Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2024 – 09:42 PM EDT

PDB ID	:	6MGI
Title	:	Photosynthetic phosphoenolpyruvate carboxylase isoenzyme from maize complexed with the allosteric activator glucose-6-phosphate in its allosteric site
Authors	:	Gonzalez-Segura, L.; Munoz-Clares, R.A.
Deposited on	:	2018-09-13
Resolution	:	2.99 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:

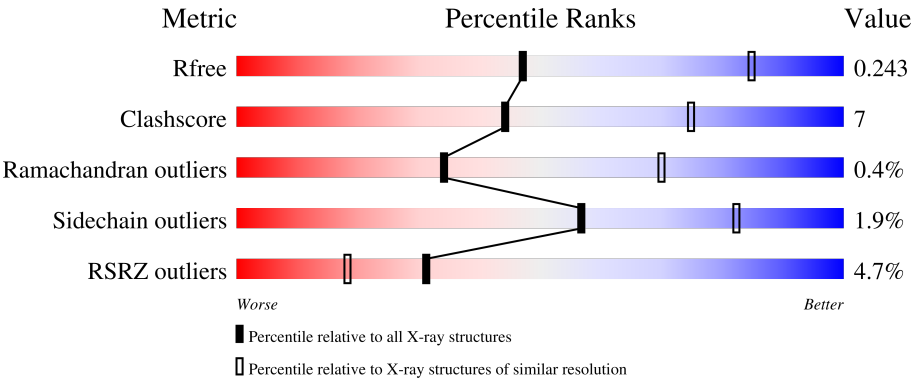
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 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 <=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	970	3% 80% 14% 6%
1	B	970	6% 75% 18% · 6%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PGA	A	1007	-	-	-	X

2 Entry composition

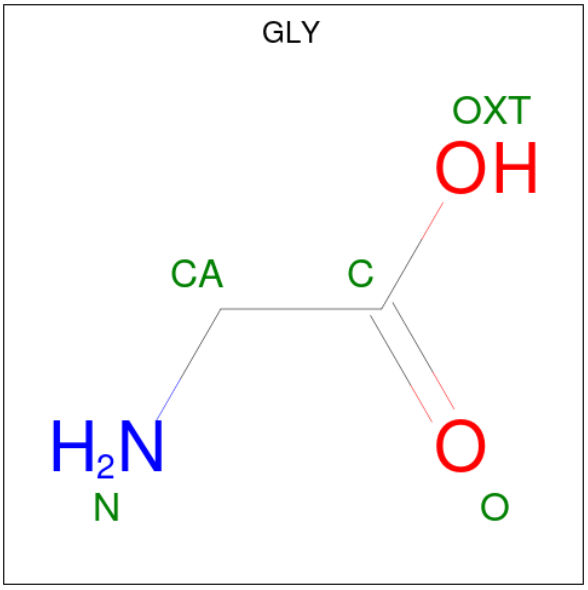
There are 7 unique types of molecules in this entry. The entry contains 14680 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphoenolpyruvate carboxylase.

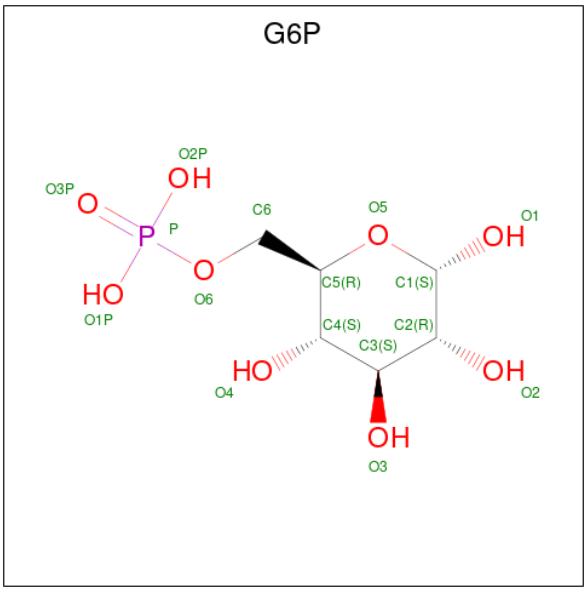
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	915	Total	C	N	O	S	0	0	0
			7298	4637	1267	1364	30			
1	B	911	Total	C	N	O	S	0	0	0
			7265	4617	1261	1357	30			

