



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:58 am BST

PDB ID : 1GKP  
Title : D-Hydantoinase (Dihydropyrimidinase) from *Thermus* sp. in space group C2221  
Authors : Abendroth, J.; Niefind, K.; Schomburg, D.  
Deposited on : 2001-08-20  
Resolution : 1.29 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

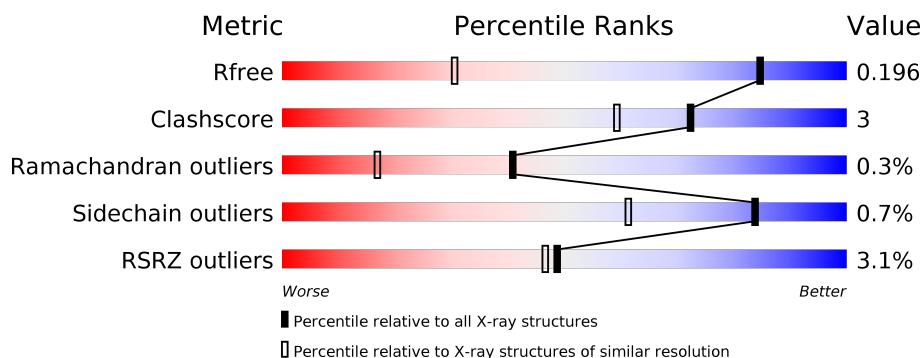
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.29 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))
$R_{free}$	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	458	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	B	458	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	C	458	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	D	458	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	E	458	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	F	458	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>10%</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
3	SO4	E	1464	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25259 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 HYDANTOINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3576	2277	606	678	15			
1	B	458	Total	C	N	O	S	0	0	0
			3576	2277	606	678	15			
1	C	458	Total	C	N	O	S	0	0	0
			3576	2277	606	678	15			
1	D	458	Total	C	N	O	S	0	0	0
			3576	2277	606	678	15			
1	E	458	Total	C	N	O	S	0	0	0
			3576	2277	606	678	15			
1	F	458	Total	C	N	O	S	0	0	0
			3576	2277	606	678	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	KCX	LYS	modified residue	PDB 1GKP
B	150	KCX	LYS	modified residue	PDB 1GKP
C	150	KCX	LYS	modified residue	PDB 1GKP
D	150	KCX	LYS	modified residue	PDB 1GKP
E	150	KCX	LYS	modified residue	PDB 1GKP
F	150	KCX	LYS	modified residue	PDB 1GKP

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



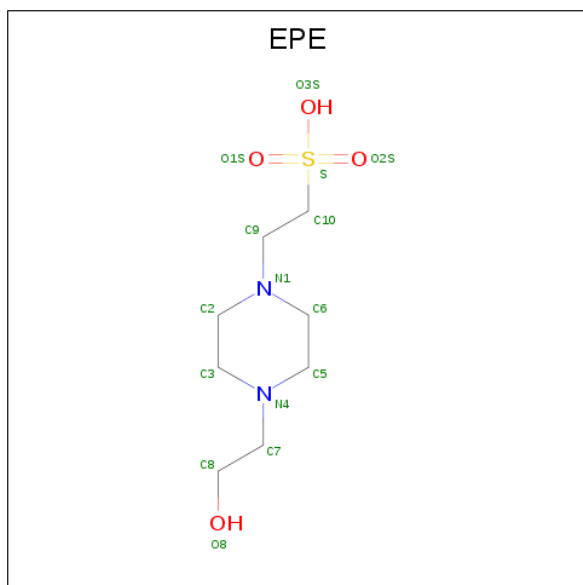
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

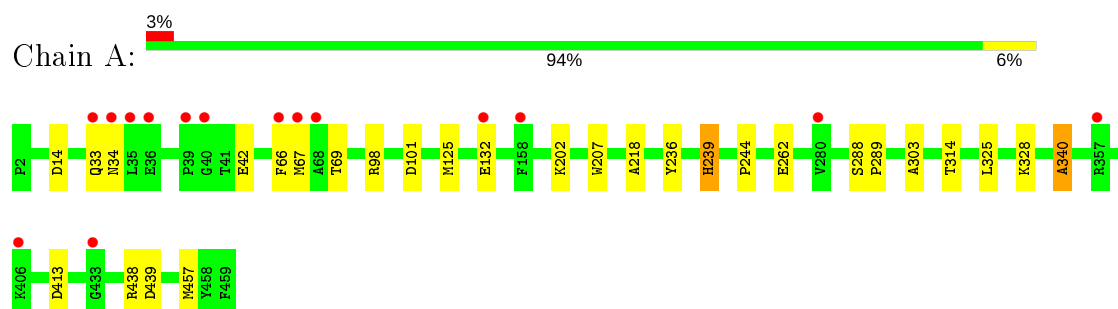
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	610	Total	O	0	0
			610	610		
5	B	589	Total	O	0	0
			589	589		
5	C	662	Total	O	0	0
			662	662		
5	D	564	Total	O	0	0
			564	564		
5	E	691	Total	O	0	0
			691	691		
5	F	600	Total	O	0	0
			600	600		

