



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:29 PM GMT

PDB ID : 5AFQ
Title : Crystal structure of RPC62 - RPC32 beta
Authors : Fribourg, S.
Deposited on : 2015-01-23
Resolution : 7.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

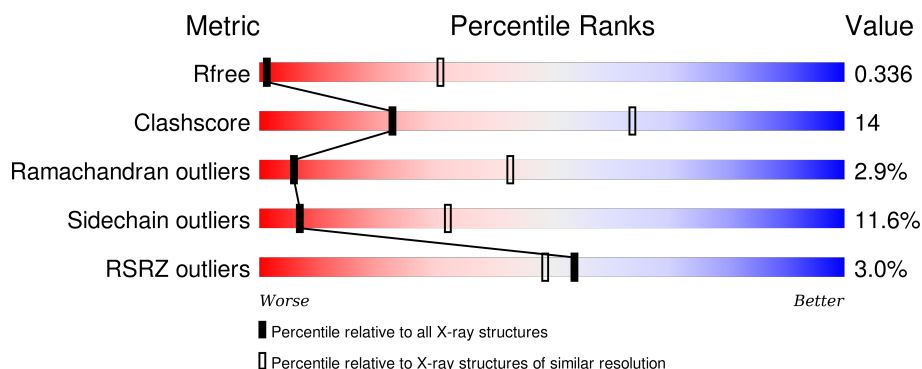
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 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}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	534	<div> <div>48%</div> <div>31%</div> <div>••</div> <div>17%</div> </div>
1	B	534	<div> <div>4%</div> <div>49%</div> <div>30%</div> <div>•</div> <div>17%</div> </div>
2	D	218	<div> <div>22%</div> <div>•</div> <div>76%</div> </div>
2	E	218	<div> <div>9%</div> <div>91%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7387 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 DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3511	2207	611	670	23			
1	B	444	Total	C	N	O	S	0	0	0
			3516	2210	612	671	23			

- Molecule 2 is a protein called RPC32 BETA (RPC7L).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	53	Total	C	N	O	0	0	0
			265	159	53	53			
2	E	19	Total	C	N	O	0	0	0
			95	57	19	19			

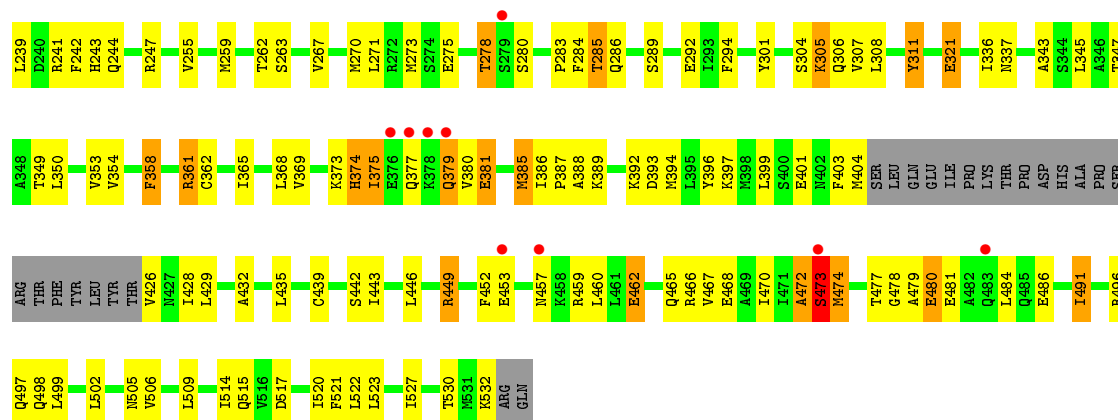
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

[illegible]

Chain B:

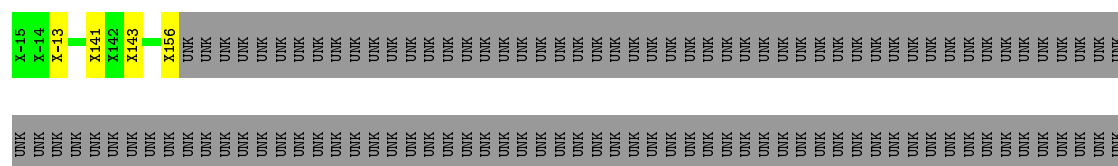
49% 30% 4% 17%

M1 T2 Q3 A4 E5 L8 C9 S10 L11 L12 H16 F17 I20 V21 G25 V26 H27 L28 N13 I29 R30 T31 G32 S33 Q34 P35 V38 T45 D48 A53 L54 C55 V56 L57 H60 N61 L62 V63 S64 Y65 Q66 K69 V72 V73 Y74 A75 E76 A77 Q78 Q79 S80 R81 R87 P88 P89 R90 Y91 I92 I93 Y94 T97 L98 L99 S100 D101 L105 L112 N113 G114 K115 V125 L129 T130 E131 T132 D135 A136 K137 T138 M139 T147 F148 L151 L156 V157 Q158 V159 R159 C160 P161 A162 V163 P160 T161 T162 T163 G164 A165 S166 S167 S168 S169 S170 S171 S172 S173 S174 S175 S176 S177 S178 S179 S180 S181 S182 S183 S184 S185 S186 S187 S188 S189 S190 S191 S192 S193 S194 S195 S196 S197 S198 S199 S200 S201 S202 S203 S204 S205 S206 S207 S208 S209 S210 S211 S212 S213 S214 S215 S216 S217 S218 S219 S220 S221 S222 S223 S224 S225 S226 S227 S228 S229 S230 S231 S232 S233 S234 S235 S236 S237 S238 S239 S240 S241 S242 S243 S244 S245 S246 S247 S248 S249 S250 S251 S252 S253 S254 S255 S256 S257 S258 S259 S260 S261 S262 S263 S264 S265 S266 S267 S268 S269 S270 S271 S272 S273 S274 S275 S276 S277 S278 S279 S280 S281 S282 S283 S284 S285 S286 S287 S288 S289 S290 S291 S292 S293 S294 S295 S296 S297 S298 S299 S300 S301 S302 S303 S304 S305 S306 S307 S308 S309 S310 S311 S312 S313 S314 S315 S316 S317 S318 S319 S320 S321 S322 S323 S324 S325 S326 S327 S328 S329 S330 S331 S332 S333 S334 S335 S336 S337 S338 S339 S340 S341 S342 S343 S344 S345 S346 S347 S348 S349 S350 S351 S352 S353 S354 S355 S356 S357 S358 S359 S360 S361 S362 S363 S364 S365 S366 S367 S368 S369 S370 S371 S372 S373 S374 S375 S376 S377 S378 S379 S380 S381 S382 S383 S384 S385 S386 S387 S388 S389 S390 S391 S392 S393 S394 S395 S396 S397 S398 S399 S400 S401 S402 S403 S404 S405 S406 S407 S408 S409 S410 S411 S412 S413 S414 S415 S416 S417 S418 S419 S420 S421 S422 S423 S424 S425 S426 S427 S428 S429 S430 S431 S432 S433 S434 S435 S436 S437 S438 S439 S440 S441 S442 S443 S444 S445 S446 S447 S448 S449 S450 S451 S452 S453 S454 S455 S456 S457 S458 S459 S460 S461 S462 S463 S464 S465 S466 S467 S468 S469 S470 S471 S472 S473 S474 S475 S476 S477 S478 S479 S480 S481 S482 S483 S484 S485 S486 S487 S488 S489 S490 S491 S492 S493 S494 S495 S496 S497 S498 S499 S500 S501 S502 S503 S504 S505 S506 S507 S508 S509 S510 S511 S512 S513 S514 S515 S516 S517 S518 S519 S520 S521 S522 S523 S524 S525 S526 S527 S528 S529 S530 S531 S532 S533 S534 S535 S536 S537 S538 S539 S540 S541 S542 S543 S544 S545 S546 S547 S548 S549 S550 S551 S552 S553 S554 S555 S556 S557 S558 S559 S560 S561 S562 S563 S564 S565 S566 S567 S568 S569 S570 S571 S572 S573 S574 S575 S576 S577 S578 S579 S580 S581 S582 S583 S584 S585 S586 S587 S588 S589 S590 S591 S592 S593 S594 S595 S596 S597 S598 S599 S600 S601 S602 S603 S604 S605 S606 S607 S608 S609 S610 S611 S612 S613 S614 S615 S616 S617 S618 S619 S620 S621 S622 S623 S624 S625 S626 S627 S628 S629 S630 S631 S632 S633 S634 S635 S636 S637 S638 S639 S640 S641 S642 S643 S644 S645 S646 S647 S648 S649 S650 S651 S652 S653 S654 S655 S656 S657 S658 S659 S660 S661 S662 S663 S664 S665 S666 S667 S668 S669 S670 S671 S672 S673 S674 S675 S676 S677 S678 S679 S680 S681 S682 S683 S684 S685 S686 S687 S688 S689 S690 S691 S692 S693 S694 S695 S696 S697 S698 S699 S700 S701 S702 S703 S704 S705 S706 S707 S708 S709 S710 S711 S712 S713 S714 S715 S716 S717 S718 S719 S720 S721 S722 S723 S724 S725 S726 S727 S728 S729 S730 S731 S732 S733 S734 S735 S736 S737 S738 S739 S740 S741 S742 S743 S744 S745 S746 S747 S748 S749 S750 S751 S752 S753 S754 S755 S756 S757 S758 S759 S760 S761 S762 S763 S764 S765 S766 S767 S768 S769 S770 S771 S772 S773 S774 S775 S776 S777 S778 S779 S780 S781 S782 S783 S784 S785 S786 S787 S788 S789 S790 S791 S792 S793 S794 S795 S796 S797 S798 S799 S800 S801 S802 S803 S804 S805 S806 S807 S808 S809 S810 S811 S812 S813 S814 S815 S816 S817 S818 S819 S820 S821 S822 S823 S824 S825 S826 S827 S828 S829 S830 S831 S832 S833 S834 S835 S836 S837 S838 S839 S840 S841 S842 S843 S844 S845 S846 S847 S848 S849 S850 S851 S852 S853 S854 S855 S856 S857 S858 S859 S860 S861 S862 S863 S864 S865 S866 S867 S868 S869 S870 S871 S872 S873 S874 S875 S876 S877 S878 S879 S880 S881 S882 S883 S884 S885 S886 S887 S888 S889 S890 S891 S892 S893 S894 S895 S896 S897 S898 S899 S900 S901 S902 S903 S904 S905 S906 S907 S908 S909 S910 S911 S912 S913 S914 S915 S916 S917 S918 S919 S920 S921 S922 S923 S924 S925 S926 S927 S928 S929 S930 S931 S932 S933 S934 S935 S936 S937 S938 S939 S940 S941 S942 S943 S944 S945 S946 S947 S948 S949 S950 S951 S952 S953 S954 S955 S956 S957 S958 S959 S960 S961 S962 S963 S964 S965 S966 S967 S968 S969 S970 S971 S972 S973 S974 S975 S976 S977 S978 S979 S980 S981 S982 S983 S984 S985 S986 S987 S988 S989 S990 S991 S992 S993 S994 S995 S996 S997 S998 S999 S1000 S1001 S1002 S1003 S1004 S1005 S1006 S1007 S1008 S1009 S1010 S1011 S1012 S1013 S1014 S1015 S1016 S1017 S1018 S1019 S1020 S1021 S1022 S1023 S1024 S1025 S1026 S1027 S1028 S1029 S1030 S1031 S1032 S1033 S1034 S1035 S1036 S1037 S1038 S1039 S1040 S1041 S1042 S1043 S1044 S1045 S1046 S1047 S1048 S1049 S1050 S1051 S1052 S1053 S1054 S10



