



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:49 AM UTC

PDB ID : 3JRK / pdb_00003jrk
Title : A putative tagatose 1,6-diphosphate aldolase from *Streptococcus pyogenes*
Authors : Fan, Y.; Volkart, L.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2009-09-08
Resolution : 1.97 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 types of validation reports are described at

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

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

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

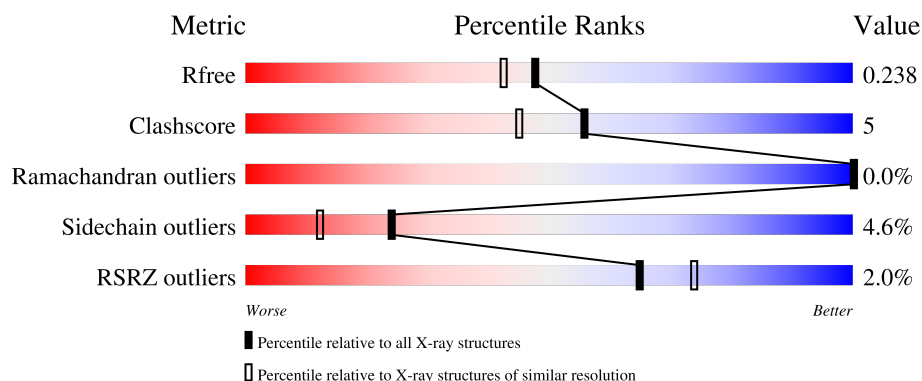
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	91% 8% .
1	B	322	94% 6%
1	C	322	87% 10% .
1	D	322	% 85% 13% .
1	E	322	5% 85% 12% .

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Mol	Chain	Length	Quality of chain
1	F	322	% 93% 6%
1	G	322	2% 88% 10%
1	H	322	7% 86% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21833 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 Tagatose 1,6-diphosphate aldolase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	Se	0	3	0
			2563	1624	425	505	3	6			
1	B	322	Total	C	N	O	S	Se	0	0	0
			2535	1609	418	499	3	6			
1	C	322	Total	C	N	O	S	Se	0	2	0
			2553	1619	420	505	3	6			
1	D	322	Total	C	N	O	S	Se	0	5	0
			2574	1630	423	512	3	6			
1	E	322	Total	C	N	O	S	Se	0	4	0
			2574	1630	428	507	3	6			
1	F	321	Total	C	N	O	S	Se	0	2	0
			2546	1614	422	502	3	5			
1	G	322	Total	C	N	O	S	Se	0	3	0
			2563	1624	424	506	3	6			
1	H	319	Total	C	N	O	S	Se	0	0	0
			2509	1593	414	494	3	5			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	281	Total	O	0	0
			281	281		
3	B	248	Total	O	0	0
			248	248		
3	C	167	Total	O	0	0
			167	167		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	143	Total 143	O 143	0	0
3	E	185	Total 185	O 185	0	0
3	F	176	Total 176	O 176	0	0
3	G	70	Total 70	O 70	0	0
3	H	92	Total 92	O 92	0	0

3 Residue-property plots

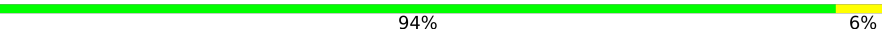
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Tagatose 1,6-diphosphate aldolase 2

Chain A: 



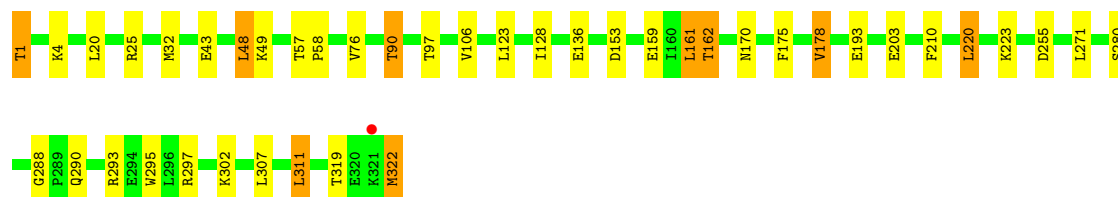
- Molecule 1: Tagatose 1,6-diphosphate aldolase 2

Chain B: 



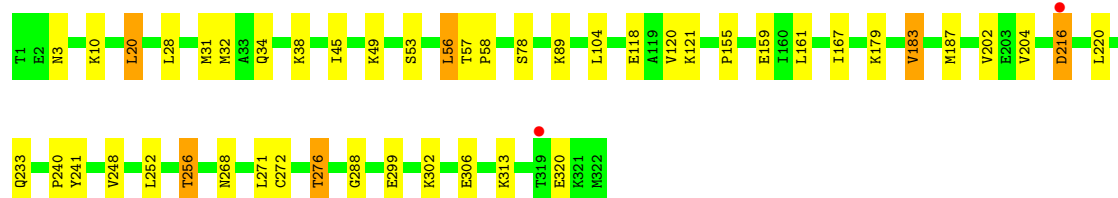
- Molecule 1: Tagatose 1,6-diphosphate aldolase 2

