



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:16 am BST

PDB ID : 6ET0
Title : Crystal structure of PqsBC (C129A) mutant from *Pseudomonas aeruginosa* (crystal form 1)
Authors : Witzgall, F.; Blankenfeldt, W.
Deposited on : 2017-10-25
Resolution : 1.53 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

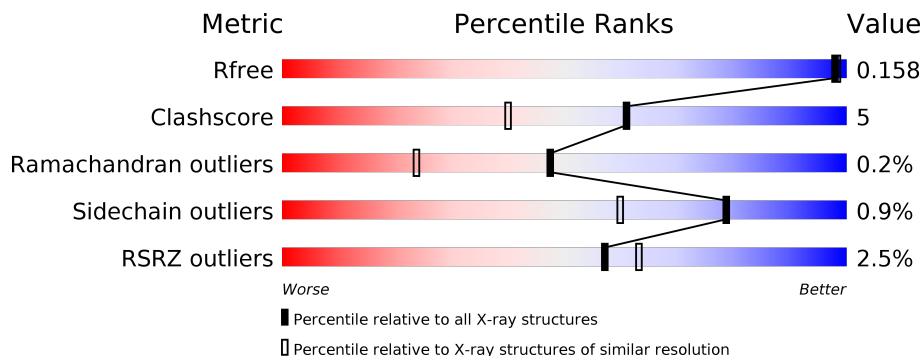
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	
1	C	365	
2	B	283	
2	D	283	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22493 atoms, of which 10595 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 PqsC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	352	5720	1819	2872	483	526	20	0	24	0
1	C	352	5768	1843	2906	475	524	20	0	31	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q9I4X1
A	-15	GLY	-	expression tag	UNP Q9I4X1
A	-14	HIS	-	expression tag	UNP Q9I4X1
A	-13	HIS	-	expression tag	UNP Q9I4X1
A	-12	HIS	-	expression tag	UNP Q9I4X1
A	-11	HIS	-	expression tag	UNP Q9I4X1
A	-10	HIS	-	expression tag	UNP Q9I4X1
A	-9	HIS	-	expression tag	UNP Q9I4X1
A	-8	ALA	-	expression tag	UNP Q9I4X1
A	-7	GLU	-	expression tag	UNP Q9I4X1
A	-6	ASN	-	expression tag	UNP Q9I4X1
A	-5	LEU	-	expression tag	UNP Q9I4X1
A	-4	TYR	-	expression tag	UNP Q9I4X1
A	-3	PHE	-	expression tag	UNP Q9I4X1
A	-2	GLN	-	expression tag	UNP Q9I4X1
A	-1	GLY	-	expression tag	UNP Q9I4X1
A	0	HIS	-	expression tag	UNP Q9I4X1
A	129	ALA	CYS	engineered mutation	UNP Q9I4X1
C	-16	MET	-	initiating methionine	UNP Q9I4X1
C	-15	GLY	-	expression tag	UNP Q9I4X1
C	-14	HIS	-	expression tag	UNP Q9I4X1
C	-13	HIS	-	expression tag	UNP Q9I4X1
C	-12	HIS	-	expression tag	UNP Q9I4X1
C	-11	HIS	-	expression tag	UNP Q9I4X1
C	-10	HIS	-	expression tag	UNP Q9I4X1

