



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:43 PM UTC

PDB ID : 2OOG / pdb_00002oog
Title : Crystal structure of glycerophosphoryl diester phosphodiesterase from *Staphylococcus aureus*
Authors : Patskovsky, Y.; Fedorov, E.; Toro, R.; Sauder, J.M.; Smith, D.; Freeman, J.; Maletic, M.; Powell, A.; Gheyi, T.; Wasserman, S.R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-01-25
Resolution : 2.20 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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

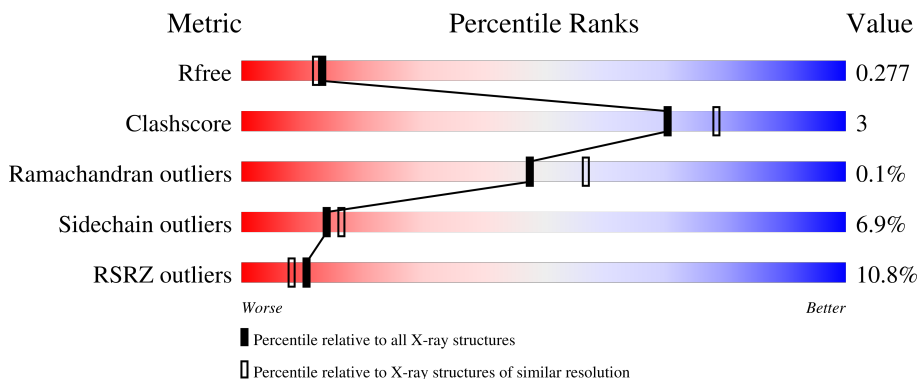
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	287	
1	B	287	
1	C	287	
1	D	287	

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Mol	Chain	Length	Quality of chain
1	E	287	
1	F	287	

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
4	GOL	A	476	-	-	X	-
4	GOL	E	467	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14474 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 Glycerophosphoryl diester phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	Total 2238	C 1418	N 392	O 424	S 4	0	10	0
1	B	267	Total 2233	C 1413	N 392	O 424	S 4	0	9	0
1	C	267	Total 2216	C 1400	N 393	O 419	S 4	0	5	0
1	D	268	Total 2223	C 1406	N 392	O 421	S 4	0	6	0
1	E	267	Total 2200	C 1392	N 386	O 418	S 4	0	3	0
1	F	267	Total 2203	C 1392	N 389	O 418	S 4	0	3	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLU	-	expression tag	UNP Q7A6H7
A	311	GLY	-	expression tag	UNP Q7A6H7
A	312	HIS	-	expression tag	UNP Q7A6H7
A	313	HIS	-	expression tag	UNP Q7A6H7
A	314	HIS	-	expression tag	UNP Q7A6H7
A	315	HIS	-	expression tag	UNP Q7A6H7
A	316	HIS	-	expression tag	UNP Q7A6H7
A	317	HIS	-	expression tag	UNP Q7A6H7
B	310	GLU	-	expression tag	UNP Q7A6H7
B	311	GLY	-	expression tag	UNP Q7A6H7
B	312	HIS	-	expression tag	UNP Q7A6H7
B	313	HIS	-	expression tag	UNP Q7A6H7
B	314	HIS	-	expression tag	UNP Q7A6H7
B	315	HIS	-	expression tag	UNP Q7A6H7
B	316	HIS	-	expression tag	UNP Q7A6H7
B	317	HIS	-	expression tag	UNP Q7A6H7
C	310	GLU	-	expression tag	UNP Q7A6H7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	311	GLY	-	expression tag	UNP Q7A6H7
C	312	HIS	-	expression tag	UNP Q7A6H7
C	313	HIS	-	expression tag	UNP Q7A6H7
C	314	HIS	-	expression tag	UNP Q7A6H7
C	315	HIS	-	expression tag	UNP Q7A6H7
C	316	HIS	-	expression tag	UNP Q7A6H7
C	317	HIS	-	expression tag	UNP Q7A6H7
D	310	GLU	-	expression tag	UNP Q7A6H7
D	311	GLY	-	expression tag	UNP Q7A6H7
D	312	HIS	-	expression tag	UNP Q7A6H7
D	313	HIS	-	expression tag	UNP Q7A6H7
D	314	HIS	-	expression tag	UNP Q7A6H7
D	315	HIS	-	expression tag	UNP Q7A6H7
D	316	HIS	-	expression tag	UNP Q7A6H7
D	317	HIS	-	expression tag	UNP Q7A6H7
E	310	GLU	-	expression tag	UNP Q7A6H7
E	311	GLY	-	expression tag	UNP Q7A6H7
E	312	HIS	-	expression tag	UNP Q7A6H7
E	313	HIS	-	expression tag	UNP Q7A6H7
E	314	HIS	-	expression tag	UNP Q7A6H7
E	315	HIS	-	expression tag	UNP Q7A6H7
E	316	HIS	-	expression tag	UNP Q7A6H7
E	317	HIS	-	expression tag	UNP Q7A6H7
F	310	GLU	-	expression tag	UNP Q7A6H7
F	311	GLY	-	expression tag	UNP Q7A6H7
F	312	HIS	-	expression tag	UNP Q7A6H7
F	313	HIS	-	expression tag	UNP Q7A6H7
F	314	HIS	-	expression tag	UNP Q7A6H7
F	315	HIS	-	expression tag	UNP Q7A6H7
F	316	HIS	-	expression tag	UNP Q7A6H7
F	317	HIS	-	expression tag	UNP Q7A6H7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

