



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:09 PM GMT

PDB ID : 4NXU
Title : Crystal structure of the cytosolic domain of human MiD51
Authors : Richter, V.; Kvansakul, M.; Ryan, M.T.
Deposited on : 2013-12-09
Resolution : 2.30 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

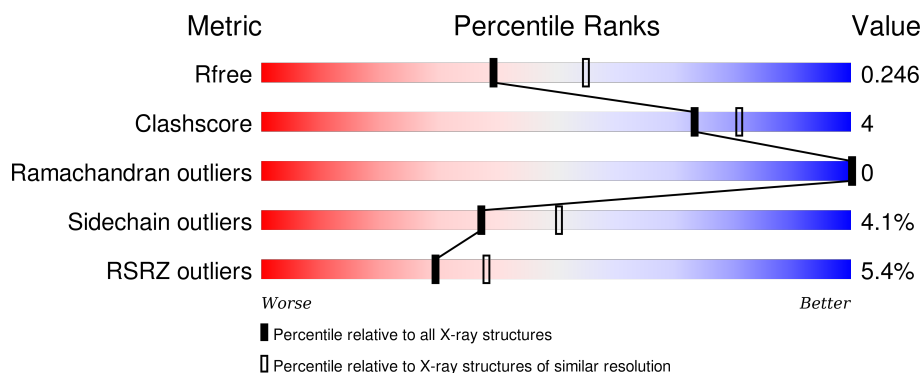
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	347	 3% 84% 10% • 6%
1	B	347	 2% 85% 9% • 5%
1	C	347	 4% 86% 7% • •
1	D	347	 11% 77% 16% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	502	-	-	-	X
3	SO4	C	504	-	-	X	-
3	SO4	C	505	-	-	-	X
4	GOL	B	502	-	-	-	X
4	GOL	C	502	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20858 atoms, of which 10206 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 Mitochondrial dynamic protein MID51.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	327	Total	C	H	N	O	S	0	1	0
			5085	1634	2543	425	471	12			
1	B	328	Total	C	H	N	O	S	0	0	0
			5146	1646	2576	435	478	11			
1	C	332	Total	C	H	N	O	S	0	0	0
			5145	1652	2572	436	474	11			
1	D	326	Total	C	H	N	O	S	0	0	0
			4937	1606	2451	412	457	11			

There are 8 discrepancies between the modelled and reference sequences:

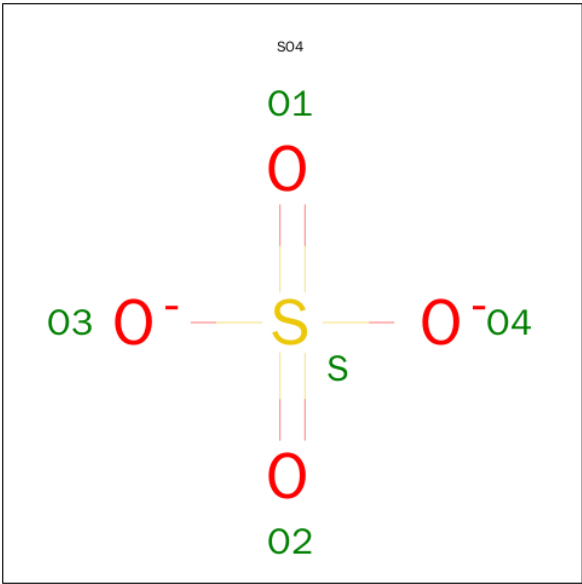
Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLY	-	EXPRESSION TAG	UNP Q9NQG6
A	118	SER	-	EXPRESSION TAG	UNP Q9NQG6
B	117	GLY	-	EXPRESSION TAG	UNP Q9NQG6
B	118	SER	-	EXPRESSION TAG	UNP Q9NQG6
C	117	GLY	-	EXPRESSION TAG	UNP Q9NQG6
C	118	SER	-	EXPRESSION TAG	UNP Q9NQG6
D	117	GLY	-	EXPRESSION TAG	UNP Q9NQG6
D	118	SER	-	EXPRESSION TAG	UNP Q9NQG6

