



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:29 AM GMT

PDB ID : 2XAE  
Title : CRYSTAL STRUCTURE OF HUMAN KINESIN EG5 IN COMPLEX WITH  
(R)-2-AMINO-3-((S)-2-METHYL-1,1-DIPHENYLBUTYLTHIO)PROPANO  
IC ACID  
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C.; Popowycz, F.; Joseph, B.; Kozielski, F.  
Deposited on : 2010-03-31  
Resolution : 2.60 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 (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

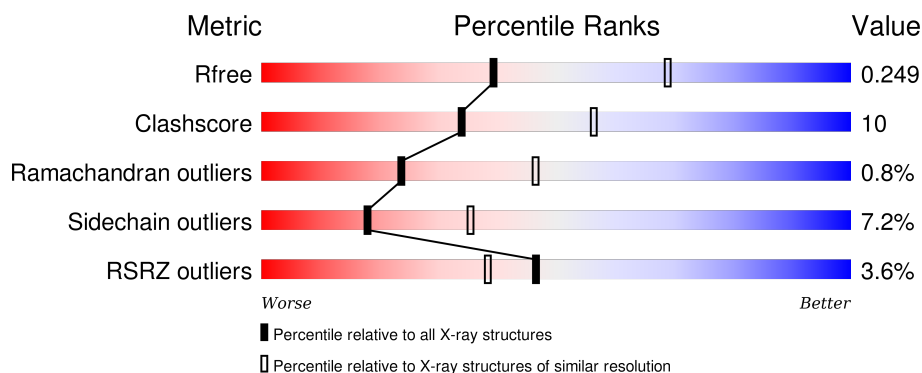
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	368	<div> <div>2%</div> <div>68%</div> <div>19%</div> <div>•</div> <div>11%</div> </div>
1	B	368	<div> <div>2%</div> <div>70%</div> <div>16%</div> <div>•</div> <div>11%</div> </div>
1	C	368	<div> <div>5%</div> <div>62%</div> <div>24%</div> <div>•</div> <div>11%</div> </div>

## 2 Entry composition [i](#)

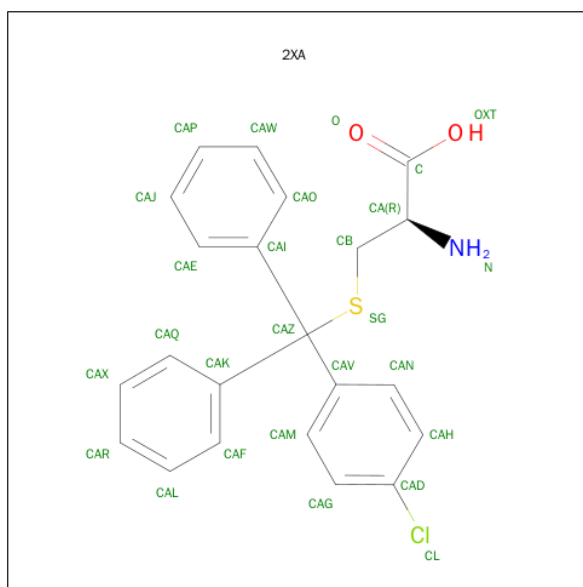
There are 7 unique types of molecules in this entry. The entry contains 8313 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	6	0
			2584	1626	452	494	12			
1	B	328	Total	C	N	O	S	0	7	0
			2604	1639	453	501	11			
1	C	329	Total	C	N	O	S	0	2	0
			2578	1618	444	506	10			

- Molecule 2 is (2R)-2-AMINO-3-[(4-CHLOROPHENYL)-DIPHENYL-METHYL]SULFANY L-PROPANOIC ACID (three-letter code: 2XA) (formula: C<sub>22</sub>H<sub>20</sub>ClNO<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			27	22	1	1	2	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			27	22	1	1	2	1		
2	C	1	Total	C	Cl	N	O	S	0	0
			27	22	1	1	2	1		

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | C     | 1        | Total Mg<br>1 1 | 0       | 0       |

