Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 08:40 AM EDT

PDB ID	:	7KLQ
Title	:	Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H59A mutant with pyruvate bound in the active site
Authors	:	Saran, S.; Sanders, D.A.R.
Deposited on	:	2020-10-31
Resolution	:	2.50 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:

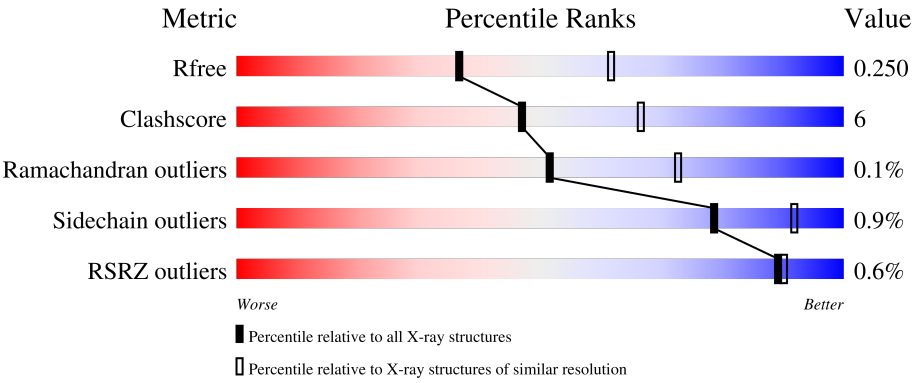
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.50 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.



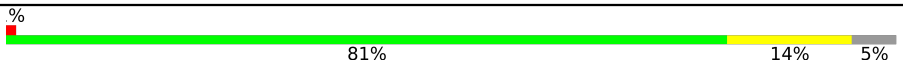
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	310	79% 16% 5%
1	B	310	84% 11% • 5%
1	C	310	82% 13% 5%
1	D	310	% 84% 11% 5%
1	E	310	% 78% 17% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	310	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14471 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 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2271	1445	376	437	13			
1	B	296	Total	C	N	O	S	0	0	0
			2267	1442	375	437	13			
1	C	296	Total	C	N	O	S	0	0	0
			2260	1439	373	435	13			
1	D	296	Total	C	N	O	S	0	0	0
			2260	1438	372	437	13			
1	E	296	Total	C	N	O	S	0	0	0
			2270	1444	376	437	13			
1	F	296	Total	C	N	O	S	0	0	0
			2256	1436	371	436	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	59	ALA	HIS	conflict	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4

Continued on next page...

Continued from previous page...

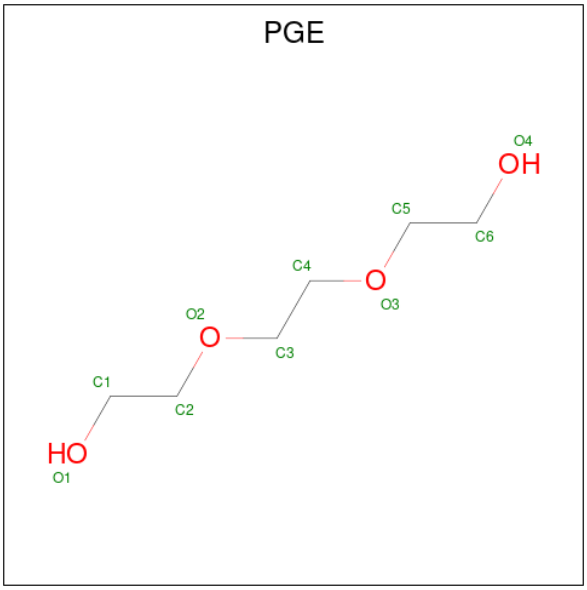
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	59	ALA	HIS	conflict	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	59	ALA	HIS	conflict	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	59	ALA	HIS	conflict	UNP Q9PPB4
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	59	ALA	HIS	conflict	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	59	ALA	HIS	conflict	UNP Q9PPB4

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



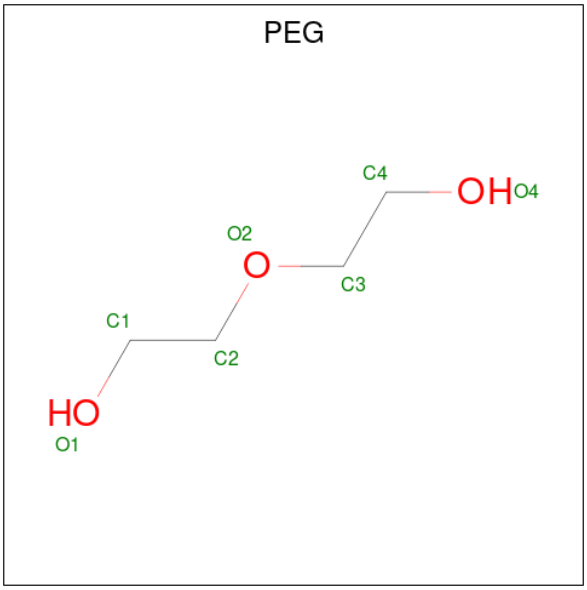
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

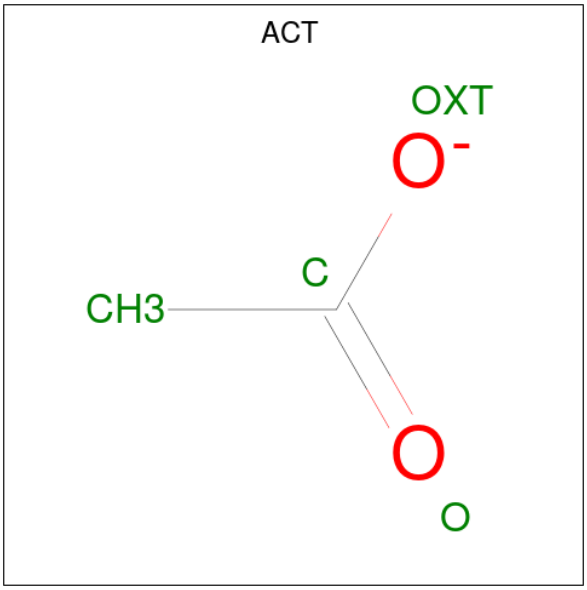
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

