



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 09:15 AM EDT

PDB ID : 6WON  
Title : Crystal structure of acetoin dehydrogenase YohF from *Salmonella typhimurium*  
Authors : Stogios, P.J.; Skarina, T.; Mesa, N.; Endres, M.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2020-04-25  
Resolution : 2.13 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

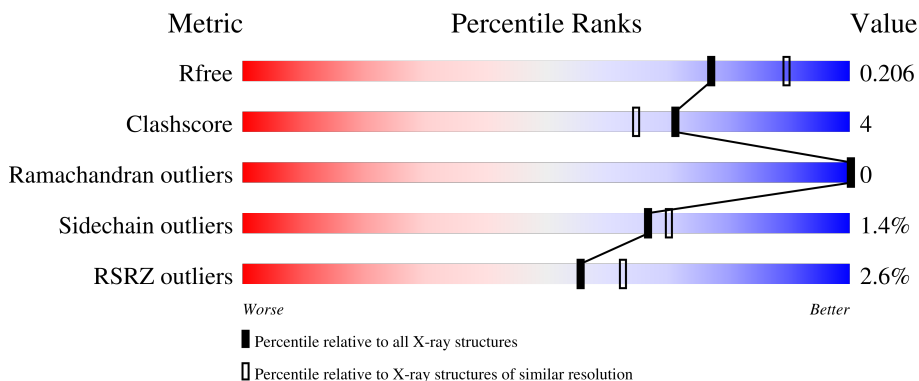
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 Å.

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



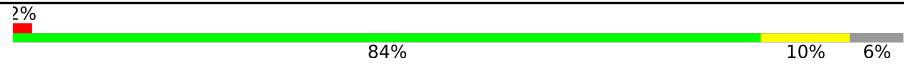

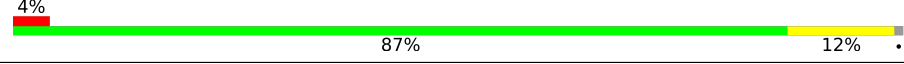
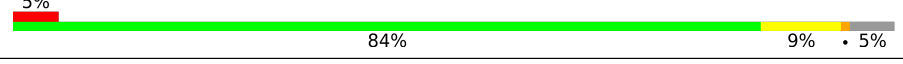
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	255	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">87% 7% 5%</p>
1	B	255	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">86% 9% .</p>
1	C	255	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">89% 7% .</p>
1	D	255	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">89% 6% 5%</p>

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Mol	Chain	Length	Quality of chain
1	E	255	 <p>2% 84% 10% 6%</p>
1	F	255	 <p>4% 86% 9% 5%</p>
1	G	255	 <p>4% 87% 12% 5%</p>
1	H	255	 <p>5% 84% 9% 5%</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15700 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 YohF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	241	Total 1790	C 1129	N 315	O 337	S 9	0	0	0
1	B	244	Total 1809	C 1138	N 320	O 342	S 9	0	0	0
1	C	244	Total 1809	C 1138	N 320	O 342	S 9	0	0	0
1	D	241	Total 1791	C 1129	N 315	O 339	S 8	0	0	0
1	E	239	Total 1775	C 1119	N 313	O 335	S 8	0	0	0
1	F	243	Total 1803	C 1136	N 318	O 340	S 9	0	0	0
1	G	253	Total 1882	C 1181	N 330	O 360	S 11	0	0	0
1	H	241	Total 1791	C 1128	N 316	O 338	S 9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

