



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:09 PM UTC

PDB ID : 5AFQ / pdb_00005afq
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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

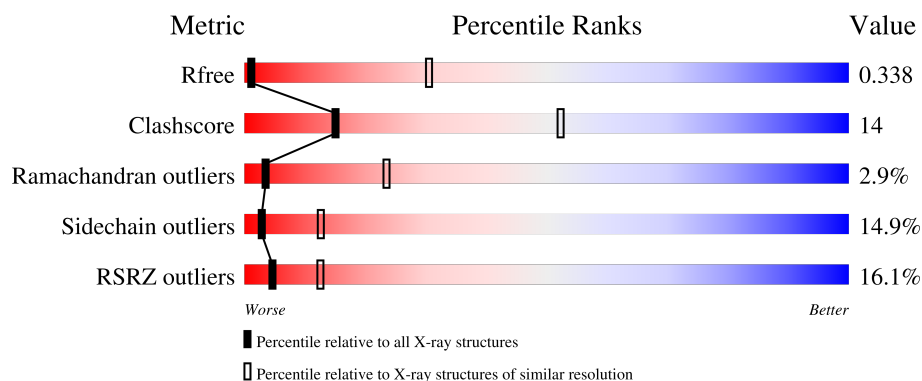
1 Overall quality at a glance

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}	180053	1167 (10.00-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	534	17% 46% 31% • • 17%
1	B	534	10% 46% 31% 6% 17%
2	D	218	22% • 76%
2	E	218	9% 91%

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			

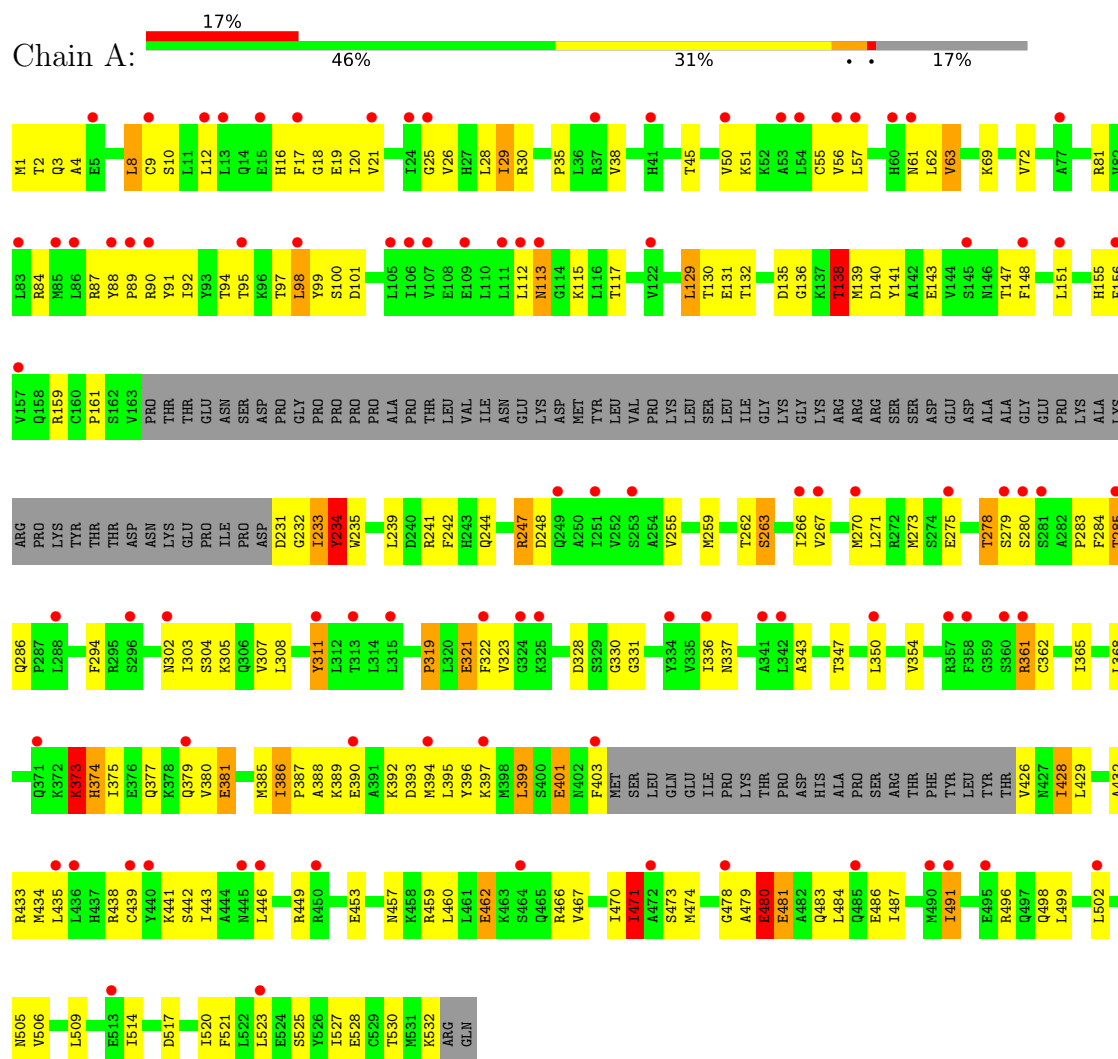
- Molecule 2 is a protein called RPC32 BETA (RPC7L).

