein homolog



SER THR SER SER ASN ALA GLY LEU S253 Q256 L257 L258 D259 E260 M261 R262 E263 D264 L271 L274 L281 P284 C285 R297 C298 T301 V305 Y306 T307 V308 L313 I322 L326 GLY PRO CYS GLN ARG THR GLN GLY PRO GLU LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.88Å 70.98Å 103.79Å 76.76° 84.61° 70.55°	Depositor
Resolution (Å)	36.44 – 2.90 36.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.7 (36.44-2.90) 89.8 (36.44-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.250 , 0.307 0.248 , 0.304	Depositor DCC
R_{free} test set	1848 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.6	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	0.91	EDS
Total number of atoms	11776	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.09% 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](#)

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	0.28	0/2443	0.51	0/3314
1	D	0.28	0/2443	0.51	0/3314
1	G	0.31	0/2443	0.50	0/3314
1	J	0.30	0/2443	0.51	0/3314
2	B	0.49	0/558	0.59	0/760
2	E	0.31	0/558	0.58	0/760
2	H	0.45	0/558	0.59	0/760
2	K	0.25	0/558	0.44	0/760
All	All	0.31	0/12004	0.52	0/16296

There are no bond length outliers.

There are no bond angle outliers.

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	2393	0	2404	87	0
1	D	2393	0	2404	90	0
1	G	2393	0	2404	80	0
1	J	2393	0	2404	87	0
2	B	550	0	537	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	550	0	537	30	0
2	H	550	0	537	28	0
2	K	550	0	537	17	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
All	All	11776	0	11764	383	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 16.

