



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:22 AM GMT

PDB ID : 3JRK
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

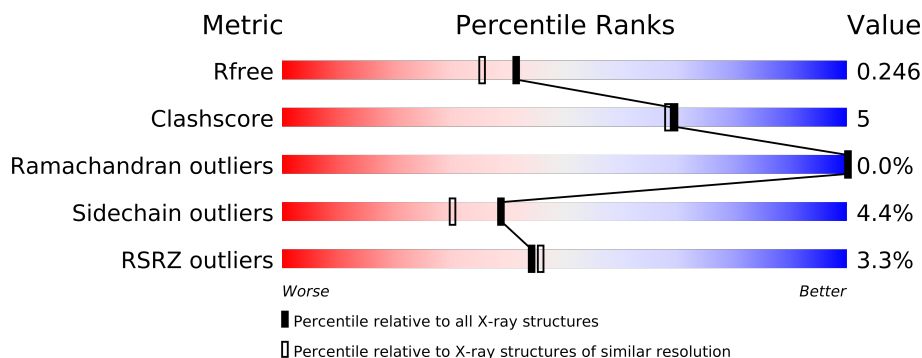
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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}	66092	6577 (2.00-1.96)
Clashscore	79885	8091 (2.00-1.96)
Ramachandran outliers	78287	7989 (2.00-1.96)
Sidechain outliers	78261	7987 (2.00-1.96)
RSRZ outliers	66119	6578 (2.00-1.96)

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. 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	322	
1	B	322	
1	C	322	
1	D	322	
1	E	322	
1	F	322	
1	G	322	
1	H	322	

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	GOL	A	323	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	324	-	X
2	GOL	B	323	-	X
2	GOL	B	324	-	X
2	GOL	C	323	-	X
2	GOL	D	323	-	X
2	GOL	D	324	-	X
2	GOL	E	323	-	X
2	GOL	F	323	-	X

2 Entry composition

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

Chain A: 



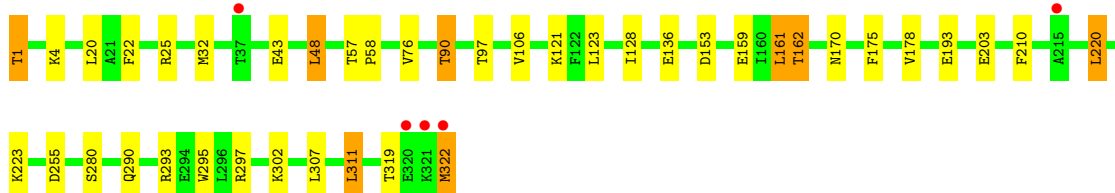
- Molecule 1: Tagatose 1,6-diphosphate aldolase 2

Chain B: 



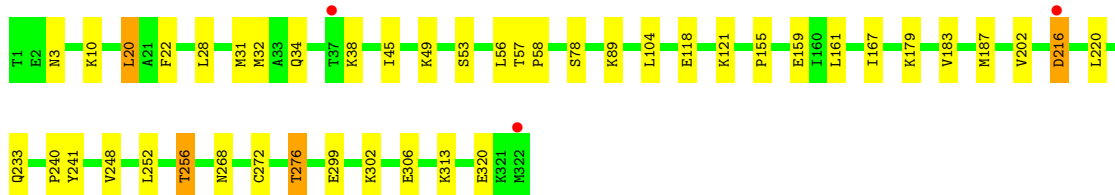
- Molecule 1: Tagatose 1,6-diphosphate aldolase 2

Chain C: 



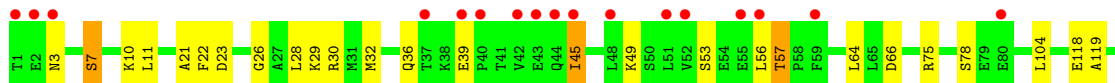
- Molecule 1: Tagatose 1,6-diphosphate aldolase 2

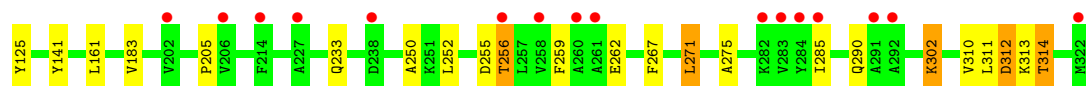
Chain D: 