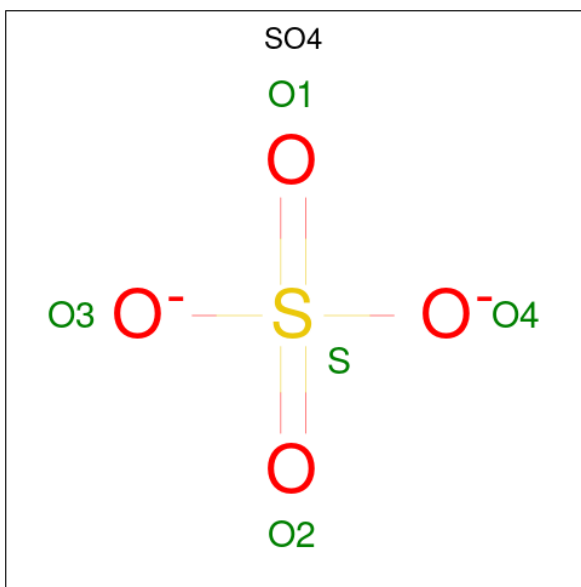
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP Q8ZNM5
A	0	GLY	-	expression tag	UNP Q8ZNM5
B	-1	GLN	-	expression tag	UNP Q8ZNM5
B	0	GLY	-	expression tag	UNP Q8ZNM5
C	-1	GLN	-	expression tag	UNP Q8ZNM5
C	0	GLY	-	expression tag	UNP Q8ZNM5
D	-1	GLN	-	expression tag	UNP Q8ZNM5
D	0	GLY	-	expression tag	UNP Q8ZNM5
E	-1	GLN	-	expression tag	UNP Q8ZNM5
E	0	GLY	-	expression tag	UNP Q8ZNM5
F	-1	GLN	-	expression tag	UNP Q8ZNM5
F	0	GLY	-	expression tag	UNP Q8ZNM5
G	-1	GLN	-	expression tag	UNP Q8ZNM5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLY	-	expression tag	UNP Q8ZNM5
H	-1	GLN	-	expression tag	UNP Q8ZNM5
H	0	GLY	-	expression tag	UNP Q8ZNM5

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



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	172	Total O 174 174	0	2
4	B	161	Total O 163 163	0	2

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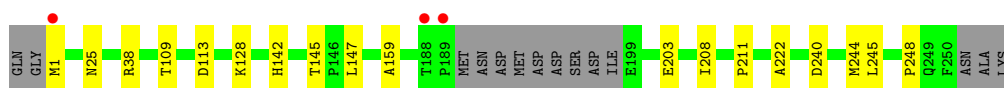
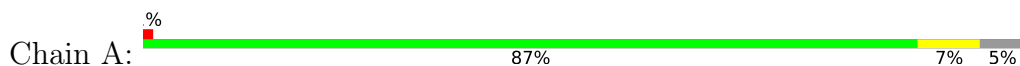
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	C	152	Total 152	O 152	0	0
4	D	182	Total 184	O 184	0	2
4	E	154	Total 156	O 156	0	2
4	F	151	Total 153	O 153	0	2
4	G	155	Total 155	O 155	0	0
4	H	101	Total 102	O 102	0	1

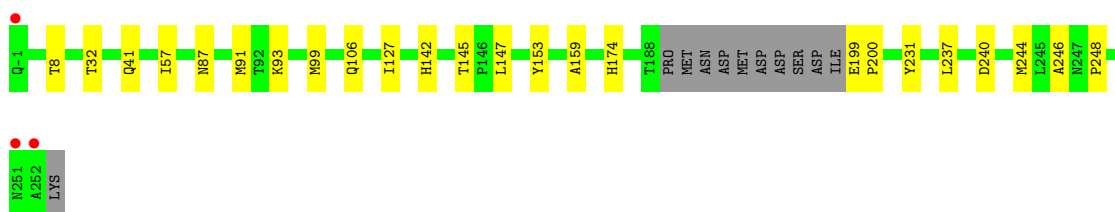
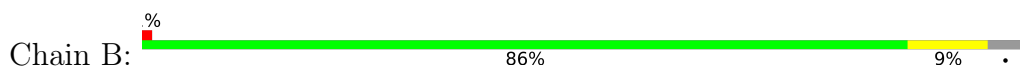
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