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



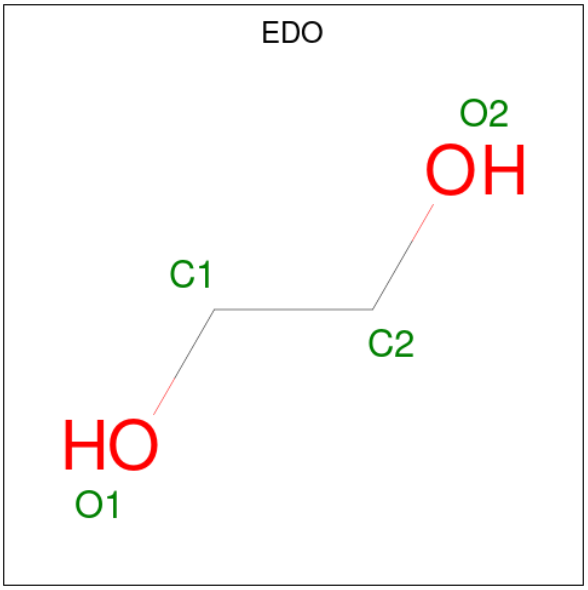
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	B	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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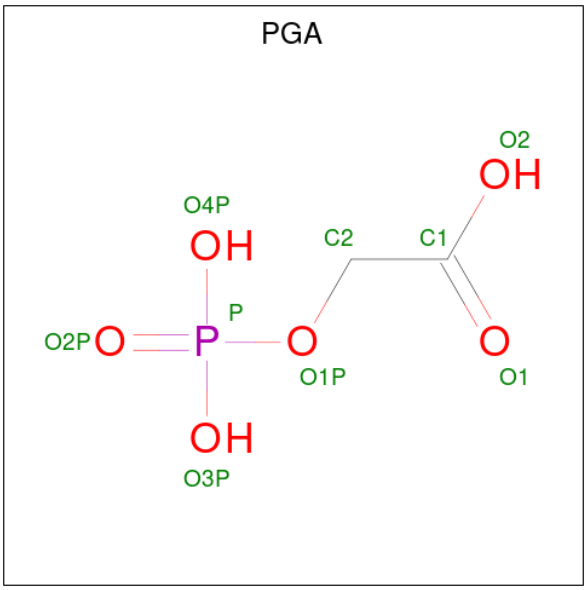
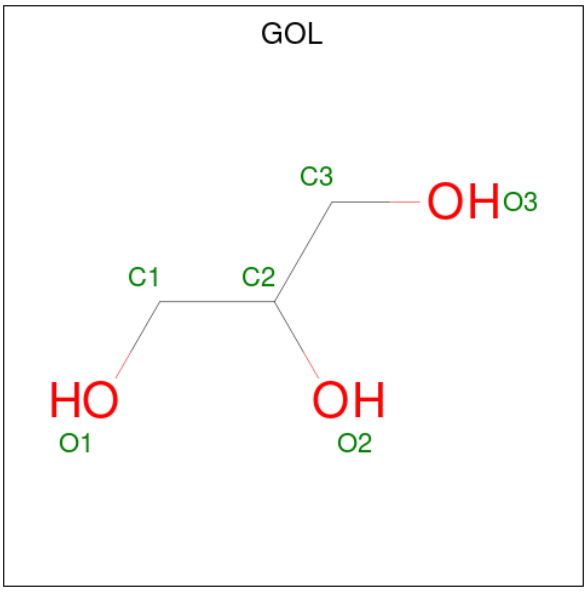
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: $C_2H_5O_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O P 9 2 6 1	0	0
5	B	1	Total C O P 9 2 6 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

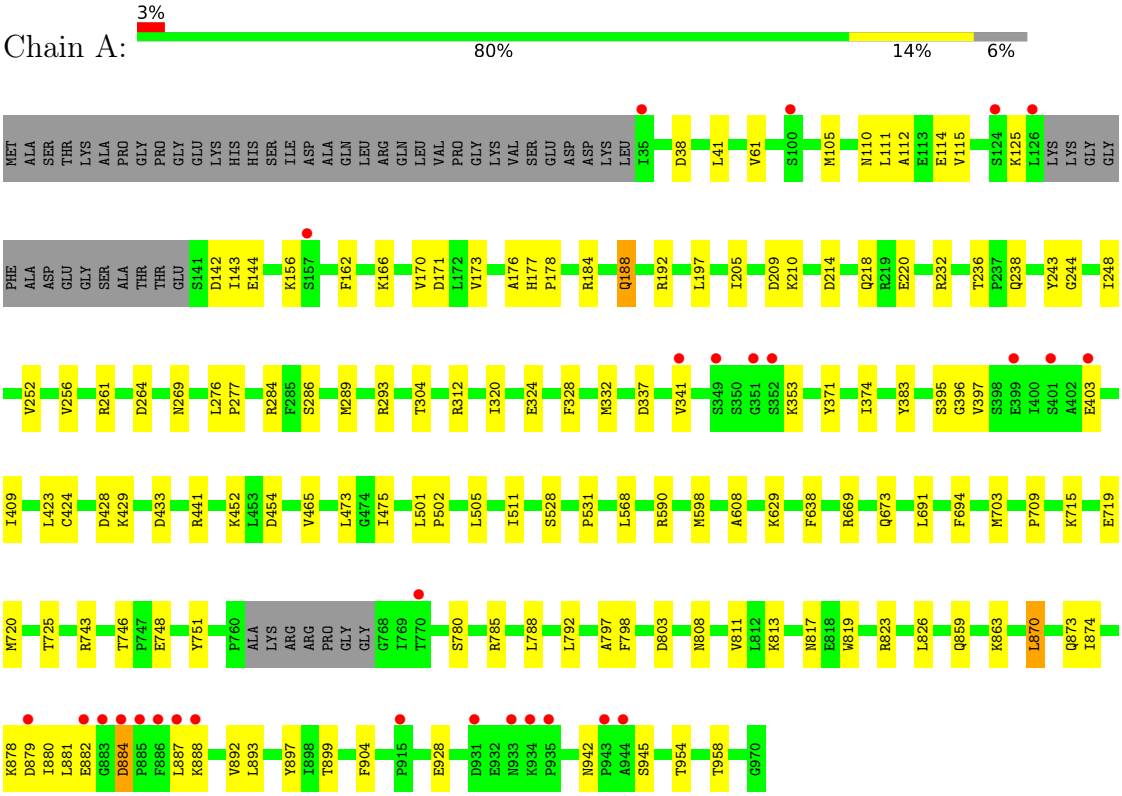
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	13	Total O 13 13	0	0
7	B	8	Total O 8 8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

