



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2017 – 09:45 AM EDT

PDB ID : 5E84
Title : ATP-bound state of BiP
Authors : Liu, Q.; Yang, J.; Nune, M.; Zong, Y.; Zhou, L.
Deposited on : unknown
Resolution : 2.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
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-20029824

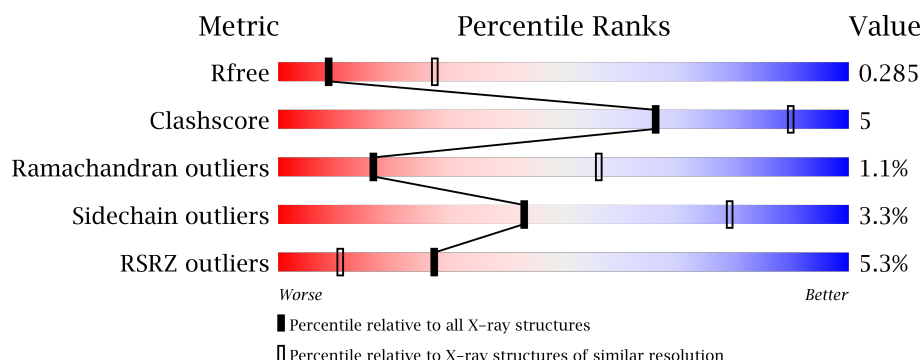
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 ≥ 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	606	<div> <div>4%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	B	606	<div> <div>7%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	C	606	<div> <div>7%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	D	606	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	E	606	<div> <div>5%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	606	

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
4	MG	A	805	-	-	-	X
4	MG	D	804	-	-	X	-
5	SO4	A	808	-	-	X	-
5	SO4	C	806	-	-	X	-
5	SO4	D	808	-	-	X	-
5	SO4	E	806	-	-	X	-
5	SO4	F	806	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28484 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 78 kDa glucose-regulated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	8	0	0
			4710	2955	806	938	11			
1	B	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			
1	C	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			
1	D	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			
1	E	606	Total	C	N	O	S	8	0	0
			4696	2945	805	935	11			
1	F	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			

There are 54 discrepancies between the modelled and reference sequences:

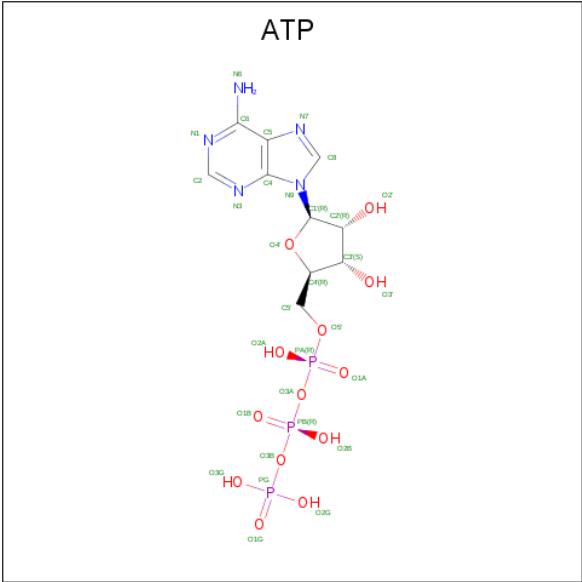
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP P11021
A	229	ALA	THR	conflict	UNP P11021
A	?	-	THR	deletion	UNP P11021
A	?	-	ALA	deletion	UNP P11021
A	?	-	SER	deletion	UNP P11021
A	?	-	ASP	deletion	UNP P11021
A	453	VAL	ASN	conflict	UNP P11021
A	454	GLY	GLN	conflict	UNP P11021
A	455	GLY	PRO	conflict	UNP P11021
B	24	SER	-	expression tag	UNP P11021
B	229	ALA	THR	conflict	UNP P11021
B	?	-	THR	deletion	UNP P11021
B	?	-	ALA	deletion	UNP P11021
B	?	-	SER	deletion	UNP P11021
B	?	-	ASP	deletion	UNP P11021
B	453	VAL	ASN	conflict	UNP P11021
B	454	GLY	GLN	conflict	UNP P11021

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Chain	Residue	Modelled	Actual	Comment	Reference
B	455	GLY	PRO	conflict	UNP P11021
C	24	SER	-	expression tag	UNP P11021
C	229	ALA	THR	conflict	UNP P11021
C	?	-	THR	deletion	UNP P11021
C	?	-	ALA	deletion	UNP P11021
C	?	-	SER	deletion	UNP P11021
C	?	-	ASP	deletion	UNP P11021
C	453	VAL	ASN	conflict	UNP P11021
C	454	GLY	GLN	conflict	UNP P11021
C	455	GLY	PRO	conflict	UNP P11021
D	24	SER	-	expression tag	UNP P11021
D	229	ALA	THR	conflict	UNP P11021
D	?	-	THR	deletion	UNP P11021
D	?	-	ALA	deletion	UNP P11021
D	?	-	SER	deletion	UNP P11021
D	?	-	ASP	deletion	UNP P11021
D	453	VAL	ASN	conflict	UNP P11021
D	454	GLY	GLN	conflict	UNP P11021
D	455	GLY	PRO	conflict	UNP P11021
E	24	SER	-	expression tag	UNP P11021
E	229	ALA	THR	conflict	UNP P11021
E	?	-	THR	deletion	UNP P11021
E	?	-	ALA	deletion	UNP P11021
E	?	-	SER	deletion	UNP P11021
E	?	-	ASP	deletion	UNP P11021
E	453	VAL	ASN	conflict	UNP P11021
E	454	GLY	GLN	conflict	UNP P11021
E	455	GLY	PRO	conflict	UNP P11021
F	24	SER	-	expression tag	UNP P11021
F	229	ALA	THR	conflict	UNP P11021
F	?	-	THR	deletion	UNP P11021
F	?	-	ALA	deletion	UNP P11021
F	?	-	SER	deletion	UNP P11021
F	?	-	ASP	deletion	UNP P11021
F	453	VAL	ASN	conflict	UNP P11021
F	454	GLY	GLN	conflict	UNP P11021
F	455	GLY	PRO	conflict	UNP P11021

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

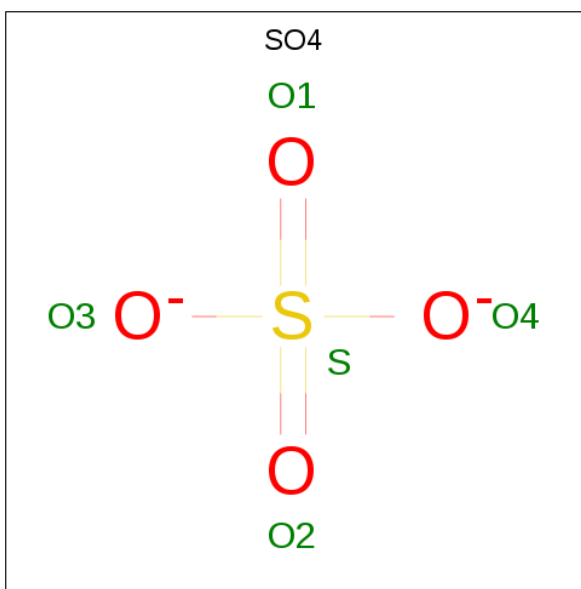
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	Zn	0	0
			3	3		
3	E	3	Total	Zn	0	0
			3	3		
3	B	3	Total	Zn	0	0
			3	3		
3	C	3	Total	Zn	0	0
			3	3		
3	A	3	Total	Zn	0	0
			3	3		
3	F	3	Total	Zn	0	0
			3	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	Mg	0	0
			3	3		
4	E	1	Total	Mg	0	0
			1	1		
4	B	3	Total	Mg	0	0
			3	3		
4	C	1	Total	Mg	0	0
			1	1		
4	A	3	Total	Mg	0	0
			3	3		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