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			

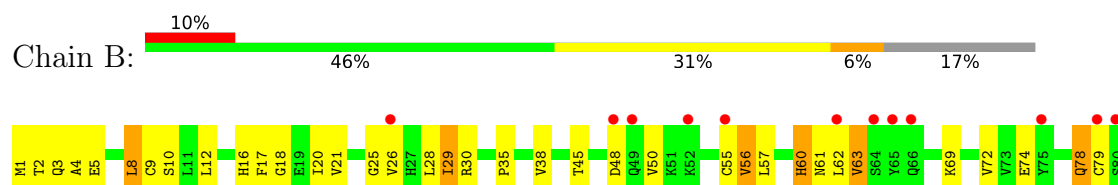
3 Residue-property plots

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: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3



• Molecule 1: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3



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 30.75 – 7.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.75-7.00) 97.6 (30.75-7.00)	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 0.295 , 0.338	Depositor DCC
R_{free} test set	342 reflections (9.47%)	wwPDB-VP
Wilson B-factor (Å ²)	452.8	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 476.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.70	0/3558	1.41	19/4798 (0.4%)
1	B	0.71	0/3563	1.47	24/4805 (0.5%)
All	All	0.70	0/7121	1.44	43/9603 (0.4%)

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 (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	472	ALA	CA-C-N	11.73	142.81	121.70
1	B	472	ALA	C-N-CA	11.73	142.81	121.70
1	B	374	HIS	CA-C-N	9.39	138.60	121.70
1	B	374	HIS	C-N-CA	9.39	138.60	121.70
1	B	472	ALA	CA-C-O	-8.45	111.95	120.82
1	A	322	PHE	N-CA-C	-7.15	104.42	113.72
1	B	322	PHE	N-CA-C	-7.09	104.51	113.72
1	B	140	ASP	CA-CB-CG	6.92	119.52	112.60
1	B	480	GLU	CA-C-N	6.89	129.51	120.28
1	B	480	GLU	C-N-CA	6.89	129.51	120.28
1	A	480	GLU	CA-C-N	6.85	129.46	120.28
1	A	480	GLU	C-N-CA	6.85	129.46	120.28
1	A	233	ILE	CA-C-N	6.80	134.53	121.54
1	A	233	ILE	C-N-CA	6.80	134.53	121.54
1	B	403	PHE	N-CA-C	-6.73	105.36	113.97
1	A	373	LYS	CA-C-N	6.51	133.41	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	LYS	C-N-CA	6.51	133.41	121.70
1	A	247	ARG	N-CA-C	-6.10	103.58	111.02
1	B	247	ARG	N-CA-C	-6.05	103.64	111.02
1	B	233	ILE	CA-C-N	5.81	132.63	121.54
1	B	233	ILE	C-N-CA	5.81	132.63	121.54
1	B	248	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	18	GLY	CA-C-N	5.67	127.88	120.28
1	A	18	GLY	C-N-CA	5.67	127.88	120.28
1	A	248	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	471	ILE	N-CA-C	-5.43	107.19	112.29
1	A	471	ILE	N-CA-C	-5.34	107.27	112.29
1	A	231	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	438	ARG	CB-CG-CD	5.25	123.37	111.30
1	B	18	GLY	CA-C-N	5.21	127.26	120.28
1	B	18	GLY	C-N-CA	5.21	127.26	120.28
1	B	231	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	322	PHE	CA-CB-CG	5.12	118.92	113.80
1	B	472	ALA	N-CA-C	5.11	116.54	111.07
1	A	319	PRO	CA-C-N	5.10	127.38	120.44
1	A	319	PRO	C-N-CA	5.10	127.38	120.44
1	A	113	ASN	N-CA-C	-5.09	105.98	113.61
1	A	328	ASP	CA-C-N	5.07	130.83	121.70
1	A	328	ASP	C-N-CA	5.07	130.83	121.70
1	B	328	ASP	CA-C-N	5.07	130.83	121.70
1	B	328	ASP	C-N-CA	5.07	130.83	121.70
1	B	471	ILE	CA-C-N	5.06	127.01	120.44
1	B	471	ILE	C-N-CA	5.06	127.01	120.44