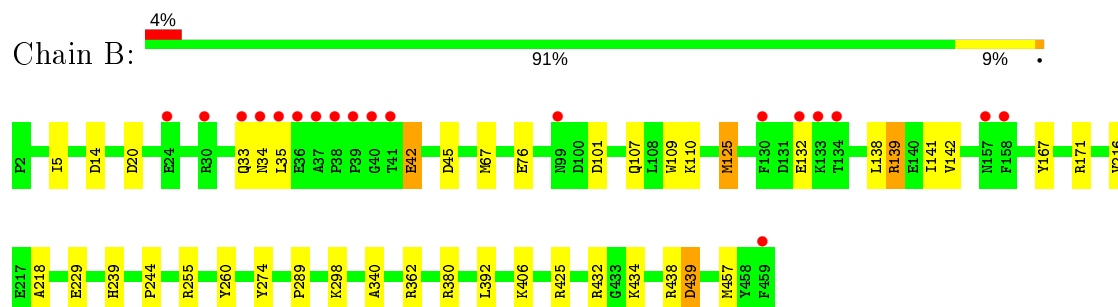
### 3 Residue-property plots [i](#)

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.

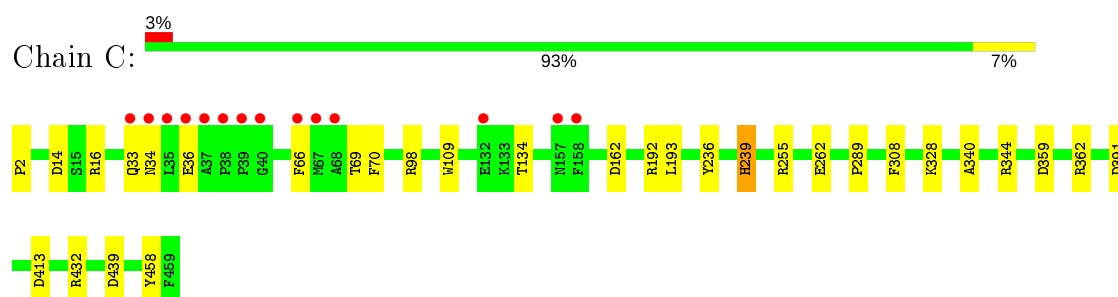
#### • Molecule 1: HYDANTOINASE



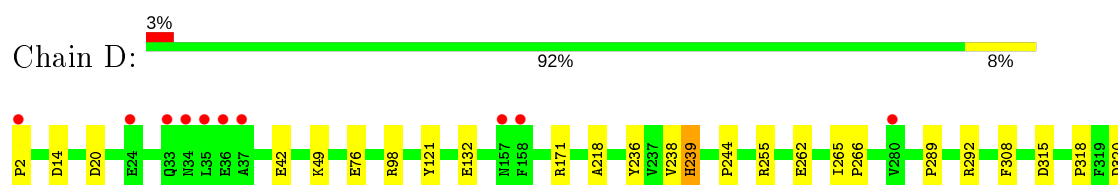
#### • Molecule 1: HYDANTOINASE



#### • Molecule 1: HYDANTOINASE

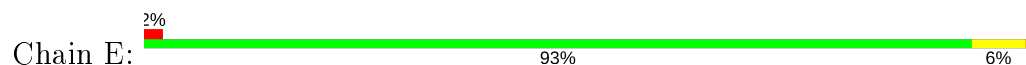


#### • Molecule 1: HYDANTOINASE

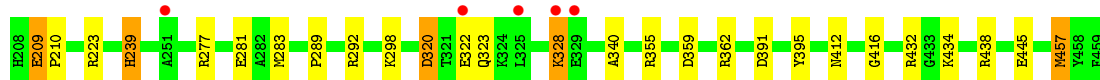
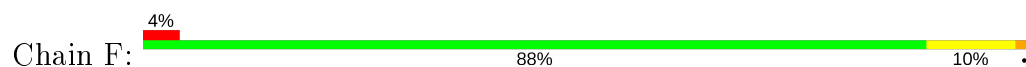




• Molecule 1: HYDANTOINASE



• Molecule 1: HYDANTOINASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.20Å 215.90Å 207.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.29 48.25 – 1.29	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-1.29) 99.7 (48.25-1.29)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 1.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.153 , 0.184 0.166 , 0.196	Depositor DCC
$R_{free}$ test set	13809 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.009 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	25259	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% 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: ZN, EPE, SO4, KCX