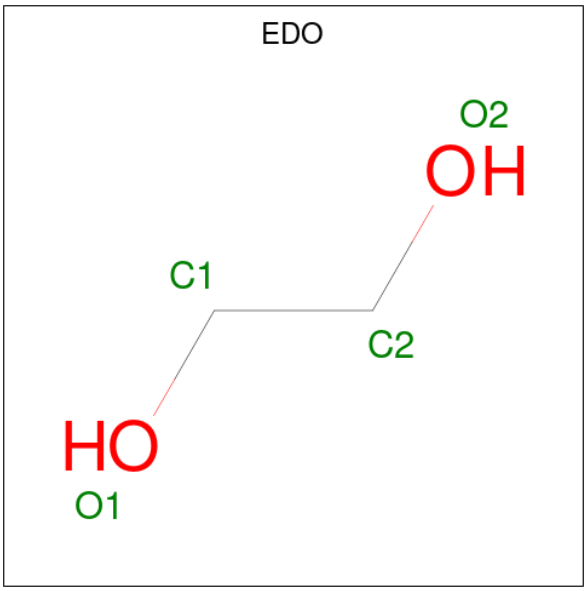
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Mg 2 2	0	0
4	E	1	Total Mg 1 1	0	0

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



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	125	Total O 125 125	0	0
7	B	124	Total O 124 124	0	0
7	C	143	Total O 143 143	0	0
7	D	127	Total O 127 127	0	0

Continued on next page...

Continued from previous page...

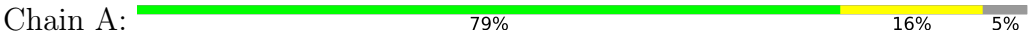
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	125	Total O 125 125	0	0
7	F	117	Total O 117 117	0	0

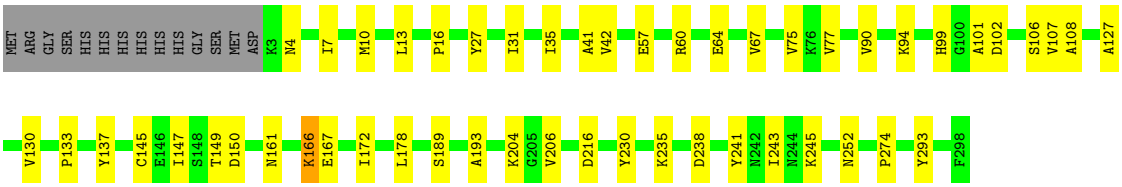
3 Residue-property plots (i)

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: 4-hydroxy-tetrahydrodipicolinate synthase

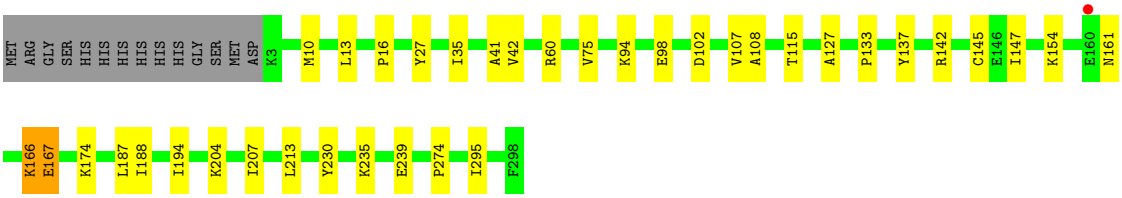
Chain A:





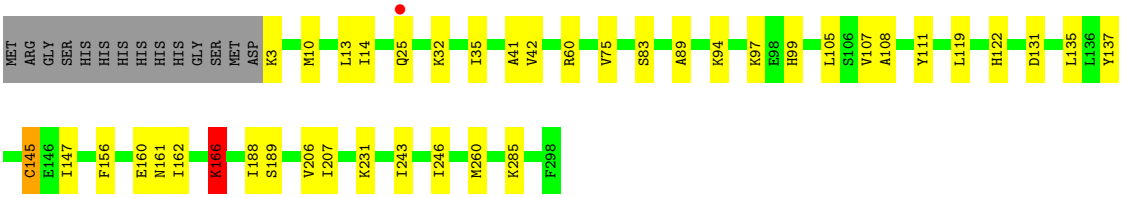
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B:



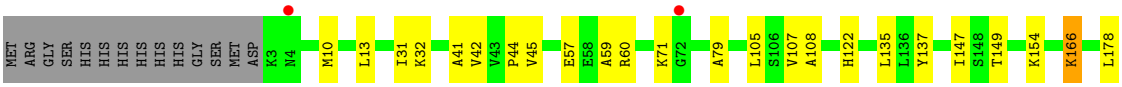
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain C:

