Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 02:07 PM JST

PDB ID	:	7XYY
Title	:	TRIM E3 ubiquitin ligase WT
Authors	:	Park, S.H.; Song, H.K.
Deposited on	:	2022-06-02
Resolution	:	7.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

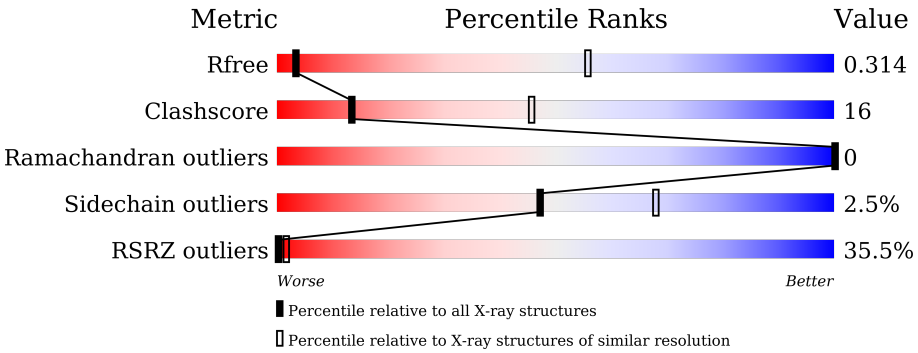
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 7.10 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	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	477	29% 54% 25% . 20%
1	B	477	27% 49% 30% . 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6034 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 Tripartite motif-containing protein 72.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total 3015	C 1904	N 541	O 553	S 17	0	0	0
1	B	382	Total 3015	C 1904	N 541	O 553	S 17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q1XH17
B	1	GLY	-	expression tag	UNP Q1XH17

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

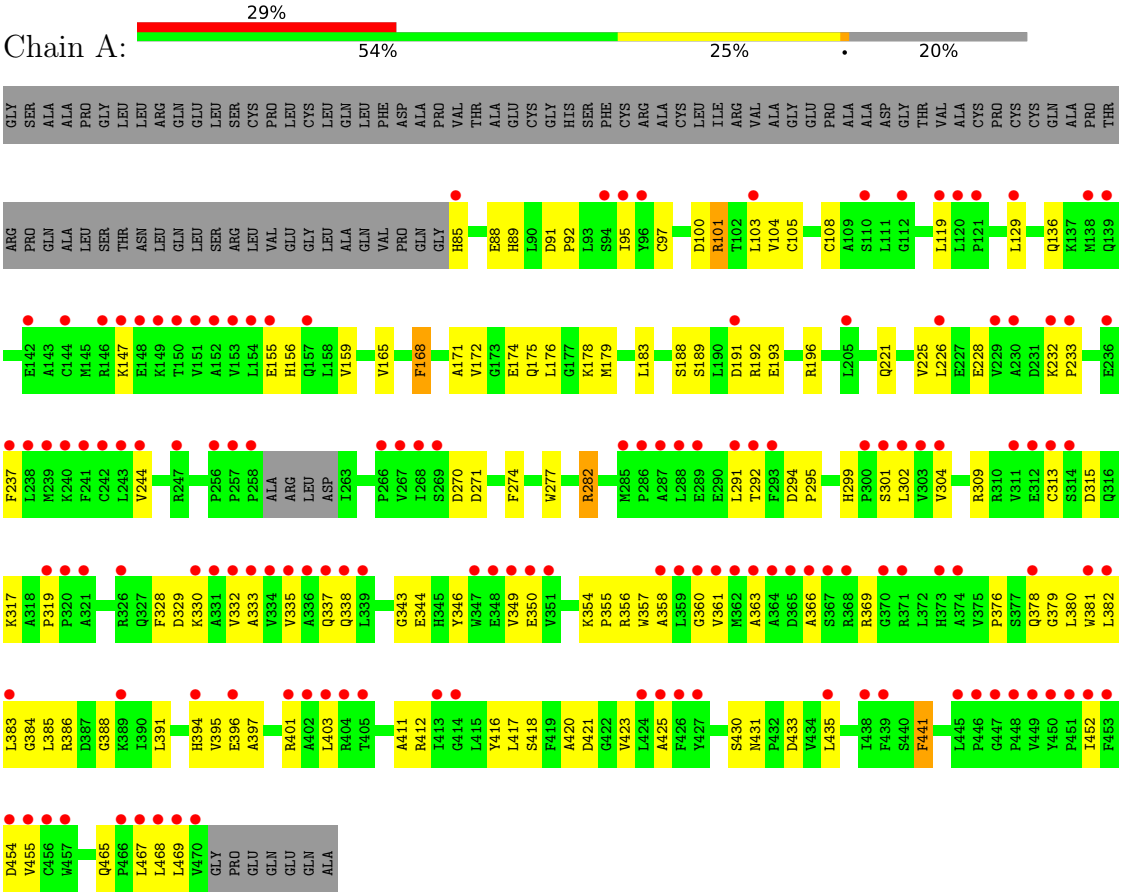
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0

3 Residue-property plots (i)

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.

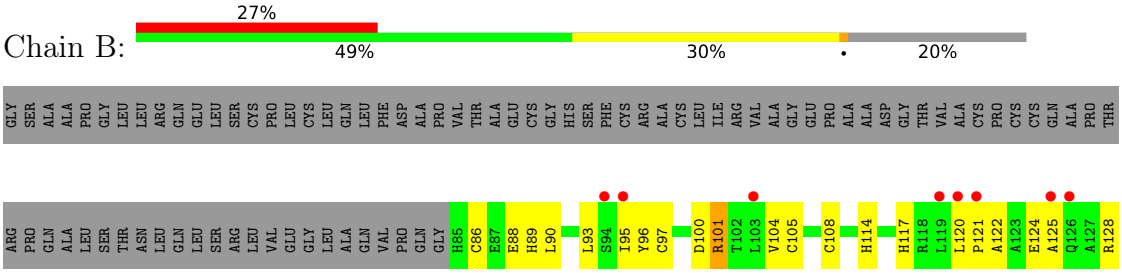
• Molecule 1: Tripartite motif-containing protein 72

