



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 17, 2018 – 11:31 PM EST

PDB ID : 3O08  
Title : Crystal structure of dimeric KIHxk1 in crystal form I  
Authors : Kuettner, E.B.; Kettner, K.; Keim, A.; Kriegel, T.M.; Strater, N.  
Deposited on : 2010-07-19  
Resolution : 2.00 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 : rb-20030736  
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) : rb-20030736

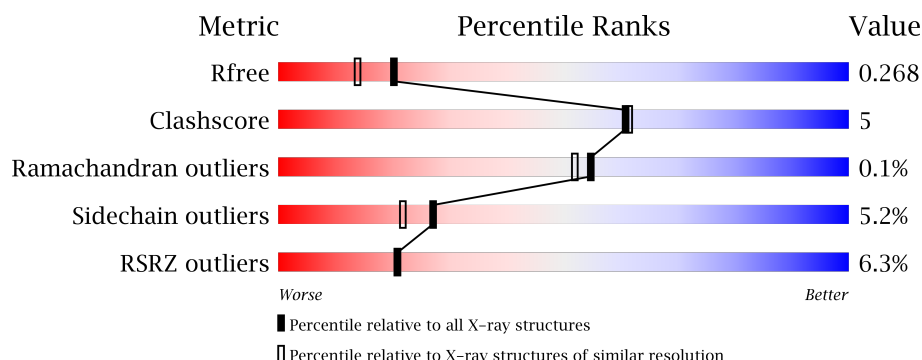
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	485	<div> <div>4%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	B	485	<div> <div>9%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>

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	488	-	-	-	X
2	SO4	A	493	-	-	-	X
2	SO4	B	488	-	-	-	X
2	SO4	B	494	-	-	X	X
2	SO4	B	495	-	-	-	X
3	NHE	B	486[A]	-	-	-	X
3	NHE	B	486[B]	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7928 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 Hexokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3665	2332	602	715	16			
1	B	479	Total	C	N	O	S	0	1	0
			3727	2371	616	724	16			

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



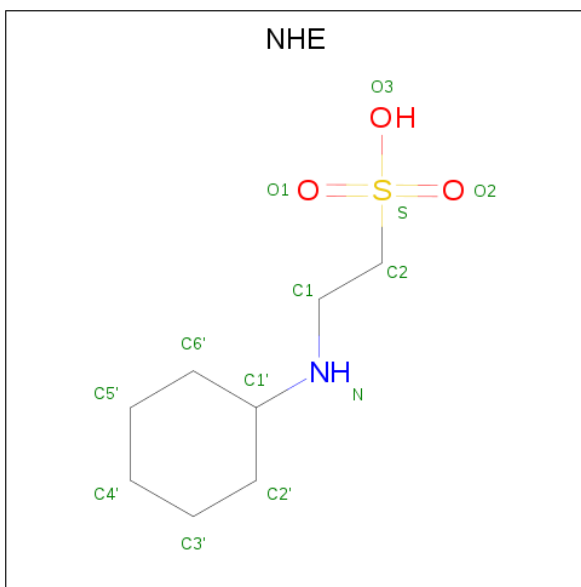
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	1
			26	16	2	6	2		