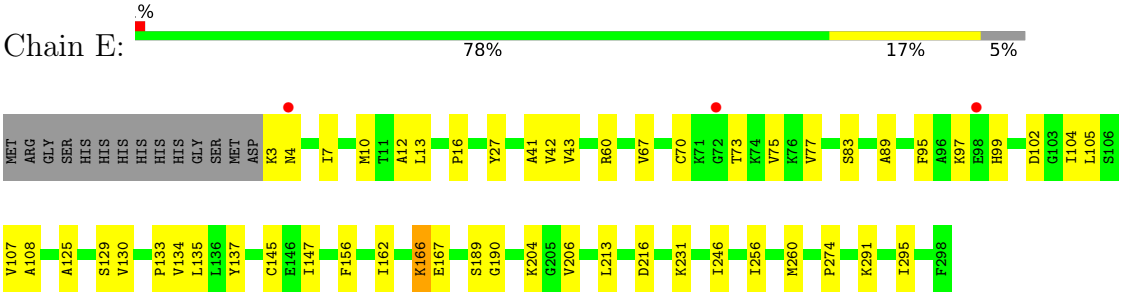


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

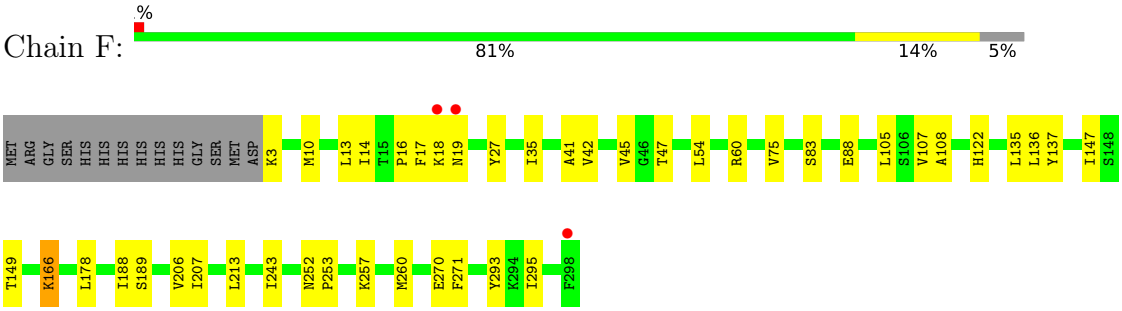
Chain D:



• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	84.97Å 231.83Å 202.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.76 – 2.50 22.76 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (22.76-2.50) 99.6 (22.76-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.23 (at 2.50Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.205 , 0.250 0.205 , 0.250	Depositor DCC
R_{free} test set	3482 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	9.9	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	14471	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: MG, ACT, KPI, PEG, PGE, 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	0.37	2/2294 (0.1%)	0.50	0/3102
1	B	0.26	0/2290	0.47	0/3098
1	C	0.43	0/2283	0.50	0/3089
1	D	0.30	0/2283	0.47	0/3090
1	E	0.33	1/2293 (0.0%)	0.47	0/3101
1	F	0.29	0/2279	0.47	0/3085
All	All	0.34	3/13722 (0.0%)	0.48	0/18565

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	0	1
1	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	GLU	CD-OE1	-6.57	1.18	1.25
1	A	167	GLU	CD-OE2	-6.12	1.19	1.25
1	E	167	GLU	CD-OE2	-5.62	1.19	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	KPI	Mainchain
1	C	166	KPI	Mainchain

