



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:57 PM UTC

PDB ID : 3VGK / pdb_00003vgk
Title : Crystal structure of a ROK family glucokinase from *Streptomyces griseus*
Authors : Miyazono, K.; Tabei, N.; Morita, S.; Ohnishi, Y.; Horinouchi, S.; Tanokura, M.
Deposited on : 2011-08-15
Resolution : 3.25 Å(reported)

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

We welcome your comments at 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

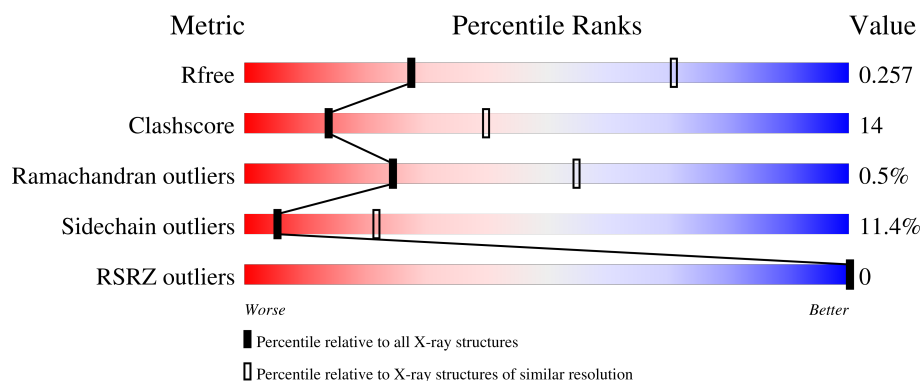
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	321	 69% 26% . .
1	B	321	 69% 26% . .
1	C	321	 69% 24% . .
1	D	321	 62% 31% . .
1	E	321	 66% 26% 5% .

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Mol	Chain	Length	Quality of chain
1	F	321	68%27%
1	G	321	60%32%
1	H	321	60%31%5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18142 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 Glucokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2267	1420	414	428	5			
1	B	312	Total	C	N	O	S	0	0	0
			2271	1422	415	429	5			
1	C	310	Total	C	N	O	S	0	0	0
			2263	1418	413	427	5			
1	D	311	Total	C	N	O	S	0	0	0
			2267	1420	414	428	5			
1	E	310	Total	C	N	O	S	0	0	0
			2263	1418	413	427	5			
1	F	310	Total	C	N	O	S	0	0	0
			2263	1418	413	427	5			
1	G	311	Total	C	N	O	S	0	0	0
			2267	1420	414	428	5			
1	H	310	Total	C	N	O	S	0	0	0
			2263	1418	413	427	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	LEU	-	expression tag	UNP B1VZT1
A	315	GLU	-	expression tag	UNP B1VZT1
A	316	HIS	-	expression tag	UNP B1VZT1
A	317	HIS	-	expression tag	UNP B1VZT1
A	318	HIS	-	expression tag	UNP B1VZT1
A	319	HIS	-	expression tag	UNP B1VZT1
A	320	HIS	-	expression tag	UNP B1VZT1
A	321	HIS	-	expression tag	UNP B1VZT1
B	314	LEU	-	expression tag	UNP B1VZT1
B	315	GLU	-	expression tag	UNP B1VZT1
B	316	HIS	-	expression tag	UNP B1VZT1
B	317	HIS	-	expression tag	UNP B1VZT1
B	318	HIS	-	expression tag	UNP B1VZT1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	319	HIS	-	expression tag	UNP B1VZT1
B	320	HIS	-	expression tag	UNP B1VZT1
B	321	HIS	-	expression tag	UNP B1VZT1
C	314	LEU	-	expression tag	UNP B1VZT1
C	315	GLU	-	expression tag	UNP B1VZT1
C	316	HIS	-	expression tag	UNP B1VZT1
C	317	HIS	-	expression tag	UNP B1VZT1
C	318	HIS	-	expression tag	UNP B1VZT1
C	319	HIS	-	expression tag	UNP B1VZT1
C	320	HIS	-	expression tag	UNP B1VZT1
C	321	HIS	-	expression tag	UNP B1VZT1
D	314	LEU	-	expression tag	UNP B1VZT1
D	315	GLU	-	expression tag	UNP B1VZT1
D	316	HIS	-	expression tag	UNP B1VZT1
D	317	HIS	-	expression tag	UNP B1VZT1
D	318	HIS	-	expression tag	UNP B1VZT1
D	319	HIS	-	expression tag	UNP B1VZT1
D	320	HIS	-	expression tag	UNP B1VZT1
D	321	HIS	-	expression tag	UNP B1VZT1
E	314	LEU	-	expression tag	UNP B1VZT1
E	315	GLU	-	expression tag	UNP B1VZT1
E	316	HIS	-	expression tag	UNP B1VZT1
E	317	HIS	-	expression tag	UNP B1VZT1
E	318	HIS	-	expression tag	UNP B1VZT1
E	319	HIS	-	expression tag	UNP B1VZT1
E	320	HIS	-	expression tag	UNP B1VZT1
E	321	HIS	-	expression tag	UNP B1VZT1
F	314	LEU	-	expression tag	UNP B1VZT1
F	315	GLU	-	expression tag	UNP B1VZT1
F	316	HIS	-	expression tag	UNP B1VZT1
F	317	HIS	-	expression tag	UNP B1VZT1
F	318	HIS	-	expression tag	UNP B1VZT1
F	319	HIS	-	expression tag	UNP B1VZT1
F	320	HIS	-	expression tag	UNP B1VZT1
F	321	HIS	-	expression tag	UNP B1VZT1
G	314	LEU	-	expression tag	UNP B1VZT1
G	315	GLU	-	expression tag	UNP B1VZT1
G	316	HIS	-	expression tag	UNP B1VZT1
G	317	HIS	-	expression tag	UNP B1VZT1
G	318	HIS	-	expression tag	UNP B1VZT1
G	319	HIS	-	expression tag	UNP B1VZT1
G	320	HIS	-	expression tag	UNP B1VZT1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	321	HIS	-	expression tag	UNP B1VZT1
H	314	LEU	-	expression tag	UNP B1VZT1
H	315	GLU	-	expression tag	UNP B1VZT1
H	316	HIS	-	expression tag	UNP B1VZT1
H	317	HIS	-	expression tag	UNP B1VZT1
H	318	HIS	-	expression tag	UNP B1VZT1
H	319	HIS	-	expression tag	UNP B1VZT1
H	320	HIS	-	expression tag	UNP B1VZT1
H	321	HIS	-	expression tag	UNP B1VZT1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