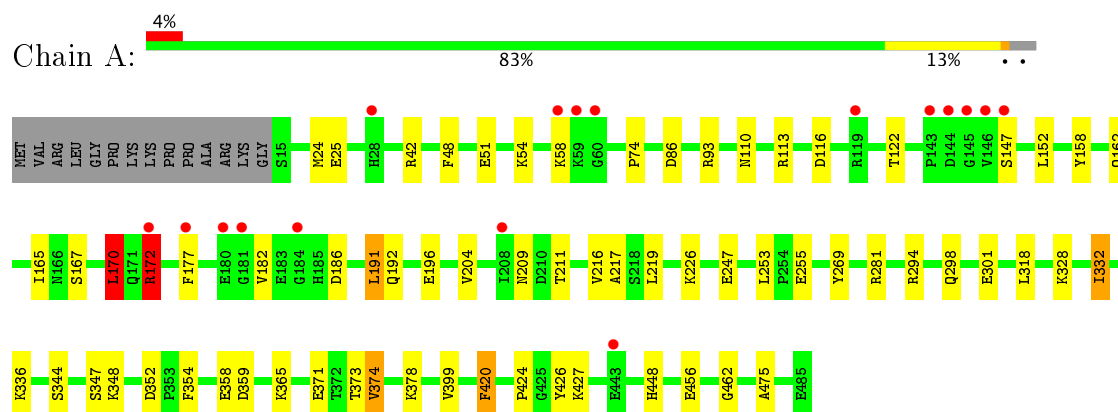
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	212	Total	O	0	0
			212	212		
4	B	188	Total	O	0	0
			188	188		

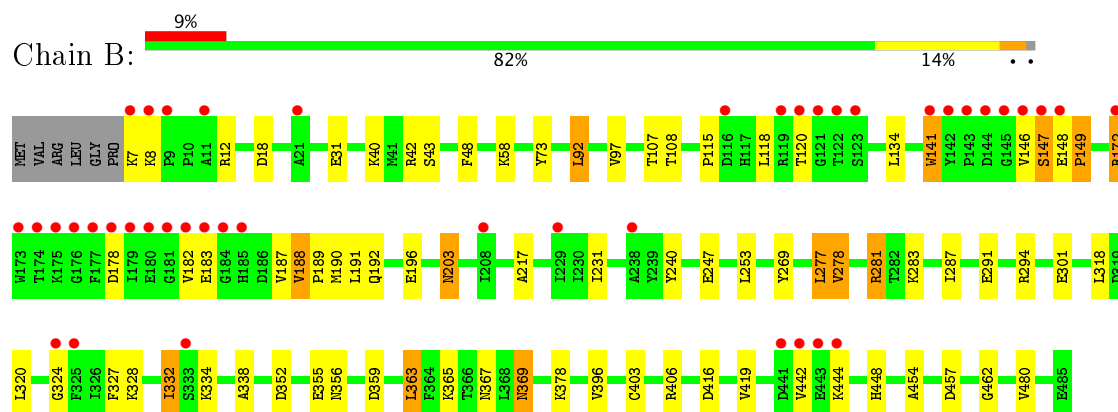
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Hexokinase



#### • Molecule 1: Hexokinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.69 Å   113.22 Å   91.23 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.97 – 2.00 29.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.97-2.00) 99.9 (29.98-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.185   ,   0.244 0.212   ,   0.268	Depositor DCC
$R_{free}$ test set	1033 reflections (1.51%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.13	8/3738 (0.2%)	1.00	6/5062 (0.1%)
1	B	1.10	9/3807 (0.2%)	1.00	11/5153 (0.2%)
All	All	1.11	17/7545 (0.2%)	1.00	17/10215 (0.2%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	TYR	CD1-CE1	6.56	1.49	1.39
1	B	240	TYR	CD2-CE2	6.29	1.48	1.39
1	A	399	VAL	CB-CG1	6.28	1.66	1.52
1	A	216	VAL	CB-CG1	6.00	1.65	1.52
1	B	480	VAL	CB-CG1	5.41	1.64	1.52
1	B	301	GLU	CD-OE1	5.29	1.31	1.25
1	B	278	VAL	CB-CG2	-5.29	1.41	1.52
1	A	420	PHE	CD1-CE1	5.27	1.49	1.39
1	B	403	CYS	CB-SG	5.26	1.91	1.82
1	B	454	ALA	CA-CB	5.17	1.63	1.52
1	A	475	ALA	CA-CB	5.15	1.63	1.52
1	A	51	GLU	CD-OE2	-5.14	1.20	1.25
1	A	298	GLN	CG-CD	5.10	1.62	1.51
1	B	141	TRP	CB-CG	5.07	1.59	1.50
1	A	301	GLU	CD-OE1	5.02	1.31	1.25
1	B	338	ALA	CA-CB	5.02	1.62	1.52
1	B	188	VAL	CB-CG2	5.01	1.63	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	ARG	NE-CZ-NH2	-11.65	114.48	120.30
1	A	172	ARG	NE-CZ-NH2	-7.99	116.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	B	416	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	281	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	172	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	A	186	ASP	CB-CG-OD1	6.45	124.11	118.30
1	B	363	LEU	CB-CG-CD2	6.30	121.72	111.00
1	B	42	ARG	CG-CD-NE	-5.58	100.08	111.80
1	B	31	GLU	CA-CB-CG	-5.54	101.20	113.40
1	B	42	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	277	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	363	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	42	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	170	LEU	CB-CG-CD2	5.29	119.99	111.00
1	B	318	LEU	CB-CG-CD2	-5.15	102.25	111.00
1	B	12	ARG	NE-CZ-NH1	-5.09	117.75	120.30