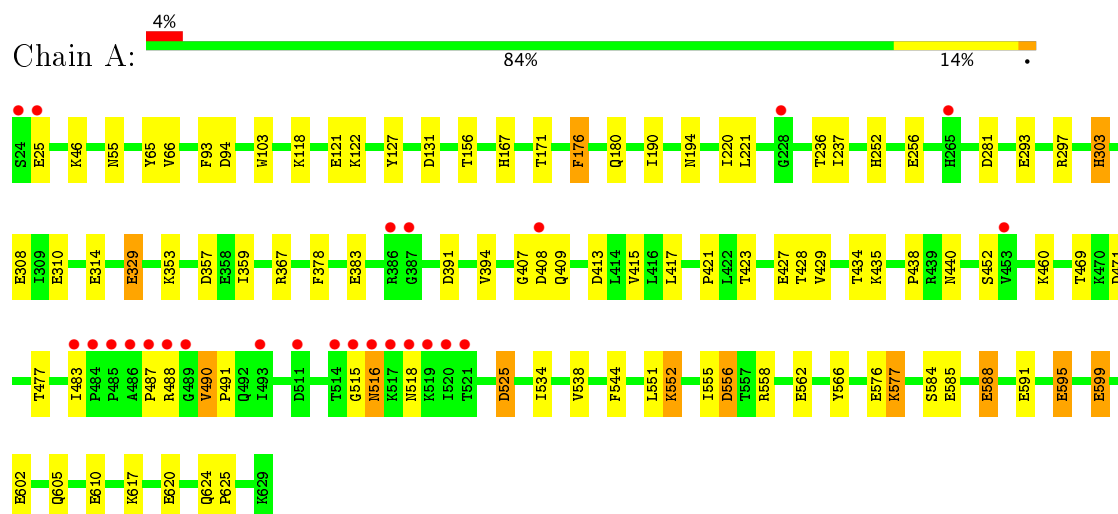
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	5	Total	O	0	0
			5	5		
6	C	4	Total	O	0	0
			4	4		
6	D	4	Total	O	0	0
			4	4		
6	E	9	Total	O	0	0
			9	9		
6	F	3	Total	O	0	0
			3	3		

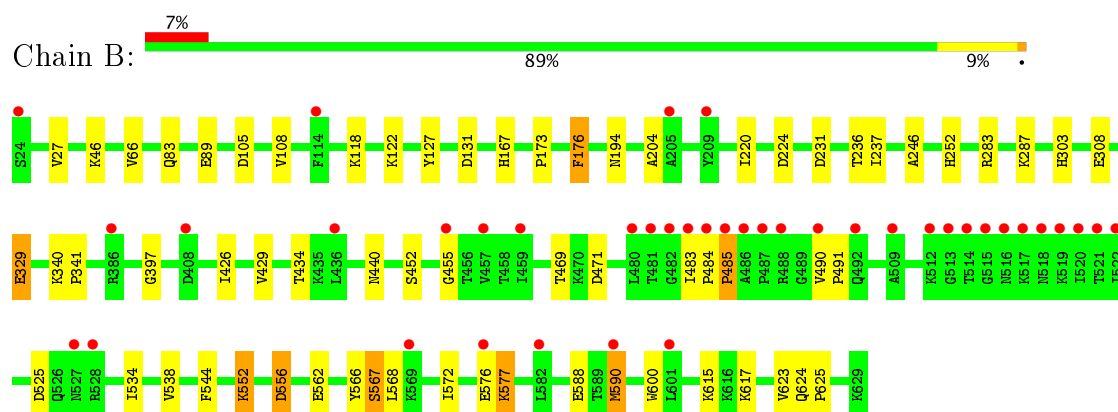
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

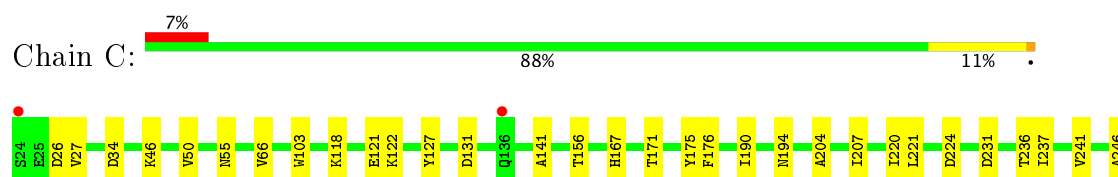
- Molecule 1: 78 kDa glucose-regulated protein

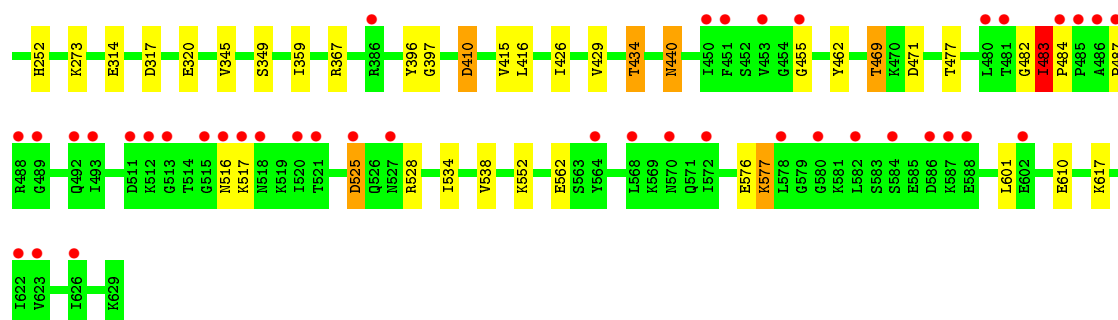


- Molecule 1: 78 kDa glucose-regulated protein

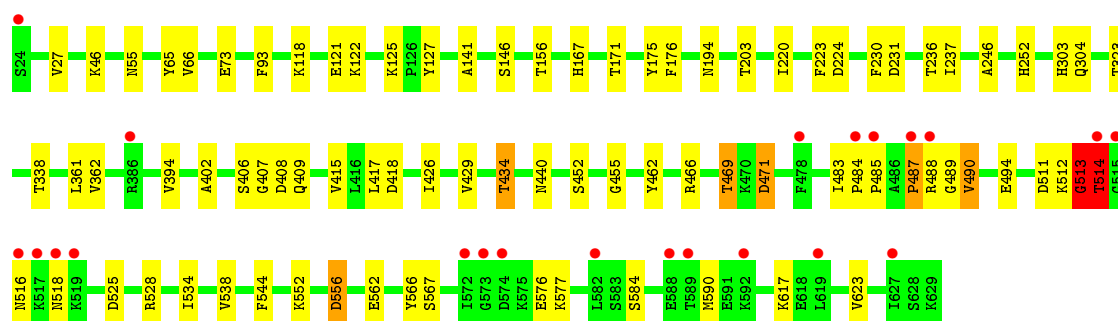
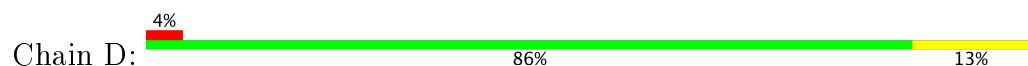


- Molecule 1: 78 kDa glucose-regulated protein

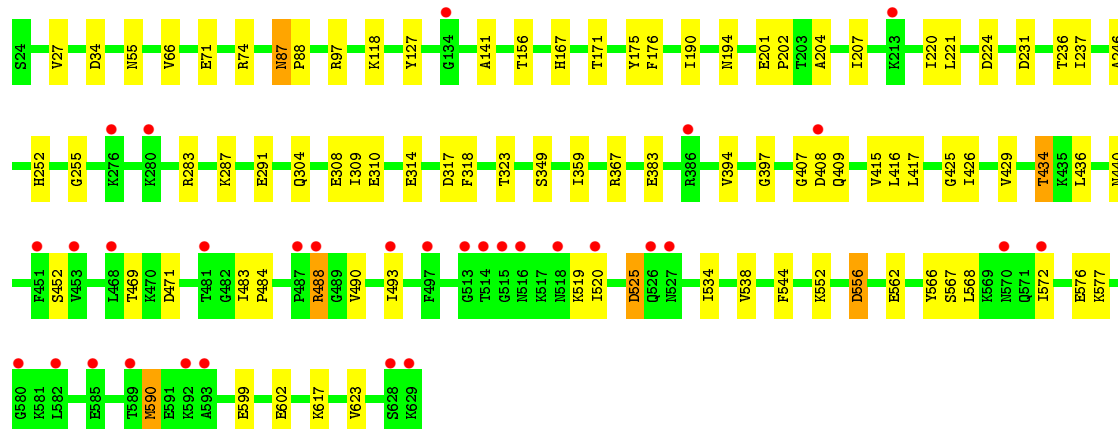
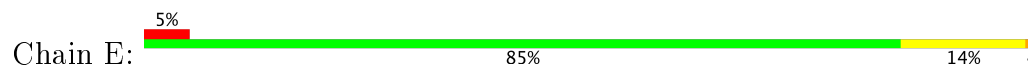




