Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 01:13 am GMT

PDB ID	:	6G1D
Title	:	Corynebacterium glutamicum OxyR C206 mutant
Authors	:	Young, D.R.; Pedre, B.P.; Messens, J.M.
Deposited on	:	2018-03-21
Resolution	:	1.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

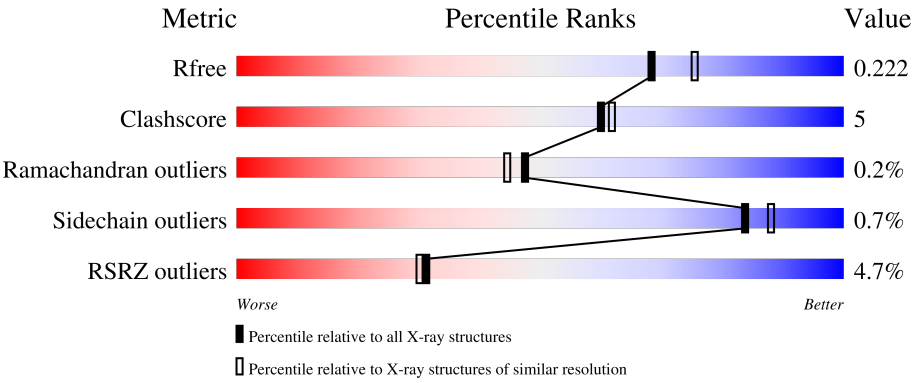
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	329	2% 87% 9%
1	B	329	7% 87% 8% 5%
1	C	329	5% 87% 6% 6%
1	D	329	4% 86% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	403	-	X	-	-
4	SO4	B	402	-	X	-	-
5	PEG	C	407	-	-	-	X
5	PEG	D	403	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10453 atoms, of which 46 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.

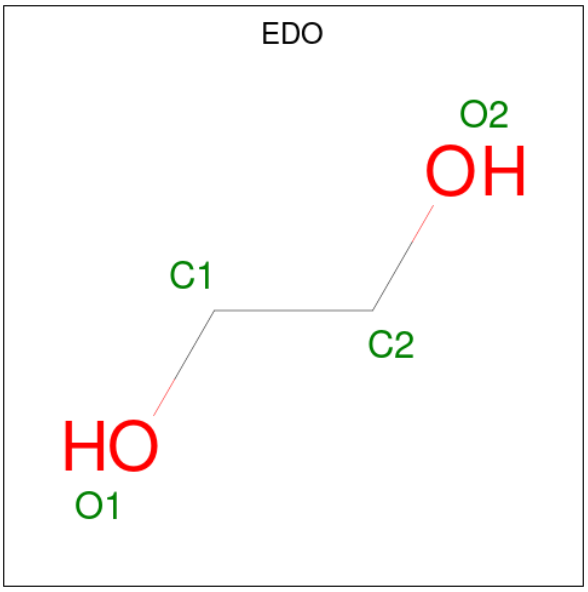
- Molecule 1 is a protein called Hydrogen peroxide-inducible genes activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	310	Total	C	N	O	S	0	12	0
			2400	1522	406	464	8			
1	D	318	Total	C	N	O	S	0	10	0
			2435	1547	409	470	9			
1	B	313	Total	C	N	O	S	17	13	0
			2411	1531	400	472	8			
1	A	315	Total	C	N	O	S	12	10	0
			2423	1537	408	469	9			

There are 12 discrepancies between the modelled and reference sequences:

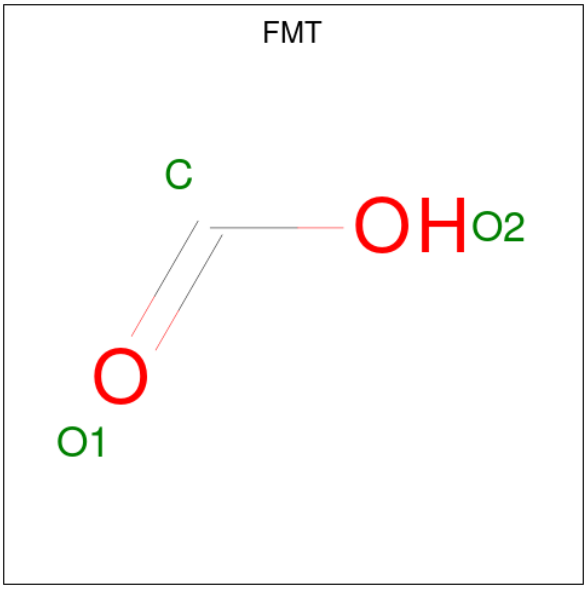
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP A0A2H5I9R9
C	0	HIS	-	expression tag	UNP A0A2H5I9R9
C	206	SER	CYS	engineered mutation	UNP A0A2H5I9R9
D	-1	SER	-	expression tag	UNP A0A2H5I9R9
D	0	HIS	-	expression tag	UNP A0A2H5I9R9
D	206	SER	CYS	engineered mutation	UNP A0A2H5I9R9
B	-1	SER	-	expression tag	UNP A0A2H5I9R9
B	0	HIS	-	expression tag	UNP A0A2H5I9R9
B	206	SER	CYS	engineered mutation	UNP A0A2H5I9R9
A	-1	SER	-	expression tag	UNP A0A2H5I9R9
A	0	HIS	-	expression tag	UNP A0A2H5I9R9
A	206	SER	CYS	engineered mutation	UNP A0A2H5I9R9

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



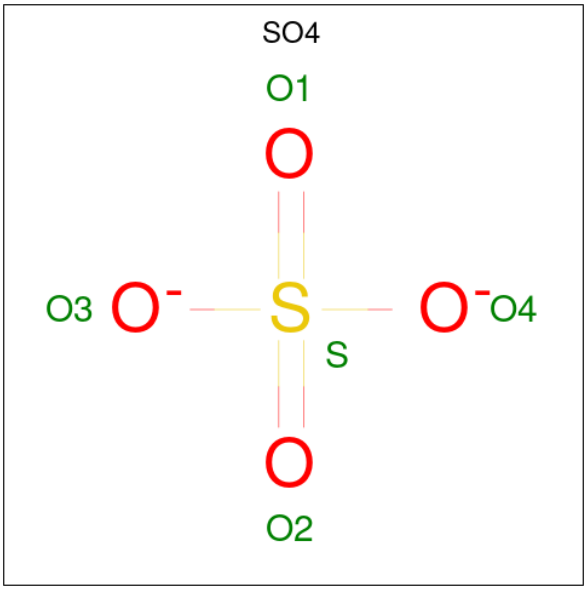
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	D	1	Total C H O 10 2 6 2	0	0
2	A	1	Total C H O 10 2 6 2	0	0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



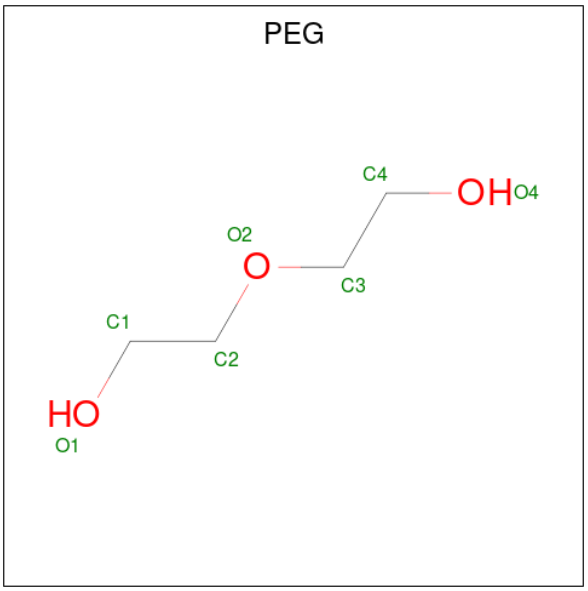
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 3 1 2	0	0
3	B	1	Total C H O 5 1 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

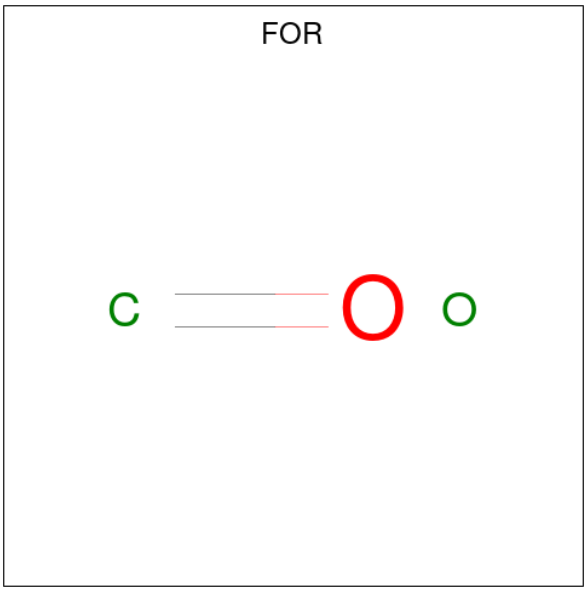


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C H O 17 4 10 3	0	0
5	D	1	Total C H O 17 4 10 3	0	0