All (383) 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:408:THR:CG2	1:A:409:PRO:HD2	1.61	1.31
1:G:359:GLN:OE1	1:G:608:LYS:HE2	1.48	1.09
1:J:375:PHE:HD1	2:K:297:ARG:HG2	1.17	1.05
1:J:375:PHE:CD1	2:K:297:ARG:HG2	1.91	1.05
1:A:408:THR:HG23	1:A:409:PRO:HD2	1.08	1.04
1:G:606:PHE:HZ	1:G:608:LYS:HE3	1.25	1.00
1:A:408:THR:CG2	1:A:409:PRO:CD	2.39	1.00
1:G:359:GLN:HB3	1:G:608:LYS:HG2	1.41	1.00
1:A:412:LYS:HD3	1:A:419:TYR:HE2	1.28	0.98
1:A:426:THR:HG22	2:B:281:LEU:HD23	1.51	0.92
1:A:426:THR:HG22	2:B:281:LEU:CD2	2.01	0.90
1:G:414:GLN:OE1	1:G:414:GLN:O	1.89	0.90
1:J:605:CYS:HB3	1:J:627:THR:HG21	1.54	0.89
1:A:408:THR:HG22	1:A:409:PRO:CD	2.03	0.87
1:G:606:PHE:CZ	1:G:608:LYS:HE3	2.11	0.86
1:G:359:GLN:CB	1:G:608:LYS:HG2	2.05	0.85
1:D:481:GLU:OE1	1:D:482:ASP:OD1	1.94	0.85
1:D:481:GLU:OE1	1:D:482:ASP:CG	2.15	0.84
1:A:413:LEU:C	1:A:415:ASN:H	1.79	0.84
1:A:410:ASP:HB2	1:A:478:SER:HB3	1.60	0.84
2:E:258:LEU:HA	2:E:261:MET:CE	2.08	0.84
1:D:485:LEU:HD11	1:D:533:LEU:HD13	1.60	0.82
1:G:359:GLN:OE1	1:G:608:LYS:CE	2.26	0.82
2:E:263:GLU:HA	2:E:266:GLU:HG3	1.62	0.81
1:G:465:LYS:HB3	2:H:278:CYS:HB3	1.63	0.81
1:J:595:ILE:HG22	1:J:596:LYS:H	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:LEU:HD21	1:D:512:ILE:HD11	1.61	0.80
1:G:432:ARG:NH2	2:H:285:CYS:SG	2.56	0.79
1:A:412:LYS:CE	1:A:416:THR:HG21	2.13	0.78
1:A:412:LYS:CE	1:A:416:THR:CG2	2.60	0.78
1:J:563:ASP:HB3	1:J:569:PRO:HA	1.65	0.78
1:A:412:LYS:HD2	1:A:416:THR:HG22	1.65	0.77
1:D:413:LEU:HD12	1:D:423:ILE:HD13	1.66	0.77
1:J:338:THR:HG21	1:J:564:LYS:HE3	1.67	0.77
1:A:412:LYS:HD3	1:A:419:TYR:CE2	2.19	0.75
1:D:426:THR:HB	1:D:429:GLN:HG3	1.69	0.75
1:D:476:VAL:HG12	1:D:485:LEU:HD23	1.69	0.74
1:A:412:LYS:CD	1:A:419:TYR:HE2	1.99	0.74
1:G:440:LYS:HG2	1:G:445:LEU:HG	1.71	0.73
1:J:375:PHE:CE1	2:K:297:ARG:HA	2.24	0.73
1:D:413:LEU:O	1:D:421:SER:HB2	1.89	0.72
2:K:256:GLN:HA	2:K:259:ASP:HB2	1.70	0.72
1:J:427:LYS:HD3	1:J:428:ASN:N	2.05	0.71
1:G:462:GLU:HG2	2:H:279:LEU:HA	1.71	0.70
1:J:375:PHE:CD1	2:K:297:ARG:CG	2.72	0.70
1:D:439:VAL:HG21	1:D:452:LEU:HD23	1.72	0.70
1:D:447:LEU:HD22	1:D:448:SER:H	1.57	0.70
1:J:602:TRP:O	1:J:603:LEU:HD23	1.91	0.70
1:J:569:PRO:HG2	1:J:572:GLU:HB2	1.72	0.70
1:D:413:LEU:HD23	1:D:413:LEU:H	1.55	0.70
1:A:376:GLN:OE1	2:B:305:VAL:HB	1.91	0.69
1:A:412:LYS:HE3	1:A:416:THR:HG21	1.74	0.69
1:J:454:LEU:HD23	1:J:474:ILE:HB	1.75	0.69
1:J:335:THR:HG23	1:J:603:LEU:HD13	1.75	0.69
2:E:258:LEU:HA	2:E:261:MET:HE2	1.74	0.68
1:A:410:ASP:CB	1:A:478:SER:HB3	2.23	0.68
2:E:320:GLN:HA	2:E:323:LEU:HB2	1.75	0.68
1:G:429:GLN:NE2	2:H:283:GLY:O	2.27	0.68
1:A:412:LYS:CD	1:A:419:TYR:CE2	2.77	0.67
1:D:472:SER:HB3	1:D:493:LEU:HD11	1.77	0.67
1:G:439:VAL:HG21	1:G:452:LEU:HD23	1.77	0.66
1:A:413:LEU:C	1:A:415:ASN:N	2.47	0.66
1:D:336:ILE:HD12	1:D:336:ILE:O	1.95	0.66
1:D:485:LEU:CD2	1:D:512:ILE:HD11	2.24	0.66
1:D:447:LEU:HG	2:H:321:LEU:HD13	1.77	0.66
1:A:367:ARG:NH2	1:A:549:ASP:OD2	2.28	0.65
1:D:420:ASP:HB2	1:D:445:LEU:HD21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:LYS:HB3	2:E:278:CYS:HB3	1.79	0.65
1:A:545:THR:HG1	2:B:306:TYR:HH	1.46	0.64
1:A:465:LYS:HG3	2:B:278:CYS:HB3	1.80	0.64
1:G:493:LEU:HD13	1:G:529:VAL:HG11	1.80	0.64
1:A:485:LEU:HD11	1:A:533:LEU:HD13	1.80	0.64
1:A:368:SER:HB3	1:A:547:THR:HB	1.79	0.63
1:J:585:MET:HA	1:J:588:ASP:HB2	1.79	0.63
1:A:421:SER:OG	1:A:437:HIS:ND1	2.26	0.63
1:J:595:ILE:HG21	1:J:599:ALA:HB3	1.80	0.63
1:G:332:LEU:HD23	1:G:332:LEU:O	1.98	0.63
1:G:563:ASP:OD1	1:G:563:ASP:N	2.28	0.63
1:G:485:LEU:HD21	1:G:533:LEU:HD13	1.80	0.63
1:D:429:GLN:HE22	1:D:432:ARG:HH21	1.45	0.62
1:G:606:PHE:HZ	1:G:608:LYS:CE	2.07	0.62
2:E:262:ARG:HG2	2:E:264:ASP:HB3	1.80	0.62
1:D:422:LYS:HZ2	2:E:272:VAL:HG21	1.64	0.62
1:D:607:ILE:HD12	1:D:622:TYR:HD2	1.63	0.62
1:J:396:ASP:HB3	2:E:298:CYS:HB3	1.81	0.62
1:A:412:LYS:HE3	1:A:416:THR:CG2	2.28	0.62
1:D:484:GLU:HG3	1:D:511:SER:HA	1.82	0.62
2:E:261:MET:HG2	2:E:266:GLU:HG2	1.80	0.61
1:J:380:LEU:HG	1:J:391:VAL:HG22	1.82	0.61
1:G:596:LYS:HG2	1:G:597:ILE:N	2.14	0.61
1:G:358:GLN:N	1:G:609:SER:OG	2.34	0.61
1:G:577:ASP:OD1	2:H:292:HIS:ND1	2.34	0.61
1:A:412:LYS:NZ	1:A:421:SER:CB	2.63	0.61
1:D:544:MET:HB2	1:D:559:LEU:HB3	1.82	0.61
1:A:412:LYS:HE2	1:A:416:THR:HG21	1.82	0.60
1:A:426:THR:HG22	2:B:281:LEU:HD22	1.79	0.60
1:D:415:ASN:C	1:D:417:SER:H	2.05	0.60
1:D:459:THR:HG1	1:D:461:SER:HG	1.39	0.60
1:J:376:GLN:HE21	2:K:305:VAL:HG13	1.67	0.60
2:E:258:LEU:HA	2:E:261:MET:HE1	1.81	0.60
1:A:335:THR:HG23	1:A:603:LEU:HD22	1.83	0.60
1:A:412:LYS:HD2	1:A:416:THR:CG2	2.31	0.60
2:B:254:LEU:HA	2:B:257:LEU:HB3	1.84	0.59
1:A:412:LYS:CD	1:A:416:THR:HG22	2.31	0.59
1:D:481:GLU:CD	1:D:482:ASP:OD1	2.41	0.59
1:A:413:LEU:O	1:A:415:ASN:N	2.34	0.59
1:A:408:THR:HG22	1:A:409:PRO:N	2.18	0.59
1:D:452:LEU:HD12	1:D:472:SER:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ARG:HG3	1:A:597:ILE:HD13	1.84	0.59
1:G:434:VAL:HG11	2:H:279:LEU:CD2	2.33	0.59
1:G:359:GLN:CD	1:G:608:LYS:HE2	2.22	0.58
1:G:349:CYS:HB3	1:G:552:THR:HB	1.83	0.58
1:J:439:VAL:HG21	1:J:452:LEU:HD23	1.86	0.58
2:B:253:SER:O	2:B:257:LEU:N	2.34	0.58
1:D:507:SER:HB3	1:D:535:ILE:HA	1.85	0.58
1:J:335:THR:H	1:J:603:LEU:HD22	1.68	0.58
2:K:258:LEU:HD12	2:K:258:LEU:H	1.69	0.58
1:G:359:GLN:HB3	1:G:608:LYS:CG	2.26	0.57
1:A:340:HIS:HB3	1:A:343:LEU:HD12	1.86	0.57
1:G:580:GLN:OE1	2:H:291:THR:OG1	2.22	0.57
1:G:420:ASP:HB2	1:G:445:LEU:HD11	1.85	0.57
1:A:531:GLU:OE2	1:J:519:VAL:N	2.30	0.57
1:D:478:SER:HA	1:D:483:LEU:HD12	1.87	0.57
1:A:426:THR:CG2	2:B:281:LEU:HD23	2.32	0.57
1:J:335:THR:N	1:J:603:LEU:HD22	2.20	0.57
1:A:371:PRO:HB3	2:B:306:TYR:HB2	1.87	0.56
1:D:337:LEU:HD23	1:D:606:PHE:HB2	1.88	0.56
1:A:412:LYS:HZ2	1:A:421:SER:CB	2.17	0.56
1:J:373:ARG:HB3	1:J:375:PHE:CE2	2.41	0.56
1:J:334:ALA:O	1:J:630:ALA:N	2.28	0.56
1:J:555:LEU:HD22	1:J:556:GLU:N	2.21	0.56
1:J:595:ILE:HG22	1:J:596:LYS:N	2.19	0.55