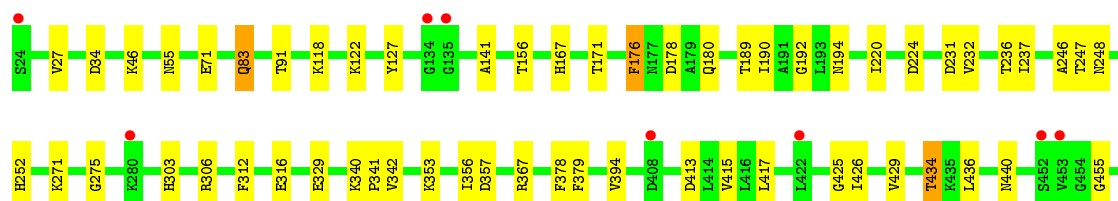
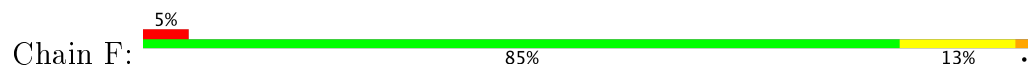
- Molecule 1: 78 kDa glucose-regulated protein

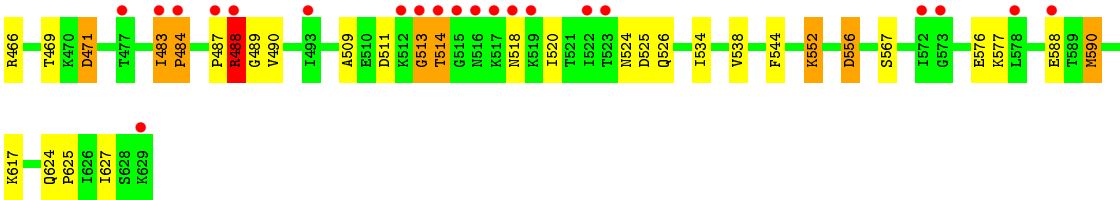


- Molecule 1: 78 kDa glucose-regulated protein



- Molecule 1: 78 kDa glucose-regulated protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	222.47Å 222.47Å 209.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.76 – 2.99 39.65 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.76-2.99) 97.6 (39.65-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.42 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.243 , 0.287 0.241 , 0.285	Depositor DCC
R_{free} test set	5907 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.309 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28484	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: MG, ZN, ATP, 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	0.75	9/4777 (0.2%)	0.86	7/6446 (0.1%)
1	B	0.60	4/4767 (0.1%)	0.73	5/6432 (0.1%)
1	C	0.56	1/4767 (0.0%)	0.71	2/6432 (0.0%)
1	D	0.67	3/4767 (0.1%)	0.78	8/6432 (0.1%)
1	E	0.66	1/4763 (0.0%)	0.73	4/6428 (0.1%)
1	F	0.61	3/4767 (0.1%)	0.75	6/6432 (0.1%)
All	All	0.65	21/28608 (0.1%)	0.76	32/38602 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	3
1	D	2	2
1	F	0	3
All	All	2	9

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	576	GLU	CB-CG	25.85	2.01	1.52
1	D	577	LYS	CB-CG	-17.80	1.04	1.52
1	F	577	LYS	CB-CG	-13.61	1.15	1.52
1	B	577	LYS	CB-CG	-13.20	1.17	1.52
1	D	576	GLU	CB-CG	-12.78	1.27	1.52
1	B	576	GLU	CB-CG	10.76	1.72	1.52
1	C	577	LYS	CB-CG	-9.90	1.25	1.52
1	A	599	GLU	CG-CD	9.70	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	595	GLU	CD-OE2	9.02	1.35	1.25
1	A	588	GLU	CD-OE2	8.54	1.35	1.25
1	A	329	GLU	CD-OE2	7.81	1.34	1.25
1	F	556	ASP	CB-CG	7.76	1.68	1.51
1	F	576	GLU	CB-CG	6.94	1.65	1.52
1	A	576	GLU	CB-CG	-6.90	1.39	1.52
1	A	329	GLU	CB-CG	6.21	1.64	1.52
1	B	556	ASP	CB-CG	6.13	1.64	1.51
1	D	556	ASP	CB-CG	5.99	1.64	1.51
1	A	577	LYS	CB-CG	-5.94	1.36	1.52
1	B	329	GLU	CD-OE2	5.40	1.31	1.25
1	A	588	GLU	CG-CD	5.37	1.60	1.51
1	A	595	GLU	CG-CD	5.08	1.59	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	556	ASP	CB-CG-OD1	11.50	128.65	118.30
1	A	556	ASP	CB-CG-OD1	11.41	128.57	118.30
1	D	577	LYS	CA-CB-CG	9.73	134.82	113.40
1	A	599	GLU	OE1-CD-OE2	-9.65	111.72	123.30
1	E	576	GLU	CA-CB-CG	-9.10	93.39	113.40
1	E	556	ASP	CB-CG-OD1	9.06	126.45	118.30
1	B	556	ASP	CB-CG-OD1	8.62	126.06	118.30
1	D	576	GLU	CA-CB-CG	-8.18	95.39	113.40
1	B	576	GLU	CA-CB-CG	-8.12	95.53	113.40
1	A	599	GLU	CG-CD-OE1	7.38	133.06	118.30
1	C	576	GLU	CA-CB-CG	7.31	129.48	113.40
1	D	556	ASP	CB-CG-OD1	7.15	124.74	118.30
1	D	513	GLY	N-CA-C	6.84	130.21	113.10
1	A	329	GLU	CG-CD-OE2	6.59	131.48	118.30
1	F	556	ASP	OD1-CG-OD2	-6.15	111.62	123.30
1	B	577	LYS	CA-CB-CG	5.80	126.17	113.40
1	A	329	GLU	CG-CD-OE1	-5.78	106.74	118.30
1	D	576	GLU	CB-CG-CD	-5.63	98.99	114.20
1	B	556	ASP	OD1-CG-OD2	-5.55	112.75	123.30
1	B	576	GLU	CB-CG-CD	-5.53	99.28	114.20
1	F	489	GLY	N-CA-C	5.51	126.89	113.10
1	A	357	ASP	CB-CG-OD1	5.48	123.23	118.30
1	F	488	ARG	N-CA-C	-5.25	96.82	111.00
1	F	178	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	487	PRO	N-CA-C	5.22	125.66	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	367	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	E	367	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	F	367	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	314	GLU	CB-CA-C	5.04	120.47	110.40
1	D	556	ASP	OD1-CG-OD2	-5.03	113.74	123.30
1	E	97	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	D	514	THR	N-CA-C	5.02	124.56	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	488	ARG	CA
1	D	514	THR	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	488	ARG	Peptide
1	C	482	GLY	Peptide
1	C	483	ILE	Peptide
1	C	484	PRO	Peptide
1	D	487	PRO	Peptide
1	D	513	GLY	Peptide
1	F	488	ARG	Peptide
1	F	513	GLY	Peptide
1	F	518	ASN	Peptide

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	4710	0	4736	47	4
1	B	4700	0	4713	33	2
1	C	4700	0	4713	37	1
1	D	4700	0	4713	52	0
1	E	4696	0	4702	51	4
1	F	4700	0	4713	58	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	1	0
2	E	31	0	12	1	0
2	F	31	0	12	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	3	0	0	1	2
4	B	3	0	0	0	0
4	C	1	0	0	0	1
4	D	3	0	0	0	2
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	5	0	0	6	0
5	B	5	0	0	1	0
5	C	5	0	0	6	0
5	D	5	0	0	5	0
5	E	5	0	0	7	0
5	F	5	0	0	5	0
6	A	7	0	0	2	0
6	B	5	0	0	4	1
6	C	4	0	0	0	0
6	D	4	0	0	1	0
6	E	9	0	0	3	0
6	F	3	0	0	1	0
All	All	28484	0	28362	262	12