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

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

- Molecule 7 is FORMYL GROUP (three-letter code: FOR) (formula: CH_2O).



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

- Molecule 8 is water.

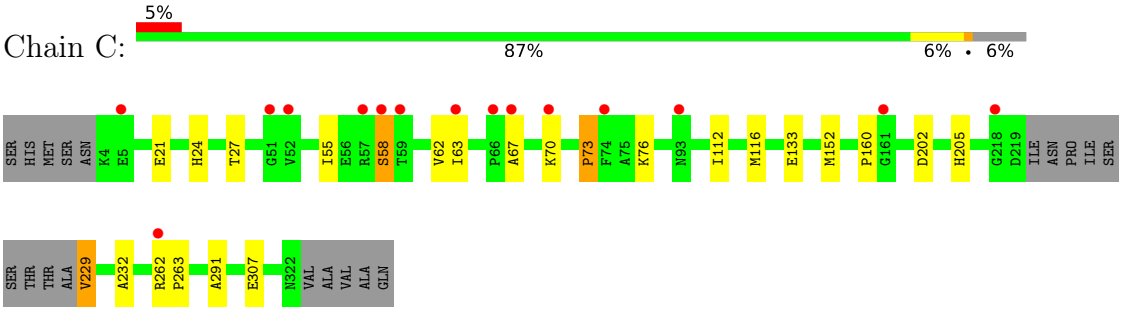
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	167	Total O 167 167	0	0
8	D	155	Total O 155 155	0	0
8	B	149	Total O 149 149	0	0
8	A	197	Total O 197 197	0	0

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.

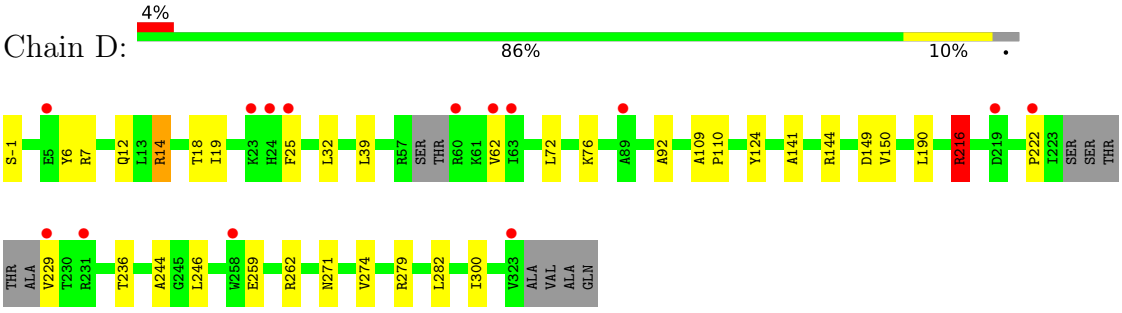
• Molecule 1: Hydrogen peroxide-inducible genes activator

Chain C:



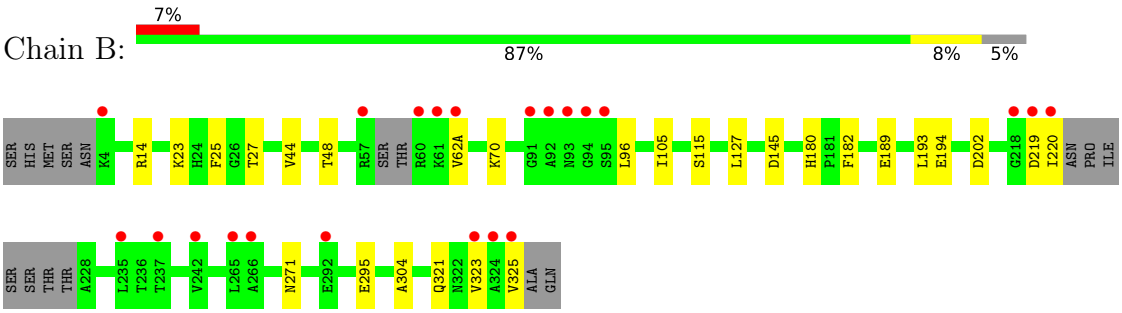
• Molecule 1: Hydrogen peroxide-inducible genes activator