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	2271	0	2307	34	0
1	B	2267	0	2296	30	0
1	C	2260	0	2291	26	0
1	D	2260	0	2284	24	0
1	E	2270	0	2305	37	0
1	F	2256	0	2277	27	0
2	A	20	0	28	2	0
2	B	10	0	14	1	0
2	D	10	0	14	2	0
3	A	7	0	10	3	0
3	B	14	0	20	2	0
3	C	7	0	10	0	0
3	D	7	0	10	2	0
3	F	7	0	10	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	E	1	0	0	0	0
5	A	4	0	3	1	0
5	B	4	0	3	0	0
6	A	12	0	17	1	0
6	B	8	0	12	3	0
6	D	4	0	6	0	0
6	F	8	0	12	0	0
7	A	125	0	0	0	0
7	B	124	0	0	0	0
7	C	143	0	0	2	0
7	D	127	0	0	1	0
7	E	125	0	0	2	0
7	F	117	0	0	2	0
All	All	14471	0	13929	172	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 (172) 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:166:KPI:HA	1:B:167:GLU:HB2	1.55	0.88
3:B:303:PEG:H21	6:B:307:EDO:H11	1.60	0.83
1:C:60:ARG:HG3	1:C:99:HIS:NE2	1.95	0.81
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.66	0.78
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.69	0.74
1:A:67:VAL:HG22	1:A:77:VAL:HG21	1.72	0.72
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.72	0.71
1:E:4:ASN:HB2	1:E:133:PRO:HG3	1.73	0.71
1:E:231:LYS:NZ	7:E:401:HOH:O	2.22	0.70
1:F:19:ASN:ND2	7:F:401:HOH:O	2.24	0.70
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.74	0.69
1:B:137:TYR:HA	1:B:166:KPI:O	1.92	0.69
1:D:285:LYS:NZ	7:D:401:HOH:O	2.20	0.69
1:E:13:LEU:HD11	1:E:42:VAL:HB	1.75	0.68
1:A:127:ALA:O	1:A:161:ASN:ND2	2.26	0.67
1:E:73:THR:HG23	1:E:75:VAL:H	1.59	0.67
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.75	0.67
1:A:193:ALA:H	3:A:303:PEG:H11	1.60	0.67
1:A:57:GLU:OE1	1:A:60:ARG:NH2	2.28	0.66
1:A:238:ASP:O	6:A:308:EDO:H11	1.95	0.65
1:C:189:SER:HB3	1:C:206:VAL:HG12	1.78	0.64
1:E:189:SER:HB3	1:E:206:VAL:HG12	1.79	0.64
1:A:189:SER:HB3	1:A:206:VAL:HG12	1.78	0.64
1:C:137:TYR:CE1	1:C:166:KPI:HEA	2.33	0.62
1:F:10:MET:HG2	1:F:41:ALA:HB3	1.82	0.62
1:F:189:SER:HB3	1:F:206:VAL:HG12	1.79	0.62
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.82	0.61
1:E:291:LYS:NZ	7:E:406:HOH:O	2.34	0.61
1:B:108:ALA:HB2	1:B:147:ILE:HD11	1.83	0.61
1:C:60:ARG:HG3	1:C:99:HIS:CD2	2.35	0.61
1:A:150:ASP:H	2:A:302:PGE:H62	1.65	0.60
1:B:35:ILE:HG12	1:B:75:VAL:HG21	1.83	0.60
1:D:189:SER:HB3	1:D:206:VAL:HG12	1.84	0.60
1:A:60:ARG:HG3	1:A:99:HIS:NE2	2.16	0.60
1:B:115:THR:HB	6:B:307:EDO:H12	1.83	0.60
1:D:32:LYS:HG3	3:D:302:PEG:H22	1.84	0.60
1:D:108:ALA:HB2	1:D:147:ILE:HD11	1.85	0.59
1:A:77:VAL:HG23	1:A:102:ASP:H	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LYS:NZ	1:C:156:PHE:O	2.37	0.57
1:D:32:LYS:HG3	3:D:302:PEG:H32	1.87	0.57
1:D:57:GLU:HG3	1:D:60:ARG:NH1	2.20	0.56
1:D:57:GLU:HG3	1:D:60:ARG:HH11	1.70	0.56
1:F:35:ILE:HG12	1:F:75:VAL:HG21	1.86	0.56
1:D:137:TYR:CE1	1:D:166:KPI:HEA	2.40	0.56
1:A:149:THR:HB	2:A:302:PGE:H52	1.86	0.56
1:D:149:THR:HG23	1:D:178:LEU:HD23	1.88	0.55
1:B:13:LEU:HD11	1:B:42:VAL:HB	1.88	0.55
1:E:10:MET:HG2	1:E:41:ALA:HB3	1.87	0.55
1:F:137:TYR:CE1	1:F:166:KPI:HEA	2.41	0.55
1:A:108:ALA:HB2	1:A:147:ILE:HD11	1.88	0.55
1:A:130:VAL:O	1:A:161:ASN:ND2	2.40	0.54
1:B:145:CYS:HA	3:B:303:PEG:H42	1.89	0.54
1:E:3:LYS:NZ	1:E:156:PHE:O	2.39	0.54
1:C:97:LYS:NZ	1:C:131:ASP:OD1	2.38	0.54
1:A:90:VAL:HG12	1:A:94:LYS:HE2	1.90	0.54
1:C:25:GLN:HB2	7:C:409:HOH:O	2.07	0.54
1:E:166:KPI:H1A	1:E:190:GLY:O	2.07	0.54
1:F:13:LEU:HD11	1:F:42:VAL:HB	1.90	0.54
1:C:105:LEU:HD13	1:C:135:LEU:HD23	1.90	0.53
1:C:10:MET:HG2	1:C:41:ALA:HB3	1.90	0.53
1:C:108:ALA:HB2	1:C:147:ILE:HD11	1.90	0.53
1:E:7:ILE:HB	1:E:204:LYS:O	2.09	0.53
1:B:10:MET:HG2	1:B:41:ALA:HB3	1.91	0.53
1:E:67:VAL:HA	1:E:77:VAL:HG21	1.91	0.53
1:C:13:LEU:HD11	1:C:42:VAL:HB	1.91	0.52
1:A:149:THR:HG23	1:A:178:LEU:HD23	1.92	0.52
1:B:166:KPI:HB	1:B:188:ILE:HB	1.92	0.52
1:E:60:ARG:HG3	1:E:99:HIS:NE2	2.25	0.51
1:F:45:VAL:HG23	1:F:54:LEU:HD12	1.92	0.51
1:B:60:ARG:O	1:B:60:ARG:HG2	2.09	0.51
1:A:60:ARG:HD3	1:A:64:GLU:OE1	2.11	0.51
1:B:167:GLU:HG3	1:B:187:LEU:HD11	1.93	0.51
1:B:235:LYS:O	1:B:239:GLU:HB2	2.11	0.51
1:E:134:VAL:HG23	1:E:162:ILE:HA	1.92	0.51
1:D:10:MET:HG2	1:D:41:ALA:HB3	1.93	0.51
1:F:149:THR:HG23	1:F:178:LEU:HD23	1.93	0.50
1:D:45:VAL:HG11	1:D:59:ALA:HA	1.93	0.50
1:D:268:SER:OG	1:D:270:GLU:HG3	2.12	0.50
1:B:235:LYS:NZ	1:B:239:GLU:OE2	2.38	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:LEU:HD11	1:F:295:ILE:HD13	1.94	0.50
1:D:13:LEU:HD11	1:D:42:VAL:HB	1.94	0.49