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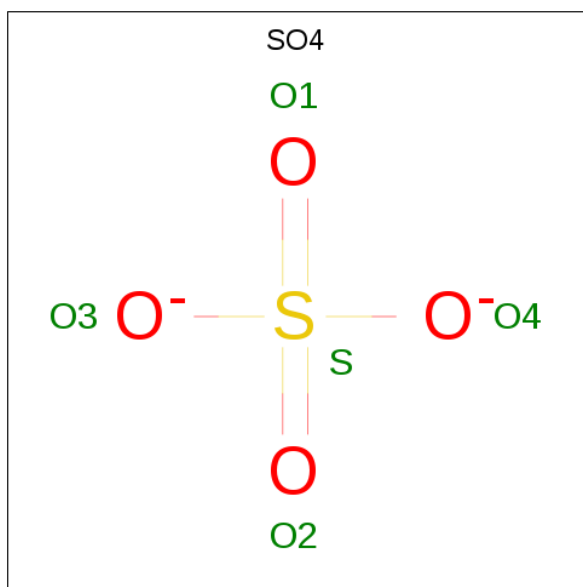
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	HIS	-	expression tag	UNP Q9I4X1
C	-8	ALA	-	expression tag	UNP Q9I4X1
C	-7	GLU	-	expression tag	UNP Q9I4X1
C	-6	ASN	-	expression tag	UNP Q9I4X1
C	-5	LEU	-	expression tag	UNP Q9I4X1
C	-4	TYR	-	expression tag	UNP Q9I4X1
C	-3	PHE	-	expression tag	UNP Q9I4X1
C	-2	GLN	-	expression tag	UNP Q9I4X1
C	-1	GLY	-	expression tag	UNP Q9I4X1
C	0	HIS	-	expression tag	UNP Q9I4X1
C	129	ALA	CYS	engineered mutation	UNP Q9I4X1

- Molecule 2 is a protein called PqsB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	278	Total	C	H	N	O	S	0	31	0
			4671	1458	2391	401	412	9			
2	D	283	Total	C	H	N	O	S	0	18	0
			4560	1428	2312	396	415	9			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



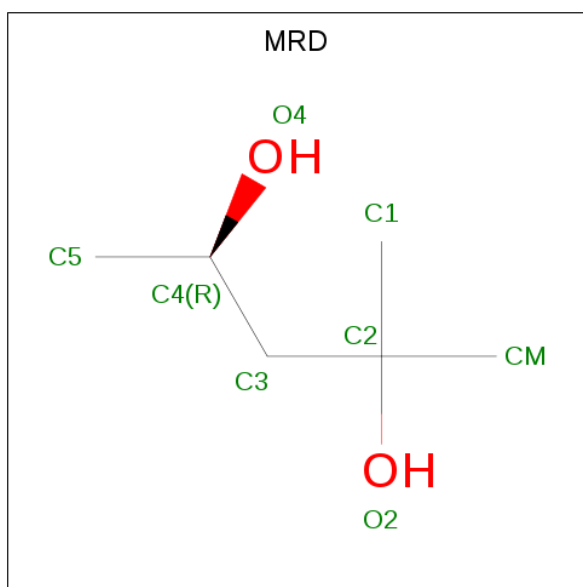
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	Total	O	S	0	0
			5	4	1		

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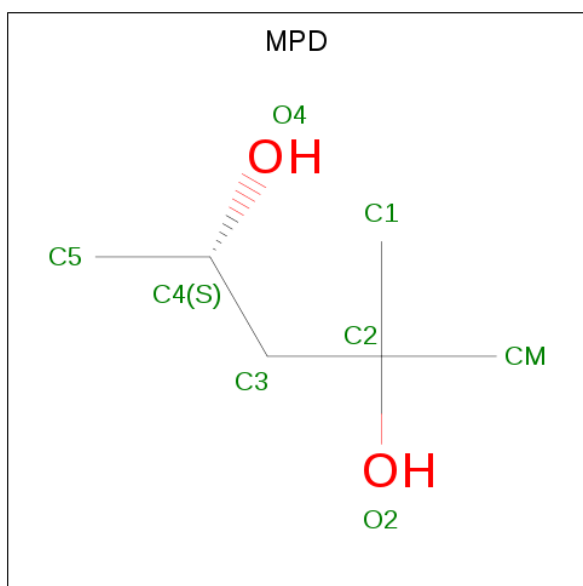
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0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

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	44	12	28	4	0	1
4	C	1	44	12	28	4	0	1

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



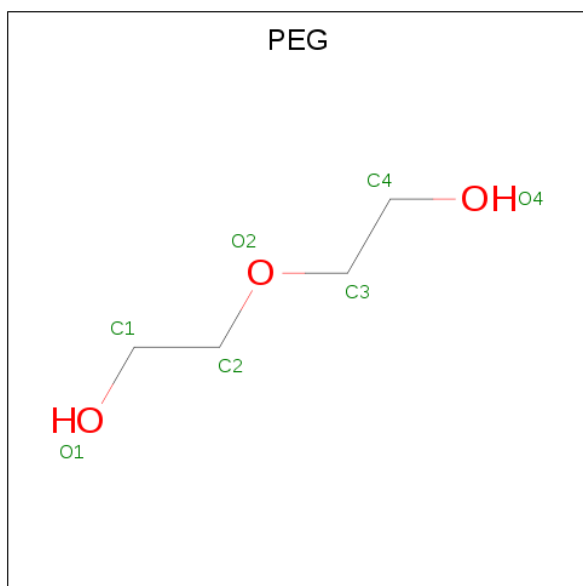
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	22	6	14	2	0	0