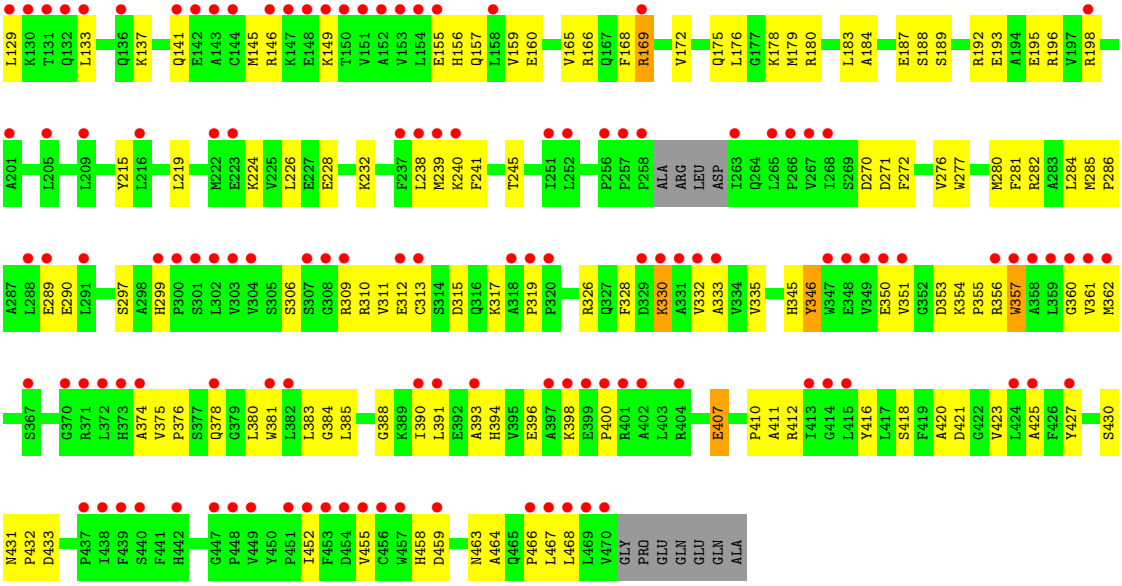
Chain A:



• Molecule 1: Tripartite motif-containing protein 72

Chain B:




L129 K130 T131 Q132 L133 Q136 K137 Q141 E142 A143 C144 M145 R146 K147 E148 K149 T150 V151 A152 V153 L154 E155 H156 Q157 L158 V159 E160 V165 R166 Q167 F168 R169 V172 Q175 L176 G177 K178 M179 R180 L183 A184 E187 S188 S189 R192 E193 A194 E195 R196 V197 R198
A201 L205 L209 Y215 L216 L219 M222 E223 K224 V225 L226 E227 E228 K232 F237 L238 M239 K240 F241 T245 I251 L252 P255 P257 P258 ALA ARG LEU ASP I263 Q264 L265 P266 V267 I268 S269 D270 D271 F272 V276 W277 M280 F281 R282 A283 L284 M285 P286
A287 L288 E289 E290 L291 S297 A298 H299 P300 S301 L302 V303 V304 S305 S306 S307 G308 R309 R310 V311 E312 C313 S314 D315 Q316 K317 A318 P319 P320 R326 Q327 F328 D329 K330 A331 V332 A333 V334 V335 H345 Y346 W347 E348 V349 E350 V351 G352 D353 K354 P355 R356 W357 A358 L359 G360 V361 M362
S367 G370 R371 L372 H373 A374 V375 P376 S377 Q378 G379 L380 W381 L382 L383 G384 L385 G388 K389 I390 L391 E392 A393 H394 V395 E396 A397 K398 E399 P400 R401 A402 L403 R404 E407 P410 A411 R412 I413 G414 L415 Y416 L417 S418 F419 A420 D421 G422 V423 L424 A425 F426 Y427 S430
N431 P432 D433 P437 I438 F439 S440 F441 H442 G447 P448 V449 Y450 P451 I452 F453 D454 V455 C456 W457 H458 D459 N463 A464 Q465 P466 L467 L468 L469 V470 GLY PRO GLU GLN GLU GLN ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	367.04Å 98.06Å 103.20Å 90.00° 101.32° 90.00°	Depositor
Resolution (Å)	49.03 – 7.10 49.03 – 7.04	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.03-7.10) 68.5 (49.03-7.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 7.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.269 , 0.314 0.270 , 0.314	Depositor DCC
R_{free} test set	553 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å^2)	248.5	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 493.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	6034	wwPDB-VP
Average B, all atoms (Å^2)	295.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.25	0/3079	0.56	0/4165
1	B	0.25	0/3079	0.57	0/4165
All	All	0.25	0/6158	0.56	0/8330

