



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:17 am GMT

PDB ID : 2NCD  
Title : NCD (NON-CLARET DISJUNCTIONAL) DIMER FROM D.  
MELANOGASTER  
Authors : Sablin, E.P.; Case, R.B.; Dai, S.C.; Hart, C.L.; Ruby, A.; Vale, R.D.; Fletter-  
ick, R.J.  
Deposited on : 1999-06-04  
Resolution : 2.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

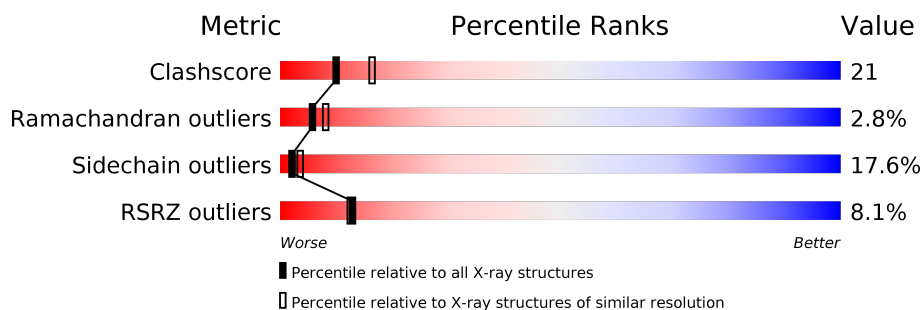
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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  $\geq 3$ , 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	420	

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
2	SO4	A	1110	-	X	-	-
2	SO4	A	1111	-	-	-	X
2	SO4	A	1112	-	X	-	-
2	SO4	A	1113	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	A	800	-	-	-	X

## 2 Entry composition [i](#)

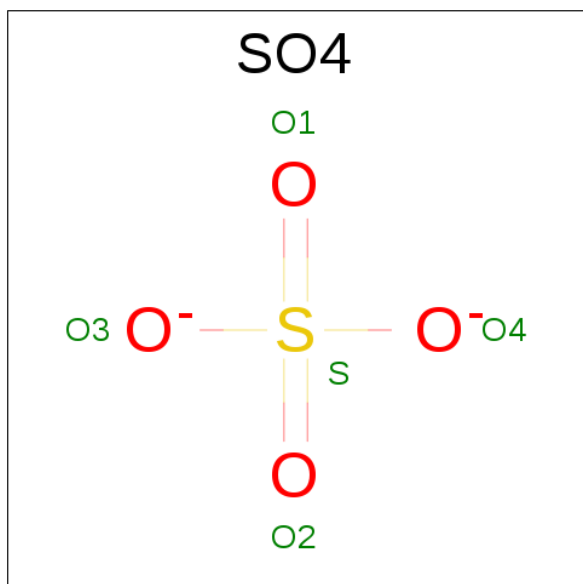
There are 4 unique types of molecules in this entry. The entry contains 2952 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (Kinesin motor NCD).

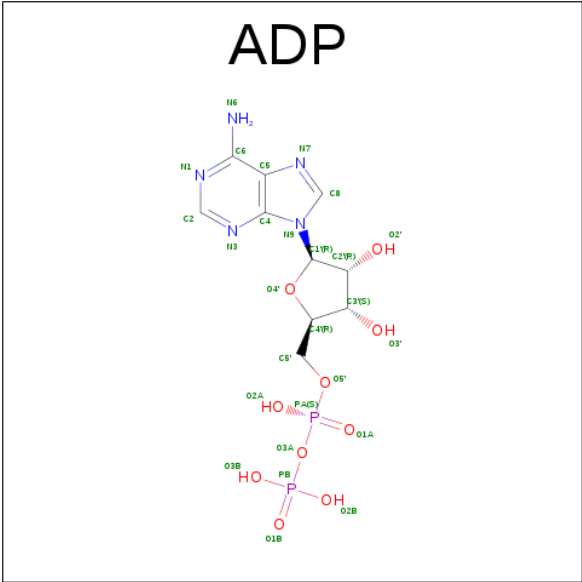
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2851	1772	502	557	20	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