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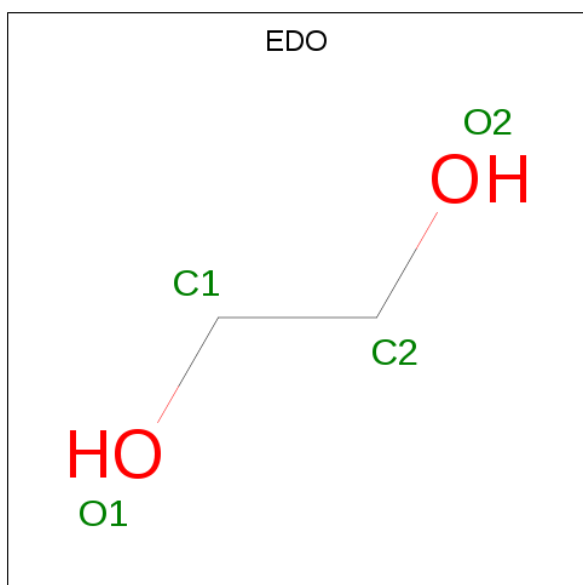
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	C	1	44	12	28	4	0	1

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	B	1	17	4	10	3	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	H	O	0	0
			10	2	6	2		

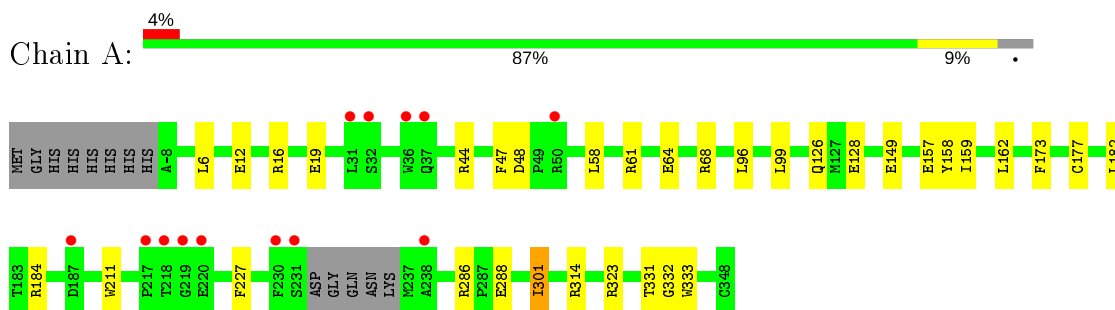
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	410	Total	O	0	1
			410	410		
8	B	317	Total	O	0	1
			317	317		
8	C	407	Total	O	0	0
			407	407		
8	D	384	Total	O	0	4
			384	384		

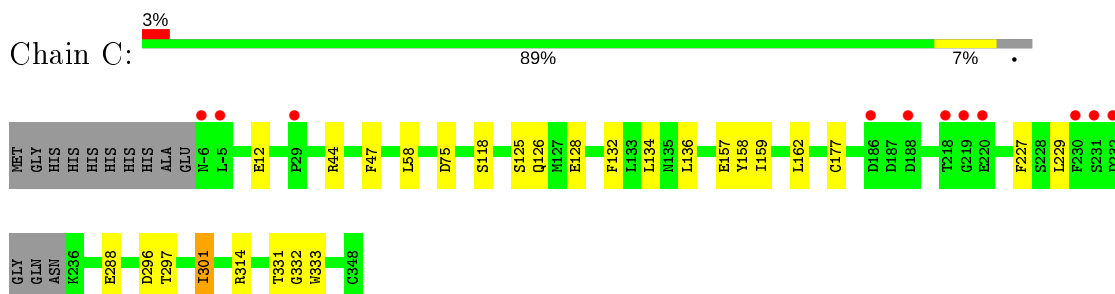
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

