



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:21 AM BST

PDB ID : 1W3T
Title : Sulfolobus solfataricus 2-keto-3-deoxygluconate (KDG) aldolase complex with D-KDGal, D-Glyceraldehyde and pyruvate
Authors : Theodossis, A.; Walden, H.; Westwick, E.J.; Connaris, H.; Lambie, H.J.; Hough, D.W.; Danson, M.J.; Taylor, G.L.
Deposited on : 2004-07-19
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

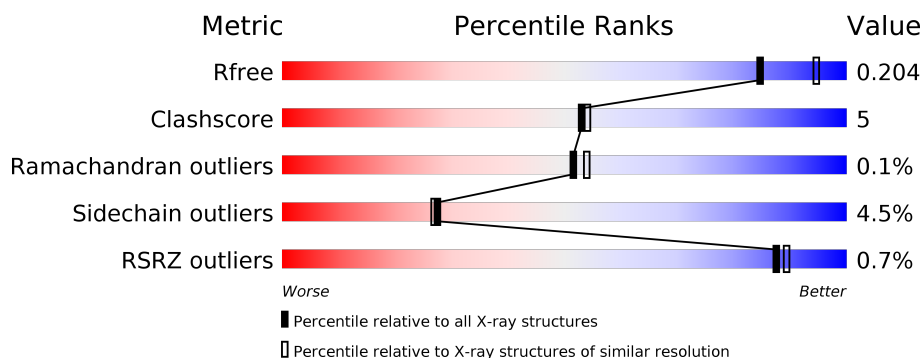
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 ≥ 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	294	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 87%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> • </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 87% 10% </div> </div>
1	B	294	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> • </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 84% 14% </div> </div>
1	C	294	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 83%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> • </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 83% 15% </div> </div>
1	D	294	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 86%; height: 10px; background-color: green;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> • </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 86% 12% </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RSH	A	1295	X	-	-	-
2	RSH	B	1295	X	-	-	-
2	RSH	C	1295	X	-	-	-
2	RSH	D	1295	X	-	-	-
4	3GR	A	1297	X	X	-	-
4	3GR	B	1297	X	-	-	-
4	3GR	C	1297	X	X	-	-
4	3GR	D	1297	X	X	-	-
5	GOL	D	1298	-	-	X	-

2 Entry composition [i](#)

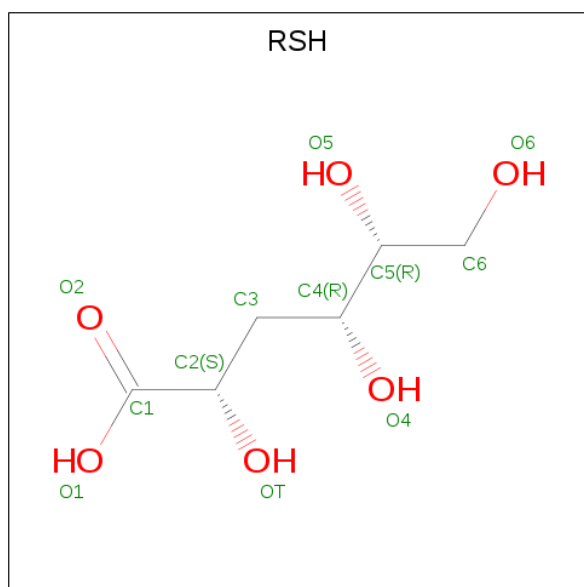
There are 6 unique types of molecules in this entry. The entry contains 10322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-KETO-3-DEOXY GLUCONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	2	0
			2340	1511	381	441	7			
1	B	293	Total	C	N	O	S	0	3	0
			2350	1517	385	441	7			
1	C	293	Total	C	N	O	S	0	3	0
			2351	1517	385	442	7			
1	D	293	Total	C	N	O	S	0	3	0
			2350	1517	385	441	7			

- Molecule 2 is 3-DEOXY-D-LYXO-HEXONIC ACID (three-letter code: RSH) (formula: $C_6H_{12}O_6$).