Chain C: 

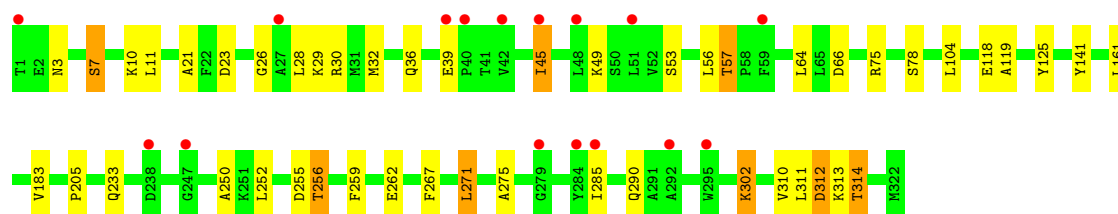
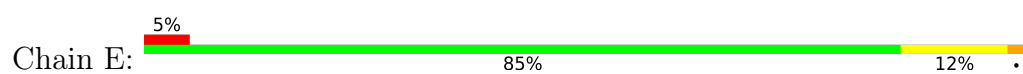


- Molecule 1: Tagatose 1,6-diphosphate aldolase 2

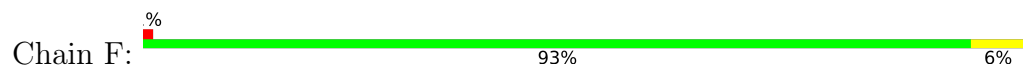
Chain D: 



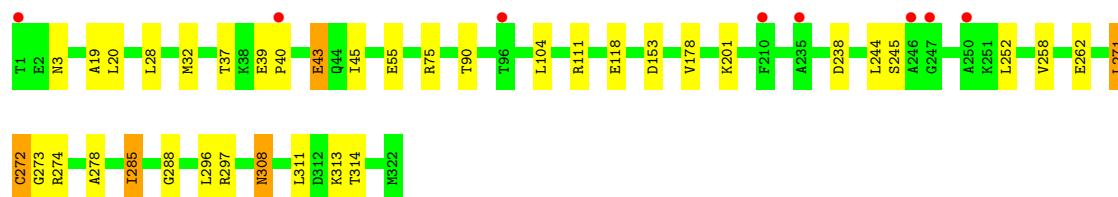
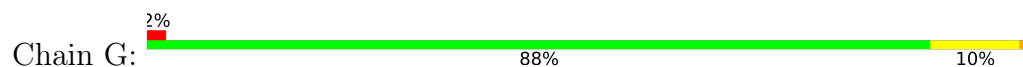
- Molecule 1: Tagatose 1,6-diphosphate aldolase 2



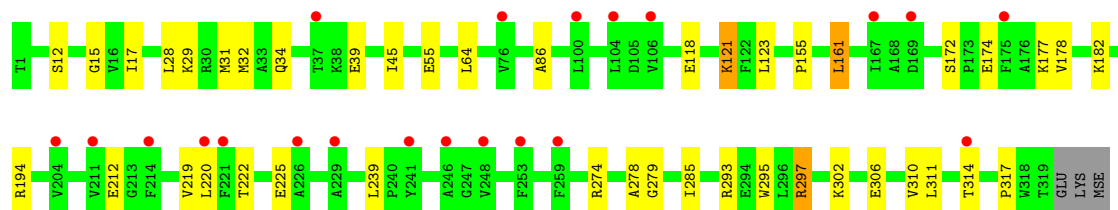
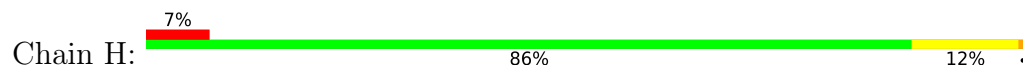
- Molecule 1: Tagatose 1,6-diphosphate aldolase 2