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	B	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	C	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	D	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C H O 14 3 8 3	0	0
4	C	1	Total C H O 14 3 8 3	0	0

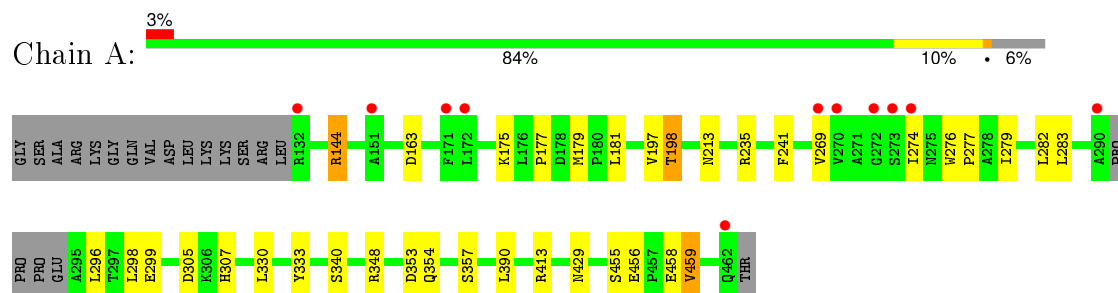
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	113	Total O 113 113	0	0
5	B	99	Total O 99 99	0	0
5	C	85	Total O 85 85	0	0
5	D	44	Total O 44 44	0	0

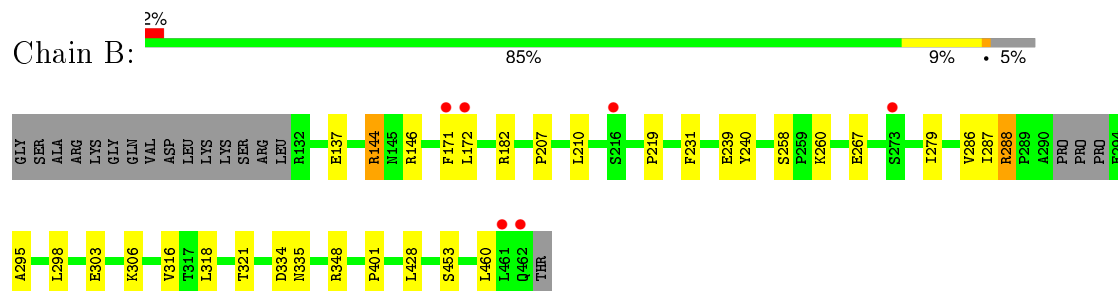
3 Residue-property plots [i](#)

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.

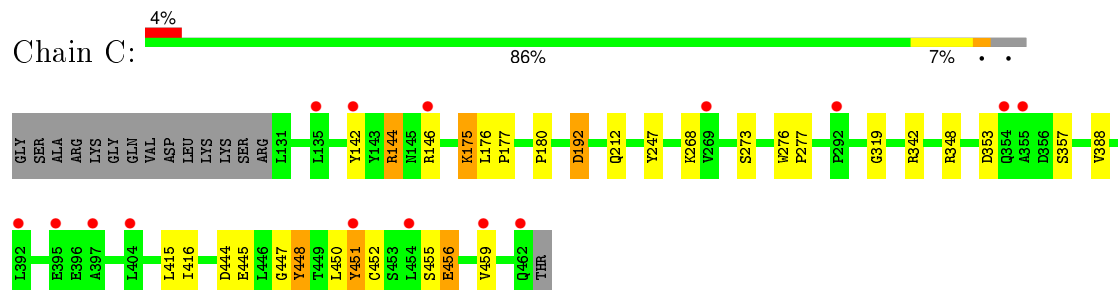
- Molecule 1: Mitochondrial dynamic protein MID51