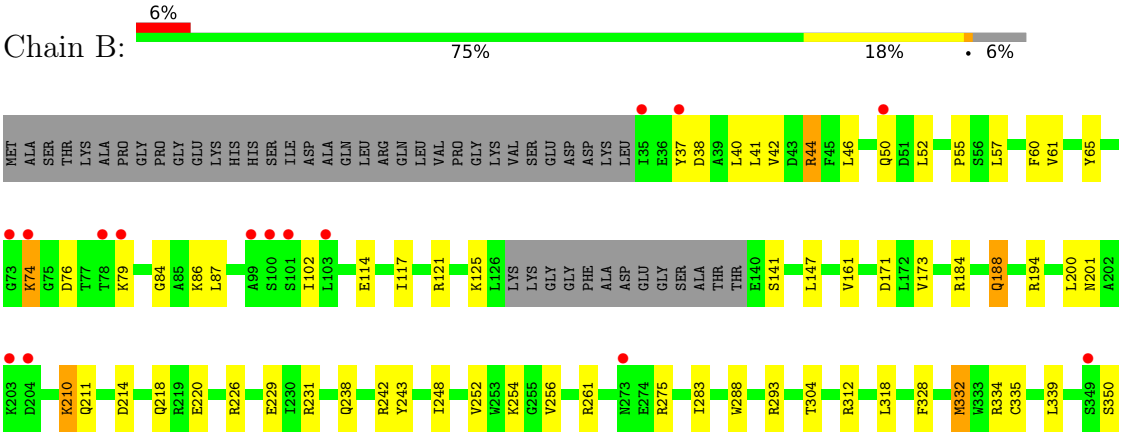
• Molecule 1: Phosphoenolpyruvate carboxylase

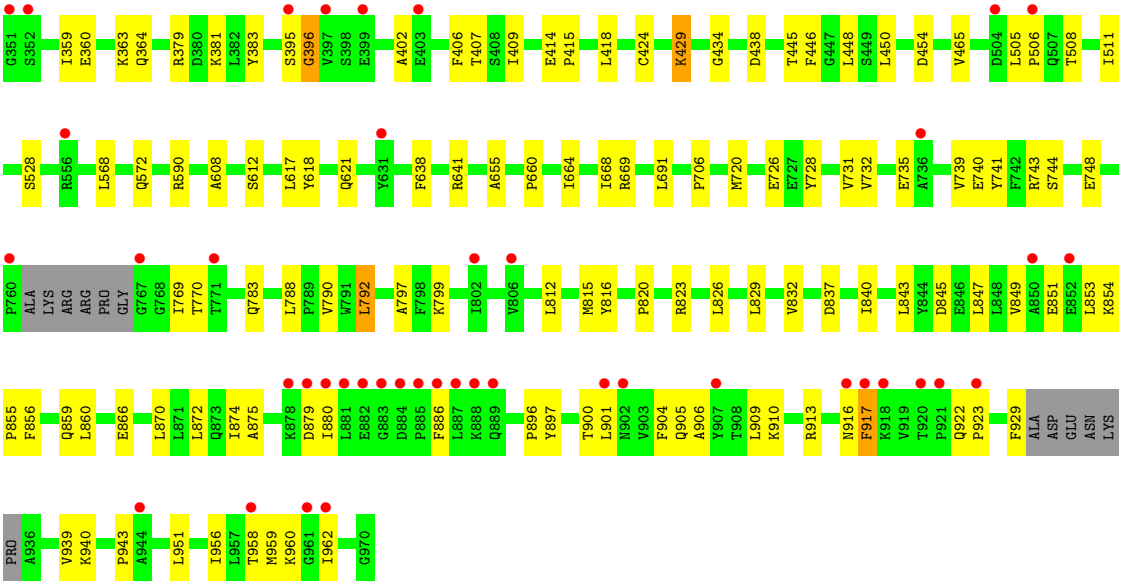
Chain A:



• Molecule 1: Phosphoenolpyruvate carboxylase

Chain B:




G351 S352 I359 E360 K363 Q364 R379 D380 K381 L382 Y383 S395 G396 V397 S398 E399 A402 E403 F406 T407 S408 I409 E414 P415 L418 C424 K429 G434 D438 T445 F446 G447 L448 S449 L450 D454 V465 D504 L505 P506 Q507 T508 I511
S528 R556 L568 Q572 R590 A608 S612 L617 Y618 Q621 Y631 F638 R641 A655 P660 I664 I668 R669 L691 P706 M720 E726 E727 Y728 V731 V732 E735 A736 V739 E740 Y741 F742 R743 S744 E748
P760 ALA LYS ARG ARG PRO GLY G767 G768 I769 T770 T771 Q783 L788 P789 V790 W791 L792 A797 F798 K799 I802 V806 L812 M815 Y816 P820 R823 L826 L829 V832 D837 I840 L843 Y844 D845 E846 L847 L848 V849 A850 E851 E852 L853 K854
P855 F856 Q859 L860 E866 L870 L871 L872 Q873 I874 A875 K878 D879 I880 L881 E882 G883 D884 P885 F886 L887 K888 Q889 P896 Y897 T900 L901 N902 V903 F904 Q905 A906 Y907 T908 L909 K910 R913 N916 F917 K918 V919 T920 P921 Q922 P923 F929 ALA ASP GLU ASN LYS
PRO A936 V939 K940 P943 A944 L951 I956 L957 T958 M959 K960 G961 I962 G970