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	1.05	4/3646 (0.1%)	1.07	8/4934 (0.2%)
1	B	1.04	8/3646 (0.2%)	1.05	13/4934 (0.3%)
1	C	0.95	0/3646	1.02	16/4934 (0.3%)
1	D	1.02	2/3646 (0.1%)	1.03	14/4934 (0.3%)
1	E	1.02	5/3646 (0.1%)	1.01	8/4934 (0.2%)
1	F	1.16	8/3646 (0.2%)	1.13	20/4934 (0.4%)
All	All	1.04	27/21876 (0.1%)	1.05	79/29604 (0.3%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	283	MET	SD-CE	-8.38	1.30	1.77
1	F	209	GLU	CD-OE2	7.47	1.33	1.25
1	B	167	TYR	CE1-CZ	-7.25	1.29	1.38
1	B	216	VAL	CB-CG1	-7.18	1.37	1.52
1	A	303	ALA	CA-CB	-6.89	1.38	1.52
1	E	362	ARG	CZ-NH1	6.86	1.42	1.33
1	A	262	GLU	CD-OE2	6.60	1.32	1.25
1	E	216	VAL	CB-CG1	-6.06	1.40	1.52
1	F	167	TYR	CD2-CE2	5.94	1.48	1.39
1	F	118	TYR	CD2-CE2	5.91	1.48	1.39
1	F	207	TRP	CB-CG	-5.87	1.39	1.50
1	B	298	LYS	CE-NZ	-5.85	1.34	1.49
1	B	76	GLU	CG-CD	-5.82	1.43	1.51
1	A	236	TYR	CE1-CZ	-5.68	1.31	1.38
1	F	298	LYS	CE-NZ	-5.66	1.34	1.49
1	F	395	TYR	CD1-CE1	-5.61	1.30	1.39
1	E	458	TYR	CE1-CZ	-5.59	1.31	1.38
1	D	121	TYR	CE1-CZ	-5.54	1.31	1.38
1	A	125	MET	SD-CE	-5.38	1.47	1.77
1	E	229	GLU	CD-OE1	-5.35	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	260	TYR	CG-CD1	-5.32	1.32	1.39
1	E	268	PHE	CG-CD1	-5.20	1.30	1.38
1	B	125	MET	CG-SD	-5.16	1.67	1.81
1	F	78	GLY	C-O	5.15	1.31	1.23
1	D	238	VAL	CB-CG2	-5.13	1.42	1.52
1	B	274	TYR	CD2-CE2	-5.05	1.31	1.39
1	B	167	TYR	CG-CD2	-5.04	1.32	1.39

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	283	MET	CG-SD-CE	-14.73	76.64	100.20
1	B	362	ARG	NE-CZ-NH1	-10.29	115.16	120.30
1	D	359	ASP	CB-CG-OD2	9.84	127.15	118.30
1	E	362	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	C	362	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	B	380	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	F	432	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	F	120	ASP	CB-CG-OD2	7.91	125.42	118.30
1	E	162	ASP	CB-CG-OD1	7.76	125.28	118.30
1	C	439	ASP	CB-CG-OD2	7.62	125.16	118.30
1	C	162	ASP	CB-CG-OD1	7.59	125.13	118.30
1	A	413	ASP	CB-CG-OD2	7.37	124.94	118.30
1	E	255	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	C	255	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	F	362	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	98	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	C	16	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	D	362	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	E	255	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	E	359	ASP	CB-CG-OD2	6.30	123.97	118.30
1	F	320	ASP	CB-CG-OD2	6.27	123.94	118.30
1	D	432	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	98	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	F	92	GLU	OE1-CD-OE2	6.23	130.77	123.30
1	B	139	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	457	MET	CA-CB-CG	6.19	123.83	113.30
1	B	457	MET	CA-CB-CG	6.19	123.82	113.30
1	D	255	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	B	101	ASP	CB-CG-OD2	6.14	123.83	118.30
1	C	308	PHE	CB-CG-CD1	6.08	125.06	120.80
1	F	34	ASN	CB-CA-C	-6.06	98.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	344	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	F	355	ARG	NE-CZ-NH1	-5.99	117.30	120.30
1	D	320	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	439	ASP	CB-CG-OD2	5.95	123.65	118.30
1	C	308	PHE	CB-CG-CD2	-5.92	116.65	120.80
1	A	101	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	98	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	E	344	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	439	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	432	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	F	223	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	344	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	C	413	ASP	CB-CG-OD2	5.72	123.44	118.30
1	B	229	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	C	98	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	380	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	F	98	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	171	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	F	162	ASP	CB-CG-OD1	5.45	123.20	118.30
1	D	98	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	F	139	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	D	292	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	D	308	PHE	CB-CG-CD2	-5.35	117.06	120.80
1	A	34	ASN	CB-CA-C	-5.35	99.70	110.40
1	B	255	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	45	ASP	CB-CG-OD1	5.33	123.10	118.30
1	F	391	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	D	20	ASP	CB-CG-OD1	5.32	123.08	118.30
1	D	315	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	362	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	20	ASP	CB-CG-OD1	5.31	123.08	118.30
1	F	298	LYS	CD-CE-NZ	5.29	123.86	111.70
1	C	255	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	F	16	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	F	70	PHE	CB-CA-C	-5.24	99.92	110.40
1	C	391	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	149	PHE	CB-CG-CD1	5.21	124.45	120.80
1	B	380	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	C	458	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	F	457	MET	CA-CB-CG	5.17	122.09	113.30
1	B	171	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	359	ASP	CB-CG-OD1	5.10	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	359	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	A	262	GLU	OE1-CD-OE2	-5.09	117.20	123.30
1	F	185	GLU	OE1-CD-OE2	5.06	129.37	123.30
1	F	292	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	432	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	F	359	ASP	CB-CG-OD2	5.03	122.83	118.30

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	3576	0	3512	14	0
1	B	3576	0	3512	28	0
1	C	3576	0	3512	24	0
1	D	3576	0	3512	23	0
1	E	3576	0	3512	22	0
1	F	3576	0	3512	36	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	10	0	0	0	0
3	D	5	0	0	1	0
3	E	15	0	0	1	9
3	F	5	0	0	0	0
4	D	15	0	17	0	0
4	F	15	0	17	0	0
5	A	610	0	0	3	6
5	B	589	0	0	22	5
5	C	662	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	564	0	0	14	3
5	E	691	0	0	12	1
5	F	600	0	0	13	0
All	All	25259	0	21106	143	22

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 3.

