Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 02:14 PM EDT

PDB ID	:	3GP3
Title	:	Crystal structure of phosphoglyceromutase from Burkholderia pseudomallei with 2-phosphoserine
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2009-03-20
Resolution	:	1.50 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 (i)) were used in the production of this report:

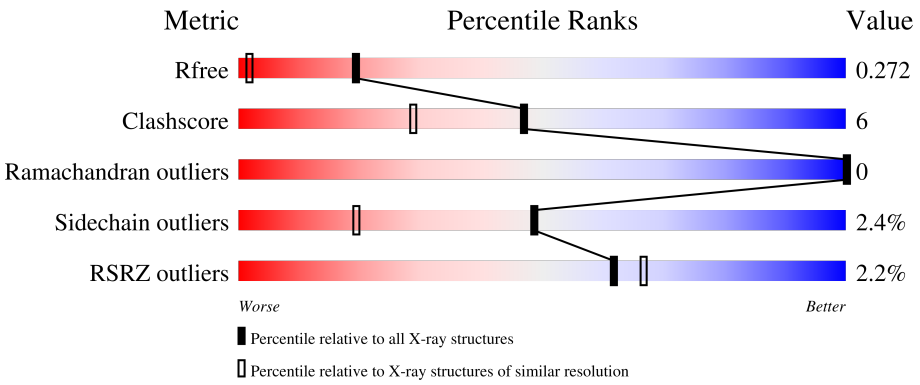
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	257	2% 77% 11% • 11%
1	B	257	3% 79% 9% • 11%
1	C	257	2% 76% 12% • 11%
1	D	257	2% 78% 11% • 11%

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
3	PO3	A	251	-	-	X	-
3	PO3	B	251	-	-	X	-
3	PO3	C	252	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8274 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 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	229	1858	1188	328	338	4	0	5	0
1	B	229	1850	1180	329	337	4	0	4	0
1	C	230	1875	1193	334	344	4	0	5	0
1	D	230	1841	1173	326	338	4	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q63XU7
A	-6	ALA	-	expression tag	UNP Q63XU7
A	-5	HIS	-	expression tag	UNP Q63XU7
A	-4	HIS	-	expression tag	UNP Q63XU7
A	-3	HIS	-	expression tag	UNP Q63XU7
A	-2	HIS	-	expression tag	UNP Q63XU7
A	-1	HIS	-	expression tag	UNP Q63XU7
A	0	HIS	-	expression tag	UNP Q63XU7
B	-7	MET	-	expression tag	UNP Q63XU7
B	-6	ALA	-	expression tag	UNP Q63XU7
B	-5	HIS	-	expression tag	UNP Q63XU7
B	-4	HIS	-	expression tag	UNP Q63XU7
B	-3	HIS	-	expression tag	UNP Q63XU7
B	-2	HIS	-	expression tag	UNP Q63XU7
B	-1	HIS	-	expression tag	UNP Q63XU7
B	0	HIS	-	expression tag	UNP Q63XU7
C	-7	MET	-	expression tag	UNP Q63XU7
C	-6	ALA	-	expression tag	UNP Q63XU7
C	-5	HIS	-	expression tag	UNP Q63XU7
C	-4	HIS	-	expression tag	UNP Q63XU7
C	-3	HIS	-	expression tag	UNP Q63XU7