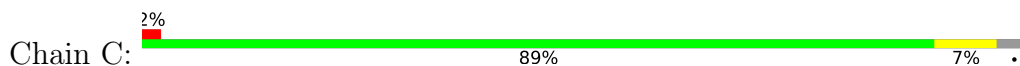
- Molecule 1: YohF



- Molecule 1: YohF



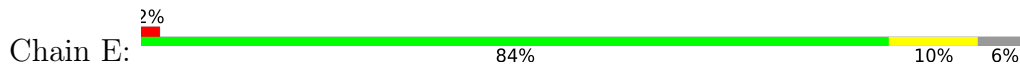
- Molecule 1: YohF

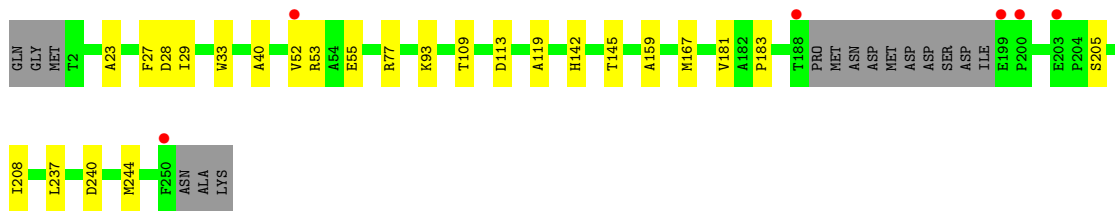


- Molecule 1: YohF

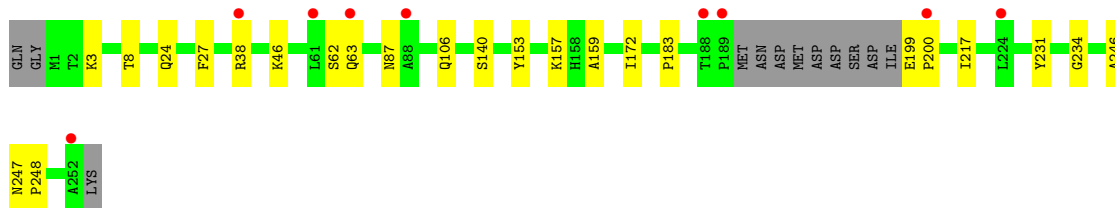
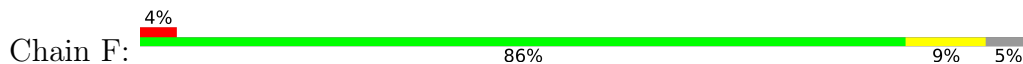


- Molecule 1: YohF

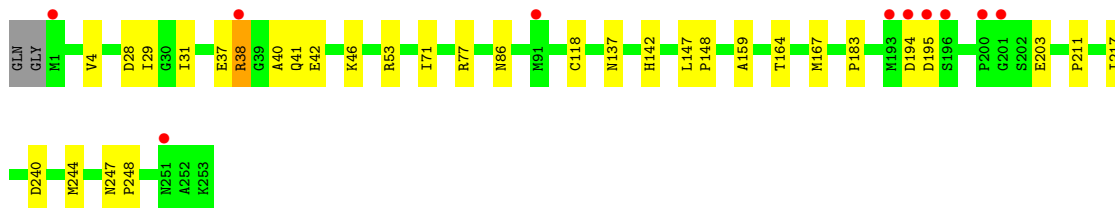
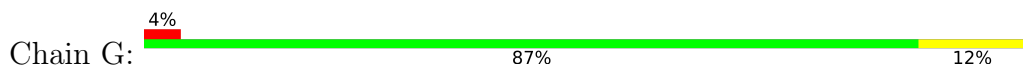




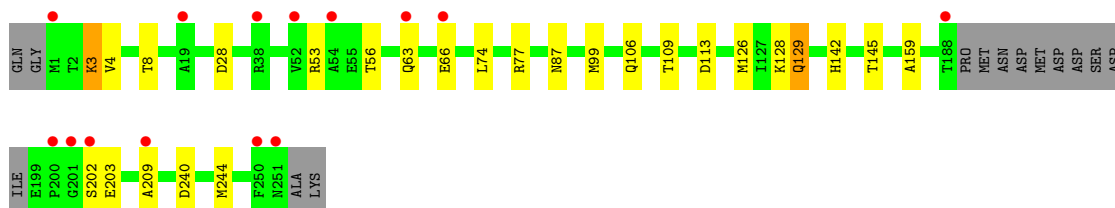
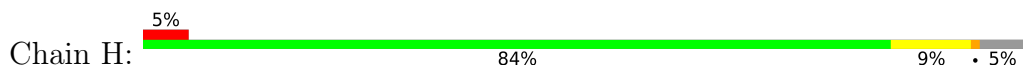
● Molecule 1: YohF



