



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:56 AM GMT

PDB ID : 1W3N  
Title : SULFOLOBUS SOLFATARICUS 2-KETO-3-DEOXYGLUCONATE(KDG)  
ALDOLASE COMPLEX WITH D-KDG  
Authors : Theodossis, A.; Walden, H.; Westwick, E.J.; Connaris, H.; Lambie, H.J.;  
Hough, D.W.; Danson, M.J.; Taylor, G.L.  
Deposited on : 2004-07-17  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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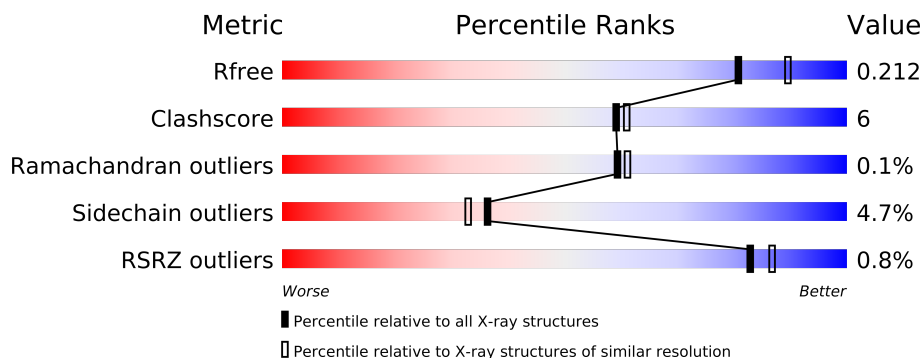
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	294	
1	B	294	
1	C	294	
1	D	294	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SSH	B	1295	-	X
2	SSH	D	1295	-	X
3	GOL	D	1296	-	X

## 2 Entry composition i

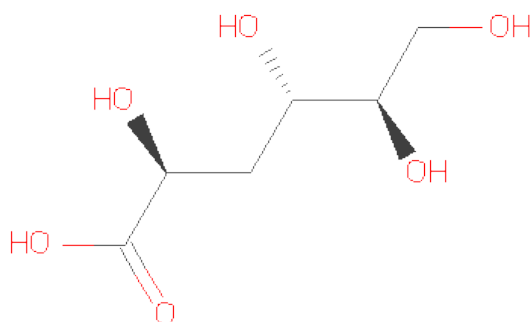
There are 4 unique types of molecules in this entry. The entry contains 10314 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2-KETO-3-DEOXY GLUCONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	3	0
			2349	1516	382	444	7			
1	B	293	Total	C	N	O	S	0	4	0
			2359	1522	386	444	7			
1	C	293	Total	C	N	O	S	0	6	0
			2376	1533	390	446	7			
1	D	293	Total	C	N	O	S	0	4	0
			2356	1521	384	444	7			

- Molecule 2 is 3-DEOXY-D-ARABINO-HEXONICACID (three-letter code: SSH) (formula:  $C_6H_{12}O_6$ ).



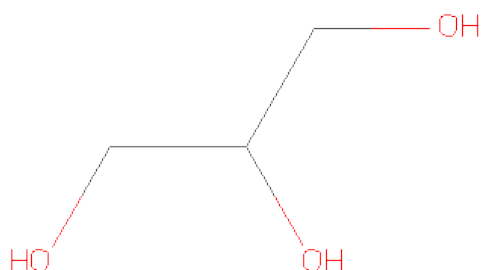
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

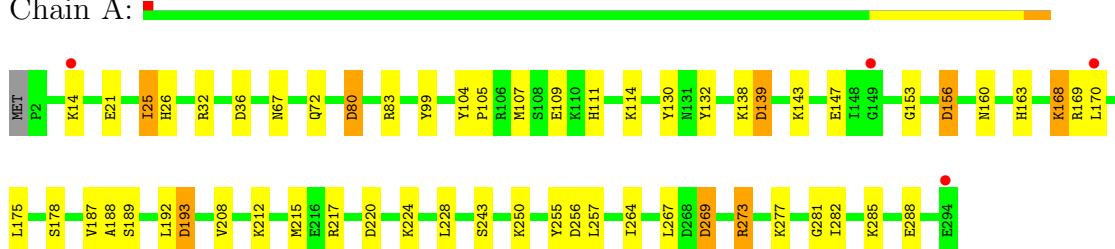
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	182	Total	O	0	0
			182	182		
4	B	226	Total	O	0	0
			226	226		
4	C	195	Total	O	0	0
			195	195		
4	D	209	Total	O	0	0
			209	209		