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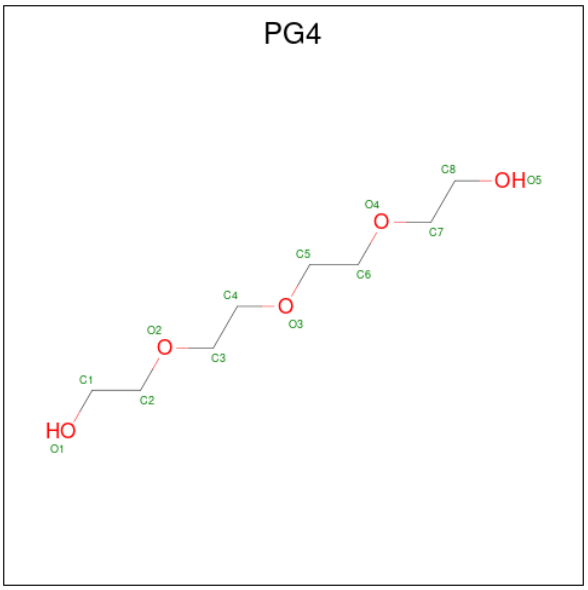
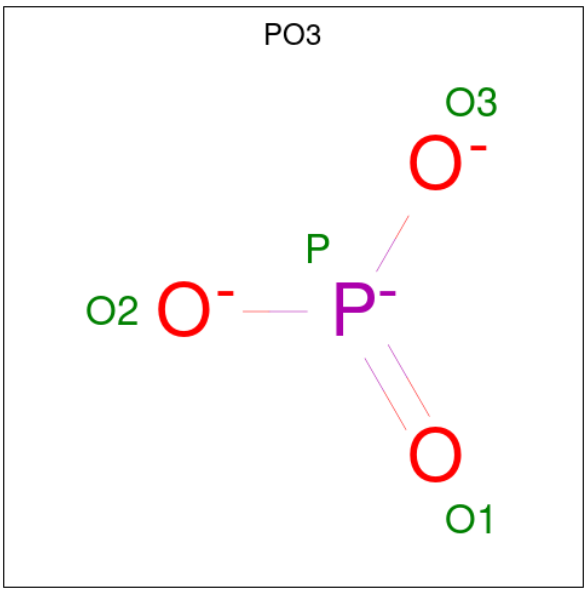
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q63XU7
C	-1	HIS	-	expression tag	UNP Q63XU7
C	0	HIS	-	expression tag	UNP Q63XU7
D	-7	MET	-	expression tag	UNP Q63XU7
D	-6	ALA	-	expression tag	UNP Q63XU7
D	-5	HIS	-	expression tag	UNP Q63XU7
D	-4	HIS	-	expression tag	UNP Q63XU7
D	-3	HIS	-	expression tag	UNP Q63XU7
D	-2	HIS	-	expression tag	UNP Q63XU7
D	-1	HIS	-	expression tag	UNP Q63XU7
D	0	HIS	-	expression tag	UNP Q63XU7

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



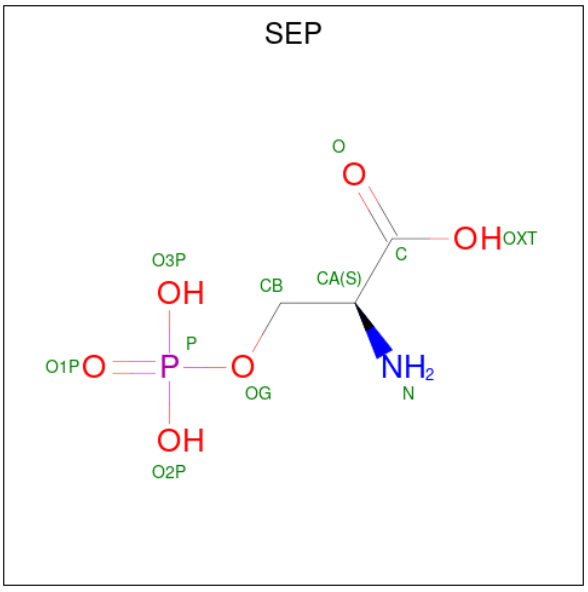
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	8	5	0	0
2	B	1	13	8	5	0	0
2	C	1	13	8	5	0	0
2	C	1	13	8	5	0	0
2	D	1	13	8	5	0	0
2	D	1	13	8	5	0	0

- Molecule 3 is PHOSPHITE ION (three-letter code: PO3) (formula: O_3P).



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

- Molecule 4 is PHOSPHOSERINE (three-letter code: SEP) (formula: $C_3H_8NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	11	3	1	6	1	0	0
4	B	1	11	3	1	6	1	0	0
4	C	1	11	3	1	6	1	0	0
4	D	1	11	3	1	6	1	0	0

- Molecule 5 is water.

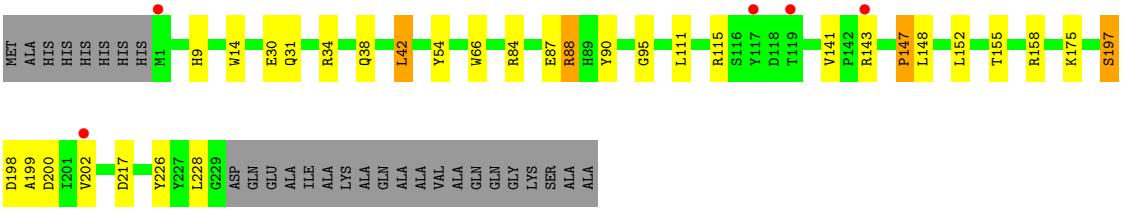
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	192	192	192	0	0
5	B	174	174	174	0	0
5	C	171	171	171	0	0
5	D	175	175	175	0	0

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.