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

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	3015	0	3025	94	0
1	B	3015	0	3025	114	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	6034	0	6050	195	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 (195) 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:91:ASP:HB2	1:A:105:CYS:HB2	1.52	0.91
1:A:366:ALA:HB3	1:A:380:LEU:HD13	1.60	0.84
1:B:374:ALA:HB1	1:B:380:LEU:HB3	1.60	0.82
1:B:357:TRP:HB3	1:B:455:VAL:HG23	1.61	0.81
1:A:420:ALA:HB3	1:B:270:ASP:HB2	1.64	0.78
1:B:416:TYR:HB3	1:B:425:ALA:HB3	1.67	0.76
1:A:333:ALA:HA	1:A:454:ASP:HB2	1.67	0.75
1:B:311:VAL:O	1:B:466:PRO:HA	1.85	0.75
1:A:416:TYR:HB3	1:A:425:ALA:HB3	1.69	0.74
1:B:385:LEU:HA	1:B:390:ILE:O	1.87	0.74
1:A:354:LYS:HB3	1:A:357:TRP:HE1	1.54	0.73
1:B:361:VAL:O	1:B:380:LEU:HA	1.89	0.73
1:A:105:CYS:H	1:A:108:CYS:HB2	1.54	0.72
1:B:335:VAL:HG12	1:B:452:ILE:HD12	1.71	0.71
1:A:344:GLU:HA	1:A:417:LEU:O	1.90	0.71
1:B:105:CYS:H	1:B:108:CYS:HB2	1.59	0.68
1:A:295:PRO:HB3	1:A:304:VAL:HG11	1.74	0.68
1:B:93:LEU:HD23	1:B:105:CYS:HB3	1.76	0.67
1:A:226:LEU:HD21	1:A:244:VAL:HG11	1.75	0.67
1:B:317:LYS:HG3	1:B:319:PRO:HD3	1.76	0.67
1:A:191:ASP:HB3	1:B:169:ARG:HH21	1.60	0.66
1:B:104:VAL:HG11	1:B:114:HIS:CD2	2.29	0.66
1:B:376:PRO:HB2	1:B:396:GLU:HB2	1.78	0.65
1:A:411:ALA:HB3	1:A:430:SER:HA	1.77	0.65
1:A:395:VAL:HG22	1:A:401:ARG:HB2	1.79	0.64
1:A:418:SER:OG	1:B:270:ASP:OD2	2.15	0.63
1:A:172:VAL:O	1:A:176:LEU:HG	1.98	0.63
1:B:354:LYS:HB3	1:B:357:TRP:HE1	1.65	0.62
1:A:301:SER:HB3	1:A:332:VAL:HG21	1.82	0.61
1:A:292:THR:OG1	1:A:338:GLN:OE1	2.15	0.61
1:B:179:MET:O	1:B:183:LEU:HG	2.01	0.61
1:A:363:ALA:HB3	1:A:379:GLY:HA3	1.84	0.60
1:B:272:PHE:O	1:B:276:VAL:HB	2.02	0.60
1:A:97:CYS:O	1:A:101:ARG:N	2.35	0.60
1:B:385:LEU:HD12	1:B:391:LEU:HG	1.84	0.60
1:B:277:TRP:HA	1:B:280:MET:HG2	1.83	0.59
1:A:354:LYS:HB3	1:A:357:TRP:NE1	2.16	0.59
1:B:189:SER:HA	1:B:192:ARG:HE	1.68	0.59
1:A:232:LYS:HB3	1:A:233:PRO:HD2	1.84	0.59
1:B:184:ALA:O	1:B:187:GLU:HG3	2.04	0.58
1:B:95:ILE:HA	1:B:120:LEU:O	2.04	0.58
1:B:96:TYR:HB3	1:B:120:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:HA	1:A:435:LEU:HD12	1.86	0.57
1:B:362:MET:HA	1:B:380:LEU:HG	1.86	0.57
1:A:193:GLU:OE1	1:A:196:ARG:NH1	2.35	0.56
1:B:286:PRO:HG2	1:B:346:TYR:HB3	1.88	0.56
1:A:189:SER:O	1:A:193:GLU:HG2	2.06	0.56
1:B:289:GLU:HG3	1:B:345:HIS:HB3	1.87	0.56
1:B:313:CYS:HB3	1:B:464:ALA:HA	1.87	0.55
1:A:129:LEU:HD11	1:B:238:LEU:HA	1.88	0.55
1:B:100:ASP:OD2	1:B:117:HIS:CE1	2.59	0.55
1:B:299:HIS:HB3	1:B:332:VAL:HG23	1.89	0.55
1:A:179:MET:O	1:A:183:LEU:HG	2.05	0.55
1:B:354:LYS:HB3	1:B:357:TRP:NE1	2.21	0.55
1:A:346:TYR:HB2	1:A:416:TYR:HD2	1.72	0.55
1:A:171:ALA:O	1:A:175:GLN:HG2	2.07	0.55
1:A:349:VAL:O	1:A:412:ARG:HG3	2.07	0.54
1:A:354:LYS:NZ	1:A:465:GLN:H	2.05	0.54
1:B:129:LEU:O	1:B:133:LEU:HD13	2.08	0.54
1:A:103:LEU:HD11	1:B:239:MET:HB2	1.90	0.53
1:A:356:ARG:HB2	1:A:386:ARG:HG2	1.91	0.53
1:B:458:HIS:HA	1:B:463:ASN:HB3	1.91	0.53
1:A:366:ALA:HB2	1:A:378:GLN:HB3	1.90	0.53
1:A:277:TRP:CD1	1:B:284:LEU:HD21	2.44	0.53
1:A:228:GLU:O	1:A:232:LYS:HG2	2.08	0.53
1:A:344:GLU:HB3	1:A:418:SER:HB2	1.91	0.53
1:A:382:LEU:HB2	1:A:394:HIS:HB2	1.90	0.53
1:A:271:ASP:HB2	1:B:421:ASP:OD2	2.09	0.53
1:B:155:GLU:O	1:B:159:VAL:HG13	2.08	0.52
1:B:145:MET:O	1:B:149:LYS:HG2	2.10	0.52
1:B:86:CYS:HB3	1:B:90:LEU:N	2.24	0.52
1:B:354:LYS:HE3	1:B:455:VAL:HG11	1.91	0.52
1:A:344:GLU:OE1	1:A:416:TYR:OH	2.26	0.52
1:B:356:ARG:NH1	1:B:459:ASP:OD2	2.27	0.52
1:A:335:VAL:HG12	1:A:452:ILE:HB	1.91	0.52
1:A:277:TRP:CD2	1:B:284:LEU:HD11	2.45	0.51
1:A:376:PRO:HB3	1:A:381:TRP:CD1	2.46	0.51
1:B:122:ALA:HA	1:B:125:ALA:HB3	1.92	0.51
1:B:394:HIS:HA	1:B:400:PRO:HB3	1.93	0.51
1:A:395:VAL:HB	1:A:397:ALA:HB3	1.93	0.51
1:A:175:GLN:O	1:A:179:MET:HG2	2.10	0.51
1:A:343:GLY:O	1:A:418:SER:HA	2.11	0.50
1:A:174:GLU:O	1:A:178:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:TYR:HB2	1:B:416:TYR:HD1	1.76	0.50
1:B:241:PHE:O	1:B:245:THR:OG1	2.29	0.50
1:B:189:SER:O	1:B:193:GLU:HG2	2.10	0.50
1:B:281:PHE:CD1	1:B:284:LEU:HD12	2.48	0.49
1:B:100:ASP:O	1:B:101:ARG:HG2	2.12	0.49
1:B:156:HIS:O	1:B:159:VAL:HG22	2.13	0.49
1:B:188:SER:O	1:B:192:ARG:HG3	2.13	0.49
1:B:282:ARG:HD3	1:B:432:PRO:O	2.12	0.49
1:B:289:GLU:OE1	1:B:290:GLU:N	2.45	0.49
1:A:221:GLN:O	1:A:225:VAL:HG23	2.12	0.49
1:B:312:GLU:HB3	1:B:466:PRO:HB3	1.95	0.48
1:A:274:PHE:CE2	1:B:423:VAL:HG11	2.48	0.48
1:B:124:GLU:O	1:B:128:ARG:HG2	2.13	0.48
1:B:310:ARG:HA	1:B:467:LEU:O	2.13	0.48
1:B:385:LEU:HD21	1:B:388:GLY:HA2	1.95	0.48