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	152.09Å 170.68Å 244.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.99 29.62 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.62-2.99) 97.1 (29.62-2.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.208 , 0.243 0.208 , 0.243	Depositor DCC
R_{free} test set	3168 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 27.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14680	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: G6P, PGA, GOL, EDO

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	0.26	0/7453	0.41	0/10096
1	B	0.25	0/7418	0.42	0/10046
All	All	0.26	0/14871	0.41	0/20142

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7298	0	7294	81	0
1	B	7265	0	7261	116	0
2	A	5	0	2	0	0
2	B	5	0	2	0	0
3	A	16	0	11	0	0
3	B	16	0	11	1	0
4	A	16	0	24	0	0
4	B	8	0	12	0	0
5	A	9	0	2	0	0
5	B	9	0	2	0	0
6	B	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	13	0	0	0	0
7	B	8	0	0	0	0
All	All	14680	0	14637	192	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 7.

All (192) 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:A:887:LEU:HD23	1:A:887:LEU:H	1.26	0.99
1:B:837:ASP:HB3	1:B:840:ILE:HD13	1.47	0.96
1:A:880:ILE:HG22	1:A:881:LEU:HG	1.57	0.87
1:A:887:LEU:HD23	1:A:887:LEU:N	1.93	0.84
1:B:359:ILE:HG22	1:B:360:GLU:HG2	1.67	0.77
1:A:403:GLU:N	1:A:403:GLU:OE1	2.19	0.75
1:B:434:GLY:HA3	6:B:1005:GOL:H31	1.71	0.71
1:B:728:TYR:HA	1:B:792:LEU:HD12	1.73	0.69
1:B:840:ILE:H	1:B:840:ILE:HD12	1.57	0.68
1:B:465:VAL:HG22	1:B:511:ILE:HG23	1.76	0.68
1:B:706:PRO:HB3	1:B:820:PRO:HG2	1.77	0.67
1:A:264:ASP:OD2	1:A:441:ARG:NH2	2.28	0.66
1:A:870:LEU:O	1:A:873:GLN:N	2.28	0.66
1:A:887:LEU:H	1:A:887:LEU:CD2	2.05	0.66
1:B:720:MET:HB3	1:B:797:ALA:HB1	1.78	0.65
1:A:264:ASP:OD1	1:A:276:LEU:N	2.22	0.64
1:B:905:GLN:HB2	1:B:958:THR:HG21	1.78	0.64
1:A:261:ARG:NH2	1:A:433:ASP:O	2.30	0.64
1:A:715:LYS:O	1:A:719:GLU:HG3	1.97	0.64
1:B:840:ILE:HD12	1:B:840:ILE:N	2.11	0.64
1:B:837:ASP:CB	1:B:840:ILE:HD13	2.26	0.63
1:A:428:ASP:OD1	1:B:226:ARG:HD2	1.99	0.63
1:B:50:GLN:HG3	1:B:55:PRO:HA	1.79	0.62
1:A:395:SER:O	1:A:397:VAL:N	2.26	0.62
1:B:84:GLY:HA2	1:B:87:LEU:HD12	1.81	0.61
1:A:184:ARG:NH2	1:B:360:GLU:OE1	2.34	0.60
1:B:851:GLU:HA	1:B:854:LYS:HD2	1.84	0.60
1:B:741:TYR:HD1	1:B:849:VAL:HG21	1.66	0.60
1:B:74:LYS:HG2	1:B:76:ASP:HB2	1.83	0.59
1:B:395:SER:OG	1:B:396:GLY:N	2.35	0.59
1:A:878:LYS:HG2	1:A:882:GLU:CD	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:HD11	1:B:44:ARG:HH21	1.67	0.58
1:A:184:ARG:HH22	1:B:360:GLU:CD	2.06	0.58
1:B:505:LEU:HD12	1:B:506:PRO:HD2	1.86	0.57
1:A:884:ASP:HB3	1:A:887:LEU:HD21	1.85	0.57
1:B:816:TYR:CE2	1:B:875:ALA:HA	2.39	0.57
1:B:896:PRO:O	1:B:900:THR:HG23	2.05	0.57
1:A:320:ILE:O	1:A:324:GLU:HG3	2.05	0.56
1:B:872:LEU:HD21	1:B:880:ILE:HD13	1.87	0.56
1:B:568:LEU:HD22	1:B:608:ALA:HB2	1.88	0.56
1:B:409:ILE:HD13	1:B:448:LEU:HG	1.88	0.56
1:A:214:ASP:OD2	1:A:218:GLN:NE2	2.37	0.56
1:B:248:ILE:HA	1:B:252:VAL:HB	1.88	0.55
1:A:473:LEU:HB2	1:A:475:ILE:HD12	1.87	0.55
1:B:905:GLN:CB	1:B:958:THR:HG21	2.37	0.54
1:B:214:ASP:OD2	1:B:218:GLN:NE2	2.37	0.54
1:A:743:ARG:NH1	1:A:748:GLU:OE1	2.38	0.54
1:A:884:ASP:CB	1:A:887:LEU:HD21	2.38	0.54