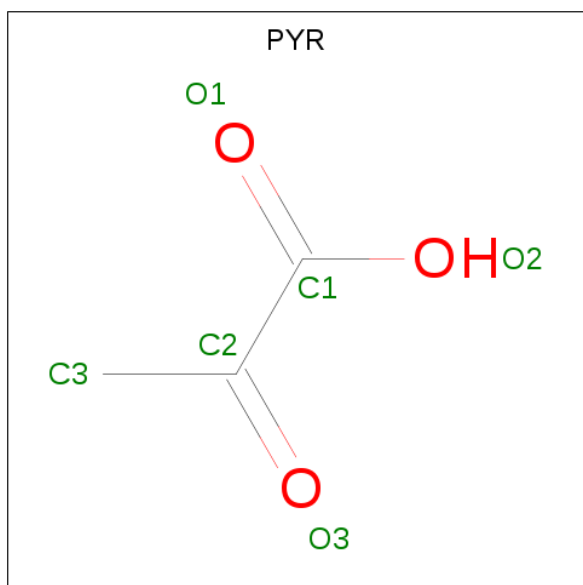
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		

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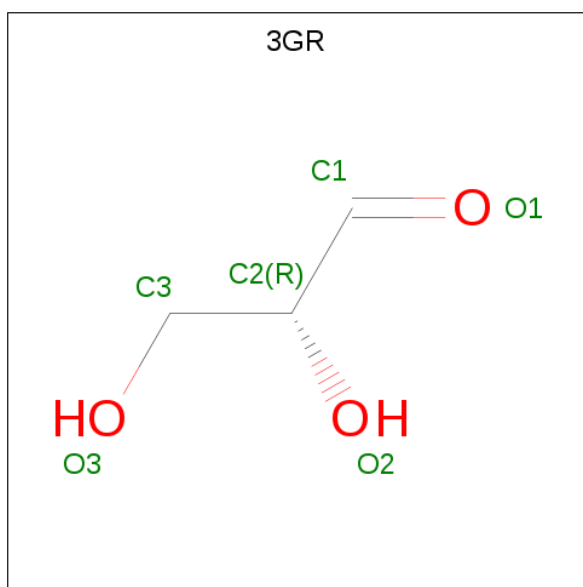
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	C	1	Total	C	O	0	0
			5	3	2		
3	D	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is D-Glyceraldehyde (three-letter code: 3GR) (formula: $C_3H_6O_3$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

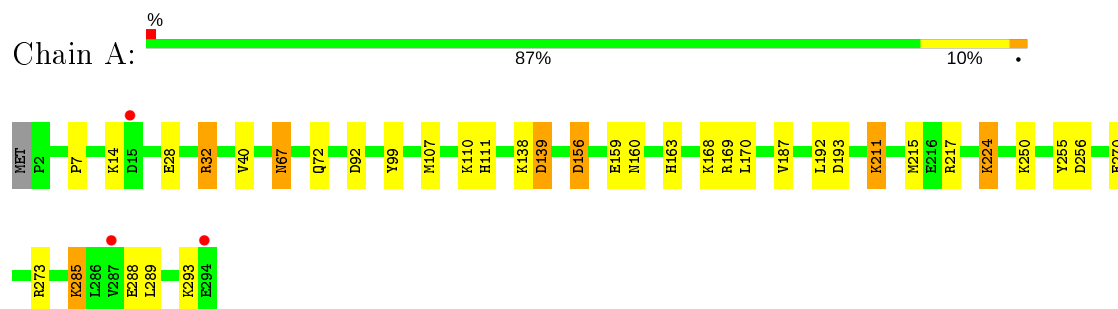
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	188	Total	O	0	0
			188	188		
6	B	224	Total	O	0	0
			224	224		
6	C	193	Total	O	0	0
			193	193		
6	D	214	Total	O	0	0
			214	214		

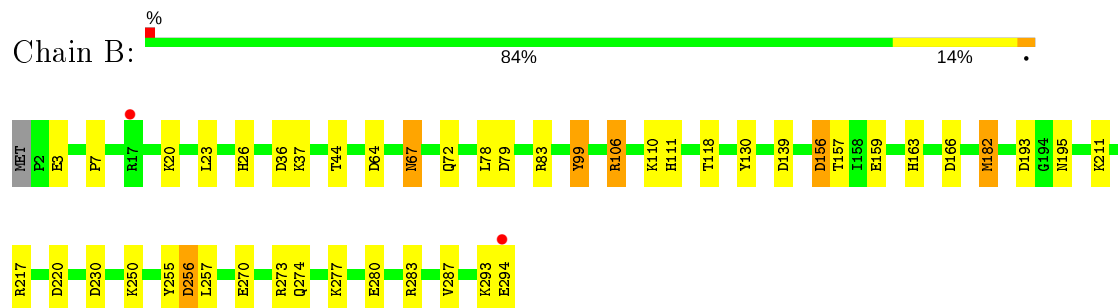
3 Residue-property plots

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.