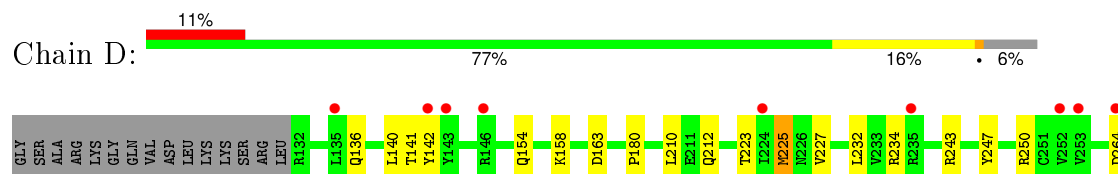
- Molecule 1: Mitochondrial dynamic protein MID51

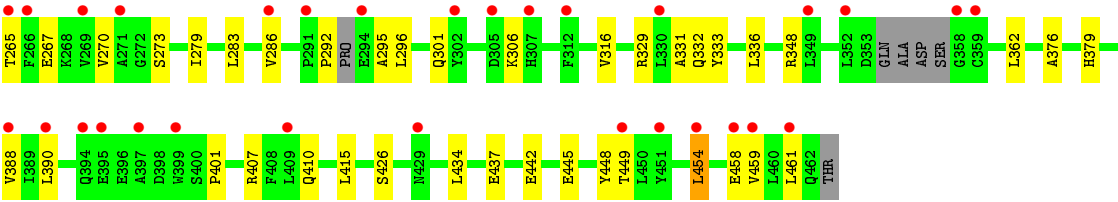


- Molecule 1: Mitochondrial dynamic protein MID51



- Molecule 1: Mitochondrial dynamic protein MID51





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.57Å 79.27Å 79.38Å 65.44° 84.18° 63.35°	Depositor
Resolution (Å)	39.19 – 2.30 45.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (39.19-2.30) 79.3 (45.67-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.216 , 0.248 0.215 , 0.246	Depositor DCC
R_{free} test set	2956 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 62141 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20858	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.90% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, ADP

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	0.30	0/2600	0.49	0/3547
1	B	0.33	0/2625	0.53	0/3578
1	C	0.28	0/2632	0.52	1/3595 (0.0%)
1	D	0.29	0/2542	0.51	0/3477
All	All	0.30	0/10399	0.51	1/14197 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	348	ARG	NE-CZ-NH1	6.50	123.55	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2542	2543	2543	20	2
1	B	2570	2576	2577	24	0
1	C	2573	2572	2569	18	1
1	D	2486	2451	2451	29	1
2	A	27	12	12	1	0
2	B	27	12	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	12	12	0	0
2	D	27	12	12	0	0
3	A	5	0	0	0	0
3	C	15	0	0	0	2
4	B	6	8	8	3	0
4	C	6	8	8	0	0
5	A	113	0	0	0	0
5	B	99	0	0	0	0
5	C	85	0	0	0	0
5	D	44	0	0	2	0
All	All	10652	10206	10204	84	3

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 4.