1:A:188:SER:O	1:A:192:ARG:HG2	2.13	0.48
1:A:299:HIS:HB3	1:A:332:VAL:HG23	1.96	0.48
1:A:346:TYR:HB2	1:A:416:TYR:CD2	2.48	0.48
1:B:165:VAL:HA	1:B:168:PHE:CE2	2.49	0.48
1:B:315:ASP:N	1:B:315:ASP:OD1	2.47	0.48
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.73	0.48
1:B:350:GLU:HG3	1:B:351:VAL:N	2.28	0.48
1:B:375:VAL:HG23	1:B:378:GLN:HB2	1.95	0.48
1:A:358:ALA:HA	1:A:384:GLY:HA2	1.96	0.47
1:A:391:LEU:HB3	1:A:403:LEU:HD12	1.96	0.47
1:A:100:ASP:O	1:A:101:ARG:HG2	2.15	0.47
1:A:155:GLU:O	1:A:159:VAL:HG13	2.14	0.47
1:A:302:LEU:HD22	1:A:313:CYS:HB2	1.96	0.47
1:B:193:GLU:OE1	1:B:196:ARG:NH1	2.42	0.47
1:B:195:GLU:OE2	1:B:198:ARG:NH1	2.47	0.47
1:A:165:VAL:HA	1:A:168:PHE:CD2	2.50	0.47
1:B:425:ALA:HB1	1:B:427:TYR:CE2	2.50	0.46
1:A:354:LYS:HZ1	1:A:465:GLN:H	1.63	0.46
1:B:385:LEU:HB2	1:B:391:LEU:HG	1.96	0.46
1:A:156:HIS:O	1:A:159:VAL:HG22	2.14	0.46
1:A:191:ASP:HB3	1:B:169:ARG:NH2	2.29	0.46
1:B:467:LEU:HA	1:B:467:LEU:HD23	1.54	0.46
1:B:104:VAL:HG11	1:B:114:HIS:HD2	1.78	0.46
1:A:396:GLU:HB2	1:A:441:PHE:HZ	1.81	0.46
1:A:349:VAL:HB	1:A:467:LEU:HD21	1.98	0.46
1:B:351:VAL:HG21	1:B:410:PRO:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ASN:HB3	1:A:433:ASP:OD1	2.15	0.46
1:A:175:GLN:HA	1:A:178:LYS:NZ	2.31	0.45
1:B:104:VAL:HB	1:B:108:CYS:HB3	1.98	0.45
1:B:411:ALA:HB3	1:B:430:SER:HA	1.99	0.45
1:A:421:ASP:OD2	1:B:271:ASP:N	2.50	0.45
1:B:328:PHE:CE1	1:B:333:ALA:HB3	2.52	0.45
1:A:291:LEU:HD13	1:A:469:LEU:HD12	1.98	0.45
1:A:299:HIS:HB3	1:A:332:VAL:HA	1.99	0.45
1:B:97:CYS:O	1:B:101:ARG:N	2.49	0.45
1:B:282:ARG:O	1:B:285:MET:HG2	2.17	0.45
1:A:385:LEU:HD21	1:A:388:GLY:HA2	1.98	0.44
1:A:350:GLU:HB2	1:A:412:ARG:HD3	1.98	0.44
1:B:281:PHE:HD1	1:B:284:LEU:HD12	1.80	0.44
1:B:418:SER:HB3	1:B:423:VAL:HB	1.98	0.44
1:A:232:LYS:HD3	1:A:232:LYS:HA	1.61	0.44
1:A:174:GLU:OE2	1:A:178:LYS:HD3	2.18	0.44
1:A:317:LYS:HG3	1:A:319:PRO:HD3	1.99	0.44
1:A:88:GLU:OE1	1:A:89:HIS:NE2	2.50	0.44
1:B:175:GLN:O	1:B:179:MET:HG2	2.17	0.44
1:B:384:GLY:O	1:B:391:LEU:HA	2.18	0.44
1:B:431:ASN:HB3	1:B:433:ASP:OD1	2.17	0.44
1:B:286:PRO:HG3	1:B:416:TYR:HE1	1.83	0.43
1:B:309:ARG:O	1:B:468:LEU:HA	2.18	0.43
1:A:315:ASP:OD1	1:A:315:ASP:N	2.49	0.43
1:B:383:LEU:HD13	1:B:393:ALA:HB2	2.00	0.43
1:A:354:LYS:HG2	1:A:355:PRO:HD2	1.99	0.43
1:B:165:VAL:HA	1:B:168:PHE:CD2	2.53	0.43
1:B:360:GLY:HA3	1:B:381:TRP:O	2.19	0.43
1:B:114:HIS:HA	1:B:117:HIS:CE1	2.53	0.43
1:B:122:ALA:HA	1:B:125:ALA:CB	2.48	0.43
1:B:282:ARG:HB2	1:B:433:ASP:HA	2.00	0.43
1:A:354:LYS:HD3	1:A:455:VAL:HG21	2.01	0.43
1:B:224:LYS:C	1:B:226:LEU:H	2.22	0.43
1:B:178:LYS:HB2	1:B:178:LYS:HE2	1.84	0.43
1:B:176:LEU:HD22	1:B:180:ARG:CZ	2.48	0.42
1:A:175:GLN:HA	1:A:178:LYS:HZ2	1.84	0.42
1:B:141:GLN:O	1:B:145:MET:HG2	2.20	0.42
1:B:176:LEU:HD22	1:B:180:ARG:NE	2.35	0.42
1:A:270:ASP:HB2	1:B:420:ALA:HB2	2.01	0.42
1:B:193:GLU:CD	1:B:196:ARG:HH12	2.23	0.42
1:B:355:PRO:HG2	1:B:463:ASN:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:HD3	1:A:147:LYS:HA	1.78	0.42
1:A:423:VAL:HG21	1:B:270:ASP:HB3	2.02	0.42
1:A:85:HIS:HB3	1:A:92:PRO:HA	2.02	0.42
1:B:88:GLU:OE1	1:B:89:HIS:NE2	2.53	0.42
1:B:121:PRO:HG2	1:B:124:GLU:HB2	2.01	0.42
1:A:299:HIS:O	1:A:301:SER:N	2.46	0.41
1:A:95:ILE:HB	1:A:104:VAL:HG23	2.03	0.41
1:A:360:GLY:HA3	1:A:381:TRP:O	2.20	0.41
1:B:232:LYS:HD3	1:B:232:LYS:HA	1.57	0.41
1:B:407:GLU:H	1:B:407:GLU:CD	2.24	0.41
1:B:412:ARG:NH2	1:B:432:PRO:HD3	2.35	0.41
1:B:133:LEU:HB3	1:B:137:LYS:NZ	2.36	0.41
1:B:330:LYS:HD3	1:B:330:LYS:HA	1.84	0.41
1:A:309:ARG:O	1:A:468:LEU:HA	2.20	0.41
1:B:297:SER:HB3	1:B:326:ARG:HH11	1.85	0.41
1:A:328:PHE:HA	1:A:369:ARG:HH12	1.85	0.41
1:B:157:GLN:O	1:B:160:GLU:HG2	2.20	0.41
1:B:215:TYR:O	1:B:219:LEU:HG	2.20	0.41
1:A:294:ASP:HB2	1:A:337:GLN:HG3	2.02	0.41
1:A:356:ARG:HA	1:A:385:LEU:O	2.21	0.41
1:A:361:VAL:HG23	1:A:381:TRP:HB2	2.02	0.41
1:B:172:VAL:O	1:B:176:LEU:HG	2.21	0.41
1:B:228:GLU:O	1:B:232:LYS:HB2	2.21	0.41
1:B:353:ASP:OD1	1:B:353:ASP:N	2.44	0.41
1:A:330:LYS:HB3	1:A:330:LYS:HE3	1.88	0.41
1:A:383:LEU:HD11	1:A:391:LEU:HD22	2.03	0.40
1:A:329:ASP:OD1	1:A:330:LYS:N	2.50	0.40
1:B:133:LEU:O	1:B:137:LYS:HG3	2.21	0.40
1:A:95:ILE:HG21	1:A:119:LEU:HG	2.03	0.40
1:B:306:SER:HB3	1:B:310:ARG:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	378/477 (79%)	335 (89%)	43 (11%)	0	100	100
1	B	378/477 (79%)	338 (89%)	40 (11%)	0	100	100
All	All	756/954 (79%)	673 (89%)	83 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	326/399 (82%)	320 (98%)	6 (2%)	59	77
1	B	326/399 (82%)	316 (97%)	10 (3%)	40	62
All	All	652/798 (82%)	636 (98%)	16 (2%)	47	68