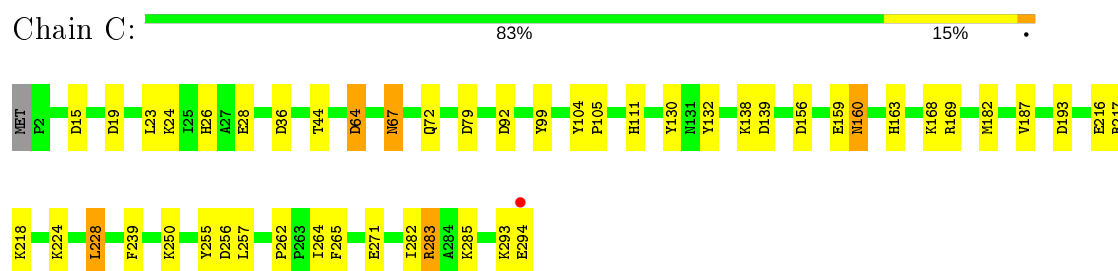
• Molecule 1: 2-KETO-3-DEOXY GLUCONATE ALDOLASE



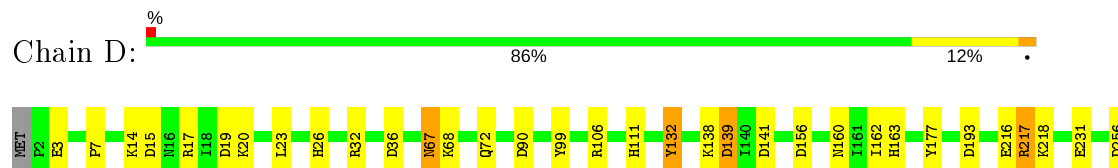
• Molecule 1: 2-KETO-3-DEOXY GLUCONATE ALDOLASE



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



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.43 Å 131.73 Å 132.86 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 39.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.10) 99.9 (39.80-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.06 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.150 , 0.204 0.152 , 0.204	Depositor DCC
R_{free} test set	8678 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10322	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PYR, 3GR, RSH

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	0.96	1/2386 (0.0%)	0.91	5/3226 (0.2%)
1	B	1.05	2/2396 (0.1%)	0.98	11/3240 (0.3%)
1	C	0.98	2/2397 (0.1%)	1.06	12/3240 (0.4%)
1	D	1.07	3/2396 (0.1%)	0.97	9/3240 (0.3%)
All	All	1.02	8/9575 (0.1%)	0.98	37/12946 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	GLU	CD-OE2	9.38	1.35	1.25
1	D	177	TYR	CD2-CE2	7.01	1.49	1.39
1	D	132	TYR	CD2-CE2	6.38	1.49	1.39
1	A	40	VAL	CB-CG2	5.85	1.65	1.52
1	C	169	ARG	CD-NE	-5.58	1.36	1.46
1	D	3	GLU	CD-OE1	-5.20	1.20	1.25
1	B	37	LYS	CD-CE	5.17	1.64	1.51
1	C	187	VAL	CB-CG2	5.08	1.63	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	ARG	NE-CZ-NH2	-19.25	110.67	120.30
1	C	169	ARG	NE-CZ-NH1	14.12	127.36	120.30
1	C	36	ASP	CB-CG-OD2	9.06	126.45	118.30
1	A	32	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	C	193	ASP	CB-CG-OD2	7.60	125.14	118.30
1	B	193	ASP	CB-CG-OD2	7.33	124.90	118.30
1	D	15	ASP	CB-CG-OD2	7.15	124.73	118.30
1	A	256	ASP	CB-CG-OD2	6.71	124.33	118.30
1	B	182	MET	CG-SD-CE	-6.46	89.86	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	ASP	CB-CG-OD2	6.44	124.09	118.30
1	B	36	ASP	CB-CG-OD2	6.34	124.01	118.30
1	D	90	ASP	CB-CG-OD2	6.33	123.99	118.30
1	B	256	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	79	ASP	CB-CG-OD1	6.32	123.99	118.30
1	C	182	MET	CG-SD-CE	-6.29	90.14	100.20
1	C	256	ASP	CB-CG-OD2	6.08	123.78	118.30
1	C	64	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	139	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	156	ASP	CB-CG-OD2	5.92	123.62	118.30
1	B	230	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	169	ARG	CG-CD-NE	-5.86	99.50	111.80
1	A	193	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	19	ASP	CB-CG-OD2	5.57	123.32	118.30
1	B	166	ASP	CB-CG-OD2	5.53	123.28	118.30
1	D	256	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	19	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	15	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	217	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	169	ARG	CD-NE-CZ	5.27	130.97	123.60
1	D	141	ASP	CB-CG-OD1	5.23	123.00	118.30
1	B	64	ASP	CB-CG-OD2	5.21	122.98	118.30
1	D	193	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	79	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	220	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	156	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	273	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	D	139	ASP	CB-CG-OD2	5.01	122.81	118.30

