



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:49 AM GMT

PDB ID : 2IXN
Title : CRYSTAL STRUCTURE OF THE PP2A PHOSPHATASE ACTIVATOR
YPA2 PTPA2
Authors : Leulliot, N.; Vicentini, G.; Jordens, J.; Quevillon-Cheruel, S.; Schiltz, M.;
Barford, D.; Van Tilbeurgh, H.; Goris, J.
Deposited on : 2006-07-09
Resolution : 2.80 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

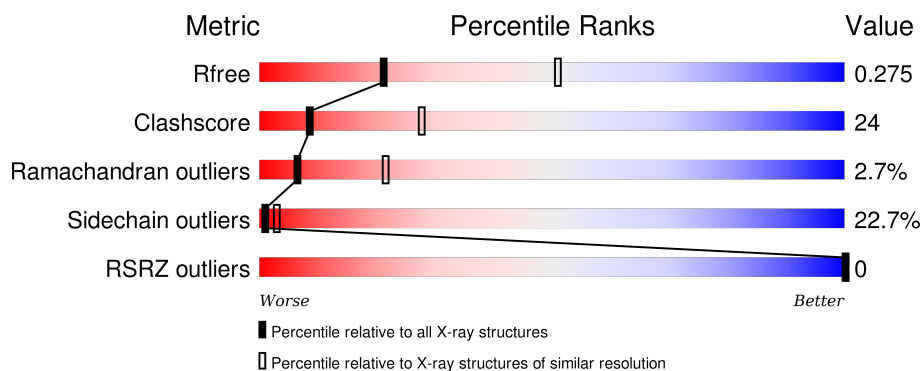
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 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	310	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 47% 33% 12% • 6% </div> </div>
1	B	310	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 47% 35% 9% • 8% </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4792 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.

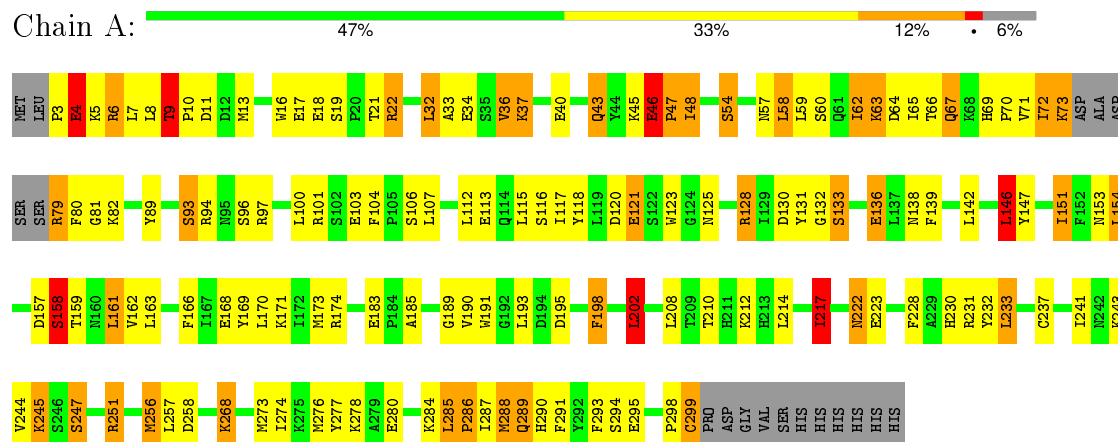
- Molecule 1 is a protein called SERINE/THREONINE-PROTEIN PHOSPHATASE 2A ACTIVATOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2418	1571	400	434	13			
1	B	286	Total	C	N	O	S	0	0	0
			2374	1543	391	427	13			

