



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:36 PM GMT

PDB ID : 3PVS
Title : Structure and biochemical activities of Escherichia coli MgsA
Authors : Page, A.N.; George, N.P.; Marceau, A.H.; Cox, M.M.; Keck, J.L.
Deposited on : 2010-12-07
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

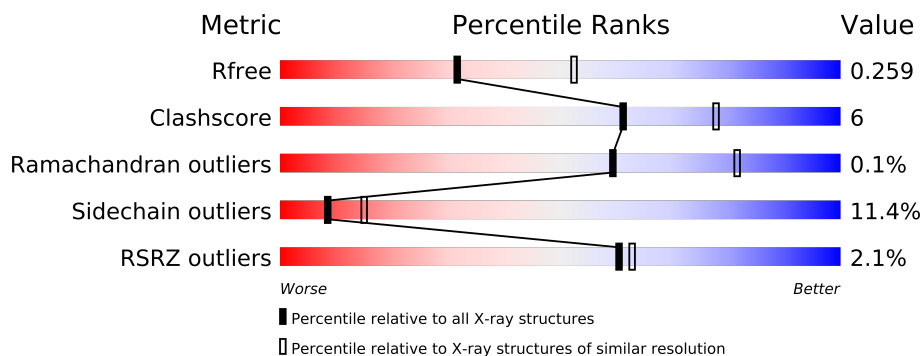
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance





The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	447	
1	B	447	
1	C	447	
1	D	447	

2 Entry composition

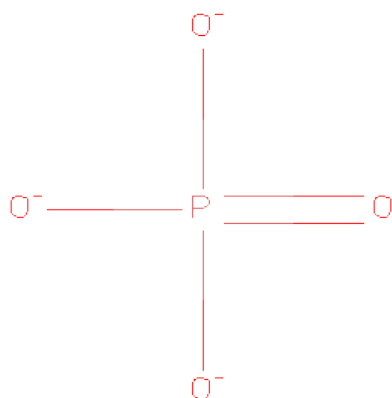
There are 3 unique types of molecules in this entry. The entry contains 13547 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Replication-associated recombination protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3224	2022	586	606	10			
1	B	417	Total	C	N	O	S	0	0	0
			3249	2038	588	613	10			
1	C	420	Total	C	N	O	S	0	0	0
			3285	2059	598	618	10			
1	D	424	Total	C	N	O	S	0	0	0
			3313	2078	600	623	12			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

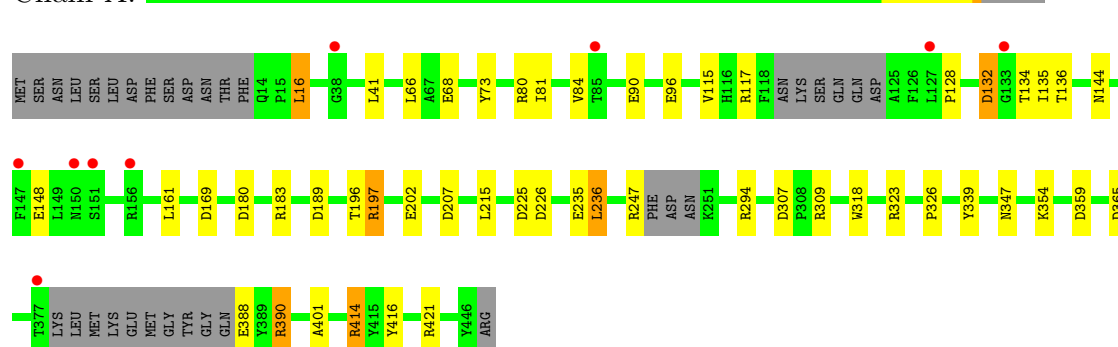
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		
3	B	130	Total	O	0	0
			130	130		
3	C	89	Total	O	0	0
			89	89		
3	D	125	Total	O	0	0
			125	125		

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.