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

Chain E: 





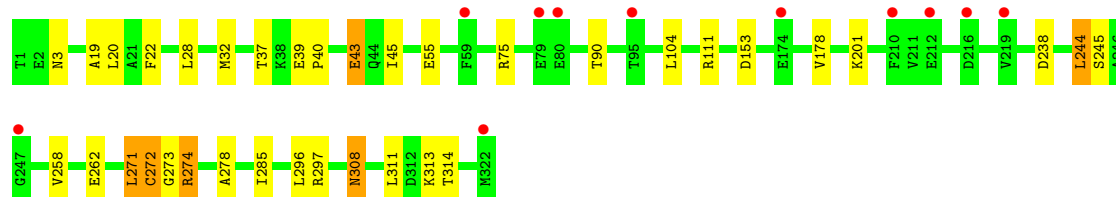
- Molecule 1: Tagatose 1,6-diphosphate aldolase 2

Chain F:



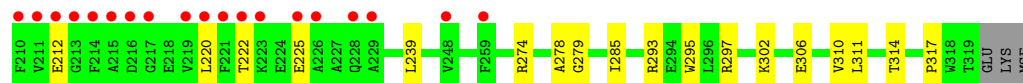
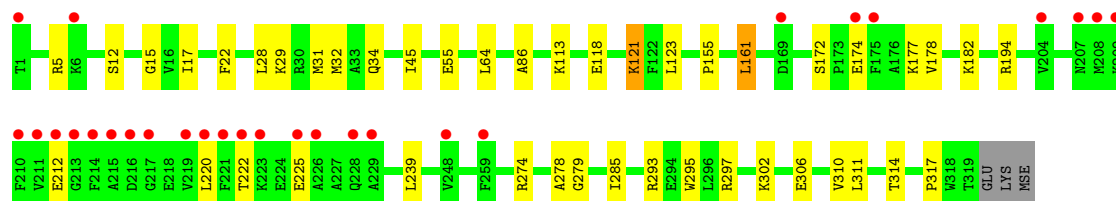
- Molecule 1: Tagatose 1,6-diphosphate aldolase 2

Chain G:



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

Chain H:



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 46.80 – 1.97	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-1.97) 95.9 (46.80-1.97)	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 0.203 , 0.246	Depositor DCC
R_{free} test set	10125 reflections (5.29%)	DCC
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 , 24.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 201445 reflections (0.000%)	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.

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	0.60	0/2603	0.63	0/3502
1	B	0.60	0/2575	0.64	1/3465 (0.0%)
1	C	0.50	0/2593	0.62	0/3489
1	D	0.55	0/2614	0.63	0/3519
1	E	0.55	0/2614	0.60	0/3516
1	F	0.53	0/2587	0.61	0/3483
1	G	0.46	0/2603	0.59	1/3502 (0.0%)
1	H	0.46	0/2550	0.54	0/3435
All	All	0.53	0/20739	0.61	2/27911 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	244	LEU	CA-CB-CG	6.03	129.16	115.30
1	B	293	ARG	NE-CZ-NH2	-5.19	117.70	120.30

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	2563	0	2536	17	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	3
1	G	2563	0	2534	20	3
1	H	2509	0	2486	26	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	191	3

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 5.