1:B:812:LEU:HA	1:B:815:MET:HE2	1.90	0.54
1:A:256:VAL:HG12	1:A:691:LEU:HD11	1.89	0.54
1:B:335:CYS:HB2	1:B:339:LEU:HD23	1.90	0.54
1:B:951:LEU:H	1:B:951:LEU:HD12	1.73	0.53
1:A:110:ASN:O	1:A:114:GLU:HG3	2.08	0.53
1:B:184:ARG:HD2	1:B:243:TYR:HB2	1.89	0.53
1:A:332:MET:HE3	1:A:423:LEU:HD21	1.91	0.53
1:A:502:PRO:HG2	1:A:505:LEU:HB2	1.91	0.52
1:B:446:PHE:HB3	1:B:450:LEU:HD23	1.92	0.52
1:A:284:ARG:HH12	1:A:452:LYS:HE3	1.74	0.52
1:A:41:LEU:HD12	1:A:112:ALA:HB2	1.91	0.52
1:B:256:VAL:HG11	1:B:445:THR:HG21	1.92	0.52
1:B:288:TRP:CD1	1:B:454:ASP:HB2	2.45	0.52
1:B:229:GLU:H	1:B:229:GLU:CD	2.14	0.52
1:B:40:LEU:O	1:B:44:ARG:HD2	2.11	0.51
1:A:176:ALA:HB2	1:A:289:MET:HG2	1.91	0.51
1:A:337:ASP:O	1:A:341:VAL:HG12	2.10	0.51
1:B:845:ASP:O	1:B:849:VAL:HG12	2.10	0.51
1:A:324:GLU:OE1	1:A:383:TYR:OH	2.23	0.50
1:A:177:HIS:ND1	1:A:673:GLN:HG2	2.26	0.50
1:B:843:LEU:O	1:B:847:LEU:HD12	2.10	0.50
1:A:156:LYS:HE3	1:A:703:MET:HB3	1.92	0.50
1:A:236:THR:HG22	1:A:238:GLN:H	1.76	0.50
1:B:741:TYR:CD1	1:B:849:VAL:HG21	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:GLU:OE1	1:B:334:ARG:NH1	2.44	0.50
1:A:465:VAL:HG22	1:A:511:ILE:HG23	1.94	0.49
1:A:942:ASN:OD1	1:A:945:SER:HB2	2.12	0.49
1:B:65:TYR:HD2	1:B:897:TYR:CE1	2.30	0.49
1:B:60:PHE:HE1	1:B:86:LYS:HG2	1.77	0.49
1:B:171:ASP:HB3	1:B:669:ARG:HG2	1.94	0.49
1:B:731:VAL:HG21	1:B:860:LEU:HD21	1.93	0.49
1:B:740:GLU:O	1:B:744:SER:OG	2.26	0.49
1:B:909:LEU:O	1:B:913:ARG:HG3	2.13	0.48
1:A:144:GLU:OE2	1:A:269:ASN:ND2	2.34	0.48
1:A:312:ARG:NH1	1:A:528:SER:HB3	2.28	0.48
1:B:840:ILE:H	1:B:840:ILE:CD1	2.24	0.48
1:B:568:LEU:O	1:B:572:GLN:HG3	2.12	0.48
1:A:746:THR:HB	1:A:780:SER:HB3	1.95	0.48
1:B:293:ARG:NH2	1:B:304:THR:OG1	2.42	0.48
1:A:248:ILE:HA	1:A:252:VAL:HB	1.96	0.47
1:A:608:ALA:HA	1:A:725:THR:HG23	1.96	0.47
1:A:785:ARG:NH2	1:A:899:THR:OG1	2.46	0.47
1:A:798:PHE:HZ	1:A:826:LEU:HD21	1.79	0.47
1:A:888:LYS:O	1:A:892:VAL:HG13	2.14	0.47
1:B:40:LEU:HD11	1:B:44:ARG:NH2	2.28	0.47
1:A:162:PHE:CE2	1:A:166:LYS:HD2	2.49	0.47
1:A:409:ILE:HD12	1:A:409:ILE:H	1.80	0.47
1:B:402:ALA:HB1	1:B:407:THR:HG21	1.97	0.47
1:B:783:GLN:HE22	1:B:959:MET:HA	1.78	0.47
1:B:816:TYR:CZ	1:B:823:ARG:NH1	2.81	0.47
1:B:866:GLU:O	1:B:870:LEU:HD12	2.15	0.47
1:B:939:VAL:HG12	1:B:940:LYS:HD2	1.97	0.47
1:A:232:ARG:NH1	1:A:942:ASN:HB2	2.30	0.47
1:A:424:CYS:SG	1:A:429:LYS:HG2	2.55	0.47
1:B:379:ARG:HG2	1:B:383:TYR:CE1	2.50	0.46
1:A:111:LEU:O	1:A:115:VAL:HG23	2.15	0.46
1:A:142:ASP:OD1	1:A:143:ILE:N	2.48	0.46
1:B:940:LYS:HA	1:B:940:LYS:HE3	1.97	0.46
1:A:41:LEU:HD21	1:A:197:LEU:HD13	1.98	0.46
1:B:847:LEU:HD13	1:B:906:ALA:HB1	1.97	0.46
1:B:283:ILE:HG21	1:B:691:LEU:HD22	1.98	0.46
1:A:173:VAL:HG22	1:A:286:SER:HB2	1.96	0.46
1:A:813:LYS:O	1:A:817:ASN:ND2	2.47	0.46
1:B:910:LYS:HG2	1:B:917:PHE:HD1	1.80	0.46
1:A:178:PRO:HB2	1:A:751:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:O	1:B:61:VAL:HG23	2.15	0.46
1:A:38:ASP:CG	1:A:893:LEU:HD21	2.36	0.46
1:A:709:PRO:HB3	1:A:819:TRP:CZ2	2.51	0.46
1:B:769:ILE:HG13	1:B:770:THR:N	2.31	0.45
1:B:910:LYS:HG2	1:B:917:PHE:CD1	2.52	0.45
1:B:739:VAL:HG22	1:B:769:ILE:HG21	1.99	0.45
1:A:598:MET:HA	1:A:638:PHE:HB3	1.98	0.45
1:B:332:MET:SD	1:B:332:MET:N	2.89	0.45
1:B:788:LEU:HD11	1:B:792:LEU:HD23	1.98	0.45
1:B:37:TYR:CE1	1:B:201:ASN:ND2	2.84	0.45