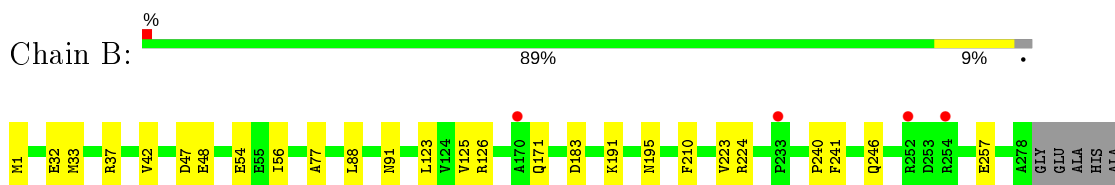
- Molecule 1: PqsC



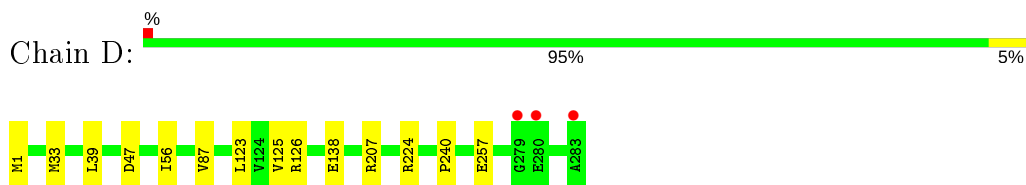
- Molecule 1: PqsC



- Molecule 2: PqsB



- Molecule 2: PqsB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.67Å 141.36Å 170.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.12 – 1.53 47.12 – 1.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.12-1.53) 99.9 (47.12-1.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.53Å)	Xtrriage
Refinement program	PHENIX dev_2875	Depositor
R, R_{free}	0.140 , 0.158 0.140 , 0.158	Depositor DCC
R_{free} test set	10963 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtrriage
Anisotropy	0.429	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	22493	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, CSO, EDO, SO4, MRD, PEG

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	0.34	0/2981	0.59	0/4042
1	C	0.34	0/3017	0.59	0/4095
2	B	0.32	0/2405	0.59	0/3262
2	D	0.35	0/2330	0.64	0/3160
All	All	0.34	0/10733	0.60	0/14559

