

Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2024 – 12:27 PM EDT

PDB ID	:	8W06
Title	:	Crystal Structure of the reconstruction of the ancestral triosephosphate iso-
		merase of the last opisthokont common ancestor obtained by maximum likeli-
		hood with PGH
Authors	:	Perez-Nino, J.A.; Rodriguez-Romero, A.; Guerra-Borrego, Y.; Fernandez-
		Velasco, D.A.
Deposited on	:	2024-02-13
Resolution	:	2.06 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 (i) 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 (1)) were used in the production of this report:

:	4.02b-467
:	2022.3.0, CSD as543be (2022)
:	1.20.1
:	3.0
:	1.1.7(2018)
:	20231227.v01 (using entries in the PDB archive December 27th 2023)
:	9.0.002 (Gargrove)
:	1.0.11
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.38.3
	: : : : : : : : : : : : : : : : : : :



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 2.06 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (2.08-2.04)

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	А	270	2% 88%	·	7%
1	В	270	87%	6%	7%
1	С	270	% 86%	6%	7%
1	D	270	85%	8%	7%
1	Е	270	% • 87%	6%	7%



Mol	Chain	Length	Quality of chain		
1	F	270	87%	6%	7%
1	G	270	84%	8%	8%
1	Н	270	13%	14%	9%



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 16891 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.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	Δ	250	Total	С	Ν	0	S	0	2	0
	A	230	1950	1234	333	376	7	0	ა	0
1	р	951	Total	С	Ν	0	S	0	2	0
	D	201	1948	1232	332	377	7	0	5	0
1	C	250	Total	С	Ν	0	S	0	4	0
		230	1955	1233	332	383	7	0	4	0
1	П	251	Total	С	Ν	0	S	0	5	0
	D	201	1976	1245	337	387	7	0	5	0
1	F	251	Total	С	Ν	0	S	0	2	0
1	Ľ	201	1948	1229	332	380	7	0	2	0
1	Б	251	Total	С	Ν	0	S	0	1	0
	Г	201	1942	1226	332	377	7	0	L	0
1	C	240	Total	С	Ν	0	S	0	0	0
	G	249	1914	1211	327	370	6	0	0	0
1	ц	246	Total	С	Ν	0	S	0	1	0
	п	240	1871	1185	323	357	6			0

• Molecule 1 is a protein called Triosephosphate isomerase.

• Molecule 2 is PHOSPHOGLYCOLOHYDROXAMIC ACID (three-letter code: PGH) (formula: C₂H₆NO₆P) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
0	Λ	1	Total	С	Ν	0	Р	0	0
	A	1	10	2	1	6	1	0	0
0	Р	1	Total	С	Ν	0	Р	0	0
	D	1	10	2	1	6	1	0	0
0	С	1	Total	С	Ν	0	Р	0	0
	U	1	10	2	1	6	1	0	0
0	Л	1	Total	С	Ν	0	Р	0	0
	D	1	10	2	1	6	1		0
0	F	1	Total	С	Ν	0	Р	0	0
	Ľ	1	10	2	1	6	1	0	0
0	Б	1	Total	С	Ν	0	Р	0	0
	Г	1	10	2	1	6	1	0	0
0	С	1	Total	С	Ν	Ο	Р	0	0
	G	L	10	2	1	6	1		U
9	Ц	1	Total	С	Ν	Ο	Р	0	0
	11		10	2	1	6	1		0

• Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	В	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	O 2	0	0

• Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	С	1	Total 10	С 6	0 4	0	0

• Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	С	1	Total 4	${ m C} 2$	O 2	0	0

• Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Na 1 1	0	0

• Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





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

• Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Е	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
8	G	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0

• Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total Cl 1 1	0	0

• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	218	Total O 218 218	0	0
10	В	196	Total O 196 196	0	0
10	С	182	Total O 182 182	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	175	Total O 175 175	0	0
10	Е	173	Total O 173 173	0	0
10	F	123	Total O 123 123	0	0
10	G	135	Total O 135 135	0	0
10	Н	67	$\begin{array}{cc} \text{Total} & \text{O} \\ 67 & 67 \end{array}$	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: Triosephosphate isomerase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	111.64Å 83.22Å 127.86Å	Depositor
a, b, c, α , β , γ	90.00° 103.49° 90.00°	Depositor
Bosolution (Å)	41.45 - 2.06	Depositor
Resolution (A)	41.45 - 2.06	EDS
% Data completeness	99.5 (41.45-2.06)	Depositor
(in resolution range)	99.5(41.45-2.06)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.09 (at 2.07 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
P. P.	0.195 , 0.235	Depositor
n, n_{free}	0.195 , 0.235	DCC
R_{free} test set	7134 reflections (5.07%)	wwPDB-VP
Wilson B-factor $(Å^2)$	28.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , 47.9	EDS
L-test for $twinning^2$	$ < L >=0.52, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16891	wwPDB-VP
Average B, all atoms $(Å^2)$	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: PEG, CL, EDO, NA, PGE, ACY, PGH, ACT

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).

Mal	Chain	Bond	lengths	Bond	angles
IVIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.47	0/1985	0.61	0/2685
1	В	0.44	0/1983	0.62	0/2684
1	С	0.42	0/1986	0.59	0/2687
1	D	0.39	0/2008	0.58	0/2717
1	Ε	0.39	0/1980	0.57	0/2679
1	F	0.38	0/1974	0.57	0/2671
1	G	0.42	0/1945	0.57	0/2632
1	Н	0.44	0/1902	0.59	0/2578
All	All	0.42	0/15763	0.59	0/21333

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 (i)

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	А	1950	0	1967	7	0
1	В	1948	0	1955	9	0
1	С	1955	0	1953	9	0
1	D	1976	0	1973	11	0
1	Е	1948	0	1951	13	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1942	0	1949	12	0
1	G	1914	0	1927	14	0
1	Н	1871	0	1861	26	0
2	А	10	0	4	0	0
2	В	10	0	4	0	0
2	С	10	0	4	0	0
2	D	10	0	4	1	0
2	Е	10	0	4	0	0
2	F	10	0	4	0	0
2	G	10	0	4	0	0
2	Н	10	0	4	0	0
3	В	4	0	3	0	0
4	С	10	0	14	1	0
5	С	4	0	3	0	0
6	D	1	0	0	0	0