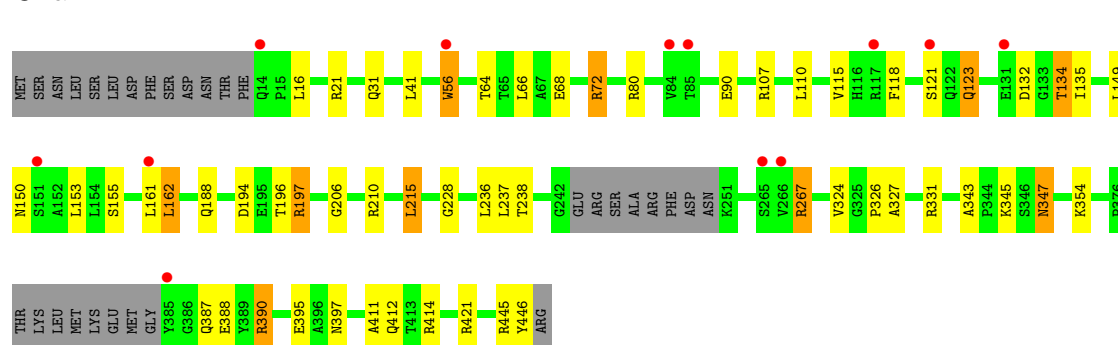
- Molecule 1: Replication-associated recombination protein A

Chain A:



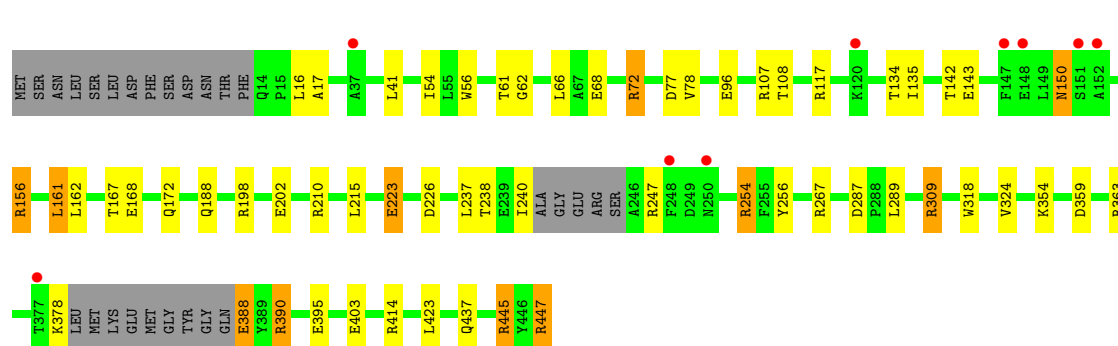
- Molecule 1: Replication-associated recombination protein A

Chain B:

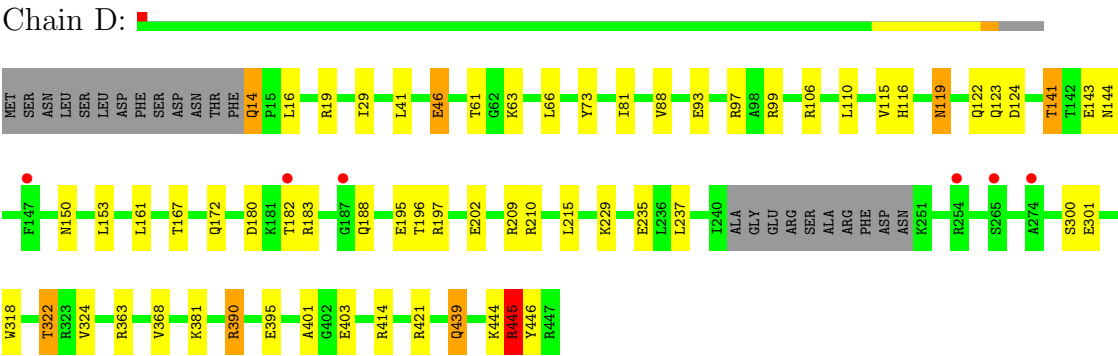


- Molecule 1: Replication-associated recombination protein A

Chain C:



● Molecule 1: Replication-associated recombination protein A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.95Å 143.69Å 163.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.98 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-2.50) 91.3 (29.98-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.195 , 0.266 0.199 , 0.259	Depositor DCC
R_{free} test set	4499 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 89737 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13547	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.73	0/3286	0.80	5/4455 (0.1%)
1	B	0.78	1/3313 (0.0%)	0.85	6/4493 (0.1%)
1	C	0.76	1/3349 (0.0%)	0.81	2/4540 (0.0%)
1	D	0.75	0/3378	0.83	3/4578 (0.1%)
All	All	0.75	2/13326 (0.0%)	0.82	16/18066 (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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	TRP	CB-CG	5.58	1.60	1.50
1	C	388	GLU	CG-CD	5.13	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	TRP	CA-CB-CG	6.66	126.36	113.70
1	B	215	LEU	CB-CG-CD2	5.86	120.96	111.00
1	D	445	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	D	197	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	445	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	421	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	421	ARG	NE-CZ-NH2	-5.41	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	16	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	267	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	162	LEU	CA-CB-CG	5.19	127.25	115.30
1	B	267	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	236	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	287	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	363	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	421	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	29	ILE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3224	0	0	20	0
1	B	3249	0	0	23	0
1	C	3285	0	0	21	0
1	D	3313	0	0	20	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
3	A	112	0	0	6	0
3	B	130	0	0	9	0
3	C	89	0	0	6	0
3	D	125	0	0	5	0
All	All	13547	0	0	76	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 6.