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2848	2872	2867	31	0
1	C	2862	2906	2904	24	0
2	B	2280	2391	2378	24	0
2	D	2248	2312	2312	10	0
3	A	20	0	0	0	0
3	B	20	0	0	1	0
3	C	15	0	0	0	0
3	D	20	0	0	1	0
4	A	16	28	28	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	16	28	28	4	0
5	A	8	14	14	4	0
5	C	16	28	28	2	0
6	B	7	10	10	2	0
7	C	4	6	6	0	0
8	A	410	0	0	10	0
8	B	317	0	0	13	1
8	C	407	0	0	8	0
8	D	384	0	0	7	1
All	All	11898	10595	10575	95	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 (95) 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)
2:B:126[B]:ARG:NH2	8:B:1001:HOH:O	1.91	0.99
1:A:68[B]:ARG:NH2	8:A:1003:HOH:O	1.96	0.95
1:A:19[B]:GLU:OE1	8:A:1001:HOH:O	1.89	0.89
1:C:296[B]:ASP:OD1	8:C:501:HOH:O	1.89	0.89
2:B:126[A]:ARG:NH2	8:B:1005:HOH:O	2.06	0.88
2:B:183:ASP:OD1	8:B:1002:HOH:O	1.93	0.85
1:C:126[B]:GLN:NE2	8:C:504:HOH:O	2.09	0.84
2:B:91[B]:ASN:OD1	8:B:1003:HOH:O	1.97	0.82
4:A:904[B]:MRD:H5C3	4:A:904[B]:MRD:HMC1	1.61	0.82
4:C:404[A]:MRD:HMC1	4:C:404[A]:MRD:H5C3	1.64	0.80
1:A:286:ARG:NH1	1:A:288:GLU:OE1	2.16	0.79
1:C:296[B]:ASP:OD2	8:C:502:HOH:O	2.02	0.78
1:A:68[B]:ARG:NH2	8:A:1004:HOH:O	2.17	0.78
1:A:331:THR:HG23	4:A:904[A]:MRD:H4	1.65	0.76
2:B:54[A]:GLU:OE2	8:B:1004:HOH:O	2.03	0.75
1:C:288[A]:GLU:OE2	8:C:503:HOH:O	2.03	0.75
1:A:128:GLU:OE2	4:A:904[B]:MRD:H5C1	1.87	0.74
3:D:304:SO4:O3	8:D:401:HOH:O	2.06	0.73
2:B:48:GLU:OE1	8:B:1006:HOH:O	2.08	0.70
1:C:128:GLU:OE2	4:C:404[A]:MRD:H5C1	1.91	0.69
2:B:257:GLU:OE2	8:B:1007:HOH:O	2.10	0.69
1:C:331:THR:HG23	4:C:404[B]:MRD:H4	1.75	0.69
1:A:323[B]:ARG:NH2	8:A:1006:HOH:O	2.26	0.68
2:D:47[A]:ASP:OD1	8:D:402:HOH:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HD13	5:A:905:MPD:H52	1.77	0.66
2:D:87[B]:VAL:HG23	8:D:523:HOH:O	1.93	0.66
1:A:173:PHE:HZ	4:A:904[A]:MRD:H5C2	1.60	0.66
2:B:48:GLU:OE2	8:B:1009:HOH:O	2.15	0.65
2:B:195[B]:ASN:OD1	8:B:1008:HOH:O	2.13	0.64
1:A:159:ILE:CD1	1:A:162[B]:LEU:HD11	2.28	0.64
2:D:257:GLU:OE2	8:D:403:HOH:O	2.15	0.63
1:C:125[A]:SER:OG	8:C:505:HOH:O	2.16	0.63
1:A:159:ILE:CD1	5:A:905:MPD:H52	2.28	0.62
1:C:296[B]:ASP:OD2	8:C:506:HOH:O	2.16	0.61
2:D:138[A]:GLU:OE2	8:D:404:HOH:O	2.17	0.60
1:A:149[B]:GLU:OE2	1:A:184:ARG:NH2	2.35	0.59
1:C:314[A]:ARG:NH2	8:C:508:HOH:O	2.36	0.58
2:D:207[B]:ARG:NE	8:D:410:HOH:O	2.36	0.58
1:C:296[B]:ASP:OD1	1:C:297:THR:HG23	2.06	0.55
1:A:16[B]:ARG:NH2	1:A:48:ASP:OD2	2.40	0.54
1:A:159:ILE:HD11	1:A:162[B]:LEU:HD11	1.89	0.54
1:A:314[A]:ARG:NH2	8:A:1009:HOH:O	2.30	0.53