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 (262) 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:303:HIS:ND1	1:F:556:ASP:OD1	1.97	0.95
1:D:556:ASP:OD2	1:F:303:HIS:CE1	2.26	0.89
1:B:552:LYS:HE2	1:B:556:ASP:OD2	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:ASP:OD2	1:F:303:HIS:ND1	2.12	0.82
1:A:415:VAL:HG11	1:D:417:LEU:HD21	1.63	0.81
1:D:303:HIS:ND1	1:F:556:ASP:CG	2.35	0.80
1:D:167:HIS:CE1	5:D:808:SO4:S	2.76	0.79
1:D:167:HIS:CE1	5:D:808:SO4:O4	2.36	0.78
1:C:167:HIS:CE1	5:C:806:SO4:O2	2.37	0.77
1:A:167:HIS:CE1	5:A:808:SO4:O4	2.38	0.76
1:D:73:GLU:OE1	1:F:306:ARG:NH2	2.17	0.76
1:A:308:GLU:OE2	6:A:901:HOH:O	2.03	0.75
1:A:167:HIS:HE1	5:A:808:SO4:S	2.12	0.73
1:B:308:GLU:OE2	6:B:901:HOH:O	2.06	0.73
1:F:466:ARG:NH1	1:F:471:ASP:OD2	2.22	0.73
1:C:194:ASN:ND2	5:C:806:SO4:O1	2.22	0.72
1:B:89:GLU:OE1	6:B:902:HOH:O	2.07	0.72
1:D:534:ILE:O	1:D:538:VAL:HG23	1.89	0.72
1:C:167:HIS:CE1	5:C:806:SO4:S	2.82	0.72
1:E:194:ASN:ND2	5:E:806:SO4:S	2.63	0.71
1:D:484:PRO:HG3	1:D:511:ASP:OD2	1.90	0.71
1:E:167:HIS:CE1	5:E:806:SO4:S	2.83	0.71
1:B:483:ILE:O	1:B:485:PRO:HD3	1.90	0.71
1:F:167:HIS:CE1	5:F:806:SO4:S	2.85	0.70
1:A:194:ASN:ND2	5:A:808:SO4:O3	2.25	0.69
1:E:417:LEU:HD21	1:F:415:VAL:HG11	1.74	0.69
1:D:556:ASP:CG	1:F:303:HIS:ND1	2.46	0.69
1:E:415:VAL:HG11	1:F:417:LEU:HD21	1.73	0.69
1:E:167:HIS:HE1	5:E:806:SO4:O3	1.76	0.69
1:F:534:ILE:O	1:F:538:VAL:HG23	1.93	0.68
1:E:308:GLU:OE2	6:E:902:HOH:O	2.13	0.68
1:E:525:ASP:OD2	6:E:901:HOH:O	2.12	0.68
1:D:194:ASN:ND2	5:D:808:SO4:O1	2.28	0.67
1:E:426:ILE:HG13	1:E:434:THR:HG23	1.75	0.67
1:A:167:HIS:CE1	5:A:808:SO4:S	2.89	0.66
1:E:167:HIS:HE1	5:E:806:SO4:S	2.18	0.66
1:F:167:HIS:CE1	5:F:806:SO4:O3	2.49	0.65
1:D:303:HIS:CE1	1:F:556:ASP:OD2	2.50	0.65
1:B:89:GLU:OE2	6:B:902:HOH:O	2.15	0.65
1:E:194:ASN:ND2	5:E:806:SO4:O3	2.29	0.65
1:A:310:GLU:OE2	4:A:805:MG:MG	1.39	0.64
1:D:246:ALA:HA	1:D:440:ASN:OD1	1.97	0.64
2:F:801:ATP:O3G	6:F:901:HOH:O	2.14	0.64
1:A:585:GLU:OE2	6:A:902:HOH:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:599:GLU:OE2	1:E:602:GLU:OE1	2.18	0.60
1:F:167:HIS:HE1	5:F:806:SO4:S	2.23	0.60
1:C:455:GLY:O	1:C:483:ILE:HG12	2.01	0.59
1:E:194:ASN:ND2	5:E:806:SO4:O1	2.35	0.59
2:D:801:ATP:O3G	6:D:901:HOH:O	2.17	0.59
1:C:127:TYR:CE2	1:C:141:ALA:HB2	2.37	0.59
1:D:466:ARG:NH1	1:D:471:ASP:OD2	2.35	0.59
1:C:534:ILE:O	1:C:538:VAL:HG23	2.02	0.59
1:F:624:GLN:HB3	1:F:625:PRO:HD3	1.85	0.58
1:A:427:GLU:OE1	1:A:460:LYS:HD2	2.04	0.58
1:A:558:ARG:NH1	1:A:605:GLN:O	2.36	0.58
1:B:590:MET:CE	1:B:623:VAL:HG13	2.34	0.58
1:E:562:GLU:HG2	1:E:566:TYR:CE2	2.38	0.58
1:B:252:HIS:ND1	1:B:252:HIS:O	2.37	0.58
1:D:167:HIS:ND1	1:D:194:ASN:HB3	2.19	0.58
1:D:407:GLY:O	1:D:409:GLN:N	2.37	0.58
1:D:303:HIS:CE1	1:F:556:ASP:CG	2.77	0.58
1:E:599:GLU:HG3	6:E:909:HOH:O	2.04	0.58
1:C:167:HIS:HE1	5:C:806:SO4:S	2.26	0.57
1:D:167:HIS:CE1	5:D:808:SO4:O2	2.57	0.57
1:E:55:ASN:HA	1:E:156:THR:HG23	1.86	0.57
1:C:55:ASN:HA	1:C:156:THR:HG23	1.85	0.56
1:E:246:ALA:HA	1:E:440:ASN:OD1	2.05	0.56
1:D:455:GLY:O	1:D:483:ILE:HD12	2.06	0.56
1:A:281:ASP:OD1	1:C:314:GLU:HG2	2.06	0.56
1:F:455:GLY:O	1:F:483:ILE:HD12	2.06	0.56
1:C:221:LEU:HD23	1:C:359:ILE:HG23	1.86	0.56
1:C:190:ILE:HA	1:C:538:VAL:HG22	1.88	0.56
1:B:194:ASN:ND2	5:B:808:SO4:O4	2.40	0.55
1:B:590:MET:HE3	1:B:623:VAL:HG13	1.87	0.55
1:F:55:ASN:HA	1:F:156:THR:HG23	1.89	0.54
1:E:252:HIS:O	1:E:252:HIS:ND1	2.40	0.54
1:A:407:GLY:O	1:A:409:GLN:N	2.40	0.54
1:C:167:HIS:ND1	1:C:194:ASN:HB3	2.23	0.54
1:F:246:ALA:HA	1:F:440:ASN:OD1	2.08	0.54
1:F:27:VAL:HA	1:F:167:HIS:CD2	2.42	0.54
1:A:452:SER:O	1:A:490:VAL:HG13	2.08	0.53
1:A:417:LEU:HD21	1:D:415:VAL:HG11	1.91	0.53
1:A:167:HIS:HE1	5:A:808:SO4:O1	1.92	0.53
1:A:190:ILE:HA	1:A:538:VAL:HG22	1.89	0.53
1:E:291:GLU:HG3	1:E:309:ILE:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:HIS:CE1	5:F:806:SO4:O1	2.62	0.53
1:A:176:PHE:CD2	1:A:180:GLN:HB3	2.45	0.52
1:E:283:ARG:O	1:E:287:LYS:HG3	2.09	0.52
1:D:167:HIS:HE1	5:D:808:SO4:S	2.29	0.52
1:D:426:ILE:HG13	1:D:434:THR:HG23	1.90	0.52
1:F:378:PHE:HD1	1:F:379:PHE:CE1	2.27	0.52
1:C:207:ILE:HD11	1:C:416:LEU:HD21	1.90	0.52
1:C:426:ILE:HG13	1:C:434:THR:HG23	1.91	0.52
1:D:304:GLN:HG3	1:D:323:THR:HG22	1.90	0.52
1:A:599:GLU:CD	1:A:602:GLU:OE1	2.48	0.52
1:A:534:ILE:O	1:A:538:VAL:HG23	2.09	0.52
1:E:304:GLN:HG3	1:E:323:THR:HG22	1.91	0.52
1:F:426:ILE:HG13	1:F:434:THR:HG23	1.92	0.52
1:B:534:ILE:O	1:B:538:VAL:HG23	2.09	0.52
1:F:340:LYS:HB2	1:F:341:PRO:HD3	1.92	0.51
1:C:483:ILE:CG2	1:C:483:ILE:O	2.58	0.51
1:E:27:VAL:HA	1:E:167:HIS:CD2	2.46	0.51
1:F:312:PHE:N	1:F:316:GLU:O	2.42	0.51
1:D:65:TYR:CD2	1:D:93:PHE:HB3	2.46	0.51
1:B:590:MET:SD	1:B:623:VAL:HG22	2.50	0.51
1:D:511:ASP:OD2	1:D:514:THR:HG23	2.11	0.50
1:E:534:ILE:O	1:E:538:VAL:HG23	2.11	0.50
1:E:167:HIS:ND1	1:E:194:ASN:HB3	2.26	0.50
1:C:483:ILE:O	1:C:483:ILE:HG23	2.09	0.50
1:E:220:ILE:HG13	1:E:237:ILE:HD12	1.92	0.50
1:E:407:GLY:O	1:E:409:GLN:N	2.44	0.50
1:E:204:ALA:O	1:E:397:GLY:HA3	2.11	0.50
1:A:624:GLN:HB3	1:A:625:PRO:HD3	1.94	0.50
1:C:27:VAL:HG12	5:C:806:SO4:O2	2.12	0.50
1:A:551:LEU:O	1:A:555:ILE:HG12	2.11	0.50
1:C:224:ASP:HB3	1:C:231:ASP:HB2	1.93	0.50
1:A:252:HIS:ND1	1:A:252:HIS:O	2.45	0.50
1:C:34:ASP:HA	1:C:171:THR:OG1	2.12	0.50
1:A:353:LYS:HD3	1:A:378:PHE:O	2.12	0.50
1:C:410:ASP:OD1	1:C:410:ASP:N	2.45	0.50
1:D:203:THR:OG1	1:D:418:ASP:OD2	2.23	0.49
1:B:483:ILE:HG23	1:B:484:PRO:HD2	1.94	0.49
1:C:204:ALA:O	1:C:397:GLY:HA3	2.12	0.49
1:F:487:PRO:O	1:F:488:ARG:HG3	2.12	0.49
1:D:127:TYR:CE2	1:D:141:ALA:HB2	2.47	0.49
1:F:194:ASN:ND2	5:F:806:SO4:O4	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ASN:HA	1:D:156:THR:HG23	1.95	0.49
1:B:220:ILE:HG13	1:B:237:ILE:HD12	1.94	0.49
1:C:462:TYR:CZ	1:C:469:THR:HG23	2.48	0.49
1:A:435:LYS:O	1:E:488:ARG:HA	2.12	0.49
1:B:167:HIS:ND1	1:B:194:ASN:HB3	2.28	0.48
1:F:167:HIS:ND1	1:F:194:ASN:HB3	2.28	0.48
1:C:122:LYS:HG3	1:C:127:TYR:CD1	2.49	0.48
1:C:220:ILE:HG13	1:C:237:ILE:HD12	1.95	0.48
1:A:25:GLU:HG3	5:A:808:SO4:O2	2.14	0.48
1:C:246:ALA:HA	1:C:440:ASN:OD1	2.14	0.48
1:D:224:ASP:HA	1:D:362:VAL:O	2.14	0.48