1:D:462:GLU:HG2	2:E:279:LEU:HA	1.88	0.55
1:G:552:THR:OG1	1:G:553:GLY:N	2.39	0.55
1:J:435:ALA:HB3	1:J:456:GLU:HB3	1.89	0.55
1:D:607:ILE:HD12	1:D:622:TYR:CD2	2.42	0.55
1:A:438:PHE:CE2	2:B:272:VAL:HG12	2.42	0.54
1:D:375:PHE:HB2	2:E:297:ARG:HG3	1.88	0.54
1:G:411:VAL:HG23	1:G:423:ILE:HD11	1.88	0.54
1:G:573:VAL:O	1:G:580:GLN:NE2	2.27	0.54
1:A:345:ARG:HD3	1:A:363:ARG:HG2	1.88	0.54
1:J:611:ASN:ND2	1:J:620:ILE:HB	2.22	0.54
1:J:555:LEU:HD21	1:J:622:TYR:CD1	2.42	0.54
1:D:592:PRO:HD2	1:D:600:TYR:CD1	2.43	0.54
1:D:425:THR:HA	1:D:433:LYS:HD3	1.89	0.54
1:G:542:PHE:N	1:G:561:ASP:O	2.32	0.54
1:D:415:ASN:OD1	1:D:417:SER:HB2	2.07	0.53
1:G:368:SER:O	1:G:547:THR:OG1	2.25	0.53
2:B:262:ARG:NH1	2:B:265:GLN:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:405:ALA:HB1	1:J:432:ARG:HD2	1.90	0.53
1:J:587:MET:HA	1:J:590:PHE:HB2	1.91	0.53
1:G:434:VAL:HG11	2:H:279:LEU:HD21	1.89	0.53
1:J:363:ARG:HB2	1:J:604:GLU:HG3	1.91	0.53
1:D:371:PRO:HD3	2:E:306:TYR:CE2	2.43	0.53
1:G:387:LEU:HD21	1:G:389:GLN:HB3	1.90	0.53
1:J:483:LEU:HB2	1:J:512:ILE:HD11	1.90	0.53
1:A:412:LYS:CD	1:A:416:THR:CG2	2.87	0.53
1:G:397:LEU:HD21	1:G:491:PRO:HD3	1.92	0.52
1:J:559:LEU:HD11	1:J:561:ASP:HB2	1.91	0.52
1:J:485:LEU:HD21	1:J:533:LEU:HD13	1.92	0.52
2:B:265:GLN:O	2:B:269:GLY:N	2.31	0.52
1:A:412:LYS:HE2	1:A:416:THR:CG2	2.37	0.52
1:G:375:PHE:O	2:H:297:ARG:NH1	2.42	0.52
1:D:374:LEU:HD21	1:D:587:MET:HG3	1.90	0.52
1:D:550:ASP:OD1	1:D:552:THR:HG22	2.09	0.52
2:B:264:ASP:O	2:B:268:GLN:HB2	2.10	0.52
1:J:351:ILE:HA	1:J:354:GLN:HB3	1.91	0.52
1:J:366:LEU:CD1	1:J:590:PHE:HB3	2.40	0.52
2:H:269:GLY:HA2	2:H:272:VAL:HG12	1.91	0.52
1:A:340:HIS:HB3	1:A:343:LEU:CD1	2.40	0.52
1:A:385:CYS:SG	1:A:387:LEU:HB2	2.50	0.52
1:A:411:VAL:O	1:A:412:LYS:HG3	2.10	0.52
1:D:336:ILE:HD11	1:D:628:THR:HG23	1.91	0.51
1:J:592:PRO:HD2	1:J:600:TYR:HD1	1.75	0.51
2:H:276:GLU:HA	2:H:279:LEU:HD12	1.92	0.51
1:A:460:LEU:HD23	2:B:288:PRO:HG3	1.93	0.51
1:D:422:LYS:NZ	2:E:272:VAL:HG21	2.26	0.51
1:A:412:LYS:CE	1:A:416:THR:HG22	2.41	0.51
1:G:580:GLN:HB2	2:H:292:HIS:HE1	1.75	0.51
1:J:357:PRO:HB3	1:J:610:TYR:HA	1.92	0.51
1:G:592:PRO:HB2	1:G:595:ILE:HD11	1.93	0.50
1:G:424:TRP:HZ3	1:G:436:VAL:HB	1.76	0.50
1:J:439:VAL:HB	1:J:452:LEU:HB3	1.92	0.50
1:D:333:SER:OG	1:D:335:THR:O	2.29	0.50
1:G:597:ILE:HA	1:G:600:TYR:CG	2.47	0.50
2:H:265:GLN:N	2:H:265:GLN:OE1	2.45	0.50
2:K:308:VAL:HB	2:K:313:LEU:HD11	1.93	0.50
1:J:555:LEU:HD22	1:J:556:GLU:H	1.76	0.50
2:B:255:SER:HA	2:K:322:ILE:HD11	1.93	0.50
2:E:262:ARG:CG	2:E:264:ASP:HB3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:LEU:HG	1:D:391:VAL:HG22	1.93	0.50
1:G:612:VAL:HG21	2:H:312:MET:HA	1.94	0.50
1:A:397:LEU:HB3	1:A:460:LEU:HD13	1.93	0.49
1:D:464:CYS:O	1:D:467:SER:OG	2.20	0.49
1:J:334:ALA:H	1:J:603:LEU:CD2	2.26	0.49
1:G:413:LEU:HD12	1:G:413:LEU:H	1.77	0.49
1:J:413:LEU:HD22	1:J:423:ILE:HD11	1.95	0.49
1:D:519:VAL:HG21	1:G:534:GLY:HA2	1.94	0.49
1:G:424:TRP:NE1	2:H:276:GLU:OE1	2.45	0.49
2:H:317:GLU:H	2:H:317:GLU:CD	2.15	0.49
1:J:427:LYS:HD3	1:J:428:ASN:H	1.78	0.49
1:A:432:ARG:NH1	1:A:457:GLY:O	2.46	0.48
2:E:319:ASP:O	2:E:323:LEU:N	2.42	0.48
1:A:412:LYS:HD2	1:A:419:TYR:CE2	2.48	0.48
1:A:451:CYS:SG	1:A:452:LEU:N	2.86	0.48
1:D:385:CYS:HB3	1:D:506:CYS:SG	2.52	0.48
1:G:555:LEU:HD11	1:G:622:TYR:CE1	2.48	0.48
1:J:489:SER:OG	1:J:504:LYS:NZ	2.45	0.48
1:D:592:PRO:HB2	1:D:595:ILE:HB	1.95	0.48
1:A:362:ILE:HD13	1:A:607:ILE:HD13	1.95	0.48
1:G:488:LEU:HB2	1:G:504:LYS:HD3	1.95	0.48
1:A:434:VAL:HG21	2:B:279:LEU:HD13	1.95	0.48
1:J:558:TYR:O	1:J:624:ILE:HG13	2.13	0.48
1:A:397:LEU:HD21	1:A:491:PRO:HD3	1.95	0.48
1:G:336:ILE:HD12	1:G:336:ILE:C	2.34	0.48
1:G:410:ASP:OD1	1:G:410:ASP:N	2.47	0.48
1:J:344:GLU:O	1:J:361:ARG:HB3	2.14	0.48
1:J:592:PRO:HD2	1:J:600:TYR:CD1	2.49	0.48
2:H:258:LEU:HA	2:H:261:MET:HE2	1.96	0.48
1:D:419:TYR:CA	1:D:438:PHE:O	2.62	0.48
1:D:419:TYR:HA	1:D:438:PHE:O	2.13	0.48
1:D:419:TYR:HB2	1:D:438:PHE:O	2.14	0.48
1:G:345:ARG:NH1	1:G:345:ARG:HB3	2.29	0.47
2:E:263:GLU:HA	2:E:266:GLU:CG	2.40	0.47
1:J:354:GLN:HG2	1:J:360:TYR:OH	2.14	0.47
1:A:424:TRP:HZ3	1:A:436:VAL:HB	1.80	0.47
1:D:406:THR:HG22	1:D:407:LYS:H	1.79	0.47
1:J:397:LEU:HB3	1:J:460:LEU:HD13	1.96	0.47
1:A:586:ILE:O	1:A:589:MET:HG3	2.15	0.47
1:G:573:VAL:HG23	1:G:579:LEU:HB3	1.96	0.47
1:J:336:ILE:O	1:J:627:THR:OG1	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:GLU:HG2	2:B:279:LEU:HA	1.97	0.47
1:D:576:ASP:HB3	1:D:579:LEU:HB2	1.96	0.47
1:G:378:VAL:HG11	1:G:574:LEU:HG	1.98	0.46
1:G:580:GLN:HG2	2:H:293:TRP:CD2	2.51	0.46
1:J:522:THR:OG1	1:J:523:SER:N	2.47	0.46
2:B:271:LEU:C	2:B:273:CYS:H	2.19	0.46
1:D:382:CYS:HB2	1:D:538:LEU:HD23	1.97	0.46
1:J:336:ILE:HG23	1:J:630:ALA:HB2	1.98	0.46
1:D:504:LYS:HE2	2:K:301:THR:OG1	2.15	0.46
1:G:448:SER:OG	1:G:449:ASN:OD1	2.27	0.46
1:G:435:ALA:HB3	1:G:456:GLU:HB3	1.98	0.46
1:J:426:THR:HG21	1:J:432:ARG:HG3	1.98	0.46
1:G:426:THR:HG22	2:H:281:LEU:HB3	1.97	0.45
1:J:424:TRP:HB2	1:J:434:VAL:HB	1.98	0.45
1:D:336:ILE:HD12	1:D:336:ILE:C	2.37	0.45
1:J:561:ASP:OD2	1:J:565:PHE:N	2.41	0.45
2:E:320:GLN:HA	2:E:323:LEU:HD12	1.97	0.45
1:A:563:ASP:HB3	1:A:569:PRO:HA	1.98	0.45
1:G:365:LYS:HD3	1:G:600:TYR:HB2	1.97	0.45
1:D:351:ILE:HG23	1:D:360:TYR:CE1	2.52	0.45
2:E:274:LEU:HA	2:E:277:SER:HB2	1.99	0.45
1:J:366:LEU:HD23	1:J:366:LEU:HA	1.84	0.45
1:J:507:SER:HB2	1:J:535:ILE:HA	1.98	0.45
1:D:429:GLN:NE2	2:E:281:LEU:HA	2.32	0.45
1:J:373:ARG:HB2	1:J:376:GLN:OE1	2.17	0.45
1:J:609:SER:HB2	1:J:622:TYR:CD2	2.52	0.45
1:G:485:LEU:HD12	1:G:485:LEU:H	1.82	0.45
2:E:286:THR:HA	2:K:284:PRO:HB3	1.99	0.45
1:A:493:LEU:HD23	1:A:500:HIS:ND1	2.32	0.45
1:D:474:ILE:CG2	1:D:485:LEU:CD2	2.95	0.45
1:J:365:LYS:HE3	1:J:365:LYS:HB2	1.76	0.45
1:J:573:VAL:O	1:J:580:GLN:NE2	2.44	0.45
1:D:429:GLN:NE2	1:D:432:ARG:HH21	2.15	0.44
1:A:408:THR:HG22	1:A:409:PRO:CG	2.44	0.44