- 
- The chemical structure of ADP (Adenosine Diphosphate) is shown. It consists of an adenine base (N1, N3, N6, N7, N9, O2, O4, O5, O6, O8, C2, C3, C4, C5, C6, C8, C9) attached to a ribose sugar (C1', C2', C3', C4', C5', O1', O2', O3', O4', O5'). The ribose sugar is linked to a diphosphate group (P1, P2, O1A, O2A, O3A, O4A, O5A, O6A, O7A, O8A, O9A, O10A, O11A, O12A, O13A, O14A, O15A, O16A, O17A, O18A, O19A, O20A, O21A, O22A, O23A, O24A, O25A, O26A, O27A, O28A, O29A, O30A, O31A, O32A, O33A, O34A, O35A, O36A, O37A, O38A, O39A, O40A, O41A, O42A, O43A, O44A, O45A, O46A, O47A, O48A, O49A, O50A, O51A, O52A, O53A, O54A, O55A, O56A, O57A, O58A, O59A, O60A, O61A, O62A, O63A, O64A, O65A, O66A, O67A, O68A, O69A, O70A, O71A, O72A, O73A, O74A, O75A, O76A, O77A, O78A, O79A, O80A, O81A, O82A, O83A, O84A, O85A, O86A, O87A, O88A, O89A, O90A, O91A, O92A, O93A, O94A, O95A, O96A, O97A, O98A, O99A, O100A, O101A, O102A, O103A, O104A, O105A, O106A, O107A, O108A, O109A, O110A, O111A, O112A, O113A, O114A, O115A, O116A, O117A, O118A, O119A, O120A, O121A, O122A, O123A, O124A, O125A, O126A, O127A, O128A, O129A, O130A, O131A, O132A, O133A, O134A, O135A, O136A, O137A, O138A, O139A, O140A, O141A, O142A, O143A, O144A, O145A, O146A, O147A, O148A, O149A, O150A, O151A, O152A, O153A, O154A, O155A, O156A, O157A, O158A, O159A, O160A, O161A, O162A, O163A, O164A, O165A, O166A, O167A, O168A, O169A, O170A, O171A, O172A, O173A, O174A, O175A, O176A, O177A, O178A, O179A, O180A, O181A, O182A, O183A, O184A, O185A, O186A, O187A, O188A, O189A, O190A, O191A, O192A, O193A, O194A, O195A, O196A, O197A, O198A, O199A, O200A, O201A, O202A, O203A, O204A, O205A, O206A, O207A, O208A, O209A, O210A, O211A, O212A, O213A, O214A, O215A, O216A, O217A, O218A, O219A, O220A, O221A, O222A, O223A, O224A, O225A, O226A, O227A, O228A, O229A, O230A, O231A, O232A, O233A, O234A, O235A, O236A, O237A, O238A, O239A, O240A, O241A, O242A, O243A, O244A, O245A, O246A, O247A, O248A, O249A, O250A, O251A, O252A, O253A, O254A, O255A, O256A, O257A, O258A, O259A, O260A, O261A, O262A, O263A, O264A, O265A, O266A, O267A, O268A, O269A, O270A, O271A, O272A, O273A, O274A, O275A, O276A, O277A, O278A, O279A, O280A, O281A, O282A, O283A, O284A, O285A, O286A, O287A, O288A, O289A, O290A, O291A, O292A, O293A, O294A, O295A, O296A, O297A, O298A, O299A, O300A, O301A, O302A, O303A, O304A, O305A, O306A, O307A, O308A, O309A, O310A, O311A, O312A, O313A, O314A, O315A, O316A, O317A, O318A, O319A, O320A, O321A, O322A, O323A, O324A, O325A, O326A, O327A, O328A, O329A, O330A, O331A, O332A, O333A, O334A, O335A, O336A, O337A, O338A, O339A, O340A, O341A, O342A, O343A, O344A, O345A, O346A, O347A, O348A, O349A, O350A, O351A, O352A, O353A, O354A, O355A, O356A, O357A, O358A, O359A, O360A, O361A, O362A, O363A, O364A, O365A, O366A, O367A, O368A, O369A, O370A, O371A, O372A, O373A, O374A, O375A, O376A, O377A, O378A, O379A, O380A, O381A, O382A, O383A, O384A, O385A, O386A, O387A, O388A, O389A, O390A, O391A, O392A, O393A, O394A, O395A, O396A, O397A, O398A, O399A, O400A, O401A, O402A, O403A, O404A, O405A, O406A, O407A, O408A, O409A, O410A, O411A, O412A, O413A, O414A, O415A, O416A, O417A, O418A, O419A, O420A, O421A, O422A, O423A, O424A, O425A, O426A, O427A, O428A, O429A, O430A, O431A, O432A, O433A, O434A, O435A, O436A, O437A, O438A, O439A, O440A, O441A, O442A, O443A, O444A, O445A, O446A, O447A, O448A, O449A, O450A, O451A, O452A, O453A, O454A, O455A, O456A, O457A, O458A, O459A, O460A, O461A, O462A, O463A, O464A, O465A, O466A, O467A, O468A, O469A, O470A, O471A, O472A, O473A, O474A, O475A, O476A, O477A, O478A, O479A, O480A, O481A, O482A, O483A, O484A, O485A, O486A, O487A, O488A, O489A, O490A, O491A, O492A, O493A, O494A, O495A, O496A, O497A, O498A, O499A, O500A, O501A, O502A, O503A, O504A, O505A, O506A, O507A, O508A, O509A, O510A, O511A, O512A, O513A, O514A, O515A, O516A, O517A, O518A, O519A, O520A, O521A, O522A, O523A, O524A, O525A, O526A, O527A, O528A, O529A, O530A, O531A, O532A, O533A, O534A, O535A, O536A, O537A, O538A, O539A, O540A, O541A, O542A, O543A, O544A, O545A, O546A, O547A, O548A, O549A, O550A, O551A, O552A, O553A, O554A, O555A, O556A, O557A, O558A, O559A, O560A, O561A, O562A, O563A, O564A, O565A, O566A, O567A, O568A, O569A, O570A, O571A, O572A, O573A, O574A, O575A, O576A, O577A, O578A, O579A, O580A, O581A, O582A, O583A, O584A, O585A, O586A, O587A, O588A, O589A, O590A, O591A, O592A, O593A, O594A, O595A, O596A, O597A, O598A, O599A, O600A, O601A, O602A, O603A, O604A, O605A, O606A, O607A, O608A, O609A, O610A, O611A, O612A, O613A, O614A, O615A, O616A, O617A, O618A, O619A, O620A, O621A, O622A, O623A, O624A, O625A, O626A, O627A, O628A, O629A, O630A, O631A, O632A, O633A, O634A, O635A, O636A, O637A, O638A, O639A, O640A, O641A, O642A, O643A, O644A, O645A, O646A, O647A, O648A, O649A, O650A, O651A, O652A, O653A, O654A, O655A, O656A, O657A, O658A, O659A, O660A, O661A, O662A, O663A, O664A, O665A, O666A, O667A, O668A, O669A, O670A, O671A, O672A, O673A