All (191) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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:E:267:PHE:CZ	1:E:314:THR:HG23	2.16	0.80
1:D:53[B]:SER:O	1:D:57[B]:THR:HG23	1.81	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:D:53[B]:SER:O	1:D:57[B]:THR:CG2	2.47	0.60
1:F:19:ALA:HB3	1:F:271:LEU:HD13	1.84	0.60
1:E:290:GLN:HB2	3:E:561:HOH:O	2.01	0.60
1:E:53:SER:O	1:E:57:THR:HB	2.01	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:3:ASN:O	1:E:7:SER:HB2	2.04	0.58
2:A:324:GOL:H12	3:A:1140:HOH:O	2.02	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:E:312[A]:ASP:OD2	1:E:312[A]:ASP:C	2.45	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:F:19:ALA:HB1	1:F:271:LEU:HD13	1.89	0.53
1:C:210:PHE:HB3	1:C:220:LEU:HB2	1.90	0.53
1:E:57:THR:HG22	1:E:78:SER:CB	2.32	0.53
1:A:36:GLN:O	2:A:324:GOL:O1	2.25	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:N	1:D:216[A]:ASP:OD1	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
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:E:21:ALA:HB2	1:E:271:LEU:HD12	1.93	0.50
1:B:23:ASP:OD1	3:B:922:HOH:O	2.19	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:53[A]:SER:O	1:D:57[A]:THR:HB	2.13	0.48
1:D:28:LEU:HG	1:D:32:MSE:HE2	1.95	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:E:57:THR:CG2	1:E:78:SER:HB3	2.36	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: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:G:308:ASN:CG	3:G:1268:HOH:O	2.54	0.46
1:A:320:GLU:HA	3:A:840:HOH:O	2.15	0.46
1:E:29:LYS:HA	1:E:32:MSE:CE	2.45	0.46
1:D:20:LEU:HD11	1:D:56:LEU:HB3	1.98	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
1:D:53[B]:SER:HA	1:D:57[B]:THR:HG23	1.98	0.45
1:C:322:MSE:HE3	1:C:322:MSE:C	2.36	0.45
1:G:238[A]:ASP:O	1:G:238[A]:ASP:OD2	2.34	0.45
1:G:311:LEU:HA	1:G:314:THR:CG2	2.40	0.45
1:F:270:VAL:HG22	1:F:311:LEU:HD21	1.99	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: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:302:LYS:O	1:H:306:GLU:HB2	2.18	0.44
1:H:64:LEU:CD1	1:H:121:LYS:HG2	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:G:311:LEU:CA	1:G:314:THR:HG22	2.42	0.44
1:E:23:ASP:HB3	1:E:64:LEU:HG	1.99	0.44
1:C:123:LEU:HD23	1:C:159:GLU:HG2	2.00	0.43
1:B:321:LYS:HE3	3:B:377:HOH:O	2.18	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:F:273:GLY:CA	3:F:907:HOH:O	2.65	0.43
1:A:15:GLY:O	1:A:317:PRO:HA	2.19	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:G:43:GLU:CD	1:G:43:GLU:H	2.21	0.42
1:C:25:ARG:CZ	1:C:90:THR:HG23	2.50	0.42
1:H:279:GLY:HA3	1:H:295:TRP:CZ2	2.54	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: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
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: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:B:118:GLU:O	1:B:155:PRO:HD2	2.20	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:D:57[B]:THR:N	1:D:58:PRO:CD	2.84	0.41
1:C:203:GLU:HB2	3:C:1160:HOH:O	2.20	0.41
1:H:86:ALA:HA	1:H:121:LYS:HG3	2.02	0.41
1:B:5:ARG:NH2	1:B:322:MSE:HG3	2.35	0.41
1:E:259:PHE:HA	1:E:262:GLU:HG2	2.03	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:E:45:ILE:HG12	1:E:45:ILE:H	1.69	0.40
1:A:121:LYS:HA	1:A:157:TYR:O	2.21	0.40
1:H:118:GLU:O	1:H:155:PRO:HD2	2.22	0.40
1:G:28:LEU:HD23	1:G:45:ILE:HG23	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:75[B]:ARG:NE	1:G:238[B]:ASP:OD2[1_554]	1.38	0.82
1:F:75[B]:ARG:CZ	1:G:238[B]:ASP:OD2[1_554]	1.99	0.21
1:F:75[B]:ARG:CD	1:G:238[B]:ASP:OD2[1_554]	2.11	0.09

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	323/322 (100%)	315 (98%)	8 (2%)	0	100	100
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%)	50	42
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%)	266 (98%)	6 (2%)	64	63
1	B	269/263 (102%)	264 (98%)	5 (2%)	69	69
1	C	271/263 (103%)	250 (92%)	21 (8%)	18	10
1	D	274/263 (104%)	258 (94%)	16 (6%)	28	19
1	E	273/263 (104%)	258 (94%)	15 (6%)	30	21
1	F	270/263 (103%)	261 (97%)	9 (3%)	50	44
1	G	272/263 (103%)	256 (94%)	16 (6%)	28	18
1	H	266/263 (101%)	257 (97%)	9 (3%)	49	42
All	All	2167/2104 (103%)	2070 (96%)	97 (4%)	39	29