1:A:597:ILE:HG23	1:A:600:TYR:CD2	2.53	0.44
1:D:426:THR:HG21	1:D:432:ARG:HG3	1.98	0.44
1:D:578:ASP:HA	1:D:581:LYS:HB2	2.00	0.44
2:E:254:LEU:HD12	2:E:254:LEU:HA	1.69	0.44
1:D:396:ASP:HB3	2:K:298:CYS:HB3	1.99	0.44
1:J:424:TRP:HB3	2:K:281:LEU:HD22	1.98	0.44
1:J:581:LYS:HB3	1:J:581:LYS:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ASP:OD1	1:A:483:LEU:N	2.50	0.44
1:D:419:TYR:CB	1:D:438:PHE:O	2.65	0.44
1:J:427:LYS:CD	1:J:428:ASN:H	2.31	0.44
1:A:455:ILE:HG21	1:A:463:ILE:CD1	2.48	0.44
1:D:437:HIS:HD2	1:D:454:LEU:O	2.01	0.44
1:D:465:LYS:CB	2:E:278:CYS:HB3	2.45	0.44
1:J:469:LYS:HB3	2:K:274:LEU:HD12	1.99	0.44
1:A:353:LYS:HA	1:A:353:LYS:HD2	1.77	0.44
1:D:347:PRO:O	1:D:351:ILE:HG13	2.18	0.44
2:E:254:LEU:HD23	2:E:257:LEU:HD22	1.99	0.44
2:H:266:GLU:H	2:H:266:GLU:HG2	1.67	0.44
1:D:426:THR:HG22	2:E:281:LEU:HD22	1.99	0.43
1:D:555:LEU:HD11	1:D:622:TYR:CE2	2.53	0.43
2:H:254:LEU:HD11	2:H:257:LEU:HB3	2.00	0.43
1:G:610:TYR:CE1	1:G:623:GLN:HG3	2.53	0.43
1:A:564:LYS:O	1:A:628:THR:OG1	2.24	0.43
1:D:419:TYR:CD1	1:D:437:HIS:HB3	2.53	0.43
1:J:452:LEU:HB2	1:J:524:TRP:CE2	2.53	0.43
1:G:492:PHE:CE1	1:G:500:HIS:HB3	2.53	0.43
1:J:424:TRP:HZ3	1:J:436:VAL:HB	1.83	0.43
1:A:365:LYS:HD3	1:A:600:TYR:HB2	2.00	0.43
1:A:412:LYS:NZ	1:A:421:SER:HB2	2.32	0.43
1:A:488:LEU:HB2	1:A:504:LYS:HG2	2.00	0.43
1:D:492:PHE:CE1	1:D:500:HIS:HB3	2.53	0.43
2:B:268:GLN:HE22	2:B:272:VAL:HG11	1.84	0.43
1:D:373:ARG:HB3	1:D:375:PHE:CE2	2.54	0.43
1:G:546:PHE:O	1:G:556:GLU:HA	2.18	0.43
2:B:317:GLU:CD	2:B:317:GLU:H	2.21	0.43
1:G:625:PHE:O	1:G:627:THR:HG23	2.19	0.43
1:A:367:ARG:HG3	1:A:597:ILE:CD1	2.48	0.43
1:D:415:ASN:C	1:D:417:SER:N	2.70	0.43
1:D:456:GLU:OE1	1:D:478:SER:HB3	2.19	0.43
1:D:476:VAL:CG1	1:D:485:LEU:HD23	2.44	0.43
1:D:565:PHE:HA	1:D:627:THR:O	2.19	0.43
1:G:592:PRO:HD2	1:G:600:TYR:CE1	2.54	0.43
1:J:395:GLY:O	1:J:399:ILE:HG12	2.19	0.43
1:A:580:GLN:HG2	2:B:293:TRP:CD2	2.53	0.43
1:A:592:PRO:HD2	1:A:600:TYR:CD1	2.54	0.43
1:D:474:ILE:CG2	1:D:485:LEU:HD21	2.49	0.43
1:G:345:ARG:NH1	1:G:363:ARG:HB3	2.34	0.43
1:J:351:ILE:HA	1:J:354:GLN:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:485:LEU:HD13	1:J:509:LEU:HD13	2.01	0.43
2:E:318:ASN:O	2:E:322:ILE:HG12	2.19	0.43
1:A:592:PRO:HD2	1:A:600:TYR:CE1	2.53	0.42
1:G:513:GLN:O	1:G:513:GLN:HG2	2.19	0.42
1:J:402:GLN:NE2	2:E:288:PRO:O	2.48	0.42
1:A:453:LEU:HD23	1:A:453:LEU:HA	1.79	0.42
1:D:335:THR:HG23	1:D:603:LEU:HG	2.00	0.42
1:J:493:LEU:HD23	1:J:500:HIS:ND1	2.34	0.42
1:D:492:PHE:CZ	1:D:530:ALA:HB2	2.53	0.42
1:G:498:ILE:HG12	1:G:572:GLU:HG2	2.00	0.42
1:J:469:LYS:HD3	2:K:274:LEU:CD1	2.49	0.42
1:J:611:ASN:ND2	1:J:618:ASN:HD21	2.16	0.42
1:A:380:LEU:HD22	1:A:538:LEU:HB2	2.00	0.42
1:J:334:ALA:HA	1:J:630:ALA:HB3	2.00	0.42
1:J:368:SER:OG	1:J:369:TYR:N	2.52	0.42
2:H:293:TRP:O	2:H:297:ARG:HB2	2.19	0.42
1:A:372:ARG:HG3	1:A:373:ARG:HG2	2.02	0.42
1:J:492:PHE:CE1	1:J:500:HIS:HB3	2.55	0.42
1:A:371:PRO:HB3	2:B:306:TYR:CB	2.49	0.42
1:G:555:LEU:HD21	1:G:622:TYR:CZ	2.53	0.42
1:G:401:PHE:HD2	1:G:460:LEU:HB2	1.84	0.42
2:B:264:ASP:OD1	2:B:264:ASP:N	2.50	0.42
1:A:510:ARG:HD3	1:A:514:ASN:ND2	2.35	0.42
1:D:426:THR:OG1	1:D:432:ARG:O	2.24	0.42
1:G:580:GLN:HA	1:G:583:VAL:HG12	2.02	0.42
1:D:419:TYR:HB3	1:D:439:VAL:HA	2.02	0.42
1:A:384:LYS:HD3	1:A:384:LYS:HA	1.90	0.42
1:J:340:HIS:HB3	1:J:343:LEU:HD23	2.02	0.42
1:D:370:LYS:HB2	1:D:370:LYS:HE3	1.82	0.41
1:D:596:LYS:HA	1:D:596:LYS:HD2	1.54	0.41
1:G:596:LYS:HG2	1:G:597:ILE:H	1.82	0.41
2:B:286:THR:OG1	2:B:287:ALA:N	2.53	0.41
1:A:410:ASP:H	1:A:478:SER:CB	2.32	0.41
2:E:261:MET:HB3	2:E:266:GLU:OE2	2.20	0.41
1:A:375:PHE:HD1	2:B:297:ARG:HG2	1.85	0.41
1:D:348:LEU:HD12	1:D:550:ASP:H	1.84	0.41
1:D:428:ASN:C	1:D:429:GLN:HG2	2.40	0.41
1:G:429:GLN:OE1	1:G:432:ARG:NH2	2.52	0.41
1:G:574:LEU:HD23	1:G:574:LEU:HA	1.87	0.41
1:J:611:ASN:HB3	1:J:618:ASN:OD1	2.21	0.41
1:A:358:GLN:HE21	1:A:358:GLN:HB2	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:271:LEU:HD23	2:H:271:LEU:HA	1.83	0.41
1:A:364:ALA:HB3	1:A:548:LEU:HB3	2.01	0.41
1:D:525:ILE:O	1:D:525:ILE:HG13	2.20	0.41
1:G:371:PRO:HD3	2:H:306:TYR:CE1	2.55	0.41
1:J:379:LYS:NZ	1:J:390:GLU:OE2	2.47	0.41
1:D:422:LYS:NZ	2:E:272:VAL:CG2	2.84	0.41
1:G:596:LYS:HE2	1:G:598:ASP:H	1.86	0.41
1:G:632:ASP:OD1	1:G:632:ASP:N	2.53	0.41
1:A:531:GLU:OE2	1:J:518:LEU:HA	2.21	0.41
1:D:419:TYR:CD1	1:D:419:TYR:O	2.74	0.41
1:G:366:LEU:HG	1:G:591:CYS:SG	2.60	0.41
1:G:380:LEU:HG	1:G:391:VAL:HG22	2.03	0.41
1:G:568:ILE:HD12	1:G:583:VAL:HB	2.03	0.41
2:E:287:ALA:HA	2:E:288:PRO:HD3	1.91	0.41
1:D:485:LEU:HD11	1:D:533:LEU:CD1	2.42	0.41
1:J:416:THR:HA	1:J:440:LYS:NZ	2.36	0.41
1:J:438:PHE:CE1	2:K:271:LEU:HB3	2.56	0.41
1:A:344:GLU:H	1:A:344:GLU:HG2	1.63	0.40
1:D:421:SER:CB	1:D:437:HIS:ND1	2.84	0.40
1:D:421:SER:OG	1:D:437:HIS:ND1	2.42	0.40
1:J:374:LEU:HA	1:J:374:LEU:HD12	1.89	0.40
1:A:371:PRO:HD3	2:B:306:TYR:CD2	2.57	0.40
1:J:371:PRO:HD3	2:K:306:TYR:CE2	2.56	0.40
1:G:367:ARG:NH1	1:G:554:VAL:HG11	2.37	0.40
1:G:426:THR:HA	2:H:281:LEU:HB3	2.02	0.40
1:G:612:VAL:HG11	2:H:312:MET:HG2	2.02	0.40
1:J:421:SER:HB3	1:J:437:HIS:ND1	2.36	0.40
2:H:309:PRO:HB2	2:H:311:SER:HB2	2.04	0.40
1:D:448:SER:HB2	1:D:470:PHE:HA	2.02	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	300/313 (96%)	276 (92%)	22 (7%)	2 (1%)	22	54
1	D	300/313 (96%)	274 (91%)	21 (7%)	5 (2%)	9	31
1	G	300/313 (96%)	271 (90%)	28 (9%)	1 (0%)	41	71
1	J	300/313 (96%)	262 (87%)	37 (12%)	1 (0%)	41	71
2	B	72/93 (77%)	68 (94%)	4 (6%)	0	100	100
2	E	72/93 (77%)	67 (93%)	5 (7%)	0	100	100
2	H	72/93 (77%)	60 (83%)	11 (15%)	1 (1%)	11	36
2	K	72/93 (77%)	67 (93%)	5 (7%)	0	100	100
All	All	1488/1624 (92%)	1345 (90%)	133 (9%)	10 (1%)	22	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	448	SER
1	A	414	GLN
2	H	263	GLU
1	A	411	VAL
1	D	339	ASP
1	G	446	PRO
1	D	446	PRO
1	D	411	VAL
1	D	597	ILE
1	J	595	ILE