● Molecule 1: YohF



● Molecule 1: YohF





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.55Å 114.17Å 219.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 2.13 29.49 – 2.13	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.49-2.13) 94.3 (29.49-2.13)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.12Å)	Xtrriage
Refinement program	PHENIX 1.15_3448	Depositor
R, $R_{free}$	0.160 , 0.207 0.160 , 0.206	Depositor DCC
$R_{free}$ test set	2000 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtrriage
Anisotropy	0.303	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15700	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

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	0.37	0/1825	0.50	0/2479
1	B	0.37	0/1843	0.51	0/2502
1	C	0.37	0/1843	0.51	0/2502
1	D	0.36	0/1825	0.50	0/2479
1	E	0.35	0/1809	0.48	0/2457
1	F	0.37	0/1838	0.53	0/2497
1	G	0.39	0/1918	0.53	0/2605
1	H	0.35	0/1825	0.50	0/2478
All	All	0.37	0/14726	0.51	0/19999

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	1790	0	1790	14	0
1	B	1809	0	1805	15	0
1	C	1809	0	1805	9	0
1	D	1791	0	1786	8	0
1	E	1775	0	1771	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1803	0	1801	15	0
1	G	1882	0	1871	25	0
1	H	1791	0	1789	12	0
2	A	5	0	0	1	0
2	F	5	0	0	0	0
3	G	1	0	0	0	0
4	A	174	0	0	2	0
4	B	163	0	0	2	0
4	C	152	0	0	0	0
4	D	184	0	0	2	0
4	E	156	0	0	1	0
4	F	153	0	0	1	0
4	G	155	0	0	4	0
4	H	102	0	0	1	0
All	All	15700	0	14418	102	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 4.