2:B:42:VAL:HG11	2:B:88:LEU:HD11	1.91	0.52
1:C:47:PHE:CE1	1:C:58[B]:LEU:HD12	2.44	0.52
2:B:47[A]:ASP:OD1	8:B:1010:HOH:O	2.19	0.52
1:A:126[A]:GLN:NE2	8:A:1018:HOH:O	2.42	0.52
1:C:12:GLU:HB3	1:C:177[B]:CYS:SG	2.50	0.52
1:C:162[B]:LEU:HD13	1:C:227:PHE:HB2	1.92	0.51
1:A:96:LEU:CB	1:A:99[B]:LEU:HD12	2.41	0.51
2:D:39:LEU:HD22	2:D:87[B]:VAL:HG11	1.93	0.51
2:B:32:GLU:OE2	6:B:904:PEG:H32	2.11	0.51
5:A:905:MPD:HM3	2:B:77:ALA:HB3	1.94	0.50
2:D:123[A]:LEU:HG	2:D:125:VAL:HG13	1.93	0.50
1:A:96:LEU:HD13	1:A:99[B]:LEU:CD1	2.42	0.49
6:B:904:PEG:C1	8:B:1018:HOH:O	2.60	0.49
5:A:905:MPD:O4	5:A:905:MPD:H12	2.14	0.48
1:A:96:LEU:HD13	1:A:99[B]:LEU:HD11	1.96	0.48
1:A:157[B]:GLU:OE1	1:A:301:ILE:HB	2.15	0.47
1:C:75[B]:ASP:OD1	1:C:118:SER:OG	2.25	0.47
2:B:126[A]:ARG:NE	8:B:1033:HOH:O	2.48	0.46
4:A:904[B]:MRD:HMC1	4:A:904[B]:MRD:C5	2.38	0.46
1:C:159[B]:ILE:HG13	1:C:301:ILE:HG12	1.97	0.45
1:A:68[A]:ARG:NH2	8:A:1026:HOH:O	2.48	0.45
2:B:123[A]:LEU:HG	2:B:125:VAL:HG13	1.98	0.45
1:C:159[B]:ILE:HG13	1:C:301:ILE:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:HB3	1:A:99[B]:LEU:HD12	1.99	0.45
1:C:332:GLY:N	1:C:333:TRP:HA	2.31	0.44
2:D:126[A]:ARG:NE	2:D:240[A]:PRO:HG2	2.32	0.44
1:A:12:GLU:HB3	1:A:177[B]:CYS:SG	2.56	0.44
1:A:332:GLY:N	1:A:333:TRP:HA	2.32	0.44
2:B:37[A]:ARG:NH1	3:B:903:SO4:O4	2.47	0.44
2:B:56[B]:ILE:HD13	2:B:123[B]:LEU:HD12	2.00	0.44
1:C:134:LEU:HD23	8:C:505:HOH:O	2.17	0.44
2:B:126[B]:ARG:NH1	2:B:240[B]:PRO:HB2	2.33	0.44
2:B:171:GLN:O	8:B:1011:HOH:O	2.21	0.43
2:B:126[B]:ARG:NH1	2:B:241:PHE:CZ	2.86	0.43
1:C:132:PHE:CE2	1:C:136[A]:LEU:HD11	2.53	0.43
1:C:227:PHE:CZ	1:C:229[B]:LEU:HG	2.54	0.43
4:C:404[A]:MRD:C5	4:C:404[A]:MRD:HMC1	2.40	0.43
1:A:314[B]:ARG:NE	8:A:1029:HOH:O	2.50	0.43
1:C:227:PHE:CD1	5:C:403[B]:MPD:H52	2.53	0.42
1:A:162[B]:LEU:HD13	1:A:227:PHE:HB2	2.00	0.42
1:A:64:GLU:OE2	8:A:1005:HOH:O	2.21	0.42
1:C:128:GLU:OE2	5:C:403[A]:MPD:H51	2.20	0.42
2:B:223:VAL:HG12	2:B:246:GLN:HB3	2.02	0.42
1:A:61:ARG:NH2	8:A:1033:HOH:O	2.51	0.42
2:D:126[A]:ARG:NH1	8:D:421[A]:HOH:O	2.52	0.42
1:A:47:PHE:CE1	1:A:58:LEU:HD12	2.56	0.41
1:C:157[A]:GLU:OE2	1:C:301:ILE:HB	2.21	0.41
2:D:56[B]:ILE:HD13	2:D:123[B]:LEU:HD12	2.01	0.41
1:A:211:TRP:CG	2:B:191:LYS:HE2	2.56	0.41
2:B:210:PHE:CD2	2:B:224[A]:ARG:HD2	2.56	0.41
1:A:6[B]:LEU:HA	1:A:182[B]:LEU:HD23	2.03	0.40
1:C:229[B]:LEU:HA	1:C:229[B]:LEU:HD23	1.98	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)
8:B:1029:HOH:O	8:D:408:HOH:O[2_455]	1.89	0.31