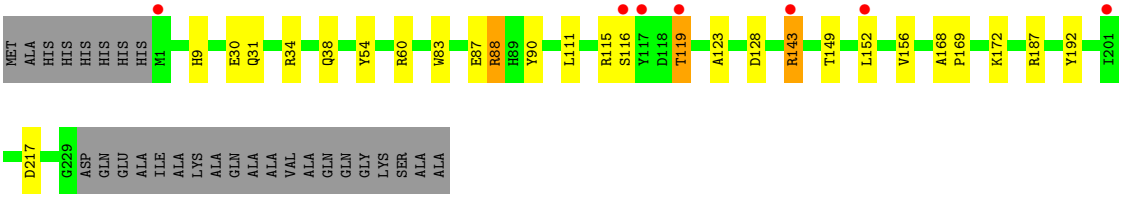
• Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase

Chain A:



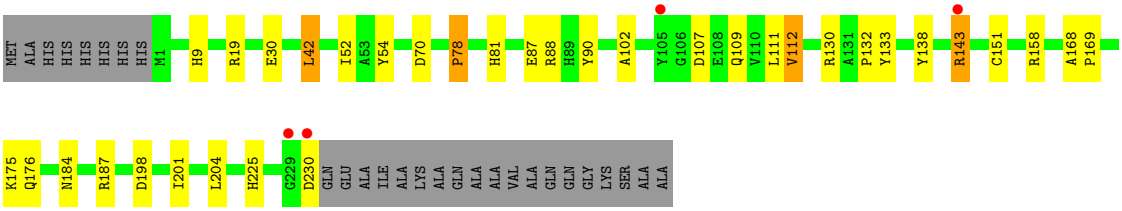
• Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase

Chain B:



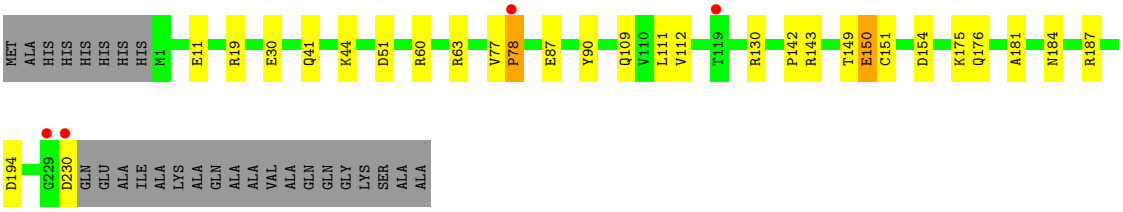
• Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase

Chain C:



• Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase

Chain D:


MET
ALA
HIS
HIS
HIS
HIS
HIS
M1
E11
R19
E30
Q41
K44
D51
R60
R63
V77
P78
E87
Y90
Q109
V110
L111
V112
T119
R130
P142
R143
T149
E150
C151
D154
K175
Q176
A181
N184
R187

D194
G229
D230
GLN
GLU
ALA
ILE
ALA
LYS
ALA
GLN
ALA
ALA
VAL
ALA
GLN
GLN
GLY
LYS
SER
ALA
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.26Å 72.05Å 78.04Å 107.96° 93.00° 104.20°	Depositor
Resolution (Å)	50.00 – 1.50 39.88 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (50.00-1.50) 94.7 (39.88-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.268 0.245 , 0.272	Depositor DCC
R_{free} test set	7460 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8274	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 90.11 % 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 2.6291e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, PG4, PO3

