



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 07:38 AM EDT

PDB ID : 5IBX
Title : 1.65 Angstrom Crystal Structure of Triosephosphate Isomerase (TIM) from *Streptococcus pneumoniae*
Authors : Minasov, G.; Shuvalova, L.; Dubrovskaya, I.; Flores, K.; Shatsman, S.; Kwon, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2016-02-22
Resolution : 1.65 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

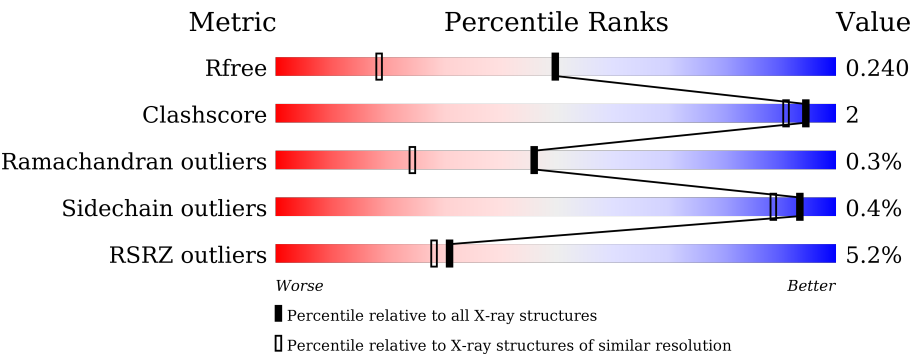
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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	255	<div><div>5%</div><div><div></div><div>91%</div><div>7%</div><div></div></div><div></div></div>
1	B	255	<div><div>3%</div><div><div></div><div>94%</div><div></div><div></div></div><div></div></div>
1	D	255	<div><div>3%</div><div><div></div><div>92%</div><div>5%</div><div></div></div><div></div></div>
1	E	255	<div><div>6%</div><div><div></div><div>96%</div><div></div><div></div></div><div></div></div>
1	H	255	<div><div>7%</div><div><div></div><div>94%</div><div>5%</div><div></div></div><div></div></div>
2	C	255	<div><div>3%</div><div><div></div><div>95%</div><div></div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	255	<div> <div>4%</div> <div>93%</div> <div>• •</div> </div>
2	G	255	<div> <div>9%</div> <div>95%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	C	301	-	-	-	X
3	NA	D	301	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17739 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 Triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	9	0
			1925	1212	320	383	10			
1	B	250	Total	C	N	O	S	0	6	0
			1897	1196	312	379	10			
1	D	249	Total	C	N	O	S	0	13	0
			1944	1230	320	384	10			
1	E	251	Total	C	N	O	S	0	7	0
			1910	1202	314	383	11			
1	H	251	Total	C	N	O	S	0	7	0
			1914	1207	317	380	10			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q04JH4
A	-1	ASN	-	expression tag	UNP Q04JH4
A	0	ALA	-	expression tag	UNP Q04JH4
B	-2	SER	-	expression tag	UNP Q04JH4
B	-1	ASN	-	expression tag	UNP Q04JH4
B	0	ALA	-	expression tag	UNP Q04JH4
D	-2	SER	-	expression tag	UNP Q04JH4
D	-1	ASN	-	expression tag	UNP Q04JH4
D	0	ALA	-	expression tag	UNP Q04JH4
E	-2	SER	-	expression tag	UNP Q04JH4
E	-1	ASN	-	expression tag	UNP Q04JH4
E	0	ALA	-	expression tag	UNP Q04JH4
H	-2	SER	-	expression tag	UNP Q04JH4
H	-1	ASN	-	expression tag	UNP Q04JH4
H	0	ALA	-	expression tag	UNP Q04JH4

- Molecule 2 is a protein called Triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	250	Total	C	N	O	S	0	9	0
			1916	1207	314	386	9			
2	F	250	Total	C	N	O	S	0	5	0
			1888	1189	311	379	9			
2	G	248	Total	C	N	O	S	0	4	0
			1865	1178	309	369	9			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP Q04JH4
C	-1	ASN	-	expression tag	UNP Q04JH4
C	0	ALA	-	expression tag	UNP Q04JH4
F	-2	SER	-	expression tag	UNP Q04JH4
F	-1	ASN	-	expression tag	UNP Q04JH4
F	0	ALA	-	expression tag	UNP Q04JH4
G	-2	SER	-	expression tag	UNP Q04JH4
G	-1	ASN	-	expression tag	UNP Q04JH4
G	0	ALA	-	expression tag	UNP Q04JH4