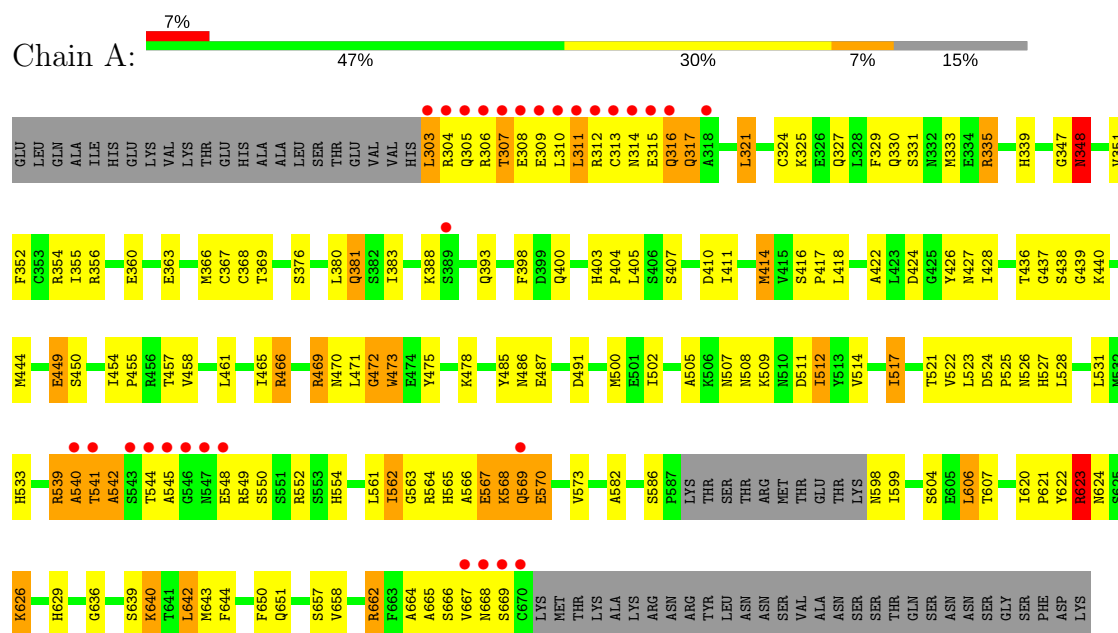
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		

### 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 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: PROTEIN (Kinesin motor NCD)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.00Å 123.00Å 121.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 34.07 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.50) 98.8 (34.07-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.01 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.226 , 0.270 0.229 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/2897	0.61	1/3909 (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	A	472	GLY	N-CA-C	-5.96	98.20	113.10

There are no chirality outliers.

There are no planarity outliers.

### 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	2851	0	2809	121	2
2	A	20	0	0	1	0
3	A	27	0	12	7	0
4	A	54	0	0	2	1
All	All	2952	0	2821	121	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 21.