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

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | A     | 1        | Total Cl<br>1 1 | 0       | 0       |

- 
- WORLD WIDE  
PDB  
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

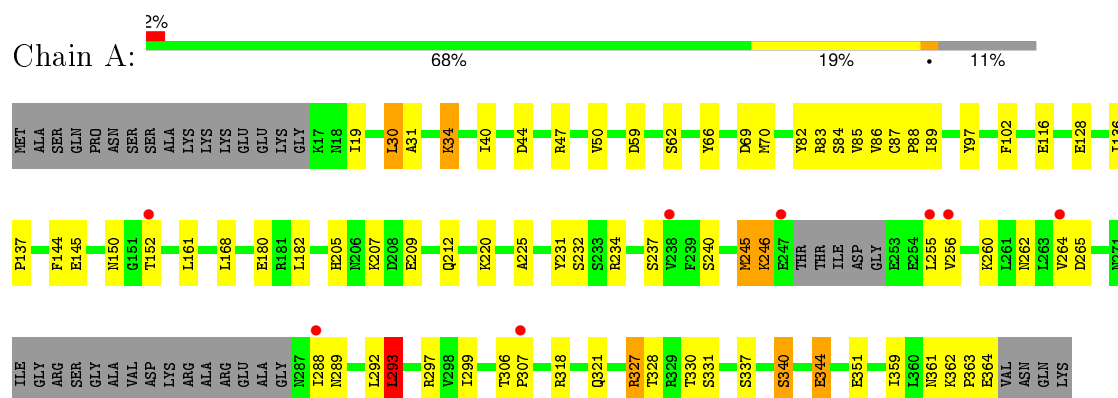
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	129	Total	O	0	0
			129	129		
7	B	156	Total	O	0	0
			156	156		
7	C	81	Total	O	0	0
			81	81		

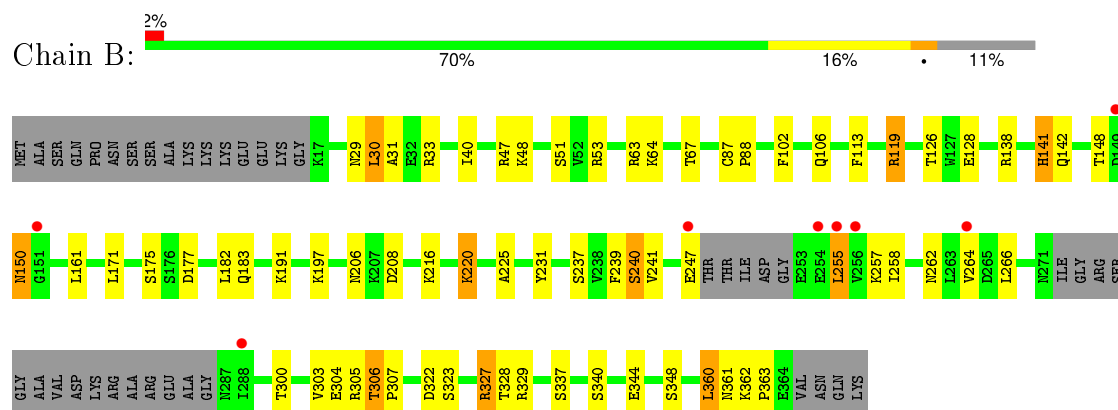
### 3 Residue-property plots [i](#)

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.

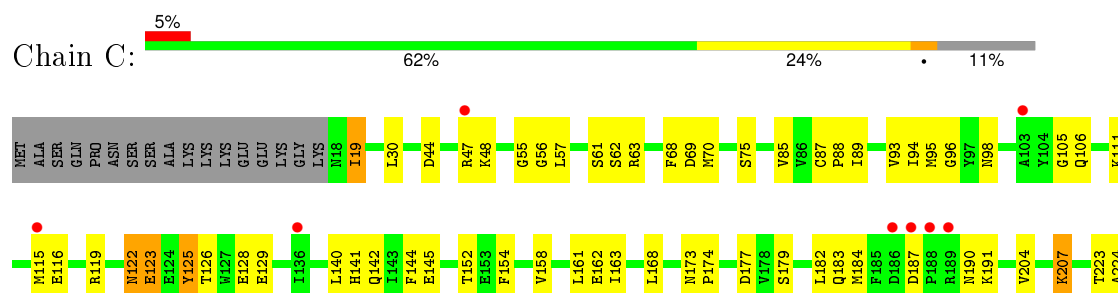
#### • Molecule 1: KINESIN-LIKE PROTEIN KIF11