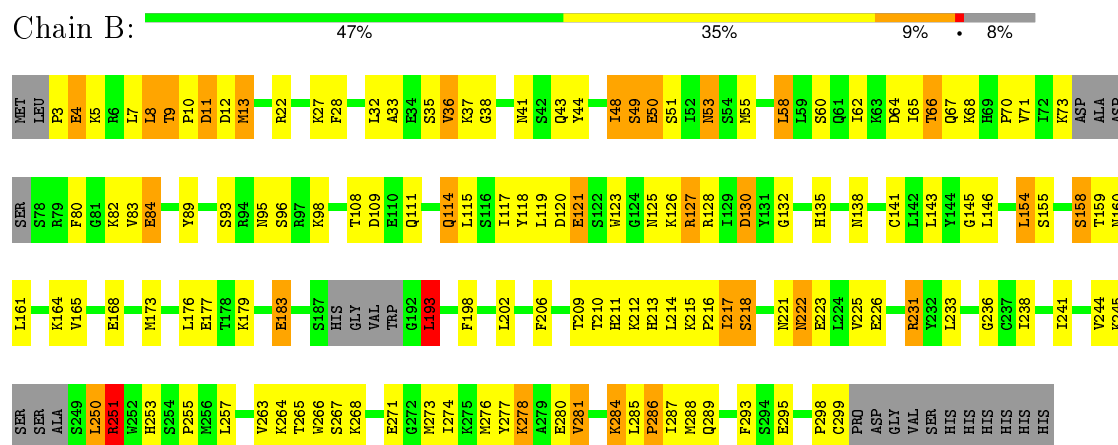
3 Residue-property plots

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 ($RSRZ > 2$). 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: SERINE/THREONINE-PROTEIN PHOSPHATASE 2A ACTIVATOR 2



• Molecule 1: SERINE/THREONINE-PROTEIN PHOSPHATASE 2A ACTIVATOR 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	157.93Å 171.04Å 53.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 53.63 – 2.56	Depositor EDS
% Data completeness (in resolution range)	93.3 (30.00-2.80) 79.8 (53.63-2.56)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.273 0.198 , 0.275	Depositor DCC
R_{free} test set	897 reflections (5.51%)	DCC
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 19063 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4792	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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	1.00	1/2484 (0.0%)	1.05	9/3349 (0.3%)
1	B	1.05	4/2436 (0.2%)	1.09	9/3279 (0.3%)
All	All	1.03	5/4920 (0.1%)	1.07	18/6628 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	GLU	CG-CD	7.00	1.62	1.51
1	B	9	THR	N-CA	6.88	1.60	1.46
1	B	121	GLU	CB-CG	-6.07	1.40	1.52
1	B	177	GLU	CB-CG	5.66	1.62	1.52
1	B	271	GLU	CG-CD	5.15	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9	THR	C-N-CD	-9.28	100.18	120.60
1	A	7	LEU	CA-CB-CG	7.27	132.03	115.30
1	A	154	LEU	CA-CB-CG	6.92	131.21	115.30
1	A	101	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	9	THR	C-N-CA	6.76	150.40	122.00
1	A	101	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	A	161	LEU	CA-CB-CG	6.73	130.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PRO	N-CA-CB	6.47	111.07	103.30
1	B	193	LEU	CA-CB-CG	6.35	129.91	115.30
1	B	251	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	130	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	250	LEU	CA-CB-CG	5.84	128.73	115.30
1	A	146	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	22	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	94	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	233	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	9	THR	N-CA-C	5.12	124.84	111.00
1	B	9	THR	CB-CA-C	-5.08	97.88	111.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ASP	Peptide
1	A	4	GLU	Peptide
1	A	9	THR	Peptide
1	B	298	PRO	Peptide
1	B	38	GLY	Peptide

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	2418	0	2388	114	0
1	B	2374	0	2353	113	0
All	All	4792	0	4741	227	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 24.