All (121) 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:347:GLY:O	1:A:348:ASN:HB2	1.69	0.92
1:A:552:ARG:HD2	1:A:599:ILE:CG2	2.09	0.83
1:A:418:LEU:HD11	1:A:642:LEU:HD13	1.60	0.82
1:A:308:GLU:HA	1:A:311:LEU:HD23	1.68	0.75
1:A:542:ALA:N	1:A:550:SER:HB2	2.00	0.75
1:A:418:LEU:HD12	1:A:642:LEU:HD22	1.71	0.72
1:A:569:GLN:O	1:A:570:GLU:HG2	1.92	0.70
1:A:461:LEU:O	1:A:465:ILE:HG13	1.91	0.69
1:A:539:ARG:HG3	1:A:541:THR:HG23	1.73	0.69
1:A:554:HIS:CD2	1:A:582:ALA:H	2.13	0.67
1:A:524:ASP:HB2	1:A:525:PRO:HD2	1.76	0.66
1:A:541:THR:HB	1:A:550:SER:OG	1.95	0.66
1:A:568:LYS:O	1:A:569:GLN:HG3	1.95	0.65
1:A:552:ARG:HD2	1:A:599:ILE:HG21	1.77	0.64
1:A:524:ASP:HB2	1:A:525:PRO:CD	2.27	0.64
1:A:303:LEU:HA	1:A:306:ARG:NH2	2.12	0.64
1:A:454:ILE:HB	1:A:455:PRO:HD3	1.80	0.64
1:A:542:ALA:HB1	1:A:545:ALA:O	1.98	0.63
1:A:440:LYS:HZ3	3:A:800:ADP:PB	2.22	0.62
1:A:352:PHE:CD1	1:A:400:GLN:HB3	2.35	0.62
1:A:554:HIS:HD2	1:A:582:ALA:H	1.48	0.62
1:A:383:ILE:HG12	1:A:651:GLN:OE1	1.99	0.61
1:A:335:ARG:NH2	1:A:424:ASP:OD2	2.34	0.60
1:A:449:GLU:CD	1:A:449:GLU:H	2.04	0.60
1:A:437:GLY:H	3:A:800:ADP:PB	2.25	0.60
1:A:376:SER:HB2	1:A:398:PHE:O	2.01	0.59
1:A:620:ILE:HB	1:A:622:TYR:CE1	2.37	0.59
1:A:565:HIS:CD2	1:A:568:LYS:HB3	2.38	0.58
1:A:539:ARG:CG	1:A:541:THR:HG23	2.34	0.58
1:A:665:ALA:O	1:A:669:SER:HB3	2.04	0.58
1:A:440:LYS:HB2	3:A:800:ADP:O3B	2.04	0.57
1:A:568:LYS:C	1:A:569:GLN:HG3	2.26	0.56
1:A:514:VAL:HB	1:A:517:ILE:HG12	1.86	0.56
1:A:461:LEU:HD21	1:A:561:LEU:HD21	1.87	0.56
1:A:667:VAL:HG12	1:A:668:ASN:N	2.20	0.56
1:A:321:LEU:HD22	1:A:325:LYS:HE3	1.87	0.56
1:A:500:MET:CE	1:A:517:ILE:HG23	2.35	0.56
1:A:473:TRP:HA	1:A:564:ARG:O	2.05	0.56
1:A:355:ILE:O	1:A:404:PRO:HA	2.06	0.56
1:A:356:ARG:HG2	1:A:438:SER:O	2.05	0.55
1:A:416:SER:OG	1:A:417:PRO:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:PHE:HD1	1:A:400:GLN:HB3	1.71	0.55
1:A:623:ARG:HB2	2:A:1110:SO4:O1	2.04	0.55
1:A:491:ASP:HB2	1:A:500:MET:CE	2.37	0.55
1:A:308:GLU:O	1:A:311:LEU:HB2	2.07	0.54
1:A:485:TYR:CE1	1:A:549:ARG:HA	2.42	0.54
1:A:514:VAL:O	1:A:517:ILE:HD11	2.07	0.54
1:A:539:ARG:O	1:A:541:THR:N	2.40	0.54
1:A:306:ARG:HB3	1:A:306:ARG:CZ	2.37	0.54
1:A:486:ASN:ND2	1:A:599:ILE:HD13	2.22	0.54
1:A:472:GLY:O	1:A:473:TRP:HB2	2.06	0.53
1:A:487:GLU:O	1:A:626:LYS:HD3	2.07	0.53
1:A:383:ILE:HG12	1:A:651:GLN:CD	2.30	0.53
1:A:303:LEU:HG	1:A:306:ARG:NH2	2.24	0.52
1:A:351:VAL:HG21	1:A:667:VAL:HG21	1.92	0.52
1:A:335:ARG:HH22	1:A:424:ASP:CG	2.12	0.52
1:A:352:PHE:CZ	1:A:414:MET:HG2	2.45	0.52
1:A:329:PHE:CE2	1:A:568:LYS:HG2	2.45	0.52
1:A:367:CYS:HA	1:A:650:PHE:HA	1.90	0.52
1:A:478:LYS:HD2	1:A:562:ILE:HD11	1.93	0.51
1:A:473:TRP:CE3	1:A:565:HIS:HB2	2.46	0.51
1:A:398:PHE:CE2	1:A:664:ALA:CB	2.94	0.51