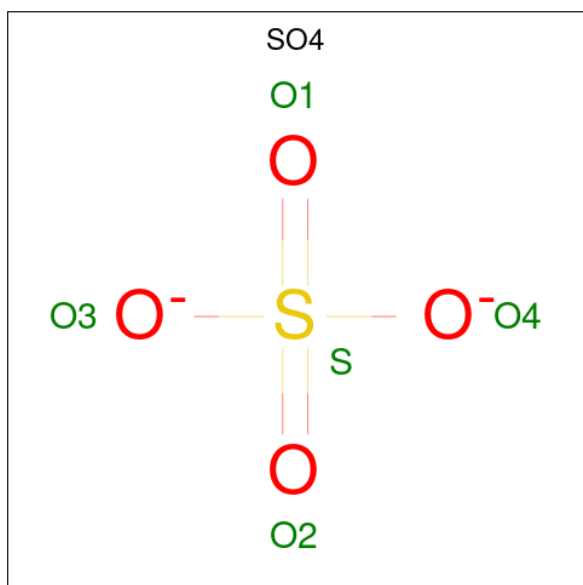
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	198	Total	O	0	0
			198	198		
5	B	211	Total	O	0	0
			211	211		
5	C	87	Total	O	0	0
			87	87		
5	D	193	Total	O	0	0
			193	193		
5	E	92	Total	O	0	0
			92	92		
5	F	110	Total	O	0	0
			110	110		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	156.31Å 183.55Å 176.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.20) 97.0 (20.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.235 , 0.280 0.231 , 0.277	Depositor DCC
R_{free} test set	3743 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtrriage
Anisotropy	0.231	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14474	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4673e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, GOL, ZN

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	0.67	0/2319	0.96	4/3128 (0.1%)
1	B	0.62	0/2311	0.89	2/3119 (0.1%)
1	C	0.56	0/2282	0.87	2/3080 (0.1%)
1	D	0.56	0/2293	0.87	2/3095 (0.1%)
1	E	0.56	0/2260	0.91	2/3052 (0.1%)
1	F	0.53	0/2263	0.92	5/3055 (0.2%)
All	All	0.59	0/13728	0.90	17/18529 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	1	3
All	All	2	10