All (84) 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:D:376:ALA:HB1	1:D:449:THR:HG21	1.66	0.78
1:B:267:GLU:HG3	1:B:295:ALA:HB1	1.67	0.75
1:A:299:GLU:OE2	1:B:288:ARG:NH1	2.21	0.74
1:A:458:GLU:HG3	1:D:331:ALA:HB3	1.72	0.70
1:C:448:TYR:HA	1:C:451:TYR:HB2	1.74	0.69
1:B:453:SER:HB2	1:B:460:LEU:CD1	2.22	0.69
1:D:407:ARG:NH2	1:D:410:GLN:OE1	2.26	0.68
1:B:453:SER:HB2	1:B:460:LEU:HD11	1.76	0.68
1:D:250:ARG:NH2	5:D:605:HOH:O	2.27	0.67
1:D:154:GLN:NE2	5:D:625:HOH:O	2.29	0.64
1:B:401:PRO:HB3	1:D:454:LEU:HD22	1.81	0.61
1:B:348:ARG:HE	1:B:428:LEU:HD21	1.65	0.61
1:D:163:ASP:HB3	1:D:283:LEU:HD22	1.86	0.58
1:C:388:VAL:HG21	1:C:415:LEU:HD13	1.87	0.57
1:C:212:GLN:OE1	1:C:319:GLY:N	2.38	0.57
1:C:456:GLU:HG3	1:C:459:VAL:HG21	1.87	0.56
1:C:416:ILE:HD11	1:C:450:LEU:HB2	1.88	0.56
1:C:416:ILE:HD11	1:C:450:LEU:CB	2.36	0.55
1:C:445:GLU:HA	1:C:448:TYR:CE1	2.41	0.55
1:C:448:TYR:O	1:C:452:CYS:N	2.30	0.55
1:D:329:ARG:NH2	1:D:442:GLU:OE2	2.41	0.53
1:D:333:TYR:HB3	1:D:336:LEU:HD12	1.90	0.53
1:B:260:LYS:HE3	1:B:334:ASP:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LYS:HG2	1:C:273:SER:HB3	1.91	0.52
1:B:171:PHE:HD2	1:B:172:LEU:HD12	1.75	0.52
1:C:444:ASP:OD1	1:C:445:GLU:N	2.43	0.51
1:D:210:LEU:HD12	1:D:316:VAL:HG13	1.93	0.51
1:A:144:ARG:HD2	1:C:448:TYR:HB3	1.93	0.50
1:A:235:ARG:HH12	1:A:241:PHE:HB2	1.77	0.50
1:B:210:LEU:HD12	1:B:316:VAL:HG13	1.93	0.50
1:B:453:SER:CB	1:B:460:LEU:HD11	2.42	0.49
1:A:274:ILE:HD11	1:A:279:ILE:HD11	1.94	0.49
1:A:276:TRP:CH2	1:A:298:LEU:HD11	2.48	0.49
1:C:180:PRO:HG2	1:C:247:TYR:HB3	1.95	0.49
1:A:197:VAL:HG12	1:A:198:THR:HG22	1.94	0.49
1:D:232:LEU:CD2	1:D:336:LEU:HD23	2.43	0.48
1:D:267:GLU:HG2	1:D:296:LEU:HD23	1.95	0.48
1:D:136:GLN:NE2	1:D:401:PRO:O	2.39	0.47
1:D:163:ASP:HB3	1:D:283:LEU:CD2	2.44	0.47
1:D:223:THR:CB	1:D:225:MET:HG2	2.43	0.47
1:B:348:ARG:HE	1:B:428:LEU:CD2	2.28	0.47
1:B:318:LEU:O	1:B:321:THR:OG1	2.32	0.47
1:B:231:PHE:CZ	4:B:502:GOL:H31	2.50	0.47