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	1.29	9/1904 (0.5%)	1.11	6/2598 (0.2%)
1	B	1.25	4/1896 (0.2%)	1.09	8/2585 (0.3%)
1	C	1.28	6/1921 (0.3%)	1.10	10/2619 (0.4%)
1	D	1.31	8/1887 (0.4%)	1.10	7/2573 (0.3%)
All	All	1.28	27/7608 (0.4%)	1.10	31/10375 (0.3%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	151	CYS	CB-SG	-12.97	1.60	1.82
1	D	77	VAL	CB-CG1	8.48	1.70	1.52
1	D	150	GLU	CA-CB	8.20	1.72	1.53
1	D	151	CYS	CB-SG	-6.63	1.71	1.82
1	C	78	PRO	CG-CD	-6.54	1.29	1.50
1	A	87	GLU	CD-OE2	-6.35	1.18	1.25
1	B	30	GLU	CD-OE2	6.28	1.32	1.25
1	A	66	TRP	CZ3-CH2	-6.13	1.30	1.40
1	D	194	ASP	CB-CG	6.05	1.64	1.51
1	C	52	ILE	CB-CG2	-5.93	1.34	1.52
1	A	30	GLU	CG-CD	5.88	1.60	1.51
1	A	147	PRO	N-CD	5.83	1.56	1.47
1	B	30	GLU	CG-CD	5.82	1.60	1.51
1	D	30	GLU	CD-OE2	5.73	1.31	1.25
1	D	78	PRO	CG-CD	5.67	1.69	1.50
1	A	30	GLU	CD-OE2	5.38	1.31	1.25
1	C	112	VAL	CB-CG2	-5.32	1.41	1.52
1	A	199	ALA	CA-CB	5.27	1.63	1.52
1	D	11	GLU	CD-OE2	5.25	1.31	1.25
1	B	83	TRP	CE3-CZ3	5.25	1.47	1.38
1	C	81	HIS	C-O	5.19	1.33	1.23
1	C	54	TYR	CE2-CZ	-5.17	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	TYR	CD1-CE1	-5.15	1.31	1.39
1	A	226	TYR	CD1-CE1	5.11	1.47	1.39
1	A	141	VAL	CB-CG1	-5.11	1.42	1.52
1	D	181	ALA	CA-CB	5.01	1.62	1.52
1	A	54	TYR	CD2-CE2	-5.00	1.31	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	158	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	C	158	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	A	198	ASP	CB-CG-OD1	8.43	125.89	118.30
1	D	150	GLU	N-CA-CB	8.16	125.28	110.60
1	A	84	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	D	187	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	C	42	LEU	CA-CB-CG	7.09	131.60	115.30
1	B	128	ASP	CB-CG-OD2	6.60	124.24	118.30
1	D	60	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	194	ASP	CB-CG-OD2	6.38	124.05	118.30
1	C	187	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	C	138	TYR	CD1-CE1-CZ	6.13	125.32	119.80
1	B	217	ASP	CB-CG-OD1	6.12	123.80	118.30
1	B	187	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	B	143[A]	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	143[B]	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	D	78	PRO	N-CD-CG	-5.97	94.24	103.20
1	A	88	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	70	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	115	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	D	63	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	87	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	A	158	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	88	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	60	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	138	TYR	CB-CG-CD2	5.25	124.15	121.00
1	C	78	PRO	CA-N-CD	-5.15	104.30	111.50
1	A	217	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	143[A]	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	143[B]	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	D	150	GLU	OE1-CD-OE2	5.04	129.35	123.30

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	A	1858	0	1846	26	0
1	B	1850	0	1834	15	0
1	C	1875	0	1854	35	0
1	D	1841	0	1820	16	0
2	A	13	0	18	4	0
2	B	13	0	18	0	0
2	C	26	0	36	4	0
2	D	26	0	36	1	0
3	A	4	0	0	2	0
3	B	4	0	0	2	0
3	C	4	0	0	2	0
3	D	4	0	0	0	0
4	A	11	0	5	0	0
4	B	11	0	5	0	0
4	C	11	0	5	0	0
4	D	11	0	5	0	0
5	A	192	0	0	1	0
5	B	174	0	0	2	0
5	C	171	0	0	19	0
5	D	175	0	0	10	0
All	All	8274	0	7482	93	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 6.