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	275/286 (96%)	270 (98%)	5 (2%)	59	85
1	D	275/286 (96%)	265 (96%)	10 (4%)	35	69
1	G	275/286 (96%)	266 (97%)	9 (3%)	38	72
1	J	275/286 (96%)	264 (96%)	11 (4%)	31	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	64/79 (81%)	60 (94%)	4 (6%)	18	46
2	E	64/79 (81%)	58 (91%)	6 (9%)	8	26
2	H	64/79 (81%)	56 (88%)	8 (12%)	4	14
2	K	64/79 (81%)	59 (92%)	5 (8%)	12	34
All	All	1356/1460 (93%)	1298 (96%)	58 (4%)	29	62

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	ARG
1	A	448	SER
1	A	469	LYS
1	A	577	ASP
1	A	591	CYS
1	D	368	SER
1	D	374	LEU
1	D	414	GLN
1	D	420	ASP
1	D	430	LYS
1	D	478	SER
1	D	527	SER
1	D	548	LEU
1	D	563	ASP
1	D	595	ILE
1	G	344	GLU
1	G	368	SER
1	G	375	PHE
1	G	414	GLN
1	G	428	ASN
1	G	447	LEU
1	G	499	HIS
1	G	508	SER
1	G	577	ASP
1	J	342	TYR
1	J	349	CYS
1	J	413	LEU
1	J	427	LYS
1	J	467	SER
1	J	516	ASN
1	J	577	ASP
1	J	584	ASP