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	101	0
1	B	3516	0	3552	99	0
2	D	265	0	60	4	0
2	E	95	0	21	0	0
All	All	7387	0	7183	200	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 (200) 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:474:MET:HE2	1:B:474:MET:HA	1.66	0.77
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:361:ARG:HG2	1:A:394:MET:HE1	1.86	0.57
1:A:443:ILE:HD11	1:A:520:ILE:HD11	1.86	0.57
1:B:304:SER:HB2	1:B:307:VAL:HG23	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:A:294:PHE:HB2	1:A:308:LEU:HD22	1.87	0.56
1:B:294:PHE:HB2	1:B: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:9:CYS:HA	1:A:12:LEU:HD12	1.86	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: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:62:LEU:HD23	1:A:81:ARG:HG3	1.88	0.55
1:A:239:LEU:HA	1:A:242:PHE:CD2	2.41	0.55
1:A:474:MET:HG2	1:A:478:GLY:O	2.08	0.54
1:A:466:ARG:O	1:A:470:ILE:HG12	2.08	0.54
1:B:435:LEU:HD23	1:B:523:LEU:HD21	1.89	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: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:B:9:CYS:O	1:B:12:LEU:HB2	2.09	0.52
1:A:89:PRO:HA	1:A:92:ILE:HD12	1.92	0.52
1:B:136:GLY:C	1:B:138:THR:H	2.17	0.52
1:A:136:GLY:C	1:A:138:THR:H	2.17	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:B:361:ARG:HG2	1:B:394:MET:HE1	1.91	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
1:B:401:GLU:HB2	1:B:403:PHE:CE1	2.44	0.50
1:A:478:GLY:C	1:A:480:GLU:H	2.20	0.50
1:B:17:PHE:HD2	1:B:21:VAL:HG11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:17:PHE:HD2	1:A:21:VAL:HG11	1.77	0.49
1:B:289:SER:OG	1:B:292:GLU:HG2	2.13	0.49
1:B:374:HIS:HA	1:B:375:ILE:C	2.37	0.49
1:A:26:VAL:HA	1:A:29:ILE:HD12	1.94	0.48
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: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: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:A:61:ASN:OD1	1:A:115:LYS:HG3	2.13	0.47
1:B:28:LEU:HD13	1:B:63:VAL:HG21	1.96	0.47
1:B:87:ARG:NH2	1:B:521:PHE:HA	2.29	0.47
1:B:478:GLY:C	1:B:480:GLU:H	2.22	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:B:505:ASN:O	1:B:509:LEU:HG	2.15	0.47
1:A:87:ARG:NH2	1:A:521:PHE:HA	2.29	0.47
1:A:129:LEU:HD23	1:A:139:MET:HG2	1.96	0.47
1:A:88:TYR:HA	1:A:91:TYR:HD2	1.80	0.47
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:B:362:CYS:HA	1:B:365:ILE:HG12	1.96	0.46
1:A:305:LYS:O	1:A:308:LEU:HB3	2.14	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:386:ILE:HB	1:A:387:PRO:HD2	2.00	0.43