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	3665	0	3646	36	0
1	B	3727	0	3721	44	0
2	A	45	0	0	2	0
2	B	65	0	0	4	0
3	B	26	0	34	2	0
4	A	212	0	0	4	0
4	B	188	0	0	3	0
All	All	7928	0	7401	78	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 5.

All (78) 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:110:ASN:HD21	1:B:355:GLU:HB2	1.42	0.84
1:B:203:ASN:H	1:B:203:ASN:HD22	1.27	0.83
1:B:294:ARG:HG3	2:B:494:SO4:O4	1.83	0.79
1:B:324:GLY:O	1:B:328:LYS:HE2	1.83	0.78
1:B:281:ARG:HD3	4:B:636:HOH:O	1.85	0.75
1:B:281:ARG:HH11	1:B:281:ARG:HG3	1.52	0.73
1:B:203:ASN:HD22	1:B:203:ASN:N	1.89	0.70
1:B:281:ARG:HH11	1:B:281:ARG:CG	2.04	0.70
1:A:162:GLN:HG2	1:A:167:SER:O	1.96	0.66
1:B:192:GLN:NE2	1:B:196:GLU:OE2	2.27	0.65
1:A:110:ASN:ND2	1:B:355:GLU:HB2	2.11	0.65
1:A:365:LYS:HE3	4:A:534:HOH:O	1.95	0.65
1:B:115:PRO:HD2	1:B:118:LEU:HD12	1.79	0.65
1:A:332:ILE:HG23	1:A:336:LYS:HE3	1.79	0.64
1:B:182:VAL:HG13	1:B:190:MET:HE1	1.78	0.64
1:B:367:ASN:ND2	2:B:497:SO4:O2	2.33	0.62
1:B:108:THR:HG21	1:B:141:TRP:CZ2	2.36	0.59
1:A:158:TYR:HH	1:A:177:PHE:HE1	1.51	0.59
1:B:97:VAL:HG22	1:B:107:THR:HG22	1.84	0.58
1:A:226:LYS:NZ	2:A:488:SO4:O3	2.37	0.58
1:A:347:SER:OG	1:A:424:PRO:HD3	2.05	0.57
1:A:74:PRO:HD2	1:A:219:LEU:HD23	1.86	0.56
3:B:486[B]:NHE:H6'2	4:B:571:HOH:O	2.04	0.56
1:B:108:THR:HG21	1:B:141:TRP:CE2	2.41	0.54
1:A:420:PHE:CZ	1:A:427:LYS:HE2	2.43	0.54
1:B:92:LEU:C	1:B:92:LEU:HD12	2.28	0.54
1:A:58:LYS:HE3	1:A:247:GLU:HG2	1.89	0.54
1:B:146:VAL:HG12	1:B:147:SER:N	2.24	0.53
1:A:448:HIS:HD2	4:A:499:HOH:O	1.92	0.53
1:A:448:HIS:HE1	4:A:658:HOH:O	1.91	0.52
1:B:18:ASP:OD2	1:B:378:LYS:NZ	2.39	0.52
1:B:183:GLU:HG3	4:B:615:HOH:O	2.10	0.52
1:A:217:ALA:HB2	1:A:462:GLY:CA	2.40	0.51
1:B:352:ASP:CG	1:B:359:ASP:HB2	2.30	0.51
1:B:172:ARG:HG2	1:B:172:ARG:HH11	1.76	0.51
1:B:182:VAL:HG13	1:B:190:MET:CE	2.40	0.50
1:A:172:ARG:HD2	1:A:172:ARG:N	2.26	0.50
1:A:209:ASN:ND2	1:A:211:THR:H	2.10	0.50
1:A:332:ILE:CG2	1:A:336:LYS:HE3	2.42	0.50