### 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 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.

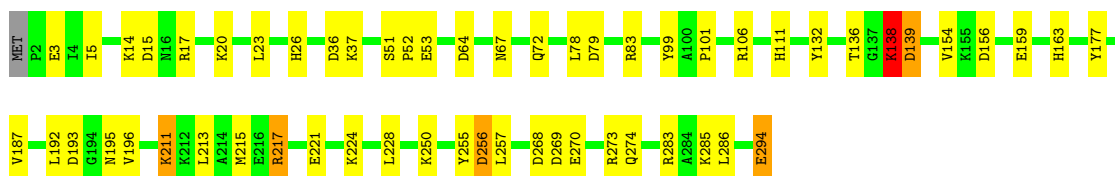
#### • Molecule 1: 2-KETO-3-DEOXY GLUCONATE ALDOLASE

Chain A:



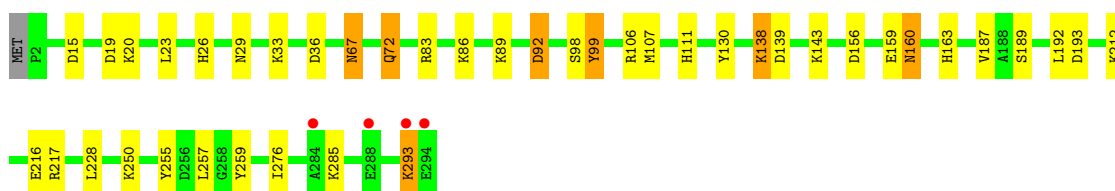
#### • Molecule 1: 2-KETO-3-DEOXY GLUCONATE ALDOLASE

Chain B:



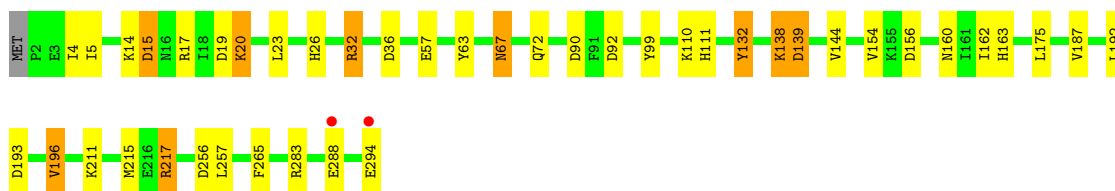
#### • Molecule 1: 2-KETO-3-DEOXY GLUCONATE ALDOLASE

Chain C:



#### • Molecule 1: 2-KETO-3-DEOXY GLUCONATE ALDOLASE

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.80Å 131.27Å 132.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 39.13 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (40.00-2.10) 96.7 (39.13-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.81 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.151 , 0.213 0.156 , 0.212	Depositor DCC
$R_{free}$ test set	8347 reflections (11.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 37.4	EDS
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 83235 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10314	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.02	0/2395	0.96	11/3238 (0.3%)
1	B	1.11	5/2405 (0.2%)	1.03	12/3252 (0.4%)
1	C	1.03	1/2422 (0.0%)	0.96	5/3273 (0.2%)
1	D	1.10	4/2402 (0.2%)	1.02	11/3248 (0.3%)
All	All	1.07	10/9624 (0.1%)	0.99	39/13011 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	LYS	CD-CE	8.08	1.71	1.51
1	B	177	TYR	CD2-CE2	7.75	1.50	1.39
1	B	3	GLU	CD-OE2	7.43	1.33	1.25
1	B	154	VAL	CB-CG1	6.18	1.65	1.52
1	D	154	VAL	CB-CG1	5.90	1.65	1.52
1	C	259	TYR	CG-CD1	5.47	1.46	1.39
1	D	63	TYR	CD2-CE2	5.42	1.47	1.39
1	B	37	LYS	CD-CE	5.36	1.64	1.51
1	D	196	VAL	CB-CG1	5.07	1.63	1.52
1	D	144	VAL	CB-CG2	5.04	1.63	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LYS	CD-CE-NZ	-12.13	83.80	111.70
1	C	36	ASP	CB-CG-OD2	10.57	127.81	118.30
1	D	15	ASP	CB-CG-OD2	10.40	127.66	118.30
1	B	36	ASP	CB-CG-OD2	8.22	125.69	118.30
1	B	15	ASP	CB-CG-OD2	8.21	125.69	118.30
1	D	36	ASP	CB-CG-OD2	7.95	125.46	118.30
1	B	269	ASP	CB-CG-OD2	7.30	124.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	ASP	CB-CG-OD2	7.26	124.84	118.30
1	B	193	ASP	CB-CG-OD2	6.93	124.54	118.30
1	D	90	ASP	CB-CG-OD2	6.91	124.52	118.30
1	D	193	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	256	ASP	CB-CG-OD2	6.87	124.48	118.30
1	D	139	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	80	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	273	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	D	19	ASP	CB-CG-OD2	6.45	124.10	118.30
1	B	64	ASP	CB-CG-OD2	6.43	124.09	118.30
1	C	15	ASP	CB-CG-OD2	6.23	123.91	118.30
1	D	256	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	273	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	156	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	269	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	32	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	C	19	ASP	CB-CG-OD2	5.79	123.52	118.30
1	B	273	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	D	217	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	36	ASP	CB-CG-OD2	5.51	123.26	118.30
1	D	217	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	83	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	139	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	32	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	139	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	268	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	220	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	79	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	193	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	217	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	175	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	C	193	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the



chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2349	0	2407	38	0
1	B	2359	0	2420	32	0
1	C	2376	0	2441	27	0
1	D	2356	0	2416	27	0
2	A	11	0	9	0	0
2	B	11	0	9	1	0
2	C	11	0	9	0	0
2	D	11	0	9	1	0
3	A	6	0	8	2	0
3	B	6	0	8	1	0
3	D	6	0	8	4	0
4	A	182	0	0	6	0
4	B	226	0	0	8	0
4	C	195	0	0	7	0
4	D	209	0	0	8	0
All	All	10314	0	9744	117	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (117) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:107:MET:SD	1:C:107:MET:CE	2.02	1.47
1:B:217:ARG:HD2	1:D:217:ARG:HD2	1.10	1.09
1:A:217:ARG:HD2	1:C:217:ARG:HD2	1.39	1.02
1:A:188:ALA:O	1:A:215[B]:MET:HE1	1.65	0.95
3:A:1296:GOL:H11	4:A:2159:HOH:O	1.69	0.91
3:B:1296:GOL:H11	4:B:2203:HOH:O	1.70	0.90
1:B:217:ARG:CD	1:D:217:ARG:HD2	2.04	0.82
1:B:217:ARG:HD2	1:D:217:ARG:CD	2.04	0.78
1:A:215[B]:MET:CE	1:A:215[B]:MET:HA	2.14	0.77
1:B:213:LEU:HD13	1:B:221:GLU:HG2	1.67	0.77
1:D:217:ARG:HG3	4:D:2061:HOH:O	1.86	0.75
1:A:156:ASP:OD1	1:A:163:HIS:HD2	1.70	0.74
1:A:215[B]:MET:HE2	1:A:215[B]:MET:HA	1.70	0.73
1:D:215[A]:MET:HE3	4:D:2155:HOH:O	1.87	0.73
1:A:83:ARG:NH1	4:A:2058:HOH:O	2.21	0.73
1:C:20:LYS:HD3	4:C:2044:HOH:O	1.89	0.71
1:B:156:ASP:OD1	1:B:163:HIS:HD2	1.75	0.70
1:D:15:ASP:OD1	4:D:2009:HOH:O	2.09	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:283[B]:ARG:HH22	1:B:294:GLU:HG2	1.58	0.69
1:D:32:ARG:HD2	4:D:2023:HOH:O	1.93	0.66
1:B:159:GLU:HG2	1:D:162:ILE:HD12	1.77	0.65
4:B:2204:HOH:O	1:C:111:HIS:HE1	1.81	0.64
1:D:139:ASP:OD2	1:D:163:HIS:HE1	1.81	0.64
1:D:57:GLU:OE2	4:D:2050:HOH:O	2.15	0.63
1:A:281:GLY:O	1:A:285:LYS:HD3	2.01	0.61
1:C:276[B]:ILE:HD11	4:C:2075:HOH:O	2.00	0.61
1:B:20:LYS:HD3	4:B:2059:HOH:O	2.00	0.61
1:B:139:ASP:OD2	1:B:163:HIS:HE1	1.84	0.60
1:D:20:LYS:HD2	4:D:2050:HOH:O	2.01	0.60
1:C:156:ASP:OD1	1:C:163:HIS:HD2	1.84	0.60
1:D:156:ASP:OD1	1:D:163:HIS:HD2	1.84	0.60
1:B:250:LYS:NZ	1:B:256:ASP:HB3	2.17	0.59
1:A:111:HIS:HD2	3:D:1296:GOL:C1	2.16	0.59
4:A:2165:HOH:O	1:D:111:HIS:HE1	1.84	0.59
1:A:217:ARG:HH11	1:C:217:ARG:HH11	1.51	0.58
1:D:67:ASN:C	1:D:67:ASN:HD22	2.06	0.58
1:D:26:HIS:HB2	1:D:257:LEU:HD21	1.87	0.56
1:A:217:ARG:CD	1:C:217:ARG:HD2	2.26	0.56
1:B:106:ARG:NH1	4:B:2099:HOH:O	2.39	0.56
1:C:276[B]:ILE:CD1	4:C:2075:HOH:O	2.52	0.56
1:A:111:HIS:HD2	3:D:1296:GOL:H11	1.69	0.56
1:C:293:LYS:HG2	4:C:2192:HOH:O	2.05	0.56
1:B:159:GLU:HB3	1:D:160:ASN:OD1	2.05	0.55
1:A:160:ASN:N	4:A:2109:HOH:O	2.38	0.55
1:C:86:LYS:O	1:C:89:LYS:HG2	2.07	0.55
1:D:283:ARG:HD3	4:D:2206:HOH:O	2.07	0.54
1:A:111:HIS:HE1	4:D:2189:HOH:O	1.91	0.54
1:A:80:ASP:OD1	1:A:83:ARG:NH2	2.40	0.53
1:A:107:MET:N	4:A:2070:HOH:O	2.40	0.53
1:D:4:ILE:HG12	1:D:211:LYS:HE3	1.92	0.52
1:A:208:VAL:O	1:A:212:LYS:HG3	2.09	0.52
1:B:270:GLU:HG3	1:B:274:GLN:HE21	1.75	0.51
1:B:111:HIS:HE1	4:C:2180:HOH:O	1.93	0.51
1:D:211:LYS:O	1:D:215[A]:MET:HG3	2.11	0.51
1:C:139:ASP:OD2	1:C:163:HIS:HE1	1.94	0.51
1:A:111:HIS:HD2	3:D:1296:GOL:O1	1.94	0.50
1:C:29:ASN:O	1:C:33:LYS:HG3	2.11	0.50
1:A:269:ASP:HB3	1:A:273:ARG:NH2	2.27	0.50