7	D	4	0	6	0	0
8	Е	7	0	10	0	0
8	G	7	0	10	0	0
9	F	1	0	0	0	0
10	А	218	0	0	0	0
10	В	196	0	0	2	0
10	С	182	0	0	0	0
10	D	175	0	0	0	0
10	Е	173	0	0	4	0
10	F	123	0	0	1	0
10	G	135	0	0	0	0
10	Н	67	0	0	0	0
All	All	16891	0	15614	96	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.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:153:ILE:HD11	1:H:158:TRP:CE2	2.16	0.80
1:H:220:GLU:HA	1:H:223:LYS:HD2	1.74	0.69
1:H:28:ASN:HA	1:H:55:ARG:HD2	1.73	0.68
1:F:48:PRO:O	1:F:52[A]:GLN:HG2	1.99	0.61
1:E:147:LYS:HD3	10:E:428:HOH:O	2.01	0.60
1:G:42:PRO:HG2	1:G:47:LEU:HD23	1.86	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:F:121:LYS:HG2	1:F:160:LYS:HE2	1.84	0.58
1:C:42:PRO:HG2	1:C:47:LEU:HD23	1.86	0.57
1:D:109:ALA:HB1	1:D:152:LYS:HD2	1.85	0.57
1:G:16:THR:H	1:G:19:SER:HB2	1.69	0.57
1:H:55:ARG:HB2	1:H:57:ASP:OD1	2.05	0.56
1:E:6:PHE:O	1:E:229:GLY:HA3	2.07	0.55
1:F:160:LYS:HD3	10:F:431:HOH:O	2.07	0.55
1:G:17:ILE:HD11	1:H:85:LEU:HD12	1.89	0.55
1:H:219:LYS:HG3	1:H:247:ALA:O	2.07	0.55
1:E:11:TRP:CZ3	1:E:42:PRO:HB3	2.42	0.55
1:E:72:ALA:HA	1:F:12:LYS:HD3	1.89	0.55
1:H:153:ILE:HD11	1:H:158:TRP:CD2	2.42	0.54
1:D:184:GLU:O	1:D:188:GLU:HG2	2.07	0.54
1:E:85:LEU:HD22	1:F:45:ILE:HD11	1.89	0.54
1:H:123:ILE:HA	1:H:162:VAL:HG13	1.89	0.54
1:G:11:TRP:CZ3	1:G:42:PRO:HB3	2.42	0.53
1:D:139:MET:HE3	1:D:139:MET:HA	1.91	0.53
1:A:28:ASN:HA	1:A:55:ARG:HD2	1.92	0.52
1:H:116:LEU:HD13	1:H:157:ASP:HB3	1.93	0.51
1:H:59[B]:GLN:HG2	1:H:88:PRO:HG2	1.93	0.51
1:G:28:ASN:HA	1:G:55:ARG:HD2	1.92	0.51
1:D:199:ALA:O	1:D:203:GLU:HG2	2.12	0.50
1:G:11:TRP:CE3	1:G:42:PRO:HB3	2.46	0.50
1:H:57:ASP:OD1	1:H:57:ASP:N	2.45	0.50
1:A:246:ASN:HB3	1:A:249:GLN:HG2	1.94	0.50
1:B:42:PRO:HG2	1:B:47:LEU:HD23	1.94	0.49
1:B:56:LYS:HE2	10:B:483:HOH:O	2.12	0.49
1:H:176:VAL:HG22	1:H:177:ALA:O	2.13	0.49
1:H:11:TRP:CZ3	1:H:20:ILE:HD12	2.47	0.49
1:H:7:VAL:HG21	1:H:245:ILE:HA	1.94	0.48
1:B:17:ILE:HG22	1:B:21:LYS:HD2	1.93	0.48
1:G:13:MET:HG3	1:H:76:GLU:O	2.13	0.48
1:E:135:ALA:CB	1:E:137:LYS:HE3	2.44	0.48
1:E:237:LEU:HD12	10:E:525:HOH:O	2.14	0.47
1:D:89:TRP:CE2	1:D:121:LYS:HE3	2.49	0.47
1:G:78:SER:OG	1:G:81:MET:HG3	2.15	0.47
1:H:41:ALA:HB2	1:H:61:ALA:HB3	1.95	0.47
1:E:69:ALA:HB2	1:E:114:TYR:OH	2.14	0.47
1:H:167:PRO:HB2	1:H:169:TRP:CE2	2.50	0.47
1:E:135:ALA:HB1	1:E:137:LYS:HE3	1.97	0.46
1:A:6:PHE:O	1:A:229:GLY:HA3	2.15	0.46