1:A:152:LEU:HD23	1:A:152:LEU:C	2.32	0.49
1:B:356:ASN:HB2	2:B:495:SO4:O3	2.12	0.49
1:B:146:VAL:HG12	1:B:148:GLU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ARG:CG	2:B:494:SO4:O4	2.58	0.49
1:A:354:PHE:HB2	1:A:358:GLU:H	1.78	0.48
1:B:192:GLN:O	1:B:196:GLU:HG2	2.13	0.48
1:A:58:LYS:HE3	1:A:247:GLU:CG	2.43	0.48
1:B:231:ILE:HG22	1:B:419:VAL:HB	1.94	0.48
1:B:73:TYR:CZ	3:B:486[B]:NHE:H2'1	2.48	0.48
1:A:191:LEU:HD13	1:A:204:VAL:HG21	1.96	0.48
1:B:217:ALA:HB2	1:B:462:GLY:CA	2.44	0.47
1:A:170:LEU:HD12	1:A:182:VAL:HG12	1.96	0.47
1:A:158:TYR:OH	1:A:177:PHE:HE1	1.97	0.47
1:B:287:ILE:O	1:B:291:GLU:HG2	2.14	0.47
1:A:347:SER:OG	1:A:424:PRO:CD	2.62	0.47
1:A:192:GLN:O	1:A:196:GLU:HG2	2.16	0.46
1:B:442:VAL:HG11	1:B:448:HIS:CD2	2.51	0.46
1:A:58:LYS:CE	1:A:247:GLU:HG2	2.45	0.46
1:B:203:ASN:H	1:B:203:ASN:ND2	2.05	0.45
1:A:344:SER:O	1:A:348:LYS:HG3	2.18	0.44
1:A:25:GLU:OE1	1:A:25:GLU:HA	2.18	0.44
1:A:352:ASP:CG	1:A:359:ASP:HB2	2.38	0.44
1:A:365:LYS:HE2	1:A:371:GLU:OE1	2.17	0.44
1:A:374:VAL:O	1:A:378:LYS:HG3	2.17	0.44
1:B:58:LYS:HG3	1:B:247:GLU:OE2	2.18	0.43
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.88	0.43
1:B:369:ASN:HA	1:B:369:ASN:HD22	1.59	0.43
1:B:327:PHE:CD2	1:B:332:ILE:HD11	2.53	0.42
1:A:373:THR:HB	4:A:585:HOH:O	2.20	0.42
1:B:172:ARG:NH1	1:B:172:ARG:HG2	2.35	0.42
1:B:188:VAL:N	1:B:189:PRO:HD2	2.35	0.41
1:A:294:ARG:HB2	2:A:493:SO4:O2	2.20	0.41
1:B:187:VAL:HG12	1:B:190:MET:CE	2.49	0.41
1:B:320:LEU:HA	1:B:320:LEU:HD23	1.81	0.41
1:B:40:LYS:NZ	1:B:278:VAL:O	2.48	0.41
1:A:192:GLN:NE2	1:A:196:GLU:OE2	2.50	0.41
1:B:203:ASN:ND2	1:B:203:ASN:N	2.63	0.41
1:A:456:GLU:OE2	1:B:7:LYS:HE2	2.21	0.41
1:A:86:ASP:HB3	1:A:93:ARG:HB2	2.04	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	469/485 (97%)	448 (96%)	21 (4%)	0	100	100
1	B	478/485 (99%)	460 (96%)	17 (4%)	1 (0%)	51	48
All	All	947/970 (98%)	908 (96%)	38 (4%)	1 (0%)	55	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	PRO