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	H	1	Total	Na	0	0
			1	1		
3	B	2	Total	Na	0	0
			2	2		
3	C	4	Total	Na	0	0
			4	4		
3	A	1	Total	Na	0	0
			1	1		
3	F	2	Total	Na	0	0
			2	2		

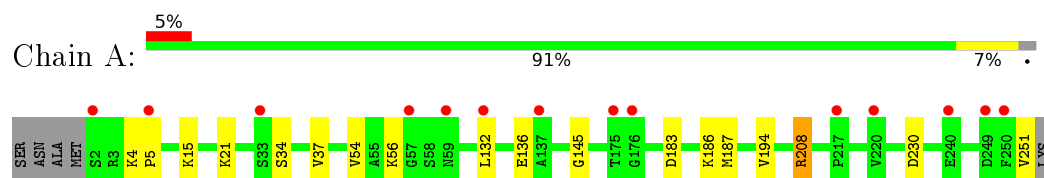
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	282	Total 292	O 292	0	13
4	B	343	Total 356	O 356	0	14
4	C	326	Total 340	O 340	0	18
4	D	308	Total 322	O 322	0	19
4	E	310	Total 318	O 318	0	10
4	F	304	Total 311	O 311	0	7
4	G	210	Total 225	O 225	0	16
4	H	289	Total 303	O 303	0	14

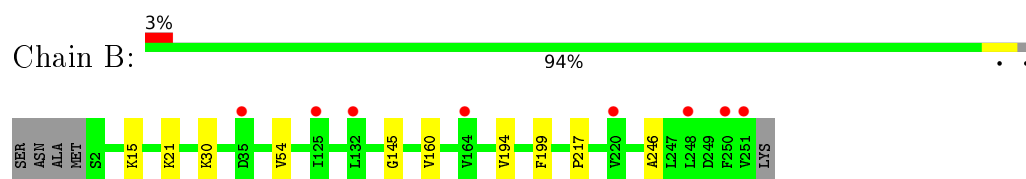
3 Residue-property plots [i](#)

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

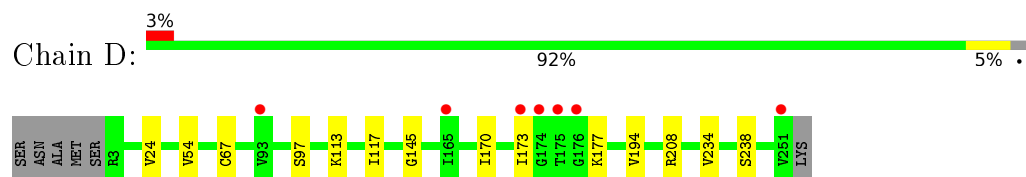
- Molecule 1: Triosephosphate isomerase



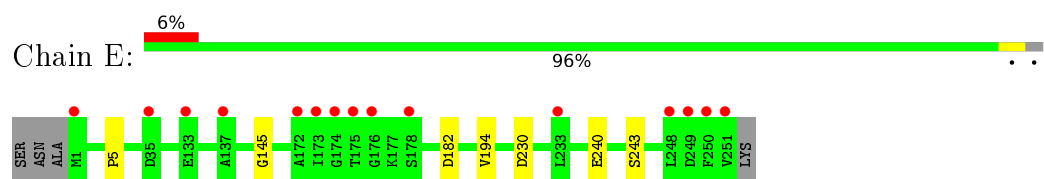
- Molecule 1: Triosephosphate isomerase



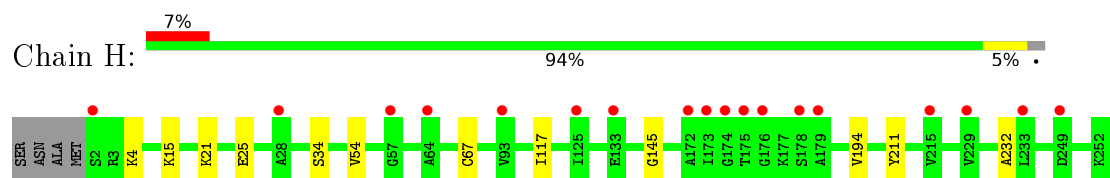
- Molecule 1: Triosephosphate isomerase



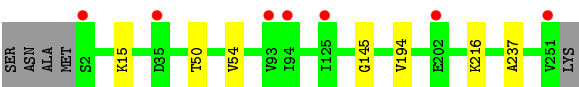
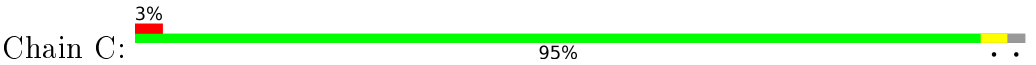
- Molecule 1: Triosephosphate isomerase