All (143) 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:398:GLN:HG2	5:D:2482:HOH:O	1.26	1.34
1:B:67:MET:HG3	5:B:2207:HOH:O	1.25	1.32
1:E:30:ARG:HD3	5:E:2075:HOH:O	1.36	1.24
1:F:193:LEU:HD12	5:F:2321:HOH:O	1.06	1.23
1:E:362:ARG:NH2	5:E:2554:HOH:O	1.70	1.23
1:B:138:LEU:O	5:B:2232:HOH:O	1.81	0.98
1:B:42:GLU:OE2	1:B:438:ARG:NH1	1.96	0.97
1:A:42:GLU:OE2	1:A:438:ARG:NH1	1.99	0.94
1:F:112:LYS:NZ	5:F:2193:HOH:O	2.00	0.92
1:F:42:GLU:OE2	1:F:438:ARG:NH1	2.01	0.92
1:B:132:GLU:OE2	5:B:2223:HOH:O	1.90	0.90
3:B:1462:SO4:O3	5:B:2587:HOH:O	1.91	0.88
1:E:358:LEU:N	5:E:2545:HOH:O	2.07	0.88
1:F:63:TYR:CE1	1:F:112:LYS:HE3	2.08	0.87
1:D:411:ASN:ND2	5:D:2503:HOH:O	2.10	0.84
1:A:14:ASP:OD1	5:A:2018:HOH:O	1.95	0.84
1:B:132:GLU:OE1	5:B:2223:HOH:O	1.97	0.83
1:B:132:GLU:CD	5:B:2223:HOH:O	2.18	0.82
1:C:328:LYS:HE2	5:C:2511:HOH:O	1.79	0.81
1:A:66:PHE:HD2	1:A:69:THR:HG22	1.46	0.79
1:C:33:GLN:OE1	1:C:33:GLN:HA	1.79	0.78
1:C:134:THR:HG21	5:C:2260:HOH:O	1.82	0.78
1:B:139:ARG:HA	5:B:2232:HOH:O	1.82	0.78
3:D:1462:SO4:O3	5:D:2558:HOH:O	2.01	0.78
1:D:76:GLU:OE2	5:D:2113:HOH:O	2.01	0.77
1:F:70:PHE:O	1:F:323:GLN:NE2	2.17	0.77
1:A:325:LEU:O	1:A:328:LYS:HE3	1.85	0.75
1:D:398:GLN:NE2	5:D:2482:HOH:O	2.20	0.74
1:F:193:LEU:CD1	5:F:2321:HOH:O	1.84	0.73
1:F:416:GLY:O	5:F:2536:HOH:O	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:TYR:CE1	1:F:112:LYS:CE	2.73	0.72
1:C:66:PHE:HD2	1:C:69:THR:HG22	1.55	0.72
1:B:14:ASP:HB3	5:B:2019:HOH:O	1.90	0.71
1:D:14:ASP:HB3	5:D:2017:HOH:O	1.90	0.71
1:B:34:ASN:O	5:B:2056:HOH:O	2.09	0.71
3:A:1462:SO4:O1	5:A:2609:HOH:O	2.09	0.70
1:F:434:LYS:NZ	1:F:445:GLU:OE1	2.25	0.70
1:C:193:LEU:HD11	5:E:2409:HOH:O	1.92	0.69
1:D:76:GLU:HG2	5:D:2111:HOH:O	1.92	0.69
1:B:142:VAL:CG2	5:B:2232:HOH:O	2.40	0.68
1:B:14:ASP:OD1	5:B:2018:HOH:O	2.10	0.68
1:A:14:ASP:HB3	5:B:2019:HOH:O	1.93	0.68
1:B:107:GLN:OE1	5:B:2173:HOH:O	2.09	0.68
1:F:14:ASP:HB3	5:F:2024:HOH:O	1.94	0.68
1:A:33:GLN:HG2	5:B:2049:HOH:O	1.93	0.67
1:F:26:GLU:OE2	5:F:2050:HOH:O	2.12	0.67
1:C:14:ASP:OD1	5:C:2019:HOH:O	2.13	0.67
1:B:35:LEU:HA	5:B:2056:HOH:O	1.95	0.67
1:B:142:VAL:HB	5:B:2232:HOH:O	1.95	0.66
1:E:357:ARG:C	5:E:2545:HOH:O	2.34	0.65
1:B:42:GLU:CD	1:B:438:ARG:HH12	1.98	0.65
3:E:1462:SO4:O1	5:E:2682:HOH:O	2.12	0.65
1:A:239:HIS:CE1	1:A:289:PRO:HD3	2.32	0.64
1:C:33:GLN:HG2	5:D:2045:HOH:O	1.97	0.64
1:E:14:ASP:OD1	5:E:2027:HOH:O	2.14	0.64
1:C:14:ASP:HB3	5:D:2017:HOH:O	1.96	0.64
1:E:14:ASP:HB3	5:F:2024:HOH:O	1.99	0.62
1:F:66:PHE:HE1	5:F:2446:HOH:O	1.83	0.62
1:F:66:PHE:CE1	5:F:2446:HOH:O	2.51	0.61
1:B:239:HIS:CE1	1:B:289:PRO:HD3	2.35	0.61
1:F:239:HIS:CE1	1:F:289:PRO:HD3	2.35	0.61
1:D:132:GLU:CD	1:D:132:GLU:H	2.05	0.60
1:D:42:GLU:OE2	1:D:438:ARG:NH1	2.34	0.60
1:C:239:HIS:CE1	1:C:289:PRO:HD3	2.36	0.60
1:E:239:HIS:CE1	1:E:289:PRO:HD3	2.38	0.59
1:D:239:HIS:CE1	1:D:289:PRO:HD3	2.37	0.59
1:B:125:MET:HG2	1:B:141:ILE:HG21	1.84	0.58
1:B:142:VAL:HG23	5:B:2232:HOH:O	2.04	0.58
1:C:33:GLN:O	1:C:34:ASN:C	2.41	0.57
1:D:42:GLU:OE2	1:D:438:ARG:NH2	2.37	0.57