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	43	GLU
1	A	96	THR
1	A	121	LYS
1	A	153	ASP
1	A	287	GLU
1	B	22	PHE
1	B	48	LEU
1	B	80	GLU
1	B	123	LEU
1	B	266	LYS
1	C	1	THR
1	C	20	LEU
1	C	22	PHE
1	C	43	GLU
1	C	48	LEU
1	C	76	VAL

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Mol	Chain	Res	Type
1	C	90	THR
1	C	106	VAL
1	C	121	LYS
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	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	22	PHE
1	D	38	LYS
1	D	49	LYS
1	D	104	LEU
1	D	161	LEU
1	D	216[A]	ASP
1	D	216[B]	ASP
1	D	220	LEU
1	D	256	THR
1	D	276	THR
1	D	299	GLU
1	D	313	LYS
1	D	320	GLU
1	E	7	SER
1	E	22	PHE
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

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Mol	Chain	Res	Type
1	E	311	LEU
1	E	312[A]	ASP
1	E	312[B]	ASP
1	E	314	THR
1	F	22	PHE
1	F	37	THR
1	F	42	VAL
1	F	48	LEU
1	F	123	LEU
1	F	153	ASP
1	F	257	LEU
1	F	271	LEU
1	F	311	LEU
1	G	3	ASN
1	G	20	LEU
1	G	22	PHE
1	G	37	THR
1	G	43	GLU
1	G	90	THR
1	G	104	LEU
1	G	153	ASP
1	G	178	VAL
1	G	244	LEU
1	G	271	LEU
1	G	272	CYS
1	G	274	ARG
1	G	296	LEU
1	G	308	ASN
1	G	313	LYS
1	H	5	ARG
1	H	22	PHE
1	H	113	LYS
1	H	121	LYS
1	H	161	LEU
1	H	172	SER
1	H	220	LEU
1	H	225	GLU
1	H	239	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	132	GLN
1	C	170	ASN
1	D	137	GLN
1	D	268	ASN
1	E	132	GLN
1	E	233	GLN
1	F	137	GLN
1	G	137	GLN
1	G	303	ASN
1	H	137	GLN
1	H	290	GLN
1	H	303	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 ⓘ

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	A	323	-	5,5,5	0.28	0	5,5,5	0.42	0
2	GOL	A	324	-	5,5,5	0.35	0	5,5,5	0.27	0
2	GOL	B	323	-	5,5,5	0.38	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	324	-	5,5,5	0.31	0	5,5,5	0.39	0
2	GOL	C	323	-	5,5,5	0.31	0	5,5,5	0.23	0
2	GOL	D	323	-	5,5,5	0.61	0	5,5,5	0.80	0
2	GOL	D	324	-	5,5,5	0.47	0	5,5,5	0.53	0
2	GOL	E	323	-	5,5,5	0.33	0	5,5,5	0.65	0
2	GOL	F	323	-	5,5,5	0.33	0	5,5,5	0.25	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	A	323	-	-	0/4/4/4	0/0/0/0
2	GOL	A	324	-	-	0/4/4/4	0/0/0/0
2	GOL	B	323	-	-	0/4/4/4	0/0/0/0
2	GOL	B	324	-	-	0/4/4/4	0/0/0/0
2	GOL	C	323	-	-	0/4/4/4	0/0/0/0
2	GOL	D	323	-	-	0/4/4/4	0/0/0/0
2	GOL	D	324	-	-	0/4/4/4	0/0/0/0
2	GOL	E	323	-	-	0/4/4/4	0/0/0/0
2	GOL	F	323	-	-	0/4/4/4	0/0/0/0