### 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	401/412 (97%)	383 (96%)	18 (4%)	32	27
1	B	408/412 (99%)	384 (94%)	24 (6%)	23	17
All	All	809/824 (98%)	767 (95%)	42 (5%)	27	22

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	48	PHE
1	A	54	LYS
1	A	113	ARG
1	A	116	ASP

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Mol	Chain	Res	Type
1	A	122	THR
1	A	147	SER
1	A	165	ILE
1	A	170	LEU
1	A	172	ARG
1	A	191	LEU
1	A	253	LEU
1	A	255	GLU
1	A	269	TYR
1	A	318	LEU
1	A	328	LYS
1	A	332	ILE
1	A	374	VAL
1	B	8	LYS
1	B	43	SER
1	B	48	PHE
1	B	92	LEU
1	B	120	THR
1	B	147	SER
1	B	149	PRO
1	B	172	ARG
1	B	178	ASP
1	B	191	LEU
1	B	203	ASN
1	B	253	LEU
1	B	269	TYR
1	B	277	LEU
1	B	281	ARG
1	B	283	LYS
1	B	332	ILE
1	B	334	LYS
1	B	363	LEU
1	B	365	LYS
1	B	369	ASN
1	B	396	VAL
1	B	444	LYS
1	B	457	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN

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Mol	Chain	Res	Type
1	A	110	ASN
1	A	209	ASN
1	A	298	GLN
1	A	356	ASN
1	A	439	ASN
1	A	448	HIS
1	A	471	GLN
1	B	117	HIS
1	B	203	ASN
1	B	369	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 ⓘ