1:A:541:THR:C	1:A:550:SER:HB2	2.30	0.51
1:A:457:THR:O	1:A:461:LEU:HB2	2.11	0.51
1:A:354:ARG:CZ	1:A:411:ILE:HD13	2.41	0.51
1:A:512:ILE:HD11	1:A:629:HIS:NE2	2.27	0.50
1:A:428:ILE:HD12	1:A:640:LYS:HB2	1.93	0.50
1:A:486:ASN:O	1:A:487:GLU:HB2	2.12	0.49
1:A:548:GLU:HG2	1:A:548:GLU:O	2.11	0.49
1:A:562:ILE:HG23	1:A:573:VAL:HG22	1.93	0.49
1:A:502:ILE:CG2	1:A:512:ILE:HG12	2.42	0.49
1:A:407:SER:O	1:A:410:ASP:HB2	2.13	0.48
1:A:458:VAL:HG22	1:A:528:LEU:HD23	1.94	0.48
1:A:458:VAL:HG22	1:A:528:LEU:CD2	2.42	0.48
1:A:312:ARG:O	1:A:315:GLU:HB2	2.13	0.48
1:A:381:GLN:NE2	1:A:388:LYS:HE3	2.28	0.48
1:A:526:ASN:HB2	4:A:954:HOH:O	2.13	0.47
1:A:439:GLY:N	3:A:800:ADP:O1A	2.47	0.47
1:A:522:VAL:HG11	1:A:528:LEU:HB2	1.96	0.47
1:A:486:ASN:HD22	1:A:599:ILE:HA	1.79	0.47
1:A:428:ILE:CD1	1:A:640:LYS:HB2	2.45	0.47
1:A:511:ASP:OD1	1:A:512:ILE:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ALA:O	1:A:567:GLU:CB	2.63	0.46
1:A:422:ALA:HA	1:A:426:TYR:O	2.16	0.46
1:A:339:HIS:HD2	4:A:942:HOH:O	1.99	0.45
1:A:466:ARG:O	1:A:469:ARG:HB2	2.17	0.45
1:A:475:TYR:CE1	1:A:563:GLY:HA3	2.52	0.45
1:A:622:TYR:C	1:A:624:ASN:H	2.18	0.45
1:A:427:ASN:O	1:A:428:ILE:HD13	2.16	0.45
1:A:491:ASP:HB2	1:A:500:MET:HE3	1.99	0.45
1:A:403:HIS:CG	1:A:404:PRO:HD2	2.52	0.45
1:A:439:GLY:C	3:A:800:ADP:O2A	2.56	0.44
1:A:411:ILE:HG23	1:A:644:PHE:CE2	2.53	0.44
1:A:436:THR:HA	3:A:800:ADP:O1B	2.18	0.44
1:A:542:ALA:H	1:A:550:SER:HB2	1.82	0.44
1:A:541:THR:CA	1:A:550:SER:HB2	2.47	0.44
1:A:324:CYS:O	1:A:327:GLN:HB2	2.18	0.44
1:A:552:ARG:HD2	1:A:599:ILE:HG22	1.97	0.43
1:A:539:ARG:O	1:A:540:ALA:C	2.56	0.43
1:A:440:LYS:NZ	3:A:800:ADP:O3B	2.49	0.43
1:A:303:LEU:CG	1:A:306:ARG:HH21	2.32	0.43
1:A:311:LEU:C	1:A:313:CYS:H	2.21	0.43
1:A:312:ARG:HA	1:A:315:GLU:HG3	2.01	0.43
1:A:313:CYS:HA	1:A:316:GLN:OE1	2.18	0.43
1:A:312:ARG:O	1:A:316:GLN:HG3	2.19	0.42
1:A:444:MET:O	1:A:454:ILE:HG13	2.18	0.42
1:A:307:THR:HG23	1:A:307:THR:O	2.19	0.42
1:A:539:ARG:HG3	1:A:539:ARG:O	2.19	0.42
1:A:541:THR:HG22	1:A:550:SER:HA	2.02	0.42
1:A:527:HIS:O	1:A:531:LEU:HG	2.19	0.42
1:A:502:ILE:HG22	1:A:512:ILE:HG12	2.02	0.42
1:A:356:ARG:NH1	1:A:437:GLY:O	2.42	0.42
1:A:606:LEU:HD22	1:A:606:LEU:O	2.20	0.41
1:A:658:VAL:O	1:A:662:ARG:HB2	2.20	0.41
1:A:621:PRO:O	1:A:624:ASN:HB2	2.19	0.41
1:A:662:ARG:O	1:A:665:ALA:HB3	2.21	0.41
1:A:311:LEU:C	1:A:313:CYS:N	2.73	0.40
1:A:314:ASN:HA	1:A:317:GLN:HB2	2.03	0.40
1:A:500:MET:HE1	1:A:517:ILE:HG23	2.02	0.40
1:A:303:LEU:HA	1:A:306:ARG:HH21	1.84	0.40
1:A:505:ALA:CB	1:A:511:ASP:HB3	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:314:ASN:ND2	1:A:314:ASN:ND2[9_555]	1.74	0.46
1:A:303:LEU:CD2	1:A:303:LEU:CD2[9_555]	1.91	0.29
4:A:943:HOH:O	4:A:944:HOH:O[12_566]	2.15	0.05