All (227) 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:217:ILE:CD1	1:A:217:ILE:CG1	1.75	1.54
1:B:4:GLU:H	1:B:4:GLU:CD	1.47	1.17
1:B:123:TRP:HE3	1:B:173:MET:CE	1.58	1.16
1:A:123:TRP:CE3	1:A:173:MET:HE1	1.90	1.07
1:B:123:TRP:CE3	1:B:173:MET:CE	2.38	1.07
1:B:123:TRP:HE3	1:B:173:MET:HE1	1.02	1.06
1:B:4:GLU:N	1:B:4:GLU:CD	2.05	1.05
1:A:123:TRP:HE3	1:A:173:MET:HE1	1.17	1.05
1:A:40:GLU:HB2	1:A:43:GLN:HE22	1.23	1.03
1:A:285:LEU:HB3	1:A:286:PRO:HD3	1.41	1.03
1:B:123:TRP:CE3	1:B:173:MET:HE1	1.94	1.02
1:B:50:GLU:CD	1:B:50:GLU:H	1.65	0.99
1:B:265:THR:HG22	1:B:267:SER:H	1.29	0.96
1:A:79:ARG:CD	1:A:80:PHE:H	1.78	0.94
1:A:40:GLU:HB2	1:A:43:GLN:NE2	1.85	0.91
1:A:285:LEU:HB3	1:A:286:PRO:CD	2.01	0.91
1:B:123:TRP:CE3	1:B:173:MET:HE3	2.08	0.88
1:A:121:GLU:HB3	1:A:138:ASN:HD22	1.40	0.85
1:B:4:GLU:N	1:B:4:GLU:OE2	2.04	0.84
1:A:123:TRP:CE3	1:A:173:MET:CE	2.61	0.83
1:B:50:GLU:CD	1:B:50:GLU:N	2.31	0.83
1:A:121:GLU:HB3	1:A:138:ASN:ND2	1.95	0.81
1:B:66:THR:O	1:B:68:LYS:N	2.18	0.77
1:B:132:GLY:H	1:B:135:HIS:HD2	1.31	0.76
1:B:127:ARG:CG	1:B:127:ARG:HH11	2.00	0.75
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.51	0.75
1:A:222:ASN:HD22	1:A:222:ASN:N	1.84	0.75
1:A:228:PHE:HE2	1:A:231:ARG:HH21	1.35	0.74
1:A:146:LEU:HB3	1:A:151:ILE:HG22	1.70	0.73
1:B:217:ILE:N	1:B:217:ILE:HD13	2.04	0.73
1:A:46:GLU:HB3	1:A:47:PRO:CD	2.18	0.73
1:B:217:ILE:H	1:B:217:ILE:HD13	1.53	0.73
1:A:251:ARG:CG	1:A:251:ARG:HH11	2.01	0.72
1:A:46:GLU:O	1:A:47:PRO:C	2.27	0.72
1:A:79:ARG:HD3	1:A:80:PHE:H	1.56	0.70
1:A:79:ARG:CD	1:A:80:PHE:N	2.53	0.70
1:A:285:LEU:HD12	1:A:289:GLN:HG2	1.73	0.69
1:A:125:ASN:HD22	1:A:128:ARG:H	1.38	0.69
1:A:123:TRP:HE3	1:A:173:MET:CE	1.97	0.68
1:B:216:PRO:HB2	1:B:217:ILE:HD13	1.75	0.68
1:A:79:ARG:HD3	1:A:80:PHE:N	2.09	0.68
1:A:79:ARG:HD2	1:A:80:PHE:H	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:SER:HB2	1:B:159:THR:OG1	1.94	0.68
1:B:244:VAL:O	1:B:244:VAL:CG1	2.41	0.67
1:B:285:LEU:HB3	1:B:286:PRO:CD	2.25	0.66
1:B:50:GLU:N	1:B:50:GLU:OE1	2.28	0.66
1:B:108:THR:OG1	1:B:111:GLN:HG3	1.95	0.66
1:B:11:ASP:OD1	1:B:11:ASP:N	2.27	0.66
1:B:244:VAL:O	1:B:244:VAL:HG13	1.95	0.66
1:B:277:TYR:CD1	1:B:281:VAL:HG21	2.31	0.65
1:A:62:ILE:HD12	1:A:123:TRP:CZ2	2.31	0.65
1:A:16:TRP:O	1:A:19:SER:OG	2.13	0.65
1:B:265:THR:CG2	1:B:267:SER:H	2.09	0.64
1:A:33:ALA:O	1:A:36:VAL:HG12	2.00	0.62
1:A:46:GLU:HA	1:A:46:GLU:OE2	1.92	0.62
1:A:58:LEU:C	1:A:58:LEU:HD23	2.20	0.62
1:B:211:HIS:HD2	1:B:213:HIS:H	1.46	0.62
1:B:28:PHE:O	1:B:32:LEU:HD12	2.00	0.62
1:A:46:GLU:HB3	1:A:47:PRO:HD3	1.81	0.61