All (76) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:322:THR:CG2	3:D:455:HOH:O	2.15	0.95
1:C:388:GLU:CG	3:C:534:HOH:O	2.17	0.90
1:C:62:GLY:N	2:C:448:PO4:O4	2.07	0.86
1:A:183:ARG:N	3:A:550:HOH:O	2.11	0.84
1:B:324:VAL:O	3:B:541:HOH:O	1.98	0.81
1:C:56:TRP:CE3	1:C:161:LEU:CD1	2.64	0.81
1:A:96:GLU:OE2	1:D:46:GLU:OE2	2.01	0.78
1:D:390:ARG:NH2	1:D:401:ALA:O	2.20	0.74
1:C:254:ARG:NH1	3:C:499:HOH:O	2.22	0.72
1:B:446:TYR:O	3:B:544:HOH:O	2.08	0.70
1:D:119:ASN:ND2	1:D:122:GLN:OE1	2.26	0.69
1:B:390:ARG:NH1	1:B:395:GLU:OE2	2.27	0.68
1:B:72:ARG:NH1	1:B:72:ARG:CG	2.58	0.67
1:A:73:TYR:OH	1:C:96:GLU:OE2	2.13	0.66
1:B:228:GLY:O	3:B:523:HOH:O	2.13	0.65
1:A:132:ASP:N	1:A:132:ASP:OD2	2.30	0.65
1:B:327:ALA:O	3:B:520:HOH:O	2.15	0.63
1:C:403:GLU:OE2	1:C:445:ARG:CD	2.47	0.63
1:A:226:ASP:OD2	1:C:267:ARG:NH2	2.31	0.62
1:B:397:ASN:ND2	3:B:517:HOH:O	2.33	0.61
1:B:68:GLU:OE2	1:B:80:ARG:NH1	2.35	0.60
1:D:116:HIS:ND1	1:D:141:THR:CG2	2.65	0.59
1:A:128:PRO:O	1:A:132:ASP:OD2	2.19	0.59
1:D:403:GLU:OE2	1:D:445:ARG:CG	2.51	0.58
1:B:326:PRO:O	1:B:327:ALA:C	2.42	0.58
1:B:132:ASP:OD2	1:B:134:THR:CG2	2.52	0.57
1:C:72:ARG:CG	1:C:72:ARG:NH1	2.69	0.56
1:D:421:ARG:NH2	3:D:518:HOH:O	2.37	0.56
1:A:96:GLU:OE2	1:D:73:TYR:OH	2.25	0.54
1:D:124:ASP:OD1	1:D:150:ASN:ND2	2.41	0.54
1:A:388:GLU:CA	3:A:558:HOH:O	2.56	0.54
1:A:180:ASP:CG	3:A:550:HOH:O	2.45	0.53
1:A:169:ASP:OD2	3:A:516:HOH:O	2.18	0.53
1:B:206:GLY:N	3:B:526:HOH:O	2.42	0.53
1:B:194:ASP:N	3:B:563:HOH:O	2.42	0.53
1:A:390:ARG:NH2	1:A:401:ALA:O	2.43	0.52
1:C:390:ARG:NH1	1:C:395:GLU:OE1	2.42	0.52
1:B:64:THR:N	2:B:448:PO4:O2	2.43	0.52
1:A:323:ARG:NH1	1:C:318:TRP:CD1	2.79	0.51
1:C:447:ARG:C	3:C:522:HOH:O	2.49	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:294:ARG:NH2	3:A:454:HOH:O	2.44	0.50
1:D:63:LYS:NZ	3:D:459:HOH:O	2.44	0.50
1:C:390:ARG:NH1	1:C:390:ARG:CG	2.74	0.50
1:B:72:ARG:NH2	3:B:481:HOH:O	2.45	0.49
1:B:331:ARG:NE	1:D:300:SER:OG	2.45	0.49
1:B:21:ARG:CD	1:B:68:GLU:OE1	2.60	0.49
1:D:446:TYR:N	3:D:539:HOH:O	2.44	0.49
1:C:56:TRP:NE1	1:C:142:THR:O	2.46	0.48
1:A:247:ARG:CD	3:A:547:HOH:O	2.61	0.48
1:C:150:ASN:N	1:C:150:ASN:OD1	2.47	0.48
1:C:17:ALA:N	3:C:479:HOH:O	2.46	0.47
1:B:267:ARG:NH2	1:C:226:ASP:OD2	2.47	0.47
1:C:156:ARG:NH1	1:C:156:ARG:CG	2.77	0.47
1:A:207:ASP:C	1:A:207:ASP:OD1	2.54	0.46
1:C:309:ARG:CB	1:C:309:ARG:NH2	2.78	0.46
1:D:209:ARG:NH2	2:D:448:PO4:O4	2.48	0.46
1:C:254:ARG:NH1	3:C:472:HOH:O	2.48	0.45
1:B:31:GLN:OE1	1:B:31:GLN:CA	2.64	0.45
1:A:318:TRP:CD1	1:A:318:TRP:C	2.91	0.44
1:B:411:ALA:O	1:B:412:GLN:CB	2.64	0.44
1:D:439:GLN:O	1:D:444:LYS:NZ	2.50	0.44
1:B:123:GLN:OE1	1:B:149:LEU:CA	2.66	0.44
1:A:189:ASP:OD1	1:C:256:TYR:OH	2.36	0.44
1:D:180:ASP:OD1	1:D:183:ARG:N	2.51	0.43
1:B:194:ASP:OD1	1:B:197:ARG:NH1	2.52	0.43
1:D:123:GLN:NE2	1:D:150:ASN:N	2.67	0.43
1:A:414:ARG:NH1	1:A:416:TYR:O	2.51	0.43
1:B:343:ALA:O	1:B:345:LYS:NZ	2.51	0.43
1:A:307:ASP:OD2	1:A:339:TYR:OH	2.36	0.43
1:D:368:VAL:N	3:D:513:HOH:O	2.51	0.42
1:A:197:ARG:NH1	1:A:197:ARG:CG	2.83	0.42
1:B:347:ASN:ND2	3:B:519:HOH:O	2.52	0.41
1:D:318:TRP:C	1:D:318:TRP:CD1	2.94	0.41
1:C:223:GLU:N	3:C:508:HOH:O	2.54	0.40
1:D:14:GLN:O	1:D:19:ARG:NH1	2.53	0.40
1:D:390:ARG:CG	1:D:395:GLU:OE2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	406/447 (91%)	387 (95%)	18 (4%)	1 (0%)	56	79
1	B	411/447 (92%)	390 (95%)	21 (5%)	0	100	100
1	C	414/447 (93%)	401 (97%)	13 (3%)	0	100	100
1	D	420/447 (94%)	408 (97%)	12 (3%)	0	100	100
All	All	1651/1788 (92%)	1586 (96%)	64 (4%)	1 (0%)	59	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	PRO