5:E:2070:HOH:O	1:F:33:GLN:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:TYR:CD1	1:F:112:LYS:HE3	2.39	0.56
1:F:209:GLU:HB3	1:F:210:PRO:HD3	1.88	0.55
1:E:14:ASP:OD1	1:F:14:ASP:OD1	2.25	0.54
1:B:132:GLU:HA	5:B:2228:HOH:O	2.08	0.53
1:E:425:ARG:NH1	5:E:2624:HOH:O	2.42	0.53
1:E:399:TYR:CD1	1:E:425:ARG:HD3	2.44	0.53
1:C:14:ASP:CG	5:C:2019:HOH:O	2.47	0.52
1:D:398:GLN:CG	5:D:2482:HOH:O	2.07	0.52
1:B:218:ALA:HB2	1:B:244:PRO:HB2	1.90	0.52
1:A:288:SER:HA	1:A:289:PRO:C	2.29	0.52
1:B:142:VAL:CB	5:B:2232:HOH:O	2.53	0.52
1:B:5:ILE:HD12	1:B:392:LEU:HD13	1.92	0.51
1:F:63:TYR:CD1	1:F:112:LYS:CD	2.93	0.51
1:F:209:GLU:N	1:F:210:PRO:CD	2.74	0.51
1:F:322:GLU:OE2	5:F:2436:HOH:O	2.19	0.51
1:E:14:ASP:OD1	1:F:14:ASP:CG	2.49	0.51
1:C:70:PHE:HE1	5:C:2127:HOH:O	1.94	0.51
1:F:277:ARG:NH1	1:F:281:GLU:OE2	2.44	0.50
1:D:49:LYS:NZ	5:D:2071:HOH:O	2.36	0.49
1:C:192:ARG:NH2	5:C:2361:HOH:O	2.41	0.49
1:D:218:ALA:HB2	1:D:244:PRO:HB2	1.95	0.49
1:C:66:PHE:HD2	1:C:69:THR:CG2	2.25	0.49
1:E:18:LYS:O	1:E:33:GLN:NE2	2.46	0.48
1:F:35:LEU:O	1:F:36:GLU:HB2	2.12	0.48
1:D:2:PRO:N	5:D:2001:HOH:O	2.46	0.48
5:D:2327:HOH:O	1:F:193:LEU:HD11	2.12	0.48
1:C:14:ASP:OD1	1:D:14:ASP:OD1	2.30	0.48
1:F:63:TYR:CD1	1:F:112:LYS:CE	2.97	0.48
1:C:66:PHE:O	1:C:66:PHE:CD2	2.66	0.48
1:C:36:GLU:N	5:C:2065:HOH:O	2.33	0.47
1:A:66:PHE:O	1:A:67:MET:C	2.53	0.46
1:F:28:ILE:HD12	5:F:2495:HOH:O	2.15	0.46
1:B:33:GLN:OE1	1:B:33:GLN:HA	2.17	0.45
1:F:328:LYS:HB3	1:F:328:LYS:HE3	1.74	0.45
1:B:406:LYS:NZ	5:B:2511:HOH:O	2.50	0.45
1:A:66:PHE:O	1:A:66:PHE:CD2	2.69	0.44
1:B:425:ARG:NH2	5:B:2536:HOH:O	2.49	0.44
1:F:209:GLU:N	1:F:210:PRO:HD2	2.32	0.44
1:C:134:THR:CG2	5:C:2260:HOH:O	2.54	0.44
1:E:14:ASP:CG	1:F:14:ASP:CG	2.75	0.44
1:C:2:PRO:N	5:C:2001:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:ALA:HB2	1:E:244:PRO:HB2	1.99	0.44
1:B:132:GLU:CD	1:B:132:GLU:H	2.21	0.43
1:F:156:LYS:HB2	1:F:187:ALA:HB1	2.00	0.43
1:C:14:ASP:CG	1:D:14:ASP:OD1	2.56	0.43
1:E:244:PRO:HG3	5:E:2159:HOH:O	2.17	0.43
1:A:14:ASP:CG	5:A:2018:HOH:O	2.45	0.43
1:E:14:ASP:OD1	1:F:14:ASP:OD2	2.36	0.43
1:D:265:ILE:N	1:D:266:PRO:HD2	2.34	0.43
1:E:439:ASP:HB3	5:E:2640:HOH:O	2.18	0.43
1:A:218:ALA:HB2	1:A:244:PRO:HB2	2.01	0.42
1:B:434:LYS:HE2	1:B:434:LYS:HB2	1.89	0.42
1:E:30:ARG:HD2	1:E:35:LEU:HD22	2.00	0.42
1:E:434:LYS:HE2	1:E:434:LYS:HB2	1.85	0.42
1:F:69:THR:OG1	5:F:2119:HOH:O	1.81	0.42
1:C:14:ASP:OD2	5:C:2019:HOH:O	2.21	0.42
1:D:446:LYS:HA	5:D:2537:HOH:O	2.18	0.42
1:F:320:ASP:OD1	1:F:412:ASN:HA	2.20	0.42
1:E:399:TYR:CE1	1:E:425:ARG:HD3	2.53	0.42
1:D:326:LEU:HA	1:D:326:LEU:HD23	1.86	0.42
1:D:236:TYR:CZ	1:D:262:GLU:HB2	2.55	0.42
1:C:236:TYR:CZ	1:C:262:GLU:HB2	2.55	0.41
5:E:2560:HOH:O	1:F:14:ASP:HB3	2.21	0.41
1:A:202:LYS:HB3	1:A:207:TRP:CD1	2.56	0.41
1:C:14:ASP:CG	1:D:14:ASP:CG	2.78	0.41
1:D:132:GLU:N	1:D:132:GLU:CD	2.74	0.41
1:F:36:GLU:HG3	5:F:2063:HOH:O	2.19	0.41
1:B:439:ASP:HB3	5:B:2552:HOH:O	2.21	0.41
1:C:14:ASP:OD1	1:D:14:ASP:CG	2.59	0.40
1:E:288:SER:HA	1:E:289:PRO:C	2.41	0.40
1:A:314:THR:HB	1:A:340:ALA:HB3	2.02	0.40
1:E:10:ILE:O	1:E:16:ARG:HA	2.22	0.40