1:B:132:GLY:H	1:B:135:HIS:CD2	2.17	0.61
1:B:8:LEU:HD12	1:B:12:ASP:HB3	1.83	0.61
1:B:277:TYR:CE1	1:B:281:VAL:HG21	2.36	0.61
1:B:66:THR:C	1:B:68:LYS:H	2.04	0.60
1:B:217:ILE:H	1:B:217:ILE:CD1	2.12	0.60
1:A:193:LEU:HD22	1:A:257:LEU:HD23	1.83	0.60
1:A:285:LEU:CD1	1:A:289:GLN:HG2	2.32	0.60
1:A:128:ARG:HH11	1:A:128:ARG:HG2	1.66	0.60
1:A:268:LYS:HD2	1:A:268:LYS:O	2.02	0.59
1:A:285:LEU:O	1:A:289:GLN:HG3	2.02	0.59
1:A:40:GLU:CB	1:A:43:GLN:HE22	2.08	0.59
1:B:285:LEU:HB3	1:B:286:PRO:HD2	1.84	0.59
1:B:125:ASN:HD22	1:B:128:ARG:H	1.50	0.59
1:A:202:LEU:HA	1:A:273:MET:HG2	1.85	0.59
1:A:13:MET:HE3	1:A:285:LEU:HD22	1.86	0.58
1:A:73:LYS:HA	1:A:73:LYS:HE3	1.86	0.58
1:A:96:SER:O	1:A:100:LEU:HD12	2.04	0.57
1:A:191:TRP:HB3	1:A:256:MET:HG2	1.86	0.57
1:A:214:LEU:HD21	1:A:228:PHE:CE1	2.39	0.57
1:A:125:ASN:HD22	1:A:128:ARG:N	2.02	0.57
1:A:298:PRO:O	1:A:299:CYS:HB2	2.03	0.57
1:A:6:ARG:HD2	1:A:290:HIS:HA	1.87	0.57
1:B:48:ILE:H	1:B:48:ILE:HD12	1.69	0.57
1:A:251:ARG:HG3	1:A:251:ARG:HH11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ASN:ND2	1:B:128:ARG:H	2.03	0.56
1:B:32:LEU:H	1:B:32:LEU:HD12	1.68	0.56
1:A:251:ARG:HD3	1:A:258:ASP:OD2	2.04	0.56
1:B:211:HIS:CD2	1:B:214:LEU:H	2.23	0.56
1:B:231:ARG:HG2	1:B:231:ARG:HH11	1.71	0.56
1:B:123:TRP:CZ3	1:B:173:MET:HE3	2.40	0.56
1:B:193:LEU:HD13	1:B:257:LEU:HD21	1.88	0.56
1:B:114:GLN:HG2	1:B:295:GLU:HG2	1.88	0.55
1:A:168:GLU:OE2	1:A:168:GLU:HA	2.05	0.55
1:A:159:THR:HG22	1:A:163:LEU:HD12	1.88	0.55
1:A:93:SER:HA	1:A:120:ASP:OD1	2.07	0.54
1:B:35:SER:HB3	1:B:158:SER:OG	2.08	0.54
1:B:127:ARG:CB	1:B:127:ARG:HH11	2.20	0.54
1:B:202:LEU:HD23	1:B:273:MET:HB3	1.89	0.54
1:B:33:ALA:O	1:B:36:VAL:HG12	2.07	0.54
1:A:36:VAL:HG13	1:A:36:VAL:O	2.07	0.53
1:B:8:LEU:HD23	1:B:288:MET:HB3	1.91	0.53
1:B:217:ILE:N	1:B:217:ILE:CD1	2.69	0.52
1:B:265:THR:HG22	1:B:266:TRP:N	2.23	0.52
1:A:65:ILE:O	1:A:65:ILE:CG2	2.57	0.52
1:B:265:THR:HG22	1:B:267:SER:N	2.12	0.52
1:B:253:HIS:O	1:B:255:PRO:HD3	2.10	0.52
1:A:193:LEU:HD22	1:A:257:LEU:CD2	2.39	0.51
1:A:9:THR:HB	1:A:10:PRO:HD3	1.92	0.51
1:A:34:GLU:O	1:A:37:LYS:HB2	2.10	0.51
1:A:245:LYS:O	1:A:245:LYS:HD3	2.11	0.51
1:A:217:ILE:HD13	1:A:217:ILE:H	1.75	0.51
1:A:66:THR:OG1	1:A:67:GLN:N	2.43	0.51
1:B:50:GLU:OE1	1:B:51:SER:N	2.45	0.50
1:B:159:THR:O	1:B:159:THR:CG2	2.59	0.50
1:A:277:TYR:O	1:A:278:LYS:C	2.50	0.50
1:B:284:LYS:HE3	1:B:284:LYS:HA	1.92	0.50
1:B:127:ARG:HB3	1:B:127:ARG:HH11	1.75	0.50
1:B:4:GLU:HB3	1:B:293:PHE:O	2.11	0.50
1:A:46:GLU:O	1:A:48:ILE:N	2.44	0.50
1:B:44:TYR:CE2	1:B:164:LYS:HE3	2.47	0.50
1:B:117:ILE:O	1:B:120:ASP:HB2	2.11	0.50