1:A:13:LEU:HD11	1:A:42:VAL:HB	1.93	0.49
1:F:108:ALA:HB2	1:F:147:ILE:HD11	1.94	0.49
1:B:147:ILE:O	1:B:174:LYS:NZ	2.35	0.49
1:F:83:SER:OG	1:F:88:GLU:OE1	2.29	0.49
1:A:245:LYS:NZ	3:A:303:PEG:H32	2.27	0.48
1:B:127:ALA:O	1:B:161:ASN:ND2	2.46	0.48
1:E:83:SER:HB3	1:E:89:ALA:HB2	1.95	0.48
1:F:166:KPI:HDA	1:F:207:ILE:HB	1.94	0.48
1:F:243:ILE:HB	1:F:293:TYR:CE2	2.48	0.48
1:B:142:ARG:HD2	1:C:111:TYR:O	2.14	0.48
1:C:166:KPI:HDA	1:C:207:ILE:HB	1.95	0.48
1:C:3:LYS:NZ	1:C:162:ILE:O	2.47	0.48
1:C:83:SER:HB3	1:C:89:ALA:HB2	1.95	0.48
1:E:108:ALA:HB2	1:E:147:ILE:HD11	1.96	0.48
1:F:3:LYS:N	7:F:412:HOH:O	2.46	0.48
1:F:188:ILE:HG21	1:F:207:ILE:HG13	1.96	0.48
1:D:105:LEU:HD13	1:D:135:LEU:HD23	1.95	0.48
1:E:125:ALA:O	1:E:129:SER:HB3	2.14	0.48
1:D:188:ILE:HG21	1:D:207:ILE:HG13	1.97	0.47
1:A:252:ASN:HB3	5:A:305:ACT:H1	1.95	0.47
1:A:10:MET:HG2	1:A:41:ALA:HB3	1.96	0.47
1:D:243:ILE:HA	1:D:246:ILE:HG22	1.96	0.47
1:B:204:LYS:HZ3	6:B:308:EDO:H22	1.78	0.47
1:A:35:ILE:HG12	1:A:75:VAL:HG21	1.97	0.47
1:A:77:VAL:HG23	1:A:101:ALA:HA	1.96	0.47
1:A:230:TYR:CD2	1:B:230:TYR:HD2	2.33	0.46
1:A:243:ILE:HB	1:A:293:TYR:CE2	2.50	0.46
1:C:119:LEU:HD11	1:C:145:CYS:SG	2.55	0.46
1:E:60:ARG:HB2	1:E:95:PHE:CZ	2.49	0.46
1:F:105:LEU:HD13	1:F:135:LEU:HD23	1.96	0.46
1:B:154:LYS:HD3	2:B:301:PGE:H52	1.97	0.46
1:B:16:PRO:HD2	1:B:27:TYR:HD1	1.81	0.46
1:C:131:ASP:HA	1:C:161:ASN:HD21	1.80	0.46
1:E:102:ASP:O	1:E:133:PRO:HD2	2.16	0.46
1:E:104:ILE:CG1	1:E:134:VAL:HG12	2.46	0.46
1:F:16:PRO:HD2	1:F:27:TYR:HD1	1.81	0.46
1:D:166:KPI:HDA	1:D:207:ILE:HB	1.97	0.45
1:D:154:LYS:HZ2	2:D:301:PGE:H32	1.81	0.45
1:E:166:KPI:HE	1:E:190:GLY:HA3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASP:OD1	1:A:216:ASP:N	2.47	0.45
1:B:166:KPI:HGA	1:B:207:ILE:HD12	1.98	0.45
1:C:246:ILE:HD11	1:C:285:LYS:HB3	1.98	0.45
1:E:60:ARG:HB2	1:E:95:PHE:HZ	1.81	0.45
1:E:137:TYR:CE1	1:E:166:KPI:HEA	2.51	0.45
1:F:17:PHE:HB2	1:F:270:GLU:HB2	1.98	0.45
1:E:216:ASP:N	1:E:216:ASP:OD1	2.48	0.45
1:B:166:KPI:CA	1:B:167:GLU:HB2	2.36	0.45
1:F:257:LYS:HD2	1:F:271:PHE:CE2	2.52	0.45
1:C:94:LYS:NZ	7:C:406:HOH:O	2.28	0.44
1:D:44:PRO:HD2	1:D:79:ALA:HA	1.98	0.44
1:E:12:ALA:HA	1:E:43:VAL:HB	1.99	0.44
1:E:105:LEU:HD13	1:E:135:LEU:HD23	1.98	0.44
1:E:213:LEU:HD11	1:E:295:ILE:HD13	1.99	0.44
1:F:137:TYR:CD1	1:F:166:KPI:HGA	2.53	0.44
1:E:70:CYS:HB3	1:E:75:VAL:O	2.18	0.44
1:E:256:ILE:O	1:E:260:MET:HG2	2.18	0.44
1:C:35:ILE:HG12	1:C:75:VAL:HG21	1.99	0.44
1:B:102:ASP:O	1:B:133:PRO:HD2	2.18	0.44
1:A:31:ILE:HG23	1:A:42:VAL:HG11	2.00	0.44
1:C:188:ILE:HG21	1:C:207:ILE:HG13	2.00	0.44
1:A:230:TYR:HD2	1:B:230:TYR:HD2	1.64	0.43
1:F:47:THR:HB	1:F:166:KPI:O2	2.19	0.43
1:E:274:PRO:HB3	1:F:122:HIS:HB2	2.00	0.43
1:A:274:PRO:HB3	1:D:122:HIS:HB2	2.01	0.43
1:E:246:ILE:HD12	1:E:246:ILE:HA	1.91	0.43
1:A:7:ILE:HB	1:A:204:LYS:O	2.17	0.43
1:B:274:PRO:HB3	1:C:122:HIS:HB2	2.01	0.43
1:B:213:LEU:HD11	1:B:295:ILE:HD13	2.01	0.42
1:C:243:ILE:HA	1:C:246:ILE:HG22	2.01	0.42
1:B:166:KPI:O	1:B:166:KPI:HG	2.19	0.42
1:B:94:LYS:O	1:B:98:GLU:HG2	2.19	0.42
1:F:252:ASN:ND2	1:F:253:PRO:HA	2.34	0.42
1:E:16:PRO:HD2	1:E:27:TYR:HD1	1.85	0.42
1:C:10:MET:HA	1:C:41:ALA:O	2.20	0.42
1:A:16:PRO:HD2	1:A:27:TYR:HD1	1.83	0.42
1:D:196:TYR:OH	1:D:230:TYR:HB3	2.20	0.42
1:E:134:VAL:HG23	1:E:162:ILE:HG12	2.01	0.42
1:A:245:LYS:HZ1	3:A:303:PEG:H32	1.84	0.41
1:E:70:CYS:O	1:E:73:THR:HG22	2.20	0.41
1:A:172:ILE:HG23	1:B:194:ILE:HG21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:ILE:HG23	1:D:42:VAL:HG11	2.02	0.41
1:C:14:ILE:HD13	1:C:260:MET:HG3	2.03	0.41
1:E:166:KPI:HE	1:E:190:GLY:CA	2.51	0.41
1:F:14:ILE:HD13	1:F:260:MET:HG3	2.03	0.41
1:F:137:TYR:CZ	1:F:166:KPI:HEA	2.56	0.41
1:A:241:TYR:O	1:A:245:LYS:HG2	2.21	0.41
1:D:154:LYS:HD2	2:D:301:PGE:H32	2.02	0.41
1:E:129:SER:OG	1:E:130:VAL:HG23	2.21	0.40
1:A:4:ASN:HB2	1:A:133:PRO:HG3	2.01	0.40
1:E:134:VAL:CG2	1:E:162:ILE:HG12	2.51	0.40
1:F:136:LEU:O	1:F:166:KPI:N	2.54	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	293/310 (94%)	285 (97%)	8 (3%)	0	100 100
1	B	293/310 (94%)	284 (97%)	8 (3%)	1 (0%)	41 61
1	C	293/310 (94%)	286 (98%)	7 (2%)	0	100 100
1	D	293/310 (94%)	284 (97%)	9 (3%)	0	100 100
1	E	293/310 (94%)	285 (97%)	8 (3%)	0	100 100
1	F	293/310 (94%)	284 (97%)	9 (3%)	0	100 100
All	All	1758/1860 (94%)	1708 (97%)	49 (3%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	167	GLU