- Molecule 2: RPC32 BETA (RPC7L)

Chain D: 22% . 76%



- Molecule 2: RPC32 BETA (RPC7L)

Chain E:  9% 91%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	218.27Å 218.27Å 182.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.75 – 7.00 30.27 – 7.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.75-7.00) 99.3 (30.27-7.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 7.24Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.268 , 0.298 0.277 , 0.336	Depositor DCC
R_{free} test set	334 reflections (9.45%)	DCC
Wilson B-factor (Å ²)	452.8	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 393.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Outliers	0 of 3612 reflections	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	7387	wwPDB-VP
Average B, all atoms (Å ²)	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0/3558	0.72	2/4798 (0.0%)
1	B	0.40	0/3563	0.73	3/4805 (0.1%)
All	All	0.41	0/7121	0.73	5/9603 (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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	472	ALA	C-N-CA	8.45	142.81	121.70
1	A	98	LEU	CA-CB-CG	7.75	133.13	115.30
1	B	374	HIS	C-N-CA	6.76	138.60	121.70
1	B	472	ALA	CA-C-N	5.78	129.92	117.20
1	A	233	ILE	C-N-CA	5.13	134.53	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	78	GLN	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	3511	0	3550	100	0
1	B	3516	0	3552	98	0
2	D	265	0	60	4	0
2	E	95	0	21	0	0
All	All	7387	0	7183	198	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 14.