1:B:490:MET:HE2	1:B:490:MET:HB3	1.94	0.43
1:B:26:VAL:O	1:B:30:ARG:HG3	2.18	0.43
1:A:35:PRO:HB3	1:A:72:VAL:HG12	2.00	0.43
1:A:51:LYS:HD3	2:D:-13:UNK:CB	2.47	0.43
1:A:161:PRO:HB3	2:D:143:UNK:CB	2.47	0.43
1:A:401:GLU:HB2	1:A:403:PHE:CE1	2.47	0.43
1:B:241:ARG:HH11	1:B:244:GLN:HB2	1.83	0.43
1:B:56:VAL:O	1:B:60:HIS:HB2	2.18	0.43
1:B:497:GLN:OE1	1:B:497:GLN:HA	2.18	0.43
1:B:262:THR:HB	1:B:311:TYR:OH	2.17	0.43
1:A:4:ALA:O	1:A:8:LEU:HB2	2.19	0.43
1:A:84:ARG:NE	1:A:84:ARG:HA	2.34	0.43
1:A:117:THR:HB	1:A:232:GLY:HA2	2.00	0.43
1:B:35:PRO:HB3	1:B:72:VAL:HG22	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:THR:O	1:B:97:THR:HB	2.18	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:284:PHE:CD1	1:B:337:ASN:HA	2.49	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:A:481:GLU:H	1:A:481:GLU:HG3	1.53	0.42
1:B:358:PHE:HB2	1:B:362:CYS:HB3	2.00	0.42
1:A:94:THR:O	1:A:97:THR:HB	2.20	0.42
1:A:131:GLU:HG3	1:A:132:THR:HG23	2.01	0.42
1:A:241:ARG:HH11	1:A:244:GLN:HB2	1.84	0.42
1:A:263:SER:HA	1:A:266:ILE:HD12	2.01	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:B:386:ILE:HB	1:B:387:PRO:HD2	2.02	0.42
1:A:480:GLU:HB3	1:A:483:GLN:HB2	2.02	0.41
1:B:365:ILE:O	1:B:369:VAL:HG23	2.19	0.41
1:A:285:THR:HB	1:A:286:GLN:H	1.70	0.41
1:A:4:ALA:HB2	1:A:441:LYS:HD3	2.01	0.41
1:A:98:LEU:HD13	1:A:99:TYR:CG	2.54	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:B:349:THR:O	1:B:353:VAL:HG23	2.20	0.41
1:A:140:ASP:OD1	1:A:143:GLU:HB2	2.21	0.41
1:B:294:PHE:HB2	1:B:308:LEU:CD2	2.51	0.41
1:B:389:LYS:HD2	1:B:392:LYS:NZ	2.36	0.41
1:A:57:LEU:HD13	1:A:63:VAL:HG21	2.03	0.41
1:A:294:PHE:HB2	1:A:308:LEU:CD2	2.50	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:148:PHE:O	1:A:151:LEU:HB2	2.19	0.41
1:A:156:PHE:CZ	1:A:241:ARG:HG3	2.56	0.41
1:A:330:GLY:HA2	1:A:331:GLY:HA2	1.79	0.41
1:A:319:PRO:HB3	1:B:385:MET:O	2.21	0.41
1:A:389:LYS:HD2	1:A:392:LYS:NZ	2.36	0.41
1:A:525:SER:HA	1:A:528:GLU:HG2	2.03	0.41
1:B:8:LEU:HD21	1:B:443:ILE:HD12	2.03	0.41
1:B:148:PHE:O	1:B:151:LEU:HB2	2.21	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:87:ARG:HB2	1:A:91:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:MET:O	1:A:438:ARG:HG3	2.21	0.41
1:B:57:LEU:HB3	1:B:63:VAL:HB	2.03	0.40
1:B:105:LEU:HD23	1:B:125:VAL:HG13	2.04	0.40
1:B:462:GLU:O	1:B:466:ARG:HG2	2.22	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%)	3	21
1	B	438/534 (82%)	382 (87%)	45 (10%)	11 (2%)	4	26
All	All	875/1068 (82%)	759 (87%)	91 (10%)	25 (3%)	3	23