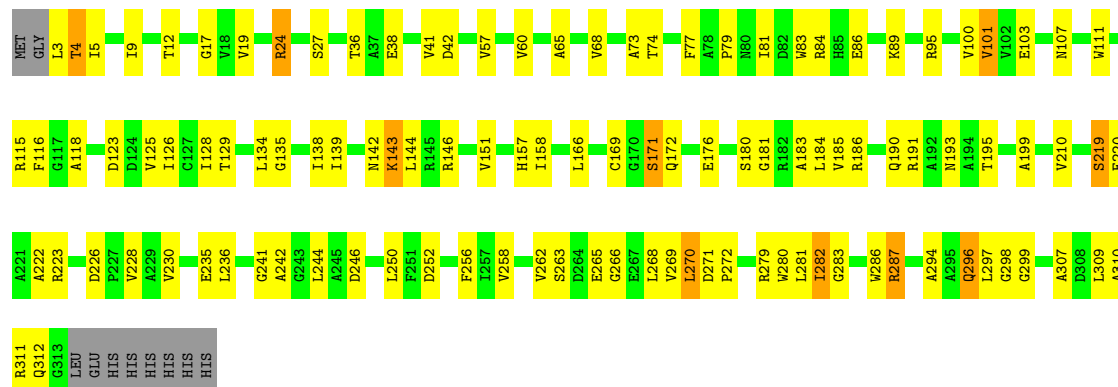
- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