All (198) 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:435:LEU:HA	1:A:438:ARG:HD2	1.44	1.00
1:A:453:GLU:HB3	1:A:502:LEU:HD11	1.54	0.88
1:B:465:GLN:O	1:B:468:GLU:HG2	1.73	0.87
1:B:404:MET:HA	1:B:426:VAL:HA	1.56	0.86
1:B:474:MET:SD	1:B:480:GLU:HG2	2.18	0.83
1:A:278:THR:HG21	1:A:285:THR:HA	1.65	0.79
1:B:278:THR:HG21	1:B:285:THR:HA	1.64	0.78
1:B:401:GLU:HB2	1:B:403:PHE:HE1	1.56	0.70
1:B:247:ARG:HH11	1:B:280:SER:HA	1.59	0.68
1:B:270:MET:HB3	1:B:336:ILE:HD11	1.74	0.68
1:B:374:HIS:HA	1:B:375:ILE:O	1.93	0.67
1:A:247:ARG:HH11	1:A:280:SER:HA	1.59	0.67
1:A:401:GLU:HB2	1:A:403:PHE:HE1	1.60	0.67
1:A:270:MET:HB3	1:A:336:ILE:HD11	1.75	0.67
1:A:381:GLU:HG3	1:A:388:ALA:HA	1.76	0.66
1:B:472:ALA:HB3	1:B:473:SER:HB2	1.77	0.65
1:B:381:GLU:HG3	1:B:388:ALA:HA	1.77	0.65
1:A:304:SER:HB3	1:A:307:VAL:HG23	1.79	0.65
1:B:374:HIS:CE1	1:B:379:GLN:HG3	2.32	0.65
1:B:255:VAL:HG21	1:B:267:VAL:HG21	1.80	0.63
1:B:347:THR:HA	1:B:350:LEU:HD12	1.79	0.63
1:A:453:GLU:HB3	1:A:502:LEU:CD1	2.25	0.63
1:A:255:VAL:HG21	1:A:267:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LEU:HA	1:B:242:PHE:HD2	1.64	0.62
1:A:239:LEU:HA	1:A:242:PHE:HD2	1.64	0.61
1:A:347:THR:HA	1:A:350:LEU:HD12	1.83	0.61
1:B:284:PHE:HD1	1:B:337:ASN:HA	1.66	0.60
1:A:284:PHE:HD1	1:A:337:ASN:HA	1.67	0.60
1:A:159:ARG:HH21	1:A:235:TRP:HZ2	1.51	0.58
1:B:354:VAL:HG13	1:B:358:PHE:HD2	1.68	0.58
1:A:361:ARG:HH12	1:A:386:ILE:HG21	1.69	0.58
1:B:304:SER:HB2	1:B:307:VAL:HG23	1.86	0.57
1:A:443:ILE:HD11	1:A:520:ILE:HD11	1.86	0.57
1:B:361:ARG:HH12	1:B:386:ILE:HG21	1.70	0.57
1:B:9:CYS:HA	1:B:12:LEU:HD12	1.87	0.57
1:A:496:ARG:HA	1:A:499:LEU:HD12	1.86	0.57
1:B:294:PHE:HB2	1:B:308:LEU:HD22	1.87	0.56
1:A:294:PHE:HB2	1:A:308:LEU:HD22	1.87	0.56
1:B:449:ARG:HH21	1:B:452:PHE:HD2	1.52	0.56
1:B:443:ILE:HD11	1:B:520:ILE:HD11	1.88	0.56
1:A:435:LEU:HD23	1:A:523:LEU:HD21	1.88	0.56
1:B:239:LEU:HA	1:B:242:PHE:CD2	2.41	0.56
1:A:9:CYS:HA	1:A:12:LEU:HD12	1.86	0.56
1:B:466:ARG:O	1:B:470:ILE:HG12	2.06	0.56
1:B:62:LEU:HD23	1:B:81:ARG:HG3	1.88	0.56
1:A:239:LEU:HA	1:A:242:PHE:CD2	2.41	0.55
1:A:62:LEU:HD23	1:A:81:ARG:HG3	1.88	0.55
1:B:474:MET:HE2	1:B:474:MET:HA	1.89	0.55
1:A:474:MET:HG2	1:A:478:GLY:O	2.08	0.54