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	2340	0	2401	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2350	0	2413	34	0
1	C	2351	0	2414	24	0
1	D	2350	0	2413	23	0
2	A	11	0	3	0	0
2	B	11	0	0	2	0
2	C	11	0	5	2	0
2	D	11	0	2	0	0
3	A	5	0	1	1	0
3	B	5	0	2	1	0
3	C	5	0	3	1	0
3	D	5	0	1	1	0
4	A	6	0	4	0	0
4	B	6	0	1	0	0
4	C	6	0	2	1	0
4	D	6	0	1	0	0
5	A	6	0	8	2	0
5	B	6	0	8	2	0
5	C	6	0	8	3	0
5	D	6	0	8	6	0
6	A	188	0	0	5	0
6	B	224	0	0	10	0
6	C	193	0	0	5	0
6	D	214	0	0	5	0
All	All	10322	0	9698	103	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 5.

All (103) 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:B:217:ARG:HD2	1:D:217:ARG:HD2	1.24	1.14
5:B:1298:GOL:H11	6:B:2194:HOH:O	1.47	1.12
1:A:217:ARG:HD2	1:C:217:ARG:HD2	1.58	0.83
1:A:270:GLU:OE1	1:A:273:ARG:NH1	2.12	0.82
1:B:111:HIS:HD2	5:C:1298:GOL:H11	1.46	0.80
1:D:67:ASN:HD21	1:D:68:LYS:HE2	1.45	0.79
1:C:67:ASN:HD22	1:C:67:ASN:H	1.31	0.79
1:A:215[A]:MET:HE3	6:A:2001:HOH:O	1.83	0.78
1:A:7:PRO:HG3	3:A:1296:PYR:H33	1.67	0.75
1:D:67:ASN:ND2	1:D:68:LYS:HE2	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2082:HOH:O	5:D:1298:GOL:H2	1.89	0.71
1:B:110:LYS:HB3	1:B:110:LYS:NZ	2.06	0.71
1:B:270:GLU:HG3	1:B:274:GLN:HE21	1.56	0.71
1:D:7:PRO:HG3	3:D:1296:PYR:H33	1.72	0.71
1:D:156:ASP:OD1	1:D:163:HIS:HD2	1.75	0.68
1:B:106:ARG:NH1	6:B:2098:HOH:O	2.26	0.68
1:B:157:THR:HG21	2:B:1295:RSH:O5	1.94	0.67
1:A:156:ASP:OD1	1:A:163:HIS:HD2	1.77	0.67
1:C:24:LYS:NZ	1:C:64:ASP:OD2	2.26	0.67
1:A:111:HIS:HD2	5:D:1298:GOL:O3	1.78	0.67
5:C:1298:GOL:H11	6:C:2173:HOH:O	1.96	0.66
1:B:156:ASP:OD1	1:B:163:HIS:HD2	1.78	0.66
1:C:26:HIS:HB2	1:C:257:LEU:HD21	1.78	0.65
1:B:20:LYS:HD3	6:B:2055:HOH:O	1.96	0.65
4:C:1297:3GR:H1C2	6:C:2093:HOH:O	1.99	0.63
1:B:283[B]:ARG:HH22	1:B:294:GLU:CB	2.11	0.63
1:B:139:ASP:OD2	1:B:163:HIS:HE1	1.83	0.62
1:B:182:MET:CE	6:B:2175:HOH:O	2.46	0.62
1:D:139:ASP:OD2	1:D:163:HIS:HE1	1.84	0.60
6:B:2195:HOH:O	1:C:111:HIS:HE1	1.85	0.60
1:C:139:ASP:OD2	1:C:163:HIS:HE1	1.84	0.60
1:D:32:ARG:HD2	6:D:2020:HOH:O	2.01	0.59
1:A:111:HIS:HE1	6:D:2193:HOH:O	1.85	0.59
1:A:107:MET:HG2	5:D:1298:GOL:H31	1.84	0.58
5:A:1298:GOL:H11	1:D:111:HIS:HD2	1.69	0.57
6:A:2175:HOH:O	1:D:111:HIS:HE1	1.87	0.57
1:C:44:THR:OG1	2:C:1295:RSH:O2	2.17	0.56
1:A:169:ARG:HG2	1:A:170:LEU:HD23	1.87	0.56
1:A:160:ASN:N	6:A:2116:HOH:O	2.38	0.56
1:B:293:LYS:O	1:B:294:GLU:CB	2.53	0.55
1:A:159:GLU:HB3	1:C:160:ASN:OD1	2.06	0.55
1:A:111:HIS:CD2	5:D:1298:GOL:O3	2.59	0.55
1:C:156:ASP:OD1	1:C:163:HIS:HD2	1.89	0.55
1:B:250:LYS:HA	1:B:255:TYR:O	2.07	0.54
1:B:111:HIS:HE1	6:C:2174:HOH:O	1.90	0.54
1:C:67:ASN:H	1:C:67:ASN:ND2	2.05	0.54
1:B:44:THR:OG1	2:B:1295:RSH:O2	2.11	0.54
1:A:224:LYS:HE3	6:A:2142:HOH:O	2.07	0.53