A 4 1	A t and D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:219:LYS:HE2	1:G:250:LYS:HD2	1.97	0.46
1:G:69:ALA:HA	1:G:80:GLU:OE1	2.15	0.46
1:C:214:ASN:HB2	1:C:240:GLU:OE2	2.15	0.46
1:E:223:LYS:NZ	10:E:408:HOH:O	2.49	0.46
1:G:116:LEU:HD13	1:G:157:ASP:HB3	1.97	0.46
4:C:302:PGE:H52	4:C:302:PGE:H32	1.64	0.45
1:F:180:GLU:H	1:F:180:GLU:CD	2.19	0.45
1:H:191:LYS:HD3	1:H:195:GLU:OE2	2.15	0.45
1:C:68:LYS:HD2	1:C:73:PHE:CZ	2.51	0.45
1:A:83[A]:LYS:HA	1:A:83[A]:LYS:HD2	1.59	0.45
1:C:109:ALA:HA	1:C:149:ILE:HG13	1.98	0.45
1:B:6:PHE:O	1:B:229:GLY:HA3	2.16	0.45
1:E:41:ALA:HA	1:E:61:ALA:O	2.17	0.45
1:G:12:LYS:HD3	1:H:72:ALA:HA	1.98	0.45
1:B:106:GLU:O	1:B:110:GLU:HG3	2.18	0.44
1:H:107:PHE:CE2	1:H:111:LYS:HE3	2.53	0.44
1:D:69:ALA:HA	1:D:80:GLU:OE1	2.18	0.44
1:F:155:GLU:H	1:F:155:GLU:CD	2.21	0.44
1:B:107:PHE:CE2	1:B:111:LYS:HE3	2.53	0.43
1:D:28:ASN:HA	1:D:55:ARG:HD2	2.01	0.43
1:F:28:ASN:HA	1:F:55:ARG:HD2	1.99	0.43
1:G:60:VAL:O	1:G:88:PRO:HD2	2.18	0.43
1:B:11:TRP:CZ3	1:B:42:PRO:HB3	2.54	0.43
1:C:209:TYR:O	1:C:230:PHE:HA	2.19	0.43
1:E:13:MET:HG3	1:F:76:GLU:O	2.18	0.43
1:C:224:GLN:HB2	1:C:227:ILE:HD12	2.00	0.42
1:F:6:PHE:O	1:F:229:GLY:HA3	2.18	0.42
1:D:68:LYS:HD2	1:D:73:PHE:CZ	2.54	0.42
1:F:199:ALA:O	1:F:203:GLU:HG3	2.19	0.42
1:D:166[A]:GLU:OE2	2:D:302:PGH:N2	2.52	0.42
1:D:39:VAL:HA	1:D:59[A]:GLN:O	2.19	0.42
1:A:126:ILE:HD13	1:A:146[A]:LEU:HG	2.00	0.42
1:C:6:PHE:O	1:C:229:GLY:HA3	2.19	0.42
1:H:60:VAL:O	1:H:88:PRO:HD2	2.20	0.42
1:B:224:GLN:NE2	10:B:416:HOH:O	2.52	0.42
1:G:6:PHE:O	1:G:229:GLY:HA3	2.19	0.42
1:C:5:PHE:CE1	1:C:229:GLY:HA2	2.55	0.41
1:D:42:PRO:HG2	1:D:47:LEU:HD23	2.01	0.41
1:A:11:TRP:CZ3	1:A:42:PRO:HB3	2.55	0.41
1:H:48:PRO:HG3	1:H:85:LEU:HD21	2.02	0.41
1:A:146[A]:LEU:HD23	1:A:146[A]:LEU:HA	1.94	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ASP:OD1	1:C:57:ASP:N	2.54	0.41
1:E:248:ARG:HD3	10:E:406:HOH:O	2.20	0.41
1:H:155:GLU:HA	1:H:158:TRP:HD1	1.86	0.41
1:B:69:ALA:HA	1:B:80:GLU:OE1	2.21	0.40
1:H:16:THR:O	1:H:20:ILE:HG12	2.21	0.40
1:H:103:GLU:CD	1:H:111:LYS:HZ2	2.25	0.40
1:F:146:LEU:HD23	1:F:146:LEU:HA	1.94	0.40
1:H:123:ILE:HG12	1:H:162:VAL:CG1	2.52	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	Perce	entiles
1	А	251/270~(93%)	241 (96%)	10 (4%)	0	100	100
1	В	252/270~(93%)	243~(96%)	9~(4%)	0	100	100
1	С	252/270~(93%)	245 (97%)	7(3%)	0	100	100
1	D	254/270~(94%)	246 (97%)	8 (3%)	0	100	100
1	Е	251/270~(93%)	245 (98%)	6 (2%)	0	100	100
1	F	250/270~(93%)	242 (97%)	8 (3%)	0	100	100
1	G	247/270~(92%)	240 (97%)	7(3%)	0	100	100
1	Н	245/270~(91%)	234 (96%)	11 (4%)	0	100	100
All	All	2002/2160~(93%)	1936 (97%)	66 (3%)	0	100	100