Chain D:



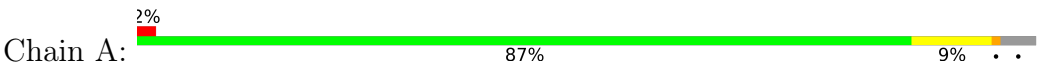
• Molecule 1: Hydrogen peroxide-inducible genes activator

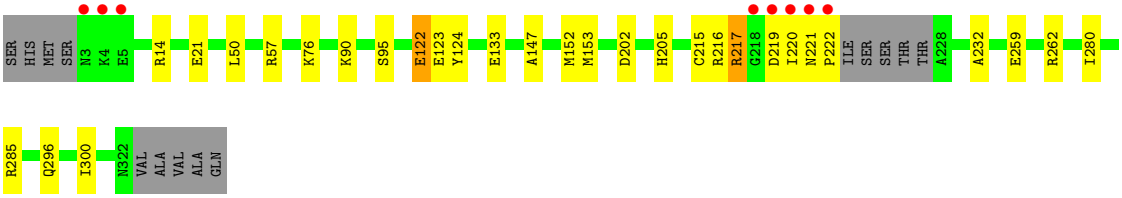
Chain B:



• Molecule 1: Hydrogen peroxide-inducible genes activator

Chain A:




SER
HIS
MET
SER
N3
K4
E5
R14
E21
L50
R57
K76
K90
S95
E122
E123
Y124
E133
A147
M152
M153
D202
H205
C215
R216
R217
G218
D219
I220
N221
P222
ILE
SER
SER
THR
THR
A228
A232
E259
R262
I280
R285
Q296
I300
N322
VAL
ALA
VAL
ALA
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.41Å 63.48Å 157.41Å 90.00° 97.79° 90.00°	Depositor
Resolution (Å)	44.86 – 1.99 49.23 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.86-1.99) 98.8 (49.23-1.99)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.200 , 0.221 0.200 , 0.222	Depositor DCC
R_{free} test set	4918 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10453	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: EDO, FMT, FOR, SO4, PEG, NA

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	0.73	2/2489 (0.1%)	0.89	9/3388 (0.3%)
1	B	0.63	0/2477	0.79	2/3374 (0.1%)
1	C	0.67	0/2467	0.91	6/3357 (0.2%)
1	D	0.69	0/2507	0.85	5/3414 (0.1%)
All	All	0.68	2/9940 (0.0%)	0.86	22/13533 (0.2%)

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	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153[A]	MET	CA-C	5.69	1.67	1.52
1	A	153[B]	MET	CA-C	5.69	1.67	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50[A]	LEU	N-CA-C	-9.79	84.56	111.00
1	A	50[B]	LEU	N-CA-C	-9.79	84.56	111.00
1	C	202[A]	ASP	CB-CG-OD2	9.19	126.57	118.30
1	C	202[B]	ASP	CB-CG-OD2	9.19	126.57	118.30
1	C	73	PRO	CA-C-N	-6.94	101.94	117.20
1	D	14	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	C	116	MET	CG-SD-CE	-6.53	89.76	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	149	ASP	CB-CG-OD2	6.36	124.02	118.30
1	A	222	PRO	N-CA-CB	6.13	110.66	103.30
1	B	14	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	153[A]	MET	CA-C-O	6.05	132.81	120.10
1	A	153[B]	MET	CA-C-O	6.05	132.81	120.10
1	C	58	SER	N-CA-C	5.97	127.11	111.00
1	D	222	PRO	N-CA-CB	5.93	110.42	103.30
1	D	216[A]	ARG	CA-C-O	5.83	132.35	120.10
1	D	216[B]	ARG	CA-C-O	5.83	132.35	120.10
1	C	229	VAL	CA-CB-CG1	5.60	119.30	110.90
1	A	202	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	202	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	14	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	14	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	202	ASP	CB-CG-OD2	-5.25	113.57	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	321[A]	GLN	Mainchain
1	B	321[B]	GLN	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	2423	0	2463	20	0
1	B	2411	0	2446	19	1
1	C	2400	0	2439	19	0
1	D	2435	0	2483	35	1
2	A	4	6	6	1	0
2	C	12	12	18	1	0
2	D	4	6	6	0	0
3	B	3	2	1	0	0
3	C	3	0	1	0	0
4	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	1	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
5	C	14	10	20	0	0
5	D	7	10	10	9	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0
8	A	197	0	0	2	0
8	B	149	0	0	2	0
8	C	167	0	0	2	0
8	D	155	0	0	3	0
All	All	10407	46	9893	89	1