1:B:231:PHE:CE1	4:B:502:GOL:H31	2.49	0.46
1:A:179:MET:CE	1:A:269:VAL:HG11	2.45	0.46
1:C:353:ASP:O	1:C:357:SER:N	2.48	0.46
1:C:192:ASP:OD2	1:C:342:ARG:NH1	2.38	0.45
1:A:456:GLU:HB3	1:A:459:VAL:HG13	1.99	0.45
1:B:144:ARG:CZ	1:D:448:TYR:HD2	2.30	0.44
1:B:171:PHE:CD2	1:B:172:LEU:HD12	2.51	0.44
1:B:287:ILE:CG2	1:B:298:LEU:HG	2.47	0.44
1:D:142:TYR:CD1	1:D:461:LEU:HB3	2.52	0.44
1:A:163:ASP:HB3	1:A:283:LEU:HD22	2.00	0.44
1:C:176:LEU:N	1:C:177:PRO:CD	2.81	0.43
1:A:179:MET:SD	1:A:181:LEU:HD11	2.58	0.43
1:A:305:ASP:OD1	1:A:305:ASP:N	2.52	0.43
1:D:329:ARG:HH22	1:D:379:HIS:CE1	2.36	0.43
1:A:353:ASP:O	1:A:357:SER:N	2.52	0.43
1:D:286:VAL:HB	1:D:301:GLN:HB3	2.00	0.43
1:D:292:PRO:HG3	1:D:295:ALA:HB2	2.00	0.43
1:A:307:HIS:CG	1:B:288:ARG:HH22	2.37	0.42
1:A:276:TRP:HB2	1:A:277:PRO:HD3	2.01	0.42
1:A:330:LEU:HB2	1:A:333:TYR:HD2	1.84	0.42
1:D:232:LEU:HD23	1:D:336:LEU:HD23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:ARG:N	1:D:437:GLU:OE1	2.53	0.42
1:A:276:TRP:HA	1:A:279:ILE:HD12	2.00	0.42
1:A:340:SER:OG	2:A:501:ADP:N1	2.48	0.42
1:D:279:ILE:HG22	1:D:283:LEU:HD12	2.00	0.42
1:B:219:PRO:HB3	4:B:502:GOL:H32	2.02	0.42
1:C:276:TRP:HB2	1:C:277:PRO:HD3	2.02	0.42
1:B:239:GLU:HG2	1:B:240:TYR:N	2.35	0.41
1:B:182:ARG:HB2	1:B:207:PRO:HG2	2.01	0.41
1:B:460:LEU:N	1:B:460:LEU:HD12	2.35	0.41
1:D:180:PRO:HG3	1:D:247:TYR:HB3	2.01	0.41
1:B:303:GLU:HB2	1:B:306:LYS:HB2	2.03	0.41
1:C:444:ASP:O	1:C:447:GLY:N	2.53	0.41
1:C:142:TYR:CZ	1:C:146:ARG:HG2	2.56	0.41
1:D:388:VAL:HG11	1:D:415:LEU:HD12	2.01	0.41
1:D:445:GLU:O	1:D:449:THR:HG23	2.22	0.40
1:A:458:GLU:HG3	1:D:331:ALA:CB	2.48	0.40
1:A:175:LYS:C	1:A:177:PRO:HD3	2.41	0.40
1:B:335:ASN:OD1	1:B:335:ASN:N	2.54	0.40
1:D:426:SER:HB2	1:D:434:LEU:HD21	2.04	0.40
1:D:333:TYR:HB3	1:D:336:LEU:CD1	2.52	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASN:HD21	3:C:504:SO4:O2[1_645]	1.55	0.05
1:A:213:ASN:ND2	3:C:504:SO4:O2[1_645]	2.15	0.05
1:C:144:ARG:O	1:D:212:GLN:NE2[1_556]	2.17	0.03