1:C:187:VAL:HG13	1:C:192:LEU:HB2	1.94	0.49
1:A:215[B]:MET:CA	1:A:215[B]:MET:CE	2.90	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168:LYS:NZ	1:A:193:ASP:OD2	2.47	0.48
1:B:211:LYS:HD3	1:B:215[A]:MET:SD	2.54	0.47
1:A:169:ARG:HG2	1:A:170:LEU:HD12	1.95	0.47
1:B:138:LYS:HZ3	1:B:138:LYS:HG3	1.14	0.47
1:A:26:HIS:HB2	1:A:257:LEU:HD21	1.96	0.47
1:B:5:ILE:HB	1:B:196:VAL:HG22	1.96	0.47
4:B:2189:HOH:O	1:C:106:ARG:HD2	2.15	0.47
1:B:213:LEU:CD1	1:B:221:GLU:HG2	2.41	0.47
1:A:139:ASP:OD2	1:A:163:HIS:HE1	1.97	0.47
1:B:17:ARG:HH11	1:B:17:ARG:HG2	1.79	0.47
1:B:250:LYS:HA	1:B:255:TYR:O	2.14	0.47
1:A:264:ILE:HA	4:A:2159:HOH:O	2.14	0.47
1:B:101:PRO:O	1:B:138:LYS:HD3	2.14	0.47
1:B:228:LEU:HD21	1:B:285:LYS:HD3	1.96	0.46
1:C:216:GLU:O	1:C:217:ARG:HB2	2.15	0.46
1:C:217:ARG:HA	1:C:217:ARG:HD3	1.78	0.45
1:B:187:VAL:HG13	1:B:192:LEU:HB2	1.96	0.45
1:A:153:GLY:HA2	1:A:175:LEU:O	2.17	0.45
1:B:136:THR:O	1:B:138:LYS:HD2	2.17	0.45
1:B:111:HIS:CD2	4:C:2179:HOH:O	2.69	0.44
1:D:5:ILE:HB	1:D:196:VAL:HG22	1.98	0.44
1:C:107:MET:CG	1:C:107:MET:CE	2.89	0.44
1:C:26:HIS:HB2	1:C:257:LEU:HD21	1.99	0.44
1:A:187:VAL:HG13	1:A:192:LEU:HB2	1.99	0.44
1:A:250:LYS:HA	1:A:255:TYR:O	2.18	0.43
1:A:111:HIS:CD2	3:D:1296:GOL:O1	2.70	0.43
1:B:26:HIS:HB2	1:B:257:LEU:HD21	2.00	0.43
1:C:276[B]:ILE:HG13	4:C:2186:HOH:O	2.19	0.43
1:A:156:ASP:OD1	1:A:163:HIS:CD2	2.61	0.43
1:D:138:LYS:HB3	1:D:138:LYS:HE3	1.86	0.43
1:A:188:ALA:HB1	1:A:215[B]:MET:HE3	2.00	0.43
1:C:138:LYS:HB3	1:C:138:LYS:HE3	1.71	0.43
1:A:114:LYS:HD3	1:D:265:PHE:CE2	2.54	0.42
1:B:195:ASN:ND2	4:B:2164:HOH:O	2.51	0.42
1:D:139:ASP:OD2	1:D:163:HIS:CE1	2.68	0.42
1:D:187:VAL:HG13	1:D:192:LEU:HB2	2.02	0.42
1:B:101:PRO:O	1:B:138:LYS:HE3	2.19	0.42
1:A:228:LEU:HD22	1:A:282:ILE:HG23	2.01	0.42
1:A:21:GLU:O	1:A:25:ILE:HD12	2.19	0.42
1:C:159:GLU:O	1:C:160:ASN:HB2	2.20	0.42
1:C:250[B]:LYS:HA	1:C:255:TYR:O	2.19	0.42
1:B:283[B]:ARG:NH2	1:B:294:GLU:HG2	2.29	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1296:GOL:O1	1:D:111:HIS:HD2	2.03	0.41
1:B:250:LYS:HZ3	1:B:256:ASP:HB3	1.84	0.41
1:C:72:GLN:OE1	1:C:98:SER:HA	2.20	0.41
1:C:99:TYR:HA	1:C:130:TYR:O	2.20	0.41
1:D:132:TYR:CE1	2:D:1295:SSH:H6C2	2.55	0.41
1:A:104:TYR:HA	1:A:105:PRO:HD3	1.91	0.41
1:D:67:ASN:HB2	1:D:92:ASP:O	2.20	0.41
1:A:189[A]:SER:HB2	1:C:189[A]:SER:O	2.20	0.41
1:A:109:GLU:OE1	1:A:147:GLU:OE1	2.38	0.41
1:B:53[B]:GLU:HG3	4:B:2058:HOH:O	2.21	0.40
1:A:243:SER:HB3	1:A:267:LEU:HD23	2.02	0.40
1:B:51:SER:HB2	1:B:52:PRO:HD2	2.03	0.40
1:A:178:SER:HB3	1:A:187:VAL:HG21	2.03	0.40
2:B:1295:SSH:O5	4:B:2225:HOH:O	2.18	0.40
1:C:67[B]:ASN:HB2	1:C:92:ASP:O	2.22	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	294/294 (100%)	287 (98%)	7 (2%)	0	100	100
1	B	295/294 (100%)	290 (98%)	5 (2%)	0	100	100
1	C	297/294 (101%)	293 (99%)	3 (1%)	1 (0%)	50	49
1	D	295/294 (100%)	288 (98%)	7 (2%)	0	100	100
All	All	1181/1176 (100%)	1158 (98%)	22 (2%)	1 (0%)	59	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	160	ASN