All (22) 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)
3:E:1464:SO4:S	3:E:1464:SO4:S[4_566]	0.52	1.68
3:E:1464:SO4:O1	3:E:1464:SO4:O2[4_566]	0.58	1.62
3:E:1464:SO4:O3	3:E:1464:SO4:O4[4_566]	0.90	1.30
5:D:2194:HOH:O	5:D:2194:HOH:O[3_556]	1.04	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:2061:HOH:O	5:D:2061:HOH:O[3_556]	1.08	1.12
3:E:1464:SO4:S	3:E:1464:SO4:O1[4_566]	1.13	1.07
5:E:2320:HOH:O	5:E:2320:HOH:O[4_566]	1.24	0.96
3:E:1464:SO4:S	3:E:1464:SO4:O3[4_566]	1.49	0.71
5:A:2296:HOH:O	5:B:2097:HOH:O[3_555]	1.68	0.52
5:B:2145:HOH:O	5:B:2145:HOH:O[3_555]	1.69	0.51
3:E:1464:SO4:S	3:E:1464:SO4:O4[4_566]	1.76	0.44
5:A:2536:HOH:O	5:D:2225:HOH:O[6_554]	1.78	0.42
3:E:1464:SO4:O1	3:E:1464:SO4:O3[4_566]	1.83	0.37
5:A:2163:HOH:O	5:A:2163:HOH:O[3_555]	1.84	0.36
5:A:2163:HOH:O	5:A:2387:HOH:O[3_555]	1.84	0.36
3:E:1464:SO4:S	3:E:1464:SO4:O2[4_566]	1.86	0.34
5:B:2145:HOH:O	5:B:2341:HOH:O[3_555]	1.90	0.30
5:B:2178:HOH:O	5:B:2401:HOH:O[3_555]	1.91	0.29
5:A:2195:HOH:O	5:A:2195:HOH:O[3_555]	1.92	0.28
5:A:2195:HOH:O	5:A:2445:HOH:O[3_555]	1.95	0.25
5:B:2178:HOH:O	5:B:2178:HOH:O[3_555]	2.14	0.06
3:E:1464:SO4:O1	3:E:1464:SO4:O4[4_566]	2.19	0.01