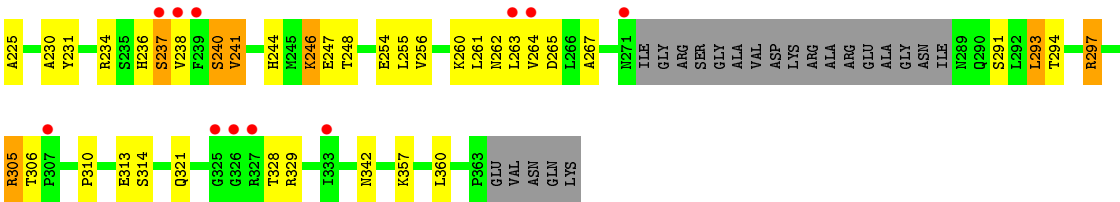


#### • Molecule 1: KINESIN-LIKE PROTEIN KIF11



#### • Molecule 1: KINESIN-LIKE PROTEIN KIF11





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.77Å 96.77Å 124.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.23 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.60) 100.0 (29.23-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.05 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.181 , 0.257 0.177 , 0.249	Depositor DCC
$R_{free}$ test set	2013 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.8	EDS
Estimated twinning fraction	0.009 for -h,-k,l 0.034 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 40185 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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, 0.375 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: 2XA, MG, SO4, ADP, CL

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	0.67	1/2640 (0.0%)	0.90	2/3569 (0.1%)
1	B	0.66	0/2665	0.91	6/3603 (0.2%)
1	C	0.59	0/2620	0.84	0/3546
All	All	0.64	1/7925 (0.0%)	0.88	8/10718 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	GLU	CG-CD	6.00	1.60	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	293	LEU	CA-CB-CG	5.70	128.42	115.30
1	A	50	VAL	CB-CA-C	-5.43	101.07	111.40
1	B	177	ASP	CB-CG-OD1	5.37	123.14	118.30
1	B	327	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	360	LEU	CA-CB-CG	5.08	126.99	115.30
1	B	119	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	119	ARG	NE-CZ-NH1	5.05	122.83	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	2584	0	2618	49	0
1	B	2604	0	2635	35	0
1	C	2578	0	2585	69	0
2	A	27	0	19	3	0
2	B	27	0	19	3	0
2	C	27	0	19	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	2	0
4	C	27	0	12	1	0
5	A	1	0	0	1	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
7	A	129	0	0	10	0
7	B	156	0	0	5	0
7	C	81	0	0	5	0
All	All	8313	0	7931	160	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 10.