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	PHE	N-CA-C	11.50	127.27	108.52
1	F	240	GLN	N-CA-C	10.74	126.38	113.28
1	B	237	PHE	N-CA-C	9.28	123.64	108.52
1	F	238	ASN	N-CA-C	7.24	121.11	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	SER	N-CA-C	6.43	116.99	109.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	237	PHE	CA
1	F	240	GLN	CA

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	PHE	Peptide
1	A	277	TYR	Peptide
1	B	277	TYR	Peptide
1	C	277	TYR	Peptide
1	D	272	PHE	Peptide

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	2238	0	2216	23	0
1	B	2233	0	2202	14	0
1	C	2216	0	2178	12	0
1	D	2223	0	2183	11	0
1	E	2200	0	2157	20	0
1	F	2203	0	2159	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	36	0	48	9	0
4	B	60	0	80	8	0
4	C	12	0	16	0	0
4	D	54	0	72	7	0
4	E	30	0	40	7	0
4	F	42	0	56	3	0
5	A	198	0	0	1	0
5	B	211	0	0	1	0
5	C	87	0	0	3	0
5	D	193	0	0	0	0
5	E	92	0	0	1	0
5	F	110	0	0	2	0
All	All	14474	0	13407	91	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 3.

The worst 5 of 91 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:194:ASN:HB2	4:B:478:GOL:H11	1.02	0.99
1:B:194:ASN:HB2	4:B:478:GOL:C1	1.94	0.97
1:B:194:ASN:CB	4:B:478:GOL:H11	1.96	0.95
1:D:202:HIS:NE2	4:D:463:GOL:H32	1.90	0.86
1:D:79:ASN:O	1:D:82:LYS:HE2	1.81	0.79

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	275/287 (96%)	267 (97%)	8 (3%)	0	100	100
1	B	274/287 (96%)	268 (98%)	4 (2%)	2 (1%)	18	19
1	C	270/287 (94%)	263 (97%)	7 (3%)	0	100	100
1	D	272/287 (95%)	265 (97%)	7 (3%)	0	100	100
1	E	268/287 (93%)	259 (97%)	9 (3%)	0	100	100
1	F	268/287 (93%)	260 (97%)	7 (3%)	1 (0%)	30	34
All	All	1627/1722 (94%)	1582 (97%)	42 (3%)	3 (0%)	48	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	147[A]	ASN
1	B	147[B]	ASN
1	F	59	HIS

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	247/254 (97%)	228 (92%)	19 (8%)	12	13
1	B	246/254 (97%)	234 (95%)	12 (5%)	22	29
1	C	242/254 (95%)	226 (93%)	16 (7%)	15	18
1	D	243/254 (96%)	229 (94%)	14 (6%)	18	22
1	E	240/254 (94%)	219 (91%)	21 (9%)	9	10
1	F	240/254 (94%)	219 (91%)	21 (9%)	9	10
All	All	1458/1524 (96%)	1355 (93%)	103 (7%)	14	16

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	237	PHE
1	E	195	ASN

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Mol	Chain	Res	Type
1	F	235	GLN
1	D	250	ILE
1	E	122	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	219	GLN
1	F	195	ASN
1	D	194	ASN
1	F	240	GLN
1	E	200	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](#)

Of 51 ligands modelled in this entry, 6 are monoatomic - leaving 45 for Mogul analysis.