- Molecule 1: Tagatose 1,6-diphosphate aldolase 2



- Molecule 1: Tagatose 1,6-diphosphate aldolase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.52Å 169.73Å 167.05Å 90.00° 94.09° 90.00°	Depositor
Resolution (Å)	50.00 – 1.97 50.00 – 1.97	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-1.97) 96.3 (50.00-1.97)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.188 , 0.230 0.200 , 0.238	Depositor DCC
R_{free} test set	10125 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21833	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.69	0/2603	0.86	3/3502 (0.1%)
1	B	0.71	0/2575	0.87	2/3465 (0.1%)
1	C	0.61	0/2593	0.86	4/3489 (0.1%)
1	D	0.65	0/2614	0.86	2/3519 (0.1%)
1	E	0.66	0/2614	0.87	0/3516
1	F	0.63	0/2587	0.85	0/3483
1	G	0.56	0/2603	0.87	2/3502 (0.1%)
1	H	0.55	0/2550	0.85	0/3435
All	All	0.63	0/20739	0.86	13/27911 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	GLY	CA-C-N	7.14	126.40	118.97
1	A	288	GLY	C-N-CA	7.14	126.40	118.97
1	B	57	THR	CA-C-N	-6.29	113.65	119.82
1	B	57	THR	C-N-CA	-6.29	113.65	119.82
1	C	178	VAL	N-CA-CB	-5.85	105.37	112.33
1	A	105	ASP	N-CA-C	5.75	118.32	111.71
1	D	288	GLY	CA-C-N	5.54	124.73	118.97
1	D	288	GLY	C-N-CA	5.54	124.73	118.97
1	C	178	VAL	CB-CA-C	5.36	116.41	110.62
1	G	288	GLY	CA-C-N	5.32	124.96	119.05
1	G	288	GLY	C-N-CA	5.32	124.96	119.05
1	C	288	GLY	CA-C-N	5.02	124.19	118.97
1	C	288	GLY	C-N-CA	5.02	124.19	118.97