1:E:519:LYS:O	1:E:520:ILE:HG12	2.14	0.48
1:E:452:SER:O	1:E:490:VAL:CG1	2.62	0.47
1:E:167:HIS:CE1	5:E:806:SO4:O1	2.66	0.47
1:F:220:ILE:HG13	1:F:237:ILE:HD12	1.96	0.47
1:B:455:GLY:O	1:B:483:ILE:HD12	2.15	0.47
1:B:567:SER:OG	1:B:568:LEU:N	2.47	0.47
1:A:591:GLU:OE1	1:A:595:GLU:OE2	2.32	0.47
1:F:552:LYS:HE2	1:F:556:ASP:OD2	2.15	0.47
1:D:484:PRO:CG	1:D:511:ASP:OD2	2.61	0.47
1:A:483:ILE:HG21	1:A:491:PRO:HG2	1.97	0.47
1:D:224:ASP:HB3	1:D:231:ASP:HB2	1.97	0.47
1:B:452:SER:O	1:B:490:VAL:CG1	2.63	0.47
1:E:425:GLY:HA2	1:E:436:LEU:HB2	1.97	0.47
1:D:224:ASP:OD1	1:D:362:VAL:HG23	2.16	0.46
1:E:74:ARG:HD3	1:E:544:PHE:CE2	2.49	0.46
1:B:426:ILE:HG13	1:B:434:THR:HG23	1.97	0.46
1:B:246:ALA:HA	1:B:440:ASN:OD1	2.16	0.46
1:A:620:GLU:O	1:A:624:GLN:HB2	2.16	0.46
1:C:252:HIS:ND1	1:C:252:HIS:O	2.49	0.46
1:F:122:LYS:HG3	1:F:127:TYR:CD1	2.51	0.46
1:D:303:HIS:CG	1:F:556:ASP:OD1	2.66	0.46
1:E:201:GLU:N	1:E:202:PRO:CD	2.79	0.46
1:E:493:ILE:HD11	1:E:520:ILE:HG13	1.97	0.46
1:A:552:LYS:HE2	1:A:556:ASP:OD2	2.16	0.46
1:D:556:ASP:OD1	1:F:303:HIS:ND1	2.48	0.46
1:A:562:GLU:HG2	1:A:566:TYR:CE2	2.51	0.46
1:B:173:PRO:O	1:B:176:PHE:HB2	2.16	0.46
1:D:402:ALA:O	1:D:406:SER:N	2.47	0.46
1:A:221:LEU:HD23	1:A:359:ILE:HG23	1.98	0.45
1:C:27:VAL:HA	1:C:167:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:PRO:HG3	1:E:488:ARG:NH2	2.31	0.45
1:D:171:THR:HG21	1:D:394:VAL:HG12	1.98	0.45
1:E:34:ASP:HA	1:E:171:THR:OG1	2.16	0.45
1:A:103:TRP:CD2	1:A:121:GLU:HB2	2.50	0.45
1:B:89:GLU:CD	6:B:902:HOH:O	2.43	0.45
1:B:122:LYS:HG3	1:B:127:TYR:CD1	2.52	0.45
1:F:378:PHE:HD1	1:F:379:PHE:CD1	2.33	0.45
1:C:103:TRP:CD1	1:C:121:GLU:OE1	2.69	0.45
1:C:525:ASP:OD1	1:C:525:ASP:N	2.49	0.45
1:F:171:THR:HG21	1:F:394:VAL:HG12	1.98	0.45
1:E:255:GLY:HA3	2:E:801:ATP:O3'	2.17	0.45
1:F:252:HIS:O	1:F:252:HIS:ND1	2.49	0.45
1:B:224:ASP:HB3	1:B:231:ASP:HB2	1.98	0.45
1:D:27:VAL:HA	1:D:167:HIS:CD2	2.52	0.45
1:F:232:VAL:HG11	1:F:342:VAL:HG22	1.99	0.44
1:F:176:PHE:CD2	1:F:180:GLN:HB3	2.52	0.44
1:F:552:LYS:CE	1:F:556:ASP:OD2	2.64	0.44
1:B:27:VAL:HA	1:B:167:HIS:CD2	2.52	0.44
1:D:121:GLU:HA	1:D:125:LYS:O	2.17	0.44
1:D:494:GLU:HB2	1:D:512:LYS:HE3	1.98	0.44
1:F:378:PHE:CD1	1:F:379:PHE:CE1	3.05	0.44
1:A:515:GLY:O	1:A:516:ASN:HB2	2.18	0.44
1:D:590:MET:SD	1:D:623:VAL:HG22	2.58	0.44
1:F:484:PRO:HG3	1:F:511:ASP:CG	2.38	0.44
1:A:55:ASN:HA	1:A:156:THR:HG23	2.00	0.44
1:F:483:ILE:HA	1:F:484:PRO:HD3	1.80	0.43
1:F:513:GLY:C	1:F:514:THR:HG23	2.38	0.43
1:C:477:THR:HB	1:C:525:ASP:HB2	2.01	0.43
1:E:127:TYR:CE2	1:E:141:ALA:HB2	2.53	0.43
1:F:34:ASP:HA	1:F:171:THR:OG1	2.18	0.43
1:D:484:PRO:HA	1:D:485:PRO:HD3	1.71	0.43
1:F:189:THR:O	1:F:192:GLY:N	2.50	0.43
1:F:425:GLY:HA2	1:F:436:LEU:HB2	2.00	0.43
1:A:220:ILE:HG13	1:A:237:ILE:HD12	2.01	0.43
1:C:241:VAL:HG22	1:C:415:VAL:CG2	2.49	0.43
1:D:452:SER:O	1:D:490:VAL:CG1	2.67	0.43
1:E:483:ILE:HG23	1:E:484:PRO:HD2	2.01	0.43
1:D:220:ILE:HG13	1:D:237:ILE:HD12	1.99	0.43
1:B:562:GLU:HG2	1:B:566:TYR:CE2	2.55	0.42
1:D:230:PHE:CZ	1:D:338:THR:HB	2.54	0.42
1:E:207:ILE:HD11	1:E:416:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:HG21	1:A:394:VAL:HG12	1.99	0.42
1:D:122:LYS:HG3	1:D:127:TYR:CD1	2.54	0.42
1:D:562:GLU:HG2	1:D:566:TYR:CE2	2.54	0.42
1:B:105:ASP:HB3	1:B:108:VAL:HG23	2.01	0.42
1:B:340:LYS:HB2	1:B:341:PRO:HD3	2.01	0.42
1:A:122:LYS:HG3	1:A:127:TYR:CD1	2.55	0.42
1:D:223:PHE:HB3	1:D:361:LEU:HD23	2.01	0.42
1:A:293:GLU:O	1:A:297:ARG:HG3	2.20	0.42
1:A:599:GLU:OE1	1:A:602:GLU:OE1	2.38	0.42
1:D:483:ILE:HG23	1:D:484:PRO:HD2	2.00	0.42
1:B:572:ILE:HD11	1:B:590:MET:HG3	2.01	0.42
1:E:221:LEU:HD23	1:E:359:ILE:HG23	2.02	0.42
1:E:252:HIS:O	1:E:252:HIS:CG	2.72	0.42
1:F:524:ASN:O	1:F:526:GLN:N	2.53	0.42
1:D:252:HIS:O	1:D:252:HIS:ND1	2.53	0.41
1:B:283:ARG:O	1:B:287:LYS:HG3	2.20	0.41
1:C:320:GLU:OE1	1:C:320:GLU:HA	2.20	0.41
1:F:83:GLN:OE1	1:F:91:THR:OG1	2.38	0.41
1:A:367:ARG:NH2	1:A:391:ASP:OD2	2.41	0.41
1:E:318:PHE:C	1:E:318:PHE:CD1	2.93	0.41
1:F:224:ASP:HB3	1:F:231:ASP:HB2	2.01	0.41
1:F:271:LYS:O	1:F:275:GLY:N	2.46	0.41
1:E:520:ILE:HA	1:E:520:ILE:HD13	1.97	0.41
1:B:204:ALA:O	1:B:397:GLY:HA3	2.21	0.41
1:C:562:GLU:CG	1:C:601:LEU:HD13	2.50	0.41
1:E:572:ILE:HD11	1:E:590:MET:HG3	2.02	0.41
1:F:127:TYR:CE2	1:F:141:ALA:HB2	2.56	0.41
1:F:248:ASN:OD1	1:F:341:PRO:HB3	2.20	0.41
1:B:600:TRP:CE2	1:B:615:LYS:HE3	2.56	0.41
1:A:423:THR:CG2	1:A:435:LYS:HG3	2.50	0.41
1:E:87:ASN:N	1:E:88:PRO:CD	2.84	0.41
1:F:356:ILE:HG13	1:F:379:PHE:HE2	1.85	0.41
1:A:65:TYR:CE2	1:A:93:PHE:HB3	2.56	0.40
1:C:562:GLU:HG3	1:C:601:LEU:HD13	2.03	0.40
1:D:462:TYR:CZ	1:D:469:THR:HG23	2.55	0.40
1:D:556:ASP:CG	1:F:303:HIS:HD1	2.24	0.40
1:F:190:ILE:HA	1:F:538:VAL:HG22	2.03	0.40
1:F:509:ALA:O	1:F:520:ILE:HG12	2.21	0.40
1:A:167:HIS:ND1	1:A:194:ASN:HB3	2.36	0.40
1:A:94:ASP:OD2	1:A:256:GLU:OE1	2.39	0.40
1:A:477:THR:HB	1:A:525:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:LYS:HB2	1:C:273:LYS:HE3	1.97	0.40
1:E:171:THR:HG21	1:E:394:VAL:HG12	2.03	0.40
1:F:353:LYS:HD3	1:F:378:PHE:O	2.20	0.40
1:A:428:THR:CG2	1:A:434:THR:HG21	2.51	0.40
1:B:252:HIS:O	1:B:252:HIS:CG	2.74	0.40
1:C:50:VAL:HB	1:C:396:TYR:CE2	2.57	0.40
1:F:590:MET:CE	1:F:627:ILE:HG23	2.52	0.40
1:B:624:GLN:HB3	1:B:625:PRO:HD3	2.03	0.40
1:C:167:HIS:HE1	5:C:806:SO4:O4	2.04	0.40
1:E:224:ASP:HB3	1:E:231:ASP:HB2	2.02	0.40
1:E:190:ILE:HA	1:E:538:VAL:HG22	2.04	0.40
1:E:568:LEU:HD13	1:E:623:VAL:HG21	2.04	0.40
1:E:590:MET:CE	1:E:623:VAL:HG13	2.51	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ASP:OD2	4:D:804:MG:MG[6_654]	1.44	0.76
4:A:803:MG:MG	4:C:803:MG:MG[2_554]	1.48	0.72
1:C:317:ASP:OD2	4:A:804:MG:MG[6_554]	1.50	0.70
1:A:303:HIS:ND1	1:A:556:ASP:OD1[6_554]	1.54	0.66
1:A:595:GLU:OE2	1:A:595:GLU:OE2[5_554]	1.62	0.58
1:E:310:GLU:OE2	4:D:804:MG:MG[6_654]	1.68	0.52
1:A:329:GLU:OE2	1:A:588:GLU:OE2[3_555]	1.73	0.47
1:A:303:HIS:CE1	1:A:556:ASP:OD1[6_554]	1.75	0.45
1:B:303:HIS:ND1	1:E:556:ASP:OD1[2_654]	1.83	0.37
1:F:329:GLU:OE2	1:F:588:GLU:OE2[2_664]	2.01	0.19
1:E:71:GLU:OE2	6:B:901:HOH:O[3_665]	2.07	0.13
1:B:329:GLU:OE2	1:B:588:GLU:OE2[3_665]	2.16	0.04