All (160) 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:83:ARG:HD2	7:A:2029:HOH:O	1.74	0.86
5:A:1368:CL:CL	7:A:2128:HOH:O	2.34	0.81
1:B:327:ARG:O	1:B:363:PRO:HA	1.83	0.79
1:C:141:HIS:HD2	1:C:142:GLN:HE21	1.31	0.76
1:A:30:LEU:HD13	1:A:31:ALA:N	2.01	0.75
1:A:234:ARG:NH1	1:A:289:ASN:OD1	2.21	0.74
1:A:87[B]:CYS:HB3	1:A:88:PRO:HD3	1.70	0.73
1:A:30:LEU:HD13	1:A:31:ALA:H	1.53	0.72
1:C:310:PRO:HB2	1:C:313:GLU:HG3	1.72	0.71
1:C:244:HIS:HD2	7:C:2053:HOH:O	1.72	0.70
1:C:98:ASN:ND2	1:C:260:LYS:HB3	2.07	0.69
4:B:1367:ADP:O3B	7:B:2155:HOH:O	2.12	0.66
1:B:87[B]:CYS:HB3	1:B:88:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:THR:O	1:A:361:ASN:ND2	2.26	0.65
1:C:246:LYS:HE2	1:C:254:GLU:HG2	1.77	0.65
1:B:141[A]:HIS:HD2	1:B:142:GLN:N	1.97	0.63
1:B:40:ILE:HD13	1:B:340:SER:HA	1.80	0.63
1:C:294:THR:HG21	1:C:314:SER:HB3	1.80	0.63
1:C:183:GLN:HE21	1:C:184:MET:H	1.48	0.61
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.83	0.61
1:C:85:VAL:O	1:C:89:ILE:HD13	2.00	0.61
1:B:30:LEU:HD13	7:B:2007:HOH:O	2.00	0.60
1:A:168:LEU:HB2	1:A:182:LEU:HB2	1.83	0.59
1:A:293:LEU:CD2	1:A:297[A]:ARG:CZ	2.80	0.59
1:A:321:GLN:NE2	7:A:2102:HOH:O	2.36	0.59
1:B:183:GLN:HG3	7:B:2040:HOH:O	2.01	0.59
1:A:318:ARG:NH1	7:A:2100:HOH:O	2.33	0.58
1:A:66:TYR:OH	1:A:351:GLU:OE2	2.21	0.58
1:C:105:GLY:O	1:C:111:LYS:HE3	2.04	0.57
1:B:47:ARG:O	1:B:48[A]:LYS:HG2	2.04	0.57
1:C:125:TYR:HB3	1:C:129:GLU:HB3	1.85	0.57
1:C:87:CYS:HB2	1:C:88:PRO:HD3	1.86	0.57
1:B:126:THR:HB	1:B:128:GLU:OE2	2.05	0.56
1:C:141:HIS:HD2	1:C:142:GLN:NE2	2.02	0.56
1:A:85:VAL:O	1:A:89:ILE:HD12	2.06	0.56
1:C:230:ALA:HB3	1:C:234:ARG:HD2	1.87	0.56
1:C:115:MET:CE	1:C:263:LEU:HB3	2.35	0.56
1:A:144:PHE:O	1:A:145:GLU:C	2.41	0.55
1:C:236:HIS:CE1	1:C:267:ALA:H	2.24	0.55
1:C:158:VAL:HG12	1:C:241:VAL:HG13	1.89	0.55
1:C:116:GLU:HB2	2:C:1364:2XA:CAH	2.37	0.55
2:A:1365:2XA:HAQ	2:A:1365:2XA:CB	2.32	0.55
1:C:69:ASP:O	1:C:70:MET:HG3	2.07	0.55
1:C:246:LYS:HE2	1:C:254:GLU:CB	2.37	0.54
2:A:1365:2XA:HAQ	2:A:1365:2XA:HB1C	1.88	0.54
1:B:150:ASN:HD22	1:B:150:ASN:N	2.05	0.54
4:A:1367:ADP:O3B	7:A:2124:HOH:O	2.19	0.54
1:B:141[A]:HIS:CD2	1:B:142:GLN:N	2.75	0.54
1:C:246:LYS:HE2	1:C:254:GLU:HB3	1.90	0.54
1:B:102:PHE:HB3	1:B:264:VAL:HB	1.91	0.53
1:C:246:LYS:HE3	1:C:247:GLU:N	2.24	0.53
1:C:225:ALA:HA	1:C:231:TYR:HB3	1.90	0.53
1:C:162:GLU:OE1	1:C:231:TYR:OH	2.23	0.53
1:B:161:LEU:C	1:B:161:LEU:HD12	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:PHE:HE1	1:B:241:VAL:HG22	1.73	0.52
1:A:34:LYS:C	1:A:34:LYS:HD2	2.29	0.52
1:A:237:SER:HB3	1:A:265:ASP:HB3	1.91	0.52
1:C:115:MET:HE1	1:C:263:LEU:HB3	1.91	0.52
1:B:306:THR:HG23	1:B:307:PRO:HD2	1.92	0.52
1:A:364:GLU:HB2	7:A:2119:HOH:O	2.09	0.52
1:C:240:SER:OG	1:C:262:ASN:ND2	2.43	0.52
1:A:97:TYR:CZ	7:A:2119:HOH:O	2.54	0.52
1:C:246:LYS:HE3	1:C:247:GLU:H	1.76	0.51
1:C:116:GLU:HB2	2:C:1364:2XA:HAH	1.92	0.51
1:A:31:ALA:O	1:A:34:LYS:HG3	2.08	0.51
1:B:247:GLU:OE1	1:B:257:LYS:HE2	2.10	0.51
1:C:237:SER:HB2	1:C:265:ASP:HB3	1.93	0.51
1:B:47:ARG:HG3	1:B:47:ARG:HH11	1.74	0.51
1:C:246:LYS:CE	1:C:254:GLU:HB3	2.40	0.51
1:A:307:PRO:HG2	7:A:2094:HOH:O	2.09	0.50
1:C:98:ASN:O	1:C:328:THR:HB	2.11	0.50
1:A:19:ILE:HD12	1:A:359:ILE:HB	1.93	0.50
1:B:87[A]:CYS:HB2	1:B:88:PRO:HD3	1.92	0.50
1:A:82:TYR:CD2	1:A:86:VAL:HB	2.47	0.50
1:C:122:ASN:O	1:C:123:GLU:C	2.50	0.50
1:C:62:SER:O	1:C:63:ARG:HD3	2.12	0.50
1:A:40:ILE:HD13	1:A:340:SER:HA	1.94	0.50
1:A:44:ASP:OD2	1:A:47:ARG:NH1	2.45	0.49
1:C:246:LYS:HE2	1:C:254:GLU:CG	2.41	0.49
1:A:30:LEU:CD1	1:A:31:ALA:H	2.22	0.49
1:B:138:ARG:O	1:B:141[A]:HIS:CD2	2.66	0.49
1:A:82:TYR:CE2	1:A:86:VAL:HB	2.47	0.49
1:C:246:LYS:NZ	1:C:254:GLU:HB3	2.27	0.49
1:A:69:ASP:O	1:A:70:MET:HG3	2.12	0.49