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 5.

All (89) 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:D:12:GLN:HE22	5:D:403:PEG:H41	0.99	1.11
1:A:57:ARG:HD2	8:A:509:HOH:O	1.50	1.08
1:D:7:ARG:O	5:D:403:PEG:H21	1.52	1.08
1:D:6:TYR:HE1	5:D:403:PEG:H42	1.17	1.05
1:C:307:GLU:OE2	2:C:403:EDO:O1	1.80	0.99
1:A:95:SER:OG	1:A:296:GLN:NE2	1.94	0.99
1:C:58:SER:CB	1:C:63:ILE:HD12	1.96	0.95
1:D:6:TYR:CE1	5:D:403:PEG:H42	2.00	0.95
1:D:12:GLN:NE2	5:D:403:PEG:H41	1.85	0.91
1:D:72[B]:LEU:HD22	1:D:76:LYS:HD2	1.66	0.78
1:D:14:ARG:HD3	8:D:634:HOH:O	1.85	0.77
1:D:7:ARG:O	5:D:403:PEG:C2	2.30	0.77
1:B:27:THR:HG21	8:B:641:HOH:O	1.86	0.75
1:B:25:PHE:CE2	1:B:62(A):VAL:HG11	2.21	0.75
1:D:6:TYR:CD1	5:D:403:PEG:H22	2.22	0.74
1:D:6:TYR:CE1	5:D:403:PEG:H22	2.24	0.73
1:D:236[B]:THR:HG22	1:D:259:GLU:OE1	1.94	0.67
1:C:160:PRO:O	8:C:501:HOH:O	2.13	0.66
1:C:205:HIS:ND1	4:C:405:SO4:O3	2.26	0.64
1:A:215:CYS:O	1:A:219:ASP:HB2	2.00	0.62
1:D:236[B]:THR:HG23	8:D:585:HOH:O	1.99	0.61
1:C:58:SER:CB	1:C:63:ILE:CD1	2.76	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262[B]:ARG:HG2	1:C:263[B]:PRO:HD2	1.81	0.61
1:C:70:LYS:HD3	1:D:92:ALA:HB1	1.83	0.61
1:C:291:ALA:HB2	8:C:603:HOH:O	2.00	0.60
1:A:95:SER:CB	1:A:296:GLN:HE22	2.14	0.60
1:A:124:TYR:CE1	1:A:300:ILE:HD11	2.36	0.60
1:A:220:ILE:H	1:A:220:ILE:HD12	1.66	0.60
1:A:21:GLU:OE2	1:A:76:LYS:HE2	2.02	0.59
1:B:96:LEU:HB3	1:B:127:LEU:HD13	1.85	0.59
1:D:229:VAL:HG12	1:D:229:VAL:O	2.03	0.58
1:D:124:TYR:CE2	1:D:300:ILE:HD11	2.40	0.57
1:B:25:PHE:CD2	1:B:62(A):VAL:HG11	2.40	0.56
1:D:150[B]:VAL:HG21	1:D:282:LEU:HG	1.87	0.56
1:C:262[B]:ARG:CG	1:C:263[B]:PRO:HD2	2.36	0.55
1:B:194:GLU:N	1:B:220:ILE:HD13	2.21	0.54
1:D:25:PHE:HD1	1:D:39:LEU:HD23	1.73	0.53
1:D:150[B]:VAL:CG2	1:D:282:LEU:HG	2.39	0.53
1:A:285:ARG:HD2	8:A:504:HOH:O	2.10	0.52
1:C:67:ALA:O	1:C:70:LYS:HG2	2.08	0.52
1:A:220:ILE:HD12	1:A:220:ILE:N	2.24	0.52
1:D:6:TYR:HE1	5:D:403:PEG:C4	2.07	0.51
1:D:19:ILE:HG22	1:D:62:VAL:HG11	1.91	0.51
1:B:96:LEU:HD12	1:B:96:LEU:N	2.26	0.51