1:B:743:ARG:NH1	1:B:748:GLU:OE1	2.50	0.45
1:B:238:GLN:O	1:B:242:ARG:HG2	2.17	0.45
1:A:808:ASN:HA	1:A:811:VAL:HG12	1.99	0.45
1:B:350:SER:O	1:B:364:GLN:NE2	2.50	0.44
1:B:956:ILE:O	1:B:960:LYS:HG3	2.18	0.44
1:A:293:ARG:NH2	1:A:304:THR:OG1	2.48	0.44
1:B:843:LEU:HG	1:B:847:LEU:HD11	1.99	0.44
1:A:188:GLN:OE1	1:A:192:ARG:NE	2.51	0.44
1:A:501:LEU:HD12	1:A:502:PRO:HD2	2.00	0.43
1:B:200:LEU:HD11	1:B:210:LYS:HG2	2.00	0.43
1:A:171:ASP:HB3	1:A:669:ARG:HG2	2.00	0.43
1:B:42:VAL:O	1:B:46:LEU:HD23	2.17	0.43
1:B:664:ILE:HG23	1:B:668:ILE:HB	1.99	0.43
1:A:720:MET:HB3	1:A:797:ALA:HB1	2.01	0.43
1:B:200:LEU:HA	1:B:200:LEU:HD12	1.82	0.43
1:B:102:ILE:HG21	1:B:901:LEU:HG	2.00	0.43
1:B:147:LEU:HG	1:B:161:VAL:HG11	2.00	0.43
1:A:205:ILE:HD11	1:A:210:LYS:HG3	2.00	0.43
1:B:261:ARG:NH2	1:B:438:ASP:OD1	2.52	0.43
1:A:454:ASP:CG	1:A:531:PRO:HD2	2.39	0.43
1:A:568:LEU:HD22	1:A:608:ALA:HB2	2.01	0.43
1:A:874:ILE:H	1:A:874:ILE:HD12	1.84	0.43
1:B:339:LEU:HD13	1:B:418:LEU:HG	2.01	0.43
1:A:244:GLY:HA3	1:A:289:MET:SD	2.59	0.43
1:B:641:ARG:CZ	1:B:655:ALA:HB1	2.48	0.43
1:B:318:LEU:HD12	1:B:450:LEU:HD11	2.01	0.43
1:B:40:LEU:HA	1:B:40:LEU:HD12	1.69	0.42
1:B:44:ARG:HH12	1:B:214:ASP:CG	2.23	0.42
1:B:508:THR:OG1	1:B:511:ILE:HD12	2.19	0.42
1:B:617:LEU:O	1:B:621:GLN:HG3	2.19	0.42
1:B:363:LYS:HE3	1:B:363:LYS:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:VAL:HG11	1:B:832:VAL:HG21	2.01	0.42
1:B:114:GLU:OE2	1:B:194:ARG:HD3	2.19	0.42
1:B:52:LEU:HD22	1:B:226:ARG:NH2	2.34	0.42
1:B:117:ILE:HD11	1:B:886:PHE:HE2	1.85	0.42
1:B:381:LYS:HB3	1:B:406:PHE:CE2	2.55	0.42
1:B:855:PRO:O	1:B:859:GLN:HG3	2.20	0.42
1:A:125:LYS:HB3	1:A:125:LYS:HE3	1.87	0.42
1:B:922:GLN:HB2	1:B:923:PRO:HD2	2.02	0.42
1:A:192:ARG:NH1	1:A:220:GLU:OE2	2.53	0.41
1:A:859:GLN:O	1:A:863:LYS:HG3	2.19	0.41
1:B:121:ARG:O	1:B:125:LYS:HG3	2.20	0.41
1:B:618:TYR:CG	1:B:660:PRO:HG3	2.54	0.41
1:A:276:LEU:HD12	1:A:277:PRO:HD2	2.01	0.41
1:A:954:THR:O	1:A:958:THR:HG23	2.21	0.41
1:B:173:VAL:HG21	1:B:638:PHE:CZ	2.55	0.41
1:A:928:GLU:CD	1:B:334:ARG:HH12	2.24	0.41
1:B:424:CYS:SG	1:B:429:LYS:HD3	2.60	0.41
1:B:728:TYR:CE1	1:B:732:VAL:HG21	2.56	0.41
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.94	0.41
1:B:188:GLN:HE21	1:B:188:GLN:HB3	1.71	0.41
1:B:254:LYS:HA	1:B:254:LYS:HD2	1.64	0.41
1:B:312:ARG:NH1	1:B:528:SER:HB3	2.36	0.41
1:B:870:LEU:O	1:B:874:ILE:HG12	2.21	0.41
1:A:788:LEU:HD11	1:A:792:LEU:HD22	2.03	0.41
1:B:231:ARG:NH1	3:B:1002:G6P:O2P	2.53	0.41
1:B:414:GLU:HB3	1:B:415:PRO:HD3	2.02	0.41
1:B:853:LEU:O	1:B:856:PHE:HB3	2.20	0.41
1:B:905:GLN:HB2	1:B:958:THR:CG2	2.50	0.41
1:A:170:VAL:HG11	1:A:694:PHE:HB3	2.03	0.41
1:B:951:LEU:HD12	1:B:951:LEU:N	2.36	0.41
1:A:61:VAL:HG11	1:A:105:MET:HE1	2.03	0.41
1:B:958:THR:O	1:B:962:ILE:HD12	2.21	0.40
1:A:184:ARG:HD3	1:A:243:TYR:HD1	1.86	0.40
1:A:353:LYS:HA	1:A:353:LYS:HD2	1.84	0.40
1:B:79:LYS:HZ2	1:B:79:LYS:HG2	1.77	0.40
1:A:371:TYR:HA	1:A:374:ILE:HG22	2.03	0.40
1:B:826:LEU:HA	1:B:829:LEU:HD12	2.04	0.40
1:A:878:LYS:HG3	1:A:879:ASP:N	2.37	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	909/970 (94%)	875 (96%)	32 (4%)	2 (0%)	47 80
1	B	903/970 (93%)	867 (96%)	31 (3%)	5 (1%)	25 61
All	All	1812/1940 (93%)	1742 (96%)	63 (4%)	7 (0%)	34 70