1:A:240:SER:OG	1:A:262:ASN:ND2	2.45	0.49
1:C:187:ASP:O	1:C:190:ASN:O	2.31	0.49
1:A:205:HIS:HB2	1:A:209:GLU:OE2	2.12	0.49
1:B:206:ASN:OD1	1:B:208:ASP:CB	2.61	0.48
1:C:294:THR:HG21	1:C:314:SER:CB	2.44	0.48
1:A:97:TYR:CE2	7:A:2119:HOH:O	2.67	0.47
1:B:240:SER:OG	1:B:262:ASN:ND2	2.47	0.47
1:A:293:LEU:HD21	1:A:297[A]:ARG:NH2	2.30	0.47
1:C:94:ILE:C	1:C:96:GLY:H	2.18	0.47
1:C:93:VAL:HG21	1:C:261:LEU:HB2	1.97	0.47
1:B:47:ARG:HG3	1:B:47:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LYS:HB3	1:C:68:PHE:O	2.15	0.46
1:C:173:ASN:CG	1:C:174:PRO:HD2	2.35	0.46
1:B:225:ALA:HA	1:B:231:TYR:HB3	1.97	0.46
1:C:106:GLN:HE22	1:C:342:ASN:HD22	1.63	0.46
1:C:183:GLN:HG3	7:C:2016:HOH:O	2.15	0.46
1:C:163:ILE:HG12	1:C:168:LEU:HD23	1.98	0.46
1:C:168:LEU:HB2	1:C:182:LEU:HB2	1.97	0.46
1:C:126:THR:OG1	1:C:129:GLU:HB2	2.16	0.45
1:B:175:SER:O	1:B:220:LYS:HE3	2.16	0.45
1:A:87[B]:CYS:HB3	1:A:88:PRO:CD	2.45	0.45
1:B:300:THR:O	1:B:303:VAL:HG22	2.17	0.45
1:B:113:PHE:CE2	4:B:1367:ADP:C6	3.04	0.45
2:B:1365:2XA:HAE	2:B:1365:2XA:HAF	1.97	0.45
1:A:327:ARG:O	1:A:363:PRO:HA	2.17	0.45
1:B:216:LYS:HB3	7:B:2076:HOH:O	2.16	0.45
1:A:240:SER:HB3	1:A:260:LYS:NZ	2.32	0.45
1:C:305:ARG:H	1:C:305:ARG:HG2	1.51	0.45
1:A:87[A]:CYS:HB2	1:A:88:PRO:HD3	2.00	0.44
2:B:1365:2XA:HAM	2:B:1365:2XA:CAF	2.46	0.44
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.79	0.44
1:A:136:ILE:N	1:A:137:PRO:HD2	2.32	0.44
1:B:48[A]:LYS:HG3	1:B:67:THR:HG23	1.98	0.44
1:C:55:GLY:O	1:C:56:GLY:C	2.54	0.44
1:C:144:PHE:CZ	1:C:204:VAL:HG12	2.53	0.44
1:A:152:THR:HB	1:A:246:LYS:O	2.18	0.44
1:B:30:LEU:HD13	1:B:31:ALA:H	1.81	0.44
1:B:102:PHE:CB	1:B:264:VAL:HB	2.48	0.44
1:C:173:ASN:OD1	1:C:174:PRO:HD2	2.17	0.44
1:C:246:LYS:HZ1	1:C:255:LEU:N	2.16	0.44
1:C:291:SER:HA	1:C:314:SER:HB2	1.99	0.44
1:C:44:ASP:OD2	1:C:47:ARG:HG3	2.18	0.43
1:A:330:THR:HG22	1:A:331:SER:N	2.34	0.43
1:C:140:LEU:HA	1:C:140:LEU:HD23	1.76	0.43
1:C:191:LYS:HG2	7:C:2036:HOH:O	2.18	0.43
1:C:238:VAL:HG22	1:C:264:VAL:HG22	1.98	0.43
1:C:119:ARG:HA	1:C:119:ARG:HD2	1.83	0.43
1:B:102:PHE:CD1	1:B:266:LEU:HD11	2.54	0.43
1:C:161:LEU:HD12	1:C:161:LEU:C	2.39	0.43
1:A:245:MET:O	1:A:256:VAL:HA	2.19	0.43
1:C:177:ASP:OD2	1:C:179:SER:OG	2.33	0.43
1:A:161:LEU:C	1:A:161:LEU:HD12	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLU:HG2	2:A:1365:2XA:CAH	2.49	0.42
1:A:225:ALA:HA	1:A:231:TYR:HB3	2.01	0.42
1:B:29:ASN:HA	1:B:33[A]:ARG:HH21	1.84	0.42
1:C:154:PHE:HA	1:C:244:HIS:O	2.18	0.42
1:C:183:GLN:CG	7:C:2016:HOH:O	2.67	0.42
1:B:53:ARG:HA	1:B:63:ARG:HD3	2.01	0.42
1:A:180:GLU:CB	1:C:57:LEU:HG	2.50	0.42
1:C:293:LEU:HD12	1:C:297:ARG:NH1	2.35	0.41
1:C:19:ILE:O	1:C:357:LYS:HE3	2.20	0.41
1:C:246:LYS:HZ1	1:C:255:LEU:C	2.23	0.41
1:C:128:GLU:OE1	1:C:141:HIS:CE1	2.74	0.41
1:B:30:LEU:CD1	7:B:2007:HOH:O	2.65	0.41
1:A:293:LEU:HD21	1:A:297[A]:ARG:CZ	2.50	0.41
2:B:1365:2XA:CAM	2:B:1365:2XA:CAF	2.97	0.41
1:A:59:ASP:OD2	1:A:62:SER:CB	2.68	0.41
1:C:111:LYS:NZ	4:C:1366:ADP:O2B	2.43	0.41
1:A:102:PHE:HB3	1:A:264:VAL:HB	2.01	0.41
1:A:306:THR:HG22	7:A:2094:HOH:O	2.20	0.41
1:B:323:SER:HA	1:B:328:THR:HB	2.02	0.41
1:C:223:THR:O	1:C:224:ALA:C	2.59	0.41
1:C:246:LYS:HZ3	1:C:254:GLU:HB3	1.86	0.41
1:A:234:ARG:HD2	1:A:288:ILE:CG1	2.51	0.40
1:C:234:ARG:HD3	7:C:2050:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/368 (89%)	316 (96%)	10 (3%)	2 (1%)	30	56
1	B	329/368 (89%)	321 (98%)	7 (2%)	1 (0%)	46	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	327/368 (89%)	308 (94%)	14 (4%)	5 (2%)	13	26
All	All	984/1104 (89%)	945 (96%)	31 (3%)	8 (1%)	24	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	LYS
1	A	150	ASN
1	A	207	LYS
1	C	123	GLU
1	C	321	GLN
1	C	95	MET
1	C	122	ASN
1	B	305	ARG