### 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	261/259 (101%)	248 (95%)	13 (5%)	34	30
1	B	262/259 (101%)	249 (95%)	13 (5%)	34	30
1	C	264/259 (102%)	252 (96%)	12 (4%)	38	35
1	D	262/259 (101%)	250 (95%)	12 (5%)	37	34
All	All	1049/1036 (101%)	999 (95%)	50 (5%)	36	32

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	25	ILE
1	A	67	ASN
1	A	72	GLN
1	A	99	TYR
1	A	130	TYR
1	A	132	TYR
1	A	138	LYS
1	A	143	LYS
1	A	168	LYS
1	A	224	LYS
1	A	277	LYS
1	A	288	GLU
1	B	14	LYS
1	B	23	LEU
1	B	67	ASN
1	B	72	GLN
1	B	78	LEU
1	B	83	ARG
1	B	99	TYR
1	B	132	TYR
1	B	138	LYS
1	B	211	LYS
1	B	224	LYS
1	B	286	LEU
1	B	294	GLU

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Mol	Chain	Res	Type
1	C	23	LEU
1	C	67[A]	ASN
1	C	67[B]	ASN
1	C	72	GLN
1	C	92	ASP
1	C	99	TYR
1	C	138	LYS
1	C	143	LYS
1	C	212	LYS
1	C	228	LEU
1	C	285	LYS
1	C	293	LYS
1	D	14	LYS
1	D	17	ARG
1	D	20	LYS
1	D	23	LEU
1	D	67	ASN
1	D	72	GLN
1	D	99	TYR
1	D	110	LYS
1	D	132	TYR
1	D	138	LYS
1	D	288	GLU
1	D	294	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	111	HIS
1	A	163	HIS
1	A	195	ASN
1	B	67	ASN
1	B	111	HIS
1	B	163	HIS
1	B	195	ASN
1	B	274	GLN
1	C	111	HIS
1	C	163	HIS
1	C	195	ASN
1	D	67	ASN
1	D	111	HIS

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Mol	Chain	Res	Type
1	D	163	HIS
1	D	171	ASN
1	D	195	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