All (102) 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:G:194:ASP:O	1:G:195:ASP:HB2	1.70	0.91
1:G:42:GLU:HG3	4:G:403:HOH:O	1.70	0.90
1:G:38:ARG:HG3	1:G:38:ARG:NH1	2.02	0.74
1:G:38:ARG:HG3	1:G:38:ARG:HH11	1.51	0.73
1:H:56:THR:O	1:H:77:ARG:NH2	2.25	0.70
1:C:159:ALA:HB2	1:D:159:ALA:HB2	1.76	0.68
1:F:106:GLN:NE2	4:F:404:HOH:O	2.31	0.62
1:E:53:ARG:NH2	1:E:77:ARG:O	2.29	0.62
1:G:159:ALA:HB2	1:H:159:ALA:HB2	1.83	0.60
1:G:38:ARG:HH11	1:G:38:ARG:CG	2.14	0.60
1:E:93:LYS:NZ	4:E:301:HOH:O	2.34	0.59
1:G:38:ARG:NH1	4:G:403:HOH:O	2.36	0.58
1:G:86:ASN:HB2	1:G:137:ASN:HD22	1.69	0.57
1:D:24:GLN:NE2	4:D:301:HOH:O	2.25	0.57
1:H:109:THR:HA	1:H:113:ASP:HB2	1.87	0.56
1:E:28:ASP:HA	1:E:52:VAL:HG13	1.87	0.56
1:H:4:VAL:HG22	1:H:28:ASP:HB2	1.87	0.56
1:A:128:LYS:NZ	4:A:401:HOH:O	2.38	0.54
1:B:41:GLN:HG2	4:B:347:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LEU:HD22	1:E:237:LEU:HD22	1.90	0.53
1:E:159:ALA:HB2	1:F:159:ALA:HB2	1.91	0.52
1:G:86:ASN:HD22	1:G:137:ASN:ND2	2.06	0.52
1:A:208:ILE:HD12	1:F:172:ILE:HD11	1.91	0.51
1:C:23:ALA:HB2	1:C:29:ILE:HG13	1.93	0.51
1:A:142:HIS:CE1	1:A:147:LEU:HB2	2.46	0.51
1:H:8:THR:O	1:H:87:ASN:HB3	2.11	0.50
1:E:142:HIS:HA	1:E:145:THR:O	2.12	0.50
1:C:199:GLU:HB3	1:C:200:PRO:HD3	1.94	0.49
1:A:208:ILE:HG21	1:F:231:TYR:CE1	2.48	0.49
1:H:106:GLN:HG3	4:H:370:HOH:O	2.12	0.49
1:G:38:ARG:HA	1:G:38:ARG:HD2	1.47	0.48
1:F:8:THR:O	1:F:87:ASN:HB3	2.14	0.48
1:C:247:ASN:HB2	1:C:248:PRO:HD2	1.96	0.48
1:E:27:PHE:O	1:E:52:VAL:HG11	2.14	0.47
1:A:240:ASP:OD2	1:A:244:MET:HG2	2.14	0.47
1:D:4:VAL:HG22	1:D:28:ASP:HB2	1.95	0.47
1:H:126:MET:HA	1:H:129:GLN:NE2	2.29	0.47
1:E:55:GLU:HB3	1:E:77:ARG:HH21	1.80	0.47
1:F:247:ASN:HB2	1:F:248:PRO:HD2	1.96	0.46
1:A:142:HIS:HA	1:A:145:THR:O	2.16	0.46
1:A:109:THR:HA	1:A:113:ASP:HB2	1.97	0.46
1:A:25:ASN:ND2	4:A:408:HOH:O	2.49	0.46
1:D:167:MET:HE2	1:D:178:VAL:HG11	1.99	0.46
1:C:240:ASP:OD2	1:C:244:MET:HG2	2.16	0.45
1:E:33:TRP:HB3	1:E:40:ALA:HB2	1.98	0.45
1:E:119:ALA:HB1	1:E:167:MET:HE1	1.98	0.45
1:G:203:GLU:CG	1:G:211:PRO:HD3	2.46	0.45
1:H:142:HIS:HA	1:H:145:THR:O	2.17	0.45
1:F:3:LYS:HE3	1:F:27:PHE:CE2	2.51	0.45
1:B:8:THR:O	1:B:87:ASN:HB3	2.17	0.45
1:B:32:THR:HA	1:B:57:ILE:O	2.17	0.45
1:G:77:ARG:NH2	4:G:405:HOH:O	2.41	0.45
1:H:240:ASP:OD2	1:H:244:MET:HG2	2.17	0.45
1:A:248:PRO:HB3	1:E:205:SER:HB2	1.98	0.44
1:C:27:PHE:O	1:C:52:VAL:HG21	2.16	0.44
1:C:142:HIS:CE1	1:C:147:LEU:HB2	2.52	0.44
1:B:91:MET:SD	1:B:93:LYS:HG3	2.57	0.44
1:D:247:ASN:HB2	1:D:248:PRO:HD2	1.99	0.44
1:G:38:ARG:O	1:G:41:GLN:N	2.50	0.44
1:C:28:ASP:HA	1:C:52:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ASP:OD2	1:D:244:MET:HG2	2.17	0.44