### 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	289/322 (90%)	272 (94%)	17 (6%)	24	47
1	B	294/322 (91%)	267 (91%)	27 (9%)	11	21
1	C	288/322 (89%)	268 (93%)	20 (7%)	19	38
All	All	871/966 (90%)	807 (93%)	64 (7%)	18	35

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	34	LYS
1	A	84	SER
1	A	128	GLU
1	A	212	GLN
1	A	220	LYS
1	A	232[A]	SER

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Mol	Chain	Res	Type
1	A	232[B]	SER
1	A	245	MET
1	A	246	LYS
1	A	255	LEU
1	A	293	LEU
1	A	327	ARG
1	A	337	SER
1	A	340	SER
1	A	344	GLU
1	A	362	LYS
1	B	30	LEU
1	B	51	SER
1	B	64	LYS
1	B	106	GLN
1	B	119	ARG
1	B	141[A]	HIS
1	B	141[B]	HIS
1	B	148	THR
1	B	150	ASN
1	B	171	LEU
1	B	182	LEU
1	B	191	LYS
1	B	197	LYS
1	B	220	LYS
1	B	237	SER
1	B	240	SER
1	B	255	LEU
1	B	258	ILE
1	B	304	GLU
1	B	306	THR
1	B	322	ASP
1	B	329	ARG
1	B	337	SER
1	B	344	GLU
1	B	348	SER
1	B	360	LEU
1	B	362	LYS
1	C	19	ILE
1	C	30	LEU
1	C	61	SER
1	C	75	SER
1	C	125	TYR

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Mol	Chain	Res	Type
1	C	145	GLU
1	C	152	THR
1	C	207	LYS
1	C	237	SER
1	C	240	SER
1	C	241	VAL
1	C	246	LYS
1	C	248	THR
1	C	256	VAL
1	C	293	LEU
1	C	297	ARG
1	C	305	ARG
1	C	306	THR
1	C	329	ARG
1	C	360	LEU

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

Mol	Chain	Res	Type
1	A	38	HIS
1	A	212	GLN
1	A	262	ASN
1	A	287	ASN
1	A	321	GLN
1	A	342	ASN
1	B	38	HIS
1	B	150	ASN
1	B	262	ASN
1	B	290	GLN
1	B	321	GLN
1	C	98	ASN
1	C	106	GLN
1	C	141	HIS
1	C	183	GLN
1	C	244	HIS
1	C	262	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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	2XA	A	1365	-	26,29,29	0.80	1 (3%)	33,40,40	1.15	1 (3%)
4	ADP	A	1367	3	22,29,29	1.21	2 (9%)	27,45,45	2.21	6 (22%)
2	2XA	B	1365	-	26,29,29	1.14	2 (7%)	33,40,40	1.27	3 (9%)
4	ADP	B	1367	3	22,29,29	1.16	2 (9%)	27,45,45	1.79	4 (14%)
6	SO4	B	1368	-	4,4,4	0.18	0	6,6,6	0.13	0
6	SO4	B	1369	-	4,4,4	0.16	0	6,6,6	0.14	0
2	2XA	C	1364	-	26,29,29	0.70	1 (3%)	33,40,40	1.12	1 (3%)
4	ADP	C	1366	3	22,29,29	1.13	1 (4%)	27,45,45	2.31	6 (22%)
6	SO4	C	1367	-	4,4,4	0.19	0	6,6,6	0.24	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	2XA	A	1365	-	-	0/24/28/28	0/3/3/3
4	ADP	A	1367	3	-	0/12/32/32	0/3/3/3
2	2XA	B	1365	-	-	0/24/28/28	0/3/3/3
4	ADP	B	1367	3	-	0/12/32/32	0/3/3/3
6	SO4	B	1368	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	B	1369	-	-	0/0/0/0	0/0/0/0
2	2XA	C	1364	-	-	0/24/28/28	0/3/3/3
4	ADP	C	1366	3	-	0/12/32/32	0/3/3/3
6	SO4	C	1367	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1367	ADP	O4'-C1'	2.44	1.44	1.41
2	C	1364	2XA	CB-SG	2.46	1.86	1.82
4	B	1367	ADP	C2-N3	2.58	1.36	1.32
2	B	1365	2XA	CAZ-SG	2.67	1.90	1.87
2	A	1365	2XA	CB-SG	3.41	1.87	1.82
4	B	1367	ADP	C5-C4	3.46	1.48	1.40
4	A	1367	ADP	C5-C4	3.74	1.48	1.40
4	C	1366	ADP	C5-C4	3.84	1.49	1.40
2	B	1365	2XA	CB-SG	4.04	1.88	1.82