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	2563	0	2536	18	0
1	B	2535	0	2514	11	0
1	C	2553	0	2524	25	0
1	D	2574	0	2538	37	0
1	E	2574	0	2546	44	0
1	F	2546	0	2520	14	0
1	G	2563	0	2534	20	0
1	H	2509	0	2486	27	0
2	A	12	0	16	3	0
2	B	12	0	16	0	0
2	C	6	0	8	0	0
2	D	12	0	16	4	0
2	E	6	0	8	1	0
2	F	6	0	8	0	0
3	A	281	0	0	5	0
3	B	248	0	0	6	0
3	C	167	0	0	2	0
3	D	143	0	0	2	0
3	E	185	0	0	4	0
3	F	176	0	0	4	0
3	G	70	0	0	2	0
3	H	92	0	0	2	0
All	All	21833	0	20270	193	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 (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136[A]:GLU:OE1	1:G:111[A]:ARG:NH2	1.80	1.13
1:D:183:VAL:HG23	1:D:187:MSE:HE3	1.17	1.08
1:H:32:MSE:HE1	1:H:45:ILE:HG12	1.42	1.00
1:D:187:MSE:HE1	1:D:233:GLN:HE21	1.30	0.94
1:E:32:MSE:HE1	1:E:45:ILE:HD13	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:THR:HG23	3:A:686:HOH:O	1.69	0.92
1:E:267:PHE:HZ	1:E:314:THR:HG23	1.38	0.89
1:D:183:VAL:HG23	1:D:187:MSE:CE	2.02	0.89
1:E:57:THR:HG22	1:E:78:SER:HB3	1.55	0.86
1:E:49:LYS:HE2	1:E:66:ASP:OD1	1.76	0.85
1:D:57[A]:THR:HG22	1:D:78:SER:HB3	1.59	0.83
1:D:187:MSE:HE1	1:D:233:GLN:NE2	1.97	0.80
1:D:53[B]:SER:O	1:D:57[B]:THR:HG23	1.81	0.80
1:E:267:PHE:CZ	1:E:314:THR:HG23	2.16	0.80
1:H:28:LEU:HG	1:H:32:MSE:HE2	1.63	0.80
1:D:32:MSE:HE1	1:D:45:ILE:HG12	1.65	0.79
1:G:311:LEU:HA	1:G:314:THR:HG22	1.63	0.79
1:E:32:MSE:HE1	1:E:45:ILE:CD1	2.13	0.77
1:E:310:VAL:O	1:E:314:THR:HB	1.84	0.77
1:E:57:THR:CG2	1:E:78:SER:H	2.01	0.74
1:E:57:THR:HG21	1:E:78:SER:H	1.53	0.74
1:H:212:GLU:HG3	1:H:222:THR:HA	1.72	0.72
1:D:89:LYS:HB2	2:D:324:GOL:H11	1.73	0.71
1:C:97:THR:HG23	3:C:360:HOH:O	1.92	0.69
1:C:25:ARG:HB2	1:C:90:THR:HG21	1.75	0.69
1:H:32:MSE:HG2	1:H:285:ILE:HD11	1.76	0.68
1:F:19:ALA:CB	1:F:271:LEU:HD13	2.24	0.68
1:B:231:ARG:NH1	3:B:731:HOH:O	2.22	0.67
1:E:256:THR:HG21	3:E:1355:HOH:O	1.95	0.66
1:E:252:LEU:O	1:E:256:THR:HG22	1.96	0.66
1:G:245:SER:HB3	1:G:272:CYS:HB2	1.76	0.66
1:H:31:MSE:O	1:H:34:GLN:HG2	1.96	0.66
1:D:183:VAL:CG2	1:D:187:MSE:HE3	2.10	0.65
1:E:252:LEU:O	1:E:256:THR:CG2	2.46	0.64
1:G:258:VAL:O	1:G:262:GLU:HG2	1.98	0.63
1:A:64:LEU:HD11	1:A:121:LYS:HG2	1.79	0.63
1:C:162:THR:HB	1:C:203:GLU:OE2	1.97	0.63
1:F:246:ALA:HA	3:F:1267:HOH:O	2.00	0.62
1:H:15:GLY:O	1:H:317:PRO:HA	2.00	0.62
1:B:170:ASN:CB	3:B:1277:HOH:O	2.47	0.62
1:A:64:LEU:CD1	1:A:121:LYS:HG2	2.29	0.62
1:C:162:THR:HG23	1:C:175:PHE:HZ	1.64	0.61
1:E:57:THR:HG21	1:E:78:SER:N	2.14	0.61
1:D:187:MSE:HE2	1:D:202:VAL:CB	2.31	0.61
1:D:256:THR:HG21	3:D:1023:HOH:O	2.00	0.61
1:D:32:MSE:HE1	1:D:45:ILE:CG1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53[B]:SER:O	1:D:57[B]:THR:CG2	2.47	0.60
1:E:290:GLN:HB2	3:E:561:HOH:O	2.01	0.60
1:F:19:ALA:HB3	1:F:271:LEU:HD13	1.84	0.60
1:E:53:SER:O	1:E:57:THR:HB	2.01	0.60
1:E:312[A]:ASP:OD2	1:E:312[A]:ASP:C	2.45	0.60
1:G:55:GLU:OE2	1:G:297:ARG:HD2	2.02	0.60
1:C:136[A]:GLU:OE1	1:G:111[A]:ARG:CZ	2.47	0.59
1:B:170:ASN:HB2	3:B:1277:HOH:O	2.01	0.59
1:D:241:TYR:H	1:D:268:ASN:HD22	1.51	0.59
1:C:123:LEU:HD21	1:C:161:LEU:HD22	1.85	0.59
1:G:201:LYS:HE3	1:G:271:LEU:HB3	1.84	0.58
2:A:324:GOL:H12	3:A:1140:HOH:O	2.02	0.58
1:E:3:ASN:O	1:E:7:SER:HB2	2.04	0.58
1:D:167:ILE:O	2:D:323:GOL:H12	2.04	0.58
1:E:75:ARG:HA	3:E:1177:HOH:O	2.03	0.57
1:D:187:MSE:HE2	1:D:202:VAL:HB	1.87	0.57
1:D:187:MSE:HE2	1:D:202:VAL:HG11	1.86	0.57
1:C:319:THR:HA	1:C:322:MSE:HE2	1.87	0.56
1:H:55:GLU:OE2	1:H:297:ARG:HD2	2.06	0.56
1:E:267:PHE:HZ	1:E:314:THR:CG2	2.16	0.56
1:E:28:LEU:HG	1:E:32:MSE:HE2	1.88	0.56
1:H:310:VAL:O	1:H:314:THR:HG22	2.06	0.56
1:E:205:PRO:HD3	1:E:233:GLN:NE2	2.21	0.55
1:D:121:LYS:HE3	1:D:159:GLU:OE1	2.06	0.55
1:B:79:GLU:HG2	3:B:1291:HOH:O	2.07	0.55
1:D:118:GLU:O	1:D:155:PRO:HD2	2.06	0.55
1:G:274:ARG:O	1:G:278:ALA:HB2	2.06	0.55
1:H:212:GLU:CG	1:H:222:THR:HA	2.36	0.54
1:F:306:GLU:HG3	3:F:1285:HOH:O	2.07	0.54
1:E:36:GLN:HG3	1:E:285:ILE:CG2	2.38	0.54
1:C:210:PHE:HB3	1:C:220:LEU:HB2	1.90	0.53
1:F:19:ALA:HB1	1:F:271:LEU:HD13	1.89	0.53
1:A:36:GLN:O	2:A:324:GOL:O1	2.25	0.53
1:E:57:THR:HG22	1:E:78:SER:CB	2.32	0.53
1:E:11:LEU:HD11	1:E:119:ALA:HB2	1.90	0.53
2:D:324:GOL:H12	3:D:1328:HOH:O	2.09	0.53
1:D:216[A]:ASP:OD1	1:D:216[A]:ASP:N	2.30	0.53
1:D:187:MSE:HE2	1:D:202:VAL:CG1	2.39	0.52
1:H:174:GLU:HA	1:H:177:LYS:HD2	1.92	0.52
1:B:20:LEU:HD12	1:B:63:ILE:HD12	1.92	0.51
1:A:43:GLU:HG2	3:A:782:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:ALA:HB3	1:G:271:LEU:HG	1.93	0.51
1:H:293:ARG:HD3	1:H:297:ARG:NH1	2.26	0.51
1:G:308:ASN:CG	3:G:1268:HOH:O	2.54	0.51
1:C:322:MSE:HE3	1:C:322:MSE:C	2.36	0.51
1:B:23:ASP:OD1	3:B:922:HOH:O	2.19	0.50
1:E:21:ALA:HB2	1:E:271:LEU:HD12	1.93	0.50
1:F:273:GLY:HA3	3:F:907:HOH:O	2.12	0.50
1:H:12:SER:HB3	1:H:17:ILE:HG13	1.94	0.50