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	246/259 (95%)	243 (99%)	3 (1%)	71 88
1	B	245/259 (95%)	245 (100%)	0	100 100
1	C	244/259 (94%)	240 (98%)	4 (2%)	62 84
1	D	244/259 (94%)	242 (99%)	2 (1%)	81 93
1	E	246/259 (95%)	244 (99%)	2 (1%)	81 93
1	F	243/259 (94%)	241 (99%)	2 (1%)	81 93
All	All	1468/1554 (94%)	1455 (99%)	13 (1%)	78 92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	145	CYS
1	A	235	LYS
1	C	32	LYS
1	C	145	CYS
1	C	160	GLU
1	C	231	LYS
1	D	71	LYS
1	D	277	SER
1	E	97	LYS
1	E	145	CYS
1	F	18	LYS
1	F	60	ARG

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

Mol	Chain	Res	Type
1	C	128	GLN
1	F	19	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KPI	D	166	1	11,13,14	1.54	2 (18%)	10,15,17	3.42	5 (50%)
1	KPI	F	166	1	11,13,14	1.53	2 (18%)	10,15,17	4.12	5 (50%)
1	KPI	B	166	1	11,13,14	1.90	2 (18%)	10,15,17	4.27	6 (60%)
1	KPI	C	166	1	11,13,14	2.29	3 (27%)	10,15,17	4.70	6 (60%)
1	KPI	A	166	1	11,13,14	1.51	1 (9%)	10,15,17	3.73	6 (60%)
1	KPI	E	166	1	11,13,14	2.55	4 (36%)	10,15,17	2.02	3 (30%)

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
1	KPI	D	166	1	-	4/13/14/16	-
1	KPI	F	166	1	-	6/13/14/16	-
1	KPI	B	166	1	-	8/13/14/16	-
1	KPI	C	166	1	-	4/13/14/16	-
1	KPI	A	166	1	-	1/13/14/16	-
1	KPI	E	166	1	-	1/13/14/16	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	166	KPI	CX2-CX1	-7.02	1.41	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	KPI	O2-CX2	5.38	1.36	1.22
1	B	166	KPI	O2-CX2	5.34	1.36	1.22
1	F	166	KPI	O-C	4.16	1.36	1.19
1	C	166	KPI	O-C	4.14	1.36	1.19
1	D	166	KPI	O-C	4.11	1.36	1.19
1	A	166	KPI	O1-CX2	-4.04	1.18	1.30
1	E	166	KPI	O1-CX2	-2.87	1.22	1.30
1	E	166	KPI	CA-N	-2.48	1.40	1.48
1	B	166	KPI	O1-CX2	-2.37	1.23	1.30
1	C	166	KPI	O1-CX2	-2.21	1.24	1.30
1	F	166	KPI	O1-CX2	2.06	1.36	1.30
1	D	166	KPI	O1-CX2	2.02	1.36	1.30
1	E	166	KPI	CB-CA	-2.02	1.50	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	166	KPI	C1-CX1-CX2	-11.16	107.32	118.17
1	F	166	KPI	C1-CX1-CX2	-10.32	108.14	118.17
1	B	166	KPI	C1-CX1-CX2	-9.67	108.76	118.17
1	A	166	KPI	O2-CX2-CX1	7.35	130.76	121.38
1	D	166	KPI	C1-CX1-CX2	-6.97	111.39	118.17
1	A	166	KPI	CE-NZ-CX1	6.12	138.38	121.70
1	C	166	KPI	CD-CE-NZ	6.01	121.60	110.66
1	D	166	KPI	O2-CX2-CX1	5.85	128.84	121.38
1	B	166	KPI	O1-CX2-CX1	5.65	128.62	116.35
1	A	166	KPI	O1-CX2-O2	-5.12	111.90	123.61
1	B	166	KPI	O2-CX2-CX1	-5.04	114.95	121.38
1	C	166	KPI	O1-CX2-CX1	4.96	127.12	116.35
1	F	166	KPI	CD-CE-NZ	4.75	119.30	110.66
1	F	166	KPI	O2-CX2-CX1	4.68	127.35	121.38
1	E	166	KPI	O2-CX2-CX1	-4.62	115.48	121.38
1	C	166	KPI	O2-CX2-CX1	-4.20	116.01	121.38
1	D	166	KPI	CD-CE-NZ	3.43	116.90	110.66
1	E	166	KPI	CG-CD-CE	-3.20	102.43	113.57
1	B	166	KPI	CD-CE-NZ	3.17	116.43	110.66
1	B	166	KPI	O1-CX2-O2	-3.14	116.43	123.61
1	A	166	KPI	CX2-CX1-NZ	3.02	122.33	114.98
1	D	166	KPI	O1-CX2-O2	-3.00	116.75	123.61
1	C	166	KPI	O1-CX2-O2	-2.95	116.86	123.61
1	D	166	KPI	C1-CX1-NZ	2.63	129.98	123.11
1	F	166	KPI	O1-CX2-O2	-2.60	117.66	123.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	KPI	C1-CX1-CX2	-2.36	115.87	118.17
1	E	166	KPI	CX2-CX1-NZ	2.17	120.27	114.98
1	F	166	KPI	C1-CX1-NZ	2.13	128.69	123.11
1	A	166	KPI	CD-CG-CB	2.12	121.12	113.62
1	B	166	KPI	CE-NZ-CX1	2.11	127.45	121.70
1	C	166	KPI	CG-CD-CE	-2.01	106.58	113.57