1:B:198:PHE:CD2	1:B:277:TYR:HD1	2.29	0.49
1:B:4:GLU:HG2	1:B:117:ILE:HG13	1.93	0.49
1:A:63:LYS:HG3	1:A:64:ASP:N	2.26	0.49
1:B:215:LYS:H	1:B:218:SER:HG	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TYR:OH	1:A:294:SER:HB3	2.12	0.49
1:A:222:ASN:ND2	1:A:222:ASN:N	2.55	0.49
1:B:154:LEU:O	1:B:155:SER:C	2.51	0.49
1:B:123:TRP:CZ3	1:B:173:MET:CE	2.93	0.48
1:B:10:PRO:HD2	1:B:11:ASP:OD1	2.12	0.48
1:B:4:GLU:CB	1:B:293:PHE:O	2.61	0.48
1:B:35:SER:CB	1:B:158:SER:OG	2.60	0.48
1:A:58:LEU:HD23	1:A:59:LEU:N	2.29	0.48
1:A:132:GLY:HA3	1:A:185:ALA:HB3	1.95	0.48
1:A:128:ARG:HH11	1:A:128:ARG:CG	2.26	0.48
1:B:233:LEU:O	1:B:236:GLY:N	2.47	0.48
1:B:138:ASN:HA	1:B:141:CYS:HB2	1.96	0.47
1:B:118:TYR:CD2	1:B:141:CYS:HB3	2.49	0.47
1:B:127:ARG:NH1	1:B:127:ARG:HB3	2.29	0.47
1:A:48:ILE:HG13	1:A:48:ILE:H	1.60	0.47
1:B:71:VAL:HG21	1:B:179:LYS:O	2.14	0.47
1:A:217:ILE:H	1:A:217:ILE:CD1	2.28	0.47
1:B:276:MET:O	1:B:280:GLU:N	2.42	0.47
1:A:202:LEU:HD12	1:A:202:LEU:C	2.35	0.46
1:B:132:GLY:N	1:B:135:HIS:HD2	2.06	0.46
1:A:202:LEU:CD1	1:A:202:LEU:C	2.83	0.46
1:A:9:THR:HB	1:A:10:PRO:CD	2.45	0.46
1:A:45:LYS:O	1:A:46:GLU:O	2.34	0.46
1:B:159:THR:HG22	1:B:159:THR:O	2.15	0.46
1:A:58:LEU:HB2	1:A:103:GLU:HG3	1.97	0.46
1:A:40:GLU:HG2	1:A:232:TYR:CZ	2.51	0.46
1:B:66:THR:C	1:B:68:LYS:N	2.64	0.45
1:A:139:PHE:O	1:A:142:LEU:HB3	2.16	0.45
1:B:130:ASP:HB2	1:B:183:GLU:O	2.17	0.45
1:A:191:TRP:O	1:A:256:MET:HG3	2.16	0.45
1:B:287:ILE:C	1:B:289:GLN:N	2.70	0.45
1:A:153:ASN:O	1:A:157:ASP:HB2	2.17	0.45
1:A:131:TYR:OH	1:A:136:GLU:HB2	2.17	0.45
1:B:251:ARG:CG	1:B:251:ARG:HH11	2.29	0.45
1:A:65:ILE:O	1:A:65:ILE:HG22	2.17	0.45
1:B:4:GLU:N	1:B:4:GLU:OE1	2.48	0.45
1:A:13:MET:O	1:A:16:TRP:HB3	2.17	0.45
1:A:146:LEU:HB3	1:A:151:ILE:CG2	2.43	0.45
1:B:287:ILE:C	1:B:289:GLN:H	2.21	0.45
1:B:115:LEU:HD21	1:B:145:GLY:HA3	1.98	0.44
1:A:32:LEU:HG	1:A:162:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:THR:HG23	1:B:176:LEU:HD21	1.99	0.44
1:A:8:LEU:O	1:A:9:THR:OG1	2.31	0.44
1:A:198:PHE:CD2	1:A:198:PHE:C	2.90	0.44
1:A:72:ILE:O	1:A:72:ILE:CG2	2.65	0.44
1:A:166:PHE:O	1:A:169:TYR:HB3	2.17	0.44
1:B:89:TYR:CD2	1:B:89:TYR:C	2.90	0.44
1:B:13:MET:HE3	1:B:285:LEU:CD1	2.48	0.44
1:B:33:ALA:HB1	1:B:206:PHE:CD1	2.52	0.44
1:B:222:ASN:HA	1:B:225:VAL:HB	2.00	0.43
1:A:4:GLU:HG3	1:A:293:PHE:O	2.18	0.43
1:B:119:LEU:HD12	1:B:119:LEU:O	2.18	0.43
1:B:127:ARG:HG2	1:B:127:ARG:NH1	2.28	0.43
1:B:285:LEU:O	1:B:289:GLN:HB2	2.18	0.43
1:B:127:ARG:NH1	1:B:127:ARG:CB	2.81	0.43
1:A:72:ILE:O	1:A:73:LYS:HB2	2.19	0.43
1:B:274:ILE:O	1:B:278:LYS:HD2	2.19	0.43