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	GLY
1	B	74	LYS
1	A	870	LEU
1	B	792	LEU
1	B	943	PRO
1	B	735	GLU
1	B	396	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	791/832 (95%)	781 (99%)	10 (1%)	69 88
1	B	787/832 (95%)	767 (98%)	20 (2%)	47 77
All	All	1578/1664 (95%)	1548 (98%)	30 (2%)	57 82

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	209	ASP
1	A	328	PHE
1	A	590	ARG
1	A	629	LYS
1	A	803	ASP
1	A	823	ARG
1	A	884	ASP
1	A	897	TYR
1	A	904	PHE
1	B	38	ASP
1	B	44	ARG
1	B	141	SER
1	B	188	GLN
1	B	210	LYS
1	B	211	GLN
1	B	220	GLU
1	B	275	ARG
1	B	328	PHE
1	B	332	MET
1	B	429	LYS
1	B	590	ARG
1	B	612	SER
1	B	726	GLU
1	B	799	LYS
1	B	879	ASP
1	B	904	PHE
1	B	916	ASN
1	B	917	PHE
1	B	929	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	B	50	GLN
1	B	188	GLN
1	B	201	ASN

5.3.3 RNA

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)

14 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	PGA	A	1007	-	8,8,8	1.24	1 (12%)	10,11,11	0.99	0
4	EDO	A	1005	-	3,3,3	0.42	0	2,2,2	0.39	0
6	GOL	B	1006	-	5,5,5	0.90	0	5,5,5	1.00	0
3	G6P	B	1002	-	16,16,16	0.51	0	24,24,24	0.72	0
6	GOL	B	1005	-	5,5,5	0.93	0	5,5,5	0.93	0
4	EDO	A	1006	-	3,3,3	0.36	0	2,2,2	0.55	0
3	G6P	A	1002	-	16,16,16	0.52	0	24,24,24	0.67	0
4	EDO	B	1004	-	3,3,3	0.42	0	2,2,2	0.35	0
4	EDO	A	1004	-	3,3,3	0.41	0	2,2,2	0.35	0
4	EDO	B	1003	-	3,3,3	0.45	0	2,2,2	0.29	0
5	PGA	B	1007	-	8,8,8	1.14	1 (12%)	10,11,11	1.01	0
2	GLY	B	1001	-	4,4,4	1.11	1 (25%)	3,4,4	1.70	2 (66%)
4	EDO	A	1003	-	3,3,3	0.46	0	2,2,2	0.29	0
2	GLY	A	1001	-	4,4,4	1.09	1 (25%)	3,4,4	1.70	1 (33%)

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	PGA	A	1007	-	-	5/6/6/6	-
4	EDO	A	1005	-	-	0/1/1/1	-
6	GOL	B	1006	-	-	0/4/4/4	-
3	G6P	B	1002	-	-	0/6/26/26	0/1/1/1
6	GOL	B	1005	-	-	0/4/4/4	-
4	EDO	A	1006	-	-	1/1/1/1	-
3	G6P	A	1002	-	-	0/6/26/26	0/1/1/1
4	EDO	B	1004	-	-	0/1/1/1	-
4	EDO	A	1004	-	-	0/1/1/1	-
4	EDO	B	1003	-	-	0/1/1/1	-
5	PGA	B	1007	-	-	2/6/6/6	-
2	GLY	B	1001	-	-	0/2/2/2	-
4	EDO	A	1003	-	-	0/1/1/1	-
2	GLY	A	1001	-	-	0/2/2/2	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PGA	O1P-C2	-2.65	1.41	1.43
5	B	1007	PGA	O1P-C2	-2.28	1.41	1.43
2	B	1001	GLY	OXT-C	-2.09	1.23	1.30
2	A	1001	GLY	OXT-C	-2.05	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	GLY	OXT-C-O	-2.13	117.99	123.30
2	B	1001	GLY	OXT-C-O	-2.08	118.12	123.30
2	B	1001	GLY	OXT-C-CA	2.03	121.52	113.45