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	166	KPI	O-C-CA-CB
1	B	166	KPI	C-CA-CB-CG
1	B	166	KPI	C1-CX1-NZ-CE
1	B	166	KPI	CX2-CX1-NZ-CE
1	B	166	KPI	NZ-CX1-CX2-O1
1	B	166	KPI	NZ-CX1-CX2-O2
1	C	166	KPI	C1-CX1-NZ-CE
1	C	166	KPI	CX2-CX1-NZ-CE
1	D	166	KPI	C1-CX1-NZ-CE
1	D	166	KPI	CX2-CX1-NZ-CE
1	F	166	KPI	C-CA-CB-CG
1	F	166	KPI	C1-CX1-NZ-CE
1	F	166	KPI	CX2-CX1-NZ-CE
1	F	166	KPI	C1-CX1-CX2-O1
1	F	166	KPI	C1-CX1-CX2-O2
1	B	166	KPI	CA-CB-CG-CD
1	E	166	KPI	CE-CD-CG-CB
1	B	166	KPI	C1-CX1-CX2-O1
1	D	166	KPI	C1-CX1-CX2-O1
1	C	166	KPI	NZ-CX1-CX2-O1
1	B	166	KPI	C1-CX1-CX2-O2
1	C	166	KPI	CE-CD-CG-CB
1	F	166	KPI	CE-CD-CG-CB
1	D	166	KPI	CE-CD-CG-CB

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	166	KPI	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	166	KPI	6	0
1	B	166	KPI	6	0
1	C	166	KPI	2	0
1	E	166	KPI	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
3	PEG	A	303	-	6,6,6	0.49	0	5,5,5	0.28	0
6	EDO	F	303	-	3,3,3	0.44	0	2,2,2	0.41	0
6	EDO	A	308	-	3,3,3	0.84	0	2,2,2	1.51	0
3	PEG	D	302	-	6,6,6	0.49	0	5,5,5	0.27	0
3	PEG	B	303	-	6,6,6	0.49	0	5,5,5	0.26	0
6	EDO	D	303	-	3,3,3	0.46	0	2,2,2	0.35	0
6	EDO	F	302	-	3,3,3	0.42	0	2,2,2	0.42	0
6	EDO	B	308	-	3,3,3	0.43	0	2,2,2	0.40	0
2	PGE	D	301	-	9,9,9	0.30	0	8,8,8	0.29	0
5	ACT	A	305	-	3,3,3	1.38	1 (33%)	3,3,3	1.36	0
2	PGE	B	301	-	9,9,9	0.28	0	8,8,8	0.34	0
3	PEG	B	302	-	6,6,6	0.48	0	5,5,5	0.28	0
3	PEG	F	301	-	6,6,6	0.50	0	5,5,5	0.23	0
3	PEG	C	301	-	6,6,6	0.49	0	5,5,5	0.19	0
2	PGE	A	302	-	9,9,9	0.32	0	8,8,8	0.28	0
6	EDO	B	307	-	3,3,3	0.42	0	2,2,2	0.38	0
5	ACT	B	306	-	3,3,3	1.35	0	3,3,3	1.50	0
6	EDO	A	306	-	3,3,3	0.46	0	2,2,2	0.37	0
6	EDO	A	307	-	3,3,3	0.46	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PGE	A	301	-	9,9,9	0.32	0	8,8,8	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	F	302	-	-	0/1/1/1	-
3	PEG	A	303	-	-	2/4/4/4	-
3	PEG	B	303	-	-	2/4/4/4	-
2	PGE	D	301	-	-	3/7/7/7	-
6	EDO	B	308	-	-	1/1/1/1	-
6	EDO	D	303	-	-	0/1/1/1	-
6	EDO	F	303	-	-	0/1/1/1	-
2	PGE	B	301	-	-	7/7/7/7	-
3	PEG	B	302	-	-	1/4/4/4	-
6	EDO	A	306	-	-	0/1/1/1	-
6	EDO	A	307	-	-	0/1/1/1	-
2	PGE	A	301	-	-	2/7/7/7	-
3	PEG	F	301	-	-	1/4/4/4	-
3	PEG	C	301	-	-	1/4/4/4	-
6	EDO	A	308	-	-	1/1/1/1	-
3	PEG	D	302	-	-	2/4/4/4	-
2	PGE	A	302	-	-	5/7/7/7	-
6	EDO	B	307	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	305	ACT	CH3-C	2.04	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	PEG	O2-C3-C4-O4
2	B	301	PGE	O2-C3-C4-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	302	PGE	O2-C3-C4-O3
2	D	301	PGE	O2-C3-C4-O3
2	A	301	PGE	O3-C5-C6-O4
2	B	301	PGE	O3-C5-C6-O4
2	B	301	PGE	O1-C1-C2-O2
2	D	301	PGE	O1-C1-C2-O2
3	B	303	PEG	O1-C1-C2-O2
3	B	303	PEG	C4-C3-O2-C2
3	D	302	PEG	C4-C3-O2-C2
2	A	302	PGE	C6-C5-O3-C4
3	C	301	PEG	C1-C2-O2-C3
2	A	302	PGE	C3-C4-O3-C5
3	A	303	PEG	C1-C2-O2-C3
2	B	301	PGE	C1-C2-O2-C3
3	B	302	PEG	C1-C2-O2-C3
2	D	301	PGE	C3-C4-O3-C5
2	A	302	PGE	C1-C2-O2-C3
2	A	301	PGE	C1-C2-O2-C3
2	B	301	PGE	C6-C5-O3-C4
2	B	301	PGE	C3-C4-O3-C5
3	D	302	PEG	C1-C2-O2-C3
2	B	301	PGE	C4-C3-O2-C2
6	A	308	EDO	O1-C1-C2-O2
6	B	308	EDO	O1-C1-C2-O2
3	F	301	PEG	O2-C3-C4-O4
2	A	302	PGE	C4-C3-O2-C2