1:B:435:LEU:HD23	1:B:523:LEU:HD21	1.89	0.54
1:A:466:ARG:O	1:A:470:ILE:HG12	2.08	0.54
1:B:374:HIS:CE1	1:B:379:GLN:CG	2.91	0.53
1:B:374:HIS:HE1	1:B:379:GLN:HG3	1.72	0.53
1:A:365:ILE:HA	1:A:368:LEU:HD12	1.91	0.53
1:B:9:CYS:O	1:B:12:LEU:HB2	2.09	0.52
1:A:362:CYS:HA	1:A:365:ILE:HG12	1.91	0.52
1:A:374:HIS:CD2	1:A:399:LEU:HG	2.44	0.52
1:A:89:PRO:HA	1:A:92:ILE:HD12	1.92	0.52
1:A:394:MET:HA	1:A:397:LYS:HD2	1.92	0.52
1:A:377:GLN:HA	1:A:380:VAL:HB	1.92	0.51
1:A:9:CYS:O	1:A:12:LEU:HB2	2.11	0.51
1:B:365:ILE:HA	1:B:368:LEU:HD12	1.92	0.51
1:A:467:VAL:HG11	1:A:491:ILE:HD11	1.93	0.50
1:B:496:ARG:HA	1:B:499:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:GLU:HB2	1:B:403:PHE:CE1	2.44	0.50
1:B:474:MET:HA	1:B:474:MET:CE	2.42	0.50
1:B:17:PHE:HD2	1:B:21:VAL:HG11	1.77	0.50
1:B:377:GLN:HA	1:B:380:VAL:HB	1.94	0.49
1:B:25:GLY:HA2	1:B:28:LEU:HD12	1.94	0.49
1:B:350:LEU:O	1:B:354:VAL:HG23	2.13	0.49
1:B:439:CYS:O	1:B:443:ILE:HG13	2.11	0.49
1:B:89:PRO:HA	1:B:92:ILE:HD12	1.94	0.49
1:A:233:ILE:HG13	1:A:234:TYR:H	1.77	0.49
1:B:35:PRO:HG2	1:B:38:VAL:HG23	1.93	0.49
1:B:289:SER:OG	1:B:292:GLU:HG2	2.13	0.49
1:A:17:PHE:HD2	1:A:21:VAL:HG11	1.77	0.49
1:A:343:ALA:O	1:A:347:THR:HG23	2.13	0.48
1:A:471:ILE:HA	1:A:474:MET:HB3	1.95	0.48
1:A:26:VAL:HA	1:A:29:ILE:HD12	1.94	0.48
1:A:271:LEU:O	1:A:275:GLU:HG3	2.13	0.48
1:B:271:LEU:O	1:B:275:GLU:HG3	2.13	0.48
1:B:343:ALA:O	1:B:347:THR:HG23	2.14	0.48
1:B:467:VAL:HG11	1:B:491:ILE:HD11	1.96	0.48
1:A:283:PRO:HB3	1:A:532:LYS:HD3	1.95	0.48
1:B:283:PRO:HB3	1:B:532:LYS:HD3	1.96	0.48
1:A:523:LEU:O	1:A:527:ILE:HG12	2.14	0.48
1:B:523:LEU:O	1:B:527:ILE:HG12	2.14	0.48
1:B:28:LEU:HD13	1:B:63:VAL:HG21	1.96	0.47
1:A:61:ASN:OD1	1:A:115:LYS:HG3	2.13	0.47
1:A:25:GLY:HA2	1:A:28:LEU:HD12	1.96	0.47
1:A:35:PRO:HG2	1:A:38:VAL:HG23	1.96	0.47
1:B:87:ARG:NH2	1:B:521:PHE:HA	2.29	0.47
1:B:394:MET:HA	1:B:397:LYS:HD2	1.96	0.47
1:B:61:ASN:OD1	1:B:115:LYS:HG3	2.15	0.47
1:B:88:TYR:HA	1:B:91:TYR:HD2	1.80	0.47
1:A:136:GLY:C	1:A:138:THR:H	2.17	0.47
1:B:505:ASN:O	1:B:509:LEU:HG	2.15	0.47
1:B:136:GLY:C	1:B:138:THR:H	2.17	0.47
1:A:129:LEU:HD23	1:A:139:MET:HG2	1.96	0.47
1:A:87:ARG:NH2	1:A:521:PHE:HA	2.29	0.47