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1366	ADP	N3-C2-N1	-8.57	122.33	128.89
4	A	1367	ADP	N3-C2-N1	-8.22	122.60	128.89
4	B	1367	ADP	N3-C2-N1	-6.08	124.24	128.89
4	A	1367	ADP	C4-C5-N7	-4.73	105.13	109.48
4	C	1366	ADP	PA-O3A-PB	-4.13	118.83	132.67
4	B	1367	ADP	C4-C5-N7	-3.91	105.88	109.48
4	C	1366	ADP	C1'-N9-C4	-3.63	121.46	126.94
4	C	1366	ADP	C4-C5-N7	-3.20	106.54	109.48
4	A	1367	ADP	PA-O3A-PB	-3.08	122.35	132.67
4	B	1367	ADP	C2'-C1'-N9	-2.41	110.61	114.29
2	B	1365	2XA	CAG-CAD-CL	-2.14	115.85	119.35
4	B	1367	ADP	O5'-C5'-C4'	-2.13	101.28	109.12
2	B	1365	2XA	CAM-CAG-CAD	-2.06	116.94	119.23
4	A	1367	ADP	C2-N1-C6	2.02	122.38	118.77
4	C	1366	ADP	O3B-PB-O2B	2.23	115.88	107.38
4	A	1367	ADP	O3B-PB-O2B	2.28	116.08	107.38
4	C	1366	ADP	C2-N1-C6	3.00	124.14	118.77
4	A	1367	ADP	C4'-O4'-C1'	3.17	113.20	109.72
2	C	1364	2XA	CB-SG-CAZ	4.15	109.32	103.26
2	A	1365	2XA	CB-SG-CAZ	4.36	109.64	103.26
2	B	1365	2XA	CB-SG-CAZ	4.48	109.80	103.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1365	2XA	3	0
4	A	1367	ADP	1	0
2	B	1365	2XA	3	0
4	B	1367	ADP	2	0
2	C	1364	2XA	2	0
4	C	1366	ADP	1	0

## 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, 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	328/368 (89%)	-0.27	8 (2%) 62 56	16, 35, 63, 74	0
1	B	328/368 (89%)	-0.29	8 (2%) 62 56	16, 33, 63, 78	0
1	C	329/368 (89%)	-0.00	19 (5%) 26 20	27, 47, 69, 82	0
All	All	985/1104 (89%)	-0.19	35 (3%) 46 38	16, 38, 66, 82	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	255	LEU	4.7
1	C	325	GLY	3.9
1	C	326	GLY	3.2
1	B	149	ASP	3.2
1	C	264	VAL	3.2
1	C	271	ASN	3.1
1	A	247	GLU	3.0
1	A	152	THR	3.0
1	C	327	ARG	2.9
1	A	256	VAL	2.9
1	A	264	VAL	2.9
1	C	238	VAL	2.8
1	C	189	ARG	2.7
1	C	187	ASP	2.6
1	B	288	ILE	2.5
1	C	186	ASP	2.5
1	C	307	PRO	2.5
1	A	255	LEU	2.4
1	C	239	PHE	2.4
1	B	264	VAL	2.4
1	C	115	MET	2.3
1	C	237	SER	2.3
1	A	288	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	136	ILE	2.3
1	B	151	GLY	2.3
1	C	103	ALA	2.3
1	B	256	VAL	2.2
1	C	47	ARG	2.2
1	C	333	ILE	2.2
1	B	254	GLU	2.2
1	C	263	LEU	2.1
1	B	247	GLU	2.1
1	A	307	PRO	2.1
1	C	188	PRO	2.0
1	A	238	VAL	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, 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(Å <sup>2</sup> )	Q<0.9
2	2XA	A	1365	27/27	0.83	0.24	1.67	47,58,76,76	0
2	2XA	C	1364	27/27	0.80	0.28	1.13	66,70,84,84	0
2	2XA	B	1365	27/27	0.85	0.20	1.03	25,42,61,61	0
6	SO4	B	1368	5/5	0.97	0.21	0.35	87,88,88,89	0
4	ADP	A	1367	27/27	0.96	0.16	0.25	21,47,55,56	0
4	ADP	C	1366	27/27	0.94	0.17	-0.31	32,69,73,73	0
4	ADP	B	1367	27/27	0.97	0.12	-0.78	17,37,47,52	0
6	SO4	B	1369	5/5	0.95	0.10	-1.13	91,91,92,92	0
5	CL	A	1368	1/1	0.87	0.10	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	1366	1/1	0.94	0.14	-	40,40,40,40	0
3	MG	B	1366	1/1	0.96	0.13	-	23,23,23,23	0
3	MG	C	1365	1/1	0.70	0.11	-	79,79,79,79	0
6	SO4	C	1367	5/5	0.97	0.21	-	87,87,87,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.