24 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	486	-	4,4,4	0.43	0	6,6,6	0.73	0
2	SO4	A	487	-	4,4,4	0.47	0	6,6,6	0.93	0
2	SO4	A	488	-	4,4,4	0.45	0	6,6,6	0.56	0
2	SO4	A	489	-	4,4,4	0.64	0	6,6,6	1.23	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	490	-	4,4,4	0.27	0	6,6,6	0.50	0
2	SO4	A	491	-	4,4,4	0.37	0	6,6,6	0.27	0
2	SO4	A	492	-	4,4,4	0.25	0	6,6,6	0.27	0
2	SO4	A	493	-	4,4,4	0.26	0	6,6,6	0.78	0
2	SO4	A	494	-	4,4,4	0.26	0	6,6,6	0.41	0
3	NHE	B	486[A]	-	13,13,13	2.02	2 (15%)	15,17,17	2.40	4 (26%)
3	NHE	B	486[B]	-	13,13,13	2.24	1 (7%)	15,17,17	3.38	3 (20%)
2	SO4	B	487	-	4,4,4	0.32	0	6,6,6	0.53	0
2	SO4	B	488	-	4,4,4	0.22	0	6,6,6	0.62	0
2	SO4	B	489	-	4,4,4	0.08	0	6,6,6	0.71	0
2	SO4	B	490	-	4,4,4	0.28	0	6,6,6	0.79	0
2	SO4	B	491	-	4,4,4	0.18	0	6,6,6	0.70	0
2	SO4	B	492	-	4,4,4	0.13	0	6,6,6	0.81	0
2	SO4	B	493	-	4,4,4	0.28	0	6,6,6	0.18	0
2	SO4	B	494	-	4,4,4	0.22	0	6,6,6	0.83	0
2	SO4	B	495	-	4,4,4	0.25	0	6,6,6	0.67	0
2	SO4	B	496	-	4,4,4	0.26	0	6,6,6	0.53	0
2	SO4	B	497	-	4,4,4	0.12	0	6,6,6	0.49	0
2	SO4	B	498	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	B	499	-	4,4,4	0.30	0	6,6,6	0.38	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	SO4	A	486	-	-	0/0/0/0	0/0/0/0
2	SO4	A	487	-	-	0/0/0/0	0/0/0/0
2	SO4	A	488	-	-	0/0/0/0	0/0/0/0
2	SO4	A	489	-	-	0/0/0/0	0/0/0/0
2	SO4	A	490	-	-	0/0/0/0	0/0/0/0
2	SO4	A	491	-	-	0/0/0/0	0/0/0/0
2	SO4	A	492	-	-	0/0/0/0	0/0/0/0
2	SO4	A	493	-	-	0/0/0/0	0/0/0/0
2	SO4	A	494	-	-	0/0/0/0	0/0/0/0
3	NHE	B	486[A]	-	-	0/7/15/15	0/1/1/1
3	NHE	B	486[B]	-	-	0/7/15/15	0/1/1/1
2	SO4	B	487	-	-	0/0/0/0	0/0/0/0
2	SO4	B	488	-	-	0/0/0/0	0/0/0/0
2	SO4	B	489	-	-	0/0/0/0	0/0/0/0
2	SO4	B	490	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	491	-	-	0/0/0/0	0/0/0/0
2	SO4	B	492	-	-	0/0/0/0	0/0/0/0
2	SO4	B	493	-	-	0/0/0/0	0/0/0/0
2	SO4	B	494	-	-	0/0/0/0	0/0/0/0
2	SO4	B	495	-	-	0/0/0/0	0/0/0/0
2	SO4	B	496	-	-	0/0/0/0	0/0/0/0
2	SO4	B	497	-	-	0/0/0/0	0/0/0/0
2	SO4	B	498	-	-	0/0/0/0	0/0/0/0
2	SO4	B	499	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	486[B]	NHE	C2-S	-7.34	1.66	1.77
3	B	486[A]	NHE	C2-S	-6.55	1.67	1.77
3	B	486[A]	NHE	O1-S	2.15	1.51	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	486[B]	NHE	O3-S-C2	-4.28	100.79	106.06
3	B	486[A]	NHE	C6'-C1'-C2'	-3.38	105.41	110.85
3	B	486[A]	NHE	O3-S-O2	-2.12	106.52	111.37
2	A	489	SO4	O4-S-O2	2.05	120.58	109.26
3	B	486[B]	NHE	O2-S-C2	4.33	110.51	106.79
3	B	486[A]	NHE	O2-S-C2	5.22	111.28	106.79
3	B	486[A]	NHE	O3-S-C2	5.49	112.81	106.06
3	B	486[B]	NHE	O1-S-C2	10.97	116.22	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	488	SO4	1	0