7 ligands 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	$\# Z  > 2$
2	SSH	A	1295	1	10,10,11	1.05	0	9,12,14	2.33	4 (44%)
3	GOL	A	1296	-	5,5,5	1.57	1 (20%)	5,5,5	1.44	1 (20%)
2	SSH	B	1295	1	10,10,11	1.13	0	9,12,14	2.99	5 (55%)
3	GOL	B	1296	-	5,5,5	1.33	0	5,5,5	1.50	1 (20%)
2	SSH	C	1295	1	10,10,11	1.60	2 (20%)	9,12,14	3.99	7 (77%)
2	SSH	D	1295	1	10,10,11	1.10	1 (10%)	9,12,14	4.87	6 (66%)
3	GOL	D	1296	-	5,5,5	1.37	0	5,5,5	1.01	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	SSH	A	1295	1	1/1/3/4	0/8/11/14	0/0/0/0
3	GOL	A	1296	-	-	0/4/4/4	0/0/0/0
2	SSH	B	1295	1	-	0/8/11/14	0/0/0/0
3	GOL	B	1296	-	-	0/4/4/4	0/0/0/0
2	SSH	C	1295	1	1/1/3/4	0/8/11/14	0/0/0/0
2	SSH	D	1295	1	-	0/8/11/14	0/0/0/0
3	GOL	D	1296	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1295	SSH	O2-C1	-4.10	1.18	1.30
3	A	1296	GOL	O2-C2	2.51	1.51	1.43
2	C	1295	SSH	O5-C5	2.21	1.48	1.43
2	D	1295	SSH	C3-C4	2.00	1.60	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1295	SSH	O5-C5-C6	-9.81	86.33	109.20
2	C	1295	SSH	O6-C6-C5	-8.97	90.98	111.05
2	D	1295	SSH	O6-C6-C5	-6.30	96.95	111.05
2	B	1295	SSH	O1-C1-C2	-5.96	111.18	128.13
2	D	1295	SSH	O5-C5-C4	-5.46	99.17	109.83
2	A	1295	SSH	O1-C1-C2	-5.13	113.54	128.13
2	D	1295	SSH	O1-C1-C2	-4.56	115.16	128.13
2	C	1295	SSH	C6-C5-C4	-4.49	104.22	112.45
2	B	1295	SSH	O6-C6-C5	-4.18	101.69	111.05
2	D	1295	SSH	O4-C4-C5	-4.07	101.89	109.83
2	B	1295	SSH	O5-C5-C4	-3.40	103.20	109.83
2	C	1295	SSH	O5-C5-C6	-3.12	101.92	109.20
2	C	1295	SSH	O2-C1-O1	3.12	129.67	122.54
2	C	1295	SSH	O4-C4-C5	-3.04	103.89	109.83
2	A	1295	SSH	O6-C6-C5	-2.73	104.95	111.05
3	B	1296	GOL	O2-C2-C3	2.71	120.58	108.22
2	C	1295	SSH	O4-C4-C3	-2.66	103.26	108.84
2	B	1295	SSH	C6-C5-C4	2.62	117.26	112.45
2	B	1295	SSH	C3-C4-C5	-2.59	109.75	113.41
2	C	1295	SSH	O1-C1-C2	-2.47	121.11	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1295	SSH	O4-C4-C3	2.41	113.91	108.84
3	A	1296	GOL	O2-C2-C3	2.32	118.77	108.22
2	A	1295	SSH	O5-C5-C6	-2.09	104.33	109.20
2	A	1295	SSH	O5-C5-C4	-2.05	105.83	109.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1295	SSH	C2
2	C	1295	SSH	C2

There are no torsion outliers.

There are no ring outliers.

## 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, 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	293/294 (99%)	-0.11	4 (1%) 72 76	13, 22, 38, 64	0
1	B	293/294 (99%)	-0.40	0 100 100	11, 18, 31, 53	0
1	C	293/294 (99%)	-0.14	4 (1%) 72 76	13, 21, 38, 65	0
1	D	293/294 (99%)	-0.33	2 (0%) 84 88	11, 18, 34, 64	0
All	All	1172/1176 (99%)	-0.24	10 (0%) 83 85	11, 20, 36, 65	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	GLU	4.4
1	C	294	GLU	3.5
1	A	170	LEU	3.0
1	C	293	LYS	2.9
1	D	294	GLU	2.6
1	A	14	LYS	2.5
1	C	288	GLU	2.4
1	A	149	GLY	2.3
1	C	284	ALA	2.1
1	D	288	GLU	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	D	1296	6/6	0.18	3.41	25,31,33,37	0
2	SSH	D	1295	11/12	0.16	3.30	2,16,23,33	0
2	SSH	B	1295	11/12	0.12	2.68	2,16,43,43	0
2	SSH	A	1295	11/12	0.15	1.30	2,24,43,44	0
2	SSH	C	1295	11/12	0.16	1.27	2,2,15,33	0
3	GOL	A	1296	6/6	0.15	1.22	28,31,33,36	0
3	GOL	B	1296	6/6	0.12	0.78	23,26,28,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.