All (93) 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:9:HIS:NE2	3:B:251:PO3:P	2.00	1.34
1:A:9:HIS:NE2	3:A:251:PO3:P	2.01	1.33
1:C:9:HIS:NE2	3:C:252:PO3:P	2.00	1.32
1:A:31[B]:GLN:NE2	5:A:602:HOH:O	1.78	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:GLU:HA	5:D:691:HOH:O	1.49	1.09
1:C:176[B]:GLN:HE21	1:C:176[B]:GLN:HA	1.19	1.04
1:A:42[A]:LEU:HD13	1:A:42[A]:LEU:O	1.62	0.99
1:A:148[B]:LEU:HD12	1:A:148[B]:LEU:N	1.83	0.93
1:D:150:GLU:HB3	1:D:154:ASP:HB2	1.55	0.89
1:C:132:PRO:HD2	5:C:532:HOH:O	1.81	0.81
1:A:42[A]:LEU:C	1:A:42[A]:LEU:CD1	2.50	0.80
1:A:38:GLN:O	1:A:42[B]:LEU:HD13	1.81	0.78
1:A:42[A]:LEU:HD13	1:A:42[A]:LEU:C	2.02	0.77
2:D:250:PG4:H52	5:D:601:HOH:O	1.84	0.77
1:A:31[B]:GLN:OE1	1:A:34:ARG:NH1	2.18	0.75
1:C:176[B]:GLN:HA	1:C:176[B]:GLN:NE2	2.01	0.74
1:D:41:GLN:HE22	1:D:44:LYS:HE2	1.52	0.73
1:C:201:ILE:CG2	5:C:668:HOH:O	2.35	0.73
1:C:132:PRO:CD	5:C:532:HOH:O	2.38	0.70
1:C:132:PRO:HG2	5:C:532:HOH:O	1.92	0.70
1:A:148[B]:LEU:N	1:A:148[B]:LEU:CD1	2.55	0.70
1:C:133:TYR:CD1	5:C:532:HOH:O	2.45	0.69
1:D:109:GLN:O	1:D:112:VAL:HG22	1.93	0.68
1:C:30:GLU:OE1	5:C:534:HOH:O	2.10	0.68
1:C:201:ILE:HG22	5:C:668:HOH:O	1.94	0.67
1:A:42[A]:LEU:O	1:A:42[A]:LEU:CD1	2.40	0.67
1:B:116:SER:CB	1:B:119:THR:HG23	2.25	0.66
1:A:175:LYS:HD3	2:A:250:PG4:H72	1.77	0.66
1:C:133:TYR:CE1	5:C:532:HOH:O	2.49	0.66
1:A:175:LYS:HZ3	2:A:250:PG4:H71	1.62	0.65
1:C:109:GLN:O	1:C:112:VAL:HG23	1.97	0.65
1:D:149:THR:O	5:D:691:HOH:O	2.16	0.63
1:B:192:TYR:OH	5:B:421:HOH:O	2.09	0.60
1:B:172:LYS:NZ	5:B:648:HOH:O	2.30	0.60
1:C:132:PRO:CG	5:C:532:HOH:O	2.49	0.60
1:C:109:GLN:O	1:C:112:VAL:CG2	2.50	0.60
1:A:147:PRO:C	1:A:148[B]:LEU:HD12	2.23	0.59
1:D:176:GLN:HG2	5:D:377:HOH:O	2.03	0.57
1:A:197:SER:OG	1:A:200:ASP:HB2	2.03	0.57
1:B:116:SER:OG	1:B:119:THR:HG23	2.05	0.56
1:C:201:ILE:HG21	5:C:668:HOH:O	2.00	0.56
1:D:175:LYS:HE2	5:D:601:HOH:O	2.04	0.56
1:A:175:LYS:NZ	2:A:250:PG4:H71	2.20	0.56
1:D:87:GLU:OE2	1:D:184:ASN:HB2	2.07	0.55
1:C:133:TYR:CG	5:C:532:HOH:O	2.59	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:GLN:NE2	5:D:386:HOH:O	2.37	0.54
1:D:142:PRO:HD3	5:D:580:HOH:O	2.08	0.54
1:C:225:HIS:CD2	2:C:251:PG4:H52	2.41	0.54
1:D:19[B]:ARG:CZ	5:D:563:HOH:O	2.55	0.54
1:C:204:LEU:HD13	2:C:251:PG4:H21	1.89	0.54
1:C:78:PRO:HD3	5:C:277:HOH:O	2.06	0.54