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	324/355 (91%)	294 (91%)	30 (9%)	13	23
1	B	327/355 (92%)	293 (90%)	34 (10%)	10	18
1	C	332/355 (94%)	287 (86%)	45 (14%)	5	10
1	D	335/355 (94%)	294 (88%)	41 (12%)	7	12
All	All	1318/1420 (93%)	1168 (89%)	150 (11%)	8	15

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	41	LEU

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Mol	Chain	Res	Type
1	A	66	LEU
1	A	68	GLU
1	A	80	ARG
1	A	81	ILE
1	A	84	VAL
1	A	90	GLU
1	A	115	VAL
1	A	117	ARG
1	A	132	ASP
1	A	134	THR
1	A	135	ILE
1	A	136	THR
1	A	144	ASN
1	A	148	GLU
1	A	161	LEU
1	A	196	THR
1	A	197	ARG
1	A	202	GLU
1	A	215	LEU
1	A	235	GLU
1	A	236	LEU
1	A	309	ARG
1	A	347	ASN
1	A	354	LYS
1	A	359	ASP
1	A	365	ASP
1	A	390	ARG
1	A	414	ARG
1	B	16	LEU
1	B	41	LEU
1	B	56	TRP
1	B	66	LEU
1	B	72	ARG
1	B	90	GLU
1	B	107	ARG
1	B	110	LEU
1	B	115	VAL
1	B	118	PHE
1	B	121	SER
1	B	123	GLN
1	B	134	THR
1	B	135	ILE

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Mol	Chain	Res	Type
1	B	150	ASN
1	B	153	LEU
1	B	155	SER
1	B	161	LEU
1	B	162	LEU
1	B	188	GLN
1	B	196	THR
1	B	197	ARG
1	B	210	ARG
1	B	215	LEU
1	B	236	LEU
1	B	237	LEU
1	B	238	THR
1	B	347	ASN
1	B	354	LYS
1	B	387	GLN
1	B	388	GLU
1	B	390	ARG
1	B	414	ARG
1	B	445	ARG
1	C	16	LEU
1	C	41	LEU
1	C	54	ILE
1	C	61	THR
1	C	66	LEU
1	C	68	GLU
1	C	72	ARG
1	C	77	ASP
1	C	78	VAL
1	C	107	ARG
1	C	108	THR
1	C	117	ARG
1	C	134	THR
1	C	135	ILE
1	C	143	GLU
1	C	150	ASN
1	C	156	ARG
1	C	161	LEU
1	C	162	LEU
1	C	167	THR
1	C	168	GLU
1	C	172	GLN