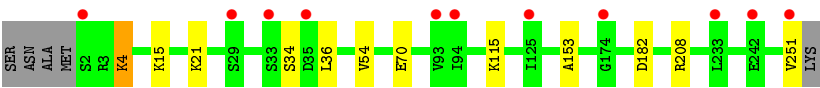
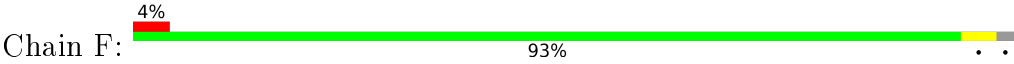
- Molecule 1: Triosephosphate isomerase



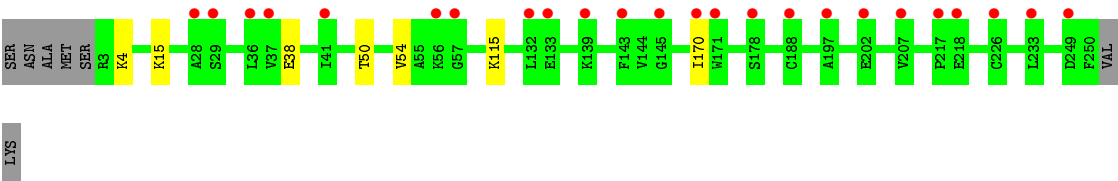
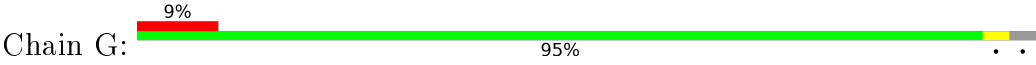
- Molecule 2: Triosephosphate isomerase



• Molecule 2: Triosephosphate isomerase



• Molecule 2: Triosephosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.84Å 84.35Å 92.46Å 75.43° 65.97° 62.03°	Depositor
Resolution (Å)	29.69 – 1.65 29.69 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.69-1.65) 94.5 (29.69-1.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.196 , 0.232 0.204 , 0.240	Depositor DCC
R_{free} test set	11243 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.4	EDS
Estimated twinning fraction	0.037 for h,h-k,h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 223818 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17739	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.56	0/1945	0.68	0/2633
1	B	0.60	0/1917	0.71	0/2596
1	D	0.59	0/1965	0.71	0/2660
1	E	0.59	0/1930	0.71	0/2612
1	H	0.57	0/1934	0.70	0/2615
2	C	0.58	0/1947	0.67	0/2640
2	F	0.53	0/1919	0.68	0/2601
2	G	0.52	0/1896	0.65	0/2568
All	All	0.57	0/15453	0.69	0/20925

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1925	0	1899	10	0
1	B	1897	0	1866	5	0
1	D	1944	0	1928	11	0
1	E	1910	0	1878	4	0
1	H	1914	0	1894	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1916	0	1874	4	0
2	F	1888	0	1852	5	0
2	G	1865	0	1844	4	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	292	0	0	1	0
4	B	356	0	0	0	0
4	C	340	0	0	0	0
4	D	322	0	0	1	0
4	E	318	0	0	0	0
4	F	311	0	0	1	0
4	G	225	0	0	2	0
4	H	303	0	0	0	0
All	All	17739	0	15035	51	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 2.