1:A:203:GLU:HG2	1:A:211:PRO:HD3	2.00	0.44
1:B:240:ASP:OD2	1:B:244:MET:HG2	2.18	0.44
1:D:120:GLN:O	1:D:124:ARG:HG3	2.18	0.44
1:G:4:VAL:HG22	1:G:28:ASP:HB2	2.00	0.44
1:B:127:ILE:HG12	1:B:174:HIS:CG	2.53	0.43
1:G:240:ASP:OD2	1:G:244:MET:HG2	2.17	0.43
1:H:203:GLU:N	1:H:209:ALA:O	2.49	0.43
1:E:181:VAL:O	1:E:183:PRO:HD3	2.17	0.43
1:E:240:ASP:OD2	1:E:244:MET:HG2	2.18	0.43
1:B:142:HIS:HA	1:B:145:THR:O	2.19	0.43
1:G:53:ARG:NH2	4:G:416:HOH:O	2.51	0.43
1:B:199:GLU:N	1:B:200:PRO:HD2	2.34	0.43
1:D:124:ARG:NH1	4:D:309:HOH:O	2.52	0.43
1:F:153:TYR:CE1	1:F:157:LYS:HE2	2.53	0.43
1:G:164:THR:HA	1:G:167:MET:HE2	2.00	0.43
1:G:183:PRO:HB3	1:G:217:ILE:CD1	2.49	0.43
1:G:203:GLU:HG3	1:G:211:PRO:HD3	2.01	0.43
1:H:63:GLN:NE2	1:H:66:GLU:OE1	2.52	0.43
1:E:23:ALA:HB2	1:E:29:ILE:HG13	2.01	0.42
1:B:153:TYR:OH	4:B:301:HOH:O	2.21	0.42
1:G:142:HIS:CE1	1:G:147:LEU:HB2	2.53	0.42
1:B:246:ALA:HB3	1:F:248:PRO:HD3	2.01	0.42
1:A:25:ASN:HD21	1:A:222:ALA:HB1	1.84	0.42
1:G:247:ASN:HB2	1:G:248:PRO:HD2	2.01	0.42
1:A:159:ALA:HB2	1:B:159:ALA:HB2	2.01	0.42
1:B:231:TYR:CE1	1:E:208:ILE:HG21	2.54	0.42
1:F:153:TYR:CZ	1:F:157:LYS:HE2	2.55	0.42
1:C:139:THR:OG1	1:C:140:SER:N	2.53	0.41
1:G:29:ILE:HG22	1:G:31:ILE:HG13	2.02	0.41
1:B:142:HIS:CE1	1:B:147:LEU:HB2	2.55	0.41
1:B:248:PRO:HD3	1:F:246:ALA:HB3	2.03	0.41
1:G:147:LEU:HD12	1:G:148:PRO:HD2	2.02	0.41
1:A:245:LEU:HD11	1:F:234:GLY:HA3	2.03	0.41
1:E:109:THR:HA	1:E:113:ASP:HB2	2.03	0.41
1:F:183:PRO:HB3	1:F:217:ILE:CD1	2.51	0.41
1:F:199:GLU:HB3	1:F:200:PRO:HD3	2.03	0.41
1:G:37:GLU:O	1:G:40:ALA:HB3	2.21	0.40
1:A:38:ARG:NH2	2:A:301:SO4:O4	2.47	0.40
1:G:71:ILE:HG13	1:G:118:CYS:SG	2.61	0.40
1:F:140:SER:HB2	1:F:157:LYS:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:LYS:HE3	1:H:3:LYS:HB2	1.65	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/255 (93%)	228 (96%)	9 (4%)	0	100	100
1	B	240/255 (94%)	229 (95%)	11 (5%)	0	100	100
1	C	240/255 (94%)	233 (97%)	7 (3%)	0	100	100
1	D	237/255 (93%)	229 (97%)	8 (3%)	0	100	100
1	E	235/255 (92%)	226 (96%)	9 (4%)	0	100	100
1	F	239/255 (94%)	230 (96%)	9 (4%)	0	100	100
1	G	251/255 (98%)	237 (94%)	14 (6%)	0	100	100
1	H	237/255 (93%)	229 (97%)	8 (3%)	0	100	100
All	All	1916/2040 (94%)	1841 (96%)	75 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/197 (94%)	184 (100%)	1 (0%)	88	91
1	B	186/197 (94%)	184 (99%)	2 (1%)	73	76
1	C	186/197 (94%)	185 (100%)	1 (0%)	88	91
1	D	185/197 (94%)	182 (98%)	3 (2%)	62	65
1	E	183/197 (93%)	183 (100%)	0	100	100
1	F	186/197 (94%)	181 (97%)	5 (3%)	44	43
1	G	196/197 (100%)	194 (99%)	2 (1%)	76	79
1	H	185/197 (94%)	178 (96%)	7 (4%)	33	30
All	All	1492/1576 (95%)	1471 (99%)	21 (1%)	67	70