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	604/606 (100%)	566 (94%)	29 (5%)	9 (2%)	12	48
1	B	604/606 (100%)	569 (94%)	32 (5%)	3 (0%)	32	74
1	C	604/606 (100%)	562 (93%)	36 (6%)	6 (1%)	18	59
1	D	604/606 (100%)	561 (93%)	34 (6%)	9 (2%)	12	48
1	E	604/606 (100%)	560 (93%)	38 (6%)	6 (1%)	18	59
1	F	604/606 (100%)	564 (93%)	32 (5%)	8 (1%)	14	51
All	All	3624/3636 (100%)	3382 (93%)	201 (6%)	41 (1%)	17	56

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	ASP
1	A	516	ASN
1	C	483	ILE
1	C	517	LYS
1	D	408	ASP
1	D	488	ARG
1	E	488	ARG
1	F	488	ARG
1	A	429	VAL
1	B	429	VAL
1	D	516	ASN
1	E	408	ASP
1	F	429	VAL
1	F	514	THR
1	F	525	ASP
1	A	440	ASN
1	A	487	PRO
1	A	518	ASN
1	A	525	ASP
1	B	485	PRO
1	B	525	ASP
1	C	440	ASN
1	C	516	ASN
1	D	429	VAL
1	D	518	ASN
1	E	429	VAL
1	E	525	ASP
1	F	71	GLU

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Mol	Chain	Res	Type
1	F	490	VAL
1	A	490	VAL
1	C	429	VAL
1	D	490	VAL
1	D	525	ASP
1	C	487	PRO
1	F	483	ILE
1	E	314	GLU
1	E	87	ASN
1	F	484	PRO
1	D	489	GLY
1	A	421	PRO
1	D	513	GLY

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	515/518 (99%)	498 (97%)	17 (3%)	43	79
1	B	511/518 (99%)	495 (97%)	16 (3%)	45	80
1	C	511/518 (99%)	490 (96%)	21 (4%)	35	73
1	D	511/518 (99%)	494 (97%)	17 (3%)	43	79
1	E	510/518 (98%)	495 (97%)	15 (3%)	48	82
1	F	511/518 (99%)	495 (97%)	16 (3%)	45	80
All	All	3069/3108 (99%)	2967 (97%)	102 (3%)	43	79

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	66	VAL
1	A	118	LYS
1	A	131	ASP
1	A	176	PHE

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Mol	Chain	Res	Type
1	A	236	THR
1	A	303	HIS
1	A	383	GLU
1	A	413	ASP
1	A	469	THR
1	A	471	ASP
1	A	544	PHE
1	A	552	LYS
1	A	577	LYS
1	A	584	SER
1	A	610	GLU
1	A	617	LYS
1	B	46	LYS
1	B	66	VAL
1	B	83	GLN
1	B	118	LYS
1	B	131	ASP
1	B	176	PHE
1	B	236	THR
1	B	469	THR
1	B	471	ASP
1	B	491	PRO
1	B	544	PHE
1	B	552	LYS
1	B	567	SER
1	B	577	LYS
1	B	590	MET
1	B	617	LYS
1	C	26	ASP
1	C	46	LYS
1	C	66	VAL
1	C	118	LYS
1	C	131	ASP
1	C	175	TYR
1	C	176	PHE
1	C	236	THR
1	C	345	VAL
1	C	349	SER
1	C	410	ASP
1	C	434	THR
1	C	469	THR
1	C	471	ASP