1:A:88:TYR:HA	1:A:91:TYR:HD2	1.80	0.47
1:B:362:CYS:HA	1:B:365:ILE:HG12	1.96	0.46
1:A:262:THR:HB	1:A:311:TYR:OH	2.16	0.46
1:B:26:VAL:HA	1:B:29:ILE:HD12	1.97	0.46
1:A:305:LYS:O	1:A:308:LEU:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASP:HA	1:B:396:TYR:CD2	2.51	0.46
1:A:481:GLU:HA	1:A:484:LEU:HD12	1.98	0.46
2:D:141:UNK:C	2:D:143:UNK:N	2.78	0.46
1:A:350:LEU:O	1:A:354:VAL:HG23	2.15	0.46
1:A:439:CYS:O	1:A:443:ILE:HG13	2.15	0.45
1:A:28:LEU:HD13	1:A:63:VAL:HG21	1.98	0.45
1:B:5:GLU:HG2	1:B:79:CYS:SG	2.56	0.45
1:A:141:TYR:CD1	2:D:156:UNK:HA	2.51	0.45
1:A:478:GLY:C	1:A:480:GLU:H	2.20	0.45
1:B:442:SER:O	1:B:446:LEU:HG	2.15	0.45
1:A:374:HIS:H	1:A:426:VAL:N	2.15	0.45
1:A:393:ASP:HA	1:A:396:TYR:CD2	2.52	0.45
1:A:284:PHE:CD1	1:A:337:ASN:HA	2.49	0.45
1:A:247:ARG:NH1	1:A:280:SER:HA	2.30	0.45
1:B:1:MET:N	1:B:2:THR:HA	2.32	0.45
1:A:99:TYR:HB3	1:A:147:THR:HG23	1.98	0.45
1:B:131:GLU:HG3	1:B:132:THR:HG23	1.99	0.45
1:B:99:TYR:HB3	1:B:147:THR:HG23	1.99	0.45
1:A:1:MET:N	1:A:2:THR:HA	2.32	0.44
1:B:506:VAL:HA	1:B:509:LEU:HD12	1.98	0.44
1:A:449:ARG:O	1:A:453:GLU:HG2	2.18	0.44
1:B:305:LYS:O	1:B:308:LEU:HB3	2.17	0.44
1:A:429:LEU:O	1:A:432:ALA:HB3	2.17	0.44
1:A:514:ILE:O	1:A:517:ASP:HB3	2.18	0.44
1:A:26:VAL:O	1:A:30:ARG:HG3	2.16	0.44
1:A:95:THR:O	1:A:98:LEU:HD12	2.17	0.44
1:A:442:SER:O	1:A:446:LEU:HG	2.18	0.44
1:B:453:GLU:O	1:B:457:ASN:HB2	2.17	0.44
1:B:374:HIS:HA	1:B:375:ILE:C	2.37	0.44
1:B:497:GLN:OE1	1:B:497:GLN:HA	2.18	0.43
1:A:386:ILE:HB	1:A:387:PRO:HD2	2.00	0.43
1:B:26:VAL:O	1:B:30:ARG:HG3	2.18	0.43
1:A:401:GLU:HB2	1:A:403:PHE:CE1	2.47	0.43
1:A:35:PRO:HB3	1:A:72:VAL:HG12	2.00	0.43
1:A:161:PRO:HB3	2:D:143:UNK:CB	2.47	0.43
1:B:241:ARG:HH11	1:B:244:GLN:HB2	1.83	0.43
1:A:51:LYS:HD3	2:D:-13:UNK:CB	2.47	0.43
1:B:56:VAL:O	1:B:60:HIS:HB2	2.18	0.43
1:B:262:THR:HB	1:B:311:TYR:OH	2.17	0.43
1:B:478:GLY:C	1:B:480:GLU:H	2.22	0.43
1:B:35:PRO:HB3	1:B:72:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:HB	1:A:232:GLY:HA2	2.00	0.43
1:A:84:ARG:HA	1:A:84:ARG:NE	2.34	0.43
1:A:4:ALA:O	1:A:8:LEU:HB2	2.19	0.43
1:A:505:ASN:O	1:A:509:LEU:HG	2.19	0.43
1:B:57:LEU:HD13	1:B:63:VAL:HG21	2.01	0.42
1:B:94:THR:O	1:B:97:THR:HB	2.18	0.42