All (51) 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:67:CYS:SG	1:D:117[B]:ILE:HD11	2.27	0.73
1:A:145:GLY:HA2	1:A:194:VAL:HG21	1.80	0.61
2:C:145:GLY:HA2	2:C:194:VAL:HG21	1.82	0.60
1:D:113:LYS:O	1:D:117[B]:ILE:HG12	2.03	0.58
1:A:21:LYS:HG3	1:A:54:VAL:HG21	1.86	0.57
1:B:145:GLY:HA2	1:B:194[A]:VAL:HG21	1.87	0.57
2:G:50:THR:O	2:G:54:VAL:HG23	2.05	0.56
1:D:177[B]:LYS:O	4:D:546[B]:HOH:O	2.17	0.56
1:A:37:VAL:HB	1:A:251:VAL:HG11	1.87	0.56
2:F:4:LYS:HE3	2:F:34:SER:O	2.07	0.54
1:D:24:VAL:HG11	1:D:54:VAL:HG13	1.90	0.53
1:H:21:LYS:HG3	1:H:54:VAL:HG21	1.90	0.53
1:D:145:GLY:HA2	1:D:194:VAL:HG21	1.92	0.52
1:D:97:SER:CB	1:D:170[B]:ILE:HD11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208[B]:ARG:HD3	4:A:410:HOH:O	2.11	0.50
1:H:4:LYS:CE	1:H:34:SER:O	2.59	0.50
1:D:170[B]:ILE:O	1:D:173[B]:ILE:HG23	2.13	0.49
1:H:4:LYS:HE3	1:H:34:SER:O	2.12	0.49
2:F:115:LYS:NZ	2:F:153:ALA:O	2.44	0.48
1:D:234[A]:VAL:HG23	1:D:238:SER:HB3	1.96	0.47
2:C:145:GLY:CA	2:C:194:VAL:HG21	2.44	0.47
1:A:4:LYS:CE	1:A:34:SER:O	2.63	0.47
1:A:183:ASP:HA	1:A:186:LYS:HE2	1.98	0.46
1:A:186:LYS:HE3	1:A:187:MET:HG2	1.96	0.46
2:F:21:LYS:HG3	2:F:54:VAL:HG21	1.98	0.46
1:E:182[A]:ASP:OD1	1:E:182[A]:ASP:O	2.34	0.46
1:H:117[B]:ILE:HD13	1:H:117[B]:ILE:HA	1.72	0.45
1:H:67:CYS:SG	1:H:117[B]:ILE:HD11	2.57	0.45
1:B:160:VAL:HG21	1:B:199:PHE:CZ	2.52	0.44
1:E:145:GLY:HA2	1:E:194:VAL:HG21	1.99	0.44
2:F:70[A]:GLU:HB3	4:F:609[A]:HOH:O	2.17	0.44
1:H:25:GLU:HG3	1:H:54:VAL:HG11	2.00	0.44
1:D:234[A]:VAL:O	1:D:234[A]:VAL:HG23	2.18	0.44
2:F:36:LEU:HB3	2:F:251:VAL:HG11	2.00	0.43
1:H:211:TYR:O	1:H:232:ALA:HA	2.18	0.43
1:A:132:LEU:O	1:A:136:GLU:HG2	2.18	0.43
1:A:56[B]:LYS:HB3	1:A:56[B]:LYS:HE2	1.82	0.43
1:B:145:GLY:CA	1:B:194[A]:VAL:HG21	2.49	0.42
1:D:97:SER:HB3	1:D:170[B]:ILE:HD11	2.02	0.42
2:G:4:LYS:HE2	2:G:38:GLU:HB2	2.02	0.42
1:E:5:PRO:HA	1:E:230:ASP:O	2.19	0.42
1:B:217:PRO:HB3	1:B:246:ALA:HB1	2.02	0.41
1:B:21:LYS:HG3	1:B:54[A]:VAL:HG21	2.02	0.41
2:G:115[A]:LYS:NZ	4:G:403:HOH:O	2.52	0.41
2:G:170[B]:ILE:HG21	4:G:590[B]:HOH:O	2.21	0.41
1:A:5:PRO:HA	1:A:230:ASP:O	2.21	0.41
2:C:216:LYS:HD2	2:C:237:ALA:HB2	2.03	0.41
2:C:50:THR:O	2:C:54:VAL:HG23	2.21	0.41
1:E:240[A]:GLU:HB3	1:E:243:SER:OG	2.21	0.40
1:H:145:GLY:HA2	1:H:194:VAL:HG21	2.02	0.40
1:D:67:CYS:SG	1:D:117[B]:ILE:CD1	3.03	0.40