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	322/322 (100%)	0.03	3 (0%) 81 84	12, 19, 29, 54	0
1	B	322/322 (100%)	0.05	2 (0%) 86 89	12, 19, 31, 55	0
1	C	322/322 (100%)	0.26	5 (1%) 68 71	17, 25, 34, 53	0
1	D	322/322 (100%)	0.17	3 (0%) 81 84	15, 25, 41, 56	0
1	E	322/322 (100%)	0.69	33 (10%) 7 7	14, 26, 49, 60	0
1	F	321/322 (99%)	0.22	1 (0%) 91 93	15, 24, 38, 53	0
1	G	322/322 (100%)	0.49	11 (3%) 43 44	17, 30, 45, 56	0
1	H	319/322 (99%)	0.65	28 (8%) 10 10	21, 34, 51, 54	0
All	All	2572/2576 (99%)	0.32	86 (3%) 44 46	12, 25, 44, 60	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	214	PHE	5.9
1	H	211	VAL	5.6
1	E	42	VAL	4.7
1	A	322	MSE	4.6
1	H	175	PHE	4.4
1	G	247	GLY	4.4
1	B	322	MSE	4.3
1	E	51	LEU	4.2
1	H	208	MSE	4.2
1	D	322	MSE	4.2
1	D	216[A]	ASP	4.2
1	E	1	THR	4.0
1	G	216	ASP	3.9
1	E	45	ILE	3.9
1	H	223	LYS	3.7
1	E	39	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	220	LEU	3.6
1	H	217	GLY	3.5
1	H	212	GLU	3.5
1	E	322	MSE	3.5
1	E	59	PHE	3.5
1	E	284	TYR	3.4
1	C	322	MSE	3.4
1	H	259	PHE	3.4
1	H	169	ASP	3.4
1	F	33	ALA	3.2
1	H	229	ALA	3.2
1	H	216	ASP	3.1
1	E	48	LEU	3.1
1	H	226	ALA	3.1
1	H	215	ALA	3.1
1	H	204	VAL	3.0
1	E	2	GLU	3.0
1	E	260	ALA	3.0
1	G	212	GLU	2.9
1	E	285	ILE	2.9
1	D	37	THR	2.9
1	G	219	VAL	2.8
1	H	210	PHE	2.8
1	A	1	THR	2.8
1	G	95	THR	2.7
1	A	320	GLU	2.7
1	C	321	LYS	2.7
1	H	225	GLU	2.7
1	H	213	GLY	2.7
1	H	209	LYS	2.7
1	E	3	ASN	2.6
1	H	1	THR	2.5
1	E	56	LEU	2.5
1	E	52	VAL	2.5
1	G	59	PHE	2.5
1	H	221	PHE	2.5
1	H	219	VAL	2.5
1	B	320	GLU	2.5
1	H	174	GLU	2.5
1	H	207	ASN	2.5
1	E	44	GLN	2.5
1	E	80	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	80	GLU	2.4
1	C	320	GLU	2.4
1	H	248	VAL	2.4
1	E	292	ALA	2.3
1	C	37	THR	2.3
1	G	210	PHE	2.3
1	E	261	ALA	2.3
1	E	55	GLU	2.3
1	E	291	ALA	2.3
1	E	43	GLU	2.3
1	E	40	PRO	2.3
1	H	222	THR	2.2
1	E	238	ASP	2.2
1	G	174	GLU	2.2
1	E	258	VAL	2.2
1	E	37	THR	2.2
1	E	282	LYS	2.1
1	E	202	VAL	2.1
1	C	215	ALA	2.1
1	E	283	VAL	2.1
1	G	322	MSE	2.1
1	G	79	GLU	2.1
1	H	6	LYS	2.0
1	E	206	VAL	2.0
1	E	214	PHE	2.0
1	H	228	GLN	2.0
1	E	227	ALA	2.0
1	E	256	THR	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 ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	E	323	6/6	0.36	14.53	54,58,60,61	0
2	GOL	A	324	6/6	0.30	13.29	53,59,60,62	0
2	GOL	B	324	6/6	0.21	9.28	78,79,79,80	0
2	GOL	C	323	6/6	0.29	8.26	80,80,81,81	0
2	GOL	A	323	6/6	0.21	8.20	74,75,76,76	0
2	GOL	D	323	6/6	0.23	5.87	47,50,52,52	0
2	GOL	B	323	6/6	0.17	4.64	64,64,64,65	0
2	GOL	D	324	6/6	0.14	2.30	37,44,47,47	0
2	GOL	F	323	6/6	0.18	2.21	68,72,72,72	0

6.5 Other polymers ⓘ

There are no such residues in this entry.