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	324/347 (93%)	315 (97%)	9 (3%)	0	100	100
1	B	324/347 (93%)	316 (98%)	8 (2%)	0	100	100
1	C	330/347 (95%)	324 (98%)	6 (2%)	0	100	100
1	D	320/347 (92%)	304 (95%)	16 (5%)	0	100	100
All	All	1298/1388 (94%)	1259 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	273/298 (92%)	262 (96%)	11 (4%)	38	52
1	B	278/298 (93%)	271 (98%)	7 (2%)	55	73
1	C	275/298 (92%)	267 (97%)	8 (3%)	50	66
1	D	260/298 (87%)	241 (93%)	19 (7%)	17	22
All	All	1086/1192 (91%)	1041 (96%)	45 (4%)	37	50

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ARG
1	A	198	THR
1	A	282	LEU
1	A	296	LEU
1	A	348	ARG
1	A	354	GLN
1	A	390	LEU
1	A	413	ARG
1	A	429	ASN
1	A	455	SER
1	A	459	VAL
1	B	137	GLU
1	B	144	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	146	ARG
1	B	258	SER
1	B	279	ILE
1	B	286	VAL
1	B	288	ARG
1	C	144	ARG
1	C	175	LYS
1	C	192	ASP
1	C	268	LYS
1	C	448	TYR
1	C	451	TYR
1	C	455	SER
1	C	456	GLU
1	D	140	LEU
1	D	141	THR
1	D	158	LYS
1	D	225	MET
1	D	227	VAL
1	D	234	ARG
1	D	243	ARG
1	D	264	ASP
1	D	265	THR
1	D	270	VAL
1	D	273	SER
1	D	306	LYS
1	D	332	GLN
1	D	348	ARG
1	D	362	LEU
1	D	390	LEU
1	D	454	LEU
1	D	458	GLU
1	D	459	VAL

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

Mol	Chain	Res	Type
1	B	275	ASN

5.3.3 RNA ⓘ

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](#)

10 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	ADP	A	501	-	22,29,29	1.11	1 (4%)	27,45,45	1.75	3 (11%)
3	SO4	A	502	-	4,4,4	0.13	0	6,6,6	0.11	0
2	ADP	B	501	-	22,29,29	1.09	1 (4%)	27,45,45	1.85	5 (18%)
4	GOL	B	502	-	5,5,5	0.97	0	5,5,5	0.78	0
2	ADP	C	501	-	22,29,29	1.05	1 (4%)	27,45,45	1.89	4 (14%)
4	GOL	C	502	-	5,5,5	0.94	0	5,5,5	0.80	0
3	SO4	C	503	-	4,4,4	0.11	0	6,6,6	0.10	0
3	SO4	C	504	-	4,4,4	0.16	0	6,6,6	0.22	0
3	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.24	0
2	ADP	D	501	-	22,29,29	1.05	1 (4%)	27,45,45	1.89	6 (22%)

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	ADP	A	501	-	-	0/12/32/32	0/3/3/3
3	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	ADP	B	501	-	-	0/12/32/32	0/3/3/3
4	GOL	B	502	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	501	-	-	0/12/32/32	0/3/3/3
4	GOL	C	502	-	-	0/4/4/4	0/0/0/0
3	SO4	C	503	-	-	0/0/0/0	0/0/0/0
3	SO4	C	504	-	-	0/0/0/0	0/0/0/0
3	SO4	C	505	-	-	0/0/0/0	0/0/0/0
2	ADP	D	501	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	ADP	C5-C4	3.30	1.47	1.40
2	C	501	ADP	C5-C4	3.30	1.47	1.40
2	A	501	ADP	C5-C4	3.36	1.48	1.40
2	B	501	ADP	C5-C4	3.39	1.48	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ADP	N3-C2-N1	-6.71	123.75	128.89
2	D	501	ADP	N3-C2-N1	-6.26	124.10	128.89
2	A	501	ADP	N3-C2-N1	-5.90	124.38	128.89
2	B	501	ADP	N3-C2-N1	-5.88	124.39	128.89
2	D	501	ADP	C4-C5-N7	-3.99	105.81	109.48
2	A	501	ADP	C4-C5-N7	-3.97	105.83	109.48
2	C	501	ADP	C4-C5-N7	-3.95	105.85	109.48
2	B	501	ADP	C4-C5-N7	-3.76	106.02	109.48
2	C	501	ADP	PA-O3A-PB	-2.89	122.98	132.67
2	D	501	ADP	C1'-N9-C4	-2.52	123.14	126.94
2	B	501	ADP	PA-O3A-PB	-2.51	124.27	132.67
2	A	501	ADP	PA-O3A-PB	-2.37	124.71	132.67
2	D	501	ADP	PA-O3A-PB	-2.34	124.83	132.67
2	B	501	ADP	O3A-PA-O5'	-2.25	96.97	102.94
2	D	501	ADP	O3A-PA-O5'	-2.16	97.20	102.94
2	C	501	ADP	O3A-PA-O5'	-2.10	97.38	102.94
2	B	501	ADP	O3B-PB-O2B	2.01	115.03	107.38
2	D	501	ADP	O2'-C2'-C3'	2.04	118.48	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ADP	1	0
4	B	502	GOL	3	0
3	C	504	SO4	0	2