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	256/255 (100%)	247 (96%)	8 (3%)	1 (0%)	39	18
1	B	253/255 (99%)	247 (98%)	5 (2%)	1 (0%)	39	18
1	D	259/255 (102%)	253 (98%)	6 (2%)	0	100	100
1	E	255/255 (100%)	247 (97%)	8 (3%)	0	100	100
1	H	255/255 (100%)	248 (97%)	6 (2%)	1 (0%)	39	18
2	C	257/255 (101%)	250 (97%)	6 (2%)	1 (0%)	39	18
2	F	253/255 (99%)	246 (97%)	6 (2%)	1 (0%)	39	18
2	G	250/255 (98%)	244 (98%)	5 (2%)	1 (0%)	39	18
All	All	2038/2040 (100%)	1982 (97%)	50 (2%)	6 (0%)	46	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	15	LYS
1	B	15	LYS
2	C	15	LYS
2	F	15	LYS
1	H	15	LYS
1	A	15	LYS

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	197/192 (103%)	195 (99%)	2 (1%)	82	68
1	B	194/192 (101%)	193 (100%)	1 (0%)	92	86
1	D	200/192 (104%)	199 (100%)	1 (0%)	92	86
1	E	196/192 (102%)	196 (100%)	0	100	100
1	H	196/192 (102%)	196 (100%)	0	100	100
2	C	198/193 (103%)	198 (100%)	0	100	100
2	F	194/193 (100%)	191 (98%)	3 (2%)	72	51
2	G	191/193 (99%)	191 (100%)	0	100	100
All	All	1566/1539 (102%)	1559 (100%)	7 (0%)	93	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208[A]	ARG
1	A	208[B]	ARG
1	B	30	LYS
1	D	208	ARG
2	F	4	LYS
2	F	182	ASP
2	F	208	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	CME	A	226	1,3	7,9,10	0.73	0	6,9,11	1.24	1 (16%)
1	CME	B	226	1,3	7,9,10	0.50	0	6,9,11	1.12	1 (16%)
1	CME	D	226	1,3	7,9,10	0.72	0	6,9,11	0.93	0
1	CME	E	226	1,3	7,9,10	0.74	0	6,9,11	1.41	2 (33%)
1	CME	H	226	1,3	7,9,10	0.69	0	6,9,11	1.28	2 (33%)

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	CME	A	226	1,3	-	0/5/8/10	0/0/0/0
1	CME	B	226	1,3	-	0/5/8/10	0/0/0/0
1	CME	D	226	1,3	-	0/5/8/10	0/0/0/0
1	CME	E	226	1,3	-	0/5/8/10	0/0/0/0
1	CME	H	226	1,3	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	CME	O-C-CA	-2.35	119.42	125.72
1	H	226	CME	O-C-CA	-2.23	119.73	125.72
1	B	226	CME	O-C-CA	-2.20	119.81	125.72
1	E	226	CME	O-C-CA	-2.14	119.99	125.72
1	H	226	CME	CB-SG-SD	2.14	108.12	103.95
1	E	226	CME	CB-SG-SD	2.47	108.75	103.95