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ARG
1	A	136	GLN
1	A	168	PHE
1	A	237	PHE
1	A	282	ARG
1	A	441	PHE
1	B	101	ARG
1	B	146	ARG
1	B	166	ARG
1	B	169	ARG
1	B	240	LYS
1	B	330	LYS
1	B	346	TYR
1	B	357	TRP
1	B	398	LYS

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Mol	Chain	Res	Type
1	B	407	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

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

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, 95^{th} 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	382/477 (80%)	1.84	140 (36%)	0	1	221, 309, 410, 462	0
1	B	382/477 (80%)	1.70	131 (34%)	0	2	148, 275, 365, 438	0
All	All	764/954 (80%)	1.77	271 (35%)	0	2	148, 296, 387, 462	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	470	VAL	9.5
1	A	454	ASP	9.3
1	A	360	GLY	8.9
1	B	348	GLU	8.8
1	A	469	LEU	8.4
1	A	447	GLY	8.3
1	B	469	LEU	7.8
1	B	360	GLY	7.2
1	B	330	LYS	6.6
1	B	371	ARG	6.5
1	B	399	GLU	6.2
1	B	454	ASP	6.1
1	A	466	PRO	6.0
1	A	448	PRO	6.0
1	A	292	THR	5.9
1	A	359	LEU	5.8
1	B	401	ARG	5.8
1	B	350	GLU	5.8
1	A	453	PHE	5.6
1	B	398	LYS	5.6
1	A	348	GLU	5.6
1	B	453	PHE	5.5
1	A	240	LYS	5.3
1	B	400	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	268	ILE	5.3
1	A	449	VAL	5.2
1	A	267	VAL	5.2
1	A	312	GLU	5.2
1	B	329	ASP	5.0
1	B	457	TRP	4.9
1	B	349	VAL	4.9
1	B	470	VAL	4.9
1	A	333	ALA	4.8
1	B	468	LEU	4.8
1	B	402	ALA	4.7
1	A	320	PRO	4.7
1	A	302	LEU	4.7
1	A	338	GLN	4.7
1	A	300	PRO	4.6
1	A	288	LEU	4.6
1	A	241	PHE	4.6
1	A	313	CYS	4.6
1	B	119	LEU	4.6
1	B	301	SER	4.6
1	B	358	ALA	4.6
1	A	119	LEU	4.5
1	A	362	MET	4.5
1	B	318	ALA	4.5
1	B	319	PRO	4.5
1	A	371	ARG	4.5
1	A	94	SER	4.4
1	A	229	VAL	4.3
1	A	147	LYS	4.3
1	B	309	ARG	4.3
1	B	466	PRO	4.2
1	B	452	ILE	4.2
1	B	267	VAL	4.2
1	B	299	HIS	4.1
1	B	359	LEU	4.1
1	B	374	ALA	4.0
1	A	450	TYR	4.0
1	A	452	ILE	4.0
1	A	381	TRP	4.0
1	A	103	LEU	4.0
1	B	390	ILE	4.0
1	B	152	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	468	LEU	3.9
1	A	321	ALA	3.9
1	B	147	LYS	3.9
1	B	370	GLY	3.9
1	A	374	ALA	3.9
1	B	456	CYS	3.9
1	A	361	VAL	3.9
1	B	361	VAL	3.8
1	A	230	ALA	3.8
1	A	336	ALA	3.8
1	A	446	PRO	3.8
1	A	367	SER	3.8
1	B	382	LEU	3.8
1	A	382	LEU	3.8
1	A	404	ARG	3.7
1	B	302	LEU	3.7
1	A	150	THR	3.7
1	B	347	TRP	3.7
1	A	457	TRP	3.7
1	A	349	VAL	3.6
1	A	332	VAL	3.6
1	A	402	ALA	3.6
1	B	300	PRO	3.6
1	A	350	GLU	3.6
1	B	291	LEU	3.6
1	B	151	VAL	3.6
1	A	151	VAL	3.6
1	A	455	VAL	3.5
1	B	268	ILE	3.5
1	B	320	PRO	3.5
1	B	154	LEU	3.5
1	A	401	ARG	3.5
1	A	467	LEU	3.5
1	A	331	ALA	3.5
1	A	363	ALA	3.5
1	A	258	PRO	3.5
1	B	94	SER	3.5
1	B	373	HIS	3.5
1	B	95	ILE	3.4
1	A	95	ILE	3.4
1	B	333	ALA	3.4
1	A	293	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	120	LEU	3.4
1	B	332	VAL	3.4
1	A	121	PRO	3.3
1	A	365	ASP	3.4
1	A	291	LEU	3.3
1	A	232	LYS	3.3
1	A	239	MET	3.3
1	B	129	LEU	3.3
1	B	150	THR	3.3
1	B	304	VAL	3.3
1	A	337	GLN	3.3
1	A	247	ARG	3.3
1	A	303	VAL	3.2
1	A	148	GLU	3.2
1	A	424	LEU	3.2
1	B	265	LEU	3.2
1	B	120	LEU	3.2
1	B	205	LEU	3.2
1	A	257	PRO	3.2
1	A	351	VAL	3.2
1	B	155	GLU	3.1
1	A	451	PRO	3.1
1	B	121	PRO	3.1
1	A	368	ARG	3.1
1	A	438	ILE	3.1
1	B	331	ALA	3.1
1	B	351	VAL	3.1
1	B	449	VAL	3.1
1	A	301	SER	3.0
1	B	131	THR	3.0
1	A	445	LEU	3.0
1	B	356	ARG	2.9
1	A	364	ALA	2.9
1	B	372	LEU	2.9
1	B	303	VAL	2.9
1	A	238	LEU	2.9
1	A	358	ALA	2.9
1	A	269	SER	2.9
1	A	266	PRO	2.9
1	B	425	ALA	2.9
1	A	396	GLU	2.9
1	B	143	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	403	LEU	2.8
1	B	148	GLU	2.8
1	A	319	PRO	2.8
1	A	149	LYS	2.8
1	B	258	PRO	2.8
1	B	438	ILE	2.8
1	B	256	PRO	2.8
1	B	362	MET	2.8
1	A	334	VAL	2.8
1	A	244	VAL	2.8
1	B	414	GLY	2.7
1	B	240	LYS	2.7
1	A	456	CYS	2.7
1	B	251	ILE	2.7
1	B	313	CYS	2.7
1	A	96	TYR	2.7
1	B	289	GLU	2.7
1	B	442	HIS	2.7
1	B	136	GLN	2.7
1	B	413	ILE	2.7
1	A	289	GLU	2.7
1	B	141	GLN	2.7
1	B	149	LYS	2.7
1	A	155	GLU	2.7
1	B	144	CYS	2.7
1	B	312	GLU	2.6
1	A	110	SER	2.6
1	B	198	ARG	2.6
1	A	226	LEU	2.6
1	B	130	LYS	2.6
1	A	347	TRP	2.6
1	A	389	LYS	2.6
1	B	308	GLY	2.6
1	B	439	PHE	2.6
1	A	285	MET	2.6
1	B	125	ALA	2.6
1	A	326	ARG	2.6
1	A	154	LEU	2.6
1	A	427	TYR	2.5
1	A	139	GLN	2.5
1	B	158	LEU	2.5
1	A	370	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	152	ALA	2.5
1	B	424	LEU	2.5
1	B	222	MET	2.5
1	B	266	PRO	2.5
1	A	425	ALA	2.5
1	B	153	VAL	2.5
1	B	448	PRO	2.5
1	A	286	PRO	2.4
1	A	304	VAL	2.4
1	A	330	LYS	2.4
1	A	112	GLY	2.4
1	B	307	SER	2.4
1	B	257	PRO	2.4
1	B	238	LEU	2.4
1	A	142	GLU	2.4
1	B	237	PHE	2.4
1	B	427	TYR	2.4
1	A	311	VAL	2.4
1	B	437	PRO	2.4
1	B	404	ARG	2.4
1	B	216	LEU	2.4
1	A	287	ALA	2.4
1	A	439	PHE	2.4
1	B	132	GLN	2.4
1	B	459	ASP	2.4
1	A	314	SER	2.4
1	B	209	LEU	2.3
1	B	239	MET	2.4
1	B	415	LEU	2.3
1	B	381	TRP	2.3
1	B	223	GLU	2.3
1	A	242	CYS	2.3
1	A	366	ALA	2.3
1	B	146	ARG	2.3
1	B	263	ILE	2.3
1	A	405	THR	2.3
1	A	435	LEU	2.3
1	A	233	PRO	2.3
1	B	378	GLN	2.3
1	B	367	SER	2.3
1	A	426	PHE	2.3
1	B	455	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	339	LEU	2.3
1	A	157	GLN	2.3
1	B	103	LEU	2.2
1	B	142	GLU	2.2
1	A	383	LEU	2.2
1	A	335	VAL	2.2
1	A	256	PRO	2.2
1	B	133	LEU	2.2
1	B	169	ARG	2.2
1	B	451	PRO	2.2
1	A	414	GLY	2.2
1	B	467	LEU	2.2
1	B	391	LEU	2.2
1	B	357	TRP	2.2
1	B	440	SER	2.1
1	B	447	GLY	2.1
1	A	153	VAL	2.1
1	B	201	ALA	2.1
1	A	138	MET	2.1
1	A	413	ILE	2.1
1	A	144	CYS	2.1
1	A	237	PHE	2.1
1	A	191	ASP	2.1
1	A	205	LEU	2.1
1	A	243	LEU	2.1
1	A	129	LEU	2.1
1	A	146	ARG	2.1
1	A	378	GLN	2.1
1	A	85	HIS	2.1
1	A	373	HIS	2.0
1	A	394	HIS	2.0
1	B	126	GLN	2.0
1	B	252	LEU	2.0
1	B	397	ALA	2.0
1	A	236	GLU	2.0
1	B	393	ALA	2.0
1	B	288	LEU	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)