1:B:3:PRO:N	1:B:4:GLU:OE2	2.52	0.43
1:B:206:PHE:HA	1:B:209:THR:HG23	2.00	0.43
1:A:222:ASN:HD22	1:A:222:ASN:H	1.60	0.42
1:B:221:ASN:C	1:B:221:ASN:OD1	2.57	0.42
1:A:60:SER:O	1:A:64:ASP:OD1	2.37	0.42
1:A:104:PHE:HB2	1:A:107:LEU:HD12	2.00	0.42
1:A:125:ASN:ND2	1:A:128:ARG:HB2	2.34	0.42
1:A:130:ASP:HB2	1:A:183:GLU:O	2.19	0.42
1:A:97:ARG:NH2	1:A:113:GLU:HG3	2.35	0.42
1:A:230:HIS:ND1	1:A:230:HIS:N	2.59	0.42
1:A:32:LEU:HA	1:A:32:LEU:HD12	1.89	0.42
1:A:72:ILE:O	1:A:72:ILE:HG22	2.20	0.42
1:A:115:LEU:O	1:A:116:SER:C	2.58	0.42
1:B:44:TYR:CZ	1:B:164:LYS:HE3	2.55	0.42
1:A:21:THR:O	1:A:22:ARG:C	2.59	0.42
1:B:62:ILE:O	1:B:65:ILE:HB	2.20	0.42
1:B:50:GLU:HA	1:B:53:ASN:HB2	2.02	0.42
1:B:285:LEU:CB	1:B:286:PRO:HD2	2.49	0.41
1:A:237:CYS:O	1:A:241:ILE:HG12	2.19	0.41
1:B:55:MET:CG	1:B:165:VAL:HG21	2.50	0.41
1:A:251:ARG:HD3	1:A:258:ASP:CG	2.40	0.41
1:B:13:MET:HE3	1:B:13:MET:HB2	1.74	0.41
1:B:160:ASN:O	1:B:164:LYS:HB2	2.20	0.41
1:B:251:ARG:CB	1:B:251:ARG:HH11	2.33	0.41
1:A:288:MET:CE	1:A:288:MET:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PHE:CD2	1:A:151:ILE:HG12	2.56	0.41
1:B:198:PHE:CD2	1:B:277:TYR:CD1	3.08	0.41
1:B:241:ILE:HG21	1:B:241:ILE:HD13	1.91	0.41
1:A:54:SER:HA	1:A:57:ASN:OD1	2.20	0.41
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.82	0.41
1:A:157:ASP:O	1:A:158:SER:C	2.59	0.41
1:B:206:PHE:HZ	1:B:274:ILE:HD11	1.85	0.41
1:B:251:ARG:HH11	1:B:251:ARG:HB3	1.85	0.41
1:B:95:ASN:O	1:B:96:SER:C	2.58	0.41
1:A:280:GLU:O	1:A:284:LYS:HG3	2.21	0.41
1:A:46:GLU:CB	1:A:47:PRO:CD	2.92	0.41
1:A:133:SER:HB2	1:A:287:ILE:HD13	2.03	0.41
1:A:284:LYS:O	1:A:285:LEU:C	2.59	0.41
1:B:71:VAL:HG11	1:B:82:LYS:HD2	2.02	0.41
1:B:58:LEU:C	1:B:58:LEU:HD23	2.41	0.41
1:A:289:GLN:H	1:A:289:GLN:HG3	1.73	0.41
1:B:49:SER:HB3	1:B:51:SER:H	1.85	0.41
1:A:157:ASP:O	1:A:159:THR:N	2.54	0.40
1:A:69:HIS:HA	1:A:70:PRO:HD3	1.84	0.40
1:B:70:PRO:O	1:B:84:GLU:HG2	2.22	0.40
1:A:4:GLU:CG	1:A:293:PHE:O	2.69	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	288/310 (93%)	248 (86%)	29 (10%)	11 (4%)	4	13
1	B	278/310 (90%)	240 (86%)	34 (12%)	4 (1%)	14	42
All	All	566/620 (91%)	488 (86%)	63 (11%)	15 (3%)	6	21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	46	GLU
1	A	158	SER
1	A	247	SER
1	B	41	ASN
1	B	67	GLN
1	A	189	GLY
1	A	244	VAL
1	B	286	PRO
1	A	81	GLY
1	A	22	ARG
1	A	47	PRO
1	A	202	LEU
1	B	84	GLU
1	A	217	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	268/285 (94%)	203 (76%)	65 (24%)	1	2
1	B	265/285 (93%)	209 (79%)	56 (21%)	1	4
All	All	533/570 (94%)	412 (77%)	121 (23%)	1	3