## 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	455/458 (99%)	433 (95%)	21 (5%)	1 (0%)	47	19
1	B	455/458 (99%)	438 (96%)	16 (4%)	1 (0%)	47	19
1	C	455/458 (99%)	435 (96%)	19 (4%)	1 (0%)	47	19
1	D	455/458 (99%)	439 (96%)	15 (3%)	1 (0%)	47	19
1	E	455/458 (99%)	438 (96%)	16 (4%)	1 (0%)	47	19
1	F	455/458 (99%)	436 (96%)	16 (4%)	3 (1%)	22	3
All	All	2730/2748 (99%)	2619 (96%)	103 (4%)	8 (0%)	41	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	34	ASN
1	B	340	ALA
1	D	340	ALA
1	F	340	ALA
1	E	340	ALA
1	F	36	GLU
1	A	340	ALA
1	C	340	ALA

### 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	373/373 (100%)	371 (100%)	2 (0%)	88	69
1	B	373/373 (100%)	370 (99%)	3 (1%)	81	58
1	C	373/373 (100%)	371 (100%)	2 (0%)	88	69
1	D	373/373 (100%)	371 (100%)	2 (0%)	88	69
1	E	373/373 (100%)	370 (99%)	3 (1%)	81	58
1	F	373/373 (100%)	370 (99%)	3 (1%)	81	58
All	All	2238/2238 (100%)	2223 (99%)	15 (1%)	84	61

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	GLU
1	A	239	HIS
1	B	42	GLU
1	B	109	TRP
1	B	110	LYS
1	C	109	TRP
1	C	239	HIS
1	D	239	HIS
1	D	318	PRO

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Mol	Chain	Res	Type
1	E	30	ARG
1	E	36	GLU
1	E	239	HIS
1	F	239	HIS
1	F	328	LYS
1	F	457	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	116	ASN
1	D	195	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	KCX	B	150	1,2	7,11,12	0.78	0	4,12,14	0.90	0
1	KCX	A	150	1,2	7,11,12	0.72	0	4,12,14	0.77	0
1	KCX	D	150	1,2	7,11,12	0.88	0	4,12,14	0.39	0
1	KCX	F	150	1,2	7,11,12	1.15	1 (14%)	4,12,14	0.23	0
1	KCX	E	150	1,2	7,11,12	1.54	2 (28%)	4,12,14	0.29	0
1	KCX	C	150	1,2	7,11,12	1.38	1 (14%)	4,12,14	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	B	150	1,2	-	0/7/10/12	-
1	KCX	A	150	1,2	-	0/7/10/12	-
1	KCX	D	150	1,2	-	0/7/10/12	-
1	KCX	F	150	1,2	-	0/7/10/12	-
1	KCX	E	150	1,2	-	0/7/10/12	-
1	KCX	C	150	1,2	-	0/7/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	150	KCX	CE-NZ	2.81	1.51	1.45
1	C	150	KCX	CE-NZ	2.25	1.50	1.45
1	E	150	KCX	O-C	2.10	1.28	1.19
1	F	150	KCX	CA-N	-2.01	1.42	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 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
3	SO4	D	1462	-	4,4,4	0.22	0	6,6,6	0.77	0
3	SO4	B	1462	-	4,4,4	0.45	0	6,6,6	0.45	0
4	EPE	F	1463	-	15,15,15	0.75	0	18,20,20	1.77	6 (33%)
3	SO4	C	1462	-	4,4,4	0.29	0	6,6,6	0.50	0
3	SO4	E	1462	-	4,4,4	0.52	0	6,6,6	0.39	0
3	SO4	E	1464	-	4,4,4	0.67	0	6,6,6	0.51	0
3	SO4	E	1463	-	4,4,4	0.40	0	6,6,6	0.26	0
4	EPE	D	1463	-	15,15,15	0.80	1 (6%)	18,20,20	2.45	9 (50%)
3	SO4	C	1463	-	4,4,4	0.19	0	6,6,6	0.65	0
3	SO4	F	1462	-	4,4,4	0.31	0	6,6,6	0.50	0
3	SO4	A	1462	-	4,4,4	0.53	0	6,6,6	0.51	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
4	EPE	D	1463	-	-	0/9/19/19	0/1/1/1
4	EPE	F	1463	-	-	0/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1463	EPE	C10-S	2.75	1.81	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1463	EPE	O1S-S-C10	-5.04	100.85	106.92
4	D	1463	EPE	O3S-S-C10	4.52	113.08	105.77
4	F	1463	EPE	O1S-S-C10	-3.86	102.27	106.92
4	F	1463	EPE	O3S-S-C10	3.48	111.40	105.77
4	D	1463	EPE	C6-C5-N4	-3.42	103.63	110.64
4	D	1463	EPE	C5-N4-C3	3.13	115.88	108.83
4	D	1463	EPE	O3S-S-O1S	3.04	118.71	111.27
4	D	1463	EPE	C5-C6-N1	-2.67	105.17	110.64
4	D	1463	EPE	C7-N4-C3	-2.66	104.42	111.23
4	F	1463	EPE	C5-N4-C3	2.65	114.78	108.83
4	F	1463	EPE	C6-C5-N4	-2.14	106.26	110.64
4	F	1463	EPE	C7-N4-C3	-2.12	105.82	111.23
4	F	1463	EPE	O2S-S-C10	2.08	109.42	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1463	EPE	C9-N1-C2	-2.03	106.05	111.23
4	D	1463	EPE	O2S-S-O1S	-2.02	106.95	113.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1462	SO4	1	0
3	B	1462	SO4	1	0
3	E	1462	SO4	1	0
3	E	1464	SO4	0	9
3	A	1462	SO4	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	457/458 (99%)	0.10	15 (3%) 46 44	12, 18, 27, 40	0
1	B	457/458 (99%)	0.06	19 (4%) 36 33	11, 18, 29, 43	0
1	C	457/458 (99%)	-0.21	14 (3%) 49 46	10, 16, 26, 44	0
1	D	457/458 (99%)	0.06	13 (2%) 53 50	12, 19, 30, 45	0
1	E	457/458 (99%)	-0.22	7 (1%) 73 75	10, 16, 25, 38	0
1	F	457/458 (99%)	0.06	17 (3%) 41 38	11, 18, 27, 44	0
All	All	2742/2748 (99%)	-0.02	85 (3%) 49 46	10, 18, 28, 45	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	158	PHE	7.6
1	F	34	ASN	6.8
1	D	34	ASN	6.5
1	A	34	ASN	5.8
1	B	158	PHE	5.5
1	B	34	ASN	5.0
1	C	158	PHE	4.9
1	A	158	PHE	4.7
1	D	35	LEU	4.7
1	A	66	PHE	4.7
1	A	68	ALA	4.6
1	C	34	ASN	4.4
1	A	36	GLU	4.3
1	D	158	PHE	4.2
1	B	35	LEU	4.1
1	F	66	PHE	4.0
1	B	40	GLY	4.0
1	C	36	GLU	3.9
1	B	36	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	36	GLU	3.9
1	F	35	LEU	3.9
1	A	35	LEU	3.8
1	B	99	ASN	3.8
1	E	34	ASN	3.7
1	B	37	ALA	3.7
1	B	130	PHE	3.7
1	C	66	PHE	3.6
1	B	39	PRO	3.5
1	D	36	GLU	3.5
1	F	70	PHE	3.4
1	E	158	PHE	3.3
1	F	325	LEU	3.3
1	B	132	GLU	3.2
1	A	357	ARG	3.1
1	C	39	PRO	3.1
1	C	37	ALA	3.0
1	A	39	PRO	3.0
1	B	41	THR	3.0
1	F	132	GLU	3.0
1	C	68	ALA	2.9
1	D	329	GLU	2.9
1	B	38	PRO	2.9
1	E	36	GLU	2.9
1	D	24	GLU	2.8
1	A	132	GLU	2.8
1	B	157	ASN	2.8
1	E	33	GLN	2.8
1	B	459	PHE	2.7
1	A	67	MET	2.7
1	C	67	MET	2.7
1	E	99	ASN	2.7
1	F	157	ASN	2.7
1	A	33	GLN	2.7
1	B	134	THR	2.7
1	B	30	ARG	2.7
1	C	157	ASN	2.6
1	F	329	GLU	2.6
1	D	37	ALA	2.6
1	D	280	VAL	2.6
1	D	157	ASN	2.5
1	F	201	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	133	LYS	2.5
1	F	203	THR	2.5
1	C	132	GLU	2.4
1	F	69	THR	2.4
1	C	38	PRO	2.4
1	E	357	ARG	2.4
1	C	33	GLN	2.4
1	C	40	GLY	2.3
1	F	322	GLU	2.3
1	D	2	PRO	2.3
1	F	328	LYS	2.3
1	D	33	GLN	2.2
1	F	251	ALA	2.2
1	C	35	LEU	2.2
1	A	406	LYS	2.2
1	A	280	VAL	2.2
1	E	132	GLU	2.2
1	B	24	GLU	2.1
1	A	433	GLY	2.1
1	F	37	ALA	2.1
1	D	328	LYS	2.1
1	B	33	GLN	2.1
1	D	357	ARG	2.0
1	A	40	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KCX	B	150	12/13	0.94	0.07	14,15,16,17	0
1	KCX	D	150	12/13	0.94	0.07	13,15,17,17	0
1	KCX	A	150	12/13	0.95	0.08	12,14,17,17	0
1	KCX	F	150	12/13	0.96	0.07	13,15,17,20	0
1	KCX	E	150	12/13	0.97	0.07	10,12,13,13	0
1	KCX	C	150	12/13	0.98	0.06	11,12,13,14	0