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Mol	Chain	Res	Type
1	C	483	ILE
1	C	525	ASP
1	C	528	ARG
1	C	552	LYS
1	C	577	LYS
1	C	610	GLU
1	C	617	LYS
1	D	46	LYS
1	D	66	VAL
1	D	118	LYS
1	D	146	SER
1	D	175	TYR
1	D	176	PHE
1	D	236	THR
1	D	434	THR
1	D	469	THR
1	D	471	ASP
1	D	514	THR
1	D	528	ARG
1	D	544	PHE
1	D	552	LYS
1	D	567	SER
1	D	584	SER
1	D	617	LYS
1	E	66	VAL
1	E	118	LYS
1	E	175	TYR
1	E	176	PHE
1	E	236	THR
1	E	349	SER
1	E	383	GLU
1	E	434	THR
1	E	469	THR
1	E	471	ASP
1	E	552	LYS
1	E	567	SER
1	E	577	LYS
1	E	590	MET
1	E	617	LYS
1	F	46	LYS
1	F	83	GLN
1	F	118	LYS

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Mol	Chain	Res	Type
1	F	176	PHE
1	F	236	THR
1	F	247	THR
1	F	357	ASP
1	F	413	ASP
1	F	434	THR
1	F	469	THR
1	F	471	ASP
1	F	544	PHE
1	F	552	LYS
1	F	567	SER
1	F	590	MET
1	F	617	LYS

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	167	HIS
1	A	194	ASN
1	B	167	HIS
1	B	194	ASN
1	C	167	HIS
1	C	194	ASN
1	D	167	HIS
1	E	167	HIS
1	E	492	GLN
1	F	167	HIS
1	F	194	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 42 ligands modelled in this entry, 30 are monoatomic - leaving 12 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	ATP	A	801	3	27,33,33	0.92	1 (3%)	25,52,52	2.05	6 (24%)
5	SO4	A	808	-	4,4,4	0.48	0	6,6,6	0.37	0
2	ATP	B	801	3	27,33,33	0.89	1 (3%)	25,52,52	1.90	5 (20%)
5	SO4	B	808	-	4,4,4	0.48	0	6,6,6	0.41	0
2	ATP	C	801	3	27,33,33	0.87	1 (3%)	25,52,52	2.12	5 (20%)
5	SO4	C	806	-	4,4,4	0.37	0	6,6,6	0.35	0
2	ATP	D	801	3	27,33,33	0.82	1 (3%)	25,52,52	1.87	4 (16%)
5	SO4	D	808	-	4,4,4	0.46	0	6,6,6	0.26	0
2	ATP	E	801	3	27,33,33	1.05	1 (3%)	25,52,52	1.81	4 (16%)
5	SO4	E	806	-	4,4,4	0.45	0	6,6,6	0.54	0
2	ATP	F	801	3	27,33,33	1.18	2 (7%)	25,52,52	1.77	5 (20%)
5	SO4	F	806	-	4,4,4	0.42	0	6,6,6	0.34	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	ATP	A	801	3	-	0/18/38/38	0/3/3/3
5	SO4	A	808	-	-	0/0/0/0	0/0/0/0
2	ATP	B	801	3	-	0/18/38/38	0/3/3/3
5	SO4	B	808	-	-	0/0/0/0	0/0/0/0
2	ATP	C	801	3	-	0/18/38/38	0/3/3/3
5	SO4	C	806	-	-	0/0/0/0	0/0/0/0
2	ATP	D	801	3	-	0/18/38/38	0/3/3/3
5	SO4	D	808	-	-	0/0/0/0	0/0/0/0
2	ATP	E	801	3	-	0/18/38/38	0/3/3/3
5	SO4	E	806	-	-	0/0/0/0	0/0/0/0
2	ATP	F	801	3	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	F	806	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	ATP	PG-O3B	2.21	1.63	1.60
2	D	801	ATP	C5-C4	2.46	1.46	1.40
2	B	801	ATP	C5-C4	2.47	1.46	1.40
2	A	801	ATP	C5-C4	2.47	1.46	1.40
2	C	801	ATP	C5-C4	2.51	1.46	1.40
2	E	801	ATP	C5-C4	2.83	1.46	1.40
2	F	801	ATP	C5-C4	3.42	1.48	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	ATP	N3-C2-N1	-8.40	121.54	128.86
2	B	801	ATP	N3-C2-N1	-7.00	122.77	128.86
2	F	801	ATP	N3-C2-N1	-6.62	123.09	128.86
2	D	801	ATP	N3-C2-N1	-6.49	123.20	128.86
2	A	801	ATP	N3-C2-N1	-6.42	123.27	128.86
2	E	801	ATP	N3-C2-N1	-5.33	124.22	128.86
2	E	801	ATP	C4'-O4'-C1'	-4.39	105.10	109.77
2	A	801	ATP	C4-C5-N7	-3.14	106.38	109.41
2	C	801	ATP	C1'-N9-C4	-3.13	121.23	126.64
2	E	801	ATP	C1'-N9-C4	-2.94	121.56	126.64
2	B	801	ATP	C1'-N9-C4	-2.90	121.63	126.64
2	A	801	ATP	C1'-N9-C4	-2.82	121.76	126.64
2	B	801	ATP	C4'-O4'-C1'	-2.79	106.80	109.77
2	A	801	ATP	C4'-O4'-C1'	-2.60	107.00	109.77
2	C	801	ATP	C4-C5-N7	-2.39	107.11	109.41
2	D	801	ATP	O4'-C4'-C5'	-2.25	101.81	109.40
2	F	801	ATP	C1'-N9-C4	-2.20	122.83	126.64
2	F	801	ATP	O3G-PG-O2G	2.04	115.83	107.61
2	B	801	ATP	N6-C6-N1	2.09	122.90	118.77
2	B	801	ATP	O3G-PG-O2G	2.12	116.18	107.61
2	E	801	ATP	C2-N1-C6	2.15	122.53	118.77
2	F	801	ATP	C2-N1-C6	2.16	122.56	118.77
2	F	801	ATP	N6-C6-N1	2.17	123.07	118.77
2	C	801	ATP	O3G-PG-O2G	2.24	116.66	107.61
2	A	801	ATP	C2'-C3'-C4'	2.34	107.17	102.62
2	C	801	ATP	C2-N1-C6	2.46	123.08	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	801	ATP	C2-N1-C6	2.47	123.09	118.77
2	D	801	ATP	N6-C6-N1	3.30	125.30	118.77
2	A	801	ATP	O3G-PG-O2G	3.50	121.74	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	808	SO4	6	0
5	B	808	SO4	1	0
5	C	806	SO4	6	0
2	D	801	ATP	1	0
5	D	808	SO4	5	0
2	E	801	ATP	1	0
5	E	806	SO4	7	0
2	F	801	ATP	1	0
5	F	806	SO4	5	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	606/606 (100%)	0.46	25 (4%)	38	15	30, 56, 111, 166	2 (0%)
1	B	606/606 (100%)	0.55	40 (6%)	19	7	47, 79, 144, 221	2 (0%)
1	C	606/606 (100%)	0.61	43 (7%)	17	6	45, 74, 148, 197	2 (0%)
1	D	606/606 (100%)	0.42	22 (3%)	43	18	40, 70, 131, 201	2 (0%)
1	E	606/606 (100%)	0.47	32 (5%)	27	11	48, 77, 131, 177	2 (0%)
1	F	606/606 (100%)	0.48	29 (4%)	31	12	47, 76, 129, 183	2 (0%)
All	All	3636/3636 (100%)	0.50	191 (5%)	27	11	30, 72, 134, 221	12 (0%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	484	PRO	12.1
1	D	516	ASN	10.5
1	C	487	PRO	10.4
1	D	517	LYS	9.3
1	A	516	ASN	9.0
1	C	516	ASN	8.8
1	D	514	THR	8.7
1	B	24	SER	8.0
1	D	573	GLY	8.0
1	A	515	GLY	7.8
1	C	517	LYS	7.8
1	B	483	ILE	7.7
1	C	488	ARG	7.6
1	C	24	SER	7.3
1	D	515	GLY	7.3
1	B	516	ASN	6.8
1	C	484	PRO	6.7
1	A	386	ARG	6.6
1	E	516	ASN	6.4