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
1	B	135	ASP
1	B	375	ILE
1	B	428	ILE
1	A	374	HIS
1	A	460	LEU

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Mol	Chain	Res	Type
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%)	334 (86%)	55 (14%)	3	13
1	B	389/476 (82%)	328 (84%)	61 (16%)	2	12
All	All	778/952 (82%)	662 (85%)	116 (15%)	3	12

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	8	LEU
1	A	10	SER
1	A	16	HIS
1	A	19	GLU
1	A	20	ILE
1	A	29	ILE
1	A	45	THR
1	A	50	VAL
1	A	55	CYS

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Mol	Chain	Res	Type
1	A	56	VAL
1	A	63	VAL
1	A	90	ARG
1	A	98	LEU
1	A	101	ASP
1	A	112	LEU
1	A	113	ASN
1	A	129	LEU
1	A	130	THR
1	A	138	THR
1	A	155	HIS
1	A	234	TYR
1	A	259	MET
1	A	263	SER
1	A	273	MET
1	A	278	THR
1	A	279	SER
1	A	302	ASN
1	A	303	ILE
1	A	311	TYR
1	A	321	GLU
1	A	323	VAL
1	A	361	ARG
1	A	373	LYS
1	A	379	GLN
1	A	381	GLU
1	A	385	MET
1	A	386	ILE
1	A	390	GLU
1	A	395	LEU
1	A	399	LEU
1	A	401	GLU
1	A	428	ILE
1	A	433	ARG
1	A	459	ARG
1	A	462	GLU
1	A	471	ILE
1	A	473	SER
1	A	480	GLU
1	A	481	GLU
1	A	486	GLU
1	A	487	ILE

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Mol	Chain	Res	Type
1	A	491	ILE
1	A	498	GLN
1	A	530	THR
1	B	3	GLN
1	B	8	LEU
1	B	10	SER
1	B	16	HIS
1	B	20	ILE
1	B	29	ILE
1	B	45	THR
1	B	48	ASP
1	B	50	VAL
1	B	55	CYS
1	B	56	VAL
1	B	60	HIS
1	B	63	VAL
1	B	78	GLN
1	B	90	ARG
1	B	101	ASP
1	B	112	LEU
1	B	113	ASN
1	B	129	LEU
1	B	162	SER
1	B	259	MET
1	B	263	SER
1	B	273	MET
1	B	278	THR
1	B	286	GLN
1	B	302	ASN
1	B	303	ILE
1	B	305	LYS
1	B	306	GLN
1	B	311	TYR
1	B	321	GLU
1	B	323	VAL
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	386	ILE

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Mol	Chain	Res	Type
1	B	390	GLU
1	B	395	LEU
1	B	399	LEU
1	B	401	GLU
1	B	428	ILE
1	B	433	ARG
1	B	438	ARG
1	B	449	ARG
1	B	459	ARG
1	B	462	GLU
1	B	463	LYS
1	B	471	ILE
1	B	473	SER
1	B	474	MET
1	B	477	THR
1	B	480	GLU
1	B	486	GLU
1	B	487	ILE
1	B	491	ILE
1	B	502	LEU
1	B	519	THR
1	B	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	146	ASN
1	A	257	ASN
1	A	286	GLN
1	A	339	HIS
1	A	374	HIS
1	A	377	GLN
1	A	451	GLN
1	A	475	GLN
1	B	113	ASN
1	B	146	ASN
1	B	257	ASN
1	B	286	GLN
1	B	306	GLN
1	B	374	HIS
1	B	377	GLN

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Mol	Chain	Res	Type
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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	20:UNK	C	140:UNK	N	40.82