1:D:109:GLN:O	1:D:112:VAL:CG2	2.56	0.53
1:D:130:ARG:HD3	5:D:699:HOH:O	2.09	0.53
1:A:175:LYS:NZ	2:A:250:PG4:C7	2.73	0.52
1:B:116:SER:HB3	1:B:119:THR:HG23	1.90	0.52
1:B:9:HIS:CE1	3:B:251:PO3:P	2.93	0.52
1:A:9:HIS:CE1	3:A:251:PO3:P	2.94	0.51
1:B:31:GLN:OE1	1:B:34:ARG:NH2	2.43	0.51
1:A:34:ARG:O	1:A:38:GLN:HG3	2.10	0.51
1:B:152:LEU:O	1:B:156:VAL:HG23	2.11	0.51
1:C:225:HIS:CE1	2:C:251:PG4:H31	2.46	0.51
1:B:34:ARG:O	1:B:38:GLN:HG3	2.11	0.50
1:C:9:HIS:CE1	3:C:252:PO3:P	2.94	0.50
1:C:175:LYS:HE2	5:C:552:HOH:O	2.12	0.49
1:A:115:ARG:HB3	1:A:202:VAL:HG13	1.94	0.49
1:C:198:ASP:HA	5:C:668:HOH:O	2.12	0.49
1:B:116:SER:OG	1:B:119:THR:CG2	2.60	0.49
1:D:150:GLU:HB3	1:D:154:ASP:CB	2.35	0.48
1:A:42[A]:LEU:C	1:A:42[A]:LEU:HD12	2.33	0.48
1:C:225:HIS:NE2	2:C:251:PG4:H31	2.28	0.48
1:D:51:ASP:O	1:D:78:PRO:HD2	2.14	0.48
1:A:42[A]:LEU:HD11	1:A:228:LEU:HB3	1.95	0.48
1:C:133:TYR:CD2	5:C:532:HOH:O	2.67	0.48
1:B:88:ARG:C	1:B:88:ARG:HD2	2.34	0.47
1:C:133:TYR:CZ	5:C:532:HOH:O	2.68	0.47
1:A:88:ARG:HD2	1:A:88:ARG:C	2.35	0.47
1:B:168:ALA:HB3	1:B:169:PRO:HD3	1.98	0.46
1:C:87:GLU:OE2	1:C:87:GLU:HA	2.15	0.46
1:C:130:ARG:HD3	5:C:542:HOH:O	2.16	0.45
1:B:87:GLU:HA	1:B:87:GLU:OE2	2.17	0.44
1:C:19[B]:ARG:CZ	5:C:656:HOH:O	2.65	0.44
1:C:87:GLU:OE2	1:C:184:ASN:HB2	2.18	0.44
1:A:42[B]:LEU:N	1:A:42[B]:LEU:CD1	2.82	0.43
1:A:152:LEU:O	1:A:155:THR:N	2.51	0.43
1:C:168:ALA:HB3	1:C:169:PRO:HD3	2.01	0.42
1:B:123:ALA:HA	1:B:149:THR:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:TYR:CE2	5:C:532:HOH:O	2.73	0.42
1:C:201:ILE:HD12	1:C:201:ILE:HA	1.95	0.41
1:D:19[B]:ARG:NH2	5:D:563:HOH:O	2.52	0.41
1:C:102:ALA:HB1	1:C:107:ASP:OD2	2.21	0.41
1:A:14:TRP:CZ3	1:A:95:GLY:HA2	2.56	0.40
1:C:88:ARG:HD2	1:C:88:ARG:C	2.42	0.40
1:A:88:ARG:HD2	1:A:88:ARG:O	2.20	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	232/257 (90%)	226 (97%)	6 (3%)	0	100	100
1	B	231/257 (90%)	225 (97%)	6 (3%)	0	100	100
1	C	233/257 (91%)	230 (99%)	3 (1%)	0	100	100
1	D	229/257 (89%)	223 (97%)	6 (3%)	0	100	100
All	All	925/1028 (90%)	904 (98%)	21 (2%)	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/211 (92%)	188 (97%)	6 (3%)	40	11
1	B	193/211 (92%)	188 (97%)	5 (3%)	46	16
1	C	196/211 (93%)	190 (97%)	6 (3%)	40	11
1	D	192/211 (91%)	188 (98%)	4 (2%)	53	23
All	All	775/844 (92%)	754 (97%)	21 (3%)	49	15