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1007	PGA	C2-O1P-P-O3P
5	B	1007	PGA	O1-C1-C2-O1P
5	B	1007	PGA	O2-C1-C2-O1P
5	A	1007	PGA	O1-C1-C2-O1P
5	A	1007	PGA	O2-C1-C2-O1P
4	A	1006	EDO	O1-C1-C2-O2
5	A	1007	PGA	C2-O1P-P-O2P
5	A	1007	PGA	C2-O1P-P-O4P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	G6P	1	0
6	B	1005	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	915/970 (94%)	0.03	28 (3%)	49	30	34, 47, 73, 134	0
1	B	911/970 (93%)	0.22	58 (6%)	19	10	32, 55, 86, 109	0
All	All	1826/1940 (94%)	0.12	86 (4%)	31	18	32, 50, 82, 134	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	ILE	6.9
1	B	921	PRO	5.3
1	A	885	PRO	5.0
1	B	944	ALA	4.3
1	B	767	GLY	4.3
1	A	886	PHE	4.3
1	B	203	LYS	4.1
1	B	918	LYS	4.1
1	B	204	ASP	4.0
1	B	883	GLY	4.0
1	B	920	THR	4.0
1	A	935	PRO	4.0
1	B	886	PHE	4.0
1	A	349	SER	3.9
1	B	100	SER	3.7
1	B	881	LEU	3.6
1	A	352	SER	3.5
1	B	885	PRO	3.5
1	B	887	LEU	3.5
1	A	931	ASP	3.4
1	A	934	LYS	3.4
1	B	504	ASP	3.4
1	B	916	ASN	3.3
1	B	889	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	73	GLY	3.2
1	A	35	ILE	3.2
1	A	887	LEU	3.1
1	B	884	ASP	3.1
1	A	883	GLY	3.1
1	B	879	ASP	3.1
1	B	74	LYS	3.0
1	A	933	ASN	3.0
1	B	961	GLY	2.8
1	B	917	PHE	2.8
1	B	958	THR	2.8
1	B	556	ARG	2.7
1	B	349	SER	2.7
1	A	944	ALA	2.7
1	A	884	ASP	2.7
1	B	962	ILE	2.6
1	A	882	GLU	2.5
1	A	943	PRO	2.5
1	B	103	LEU	2.5
1	B	878	LYS	2.4
1	B	888	LYS	2.4
1	B	101	SER	2.4
1	B	397	VAL	2.4
1	B	631	TYR	2.4
1	B	273	ASN	2.3
1	A	399	GLU	2.3
1	A	879	ASP	2.3
1	B	403	GLU	2.3
1	A	351	GLY	2.3
1	B	399	GLU	2.3
1	B	806	VAL	2.3
1	B	902	ASN	2.3
1	B	351	GLY	2.3
1	A	401	SER	2.2
1	A	403	GLU	2.2
1	B	99	ALA	2.2
1	B	771	THR	2.2
1	A	915	PRO	2.2
1	A	124	SER	2.2
1	B	923	PRO	2.2
1	B	882	GLU	2.2
1	B	79	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	736	ALA	2.2
1	B	880	ILE	2.2
1	B	506	PRO	2.2
1	A	770	THR	2.2
1	B	907	TYR	2.1
1	B	850	ALA	2.1
1	B	901	LEU	2.1
1	B	395	SER	2.1
1	B	78	THR	2.1
1	A	341	VAL	2.1
1	B	852	GLU	2.1
1	A	126	LEU	2.1
1	A	888	LYS	2.1
1	B	352	SER	2.1
1	B	802	ILE	2.1
1	B	760	PRO	2.0
1	B	50	GLN	2.0
1	A	100	SER	2.0
1	A	157	SER	2.0
1	B	37	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGA	A	1007	9/9	0.69	0.41	38,50,70,80	9
4	EDO	A	1006	4/4	0.79	0.36	43,43,43,43	0
5	PGA	B	1007	9/9	0.79	0.34	41,62,78,98	9

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLY	B	1001	5/5	0.85	0.26	60,65,79,105	0
4	EDO	A	1005	4/4	0.87	0.32	50,50,50,50	0
6	GOL	B	1006	6/6	0.87	0.23	40,46,49,50	0
6	GOL	B	1005	6/6	0.94	0.20	37,44,46,51	0
2	GLY	A	1001	5/5	0.94	0.26	36,47,51,52	0
3	G6P	B	1002	16/16	0.95	0.16	50,57,67,69	0
4	EDO	B	1003	4/4	0.96	0.33	41,43,44,47	0
4	EDO	B	1004	4/4	0.96	0.39	44,47,52,54	0
4	EDO	A	1004	4/4	0.96	0.30	40,40,41,44	0
4	EDO	A	1003	4/4	0.97	0.29	31,39,46,50	0
3	G6P	A	1002	16/16	0.97	0.13	37,47,53,57	0

6.5 Other polymers (i)

There are no such residues in this entry.