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	$\# Z > 2$
4	GOL	E	454	2	5,5,5	0.33	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	E	474	-	5,5,5	0.38	0	5,5,5	0.25	0
4	GOL	F	486	-	5,5,5	0.34	0	5,5,5	0.29	0
4	GOL	B	480	-	5,5,5	0.84	0	5,5,5	1.01	0
4	GOL	F	457	-	5,5,5	0.40	0	5,5,5	0.39	0
4	GOL	A	489	-	5,5,5	0.36	0	5,5,5	0.36	0
4	GOL	B	458	-	5,5,5	0.43	0	5,5,5	0.59	0
4	GOL	F	456	2	5,5,5	0.43	0	5,5,5	0.42	0
4	GOL	E	467	-	5,5,5	0.38	0	5,5,5	0.31	0
4	GOL	D	468	-	5,5,5	0.40	0	5,5,5	0.32	0
4	GOL	C	482	-	5,5,5	0.50	0	5,5,5	0.33	0
4	GOL	D	466	-	5,5,5	0.36	0	5,5,5	0.26	0
4	GOL	B	477	-	5,5,5	0.46	0	5,5,5	0.30	0
4	GOL	D	462	-	5,5,5	0.43	0	5,5,5	0.21	0
4	GOL	D	463	-	5,5,5	0.36	0	5,5,5	0.31	0
4	GOL	A	475	-	5,5,5	0.38	0	5,5,5	0.32	0
4	GOL	B	479	-	5,5,5	0.35	0	5,5,5	0.44	0
4	GOL	A	487	-	5,5,5	0.66	0	5,5,5	0.37	0
4	GOL	D	481	-	5,5,5	0.69	0	5,5,5	0.94	0
4	GOL	F	460	-	5,5,5	0.36	0	5,5,5	0.34	0
4	GOL	D	453	2	5,5,5	0.35	0	5,5,5	0.37	0
4	GOL	A	470	-	5,5,5	0.34	0	5,5,5	0.42	0
4	GOL	D	483	-	5,5,5	0.37	0	5,5,5	0.31	0
4	GOL	E	465	-	5,5,5	0.36	0	5,5,5	0.28	0
4	GOL	F	464	-	5,5,5	0.35	0	5,5,5	0.39	0
3	SO4	C	446	-	4,4,4	0.24	0	6,6,6	0.11	0
4	GOL	D	471	-	5,5,5	0.36	0	5,5,5	0.39	0
3	SO4	B	443	-	4,4,4	0.25	0	6,6,6	0.18	0
4	GOL	A	476	-	5,5,5	0.59	0	5,5,5	0.25	0
3	SO4	A	445	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	442	-	4,4,4	0.26	0	6,6,6	0.08	0
4	GOL	F	488	-	5,5,5	0.38	0	5,5,5	0.32	0
4	GOL	B	461	-	5,5,5	0.42	0	5,5,5	0.53	0
4	GOL	B	469	-	5,5,5	0.38	0	5,5,5	0.31	0
4	GOL	A	455	2	5,5,5	0.27	0	5,5,5	0.49	0
4	GOL	D	484	-	5,5,5	0.37	0	5,5,5	0.37	0
4	GOL	B	478	-	5,5,5	0.38	0	5,5,5	0.32	0
3	SO4	A	441	-	4,4,4	0.26	0	6,6,6	0.05	0
4	GOL	B	452	2	5,5,5	0.27	0	5,5,5	0.53	0
4	GOL	E	485	-	5,5,5	0.31	0	5,5,5	0.44	0
3	SO4	D	444	-	4,4,4	0.24	0	6,6,6	0.11	0
4	GOL	C	451	2	5,5,5	0.38	0	5,5,5	0.40	0
4	GOL	B	472	-	5,5,5	0.38	0	5,5,5	0.21	0
4	GOL	F	459	-	5,5,5	0.36	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	473	-	5,5,5	0.49	0	5,5,5	0.40	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
4	GOL	E	454	2	-	4/4/4/4	-
4	GOL	E	474	-	-	2/4/4/4	-
4	GOL	F	486	-	-	4/4/4/4	-
4	GOL	B	480	-	-	4/4/4/4	-
4	GOL	F	457	-	-	0/4/4/4	-
4	GOL	A	489	-	-	2/4/4/4	-
4	GOL	B	458	-	-	4/4/4/4	-
4	GOL	F	456	2	-	4/4/4/4	-
4	GOL	E	467	-	-	4/4/4/4	-
4	GOL	D	468	-	-	0/4/4/4	-
4	GOL	C	482	-	-	4/4/4/4	-
4	GOL	D	466	-	-	2/4/4/4	-
4	GOL	B	477	-	-	2/4/4/4	-
4	GOL	D	462	-	-	2/4/4/4	-
4	GOL	D	463	-	-	4/4/4/4	-
4	GOL	A	475	-	-	1/4/4/4	-
4	GOL	B	479	-	-	1/4/4/4	-
4	GOL	A	487	-	-	1/4/4/4	-
4	GOL	D	481	-	-	4/4/4/4	-
4	GOL	F	460	-	-	4/4/4/4	-
4	GOL	D	453	2	-	1/4/4/4	-
4	GOL	A	470	-	-	4/4/4/4	-
4	GOL	D	483	-	-	0/4/4/4	-
4	GOL	E	465	-	-	2/4/4/4	-
4	GOL	F	464	-	-	2/4/4/4	-
4	GOL	D	471	-	-	2/4/4/4	-
4	GOL	A	476	-	-	2/4/4/4	-
4	GOL	F	488	-	-	2/4/4/4	-
4	GOL	B	461	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	469	-	-	3/4/4/4	-
4	GOL	A	455	2	-	0/4/4/4	-
4	GOL	D	484	-	-	2/4/4/4	-
4	GOL	B	478	-	-	4/4/4/4	-
4	GOL	B	452	2	-	0/4/4/4	-
4	GOL	E	485	-	-	3/4/4/4	-
4	GOL	C	451	2	-	2/4/4/4	-
4	GOL	B	472	-	-	4/4/4/4	-
4	GOL	F	459	-	-	3/4/4/4	-
4	GOL	B	473	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 95 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	470	GOL	O1-C1-C2-C3
4	A	470	GOL	C1-C2-C3-O3
4	A	470	GOL	O2-C2-C3-O3
4	A	489	GOL	O1-C1-C2-C3
4	A	476	GOL	O1-C1-C2-C3