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	PEG	3	0
6	A	308	EDO	1	0
3	D	302	PEG	2	0
3	B	303	PEG	2	0
6	B	308	EDO	1	0
2	D	301	PGE	2	0
5	A	305	ACT	1	0
2	B	301	PGE	1	0
2	A	302	PGE	2	0
6	B	307	EDO	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

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	295/310 (95%)	-0.35	0 100 100	4, 10, 23, 35	0
1	B	295/310 (95%)	-0.36	1 (0%) 94 94	4, 10, 24, 37	0
1	C	295/310 (95%)	-0.31	1 (0%) 94 94	5, 11, 23, 35	0
1	D	295/310 (95%)	-0.25	2 (0%) 87 89	6, 12, 28, 40	0
1	E	295/310 (95%)	-0.11	3 (1%) 82 84	8, 17, 33, 49	0
1	F	295/310 (95%)	-0.07	3 (1%) 82 84	8, 19, 33, 44	0
All	All	1770/1860 (95%)	-0.24	10 (0%) 89 90	4, 13, 29, 49	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	72	GLY	2.9
1	C	25	GLN	2.9
1	E	4	ASN	2.8
1	F	298	PHE	2.5
1	F	18	LYS	2.5
1	F	19	ASN	2.3
1	B	160	GLU	2.3
1	E	98	GLU	2.1
1	D	4	ASN	2.1
1	D	72	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	KPI	B	166	14/15	0.77	0.27	8,12,34,40	0
1	KPI	D	166	14/15	0.87	0.19	8,10,18,21	0
1	KPI	C	166	14/15	0.88	0.19	4,10,21,25	0
1	KPI	F	166	14/15	0.88	0.18	10,14,35,37	0
1	KPI	A	166	14/15	0.89	0.17	4,8,22,23	0
1	KPI	E	166	14/15	0.91	0.16	13,18,26,27	0

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
6	EDO	B	307	4/4	0.78	0.24	13,16,22,26	0
2	PGE	A	302	10/10	0.79	0.34	14,22,31,33	0
3	PEG	A	303	7/7	0.86	0.32	13,17,28,39	0
6	EDO	B	308	4/4	0.86	0.21	13,13,14,32	0
3	PEG	F	301	7/7	0.87	0.19	11,11,15,18	0
2	PGE	B	301	10/10	0.88	0.18	12,19,22,31	0
3	PEG	B	302	7/7	0.88	0.24	15,16,24,26	0
3	PEG	D	302	7/7	0.88	0.19	25,26,30,33	0
4	MG	E	301	1/1	0.89	0.13	29,29,29,29	0
5	ACT	A	305	4/4	0.91	0.34	13,17,20,27	0
6	EDO	A	308	4/4	0.91	0.20	20,20,20,20	0
3	PEG	B	303	7/7	0.91	0.26	9,14,24,36	0
2	PGE	D	301	10/10	0.91	0.21	10,16,20,22	0
2	PGE	A	301	10/10	0.92	0.15	13,15,23,24	0
6	EDO	F	302	4/4	0.92	0.20	13,16,16,24	0
4	MG	B	305	1/1	0.94	0.08	12,12,12,12	0
6	EDO	A	307	4/4	0.94	0.25	15,18,23,24	0
6	EDO	D	303	4/4	0.94	0.24	14,16,22,25	0
3	PEG	C	301	7/7	0.94	0.15	8,10,13,14	0
5	ACT	B	306	4/4	0.95	0.11	12,12,16,19	0
6	EDO	A	306	4/4	0.95	0.23	14,16,20,30	0
6	EDO	F	303	4/4	0.95	0.24	18,19,19,21	0
4	MG	A	304	1/1	0.96	0.06	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	B	304	1/1	0.97	0.05	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.