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Mol	Chain	Res	Type
1	J	621	CYS
1	J	625	PHE
1	J	626	ASP
2	B	264	ASP
2	B	299	LYS
2	B	303	GLU
2	B	312	MET
2	E	262	ARG
2	E	263	GLU
2	E	273	CYS
2	E	276	GLU
2	E	296	SER
2	E	312	MET
2	H	259	ASP
2	H	265	GLN
2	H	266	GLU
2	H	267	HIS
2	H	268	GLN
2	H	273	CYS
2	H	279	LEU
2	H	318	ASN
2	K	253	SER
2	K	259	ASP
2	K	260	GLU
2	K	262	ARG
2	K	264	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	GLN
1	A	514	ASN
1	A	618	ASN
1	D	358	GLN
1	D	429	GLN
1	G	376	GLN
1	J	376	GLN
1	J	539	GLN
1	J	611	ASN
2	B	268	GLN
2	B	318	ASN
2	B	320	GLN

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 monosaccharides 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	302/313 (96%)	0.18	14 (4%) 32 29	40, 64, 112, 164	0
1	D	302/313 (96%)	0.36	21 (6%) 16 12	41, 68, 115, 161	0
1	G	302/313 (96%)	0.24	19 (6%) 20 16	39, 72, 105, 161	0
1	J	302/313 (96%)	0.63	32 (10%) 6 4	39, 77, 134, 158	0
2	B	74/93 (79%)	0.32	2 (2%) 54 50	48, 78, 101, 115	0
2	E	74/93 (79%)	0.26	3 (4%) 37 32	43, 79, 118, 125	0
2	H	74/93 (79%)	0.36	6 (8%) 12 9	51, 82, 107, 113	0
2	K	74/93 (79%)	0.26	2 (2%) 54 50	54, 82, 103, 171	0
All	All	1504/1624 (92%)	0.34	99 (6%) 18 14	39, 71, 121, 171	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	LEU	7.4
1	A	632	ASP	5.6
2	K	256	GLN	5.6
1	J	615	GLY	5.5
1	A	415	ASN	5.1
1	J	598	ASP	5.1
1	J	554	VAL	4.7
2	E	326	LEU	4.7
1	G	413	LEU	4.6
1	D	594	GLY	4.5
1	D	422	LYS	4.5
1	J	553	GLY	4.5
1	A	414	GLN	4.5
1	D	633	VAL	4.4
1	G	617	ASP	4.3
1	J	362	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	J	617	ASP	4.2
1	J	416	THR	4.1
1	A	633	VAL	4.1
1	J	364	ALA	4.0
1	J	353	LYS	3.8
1	A	433	LYS	3.7
1	D	417	SER	3.7
2	H	262	ARG	3.7
1	J	349	CYS	3.7
1	G	480	HIS	3.6
1	A	616	THR	3.6
1	D	433	LYS	3.5
1	A	617	ASP	3.5
1	J	597	ILE	3.5
1	J	367	ARG	3.3
1	D	593	PRO	3.3
2	H	280	THR	3.3
1	J	602	TRP	3.2
1	G	616	THR	3.2
1	J	352	LEU	3.1
1	J	618	ASN	3.1
1	J	428	ASN	3.1
1	G	605	CYS	3.0
1	J	616	THR	3.0
1	D	416	THR	2.9
1	J	337	LEU	2.9
1	G	609	SER	2.8
1	G	415	ASN	2.8
1	D	482	ASP	2.8
1	J	433	LYS	2.8
1	A	630	ALA	2.8
1	D	622	TYR	2.8
1	G	615	GLY	2.7
1	G	347	PRO	2.7
1	A	615	GLY	2.6
1	D	595	ILE	2.6
1	G	414	GLN	2.6
1	A	480	HIS	2.6
1	J	590	PHE	2.6
1	G	407	LYS	2.6
1	J	614	ASN	2.6
1	D	412	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	595	ILE	2.5
2	H	284	PRO	2.5
1	D	427	LYS	2.5
1	G	594	GLY	2.5
1	G	618	ASN	2.4
1	J	549	ASP	2.4
2	H	283	GLY	2.4
1	D	616	THR	2.4
1	G	608	LYS	2.4
1	D	407	LYS	2.4
1	J	632	ASP	2.4
1	J	348	LEU	2.4
1	A	614	ASN	2.4
1	G	343	LEU	2.4
2	H	282	GLU	2.3
1	A	332	LEU	2.3
2	B	282	GLU	2.3
1	J	633	VAL	2.3
1	J	603	LEU	2.3
1	D	342	TYR	2.3
1	G	344	GLU	2.2
1	G	345	ARG	2.2
1	G	517	SER	2.2
1	J	551	GLY	2.2
2	E	283	GLY	2.2
1	D	426	THR	2.2
2	H	266	GLU	2.1
1	G	614	ASN	2.1
1	J	601	PRO	2.1
1	D	513	GLN	2.1
2	B	284	PRO	2.1
1	D	349	CYS	2.1
1	D	414	GLN	2.1
1	J	582	SER	2.1
1	J	596	LYS	2.1
2	K	285	CYS	2.0
1	D	406	THR	2.0
2	E	256	GLN	2.0
1	J	430	LYS	2.0
1	A	613	THR	2.0
1	D	611	ASN	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 monosaccharides in this entry.