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Mol	Chain	Res	Type
1	C	188	GLN
1	C	198	ARG
1	C	202	GLU
1	C	210	ARG
1	C	215	LEU
1	C	223	GLU
1	C	237	LEU
1	C	238	THR
1	C	240	ILE
1	C	247	ARG
1	C	254	ARG
1	C	289	LEU
1	C	309	ARG
1	C	324	VAL
1	C	354	LYS
1	C	359	ASP
1	C	378	LYS
1	C	390	ARG
1	C	414	ARG
1	C	423	LEU
1	C	437	GLN
1	C	445	ARG
1	C	447	ARG
1	D	14	GLN
1	D	16	LEU
1	D	41	LEU
1	D	46	GLU
1	D	61	THR
1	D	66	LEU
1	D	81	ILE
1	D	88	VAL
1	D	93	GLU
1	D	97	ARG
1	D	99	ARG
1	D	106	ARG
1	D	110	LEU
1	D	115	VAL
1	D	119	ASN
1	D	141	THR
1	D	143	GLU
1	D	144	ASN
1	D	153	LEU

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Mol	Chain	Res	Type
1	D	161	LEU
1	D	167	THR
1	D	172	GLN
1	D	182	THR
1	D	188	GLN
1	D	195	GLU
1	D	196	THR
1	D	202	GLU
1	D	210	ARG
1	D	215	LEU
1	D	229	LYS
1	D	235	GLU
1	D	237	LEU
1	D	301	GLU
1	D	322	THR
1	D	324	VAL
1	D	363	ARG
1	D	381	LYS
1	D	390	ARG
1	D	414	ARG
1	D	439	GLN
1	D	445	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	448	-	4,4,4	0.57	0	6,6,6	0.32	0
2	PO4	B	448	-	4,4,4	0.46	0	6,6,6	0.33	0
2	PO4	C	448	-	4,4,4	0.29	0	6,6,6	0.32	0
2	PO4	D	448	-	4,4,4	0.43	0	6,6,6	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	448	-	-	0/0/0/0	0/0/0/0
2	PO4	B	448	-	-	0/0/0/0	0/0/0/0
2	PO4	C	448	-	-	0/0/0/0	0/0/0/0
2	PO4	D	448	-	-	0/0/0/0	0/0/0/0

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.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	414/447 (92%)	-0.09	9 (2%) 59 61	28, 52, 85, 104	0
1	B	417/447 (93%)	-0.10	12 (2%) 49 51	27, 51, 96, 112	0
1	C	420/447 (93%)	-0.09	9 (2%) 60 63	26, 53, 97, 118	0
1	D	424/447 (94%)	-0.16	6 (1%) 72 74	30, 45, 68, 82	0
All	All	1675/1788 (93%)	-0.11	36 (2%) 60 63	26, 50, 86, 118	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	PHE	4.8
1	C	248	PHE	3.6
1	C	120	LYS	3.5
1	C	37	ALA	3.2
1	C	147	PHE	3.2
1	C	151	SER	3.1
1	D	147	PHE	3.0
1	D	187	GLY	3.0
1	A	85	THR	2.9
1	B	161	LEU	2.8
1	D	254	ARG	2.7
1	A	133	GLY	2.7
1	B	265	SER	2.7
1	A	156	ARG	2.7
1	B	56	TRP	2.7
1	C	377	THR	2.6
1	A	151	SER	2.5
1	C	152	ALA	2.5
1	B	85	THR	2.4
1	D	274	ALA	2.4
1	A	150	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	182	THR	2.4
1	B	14	GLN	2.4
1	B	121	SER	2.3
1	D	265	SER	2.3
1	C	250	ASN	2.3
1	B	385	TYR	2.3
1	A	127	LEU	2.2
1	C	148	GLU	2.2
1	B	266	VAL	2.2
1	B	131	GLU	2.1
1	B	84	VAL	2.1
1	B	151	SER	2.1
1	A	38	GLY	2.0
1	A	377	THR	2.0
1	B	117	ARG	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PO4	B	448	5/5	0.15	1.17	60,60,61,65	0
2	PO4	A	448	5/5	0.17	0.25	55,56,59,60	0
2	PO4	D	448	5/5	0.17	0.10	45,47,48,49	0
2	PO4	C	448	5/5	0.10	-1.56	82,85,86,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.