1:B:284:PHE:CD1	1:B:337:ASN:HA	2.49	0.42
1:A:95:THR:HA	1:A:98:LEU:HD12	2.02	0.42
1:A:506:VAL:HA	1:A:509:LEU:HD12	2.01	0.42
1:B:247:ARG:NH1	1:B:280:SER:HA	2.29	0.42
1:B:514:ILE:O	1:B:517:ASP:HB3	2.19	0.42
1:B:358:PHE:HB2	1:B:362:CYS:HB3	2.00	0.42
1:A:481:GLU:HG3	1:A:481:GLU:H	1.53	0.42
1:A:131:GLU:HG3	1:A:132:THR:HG23	2.01	0.42
1:A:94:THR:O	1:A:97:THR:HB	2.20	0.42
1:A:241:ARG:HH11	1:A:244:GLN:HB2	1.84	0.42
1:B:386:ILE:HB	1:B:387:PRO:HD2	2.02	0.42
1:B:8:LEU:HD11	1:B:443:ILE:HB	2.02	0.42
1:B:156:PHE:CZ	1:B:241:ARG:HG3	2.55	0.42
1:A:263:SER:HA	1:A:266:ILE:HD12	2.01	0.42
1:B:365:ILE:O	1:B:369:VAL:HG23	2.19	0.41
1:A:480:GLU:HB3	1:A:483:GLN:HB2	2.02	0.41
1:A:285:THR:HB	1:A:286:GLN:H	1.70	0.41
1:B:4:ALA:O	1:B:8:LEU:HB2	2.20	0.41
1:B:35:PRO:HA	1:B:74:GLU:HA	2.03	0.41
1:A:98:LEU:HD13	1:A:99:TYR:CG	2.54	0.41
1:A:4:ALA:HB2	1:A:441:LYS:HD3	2.01	0.41
1:B:349:THR:O	1:B:353:VAL:HG23	2.20	0.41
1:B:294:PHE:HB2	1:B:308:LEU:CD2	2.51	0.41
1:A:140:ASP:OD1	1:A:143:GLU:HB2	2.21	0.41
1:B:389:LYS:HD2	1:B:392:LYS:NZ	2.36	0.41
1:A:294:PHE:HB2	1:A:308:LEU:CD2	2.50	0.41
1:A:57:LEU:HD13	1:A:63:VAL:HG21	2.03	0.41
1:B:129:LEU:HD23	1:B:139:MET:HG2	2.01	0.41
1:B:429:LEU:O	1:B:432:ALA:HB3	2.20	0.41
1:A:156:PHE:CZ	1:A:241:ARG:HG3	2.56	0.41
1:A:148:PHE:O	1:A:151:LEU:HB2	2.19	0.41
1:A:330:GLY:HA2	1:A:331:GLY:HA2	1.79	0.41
1:B:8:LEU:HD21	1:B:443:ILE:HD12	2.03	0.41
1:A:319:PRO:HB3	1:B:385:MET:O	2.21	0.41
1:B:148:PHE:O	1:B:151:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:SER:HA	1:A:528:GLU:HG2	2.03	0.41
1:B:345:LEU:HB3	1:B:522:LEU:HD11	2.03	0.41
1:B:481:GLU:HA	1:B:484:LEU:HD12	2.01	0.41
1:A:389:LYS:HD2	1:A:392:LYS:NZ	2.36	0.41
1:A:434:MET:O	1:A:438:ARG:HG3	2.21	0.41
1:A:87:ARG:HB2	1:A:91:TYR:CE2	2.55	0.41
1:B:57:LEU:HB3	1:B:63:VAL:HB	2.03	0.40
1:B:462:GLU:O	1:B:466:ARG:HG2	2.22	0.40
1:B:105:LEU:HD23	1:B:125:VAL:HG13	2.04	0.40
1:A:453:GLU:O	1:A:457:ASN:HB2	2.20	0.40
1:A:462:GLU:O	1:A:466:ARG:HG2	2.21	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	437/534 (82%)	377 (86%)	46 (10%)	14 (3%)	5	41
1	B	438/534 (82%)	382 (87%)	45 (10%)	11 (2%)	7	46
All	All	875/1068 (82%)	759 (87%)	91 (10%)	25 (3%)	6	43