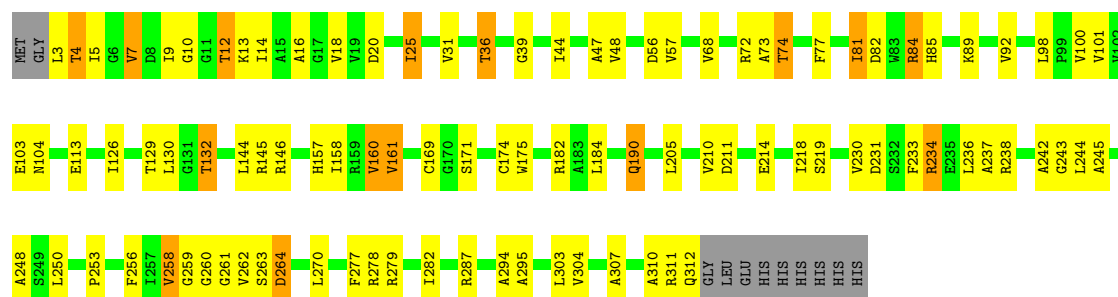
- Molecule 1: Glucokinase

Chain D:  62% 31%



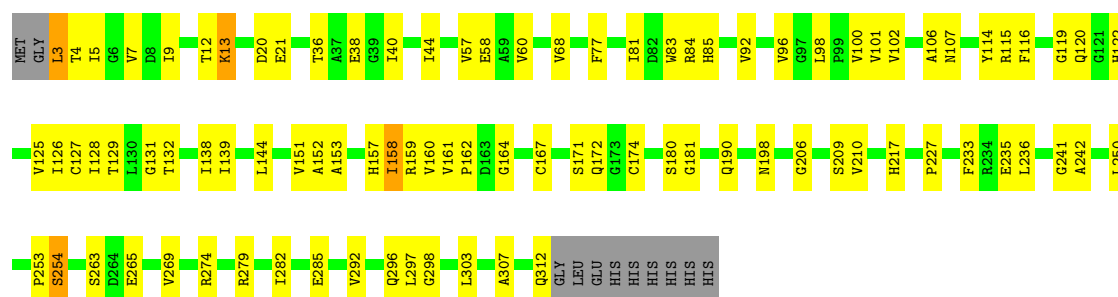
- Molecule 1: Glucokinase

Chain E:  66% 26% 5%



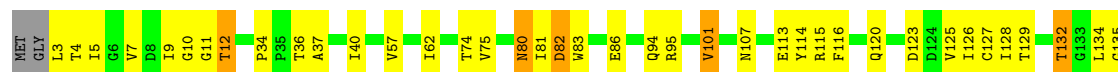
- Molecule 1: Glucokinase

Chain F:  68% 27%



- Molecule 1: Glucokinase

Chain G:  60% 32%





● Molecule 1: Glucokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.69Å 173.70Å 124.03Å 90.00° 106.69° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 20.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-3.25) 96.4 (20.00-3.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.22Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0109	Depositor
R, R_{free}	0.206 , 0.264 0.205 , 0.257	Depositor DCC
R_{free} test set	6121 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18142	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8729e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.90	1/2308 (0.0%)	0.99	2/3129 (0.1%)
1	B	0.89	1/2312 (0.0%)	0.96	1/3134 (0.0%)
1	C	0.86	2/2304 (0.1%)	0.97	3/3124 (0.1%)
1	D	0.92	1/2308 (0.0%)	1.02	4/3129 (0.1%)
1	E	0.91	2/2304 (0.1%)	1.04	5/3124 (0.2%)
1	F	0.88	0/2304	1.00	5/3124 (0.2%)
1	G	0.90	1/2308 (0.0%)	1.04	7/3129 (0.2%)
1	H	0.86	2/2304 (0.1%)	1.02	8/3124 (0.3%)
All	All	0.89	10/18452 (0.1%)	1.01	35/25017 (0.1%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	VAL	CA-CB	7.18	1.63	1.54
1	D	129	THR	CA-CB	6.94	1.62	1.53
1	E	158	ILE	CA-CB	5.74	1.60	1.54
1	B	158	ILE	CA-CB	5.56	1.60	1.54
1	H	129	THR	CA-CB	5.54	1.60	1.53

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	161	VAL	N-CA-C	10.65	118.69	108.15
1	E	132	THR	N-CA-C	-9.96	100.50	111.36
1	C	158	ILE	N-CA-C	-6.89	100.69	109.30
1	G	235	GLU	N-CA-C	-6.88	103.71	111.07
1	D	235	GLU	N-CA-C	-6.67	103.93	111.14

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	2267	0	2237	55	0
1	B	2271	0	2241	69	0
1	C	2263	0	2234	59	0
1	D	2267	0	2237	80	0
1	E	2263	0	2234	67	0
1	F	2263	0	2234	61	0
1	G	2267	0	2237	86	0
1	H	2263	0	2234	85	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	B	5	0	0	0	0
3	E	5	0	0	0	0
All	All	18142	0	17888	520	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 14.