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Mol	Chain	Res	Type	RSRZ
1	F	518	ASN	6.4
1	A	517	LYS	6.3
1	B	487	PRO	6.2
1	B	515	GLY	6.1
1	F	24	SER	6.0
1	C	572	ILE	5.9
1	F	408	ASP	5.9
1	D	487	PRO	5.7
1	F	516	ASN	5.6
1	C	584	SER	5.5
1	D	518	ASN	5.5
1	F	514	THR	5.4
1	B	488	ARG	5.2
1	B	582	LEU	5.2
1	B	520	ILE	5.2
1	B	514	THR	5.1
1	C	486	ALA	5.0
1	B	386	ARG	5.0
1	F	517	LYS	4.9
1	E	453	VAL	4.8
1	B	485	PRO	4.8
1	F	572	ILE	4.6
1	E	386	ARG	4.5
1	C	520	ILE	4.4
1	C	513	GLY	4.4
1	E	488	ARG	4.4
1	C	515	GLY	4.4
1	C	512	LYS	4.4
1	B	482	GLY	4.3
1	A	24	SER	4.3
1	F	515	GLY	4.2
1	C	587	LYS	4.2
1	E	582	LEU	4.0
1	A	520	ILE	3.9
1	D	488	ARG	3.9
1	E	408	ASP	3.8
1	B	513	GLY	3.8
1	E	493	ILE	3.7
1	E	518	ASN	3.7
1	B	576	GLU	3.7
1	B	521	THR	3.7
1	B	486	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	514	THR	3.5
1	C	493	ILE	3.5
1	A	484	PRO	3.5
1	B	590	MET	3.5
1	B	522	ILE	3.5
1	C	386	ARG	3.5
1	E	134	GLY	3.4
1	B	569	LYS	3.4
1	C	582	LEU	3.4
1	F	487	PRO	3.4
1	B	459	ILE	3.4
1	E	589	THR	3.4
1	A	486	ALA	3.3
1	F	484	PRO	3.3
1	C	481	THR	3.3
1	F	522	ILE	3.3
1	F	134	GLY	3.3
1	B	481	THR	3.2
1	C	527	ASN	3.2
1	B	519	LYS	3.2
1	A	519	LYS	3.2
1	B	408	ASP	3.2
1	C	521	THR	3.2
1	F	513	GLY	3.2
1	D	592	LYS	3.2
1	B	517	LYS	3.1
1	E	629	LYS	3.1
1	E	481	THR	3.1
1	E	570	ASN	3.1
1	B	492	GLN	3.1
1	A	488	ARG	3.1
1	D	24	SER	3.1
1	D	574	ASP	3.0
1	D	484	PRO	3.0
1	A	518	ASN	3.0
1	C	485	PRO	2.9
1	F	629	LYS	2.9
1	E	585	GLU	2.9
1	E	515	GLY	2.9
1	B	509	ALA	2.9
1	B	205	ALA	2.8
1	B	455	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	436	LEU	2.8
1	B	518	ASN	2.8
1	C	623	VAL	2.8
1	A	483	ILE	2.8
1	C	136	GLN	2.8
1	E	514	THR	2.7
1	A	387	GLY	2.7
1	C	578	LEU	2.7
1	E	628	SER	2.7
1	F	452	SER	2.7
1	C	511	ASP	2.7
1	E	572	ILE	2.6
1	E	526	GLN	2.6
1	C	564	TYR	2.6
1	F	453	VAL	2.6
1	C	586	ASP	2.6
1	D	619	LEU	2.5
1	C	622	ILE	2.5
1	D	519	LYS	2.5
1	C	489	GLY	2.5
1	C	580	GLY	2.5
1	E	592	LYS	2.5
1	E	497	PHE	2.5
1	D	386	ARG	2.5
1	F	519	LYS	2.5
1	A	25	GLU	2.4
1	A	485	PRO	2.4
1	E	487	PRO	2.4
1	E	593	ALA	2.4
1	D	588	GLU	2.4
1	C	492	GLN	2.4
1	E	276	LYS	2.4
1	A	511	ASP	2.4
1	E	580	GLY	2.4
1	B	209	TYR	2.4
1	C	568	LEU	2.4
1	B	512	LYS	2.4
1	E	213	LYS	2.4
1	D	627	ILE	2.4
1	D	485	PRO	2.3
1	E	468	LEU	2.3
1	C	588	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	572	ILE	2.3
1	C	455	GLY	2.3
1	F	488	ARG	2.3
1	F	573	GLY	2.3
1	E	527	ASN	2.3
1	B	527	ASN	2.3
1	A	487	PRO	2.3
1	C	626	ILE	2.3
1	C	451	PHE	2.3
1	C	453	VAL	2.3
1	F	477	THR	2.2
1	A	453	VAL	2.2
1	F	512	LYS	2.2
1	B	490	VAL	2.2
1	D	478	PHE	2.2
1	F	493	ILE	2.2
1	A	521	THR	2.2
1	B	601	LEU	2.2
1	C	602	GLU	2.2
1	A	265	HIS	2.2
1	B	480	LEU	2.2
1	E	520	ILE	2.2
1	A	408	ASP	2.2
1	C	480	LEU	2.2
1	B	528	ARG	2.2
1	F	588	GLU	2.2
1	A	489	GLY	2.1
1	E	513	GLY	2.1
1	E	451	PHE	2.1
1	F	483	ILE	2.1
1	C	450	ILE	2.1
1	E	280	LYS	2.1
1	C	570	ASN	2.1
1	B	457	VAL	2.1
1	C	525	ASP	2.1
1	B	114	PHE	2.1
1	F	523	THR	2.1
1	F	578	LEU	2.1
1	D	589	THR	2.1
1	F	280	LYS	2.1
1	C	518	ASN	2.1
1	A	228	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	135	GLY	2.0
1	F	422	LEU	2.0
1	A	493	ILE	2.0
1	D	582	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	805	1/1	0.99	0.25	3.12	38,38,38,38	0
3	ZN	B	802	1/1	0.96	0.24	1.84	68,68,68,68	0
3	ZN	F	802	1/1	0.85	0.25	1.08	71,71,71,71	0
3	ZN	B	803	1/1	0.98	0.21	0.81	87,87,87,87	0
2	ATP	D	801	31/31	0.98	0.22	0.67	42,48,59,61	0
3	ZN	C	802	1/1	0.97	0.21	0.63	68,68,68,68	0
2	ATP	B	801	31/31	0.97	0.21	0.35	47,54,61,65	0
2	ATP	F	801	31/31	0.97	0.21	0.34	43,53,61,66	0
2	ATP	A	801	31/31	0.97	0.23	0.34	35,42,51,57	0
2	ATP	C	801	31/31	0.97	0.21	-0.05	46,52,58,63	0
2	ATP	E	801	31/31	0.97	0.19	-0.39	45,52,59,62	0
5	SO4	D	808	5/5	0.90	0.17	-0.55	88,102,103,112	0
3	ZN	A	806	1/1	0.97	0.20	-0.93	65,65,65,65	0
5	SO4	F	806	5/5	0.96	0.16	-1.08	84,85,95,96	0
3	ZN	E	803	1/1	0.99	0.16	-1.12	65,65,65,65	0
3	ZN	C	804	1/1	0.99	0.19	-2.63	73,73,73,73	0
5	SO4	B	808	5/5	0.88	0.19	-	93,100,108,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	A	804	1/1	0.91	0.27	-	41,41,41,41	0
3	ZN	D	806	1/1	0.98	0.18	-	74,74,74,74	0
4	MG	C	803	1/1	0.99	0.21	-	23,23,23,23	0
4	MG	E	802	1/1	0.83	0.28	-	67,67,67,67	0
4	MG	D	804	1/1	0.97	0.23	-	36,36,36,36	0
3	ZN	A	807	1/1	0.95	0.26	-	78,78,78,78	0
3	ZN	D	807	1/1	0.92	0.23	-	99,99,99,99	0
3	ZN	E	805	1/1	0.89	0.22	-	107,107,107,107	0
3	ZN	F	805	1/1	0.92	0.22	-	103,103,103,103	0
4	MG	B	804	1/1	0.81	0.22	-	58,58,58,58	0
4	MG	D	805	1/1	0.97	0.23	-	43,43,43,43	0
4	MG	A	803	1/1	0.99	0.21	-	54,54,54,54	0
5	SO4	E	806	5/5	0.94	0.17	-	74,92,94,98	0
3	ZN	D	802	1/1	0.96	0.23	-	71,71,71,71	0
4	MG	D	803	1/1	0.93	0.31	-	56,56,56,56	0
5	SO4	A	808	5/5	0.91	0.22	-	78,80,86,89	0
3	ZN	F	804	1/1	0.96	0.23	-	84,84,84,84	0
4	MG	B	805	1/1	0.78	0.22	-	96,96,96,96	0
4	MG	F	803	1/1	0.98	0.25	-	55,55,55,55	0
3	ZN	C	805	1/1	0.95	0.24	-	81,81,81,81	0
3	ZN	E	804	1/1	0.94	0.19	-	84,84,84,84	0
4	MG	B	806	1/1	0.88	0.12	-	87,87,87,87	0
5	SO4	C	806	5/5	0.92	0.17	-	84,86,95,111	0
3	ZN	A	802	1/1	0.96	0.28	-	65,65,65,65	0
3	ZN	B	807	1/1	0.95	0.20	-	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.