1:B:70:LYS:HZ1	2:A:401:EDO:HO2	1.55	0.50
1:B:193:LEU:HB2	1:B:220:ILE:CD1	2.42	0.50
1:C:262[B]:ARG:HG2	1:C:263[B]:PRO:CD	2.41	0.50
1:A:205:HIS:ND1	4:A:403:SO4:O1	2.33	0.50
1:D:150[B]:VAL:HG21	1:D:282:LEU:CG	2.43	0.49
1:D:72[B]:LEU:HD22	1:D:76:LYS:CD	2.38	0.49
1:B:145:ASP:HB2	1:A:147:ALA:HB2	1.96	0.47
1:B:193:LEU:HB2	1:B:220:ILE:HD12	1.96	0.47
1:D:25:PHE:CD1	1:D:39:LEU:HD23	2.50	0.46
1:C:55:ILE:CG2	1:C:62:VAL:HG13	2.46	0.46
1:B:189:GLU:CD	1:B:271[B]:ASN:HD21	2.19	0.46
1:D:19:ILE:CG2	1:D:62:VAL:HG11	2.45	0.45
1:D:18[A]:THR:HG21	1:D:32:LEU:HD21	1.99	0.45
1:D:244:ALA:HB3	1:D:246:LEU:HD13	1.98	0.45
1:A:152:MET:HE3	1:A:280:ILE:HG21	1.98	0.45
1:C:73:PRO:O	1:C:76:LYS:HB2	2.15	0.45
1:A:122:GLU:HG2	1:A:123:GLU:HG3	1.98	0.45
1:B:44:VAL:O	1:B:48:THR:HG23	2.16	0.45
1:A:216:ARG:O	1:A:217:ARG:C	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:VAL:HG12	1:B:325:VAL:HG23	1.99	0.44
1:C:112:ILE:HG21	1:C:152:MET:HE1	1.99	0.43
1:C:133:GLU:HB3	1:A:232:ALA:HA	2.01	0.43
1:D:190:LEU:HD13	1:D:274:VAL:CG1	2.49	0.43
1:C:24:HIS:HB2	1:C:27:THR:OG1	2.19	0.42
1:D:18[A]:THR:OG1	1:D:32:LEU:HD11	2.19	0.42
1:D:271:ASN:ND2	8:D:502:HOH:O	2.50	0.42
1:A:215:CYS:O	1:A:219:ASP:N	2.52	0.42
1:B:115[B]:SER:OG	1:B:304:ALA:HA	2.20	0.42
1:D:141:ALA:HA	1:D:144:ARG:HG2	2.01	0.42
1:D:236[A]:THR:HG23	1:D:262:ARG:HH22	1.83	0.42
1:B:105:ILE:HB	4:B:402:SO4:O3	2.20	0.42
1:C:58:SER:CB	1:C:63:ILE:CG1	2.97	0.42
1:D:190:LEU:HD13	1:D:274:VAL:HG13	2.03	0.41
1:B:295:GLU:HG3	8:B:507:HOH:O	2.20	0.41
1:A:216:ARG:O	1:A:217:ARG:O	2.38	0.41
1:C:112:ILE:HG21	1:C:152:MET:CE	2.51	0.41
1:B:180:HIS:CE1	1:B:182:PHE:H	2.39	0.41
1:A:215:CYS:O	1:A:219:ASP:CB	2.66	0.41
1:B:23:LYS:HA	1:B:62(A):VAL:HG23	2.02	0.41
1:B:96:LEU:N	1:B:96:LEU:CD1	2.84	0.40
1:A:259:GLU:HA	1:A:262:ARG:HH21	1.86	0.40
1:C:232:ALA:HA	1:A:133:GLU:HB3	2.02	0.40
1:D:109:ALA:HB3	1:D:110:PRO:HD3	2.03	0.40
1:D:190:LEU:HD12	1:D:190:LEU:HA	1.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:ARG:NH1	1:B:325:VAL:CG2[1_545]	1.70	0.50