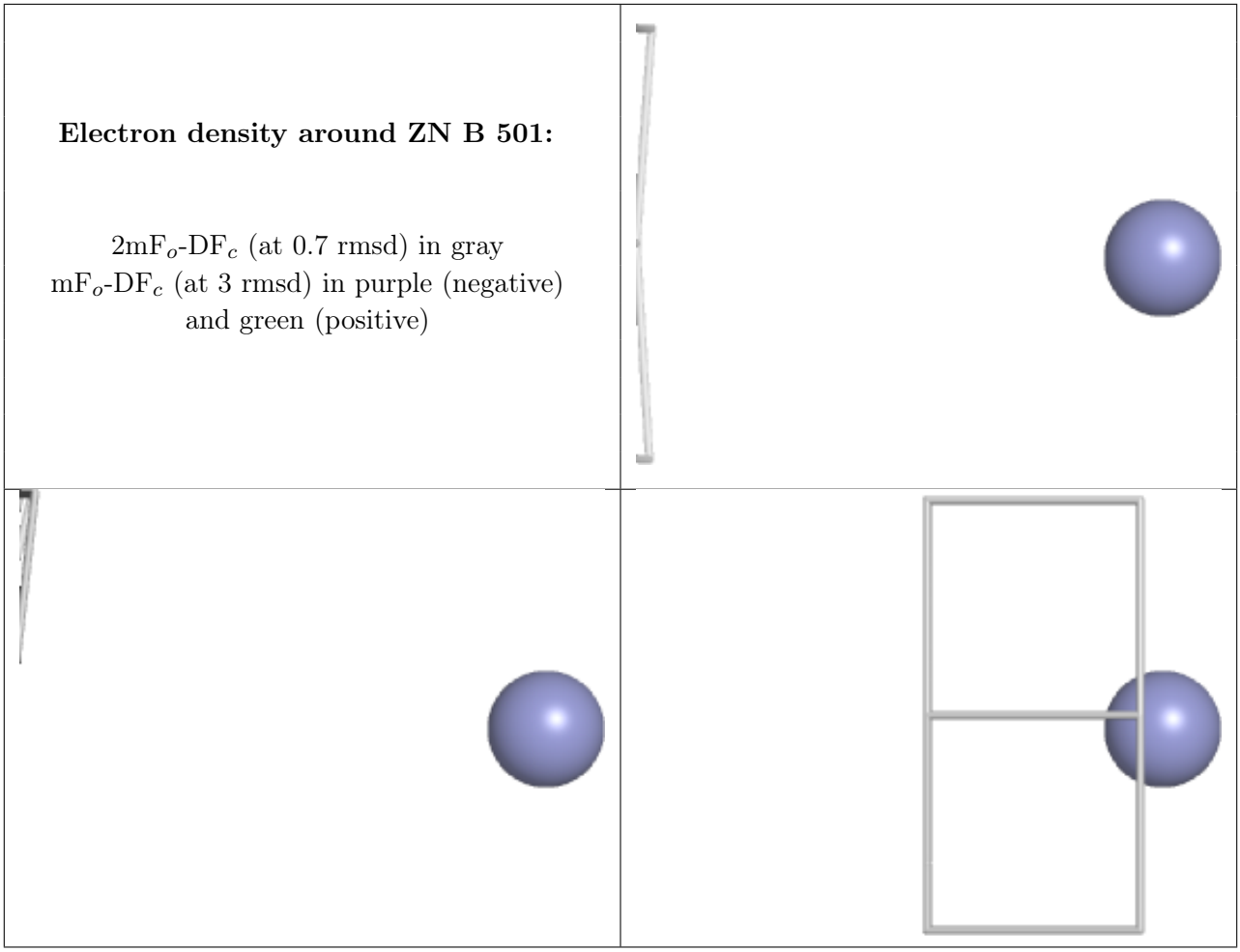
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	501	1/1	0.96	0.13	300,300,300,300	0
2	ZN	B	502	1/1	0.96	0.16	365,365,365,365	0
2	ZN	A	501	1/1	0.98	0.24	317,317,317,317	0
2	ZN	A	502	1/1	0.99	0.13	318,318,318,318	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.