## 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	354/420 (84%)	312 (88%)	32 (9%)	10 (3%)	<b>6</b> <b>8</b>

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	ALA
1	A	542	ALA
1	A	568	LYS
1	A	348	ASN
1	A	570	GLU
1	A	636	GLY
1	A	508	ASN
1	A	569	GLN
1	A	473	TRP
1	A	623	ARG

### 5.3.2 Protein sidechains [i](#)

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	324/380 (85%)	267 (82%)	57 (18%)	<b>2</b> <b>3</b>

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	LEU
1	A	304	ARG
1	A	305	GLN
1	A	307	THR
1	A	309	GLU
1	A	310	LEU
1	A	311	LEU
1	A	316	GLN
1	A	317	GLN
1	A	321	LEU
1	A	330	GLN
1	A	331	SER
1	A	333	MET
1	A	335	ARG
1	A	348	ASN
1	A	360	GLU
1	A	363	GLU
1	A	366	MET
1	A	368	CYS
1	A	369	THR
1	A	380	LEU
1	A	381	GLN
1	A	393	GLN
1	A	405	LEU
1	A	414	MET
1	A	449	GLU
1	A	450	SER
1	A	466	ARG
1	A	469	ARG
1	A	470	ASN
1	A	471	LEU
1	A	507	ASN
1	A	509	LYS
1	A	512	ILE
1	A	517	ILE
1	A	521	THR
1	A	523	LEU
1	A	533	HIS

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Mol	Chain	Res	Type
1	A	539	ARG
1	A	541	THR
1	A	544	THR
1	A	562	ILE
1	A	567	GLU
1	A	586	SER
1	A	598	ASN
1	A	604	SER
1	A	606	LEU
1	A	607	THR
1	A	623	ARG
1	A	626	LYS
1	A	639	SER
1	A	640	LYS
1	A	642	LEU
1	A	643	MET
1	A	657	SER
1	A	662	ARG
1	A	666	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	ASN
1	A	339	HIS
1	A	364	ASN
1	A	381	GLN
1	A	393	GLN
1	A	486	ASN
1	A	507	ASN
1	A	554	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	SO4	A	1110	-	4,4,4	0.39	0	6,6,6	3.25	5 (83%)
2	SO4	A	1111	-	4,4,4	0.42	0	6,6,6	3.01	3 (50%)
2	SO4	A	1112	-	4,4,4	0.40	0	6,6,6	4.50	4 (66%)
2	SO4	A	1113	-	4,4,4	0.30	0	6,6,6	2.59	3 (50%)
3	ADP	A	800	-	25,29,29	1.58	3 (12%)	24,45,45	2.98	8 (33%)