1:D:26:HIS:HB2	1:D:257:LEU:HD21	1.90	0.53
1:B:7:PRO:HG3	3:B:1296:PYR:H33	1.91	0.53
1:B:159:GLU:HG2	1:D:162:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:LYS:O	1:C:28:GLU:HG3	2.07	0.53
1:B:110:LYS:HZ3	1:B:110:LYS:HB3	1.69	0.53
1:B:293:LYS:O	1:B:294:GLU:HB2	2.11	0.51
1:D:216:GLU:OE1	1:D:218:LYS:HE3	2.10	0.50
1:C:216:GLU:OE1	1:C:218:LYS:HE3	2.12	0.50
1:C:293:LYS:HG3	6:C:2190:HOH:O	2.11	0.50
1:D:293:LYS:O	1:D:294:GLU:HB3	2.12	0.50
1:D:231:GLU:OE1	6:D:2166:HOH:O	2.19	0.49
1:D:264:ILE:HD12	5:D:1298:GOL:H32	1.93	0.49
1:D:67:ASN:HD22	1:D:67:ASN:C	2.15	0.48
1:A:139:ASP:OD2	1:A:163:HIS:HE1	1.97	0.48
1:B:67:ASN:HD22	1:B:67:ASN:C	2.17	0.47
1:A:67:ASN:C	1:A:67:ASN:HD22	2.16	0.47
1:D:264:ILE:CD1	5:D:1298:GOL:H32	2.45	0.47
1:C:239:PHE:CD2	1:C:271:GLU:HG2	2.50	0.47
1:B:277:LYS:HE3	6:B:2211:HOH:O	2.15	0.47
1:A:211:LYS:HD3	1:A:215[A]:MET:SD	2.56	0.46
1:B:195:ASN:ND2	6:B:2155:HOH:O	2.49	0.46
1:B:26:HIS:HB2	1:B:257:LEU:HD21	1.98	0.46
1:A:217:ARG:HD3	1:A:217:ARG:HA	1.78	0.46
1:D:278:LYS:HE3	6:D:2206:HOH:O	2.16	0.46
1:C:264:ILE:HA	6:C:2173:HOH:O	2.15	0.45
1:D:217:ARG:HG3	6:D:2156:HOH:O	2.16	0.45
1:B:78:LEU:HD21	1:B:118:THR:HG21	1.98	0.45
1:B:283[A]:ARG:NH2	6:B:2216:HOH:O	2.48	0.45
5:A:1298:GOL:C1	1:D:111:HIS:HD2	2.30	0.45
1:B:283[B]:ARG:O	1:B:287:VAL:HG23	2.16	0.45
2:C:1295:RSH:H4	3:C:1296:PYR:O1	2.13	0.45
1:A:28:GLU:O	1:A:32:ARG:HG3	2.17	0.45
1:C:104:TYR:HA	1:C:105:PRO:HD3	1.82	0.44
5:B:1298:GOL:H11	1:C:111:HIS:HD2	1.83	0.44
1:C:262:PRO:HB3	1:C:265:PHE:CE2	2.53	0.43
1:B:283[B]:ARG:HH22	1:B:294:GLU:HB3	1.81	0.43
1:B:159:GLU:HB3	1:D:160:ASN:OD1	2.18	0.43
1:A:250:LYS:HA	1:A:255:TYR:O	2.18	0.43
1:B:250:LYS:HD2	1:B:256:ASP:HB3	1.99	0.43
1:B:111:HIS:CD2	5:C:1298:GOL:H11	2.38	0.43
1:A:187:VAL:HG13	1:A:192:LEU:HB2	2.01	0.42
1:B:277:LYS:CE	6:B:2211:HOH:O	2.68	0.42
1:C:168:LYS:HA	1:C:168:LYS:HD3	1.83	0.42
1:C:250:LYS:HA	1:C:255:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:MET:HE3	6:B:2175:HOH:O	2.17	0.42
1:A:285:LYS:O	1:A:289:LEU:HG	2.20	0.42
1:B:99:TYR:HA	1:B:130:TYR:O	2.20	0.41
1:C:139:ASP:OD2	1:C:163:HIS:CE1	2.69	0.41
1:A:67:ASN:HB2	1:A:92:ASP:O	2.21	0.41
1:B:277:LYS:HE2	1:B:280:GLU:OE1	2.21	0.41
1:C:228:LEU:HD13	1:C:282:ILE:HG23	2.01	0.41
1:D:139:ASP:OD2	1:D:163:HIS:CE1	2.69	0.41
1:C:159:GLU:O	1:C:160:ASN:HB2	2.21	0.41
1:C:283[B]:ARG:HH12	1:C:294:GLU:HG3	1.86	0.40
1:D:156:ASP:OD1	1:D:163:HIS:CD2	2.64	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	293/294 (100%)	287 (98%)	6 (2%)	0	100	100
1	B	294/294 (100%)	287 (98%)	7 (2%)	0	100	100
1	C	294/294 (100%)	287 (98%)	6 (2%)	1 (0%)	41	41
1	D	294/294 (100%)	289 (98%)	5 (2%)	0	100	100
All	All	1175/1176 (100%)	1150 (98%)	24 (2%)	1 (0%)	51	54