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	5	LYS
1	A	6	ARG
1	A	9	THR
1	A	17	GLU
1	A	18	GLU
1	A	32	LEU
1	A	36	VAL

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Mol	Chain	Res	Type
1	A	37	LYS
1	A	43	GLN
1	A	46	GLU
1	A	48	ILE
1	A	54	SER
1	A	58	LEU
1	A	62	ILE
1	A	63	LYS
1	A	67	GLN
1	A	71	VAL
1	A	72	ILE
1	A	73	LYS
1	A	79	ARG
1	A	82	LYS
1	A	89	TYR
1	A	93	SER
1	A	106	SER
1	A	112	LEU
1	A	117	ILE
1	A	121	GLU
1	A	128	ARG
1	A	133	SER
1	A	136	GLU
1	A	146	LEU
1	A	147	TYR
1	A	151	ILE
1	A	154	LEU
1	A	158	SER
1	A	161	LEU
1	A	170	LEU
1	A	171	LYS
1	A	174	ARG
1	A	190	VAL
1	A	195	ASP
1	A	198	PHE
1	A	202	LEU
1	A	208	LEU
1	A	210	THR
1	A	212	LYS
1	A	217	ILE
1	A	222	ASN
1	A	233	LEU

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Mol	Chain	Res	Type
1	A	243	LYS
1	A	245	LYS
1	A	247	SER
1	A	251	ARG
1	A	256	MET
1	A	268	LYS
1	A	274	ILE
1	A	276	MET
1	A	285	LEU
1	A	286	PRO
1	A	288	MET
1	A	289	GLN
1	A	291	PHE
1	A	295	GLU
1	A	299	CYS
1	B	4	GLU
1	B	5	LYS
1	B	7	LEU
1	B	8	LEU
1	B	9	THR
1	B	11	ASP
1	B	13	MET
1	B	27	LYS
1	B	36	VAL
1	B	37	LYS
1	B	43	GLN
1	B	48	ILE
1	B	49	SER
1	B	50	GLU
1	B	53	ASN
1	B	58	LEU
1	B	60	SER
1	B	64	ASP
1	B	66	THR
1	B	73	LYS
1	B	80	PHE
1	B	83	VAL
1	B	93	SER
1	B	98	LYS
1	B	109	ASP
1	B	114	GLN
1	B	121	GLU