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	249/255 (97%)	0.32	14 (5%) 28 25	12, 20, 39, 53	0
1	B	249/255 (97%)	0.29	8 (3%) 51 52	13, 18, 32, 49	0
1	D	248/255 (97%)	0.26	7 (2%) 56 57	12, 19, 30, 54	0
1	E	250/255 (98%)	0.31	15 (6%) 25 22	12, 18, 36, 60	0
1	H	250/255 (98%)	0.44	18 (7%) 18 16	13, 20, 36, 59	0
2	C	250/255 (98%)	0.30	7 (2%) 56 57	13, 19, 33, 47	0
2	F	250/255 (98%)	0.40	11 (4%) 38 37	13, 23, 36, 46	0
2	G	248/255 (97%)	0.73	24 (9%) 10 8	14, 27, 45, 53	0
All	All	1994/2040 (97%)	0.38	104 (5%) 31 28	12, 20, 38, 60	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	174	GLY	7.9
1	B	251	VAL	6.5
1	H	2	SER	5.3
1	E	250	PHE	5.0
1	D	176	GLY	4.9
1	D	175	THR	4.8
1	H	173	ILE	4.6
1	H	175	THR	4.5
1	E	175	THR	4.5
1	E	1	MET	4.4
2	G	132	LEU	4.4
2	G	57	GLY	4.2
1	B	250	PHE	4.2
2	G	218	GLU	4.0
2	C	2	SER	3.9
1	A	176	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	215	VAL	3.8
2	C	251	VAL	3.8
2	F	93	VAL	3.8
2	F	251	VAL	3.8
1	E	173	ILE	3.7
1	H	249	ASP	3.6
1	A	137	ALA	3.5
1	E	176	GLY	3.5
2	C	94	ILE	3.5
1	E	251	VAL	3.4
1	A	250	PHE	3.4
1	E	174	GLY	3.3
2	G	170[A]	ILE	3.3
1	D	165[A]	ILE	3.3
1	E	137	ALA	3.2
1	A	217	PRO	3.2
1	A	220[A]	VAL	3.2
2	F	125	ILE	3.1
2	G	202	GLU	3.1
1	D	174	GLY	3.1
1	H	233	LEU	3.1
2	F	29	SER	3.1
1	E	249	ASP	3.0
1	D	173[A]	ILE	3.0
2	G	217	PRO	3.0
2	G	36	LEU	3.0
1	D	93	VAL	2.9
1	H	229	VAL	2.9
2	G	37	VAL	2.9
1	A	249	ASP	2.9
1	B	220	VAL	2.9
1	B	248	LEU	2.8
2	F	35	ASP	2.8
1	H	172	ALA	2.8
1	B	35	ASP	2.7
2	G	197	ALA	2.7
2	F	94	ILE	2.7
1	A	175	THR	2.7
2	G	233	LEU	2.7
1	H	178	SER	2.7
1	H	28	ALA	2.6
2	G	178	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	35	ASP	2.6
1	H	125	ILE	2.5
1	E	172	ALA	2.5
2	F	174	GLY	2.5
1	E	233	LEU	2.5
1	H	176	GLY	2.4
2	G	56	LYS	2.4
1	A	57	GLY	2.4
2	F	233	LEU	2.4
1	E	133	GLU	2.4
2	F	2	SER	2.4
2	G	226	CYS	2.3
1	H	57	GLY	2.3
1	H	179	ALA	2.3
2	C	202	GLU	2.3
2	G	29	SER	2.3
1	D	251	VAL	2.3
1	A	33	SER	2.3
1	A	2	SER	2.3
2	C	93	VAL	2.2
2	G	188	CYS	2.2
2	F	33	SER	2.2
1	A	5	PRO	2.2
1	B	125	ILE	2.2
1	H	93	VAL	2.2
2	G	41	ILE	2.2
2	G	139	LYS	2.2
1	E	178	SER	2.2
2	C	35	ASP	2.2
2	G	171	TRP	2.2
2	G	249	ASP	2.1
2	G	143	PHE	2.1
1	H	133	GLU	2.1
2	F	242	GLU	2.1
1	A	132	LEU	2.1
1	H	64	ALA	2.1
1	B	164	VAL	2.1
2	G	207	VAL	2.1
2	G	145	GLY	2.1
2	G	133	GLU	2.1
1	A	240	GLU	2.0
2	C	125	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	G	28	ALA	2.0
1	B	132	LEU	2.0
1	E	248	LEU	2.0
1	A	59	ASN	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. 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
1	CME	B	226	10/11	0.94	0.11	-	23,24,31,31	4
1	CME	E	226	10/11	0.96	0.08	-	21,23,27,29	0
1	CME	H	226	10/11	0.95	0.10	-	19,22,28,29	0
1	CME	A	226	10/11	0.94	0.12	-	19,22,27,28	0
1	CME	D	226	10/11	0.90	0.11	-	19,22,29,31	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. 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
3	NA	C	301	1/1	0.97	0.17	3.74	21,21,21,21	0
3	NA	D	301	1/1	0.98	0.10	2.11	18,18,18,18	0
3	NA	F	301	1/1	0.96	0.12	1.63	26,26,26,26	0
3	NA	A	301	1/1	0.98	0.13	1.62	19,19,19,19	0
3	NA	C	303	1/1	0.96	0.10	-0.22	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	H	301	1/1	0.98	0.08	-0.70	19,19,19,19	0
3	NA	B	301	1/1	0.98	0.07	-1.06	21,21,21,21	0
3	NA	E	301	1/1	0.99	0.04	-2.25	19,19,19,19	0
3	NA	G	301	1/1	0.95	0.06	-2.92	28,28,28,28	0
3	NA	F	302	1/1	0.98	0.12	-	22,22,22,22	0
3	NA	B	302	1/1	0.95	0.12	-	25,25,25,25	0
3	NA	C	302	1/1	0.99	0.05	-	18,18,18,18	0
3	NA	C	304	1/1	0.99	0.05	-	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.