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	B	99	MET
1	B	106	GLN
1	C	106	GLN
1	D	45	LYS
1	D	99	MET
1	D	134	ARG
1	F	24	GLN
1	F	38	ARG
1	F	46	LYS
1	F	62	SER
1	F	63	GLN
1	G	38	ARG
1	G	46	LYS
1	H	3	LYS
1	H	53	ARG
1	H	74	LEU
1	H	99	MET
1	H	128	LYS
1	H	129	GLN
1	H	202	SER

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

Mol	Chain	Res	Type
1	A	25	ASN

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Mol	Chain	Res	Type
1	G	137	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
2	SO4	F	301	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	A	301	-	4,4,4	0.12	0	6,6,6	0.18	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.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	241/255 (94%)	-0.39	3 (1%) 79 83	20, 29, 49, 114	0
1	B	244/255 (95%)	-0.33	3 (1%) 79 83	19, 29, 52, 108	0
1	C	244/255 (95%)	-0.38	4 (1%) 72 77	19, 31, 55, 86	0
1	D	241/255 (94%)	-0.34	2 (0%) 86 89	20, 30, 49, 91	0
1	E	239/255 (93%)	-0.23	6 (2%) 57 64	22, 34, 58, 73	0
1	F	243/255 (95%)	-0.19	9 (3%) 41 49	22, 33, 63, 108	0
1	G	253/255 (99%)	-0.18	10 (3%) 38 46	22, 34, 66, 122	0
1	H	241/255 (94%)	0.19	14 (5%) 23 29	24, 45, 76, 113	0
All	All	1946/2040 (95%)	-0.23	51 (2%) 56 62	19, 32, 63, 122	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	ASN	7.0
1	H	200	PRO	6.4
1	G	195	ASP	5.6
1	A	189	PRO	5.2
1	F	189	PRO	4.7
1	C	188	THR	4.6
1	H	201	GLY	4.4
1	E	250	PHE	4.3
1	E	200	PRO	4.3
1	F	252	ALA	4.2
1	E	188	THR	3.9
1	H	1	MET	3.9
1	B	251	ASN	3.7
1	G	38	ARG	3.7
1	G	193	MET	3.6
1	H	54	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	188	THR	3.4
1	F	188	THR	3.2
1	G	251	ASN	3.2
1	F	61	LEU	3.2
1	A	1	MET	3.1
1	H	52	VAL	3.1
1	F	200	PRO	3.0
1	G	196	SER	2.9
1	F	88	ALA	2.9
1	H	38	ARG	2.8
1	A	188	THR	2.8
1	F	38	ARG	2.8
1	H	250	PHE	2.8
1	C	252	ALA	2.5
1	C	199	GLU	2.5
1	D	197	ASP	2.5
1	G	91	MET	2.5
1	H	202	SER	2.5
1	B	252	ALA	2.4
1	G	194	ASP	2.4
1	G	201	GLY	2.3
1	H	188	THR	2.3
1	G	200	PRO	2.3
1	F	63	GLN	2.3
1	F	224	LEU	2.3
1	G	1	MET	2.3
1	E	199	GLU	2.2
1	E	203	GLU	2.2
1	H	209	ALA	2.2
1	C	187	ALA	2.1
1	H	66	GLU	2.1
1	H	63	GLN	2.0
1	H	19	ALA	2.0
1	E	52	VAL	2.0
1	B	-1	GLN	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	F	301	5/5	0.97	0.12	68,70,71,72	0
3	CL	G	301	1/1	0.97	0.21	67,67,67,67	0
2	SO4	A	301	5/5	0.99	0.11	41,42,44,45	0

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

There are no such residues in this entry.