6.4 Ligands [i](#)

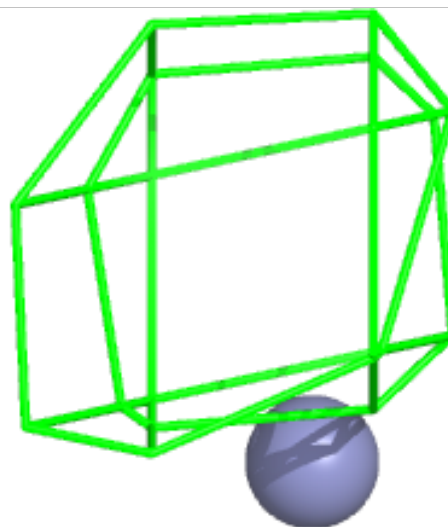
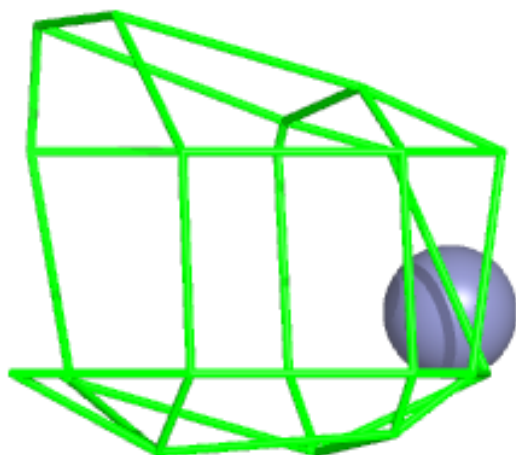
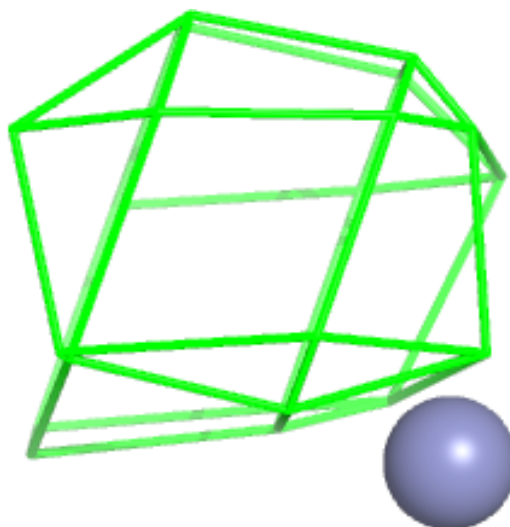
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	701	1/1	0.93	0.19	72,72,72,72	0
3	ZN	A	701	1/1	0.94	0.13	61,61,61,61	0
3	ZN	D	701	1/1	0.95	0.12	69,69,69,69	0
3	ZN	J	701	1/1	0.96	0.15	69,69,69,69	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

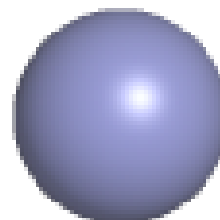
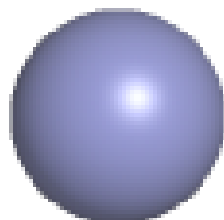
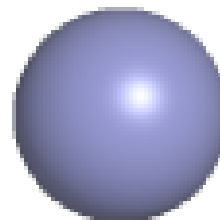
Electron density around ZN G 701:

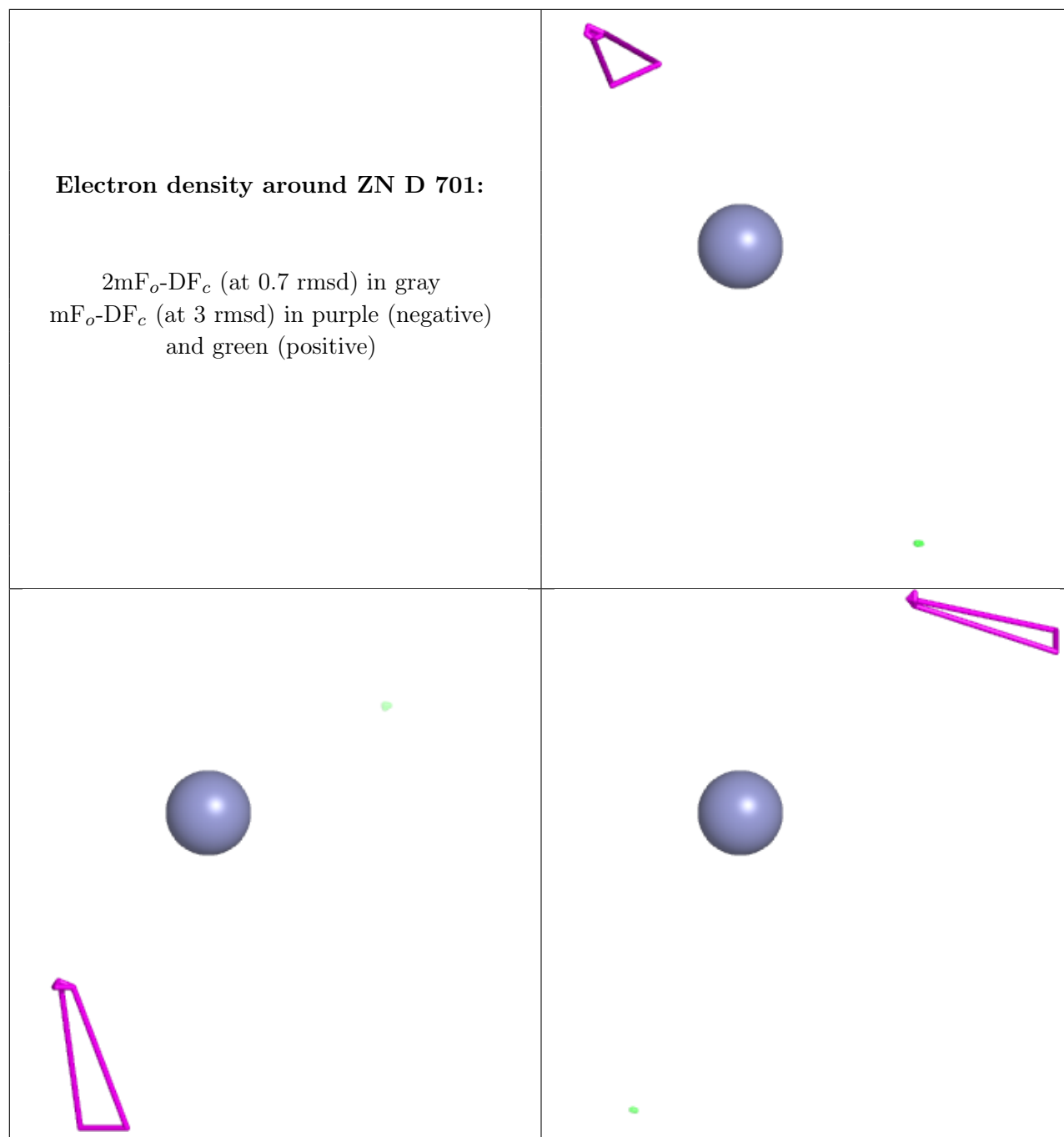
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

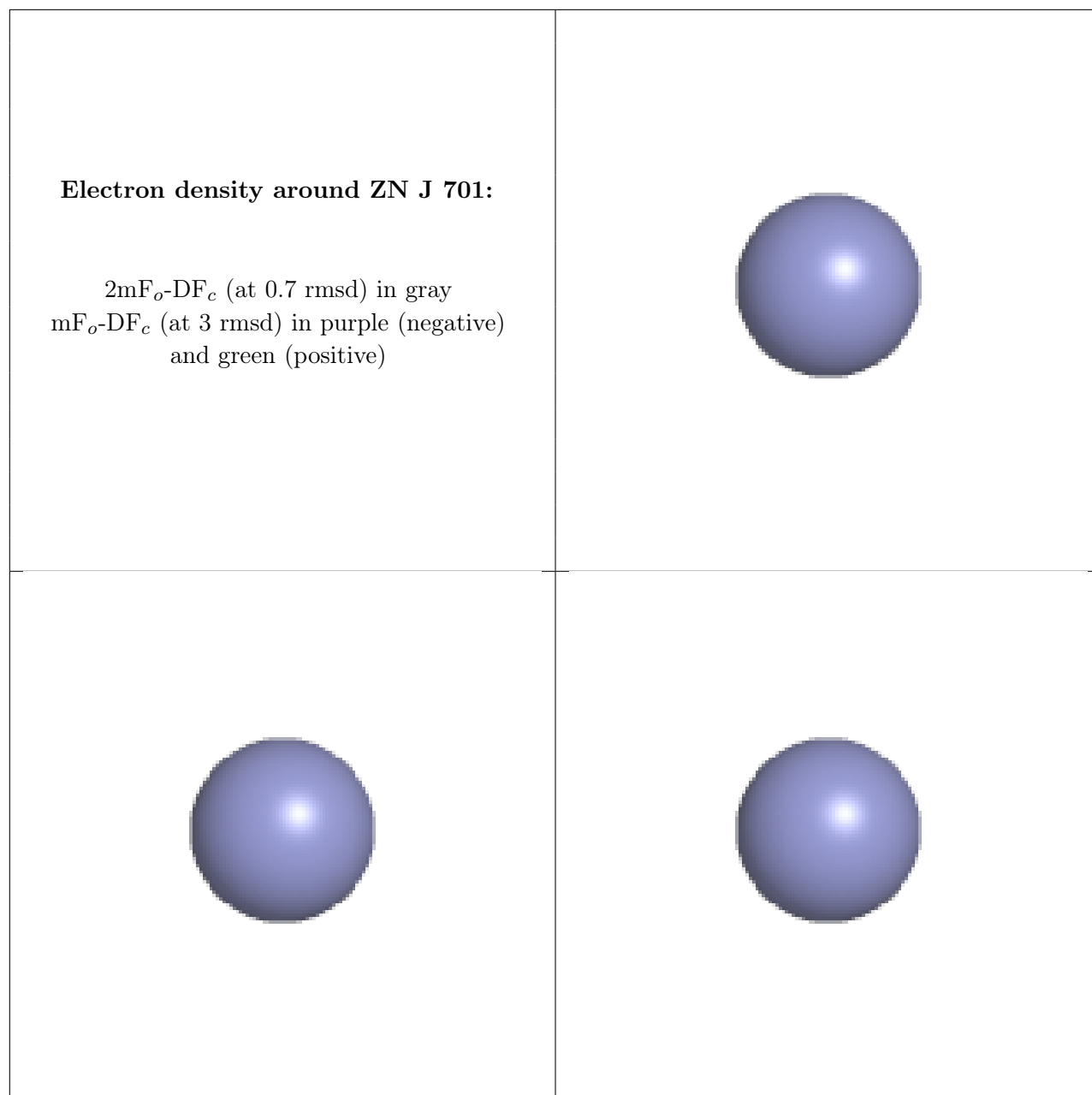


Electron density around ZN A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers [i](#)

There are no such residues in this entry.