There are no ring outliers.

15 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	474	GOL	2	0
4	B	480	GOL	1	0
4	B	458	GOL	1	0
4	E	467	GOL	4	0
4	D	468	GOL	1	0
4	D	463	GOL	3	0
4	A	487	GOL	3	0
4	D	481	GOL	3	0
4	F	460	GOL	1	0
4	A	476	GOL	6	0
4	B	478	GOL	3	0
4	E	485	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	472	GOL	1	0
4	F	459	GOL	2	0
4	B	473	GOL	2	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	267/287 (93%)	0.08	4 (1%) 72 69	22, 43, 73, 125	10 (3%)
1	B	267/287 (93%)	-0.23	5 (1%) 66 63	20, 37, 65, 113	9 (3%)
1	C	267/287 (93%)	1.35	74 (27%) 1 1	32, 64, 99, 151	5 (1%)
1	D	268/287 (93%)	0.05	5 (1%) 66 63	24, 45, 77, 124	6 (2%)
1	E	267/287 (93%)	1.08	59 (22%) 2 1	34, 66, 100, 145	3 (1%)
1	F	267/287 (93%)	0.68	26 (9%) 13 10	25, 56, 86, 135	3 (1%)
All	All	1603/1722 (93%)	0.50	173 (10%) 11 8	20, 52, 91, 151	36 (2%)

The worst 5 of 173 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	300	PHE	5.2
1	E	54	PHE	4.9
1	E	243	LYS	4.6
1	C	308	ILE	4.5
1	E	273	ILE	4.4