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	372/365 (102%)	361 (97%)	10 (3%)	1 (0%)	41	19
1	C	379/365 (104%)	366 (97%)	12 (3%)	1 (0%)	41	19
2	B	305/283 (108%)	302 (99%)	3 (1%)	0	100	100
2	D	297/283 (105%)	294 (99%)	3 (1%)	0	100	100
All	All	1353/1296 (104%)	1323 (98%)	28 (2%)	2 (0%)	47	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	ILE
1	C	301	ILE

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	310/299 (104%)	308 (99%)	2 (1%)	86	72
1	C	313/299 (105%)	311 (99%)	2 (1%)	86	72
2	B	250/222 (113%)	248 (99%)	2 (1%)	81	64
2	D	239/222 (108%)	236 (99%)	3 (1%)	69	42
All	All	1112/1042 (107%)	1103 (99%)	9 (1%)	78	64

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	158	TYR
2	B	1	MET
2	B	33	MET
1	C	44	ARG
1	C	158	TYR
2	D	1	MET
2	D	33	MET
2	D	224	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 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	$\# Z > 2$
2	CSO	D	16[A]	-	3,6,7	0.75	0	0,6,8	0.00	-
2	CSO	D	16[B]	-	3,6,7	0.74	0	0,6,8	0.00	-
2	CSO	B	16[A]	-	3,6,7	0.80	0	0,6,8	0.00	-
2	CSO	B	16[B]	-	3,6,7	0.81	0	0,6,8	0.00	-

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	CSO	D	16[A]	-	-	0/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	D	16[B]	-	-	1/1/5/7	-
2	CSO	B	16[A]	-	-	0/1/5/7	-
2	CSO	B	16[B]	-	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	16[B]	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
3	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.23	0
5	MPD	A	905	-	7,7,7	0.26	0	9,10,10	0.30	0
3	SO4	B	903	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	A	902	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	902	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	901	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	A	900	-	4,4,4	0.13	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	406	-	4,4,4	0.20	0	6,6,6	0.24	0
6	PEG	B	904	-	6,6,6	0.52	0	5,5,5	0.38	0
4	MRD	C	404[B]	-	7,7,7	0.69	0	9,10,10	0.48	0
7	EDO	C	405	-	3,3,3	0.51	0	2,2,2	0.19	0
3	SO4	A	901	-	4,4,4	0.14	0	6,6,6	0.06	0
4	MRD	C	404[A]	-	7,7,7	0.68	0	9,10,10	0.40	0
3	SO4	D	302	-	4,4,4	0.12	0	6,6,6	0.11	0
3	SO4	D	304	-	4,4,4	0.17	0	6,6,6	0.11	0
3	SO4	C	402	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	D	303	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	C	401	-	4,4,4	0.13	0	6,6,6	0.11	0
4	MRD	A	904[A]	-	7,7,7	0.67	0	9,10,10	0.37	0
3	SO4	A	903	-	4,4,4	0.15	0	6,6,6	0.13	0
5	MPD	C	403[B]	-	7,7,7	0.25	0	9,10,10	0.29	0
3	SO4	B	900	-	4,4,4	0.14	0	6,6,6	0.29	0
5	MPD	C	403[A]	-	7,7,7	0.19	0	9,10,10	0.53	0
4	MRD	A	904[B]	-	7,7,7	0.68	0	9,10,10	0.45	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	PEG	B	904	-	-	0/4/4/4	-
5	MPD	A	905	-	-	2/5/5/5	-
4	MRD	C	404[B]	-	-	0/5/5/5	-
7	EDO	C	405	-	-	1/1/1/1	-
4	MRD	C	404[A]	-	-	2/5/5/5	-
4	MRD	A	904[A]	-	-	0/5/5/5	-
5	MPD	C	403[B]	-	-	0/5/5/5	-
5	MPD	C	403[A]	-	-	4/5/5/5	-
4	MRD	A	904[B]	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	405	EDO	O1-C1-C2-O2
4	A	904[B]	MRD	O2-C2-C3-C4
5	A	905	MPD	C2-C3-C4-C5
5	C	403[A]	MPD	C2-C3-C4-C5
5	C	403[A]	MPD	C1-C2-C3-C4
4	C	404[A]	MRD	O2-C2-C3-C4
5	C	403[A]	MPD	O2-C2-C3-C4
4	C	404[A]	MRD	C2-C3-C4-C5
4	A	904[B]	MRD	C2-C3-C4-C5
5	A	905	MPD	C2-C3-C4-O4
5	C	403[A]	MPD	C2-C3-C4-O4