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	1462	5/5	0.85	0.26	34,34,38,40	0
3	SO4	E	1463	5/5	0.90	0.25	33,34,37,38	0
3	SO4	D	1462	5/5	0.92	0.20	32,32,34,40	0
3	SO4	E	1462	5/5	0.93	0.15	22,22,24,30	0
4	EPE	D	1463	15/15	0.96	0.21	30,32,35,36	0
3	SO4	A	1462	5/5	0.96	0.14	23,24,25,28	0
3	SO4	F	1462	5/5	0.97	0.12	22,22,26,27	0
3	SO4	C	1462	5/5	0.97	0.09	21,23,25,26	0
3	SO4	C	1463	5/5	0.98	0.17	24,24,26,31	0
4	EPE	F	1463	15/15	0.98	0.09	22,23,25,26	0
3	SO4	E	1464	5/5	0.98	0.38	26,27,29,29	0
2	ZN	B	1460	1/1	0.99	0.05	18,18,18,18	0
2	ZN	B	1461	1/1	0.99	0.03	18,18,18,18	0
2	ZN	A	1461	1/1	0.99	0.02	19,19,19,19	0
2	ZN	F	1461	1/1	1.00	0.03	21,21,21,21	0
2	ZN	E	1460	1/1	1.00	0.04	15,15,15,15	0
2	ZN	C	1460	1/1	1.00	0.06	16,16,16,16	0
2	ZN	D	1460	1/1	1.00	0.04	19,19,19,19	0
2	ZN	A	1460	1/1	1.00	0.05	19,19,19,19	0
2	ZN	C	1461	1/1	1.00	0.03	15,15,15,15	0
2	ZN	D	1461	1/1	1.00	0.05	20,20,20,20	0
2	ZN	F	1460	1/1	1.00	0.03	21,21,21,21	0
2	ZN	E	1461	1/1	1.00	0.02	15,15,15,15	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.