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	321/329 (98%)	315 (98%)	4 (1%)	2 (1%)	25 19
1	B	320/329 (97%)	317 (99%)	3 (1%)	0	100 100
1	C	318/329 (97%)	315 (99%)	3 (1%)	0	100 100
1	D	322/329 (98%)	318 (99%)	4 (1%)	0	100 100
All	All	1281/1316 (97%)	1265 (99%)	14 (1%)	2 (0%)	47 44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	217	ARG

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	266/273 (97%)	264 (99%)	2 (1%)	81 86
1	B	267/273 (98%)	266 (100%)	1 (0%)	91 93
1	C	264/273 (97%)	262 (99%)	2 (1%)	81 86
1	D	270/273 (99%)	267 (99%)	3 (1%)	73 78
All	All	1067/1092 (98%)	1059 (99%)	8 (1%)	84 88

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

Mol	Chain	Res	Type
1	C	21	GLU
1	C	229	VAL
1	D	-1	SER
1	D	216[A]	ARG
1	D	216[B]	ARG
1	B	219	ASP

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Mol	Chain	Res	Type
1	A	90	LYS
1	A	122	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	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)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	$\#\|Z\| > 2$
7	FOR	A	404	-	0,1,1	-	-	-		
5	PEG	C	407	-	6,6,6	0.30	0	5,5,5	0.35	0
5	PEG	C	406	-	6,6,6	0.64	0	5,5,5	0.50	0
2	EDO	D	401	-	3,3,3	0.45	0	2,2,2	0.10	0
3	FMT	B	401	-	2,2,2	0.57	0	1,1,1	0.75	0
3	FMT	C	404	-	2,2,2	0.74	0	1,1,1	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	A	401	-	3,3,3	0.38	0	2,2,2	0.27	0
4	SO4	C	405	-	4,4,4	3.50	3 (75%)	6,6,6	1.07	0
4	SO4	D	402	-	4,4,4	3.35	3 (75%)	6,6,6	1.02	0
2	EDO	C	402	-	3,3,3	0.43	0	2,2,2	0.16	0
2	EDO	C	403	-	3,3,3	0.42	0	2,2,2	0.25	0
4	SO4	B	402	-	4,4,4	3.14	3 (75%)	6,6,6	1.37	1 (16%)
4	SO4	A	403	-	4,4,4	3.07	4 (100%)	6,6,6	1.34	2 (33%)
5	PEG	D	403	-	6,6,6	0.52	0	5,5,5	0.47	0
2	EDO	C	401	-	3,3,3	0.58	0	2,2,2	0.06	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
5	PEG	C	407	-	-	3/4/4/4	-
5	PEG	C	406	-	-	2/4/4/4	-
2	EDO	D	401	-	-	1/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	C	402	-	-	1/1/1/1	-
2	EDO	C	403	-	-	1/1/1/1	-
5	PEG	D	403	-	-	3/4/4/4	-
2	EDO	C	401	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	405	SO4	O1-S	5.36	1.75	1.46
4	D	402	SO4	O2-S	4.64	1.71	1.46
4	D	402	SO4	O1-S	3.85	1.66	1.46
4	B	402	SO4	O4-S	3.61	1.77	1.47
4	C	405	SO4	O2-S	3.52	1.65	1.46
4	A	403	SO4	O2-S	3.47	1.64	1.46
4	B	402	SO4	O2-S	3.43	1.64	1.46
4	B	402	SO4	O1-S	3.38	1.64	1.46
4	A	403	SO4	O4-S	3.31	1.75	1.47
4	A	403	SO4	O1-S	3.13	1.63	1.46
4	D	402	SO4	O3-S	2.33	1.67	1.47
4	A	403	SO4	O3-S	2.23	1.66	1.47
4	C	405	SO4	O3-S	2.14	1.65	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	SO4	O4-S-O3	2.46	119.58	109.06
4	A	403	SO4	O3-S-O1	-2.07	98.52	109.31
4	B	402	SO4	O3-S-O2	-2.03	98.70	109.31

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	407	PEG	O2-C3-C4-O4
5	C	407	PEG	O1-C1-C2-O2
5	C	406	PEG	O1-C1-C2-O2
5	D	403	PEG	O1-C1-C2-O2
2	D	401	EDO	O1-C1-C2-O2
5	D	403	PEG	C1-C2-O2-C3
5	D	403	PEG	O2-C3-C4-O4
2	C	402	EDO	O1-C1-C2-O2
5	C	406	PEG	O2-C3-C4-O4
5	C	407	PEG	C4-C3-O2-C2
2	A	401	EDO	O1-C1-C2-O2
2	C	403	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	EDO	1	0
4	C	405	SO4	1	0
2	C	403	EDO	1	0
4	B	402	SO4	1	0
4	A	403	SO4	1	0
5	D	403	PEG	9	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	230:THR	C	231[B]:ARG	N	1.20