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 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(Å ²)	Q<0.9
4	GOL	B	473	6/6	0.55	0.22	105,114,121,126	0
4	GOL	A	476	6/6	0.56	0.13	92,108,116,117	0
4	GOL	B	478	6/6	0.65	0.23	79,98,125,136	0
4	GOL	F	486	6/6	0.66	0.17	78,91,111,116	0
3	SO4	A	441	5/5	0.67	0.13	95,100,125,131	0
4	GOL	B	480	6/6	0.70	0.22	69,95,105,118	0
4	GOL	E	467	6/6	0.71	0.19	70,102,105,118	0
4	GOL	C	482	6/6	0.71	0.13	70,95,99,99	0
4	GOL	A	475	6/6	0.72	0.19	67,90,96,98	0
4	GOL	B	469	6/6	0.72	0.17	60,77,98,113	0
4	GOL	B	472	6/6	0.74	0.14	78,93,99,105	0
4	GOL	E	474	6/6	0.77	0.13	101,111,119,121	0
4	GOL	F	460	6/6	0.78	0.20	97,117,121,121	0
3	SO4	D	444	5/5	0.78	0.10	73,79,104,107	0
3	SO4	B	443	5/5	0.79	0.14	73,83,96,114	0
4	GOL	E	485	6/6	0.80	0.18	55,60,70,84	0
4	GOL	E	454	6/6	0.81	0.17	54,65,77,87	0
4	GOL	D	463	6/6	0.81	0.16	45,63,89,106	0
4	GOL	F	464	6/6	0.81	0.10	63,82,88,93	0
4	GOL	D	468	6/6	0.81	0.12	49,82,87,89	0
4	GOL	A	489	6/6	0.82	0.14	94,102,108,108	0
3	SO4	C	446	5/5	0.82	0.08	77,80,103,109	0
4	GOL	F	457	6/6	0.83	0.17	39,62,84,84	0
3	SO4	A	445	5/5	0.84	0.10	77,85,104,112	0
4	GOL	F	488	6/6	0.84	0.13	56,79,94,94	0
4	GOL	B	458	6/6	0.85	0.15	46,64,70,88	0
4	GOL	D	471	6/6	0.85	0.15	52,65,80,81	0
4	GOL	D	483	6/6	0.85	0.10	89,93,102,105	0
4	GOL	A	487	6/6	0.85	0.11	80,87,93,107	0
4	GOL	D	466	6/6	0.86	0.12	58,95,100,116	0
4	GOL	B	479	6/6	0.87	0.19	68,90,106,107	0
4	GOL	D	462	6/6	0.87	0.12	44,59,87,92	0
4	GOL	E	465	6/6	0.88	0.10	43,84,89,98	0
4	GOL	F	459	6/6	0.88	0.10	52,71,84,99	0
4	GOL	D	481	6/6	0.88	0.12	64,76,84,92	0
4	GOL	D	484	6/6	0.90	0.12	57,79,86,87	0
4	GOL	A	470	6/6	0.90	0.09	56,70,80,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	C	451	6/6	0.91	0.12	58,67,89,90	0
3	SO4	A	442	5/5	0.91	0.12	57,72,80,81	0
4	GOL	B	461	6/6	0.91	0.13	57,75,86,86	0
4	GOL	B	477	6/6	0.92	0.10	36,64,80,87	0
4	GOL	F	456	6/6	0.93	0.08	43,53,53,54	0
2	ZN	F	402	1/1	0.94	0.07	76,76,76,76	0
2	ZN	E	404	1/1	0.97	0.06	73,73,73,73	0
2	ZN	C	406	1/1	0.97	0.06	76,76,76,76	0
4	GOL	A	455	6/6	0.97	0.06	30,36,45,50	0
4	GOL	B	452	6/6	0.98	0.06	19,25,34,36	0
4	GOL	D	453	6/6	0.98	0.06	34,37,43,49	0
2	ZN	D	405	1/1	0.99	0.07	60,60,60,60	0
2	ZN	B	401	1/1	0.99	0.07	46,46,46,46	0
2	ZN	A	403	1/1	1.00	0.05	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.