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42[A]	LEU
1	A	42[B]	LEU
1	A	90	TYR
1	A	111	LEU
1	A	143	ARG
1	A	197	SER
1	B	90	TYR
1	B	111	LEU
1	B	119	THR
1	B	143[A]	ARG
1	B	143[B]	ARG
1	C	42	LEU
1	C	90	TYR
1	C	111	LEU
1	C	143[A]	ARG
1	C	143[B]	ARG
1	C	230	ASP
1	D	90	TYR
1	D	111	LEU
1	D	143	ARG
1	D	230	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	41	GLN
1	D	71	GLN

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 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	$\#\|Z\| > 2$
2	PG4	D	251	-	12,12,12	0.44	0	11,11,11	0.56	0
3	PO3	D	252	-	0,3,3	-	-	0,3,3	-	-
2	PG4	D	250	-	12,12,12	0.56	0	11,11,11	0.38	0
3	PO3	B	251	-	0,3,3	-	-	0,3,3	-	-
4	SEP	C	253	-	9,10,10	1.43	2 (22%)	9,14,14	1.55	2 (22%)
2	PG4	C	250	-	12,12,12	0.44	0	11,11,11	0.61	0
2	PG4	B	250	-	12,12,12	0.56	0	11,11,11	0.45	0
3	PO3	C	252	-	0,3,3	-	-	0,3,3	-	-
2	PG4	A	250	-	12,12,12	0.61	0	11,11,11	0.73	0
3	PO3	A	251	-	0,3,3	-	-	0,3,3	-	-
4	SEP	B	252	-	9,10,10	1.73	3 (33%)	9,14,14	3.28	3 (33%)
4	SEP	A	252	-	9,10,10	1.70	2 (22%)	9,14,14	2.19	2 (22%)
2	PG4	C	251	-	12,12,12	0.56	0	11,11,11	0.99	1 (9%)
4	SEP	D	253	-	9,10,10	1.69	3 (33%)	9,14,14	1.65	2 (22%)

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	PG4	D	251	-	-	2/10/10/10	-
2	PG4	D	250	-	-	6/10/10/10	-
4	SEP	C	253	-	-	1/10/10/10	-
2	PG4	C	250	-	-	2/10/10/10	-
2	PG4	B	250	-	-	3/10/10/10	-
2	PG4	A	250	-	-	6/10/10/10	-
4	SEP	B	252	-	-	5/10/10/10	-
4	SEP	A	252	-	-	5/10/10/10	-
2	PG4	C	251	-	-	6/10/10/10	-
4	SEP	D	253	-	-	5/10/10/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	252	SEP	P-O1P	3.91	1.62	1.50
4	D	253	SEP	P-O1P	3.74	1.62	1.50
4	B	252	SEP	OXT-C	-3.19	1.20	1.30
4	C	253	SEP	P-O1P	2.70	1.58	1.50
4	A	252	SEP	P-OG	2.64	1.68	1.60
4	B	252	SEP	P-O1P	2.60	1.58	1.50
4	C	253	SEP	OXT-C	-2.52	1.22	1.30
4	D	253	SEP	P-O2P	2.12	1.62	1.54
4	D	253	SEP	OXT-C	-2.11	1.23	1.30
4	B	252	SEP	P-O3P	2.01	1.62	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	252	SEP	OG-CB-CA	8.16	115.18	108.06
4	A	252	SEP	OG-CB-CA	5.42	112.79	108.06
4	B	252	SEP	OG-P-O1P	3.66	116.32	106.44
4	D	253	SEP	O2P-P-OG	-3.25	98.20	106.67
4	C	253	SEP	O2P-P-OG	-2.89	99.13	106.67
4	B	252	SEP	O2P-P-OG	-2.80	99.37	106.67
4	D	253	SEP	O3P-P-OG	2.78	113.93	106.67
4	A	252	SEP	OG-P-O1P	-2.65	99.28	106.44
4	C	253	SEP	O3P-P-OG	2.55	113.31	106.67
2	C	251	PG4	C5-O3-C4	2.25	123.10	113.26