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	327/347 (94%)	0.20	11 (3%) 49 58	19, 38, 63, 98	0
1	B	328/347 (94%)	0.13	6 (1%) 71 78	22, 36, 58, 94	0
1	C	332/347 (95%)	0.42	15 (4%) 37 46	21, 43, 75, 102	0
1	D	326/347 (93%)	0.71	39 (11%) 6 9	35, 59, 85, 136	0
All	All	1313/1388 (94%)	0.37	71 (5%) 29 38	19, 44, 76, 136	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	SER	5.6
1	D	135	LEU	5.2
1	A	270	VAL	5.0
1	C	451	TYR	4.8
1	C	462	GLN	4.7
1	D	349	LEU	3.6
1	A	274	ILE	3.6
1	D	269	VAL	3.6
1	D	142	TYR	3.5
1	D	253	VAL	3.5
1	D	294	GLU	3.5
1	B	461	LEU	3.4
1	D	359	CYS	3.4
1	D	305	ASP	3.3
1	C	459	VAL	3.2
1	D	307	HIS	3.2
1	C	395	GLU	3.1
1	D	291	PRO	3.1
1	D	352	LEU	3.0
1	C	355	ALA	3.0
1	C	135	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	462	GLN	2.9
1	A	171	PHE	2.9
1	D	459	VAL	2.8
1	C	404	LEU	2.8
1	D	390	LEU	2.8
1	D	271	ALA	2.7
1	D	451	TYR	2.7
1	A	272	GLY	2.7
1	D	330	LEU	2.7
1	D	252	VAL	2.7
1	A	172	LEU	2.7
1	D	224	ILE	2.6
1	D	429	ASN	2.6
1	D	358	GLY	2.6
1	A	151	ALA	2.6
1	A	462	GLN	2.5
1	C	142	TYR	2.5
1	D	397	ALA	2.4
1	D	143	TYR	2.4
1	D	449	THR	2.4
1	C	354	GLN	2.4
1	C	269	VAL	2.3
1	D	312	PHE	2.3
1	D	286	VAL	2.3
1	B	172	LEU	2.3
1	D	146	ARG	2.3
1	A	290	ALA	2.3
1	C	392	LEU	2.3
1	C	454	LEU	2.3
1	A	269	VAL	2.3
1	D	266	PHE	2.3
1	D	264	ASP	2.2
1	D	458	GLU	2.2
1	C	397	ALA	2.2
1	A	132	ARG	2.2
1	D	235	ARG	2.2
1	D	461	LEU	2.2
1	B	171	PHE	2.2
1	D	388	VAL	2.2
1	C	292	PRO	2.2
1	D	395	GLU	2.2
1	D	394	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	409	LEU	2.1
1	C	146	ARG	2.1
1	D	399	TRP	2.1
1	D	454	LEU	2.0
1	D	302	TYR	2.0
1	D	265	THR	2.0
1	B	216	SER	2.0
1	B	273	SER	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](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	C	502	6/6	0.71	0.35	10.13	32,39,41,42	0
4	GOL	B	502	6/6	0.83	0.33	7.68	35,42,46,46	0
3	SO4	C	505	5/5	0.93	0.39	7.47	44,45,46,47	0
3	SO4	A	502	5/5	0.94	0.25	3.44	46,47,48,49	0
3	SO4	C	503	5/5	0.95	0.18	1.37	44,45,46,46	0
2	ADP	B	501	27/27	0.96	0.14	0.68	23,34,42,43	0
2	ADP	A	501	27/27	0.98	0.15	0.68	24,31,39,43	0
2	ADP	D	501	27/27	0.96	0.13	-0.48	42,44,53,71	0
2	ADP	C	501	27/27	0.97	0.11	-0.83	36,40,50,88	0
3	SO4	C	504	5/5	0.97	0.09	-2.18	42,43,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.