There are no Ramachandran outliers to report.



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	208/222~(94%)	207~(100%)	1 (0%)	86 88
1	В	207/222~(93%)	206 (100%)	1 (0%)	86 88
1	С	208/222~(94%)	207 (100%)	1 (0%)	86 88
1	D	211/222~(95%)	210 (100%)	1 (0%)	86 88
1	Ε	208/222~(94%)	208 (100%)	0	100 100
1	F	207/222~(93%)	205~(99%)	2(1%)	73 73
1	G	203/222~(91%)	203 (100%)	0	100 100
1	Н	194/222~(87%)	192 (99%)	2 (1%)	73 73
All	All	1646/1776~(93%)	1638 (100%)	8 (0%)	86 88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1	MET
1	В	166	GLU
1	С	1	MET
1	D	206	ARG
1	F	83	LYS
1	F	146	LEU
1	Н	156	SER
1	Н	248	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.

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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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).

Mal	Type	Chain	Dog	Link	Bond lengths		В	ond ang	les	
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	PGE	С	302	-	9,9,9	0.28	0	8,8,8	0.40	0
2	PGH	F	302	-	9,9,9	0.74	0	10,12,12	0.92	0
8	PEG	Е	302	-	6,6,6	0.16	0	$5,\!5,\!5$	0.08	0
2	PGH	G	301	-	9,9,9	0.76	0	10,12,12	0.90	0
8	PEG	G	302	-	6,6,6	0.11	0	$5,\!5,\!5$	0.12	0
2	PGH	А	301	-	9,9,9	0.81	0	10,12,12	0.94	0
2	PGH	D	302	-	9,9,9	0.79	0	10,12,12	0.88	0
2	PGH	В	301	-	9,9,9	0.81	0	10,12,12	0.95	0
3	ACY	В	302	-	3,3,3	1.66	0	3,3,3	1.71	1 (33%)
5	ACT	С	303	-	3,3,3	1.22	0	$3,\!3,\!3$	1.46	1 (33%)
2	PGH	Н	301	-	9,9,9	0.75	0	10,12,12	0.93	1 (10%)
2	PGH	Е	301	-	9,9,9	0.77	0	10,12,12	0.98	0
2	PGH	С	301	-	9,9,9	0.76	0	10,12,12	0.88	0
7	EDO	D	303	-	3,3,3	0.48	0	2,2,2	0.37	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	PGE	С	302	-	-	4/7/7/7	-
2	PGH	F	302	-	-	2/8/8/8	-
8	PEG	Е	302	-	-	1/4/4/4	-
2	PGH	G	301	-	-	1/8/8/8	-
8	PEG	G	302	-	-	3/4/4/4	-
2	PGH	А	301	-	-	2/8/8/8	-
2	PGH	D	302	-	-	4/8/8/8	-
2	PGH	В	301	-	-	2/8/8/8	-
2	PGH	Н	301	-	-	3/8/8/8	-
2	PGH	Е	301	-	-	2/8/8/8	-
2	PGH	С	301	-	-	2/8/8/8	-
7	EDO	D	303	-	-	0/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	302	ACY	O-C-CH3	-2.33	112.95	122.53
2	Н	301	PGH	O4P-P-O3P	2.01	115.34	107.80
5	С	303	ACT	OXT-C-O	2.00	129.45	122.03

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	301	PGH	N2-C1-C2-O1P
2	С	301	PGH	N2-C1-C2-O1P
2	D	302	PGH	C2-C1-N2-O2
2	D	302	PGH	O1-C1-N2-O2
2	Е	301	PGH	N2-C1-C2-O1P
2	Н	301	PGH	C2-C1-N2-O2
2	Н	301	PGH	O1-C1-N2-O2
4	С	302	PGE	C3-C4-O3-C5
4	С	302	PGE	O2-C3-C4-O3
8	G	302	PEG	O2-C3-C4-O4
8	G	302	PEG	O1-C1-C2-O2
2	D	302	PGH	C2-O1P-P-O2P
2	А	301	PGH	01-C1-C2-O1P
2	С	301	PGH	01-C1-C2-O1P
2	F	302	PGH	01-C1-C2-O1P



Mol	Chain	Res	Type	Atoms
2	В	301	PGH	01-C1-C2-O1P
2	D	302	PGH	01-C1-C2-O1P
2	Е	301	PGH	01-C1-C2-O1P
2	G	301	PGH	01-C1-C2-O1P
2	F	302	PGH	N2-C1-C2-O1P
4	С	302	PGE	O1-C1-C2-O2
4	С	302	PGE	C1-C2-O2-C3
2	В	301	PGH	C2-O1P-P-O2P
8	G	302	PEG	C1-C2-O2-C3
2	Н	301	PGH	01-C1-C2-O1P
8	Е	302	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	302	PGE	1	0
2	D	302	PGH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

