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	905	MPD	4	0
3	B	903	SO4	1	0
6	B	904	PEG	2	0
4	C	404[B]	MRD	1	0
4	C	404[A]	MRD	3	0
3	D	304	SO4	1	0
4	A	904[A]	MRD	2	0
5	C	403[B]	MPD	1	0
5	C	403[A]	MPD	1	0
4	A	904[B]	MRD	3	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, 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	352/365 (96%)	-0.43	13 (3%) 41 48	15, 23, 55, 100	0
1	C	352/365 (96%)	-0.49	11 (3%) 49 56	14, 22, 53, 104	0
2	B	277/283 (97%)	-0.46	4 (1%) 75 79	14, 20, 53, 70	0
2	D	282/283 (99%)	-0.51	3 (1%) 80 83	12, 17, 48, 86	0
All	All	1263/1296 (97%)	-0.47	31 (2%) 57 63	12, 21, 53, 104	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	SER	6.5
1	C	232	ASP	4.7
1	A	219	GLY	4.5
1	A	218	THR	4.4
1	A	37[A]	GLN	4.4
1	C	219	GLY	3.8
1	A	230	PHE	3.7
1	C	188	ASP	3.4
1	C	218	THR	3.2
1	C	231	SER	3.1
1	A	50	ARG	3.0
1	C	-5	LEU	3.0
1	C	230	PHE	3.0
2	D	283	ALA	3.0
1	A	238	ALA	2.9
2	B	233	PRO	2.9
1	A	31	LEU	2.7
2	B	252[A]	ARG	2.6
1	A	36	TRP	2.4
2	D	280	GLU	2.4
1	A	217	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	220	GLU	2.4
2	B	170	ALA	2.3
2	B	254	ARG	2.2
1	A	32	SER	2.2
1	C	-6	ASN	2.2
1	A	187	ASP	2.2
2	D	279	GLY	2.1
1	C	29	PRO	2.1
1	C	220	GLU	2.1
1	C	186	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	CSO	D	16[A]	7/8	0.97	0.09	15,20,35,42	8
2	CSO	D	16[B]	7/8	0.97	0.09	15,20,75,90	8
2	CSO	B	16[A]	7/8	0.97	0.06	17,24,37,45	8
2	CSO	B	16[B]	7/8	0.97	0.06	17,23,42,50	8

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
3	SO4	B	902	5/5	0.76	0.22	97,99,106,111	5
4	MRD	A	904[A]	8/8	0.83	0.17	34,55,70,70	22
4	MRD	A	904[B]	8/8	0.83	0.17	32,53,61,61	22
6	PEG	B	904	7/7	0.84	0.24	19,26,33,34	17

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	C	402	5/5	0.85	0.22	31,33,44,58	5
7	EDO	C	405	4/4	0.86	0.24	31,46,59,59	10
3	SO4	B	900	5/5	0.88	0.16	39,42,49,61	5
3	SO4	B	903	5/5	0.88	0.22	25,39,48,65	5
3	SO4	D	301	5/5	0.89	0.18	38,39,53,61	5
4	MRD	C	404[B]	8/8	0.89	0.14	25,35,47,47	22
3	SO4	A	903	5/5	0.89	0.18	32,35,39,51	5
5	MPD	A	905	8/8	0.89	0.17	50,69,83,83	0
4	MRD	C	404[A]	8/8	0.89	0.14	23,33,39,47	22
3	SO4	A	901	5/5	0.91	0.28	91,94,101,108	5
5	MPD	C	403[A]	8/8	0.91	0.16	26,42,53,63	22
5	MPD	C	403[B]	8/8	0.91	0.16	31,45,56,56	22
3	SO4	A	902	5/5	0.92	0.13	102,103,108,113	0
3	SO4	B	901	5/5	0.92	0.13	24,29,57,63	5
3	SO4	D	303	5/5	0.92	0.13	34,58,68,74	5
3	SO4	D	302	5/5	0.93	0.11	28,34,55,60	5
3	SO4	A	900	5/5	0.94	0.10	62,69,85,85	5
3	SO4	D	304	5/5	0.94	0.14	25,42,52,59	5
3	SO4	C	406	5/5	0.97	0.10	23,25,38,53	5
3	SO4	C	401	5/5	0.97	0.12	53,55,60,67	5

6.5 Other polymers

There are no such residues in this entry.