1:A:259:PHE:HA	1:A:262[A]:GLU:HG2	1.94	0.50
1:E:28:LEU:HD23	1:E:45:ILE:HG23	1.94	0.49
1:E:141:TYR:CE2	2:E:323:GOL:H31	2.47	0.49
1:A:1:THR:HA	3:A:1303:HOH:O	2.13	0.49
1:G:245:SER:CB	1:G:272:CYS:HB2	2.42	0.49
1:A:250:ALA:HA	1:A:275:ALA:HB1	1.95	0.48
1:E:32:MSE:HB2	3:E:763:HOH:O	2.12	0.48
1:H:123:LEU:HD11	1:H:161:LEU:HD22	1.95	0.48
1:D:28:LEU:HG	1:D:32:MSE:HE2	1.95	0.48
1:D:53[A]:SER:O	1:D:57[A]:THR:HB	2.13	0.48
1:D:252:LEU:O	1:D:256:THR:CG2	2.62	0.48
1:G:32:MSE:HG2	1:G:285:ILE:HD11	1.96	0.47
1:H:31:MSE:O	1:H:34:GLN:CG	2.62	0.47
1:D:252:LEU:O	1:D:256:THR:HG22	2.15	0.47
1:F:272:CYS:HB2	1:F:273:GLY:HA3	1.96	0.47
1:A:178:VAL:O	1:A:182:LYS:HG2	2.15	0.47
1:E:10:LYS:HD3	1:E:118:GLU:HG2	1.97	0.47
1:E:57:THR:CG2	1:E:78:SER:HB3	2.36	0.47
1:G:43:GLU:H	1:G:43:GLU:CD	2.21	0.47
1:C:223:LYS:HD2	1:E:302:LYS:HG2	1.97	0.47
1:C:162:THR:CG2	1:C:175:PHE:HZ	2.27	0.46
1:F:201:LYS:HD2	1:F:271:LEU:HD23	1.96	0.46
1:F:209:LYS:NZ	1:F:247:GLY:O	2.49	0.46
1:A:320:GLU:HA	3:A:840:HOH:O	2.15	0.46
1:D:20:LEU:HD11	1:D:56:LEU:HB3	1.98	0.46
1:E:29:LYS:HA	1:E:32:MSE:CE	2.45	0.46
1:C:136[A]:GLU:OE1	1:G:111[A]:ARG:NH1	2.48	0.46
1:E:312[A]:ASP:OD2	1:E:313:LYS:N	2.48	0.45
1:F:31:MSE:O	1:F:34:GLN:HG2	2.16	0.45
1:E:205:PRO:HD3	1:E:233:GLN:HE22	1.81	0.45
1:A:33:ALA:HB1	2:A:324:GOL:H2	1.98	0.45
1:C:32:MSE:HE3	1:C:48:LEU:HD12	1.98	0.45
1:H:174:GLU:HB3	3:H:457:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53[B]:SER:HA	1:D:57[B]:THR:HG23	1.98	0.45
1:G:238[A]:ASP:O	1:G:238[A]:ASP:OD2	2.34	0.45
1:F:270:VAL:HG22	1:F:311:LEU:HD21	1.99	0.45
1:G:311:LEU:HA	1:G:314:THR:CG2	2.40	0.45
1:D:179:LYS:O	1:D:183:VAL:HG13	2.17	0.45
1:E:57:THR:HG22	1:E:78:SER:H	1.81	0.45
1:H:29:LYS:HA	1:H:32:MSE:HE3	1.99	0.44
1:A:123:LEU:C	1:A:123:LEU:HD23	2.42	0.44
1:C:123:LEU:HD21	1:C:161:LEU:HB2	1.99	0.44
1:D:240:PRO:HA	1:D:268:ASN:ND2	2.33	0.44
1:F:123:LEU:HD22	1:F:124:LEU:N	2.32	0.44
1:H:311:LEU:HA	1:H:314:THR:HG22	1.99	0.44
1:H:64:LEU:CD1	1:H:121:LYS:HG2	2.48	0.44
1:H:302:LYS:O	1:H:306:GLU:HB2	2.18	0.44
1:B:20:LEU:HD12	1:B:63:ILE:CD1	2.47	0.44
1:A:259:PHE:O	1:A:262[A]:GLU:HG2	2.18	0.44
1:E:23:ASP:HB3	1:E:64:LEU:HG	1.99	0.44
1:G:311:LEU:CA	1:G:314:THR:HG22	2.42	0.44
1:B:321:LYS:HE3	3:B:377:HOH:O	2.18	0.43
1:C:123:LEU:HD23	1:C:159:GLU:HG2	2.00	0.43
1:C:255:ASP:OD2	1:E:255:ASP:OD2	2.35	0.43
1:C:1:THR:HG22	1:C:4:LYS:H	1.83	0.43
1:E:252:LEU:O	1:E:256:THR:HG23	2.17	0.43
1:C:293:ARG:HG2	1:C:297:ARG:NH1	2.34	0.43
1:D:272:CYS:SG	1:D:276:THR:HG22	2.58	0.43
1:H:123:LEU:C	1:H:123:LEU:HD23	2.44	0.43
1:A:15:GLY:O	1:A:317:PRO:HA	2.19	0.43
1:F:273:GLY:CA	3:F:907:HOH:O	2.65	0.43
1:D:241:TYR:H	1:D:268:ASN:ND2	2.16	0.42
1:E:26:GLY:O	1:E:30:ARG:HG3	2.19	0.42
1:D:183:VAL:CG2	1:D:187:MSE:CE	2.85	0.42
1:H:32:MSE:CG	1:H:285:ILE:HD11	2.48	0.42
1:C:25:ARG:CZ	1:C:90:THR:HG23	2.50	0.42
1:D:302:LYS:HE2	1:D:306:GLU:OE1	2.20	0.42
1:H:274:ARG:O	1:H:278:ALA:HB2	2.19	0.42
1:H:279:GLY:HA3	1:H:295:TRP:CZ2	2.54	0.42
1:A:57:THR:N	1:A:58:PRO:CD	2.82	0.42
1:C:1:THR:HG21	1:C:153:ASP:OD2	2.19	0.42
1:C:280:SER:HB3	1:C:295:TRP:CE3	2.54	0.42
1:D:31:MSE:O	1:D:34:GLN:HG2	2.19	0.42
1:G:75:ARG:NH2	3:G:995:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:VAL:O	1:F:285:ILE:HD12	2.20	0.41
1:C:57:THR:N	1:C:58:PRO:CD	2.83	0.41
1:B:118:GLU:O	1:B:155:PRO:HD2	2.20	0.41
1:D:167:ILE:O	2:D:323:GOL:C1	2.68	0.41
1:E:36:GLN:HG3	1:E:285:ILE:HG21	2.02	0.41
1:A:64:LEU:HD13	1:A:121:LYS:HG2	2.01	0.41
1:E:125:TYR:HA	1:E:161:LEU:O	2.21	0.41
1:E:250:ALA:HA	1:E:275:ALA:HB1	2.03	0.41
1:B:5:ARG:NH2	1:B:322:MSE:HG3	2.35	0.41
1:C:203:GLU:HB2	3:C:1160:HOH:O	2.20	0.41
1:D:57[B]:THR:N	1:D:58:PRO:CD	2.84	0.41
1:E:259:PHE:HA	1:E:262:GLU:HG2	2.03	0.41
1:H:86:ALA:HA	1:H:121:LYS:HG3	2.02	0.41
1:A:201:LYS:HE2	1:A:244:LEU:HB3	2.02	0.41
1:B:250:ALA:HA	1:B:275:ALA:HB1	2.02	0.41
1:H:194:ARG:HD2	3:H:602:HOH:O	2.19	0.41
1:G:39:GLU:HA	1:G:40:PRO:HD3	1.91	0.40
1:C:307:LEU:HG	1:C:311:LEU:HD22	2.02	0.40
1:D:248:VAL:HB	1:D:252:LEU:HD23	2.03	0.40
1:H:178:VAL:O	1:H:182:LYS:HG2	2.21	0.40
1:A:121:LYS:HA	1:A:157:TYR:O	2.21	0.40
1:E:45:ILE:H	1:E:45:ILE:HG12	1.69	0.40
1:G:28:LEU:HD23	1:G:45:ILE:HG23	2.03	0.40
1:H:118:GLU:O	1:H:155:PRO:HD2	2.22	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	323/322 (100%)	315 (98%)	8 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	320/322 (99%)	311 (97%)	9 (3%)	0	100	100
1	C	322/322 (100%)	317 (98%)	5 (2%)	0	100	100
1	D	325/322 (101%)	316 (97%)	9 (3%)	0	100	100
1	E	324/322 (101%)	317 (98%)	7 (2%)	0	100	100
1	F	321/322 (100%)	315 (98%)	6 (2%)	0	100	100
1	G	323/322 (100%)	311 (96%)	11 (3%)	1 (0%)	36	27
1	H	317/322 (98%)	307 (97%)	10 (3%)	0	100	100
All	All	2575/2576 (100%)	2509 (97%)	65 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	273	GLY