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	260/259 (100%)	248 (95%)	12 (5%)	27	26
1	B	261/259 (101%)	254 (97%)	7 (3%)	44	48
1	C	261/259 (101%)	248 (95%)	13 (5%)	24	23
1	D	261/259 (101%)	245 (94%)	16 (6%)	18	16
All	All	1043/1036 (101%)	995 (95%)	48 (5%)	27	26

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	67	ASN
1	A	72	GLN
1	A	99	TYR
1	A	110	LYS
1	A	138	LYS
1	A	168	LYS
1	A	211	LYS
1	A	224	LYS
1	A	285	LYS
1	A	288	GLU
1	A	293	LYS
1	B	23	LEU
1	B	67	ASN
1	B	72	GLN
1	B	83	ARG
1	B	99	TYR
1	B	106	ARG
1	B	211	LYS
1	C	23	LEU
1	C	67	ASN
1	C	72	GLN
1	C	92	ASP
1	C	99	TYR

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Mol	Chain	Res	Type
1	C	130	TYR
1	C	132	TYR
1	C	138	LYS
1	C	224	LYS
1	C	228	LEU
1	C	283[A]	ARG
1	C	283[B]	ARG
1	C	285	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	106	ARG
1	D	132	TYR
1	D	138	LYS
1	D	283[A]	ARG
1	D	283[B]	ARG
1	D	285	LYS
1	D	288	GLU
1	D	293	LYS
1	D	294	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) 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	67	ASN
1	C	111	HIS
1	C	163	HIS
1	C	195	ASN
1	D	67	ASN

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Mol	Chain	Res	Type
1	D	111	HIS
1	D	163	HIS
1	D	171	ASN
1	D	195	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](#)

16 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$
5	GOL	A	1298	-	5,5,5	1.42	0	5,5,5	0.78	0
4	3GR	C	1297	-	4,5,5	4.17	3 (75%)	4,5,5	6.73	1 (25%)
4	3GR	A	1297	-	4,5,5	4.22	3 (75%)	4,5,5	7.34	3 (75%)
5	GOL	B	1298	-	5,5,5	1.45	1 (20%)	5,5,5	1.53	1 (20%)
2	RSH	C	1295	1	7,10,11	1.48	2 (28%)	9,12,14	2.42	3 (33%)
3	PYR	C	1296	1	1,4,5	0.25	0	1,4,6	4.98	1 (100%)
3	PYR	A	1296	1	1,4,5	0.36	0	1,4,6	3.09	1 (100%)
3	PYR	B	1296	1	1,4,5	0.01	0	1,4,6	9.25	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RSH	A	1295	1	7,10,11	1.33	1 (14%)	9,12,14	1.70	3 (33%)
5	GOL	D	1298	-	5,5,5	1.31	0	5,5,5	2.17	2 (40%)
3	PYR	D	1296	1	1,4,5	0.93	0	1,4,6	4.84	1 (100%)
2	RSH	B	1295	1	7,10,11	1.33	1 (14%)	9,12,14	2.23	3 (33%)
4	3GR	D	1297	-	4,5,5	4.14	2 (50%)	4,5,5	5.40	1 (25%)
4	3GR	B	1297	-	4,5,5	4.03	2 (50%)	4,5,5	4.98	1 (25%)
2	RSH	D	1295	1	7,10,11	1.48	2 (28%)	9,12,14	1.97	2 (22%)
5	GOL	C	1298	-	5,5,5	1.79	1 (20%)	5,5,5	1.58	1 (20%)