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	315/329 (95%)	0.23	8 (2%)	57	56	28, 42, 72, 179	2 (0%)
1	B	313/329 (95%)	0.45	22 (7%)	16	15	32, 47, 84, 165	1 (0%)
1	C	310/329 (94%)	0.37	15 (4%)	30	29	31, 45, 80, 146	1 (0%)
1	D	318/329 (96%)	0.33	14 (4%)	34	33	31, 47, 85, 125	1 (0%)
All	All	1256/1316 (95%)	0.34	59 (4%)	31	30	28, 45, 82, 179	5 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	93	ASN	7.1
1	A	3	ASN	5.8
1	A	4	LYS	5.8
1	B	92	ALA	5.8
1	C	59	THR	5.7
1	B	324	ALA	5.7
1	A	220	ILE	5.5
1	B	94	GLY	5.3
1	C	58	SER	5.2
1	C	262[A]	ARG	5.2
1	B	62(A)	VAL	4.5
1	B	60	ARG	4.2
1	C	67	ALA	4.1
1	B	220	ILE	3.8
1	D	62	VAL	3.8
1	C	52	VAL	3.3
1	D	25	PHE	3.2
1	C	74	PHE	3.1
1	C	63	ILE	3.1
1	B	4	LYS	3.1
1	B	218	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	218	GLY	3.1
1	C	66	PRO	3.0
1	A	219	ASP	2.9
1	D	24	HIS	2.9
1	B	91	GLY	2.8
1	A	5	GLU	2.8
1	D	229	VAL	2.8
1	D	23	LYS	2.7
1	C	218	GLY	2.6
1	A	221	ASN	2.6
1	D	323	VAL	2.5
1	B	323	VAL	2.5
1	D	222	PRO	2.5
1	B	325	VAL	2.4
1	B	219	ASP	2.4
1	D	219	ASP	2.3
1	C	51	GLY	2.3
1	D	258	TRP	2.3
1	B	57	ARG	2.3
1	B	61	LYS	2.2
1	C	57	ARG	2.2
1	C	5	GLU	2.2
1	A	222	PRO	2.2
1	B	235	LEU	2.2
1	D	231[A]	ARG	2.2
1	D	60	ARG	2.1
1	B	237	THR	2.1
1	B	266	ALA	2.1
1	B	265	LEU	2.1
1	C	161	GLY	2.1
1	B	242	VAL	2.1
1	D	89	ALA	2.1
1	B	95	SER	2.0
1	C	93	ASN	2.0
1	D	5	GLU	2.0
1	B	292	GLU	2.0
1	D	63	ILE	2.0
1	C	70	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	C	407	7/7	0.64	2.40	25,30,30,30	17
6	NA	A	402	1/1	0.65	0.20	94,94,94,94	0
2	EDO	C	401	4/4	0.77	0.32	60,61,64,66	0
5	PEG	D	403	7/7	0.78	0.28	18,21,21,21	17
5	PEG	C	406	7/7	0.89	0.14	65,70,93,103	0
2	EDO	C	402	4/4	0.89	0.11	25,30,30,30	10
7	FOR	A	404	2/2	0.89	0.14	67,67,67,72	0
2	EDO	D	401	4/4	0.90	0.31	18,21,21,21	0
3	FMT	C	404	3/3	0.91	0.12	66,66,68,68	0
4	SO4	B	402	5/5	0.92	0.17	56,59,60,66	0
2	EDO	A	401	4/4	0.94	0.41	18,21,21,21	0
2	EDO	C	403	4/4	0.94	0.47	18,21,21,21	0
3	FMT	B	401	3/3	0.94	0.37	18,18,21,21	0
4	SO4	C	405	5/5	0.95	0.16	55,55,62,62	0
4	SO4	D	402	5/5	0.95	0.15	57,57,58,61	0
4	SO4	A	403	5/5	0.97	0.14	54,57,58,60	0

6.5 Other polymers (i)

There are no such residues in this entry.