2	A	493	SO4	1	0
3	B	486[B]	NHE	2	0
2	B	494	SO4	2	0
2	B	495	SO4	1	0
2	B	497	SO4	1	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	471/485 (97%)	0.27	17 (3%) 43 44	15, 26, 51, 72	0
1	B	479/485 (98%)	0.47	43 (8%) 10 10	13, 31, 64, 88	0
All	All	950/970 (97%)	0.37	60 (6%) 21 21	13, 28, 58, 88	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	SER	4.8
1	B	181	GLY	4.6
1	B	184	GLY	4.4
1	B	120	THR	4.4
1	B	9	PRO	4.3
1	B	178	ASP	4.2
1	A	144	ASP	4.0
1	B	122	THR	3.9
1	B	148	GLU	3.9
1	A	180	GLU	3.7
1	B	141	TRP	3.7
1	B	180	GLU	3.6
1	B	443	GLU	3.6
1	B	324	GLY	3.6
1	A	59	LYS	3.5
1	B	172	ARG	3.4
1	B	116	ASP	3.4
1	B	182	VAL	3.4
1	B	144	ASP	3.3
1	B	176	GLY	3.3
1	B	7	LYS	3.3
1	B	119	ARG	3.3
1	A	143	PRO	3.3
1	B	175	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	442	VAL	3.2
1	A	145	GLY	3.0
1	A	60	GLY	2.9
1	B	238	ALA	2.7
1	B	441	ASP	2.7
1	B	123	SER	2.7
1	B	179	ILE	2.7
1	A	184	GLY	2.6
1	B	142	TYR	2.6
1	B	333	SER	2.6
1	B	229	ILE	2.6
1	B	145	GLY	2.6
1	B	11	ALA	2.5
1	A	119	ARG	2.5
1	B	177	PHE	2.5
1	B	325	PHE	2.5
1	B	143	PRO	2.5
1	A	58	LYS	2.4
1	A	443	GLU	2.4
1	B	174	THR	2.4
1	A	28	HIS	2.4
1	B	21	ALA	2.3
1	B	444	LYS	2.3
1	B	183	GLU	2.3
1	A	177	PHE	2.2
1	A	172	ARG	2.2
1	B	146	VAL	2.2
1	B	185	HIS	2.2
1	B	8	LYS	2.1
1	A	147	SER	2.1
1	A	181	GLY	2.1
1	B	121	GLY	2.1
1	A	146	VAL	2.1
1	A	208	ILE	2.1
1	B	208	ILE	2.0
1	B	173	TRP	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, 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	SO4	B	495	5/5	0.95	0.50	15.08	20,23,25,30	5
2	SO4	A	493	5/5	0.89	0.34	8.95	14,23,24,30	5
2	SO4	B	494	5/5	0.80	0.45	8.43	4,15,24,24	5
2	SO4	A	488	5/5	0.95	0.28	6.80	16,16,21,24	5
3	NHE	B	486[A]	13/13	0.84	0.23	4.76	19,29,37,37	13
3	NHE	B	486[B]	13/13	0.84	0.23	4.63	21,28,33,34	13
2	SO4	B	488	5/5	0.92	0.20	4.05	20,22,27,28	5
2	SO4	B	487	5/5	0.98	0.15	0.70	15,22,27,27	5
2	SO4	B	499	5/5	0.95	0.17	0.15	27,29,33,34	5
2	SO4	A	486	5/5	0.98	0.10	-0.12	22,25,27,28	0
2	SO4	A	487	5/5	0.98	0.15	-0.17	23,25,27,27	5
2	SO4	B	497	5/5	0.70	0.29	-	18,22,23,23	5
2	SO4	A	490	5/5	0.94	0.19	-	18,25,27,31	5
2	SO4	B	491	5/5	0.94	0.15	-	19,22,27,29	5
2	SO4	B	492	5/5	0.88	0.15	-	29,31,38,38	5
2	SO4	B	493	5/5	0.90	0.24	-	9,20,26,28	5
2	SO4	B	490	5/5	0.96	0.19	-	19,25,25,27	5
2	SO4	A	494	5/5	0.93	0.23	-	14,16,21,22	5
2	SO4	B	496	5/5	0.86	0.36	-	16,19,23,24	5
2	SO4	B	498	5/5	0.91	0.41	-	13,19,24,24	5
2	SO4	A	492	5/5	0.87	0.35	-	19,19,21,34	5
2	SO4	A	491	5/5	0.95	0.29	-	19,21,24,25	5
2	SO4	A	489	5/5	0.93	0.18	-	15,15,29,30	5
2	SO4	B	489	5/5	0.87	0.20	-	22,30,36,36	5

### 6.5 Other polymers ⓘ

There are no such residues in this entry.