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
5	GOL	A	1298	-	-	1/4/4/4	-
4	3GR	C	1297	-	1/1/1/2	2/3/4/4	-
3	PYR	C	1296	1	-	0/0/2/4	-
5	GOL	B	1298	-	-	0/4/4/4	-
2	RSH	C	1295	1	1/1/3/4	8/9/11/14	-
4	3GR	A	1297	-	1/1/1/2	0/3/4/4	-
3	PYR	A	1296	1	-	0/0/2/4	-
3	PYR	B	1296	1	-	0/0/2/4	-
2	RSH	A	1295	1	1/1/3/4	9/9/11/14	-
5	GOL	D	1298	-	-	2/4/4/4	-
3	PYR	D	1296	1	-	0/0/2/4	-
2	RSH	B	1295	1	1/1/3/4	4/9/11/14	-
4	3GR	D	1297	-	1/1/1/2	3/3/4/4	-
4	3GR	B	1297	-	1/1/1/2	1/3/4/4	-
2	RSH	D	1295	1	1/1/3/4	4/9/11/14	-
5	GOL	C	1298	-	-	2/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1297	3GR	O1-C1	6.90	1.47	1.19
4	C	1297	3GR	O1-C1	6.77	1.46	1.19
4	D	1297	3GR	O1-C1	6.72	1.46	1.19
4	B	1297	3GR	O1-C1	6.63	1.46	1.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1297	3GR	O3-C3	-4.57	1.23	1.42
4	B	1297	3GR	O3-C3	-4.22	1.24	1.42
4	C	1297	3GR	O3-C3	-3.98	1.25	1.42
4	A	1297	3GR	O3-C3	-3.58	1.27	1.42
4	A	1297	3GR	C3-C2	3.30	1.55	1.50
2	D	1295	RSH	C3-C4	2.94	1.57	1.52
2	B	1295	RSH	C3-C4	2.81	1.57	1.52
4	C	1297	3GR	C3-C2	2.76	1.54	1.50
2	A	1295	RSH	C5-C4	2.46	1.59	1.52
5	C	1298	GOL	O2-C2	2.35	1.50	1.43
2	C	1295	RSH	C3-C4	2.34	1.56	1.52
2	D	1295	RSH	C5-C4	2.28	1.58	1.52
2	C	1295	RSH	C5-C4	2.26	1.58	1.52
5	B	1298	GOL	O2-C2	2.16	1.49	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1297	3GR	O3-C3-C2	13.79	132.52	112.40
4	C	1297	3GR	O3-C3-C2	13.20	131.65	112.40
4	D	1297	3GR	O3-C3-C2	10.74	128.06	112.40
4	B	1297	3GR	O3-C3-C2	9.69	126.53	112.40
3	B	1296	PYR	C3-C2-C1	9.25	125.38	112.59
2	C	1295	RSH	C2-C3-C4	-5.81	108.13	113.43
3	C	1296	PYR	C3-C2-C1	4.98	119.47	112.59
3	D	1296	PYR	C3-C2-C1	4.84	119.29	112.59
4	A	1297	3GR	C3-C2-C1	4.16	117.86	110.54
2	B	1295	RSH	O5-C5-C6	-3.97	99.84	109.14
2	D	1295	RSH	O5-C5-C6	-3.90	99.99	109.14
2	B	1295	RSH	O5-C5-C4	3.51	116.94	109.72
2	B	1295	RSH	O6-C6-C5	-3.22	104.07	111.07
3	A	1296	PYR	C3-C2-C1	3.09	116.87	112.59
2	D	1295	RSH	O5-C5-C4	3.04	115.97	109.72
5	D	1298	GOL	O3-C3-C2	2.99	124.53	110.20
2	A	1295	RSH	O5-C5-C6	-2.88	102.39	109.14
2	A	1295	RSH	C3-C2-C1	2.68	119.35	113.59
4	A	1297	3GR	O2-C2-C1	-2.62	104.01	109.17
5	D	1298	GOL	O2-C2-C3	2.61	120.64	109.12
2	A	1295	RSH	O5-C5-C4	2.57	115.01	109.72
5	B	1298	GOL	O2-C2-C3	2.56	120.41	109.12
2	C	1295	RSH	O5-C5-C6	-2.50	103.28	109.14
5	C	1298	GOL	O2-C2-C3	2.20	118.81	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1295	RSH	C3-C2-C1	-2.19	108.89	113.59

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	1297	3GR	C2
4	A	1297	3GR	C2
2	C	1295	RSH	C2
2	A	1295	RSH	C2
2	B	1295	RSH	C2
4	D	1297	3GR	C2
4	B	1297	3GR	C2
2	D	1295	RSH	C2