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	272/263 (103%)	265 (97%)	7 (3%)	40	32
1	B	269/263 (102%)	264 (98%)	5 (2%)	50	44
1	C	271/263 (103%)	250 (92%)	21 (8%)	12	4
1	D	274/263 (104%)	254 (93%)	20 (7%)	13	4
1	E	273/263 (104%)	259 (95%)	14 (5%)	21	10
1	F	270/263 (103%)	261 (97%)	9 (3%)	33	23
1	G	272/263 (103%)	255 (94%)	17 (6%)	16	6
1	H	266/263 (101%)	257 (97%)	9 (3%)	32	22
All	All	2167/2104 (103%)	2065 (95%)	102 (5%)	24	12

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	43	GLU
1	A	96	THR
1	A	121	LYS
1	A	153	ASP
1	A	271	LEU
1	A	287	GLU
1	B	48	LEU
1	B	80	GLU
1	B	123	LEU
1	B	266	LYS
1	B	271	LEU
1	C	1	THR
1	C	20	LEU
1	C	43	GLU
1	C	48	LEU
1	C	49	LYS
1	C	76	VAL
1	C	90	THR
1	C	106	VAL
1	C	128	ILE
1	C	161	LEU
1	C	162	THR
1	C	170	ASN
1	C	178	VAL
1	C	193[A]	GLU
1	C	193[B]	GLU
1	C	220	LEU
1	C	271	LEU
1	C	290	GLN
1	C	302	LYS
1	C	311	LEU
1	C	322	MSE
1	D	3	ASN
1	D	10	LYS
1	D	20	LEU
1	D	38	LYS
1	D	49	LYS
1	D	56	LEU
1	D	104	LEU
1	D	120	VAL
1	D	161	LEU
1	D	183	VAL