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%)	1.08	92 (20%) 2 10	300, 300, 300, 300	0
1	B	444/534 (83%)	0.90	51 (11%) 9 17	300, 300, 300, 300	0
2	D	0/218	-	-	-	-
2	E	0/218	-	-	-	-
All	All	887/1504 (58%)	0.99	143 (16%) 4 12	300, 300, 300, 300	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	ALA	5.8
1	A	148	PHE	5.0
1	B	62	LEU	4.9
1	A	53	ALA	4.8
1	B	376	GLU	4.8
1	A	21	VAL	4.7
1	A	112	LEU	4.7
1	A	334	TYR	4.7
1	B	441	LYS	4.5
1	A	280	SER	4.4
1	B	377	GLN	4.3
1	B	109	GLU	4.0
1	B	123	LYS	4.0
1	A	279	SER	3.9
1	A	523	LEU	3.7
1	A	394	MET	3.6
1	A	50	VAL	3.6
1	A	122	VAL	3.6
1	B	65	TYR	3.6
1	B	115	LYS	3.5
1	A	57	LEU	3.5
1	A	54	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	513	GLU	3.4
1	A	302	ASN	3.4
1	A	350	LEU	3.3
1	B	125	VAL	3.3
1	A	439	CYS	3.2
1	B	400	SER	3.2
1	A	15	GLU	3.2
1	B	380	VAL	3.2
1	B	375	ILE	3.2
1	A	491	ILE	3.2
1	A	56	VAL	3.2
1	B	80	SER	3.1
1	A	288	LEU	3.1
1	A	17	PHE	3.1
1	B	26	VAL	3.1
1	A	86	LEU	3.0
1	B	306	GLN	3.0
1	A	357	ARG	3.0
1	A	336	ILE	3.0
1	A	371	GLN	3.0
1	B	463	LYS	3.0
1	B	457	ASN	3.0
1	A	322	PHE	2.9
1	A	445	ASN	2.9
1	B	55	CYS	2.7
1	A	270	MET	2.7
1	A	12	LEU	2.7
1	B	145	SER	2.7
1	B	460	LEU	2.7
1	A	513	GLU	2.7
1	B	275	GLU	2.7
1	A	485	GLN	2.6
1	A	360	SER	2.6
1	A	315	LEU	2.6
1	B	378	LYS	2.6
1	A	253	SER	2.6
1	B	488	GLU	2.6
1	A	435	LEU	2.6
1	A	157	VAL	2.6
1	A	436	LEU	2.6
1	A	281	SER	2.5
1	B	403	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	106	ILE	2.5
1	A	266	ILE	2.5
1	A	342	LEU	2.5
1	A	5	GLU	2.5
1	A	490	MET	2.5
1	A	251	ILE	2.5
1	A	77	ALA	2.5
1	B	404	MET	2.5
1	A	95	THR	2.5
1	A	90	ARG	2.5
1	B	141	TYR	2.5
1	B	79	CYS	2.5
1	B	75	TYR	2.5
1	A	446	LEU	2.5
1	A	9	CYS	2.5
1	B	245	HIS	2.5
1	A	25	GLY	2.5
1	B	325	LYS	2.5
1	B	64	SER	2.4
1	B	237	ALA	2.4
1	A	145	SER	2.4
1	A	267	VAL	2.4
1	A	249	GLN	2.4
1	B	309	ASP	2.4
1	A	88	TYR	2.4
1	B	121	VAL	2.4
1	A	98	LEU	2.4
1	A	105	LEU	2.4
1	A	107	VAL	2.3
1	A	502	LEU	2.3
1	A	109	GLU	2.3
1	B	470	ILE	2.3
1	A	37	ARG	2.3
1	B	466	ARG	2.3
1	A	156	PHE	2.3
1	A	324	GLY	2.3
1	A	296	SER	2.3
1	A	464	SER	2.3
1	B	89	PRO	2.3
1	A	325	LYS	2.3
1	A	311	TYR	2.3
1	A	24	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	149	VAL	2.3
1	A	313	THR	2.2
1	A	478	GLY	2.2
1	A	403	PHE	2.2
1	A	440	TYR	2.2
1	A	358	PHE	2.2
1	A	341	ALA	2.2
1	B	274	SER	2.2
1	B	52	LYS	2.2
1	B	160	CYS	2.2
1	B	48	ASP	2.2
1	B	445	ASN	2.2
1	A	361	ARG	2.2
1	B	253	SER	2.1
1	A	390	GLU	2.1
1	A	61	ASN	2.1
1	A	285	THR	2.1
1	B	374	HIS	2.1
1	A	113	ASN	2.1
1	A	89	PRO	2.1
1	A	151	LEU	2.1
1	A	111	LEU	2.1
1	A	85	MET	2.1
1	A	83	LEU	2.1
1	A	379	GLN	2.1
1	B	49	GLN	2.1
1	A	495	GLU	2.1
1	A	60	HIS	2.0
1	B	66	GLN	2.0
1	A	13	LEU	2.0
1	B	142	ALA	2.0
1	B	240	ASP	2.0
1	A	41	HIS	2.0
1	B	132	THR	2.0
1	A	450	ARG	2.0
1	A	275	GLU	2.0
1	A	397	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.