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1297	3GR	O2-C2-C3-O3
2	C	1295	RSH	C3-C4-C5-O5
2	C	1295	RSH	C3-C4-C5-C6
2	C	1295	RSH	O4-C4-C5-O5
2	C	1295	RSH	O4-C4-C5-C6
2	C	1295	RSH	C4-C5-C6-O6
2	C	1295	RSH	O5-C5-C6-O6
2	A	1295	RSH	C1-C2-C3-C4
2	A	1295	RSH	C2-C3-C4-C5
2	A	1295	RSH	C3-C4-C5-O5
2	A	1295	RSH	C3-C4-C5-C6
2	A	1295	RSH	O4-C4-C5-O5
2	A	1295	RSH	O4-C4-C5-C6
2	A	1295	RSH	C4-C5-C6-O6
2	A	1295	RSH	O5-C5-C6-O6
5	D	1298	GOL	O1-C1-C2-C3
2	B	1295	RSH	C3-C4-C5-O5
2	B	1295	RSH	C3-C4-C5-C6
2	B	1295	RSH	O4-C4-C5-O5
2	B	1295	RSH	O4-C4-C5-C6
4	D	1297	3GR	O2-C2-C3-O3
4	D	1297	3GR	O1-C1-C2-C3
2	D	1295	RSH	C3-C4-C5-O5
2	D	1295	RSH	C3-C4-C5-C6
2	D	1295	RSH	O4-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
2	D	1295	RSH	O4-C4-C5-C6
4	C	1297	3GR	C1-C2-C3-O3
4	D	1297	3GR	C1-C2-C3-O3
2	C	1295	RSH	C2-C3-C4-C5
5	D	1298	GOL	O1-C1-C2-O2
2	A	1295	RSH	C2-C3-C4-O4
5	C	1298	GOL	O2-C2-C3-O3
5	A	1298	GOL	O2-C2-C3-O3
4	B	1297	3GR	O2-C2-C3-O3
2	C	1295	RSH	C2-C3-C4-O4
5	C	1298	GOL	C1-C2-C3-O3

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1298	GOL	2	0
4	C	1297	3GR	1	0
5	B	1298	GOL	2	0
2	C	1295	RSH	2	0
3	C	1296	PYR	1	0
3	A	1296	PYR	1	0
3	B	1296	PYR	1	0
5	D	1298	GOL	6	0
3	D	1296	PYR	1	0
2	B	1295	RSH	2	0
5	C	1298	GOL	3	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 [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	293/294 (99%)	-0.20	3 (1%) 82 85	12, 20, 35, 63	0
1	B	293/294 (99%)	-0.50	2 (0%) 87 89	10, 17, 30, 56	0
1	C	293/294 (99%)	-0.27	1 (0%) 94 94	10, 18, 35, 60	0
1	D	293/294 (99%)	-0.37	2 (0%) 87 89	9, 17, 31, 61	0
All	All	1172/1176 (99%)	-0.33	8 (0%) 87 89	9, 18, 34, 63	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	GLU	3.3
1	C	294	GLU	2.8
1	B	294	GLU	2.2
1	A	287	VAL	2.1
1	D	288	GLU	2.1
1	D	289	LEU	2.0
1	B	17	ARG	2.0
1	A	15	ASP	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

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(\AA^2)	Q<0.9
5	GOL	C	1298	6/6	0.82	0.20	27,31,35,36	0
4	3GR	B	1297	6/6	0.84	0.25	43,53,55,57	6
4	3GR	C	1297	6/6	0.86	0.18	40,48,51,51	6
4	3GR	A	1297	6/6	0.87	0.21	33,42,44,47	6
4	3GR	D	1297	6/6	0.87	0.21	42,51,53,56	6
5	GOL	D	1298	6/6	0.88	0.21	22,29,33,37	0
5	GOL	A	1298	6/6	0.89	0.22	24,30,31,36	0
5	GOL	B	1298	6/6	0.93	0.15	20,29,31,34	0
2	RSH	A	1295	11/12	0.94	0.14	2,11,14,15	11
3	PYR	B	1296	5/6	0.94	0.12	2,2,7,10	5
2	RSH	B	1295	11/12	0.94	0.18	2,4,10,12	11
2	RSH	D	1295	11/12	0.95	0.14	2,7,10,16	11
3	PYR	A	1296	5/6	0.95	0.12	2,2,9,16	5
3	PYR	D	1296	5/6	0.96	0.10	2,8,17,20	5
2	RSH	C	1295	11/12	0.96	0.13	2,10,15,15	11
3	PYR	C	1296	5/6	0.97	0.09	2,2,9,21	5

6.5 Other polymers

There are no such residues in this entry.