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Mol	Chain	Res	Type
1	D	204	VAL
1	D	216[A]	ASP
1	D	216[B]	ASP
1	D	220	LEU
1	D	256	THR
1	D	271	LEU
1	D	276	THR
1	D	299	GLU
1	D	313	LYS
1	D	320	GLU
1	E	7	SER
1	E	39	GLU
1	E	45	ILE
1	E	56	LEU
1	E	57	THR
1	E	104	LEU
1	E	183	VAL
1	E	256	THR
1	E	271	LEU
1	E	302	LYS
1	E	311	LEU
1	E	312[A]	ASP
1	E	312[B]	ASP
1	E	314	THR
1	F	3	ASN
1	F	37	THR
1	F	42	VAL
1	F	48	LEU
1	F	90	THR
1	F	123	LEU
1	F	257	LEU
1	F	271	LEU
1	F	311	LEU
1	G	3	ASN
1	G	20	LEU
1	G	37	THR
1	G	43	GLU
1	G	90	THR
1	G	104	LEU
1	G	118	GLU
1	G	153	ASP
1	G	178	VAL

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Mol	Chain	Res	Type
1	G	244	LEU
1	G	252	LEU
1	G	271	LEU
1	G	272	CYS
1	G	285	ILE
1	G	296	LEU
1	G	308	ASN
1	G	313	LYS
1	H	39	GLU
1	H	121	LYS
1	H	161	LEU
1	H	172	SER
1	H	219	VAL
1	H	220	LEU
1	H	225	GLU
1	H	239	LEU
1	H	297	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	254	GLN
1	B	132	GLN
1	B	137	GLN
1	C	170	ASN
1	C	184	ASN
1	C	290	GLN
1	D	137	GLN
1	D	233	GLN
1	D	268	ASN
1	D	290	GLN
1	E	34	GLN
1	E	132	GLN
1	E	233	GLN
1	F	137	GLN
1	G	35	HIS
1	G	137	GLN
1	G	181	HIS
1	G	228	GLN
1	G	290	GLN
1	G	303	ASN