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	135	ASP
1	A	234	TYR
1	A	373	LYS
1	A	375	ILE
1	A	428	ILE
1	B	69	LYS

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Mol	Chain	Res	Type
1	B	135	ASP
1	B	375	ILE
1	B	428	ILE
1	A	374	HIS
1	A	460	LEU
1	A	479	ALA
1	B	460	LEU
1	B	473	SER
1	A	321	GLU
1	B	321	GLU
1	B	479	ALA
1	A	138	THR
1	A	285	THR
1	B	285	THR
1	A	480	GLU
1	B	161	PRO
1	A	100	SER
1	B	138	THR

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	389/476 (82%)	347 (89%)	42 (11%)	8	35
1	B	389/476 (82%)	341 (88%)	48 (12%)	6	30
All	All	778/952 (82%)	688 (88%)	90 (12%)	7	32

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	10	SER
1	A	16	HIS
1	A	19	GLU
1	A	20	ILE

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Mol	Chain	Res	Type
1	A	45	THR
1	A	55	CYS
1	A	56	VAL
1	A	90	ARG
1	A	98	LEU
1	A	112	LEU
1	A	113	ASN
1	A	130	THR
1	A	138	THR
1	A	140	ASP
1	A	158	GLN
1	A	234	TYR
1	A	243	HIS
1	A	259	MET
1	A	263	SER
1	A	273	MET
1	A	278	THR
1	A	279	SER
1	A	301	TYR
1	A	302	ASN
1	A	311	TYR
1	A	321	GLU
1	A	361	ARG
1	A	379	GLN
1	A	381	GLU
1	A	385	MET
1	A	399	LEU
1	A	433	ARG
1	A	459	ARG
1	A	462	GLU
1	A	473	SER
1	A	480	GLU
1	A	481	GLU
1	A	486	GLU
1	A	491	ILE
1	A	498	GLN
1	A	530	THR
1	B	3	GLN
1	B	10	SER
1	B	16	HIS
1	B	20	ILE
1	B	45	THR

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Mol	Chain	Res	Type
1	B	48	ASP
1	B	55	CYS
1	B	56	VAL
1	B	60	HIS
1	B	78	GLN
1	B	90	ARG
1	B	101	ASP
1	B	112	LEU
1	B	113	ASN
1	B	158	GLN
1	B	162	SER
1	B	231	ASP
1	B	243	HIS
1	B	259	MET
1	B	263	SER
1	B	273	MET
1	B	278	THR
1	B	286	GLN
1	B	301	TYR
1	B	305	LYS
1	B	306	GLN
1	B	311	TYR
1	B	321	GLU
1	B	358	PHE
1	B	361	ARG
1	B	373	LYS
1	B	379	GLN
1	B	381	GLU
1	B	385	MET
1	B	399	LEU
1	B	449	ARG
1	B	459	ARG
1	B	462	GLU
1	B	473	SER
1	B	474	MET
1	B	477	THR
1	B	480	GLU
1	B	486	GLU
1	B	491	ILE
1	B	498	GLN
1	B	502	LEU
1	B	515	GLN

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Mol	Chain	Res	Type
1	B	530	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	A	377	GLN
1	A	451	GLN
1	B	257	ASN
1	B	374	HIS
1	B	377	GLN
1	B	451	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/534 (82%)	-0.04	3 (0%) 89 85	300, 300, 300, 300	0
1	B	444/534 (83%)	0.24	24 (5%) 29 30	300, 300, 300, 300	0
2	D	0/218	-	-	-	-
2	E	0/218	-	-	-	-
All	All	887/1504 (58%)	0.10	27 (3%) 54 49	300, 300, 300, 300	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	GLU	5.5
1	B	65	TYR	5.0
1	B	377	GLN	4.6
1	B	66	GLN	4.6
1	B	33	SER	4.1
1	B	378	LYS	3.6
1	B	64	SER	3.3
1	B	76	GLU	3.2
1	B	473	SER	3.1
1	B	53	ALA	2.8
1	B	80	SER	2.7
1	B	457	ASN	2.6
1	B	279	SER	2.5
1	B	34	GLN	2.5
1	B	74	GLU	2.5
1	B	453	GLU	2.4
1	B	231	ASP	2.3
1	B	162	SER	2.3
1	A	61	ASN	2.2
1	B	160	CYS	2.2
1	B	75	TYR	2.2
1	B	483	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	279	SER	2.1
1	A	280	SER	2.1
1	B	78	GLN	2.0
1	B	31	THR	2.0
1	B	379	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.