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	252	SEP	N-CA-CB-OG
4	A	252	SEP	C-CA-CB-OG
4	A	252	SEP	CB-OG-P-O2P
4	A	252	SEP	CB-OG-P-O3P
4	B	252	SEP	N-CA-CB-OG
4	B	252	SEP	C-CA-CB-OG
4	B	252	SEP	CB-OG-P-O2P
4	B	252	SEP	CB-OG-P-O3P
4	D	253	SEP	CB-OG-P-O2P
2	C	251	PG4	O2-C3-C4-O3
2	C	251	PG4	O3-C5-C6-O4
2	B	250	PG4	O1-C1-C2-O2
2	C	250	PG4	O1-C1-C2-O2
2	C	251	PG4	O4-C7-C8-O5
2	A	250	PG4	O1-C1-C2-O2
2	A	250	PG4	O4-C7-C8-O5
2	D	251	PG4	O2-C3-C4-O3
2	B	250	PG4	C1-C2-O2-C3
2	A	250	PG4	O3-C5-C6-O4
4	A	252	SEP	CB-OG-P-O1P
4	D	253	SEP	CB-OG-P-O1P
2	D	250	PG4	O3-C5-C6-O4
2	D	250	PG4	O2-C3-C4-O3
2	D	251	PG4	O3-C5-C6-O4
2	A	250	PG4	C5-C6-O4-C7
2	C	251	PG4	C6-C5-O3-C4
2	A	250	PG4	C8-C7-O4-C6
2	C	251	PG4	C5-C6-O4-C7
2	D	250	PG4	O4-C7-C8-O5
4	C	253	SEP	CB-OG-P-O1P
2	C	251	PG4	C1-C2-O2-C3
2	A	250	PG4	C4-C3-O2-C2
2	C	250	PG4	O4-C7-C8-O5
2	D	250	PG4	O1-C1-C2-O2
4	B	252	SEP	CB-OG-P-O1P
4	D	253	SEP	CB-OG-P-O3P
4	D	253	SEP	C-CA-CB-OG
2	D	250	PG4	C1-C2-O2-C3
4	D	253	SEP	N-CA-CB-OG
2	D	250	PG4	C3-C4-O3-C5
2	B	250	PG4	C3-C4-O3-C5

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	250	PG4	1	0
3	B	251	PO3	2	0
3	C	252	PO3	2	0
2	A	250	PG4	4	0
3	A	251	PO3	2	0
2	C	251	PG4	4	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	229/257 (89%)	0.21	5 (2%)	62	67	8, 16, 30, 35	0
1	B	229/257 (89%)	0.16	7 (3%)	49	54	8, 16, 29, 34	0
1	C	230/257 (89%)	0.17	4 (1%)	70	75	8, 17, 31, 42	0
1	D	230/257 (89%)	0.17	4 (1%)	70	75	8, 16, 31, 42	0
All	All	918/1028 (89%)	0.18	20 (2%)	62	67	8, 16, 30, 42	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	230	ASP	3.9
1	C	230	ASP	3.9
1	D	78	PRO	3.1
1	A	202	VAL	3.0
1	A	119	THR	2.8
1	B	1	MET	2.8
1	D	229	GLY	2.8
1	C	229	GLY	2.7
1	C	143[A]	ARG	2.7
1	B	117	TYR	2.6
1	A	117	TYR	2.6
1	A	143	ARG	2.4
1	B	119	THR	2.4
1	B	116	SER	2.4
1	A	1	MET	2.3
1	B	143[A]	ARG	2.3
1	B	152	LEU	2.2
1	B	201	ILE	2.2
1	D	119	THR	2.1
1	C	105	TYR	2.1

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, 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
2	PG4	A	250	13/13	0.67	0.21	39,45,54,57	0
2	PG4	D	250	13/13	0.71	0.22	40,45,55,58	0
2	PG4	C	251	13/13	0.75	0.16	38,40,46,46	0
2	PG4	C	250	13/13	0.77	0.16	38,44,50,54	0
2	PG4	B	250	13/13	0.88	0.13	35,40,45,46	0
2	PG4	D	251	13/13	0.90	0.15	28,33,43,47	0
4	SEP	A	252	11/11	0.96	0.11	18,25,28,31	0
4	SEP	C	253	11/11	0.96	0.10	23,26,30,30	0
4	SEP	B	252	11/11	0.97	0.10	17,24,28,31	0
3	PO3	B	251	4/4	0.97	0.07	14,16,16,17	0
4	SEP	D	253	11/11	0.97	0.10	20,24,27,28	0
3	PO3	A	251	4/4	0.98	0.06	16,16,16,18	0
3	PO3	C	252	4/4	0.99	0.05	16,17,17,17	0
3	PO3	D	252	4/4	0.99	0.06	15,16,16,19	0

6.5 Other polymers (i)

There are no such residues in this entry.