The worst 5 of 520 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:C:193:ASN:HD22	1:C:210:VAL:HG21	1.22	1.02
1:G:270:LEU:CD1	1:G:294:ALA:HB2	1.96	0.96
1:G:270:LEU:HD13	1:G:294:ALA:HB2	1.46	0.94
1:B:172:GLN:HE21	1:H:190:GLN:HE22	1.16	0.94
1:B:167:CYS:HG	2:B:322:ZN:ZN	0.69	0.88

There are no symmetry-related clashes.

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	309/321 (96%)	286 (93%)	23 (7%)	0	100	100
1	B	310/321 (97%)	287 (93%)	20 (6%)	3 (1%)	12	40
1	C	308/321 (96%)	279 (91%)	26 (8%)	3 (1%)	12	40
1	D	309/321 (96%)	281 (91%)	28 (9%)	0	100	100
1	E	308/321 (96%)	284 (92%)	23 (8%)	1 (0%)	36	66
1	F	308/321 (96%)	287 (93%)	20 (6%)	1 (0%)	36	66
1	G	309/321 (96%)	282 (91%)	24 (8%)	3 (1%)	12	40
1	H	308/321 (96%)	272 (88%)	34 (11%)	2 (1%)	21	51
All	All	2469/2568 (96%)	2258 (92%)	198 (8%)	13 (0%)	24	55

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	ARG
1	C	180	SER
1	H	11	GLY
1	B	156	GLY
1	B	301	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	218/227 (96%)	194 (89%)	24 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	218/227 (96%)	201 (92%)	17 (8%)	11	36
1	C	218/227 (96%)	192 (88%)	26 (12%)	5	20
1	D	218/227 (96%)	196 (90%)	22 (10%)	7	26
1	E	218/227 (96%)	196 (90%)	22 (10%)	7	26
1	F	218/227 (96%)	198 (91%)	20 (9%)	8	29
1	G	218/227 (96%)	188 (86%)	30 (14%)	3	15
1	H	218/227 (96%)	181 (83%)	37 (17%)	2	9
All	All	1744/1816 (96%)	1546 (89%)	198 (11%)	5	22

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	38	GLU
1	G	132	THR
1	F	129	THR
1	F	312	GLN
1	G	205	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	190	GLN
1	H	198	ASN
1	F	172	GLN
1	H	193	ASN
1	H	80	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	B	323	-	4,4,4	0.33	0	6,6,6	0.25	0
3	SO4	E	323	-	4,4,4	0.24	0	6,6,6	0.32	0

There are no bond length outliers.

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.

5.7 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	311/321 (96%)	-0.44	0 100 100	60, 81, 106, 116	0
1	B	312/321 (97%)	-0.44	0 100 100	60, 84, 111, 122	0
1	C	310/321 (96%)	-0.43	0 100 100	58, 84, 111, 119	0
1	D	311/321 (96%)	-0.37	0 100 100	58, 82, 107, 117	0
1	E	310/321 (96%)	-0.42	0 100 100	60, 82, 113, 125	0
1	F	310/321 (96%)	-0.44	0 100 100	62, 83, 112, 120	0
1	G	311/321 (96%)	-0.35	0 100 100	60, 84, 111, 120	0
1	H	310/321 (96%)	-0.32	0 100 100	57, 99, 160, 171	0
All	All	2485/2568 (96%)	-0.40	0 100 100	57, 84, 116, 171	0

There are no RSRZ outliers to report.

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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	323	5/5	0.82	0.13	114,115,115,115	0
3	SO4	E	323	5/5	0.87	0.11	110,110,111,112	0
2	ZN	C	322	1/1	1.00	0.02	81,81,81,81	0
2	ZN	D	322	1/1	1.00	0.03	79,79,79,79	0
2	ZN	E	322	1/1	1.00	0.02	73,73,73,73	0
2	ZN	F	322	1/1	1.00	0.03	70,70,70,70	0
2	ZN	G	322	1/1	1.00	0.03	75,75,75,75	0
2	ZN	H	322	1/1	1.00	0.03	79,79,79,79	0
2	ZN	A	322	1/1	1.00	0.03	82,82,82,82	0
2	ZN	B	322	1/1	1.00	0.04	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.