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Mol	Chain	Res	Type
1	H	137	GLN
1	H	290	GLN
1	H	303	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	GOL	F	323	-	5,5,5	0.40	0	5,5,5	0.23	0
2	GOL	B	323	-	5,5,5	0.46	0	5,5,5	0.19	0
2	GOL	D	324	-	5,5,5	0.49	0	5,5,5	0.51	0
2	GOL	C	323	-	5,5,5	0.37	0	5,5,5	0.27	0
2	GOL	D	323	-	5,5,5	0.67	0	5,5,5	0.82	0
2	GOL	E	323	-	5,5,5	0.42	0	5,5,5	0.56	0
2	GOL	A	324	-	5,5,5	0.42	0	5,5,5	0.30	0
2	GOL	B	324	-	5,5,5	0.35	0	5,5,5	0.39	0
2	GOL	A	323	-	5,5,5	0.36	0	5,5,5	0.39	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	GOL	F	323	-	-	2/4/4/4	-
2	GOL	B	323	-	-	1/4/4/4	-
2	GOL	D	324	-	-	2/4/4/4	-
2	GOL	C	323	-	-	4/4/4/4	-
2	GOL	D	323	-	-	0/4/4/4	-
2	GOL	E	323	-	-	2/4/4/4	-
2	GOL	A	324	-	-	4/4/4/4	-
2	GOL	B	324	-	-	4/4/4/4	-
2	GOL	A	323	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	323	GOL	C1-C2-C3-O3
2	A	324	GOL	C1-C2-C3-O3
2	B	324	GOL	C1-C2-C3-O3
2	C	323	GOL	O2-C2-C3-O3
2	E	323	GOL	C1-C2-C3-O3
2	F	323	GOL	O1-C1-C2-C3
2	E	323	GOL	O2-C2-C3-O3
2	F	323	GOL	O1-C1-C2-O2
2	A	324	GOL	O1-C1-C2-C3
2	B	324	GOL	O1-C1-C2-C3
2	C	323	GOL	O1-C1-C2-C3
2	C	323	GOL	C1-C2-C3-O3
2	D	324	GOL	O1-C1-C2-C3
2	A	323	GOL	O2-C2-C3-O3
2	A	324	GOL	O1-C1-C2-O2
2	A	324	GOL	O2-C2-C3-O3
2	B	324	GOL	O2-C2-C3-O3
2	C	323	GOL	O1-C1-C2-O2
2	B	324	GOL	O1-C1-C2-O2
2	D	324	GOL	O1-C1-C2-O2
2	B	323	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	324	GOL	2	0
2	D	323	GOL	2	0
2	E	323	GOL	1	0
2	A	324	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 ⓘ

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	316/322 (98%)	-0.50	0 100 100	8, 19, 29, 49	3 (0%)
1	B	316/322 (98%)	-0.51	1 (0%) 90 93	12, 19, 30, 51	0
1	C	316/322 (98%)	-0.30	1 (0%) 90 93	10, 25, 34, 50	2 (0%)
1	D	316/322 (98%)	-0.14	2 (0%) 85 90	11, 25, 41, 51	5 (1%)
1	E	316/322 (98%)	0.22	16 (5%) 33 43	10, 26, 49, 60	4 (1%)
1	F	316/322 (98%)	-0.17	2 (0%) 85 90	9, 24, 38, 53	2 (0%)
1	G	316/322 (98%)	0.39	8 (2%) 58 68	10, 30, 45, 56	3 (0%)
1	H	314/322 (97%)	0.73	21 (6%) 24 31	21, 34, 51, 54	0
All	All	2526/2576 (98%)	-0.04	51 (2%) 65 74	8, 25, 43, 60	19 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	45	ILE	3.9
1	H	211	VAL	3.3
1	H	175	PHE	3.3
1	H	37	THR	3.3
1	H	106	VAL	3.2
1	H	214	PHE	3.1
1	H	226	ALA	3.1
1	H	220	LEU	3.0
1	H	204	VAL	2.9
1	H	259	PHE	2.8
1	E	42	VAL	2.8
1	G	247	GLY	2.7
1	H	169	ASP	2.7
1	D	319	THR	2.6
1	H	221	PHE	2.6
1	E	51	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	285	ILE	2.6
1	H	229	ALA	2.6
1	H	253	PHE	2.5
1	H	314	THR	2.5
1	H	76	VAL	2.5
1	B	320	GLU	2.5
1	G	235	ALA	2.5
1	G	1	THR	2.4
1	G	210	PHE	2.4
1	E	27	ALA	2.3
1	E	284	TYR	2.3
1	E	238	ASP	2.3
1	E	48	LEU	2.3
1	G	96	THR	2.3
1	E	247	GLY	2.2
1	D	216[A]	ASP	2.2
1	F	33	ALA	2.2
1	E	39	GLU	2.2
1	E	1	THR	2.2
1	E	292	ALA	2.2
1	H	248	VAL	2.2
1	H	100	LEU	2.2
1	H	104	LEU	2.2
1	G	40	PRO	2.1
1	H	167	ILE	2.1
1	H	241	TYR	2.1
1	E	279	GLY	2.1
1	E	40	PRO	2.1
1	E	295	TRP	2.1
1	F	246	ALA	2.1
1	E	59	PHE	2.0
1	G	246	ALA	2.0
1	G	250	ALA	2.0
1	H	246	ALA	2.0
1	C	321	LYS	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	E	323	6/6	0.61	0.24	54,58,60,61	0
2	GOL	D	323	6/6	0.70	0.17	47,50,52,52	0
2	GOL	C	323	6/6	0.70	0.17	80,80,81,81	0
2	GOL	A	323	6/6	0.73	0.23	74,75,76,76	0
2	GOL	F	323	6/6	0.73	0.16	68,72,72,72	0
2	GOL	A	324	6/6	0.76	0.14	53,59,60,62	0
2	GOL	B	323	6/6	0.77	0.17	64,64,64,65	0
2	GOL	B	324	6/6	0.81	0.19	78,79,79,80	0
2	GOL	D	324	6/6	0.86	0.11	37,44,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.