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	SO4	A	1110	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1111	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1112	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1113	-	-	0/0/0/0	0/0/0/0
3	ADP	A	800	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	ADP	C5-N7	-2.28	1.31	1.39
3	A	800	ADP	C5'-C4'	2.08	1.58	1.51
3	A	800	ADP	O4'-C1'	5.60	1.49	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	ADP	N3-C2-N1	-11.38	118.95	128.86
2	A	1112	SO4	O4-S-O3	-7.86	73.53	108.96
2	A	1110	SO4	O2-S-O1	-4.63	77.31	109.64
2	A	1113	SO4	O3-S-O1	-4.06	86.88	109.26
2	A	1112	SO4	O2-S-O1	-3.78	83.24	109.64
2	A	1110	SO4	O4-S-O1	-3.64	89.20	109.26
2	A	1111	SO4	O4-S-O3	-2.69	96.86	108.96
2	A	1111	SO4	O4-S-O1	-2.62	94.83	109.26
2	A	1110	SO4	O3-S-O1	-2.34	96.38	109.26
3	A	800	ADP	O2A-PA-O5'	-2.00	98.68	108.14
3	A	800	ADP	O2A-PA-O1A	2.01	122.66	112.28
3	A	800	ADP	C2-N1-C6	2.05	122.36	118.77
3	A	800	ADP	O4'-C4'-C5'	2.11	116.53	109.40
3	A	800	ADP	C2'-C3'-C4'	2.15	106.81	102.62
2	A	1110	SO4	O4-S-O2	2.80	124.69	109.26
2	A	1113	SO4	O3-S-O2	2.98	125.68	109.26
2	A	1113	SO4	O4-S-O3	3.53	124.85	108.96
2	A	1110	SO4	O4-S-O3	3.94	126.72	108.96
2	A	1112	SO4	O4-S-O1	4.52	134.17	109.26
3	A	800	ADP	C4-C5-N7	4.62	113.87	109.41
2	A	1112	SO4	O4-S-O2	4.65	134.88	109.26
3	A	800	ADP	O5'-C5'-C4'	4.72	125.74	109.00
2	A	1111	SO4	O3-S-O2	6.01	142.40	109.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1110	SO4	1	0
3	A	800	ADP	7	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	358/420 (85%)	0.06	29 (8%) <b>13</b> <b>12</b>	3, 17, 81, 99	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	SER	7.8
1	A	544	THR	7.5
1	A	545	ALA	5.7
1	A	304	ARG	5.7
1	A	315	GLU	4.9
1	A	313	CYS	4.9
1	A	310	LEU	4.8
1	A	669	SER	4.6
1	A	670	CYS	4.5
1	A	305	GLN	4.5
1	A	306	ARG	4.5
1	A	311	LEU	3.8
1	A	303	LEU	3.6
1	A	308	GLU	3.5
1	A	541	THR	3.4
1	A	569	GLN	3.3
1	A	312	ARG	3.2
1	A	314	ASN	2.8
1	A	309	GLU	2.8
1	A	307	THR	2.7
1	A	318	ALA	2.5
1	A	540	ALA	2.5
1	A	668	ASN	2.4
1	A	316	GLN	2.4
1	A	548	GLU	2.2
1	A	547	ASN	2.1
1	A	546	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	667	VAL	2.1
1	A	389	SER	2.1

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	ADP	A	800	27/27	0.70	0.42	11.64	39,85,100,100	0
2	SO4	A	1113	5/5	0.81	0.29	6.14	90,92,100,100	0
2	SO4	A	1111	5/5	0.91	0.31	4.27	83,90,91,96	0
2	SO4	A	1110	5/5	0.94	0.22	0.92	74,75,81,87	0
2	SO4	A	1112	5/5	0.93	0.13	-0.12	60,65,70,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.