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, 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		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	250/270~(92%)	0.03	5 (2%) 64 6	7	9, 23, 39, 60	3(1%)
1	В	251/270~(92%)	0.06	4 (1%) 70 72	2	11, 25, 43, 69	3(1%)
1	С	250/270~(92%)	-0.05	3 (1%) 76 78	3	13, 25, 39, 73	4 (1%)
1	D	251/270~(92%)	0.02	3 (1%) 76 78	3	12, 26, 41, 63	5(1%)
1	Ε	251/270~(92%)	0.25	3 (1%) 76 78	3	14,30,44,57	2 (0%)
1	F	251/270~(92%)	0.35	4 (1%) 70 72	2	19, 33, 46, 68	1 (0%)
1	G	249/270~(92%)	0.19	2 (0%) 82 84	1	21,31,43,57	0
1	Н	246/270~(91%)	1.13	36 (14%) 7	7	23, 45, 61, 72	1 (0%)
All	All	1999/2160~(92%)	0.24	60 (3%) 52 5	4	9, 29, 50, 73	19 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	А	1	MET	5.6
1	С	1	MET	4.2
1	В	1	MET	4.0
1	Н	69	ALA	3.6
1	А	0	HIS	3.5
1	Н	198	SER	3.5
1	Н	197	VAL	3.4
1	Н	245	ILE	3.4
1	Н	162	VAL	3.3
1	Н	8	GLY	3.3
1	Н	89	TRP	3.2
1	С	2	ALA	3.1
1	Н	227	ILE	3.1
1	Н	166	GLU	3.1
1	Н	9	GLY	3.0
1	A	2	ALA	3.0



Mol	Mol Chain Bos Type BSBZ							
1	R	2		3.0				
1	Б F	0	HIS	$\frac{0.0}{2.0}$				
1	 Н	$\frac{0}{247}$		2.9				
1	 	247	CIV	2.0				
1		215 1	SEB	2.0				
1	 	-1	DHE	2.0 2.7				
1	 	242	I IIL VAI	2.1				
1	 Ц	180	CLU	$\frac{2.1}{2.7}$				
1	 Ц	230	180 GLU					
1	Δ	$\frac{250}{52}$	CLN	2.0				
1		170	PRO	2.0				
1		113	HIS	2.5				
1	н Н	38	VAL	2.5				
1	H	120	LEI	2.5				
1	F	_1	SER	2.5 9.4				
1	E E	-1 59	GLN	2.4				
1	н	59[A]	GLN	2.4				
1	 Н	104		2.0				
1	H	213	VAL	2.0				
1	H	232	VAL	2.3				
1	F	52[A]	GLN	2.3				
1	H	$\frac{02[11]}{222}$	ALA	2.3				
1	A	31	GLU	2.0				
1	H	39	VAL	2.2				
1	C	119	GLY	2.2				
1	H	27	LEU	2.2				
1	F	2	ALA	2.2				
1	H	155	GLU	2.2				
1	H	87	ILE	2.2				
1	D	203	GLU	2.2				
1	Н	157	ASP	2.2				
1	G	2	ALA	2.2				
1	Н	199	ALA	2.2				
1	Н	192	TRP	2.1				
1	В	0	HIS	2.1				
1	Н	216	GLY	2.1				
1	Н	219	LYS	2.1				
1	Н	205	THR	2.1				
1	Н	150	ALA	2.0				
1	G	250	LYS	2.0				
1	Н	175	LYS	2.0				
1	Н	80	GLU	2.0				



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Ε	69	ALA	2.0
1	В	139[A]	MET	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
3	ACY	В	302	4/4	0.71	0.18	$41,\!46,\!59,\!63$	0
7	EDO	D	303	4/4	0.77	0.15	42,44,47,47	0
4	PGE	С	302	10/10	0.81	0.13	37,46,54,58	0
8	PEG	G	302	7/7	0.82	0.12	43,48,57,62	0
8	PEG	Е	302	7/7	0.85	0.12	49,55,58,59	0
5	ACT	С	303	4/4	0.87	0.10	43,52,54,54	0
2	PGH	Н	301	10/10	0.87	0.12	41,45,54,55	0
6	NA	D	301	1/1	0.92	0.07	21,21,21,21	0
2	PGH	F	302	10/10	0.92	0.10	31,35,41,45	0
2	PGH	Е	301	10/10	0.94	0.08	26,35,39,39	0
2	PGH	G	301	10/10	0.94	0.08	27,33,39,41	0
2	PGH	D	302	10/10	0.95	0.08	24,25,35,36	0
2	PGH	А	301	10/10	0.95	0.09	21,25,33,34	0
2	PGH	В	301	10/10	0.96	0.06	24,27,34,37	0
2	PGH	С	301	10/10	0.97	0.07	22,27,33,37	0
9	CL	F	301	1/1	0.97	0.04	28,28,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



















6.5 Other polymers (i)

There are no such residues in this entry.