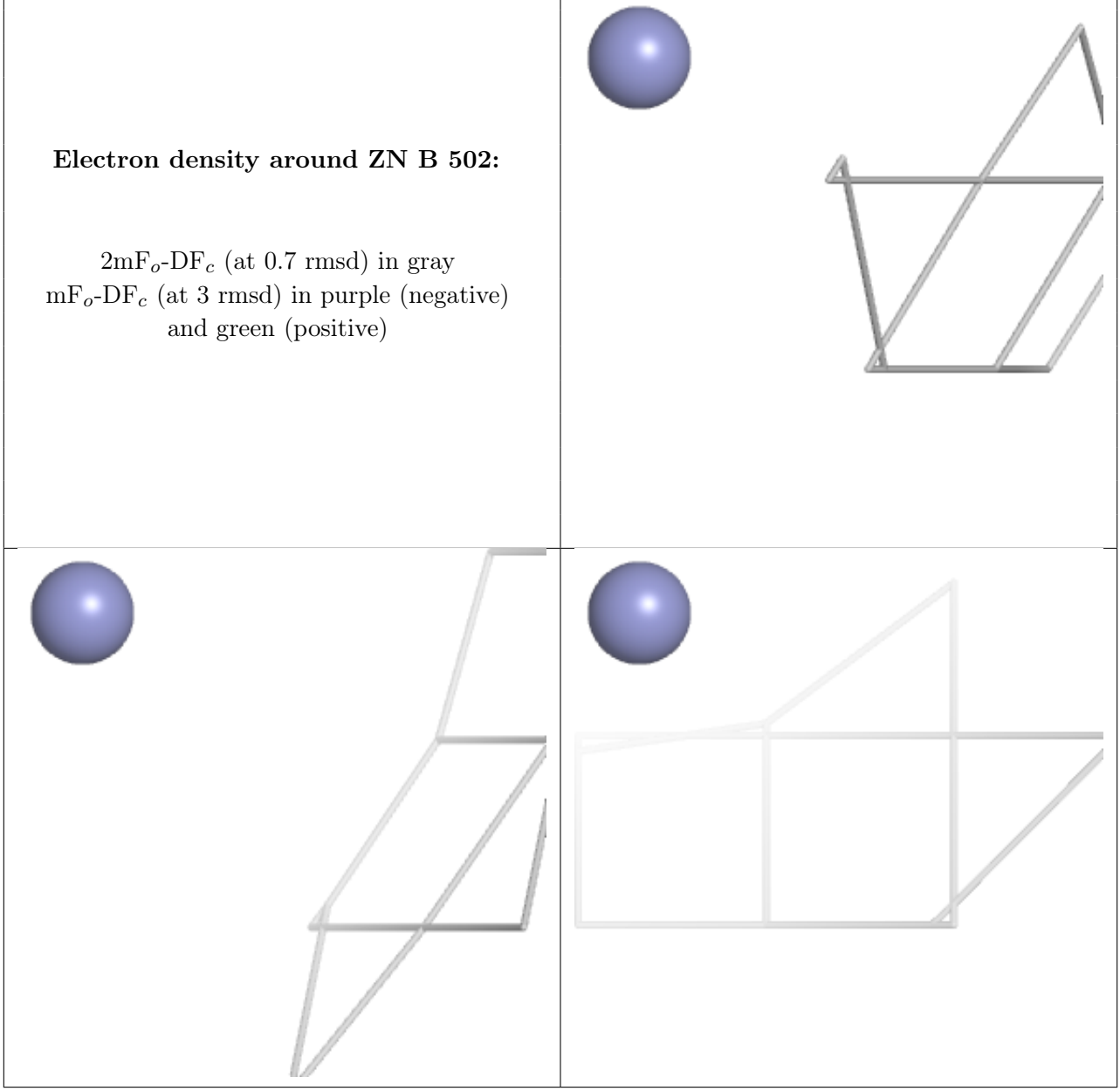
Electron density around ZN B 501:

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



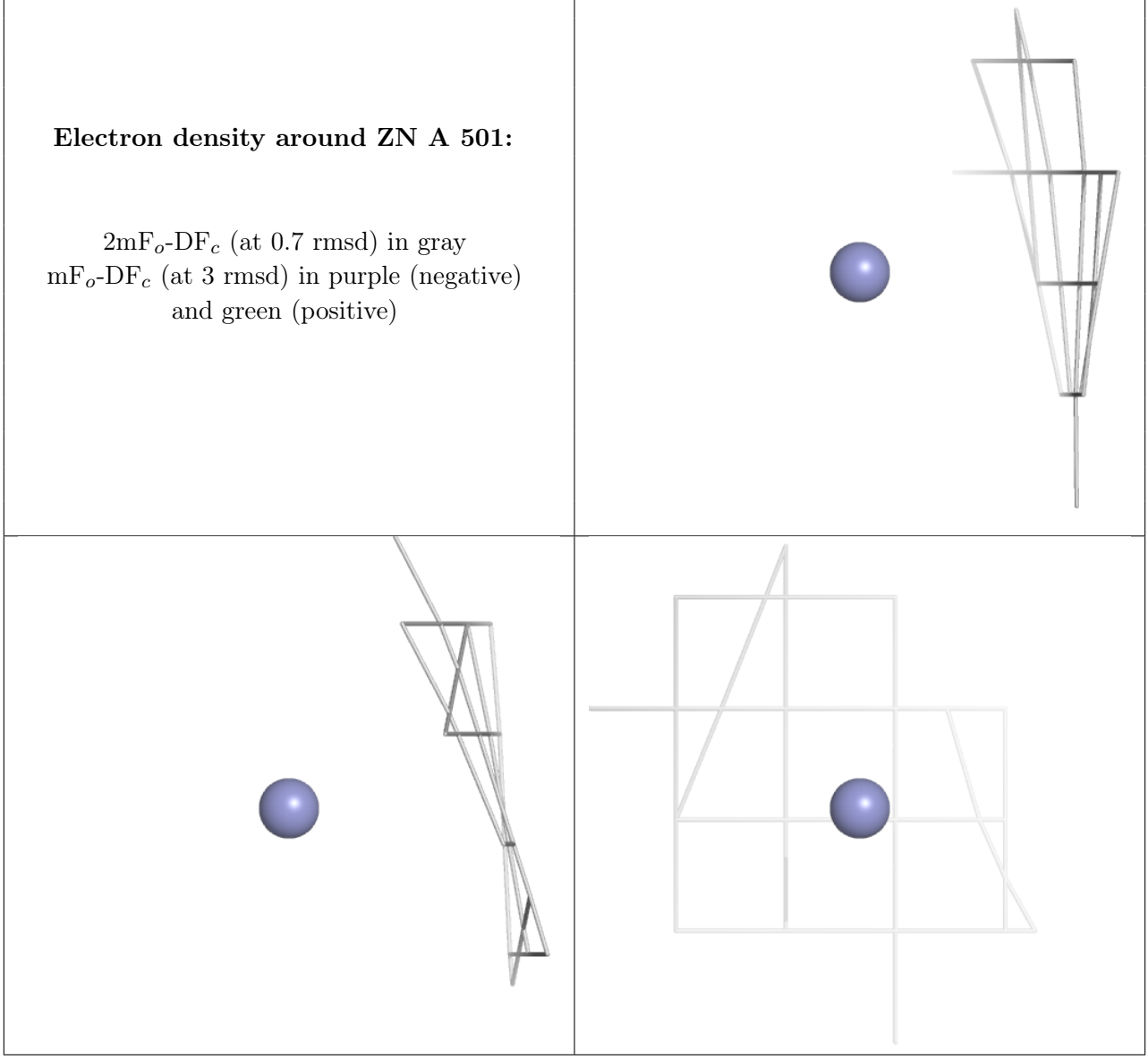
Electron density around ZN B 502:

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



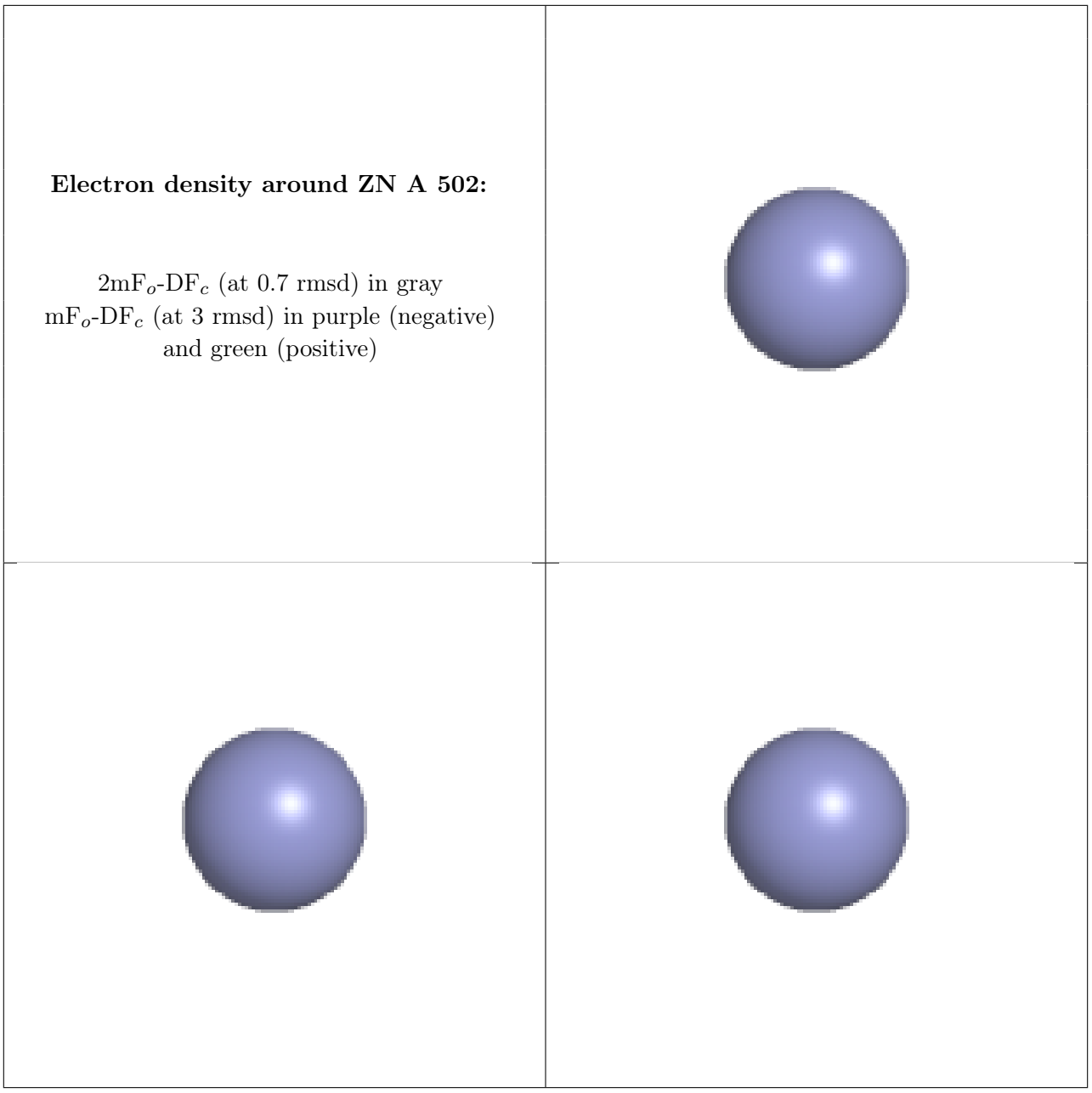
Electron density around ZN A 501:

$2mF_o$-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 502:

$2mF_o$-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.