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Mol	Chain	Res	Type
1	B	126	LYS
1	B	127	ARG
1	B	143	LEU
1	B	146	LEU
1	B	154	LEU
1	B	158	SER
1	B	161	LEU
1	B	168	GLU
1	B	183	GLU
1	B	193	LEU
1	B	210	THR
1	B	212	LYS
1	B	217	ILE
1	B	218	SER
1	B	222	ASN
1	B	223	GLU
1	B	226	GLU
1	B	231	ARG
1	B	238	ILE
1	B	245	LYS
1	B	250	LEU
1	B	251	ARG
1	B	263	VAL
1	B	264	LYS
1	B	268	LYS
1	B	278	LYS
1	B	281	VAL
1	B	284	LYS
1	B	299	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	53	ASN
1	A	69	HIS
1	A	125	ASN
1	A	135	HIS
1	A	138	ASN
1	A	156	ASN
1	A	222	ASN
1	A	289	GLN

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Mol	Chain	Res	Type
1	A	290	HIS
1	B	111	GLN
1	B	125	ASN
1	B	135	HIS
1	B	153	ASN
1	B	211	HIS
1	B	289	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	292/310 (94%)	-0.52	0 100 100	2, 14, 25, 38	0
1	B	286/310 (92%)	-0.55	0 100 100	5, 14, 24, 31	0
All	All	578/620 (93%)	-0.53	0 100 100	2, 14, 24, 38	0

There are no RSRZ outliers to report.

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.